



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 10:10 PM EDT

PDB ID : 4V94 / pdb_00004v94
Title : Molecular architecture of the eukaryotic chaperonin TRiC/CCT derived by a combination of chemical crosslinking and mass-spectrometry, XL-MS
Authors : Leitner, A.; Joachimiak, L.A.; Bracher, A.; Walzthoeni, T.; Chen, B.; Monke-meyer, L.; Pechmann, S.; Holmes, S.; Cong, Y.; Ma, B.; Ludtke, S.; Chiu, W.; Hartl, F.U.; Aebersold, R.; Frydman, J.
Deposited on : 2012-01-11
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

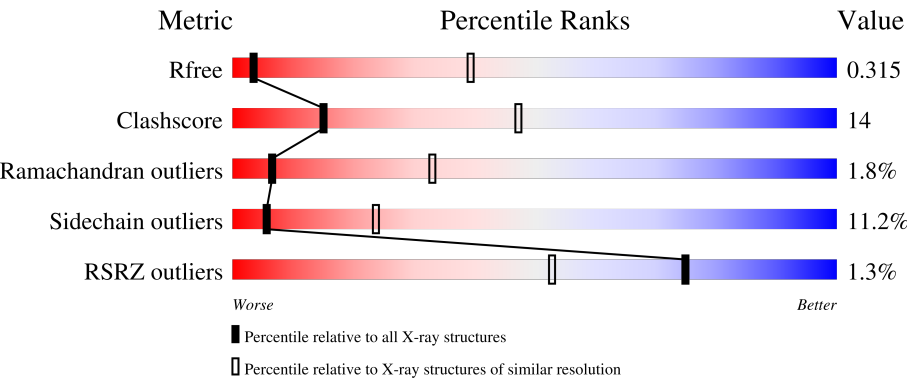
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	F	546	%66%28%5%.
1	N	546	2%72%24%..
1	f	546	2%73%23%..
1	n	546	73%23%..
2	H	568	63%25%.8%

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Mol	Chain	Length	Quality of chain
2	P	568	
2	h	568	
2	p	568	
3	G	550	
3	O	550	
3	g	550	
3	o	550	
4	E	562	
4	M	562	
4	e	562	
4	m	562	
5	B	527	
5	J	527	
5	b	527	
5	j	527	
6	D	528	
6	L	528	
6	d	528	
6	l	528	
7	A	559	
7	I	559	
7	a	559	
7	i	559	
8	C	590	
8	K	590	

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Mol	Chain	Length	Quality of chain
8	c	590	
8	k	590	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	BEF	b	603	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 120080 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	538	Total	C	N	O	S	0	0	0
			3836	2417	640	765	14			
1	N	538	Total	C	N	O	S	0	0	0
			3836	2417	640	765	14			
1	f	538	Total	C	N	O	S	0	0	0
			3836	2417	640	765	14			
1	n	538	Total	C	N	O	S	0	0	0
			3836	2417	640	765	14			

- Molecule 2 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	521	Total	C	N	O	S	0	0	0
			3619	2286	602	708	23			
2	P	521	Total	C	N	O	S	0	0	0
			3619	2286	602	708	23			
2	h	521	Total	C	N	O	S	0	0	0
			3619	2286	602	708	23			
2	p	521	Total	C	N	O	S	0	0	0
			3619	2286	602	708	23			

- Molecule 3 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	526	Total	C	N	O	S	0	0	0
			3752	2372	631	730	19			
3	O	526	Total	C	N	O	S	0	0	0
			3752	2372	631	730	19			
3	g	526	Total	C	N	O	S	0	0	0
			3752	2372	631	730	19			
3	o	526	Total	C	N	O	S	0	0	0
			3752	2372	631	730	19			

- Molecule 4 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	535	Total	C	N	O	S	0	0	0
			3798	2391	634	752	21			
4	M	535	Total	C	N	O	S	0	0	0
			3798	2391	634	752	21			
4	e	535	Total	C	N	O	S	0	0	0
			3798	2391	634	752	21			
4	m	535	Total	C	N	O	S	0	0	0
			3798	2391	634	752	21			

- Molecule 5 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	518	Total	C	N	O	S	0	0	0
			3689	2306	623	747	13			
5	J	518	Total	C	N	O	S	0	0	0
			3689	2306	623	747	13			
5	b	518	Total	C	N	O	S	0	0	0
			3689	2306	623	747	13			
5	j	518	Total	C	N	O	S	0	0	0
			3689	2306	623	747	13			

- Molecule 6 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	523	Total	C	N	O	S	0	0	0
			3685	2306	631	731	17			
6	L	523	Total	C	N	O	S	0	0	0
			3685	2306	631	731	17			
6	d	523	Total	C	N	O	S	0	0	0
			3685	2306	631	731	17			
6	l	523	Total	C	N	O	S	0	0	0
			3685	2306	631	731	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	345	ASP	GLY	engineered mutation	UNP P39078
L	345	ASP	GLY	engineered mutation	UNP P39078
d	345	ASP	GLY	engineered mutation	UNP P39078
l	345	ASP	GLY	engineered mutation	UNP P39078

- Molecule 7 is a protein called T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	A	539	Total	C	N	O	S	0	0	0
			3770	2369	638	746	17			
7	I	539	Total	C	N	O	S	0	0	0
			3770	2369	638	746	17			
7	a	539	Total	C	N	O	S	0	0	0
			3770	2369	638	746	17			
7	i	539	Total	C	N	O	S	0	0	0
			3770	2369	638	746	17			

- Molecule 8 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	C	513	Total	C	N	O	S	0	0	0
			3615	2270	620	699	26			
8	K	513	Total	C	N	O	S	0	0	0
			3615	2270	620	699	26			
8	c	513	Total	C	N	O	S	0	0	0
			3615	2270	620	699	26			
8	k	513	Total	C	N	O	S	0	0	0
			3615	2270	620	699	26			

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1001	GLY	-	SEE REMARK 999	UNP P39077
C	1002	SER	-	SEE REMARK 999	UNP P39077
C	1003	GLY	-	SEE REMARK 999	UNP P39077
C	1004	SER	-	SEE REMARK 999	UNP P39077
C	1005	GLY	-	SEE REMARK 999	UNP P39077
C	1006	TRP	-	SEE REMARK 999	UNP P39077
C	1007	SER	-	SEE REMARK 999	UNP P39077
C	1008	HIS	-	SEE REMARK 999	UNP P39077
C	1009	PRO	-	SEE REMARK 999	UNP P39077
C	1010	GLN	-	SEE REMARK 999	UNP P39077
C	1011	PHE	-	SEE REMARK 999	UNP P39077
C	1012	GLU	-	SEE REMARK 999	UNP P39077
C	1013	LYS	-	SEE REMARK 999	UNP P39077
C	1014	GLY	-	SEE REMARK 999	UNP P39077
C	1015	SER	-	SEE REMARK 999	UNP P39077
C	1016	GLY	-	SEE REMARK 999	UNP P39077
C	1017	LYS	-	SEE REMARK 999	UNP P39077
C	1018	ARG	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1019	ARG	-	SEE REMARK 999	UNP P39077
C	1020	TRP	-	SEE REMARK 999	UNP P39077
C	1021	LYS	-	SEE REMARK 999	UNP P39077
C	1022	LYS	-	SEE REMARK 999	UNP P39077
C	1023	ASN	-	SEE REMARK 999	UNP P39077
C	1024	PHE	-	SEE REMARK 999	UNP P39077
C	1025	ILE	-	SEE REMARK 999	UNP P39077
C	1026	ALA	-	SEE REMARK 999	UNP P39077
C	1027	VAL	-	SEE REMARK 999	UNP P39077
C	1028	SER	-	SEE REMARK 999	UNP P39077
C	1029	ALA	-	SEE REMARK 999	UNP P39077
C	1030	ALA	-	SEE REMARK 999	UNP P39077
C	1031	ASN	-	SEE REMARK 999	UNP P39077
C	1032	ARG	-	SEE REMARK 999	UNP P39077
C	1033	PHE	-	SEE REMARK 999	UNP P39077
C	1034	LYS	-	SEE REMARK 999	UNP P39077
C	1035	LYS	-	SEE REMARK 999	UNP P39077
C	1036	ILE	-	SEE REMARK 999	UNP P39077
C	1037	SER	-	SEE REMARK 999	UNP P39077
C	1038	SER	-	SEE REMARK 999	UNP P39077
C	1039	SER	-	SEE REMARK 999	UNP P39077
C	1040	GLY	-	SEE REMARK 999	UNP P39077
C	1041	ALA	-	SEE REMARK 999	UNP P39077
C	1042	LEU	-	SEE REMARK 999	UNP P39077
C	1043	GLY	-	SEE REMARK 999	UNP P39077
C	1044	SER	-	SEE REMARK 999	UNP P39077
C	1045	GLY	-	SEE REMARK 999	UNP P39077
C	1046	HIS	-	SEE REMARK 999	UNP P39077
C	1047	HIS	-	SEE REMARK 999	UNP P39077
C	1048	HIS	-	SEE REMARK 999	UNP P39077
C	1049	HIS	-	SEE REMARK 999	UNP P39077
C	1050	HIS	-	SEE REMARK 999	UNP P39077
C	1051	HIS	-	SEE REMARK 999	UNP P39077
C	1052	HIS	-	SEE REMARK 999	UNP P39077
C	1053	HIS	-	SEE REMARK 999	UNP P39077
C	1054	GLY	-	SEE REMARK 999	UNP P39077
C	1055	SER	-	SEE REMARK 999	UNP P39077
C	1056	GLY	-	SEE REMARK 999	UNP P39077
K	1001	GLY	-	SEE REMARK 999	UNP P39077
K	1002	SER	-	SEE REMARK 999	UNP P39077
K	1003	GLY	-	SEE REMARK 999	UNP P39077
K	1004	SER	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1005	GLY	-	SEE REMARK 999	UNP P39077
K	1006	TRP	-	SEE REMARK 999	UNP P39077
K	1007	SER	-	SEE REMARK 999	UNP P39077
K	1008	HIS	-	SEE REMARK 999	UNP P39077
K	1009	PRO	-	SEE REMARK 999	UNP P39077
K	1010	GLN	-	SEE REMARK 999	UNP P39077
K	1011	PHE	-	SEE REMARK 999	UNP P39077
K	1012	GLU	-	SEE REMARK 999	UNP P39077
K	1013	LYS	-	SEE REMARK 999	UNP P39077
K	1014	GLY	-	SEE REMARK 999	UNP P39077
K	1015	SER	-	SEE REMARK 999	UNP P39077
K	1016	GLY	-	SEE REMARK 999	UNP P39077
K	1017	LYS	-	SEE REMARK 999	UNP P39077
K	1018	ARG	-	SEE REMARK 999	UNP P39077
K	1019	ARG	-	SEE REMARK 999	UNP P39077
K	1020	TRP	-	SEE REMARK 999	UNP P39077
K	1021	LYS	-	SEE REMARK 999	UNP P39077
K	1022	LYS	-	SEE REMARK 999	UNP P39077
K	1023	ASN	-	SEE REMARK 999	UNP P39077
K	1024	PHE	-	SEE REMARK 999	UNP P39077
K	1025	ILE	-	SEE REMARK 999	UNP P39077
K	1026	ALA	-	SEE REMARK 999	UNP P39077
K	1027	VAL	-	SEE REMARK 999	UNP P39077
K	1028	SER	-	SEE REMARK 999	UNP P39077
K	1029	ALA	-	SEE REMARK 999	UNP P39077
K	1030	ALA	-	SEE REMARK 999	UNP P39077
K	1031	ASN	-	SEE REMARK 999	UNP P39077
K	1032	ARG	-	SEE REMARK 999	UNP P39077
K	1033	PHE	-	SEE REMARK 999	UNP P39077
K	1034	LYS	-	SEE REMARK 999	UNP P39077
K	1035	LYS	-	SEE REMARK 999	UNP P39077
K	1036	ILE	-	SEE REMARK 999	UNP P39077
K	1037	SER	-	SEE REMARK 999	UNP P39077
K	1038	SER	-	SEE REMARK 999	UNP P39077
K	1039	SER	-	SEE REMARK 999	UNP P39077
K	1040	GLY	-	SEE REMARK 999	UNP P39077
K	1041	ALA	-	SEE REMARK 999	UNP P39077
K	1042	LEU	-	SEE REMARK 999	UNP P39077
K	1043	GLY	-	SEE REMARK 999	UNP P39077
K	1044	SER	-	SEE REMARK 999	UNP P39077
K	1045	GLY	-	SEE REMARK 999	UNP P39077
K	1046	HIS	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1047	HIS	-	SEE REMARK 999	UNP P39077
K	1048	HIS	-	SEE REMARK 999	UNP P39077
K	1049	HIS	-	SEE REMARK 999	UNP P39077
K	1050	HIS	-	SEE REMARK 999	UNP P39077
K	1051	HIS	-	SEE REMARK 999	UNP P39077
K	1052	HIS	-	SEE REMARK 999	UNP P39077
K	1053	HIS	-	SEE REMARK 999	UNP P39077
K	1054	GLY	-	SEE REMARK 999	UNP P39077
K	1055	SER	-	SEE REMARK 999	UNP P39077
K	1056	GLY	-	SEE REMARK 999	UNP P39077
c	1001	GLY	-	SEE REMARK 999	UNP P39077
c	1002	SER	-	SEE REMARK 999	UNP P39077
c	1003	GLY	-	SEE REMARK 999	UNP P39077
c	1004	SER	-	SEE REMARK 999	UNP P39077
c	1005	GLY	-	SEE REMARK 999	UNP P39077
c	1006	TRP	-	SEE REMARK 999	UNP P39077
c	1007	SER	-	SEE REMARK 999	UNP P39077
c	1008	HIS	-	SEE REMARK 999	UNP P39077
c	1009	PRO	-	SEE REMARK 999	UNP P39077
c	1010	GLN	-	SEE REMARK 999	UNP P39077
c	1011	PHE	-	SEE REMARK 999	UNP P39077
c	1012	GLU	-	SEE REMARK 999	UNP P39077
c	1013	LYS	-	SEE REMARK 999	UNP P39077
c	1014	GLY	-	SEE REMARK 999	UNP P39077
c	1015	SER	-	SEE REMARK 999	UNP P39077
c	1016	GLY	-	SEE REMARK 999	UNP P39077
c	1017	LYS	-	SEE REMARK 999	UNP P39077
c	1018	ARG	-	SEE REMARK 999	UNP P39077
c	1019	ARG	-	SEE REMARK 999	UNP P39077
c	1020	TRP	-	SEE REMARK 999	UNP P39077
c	1021	LYS	-	SEE REMARK 999	UNP P39077
c	1022	LYS	-	SEE REMARK 999	UNP P39077
c	1023	ASN	-	SEE REMARK 999	UNP P39077
c	1024	PHE	-	SEE REMARK 999	UNP P39077
c	1025	ILE	-	SEE REMARK 999	UNP P39077
c	1026	ALA	-	SEE REMARK 999	UNP P39077
c	1027	VAL	-	SEE REMARK 999	UNP P39077
c	1028	SER	-	SEE REMARK 999	UNP P39077
c	1029	ALA	-	SEE REMARK 999	UNP P39077
c	1030	ALA	-	SEE REMARK 999	UNP P39077
c	1031	ASN	-	SEE REMARK 999	UNP P39077
c	1032	ARG	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
c	1033	PHE	-	SEE REMARK 999	UNP P39077
c	1034	LYS	-	SEE REMARK 999	UNP P39077
c	1035	LYS	-	SEE REMARK 999	UNP P39077
c	1036	ILE	-	SEE REMARK 999	UNP P39077
c	1037	SER	-	SEE REMARK 999	UNP P39077
c	1038	SER	-	SEE REMARK 999	UNP P39077
c	1039	SER	-	SEE REMARK 999	UNP P39077
c	1040	GLY	-	SEE REMARK 999	UNP P39077
c	1041	ALA	-	SEE REMARK 999	UNP P39077
c	1042	LEU	-	SEE REMARK 999	UNP P39077
c	1043	GLY	-	SEE REMARK 999	UNP P39077
c	1044	SER	-	SEE REMARK 999	UNP P39077
c	1045	GLY	-	SEE REMARK 999	UNP P39077
c	1046	HIS	-	SEE REMARK 999	UNP P39077
c	1047	HIS	-	SEE REMARK 999	UNP P39077
c	1048	HIS	-	SEE REMARK 999	UNP P39077
c	1049	HIS	-	SEE REMARK 999	UNP P39077
c	1050	HIS	-	SEE REMARK 999	UNP P39077
c	1051	HIS	-	SEE REMARK 999	UNP P39077
c	1052	HIS	-	SEE REMARK 999	UNP P39077
c	1053	HIS	-	SEE REMARK 999	UNP P39077
c	1054	GLY	-	SEE REMARK 999	UNP P39077
c	1055	SER	-	SEE REMARK 999	UNP P39077
c	1056	GLY	-	SEE REMARK 999	UNP P39077
k	1001	GLY	-	SEE REMARK 999	UNP P39077
k	1002	SER	-	SEE REMARK 999	UNP P39077
k	1003	GLY	-	SEE REMARK 999	UNP P39077
k	1004	SER	-	SEE REMARK 999	UNP P39077
k	1005	GLY	-	SEE REMARK 999	UNP P39077
k	1006	TRP	-	SEE REMARK 999	UNP P39077
k	1007	SER	-	SEE REMARK 999	UNP P39077
k	1008	HIS	-	SEE REMARK 999	UNP P39077
k	1009	PRO	-	SEE REMARK 999	UNP P39077
k	1010	GLN	-	SEE REMARK 999	UNP P39077
k	1011	PHE	-	SEE REMARK 999	UNP P39077
k	1012	GLU	-	SEE REMARK 999	UNP P39077
k	1013	LYS	-	SEE REMARK 999	UNP P39077
k	1014	GLY	-	SEE REMARK 999	UNP P39077
k	1015	SER	-	SEE REMARK 999	UNP P39077
k	1016	GLY	-	SEE REMARK 999	UNP P39077
k	1017	LYS	-	SEE REMARK 999	UNP P39077
k	1018	ARG	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
k	1019	ARG	-	SEE REMARK 999	UNP P39077
k	1020	TRP	-	SEE REMARK 999	UNP P39077
k	1021	LYS	-	SEE REMARK 999	UNP P39077
k	1022	LYS	-	SEE REMARK 999	UNP P39077
k	1023	ASN	-	SEE REMARK 999	UNP P39077
k	1024	PHE	-	SEE REMARK 999	UNP P39077
k	1025	ILE	-	SEE REMARK 999	UNP P39077
k	1026	ALA	-	SEE REMARK 999	UNP P39077
k	1027	VAL	-	SEE REMARK 999	UNP P39077
k	1028	SER	-	SEE REMARK 999	UNP P39077
k	1029	ALA	-	SEE REMARK 999	UNP P39077
k	1030	ALA	-	SEE REMARK 999	UNP P39077
k	1031	ASN	-	SEE REMARK 999	UNP P39077
k	1032	ARG	-	SEE REMARK 999	UNP P39077
k	1033	PHE	-	SEE REMARK 999	UNP P39077
k	1034	LYS	-	SEE REMARK 999	UNP P39077
k	1035	LYS	-	SEE REMARK 999	UNP P39077
k	1036	ILE	-	SEE REMARK 999	UNP P39077
k	1037	SER	-	SEE REMARK 999	UNP P39077
k	1038	SER	-	SEE REMARK 999	UNP P39077
k	1039	SER	-	SEE REMARK 999	UNP P39077
k	1040	GLY	-	SEE REMARK 999	UNP P39077
k	1041	ALA	-	SEE REMARK 999	UNP P39077
k	1042	LEU	-	SEE REMARK 999	UNP P39077
k	1043	GLY	-	SEE REMARK 999	UNP P39077
k	1044	SER	-	SEE REMARK 999	UNP P39077
k	1045	GLY	-	SEE REMARK 999	UNP P39077
k	1046	HIS	-	SEE REMARK 999	UNP P39077
k	1047	HIS	-	SEE REMARK 999	UNP P39077
k	1048	HIS	-	SEE REMARK 999	UNP P39077
k	1049	HIS	-	SEE REMARK 999	UNP P39077
k	1050	HIS	-	SEE REMARK 999	UNP P39077
k	1051	HIS	-	SEE REMARK 999	UNP P39077
k	1052	HIS	-	SEE REMARK 999	UNP P39077
k	1053	HIS	-	SEE REMARK 999	UNP P39077
k	1054	GLY	-	SEE REMARK 999	UNP P39077
k	1055	SER	-	SEE REMARK 999	UNP P39077
k	1056	GLY	-	SEE REMARK 999	UNP P39077

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

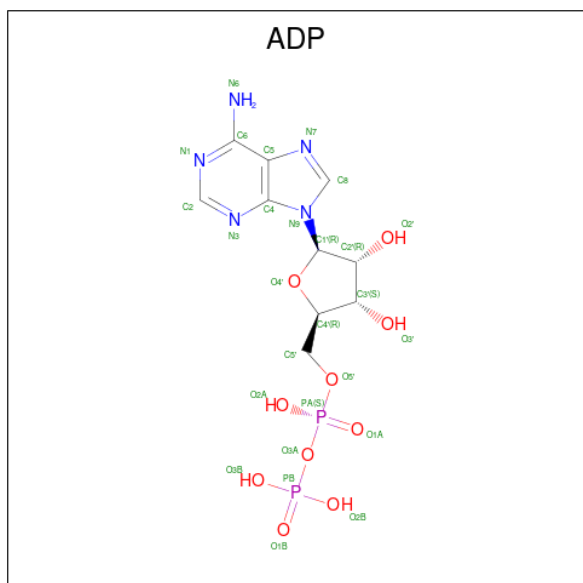
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	F	1	Total Mg 1 1	0	0
9	H	1	Total Mg 1 1	0	0
9	G	1	Total Mg 1 1	0	0
9	E	1	Total Mg 1 1	0	0
9	B	1	Total Mg 1 1	0	0
9	D	1	Total Mg 1 1	0	0
9	A	1	Total Mg 1 1	0	0
9	C	1	Total Mg 1 1	0	0
9	N	1	Total Mg 1 1	0	0
9	P	1	Total Mg 1 1	0	0
9	O	1	Total Mg 1 1	0	0
9	M	1	Total Mg 1 1	0	0
9	J	1	Total Mg 1 1	0	0
9	L	1	Total Mg 1 1	0	0
9	I	1	Total Mg 1 1	0	0
9	K	1	Total Mg 1 1	0	0
9	f	1	Total Mg 1 1	0	0
9	h	1	Total Mg 1 1	0	0
9	g	1	Total Mg 1 1	0	0
9	e	1	Total Mg 1 1	0	0
9	b	1	Total Mg 1 1	0	0
9	d	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	a	1	Total	Mg	0	0
			1	1		
9	c	1	Total	Mg	0	0
			1	1		
9	n	1	Total	Mg	0	0
			1	1		
9	p	1	Total	Mg	0	0
			1	1		
9	o	1	Total	Mg	0	0
			1	1		
9	m	1	Total	Mg	0	0
			1	1		
9	j	1	Total	Mg	0	0
			1	1		
9	l	1	Total	Mg	0	0
			1	1		
9	i	1	Total	Mg	0	0
			1	1		
9	k	1	Total	Mg	0	0
			1	1		

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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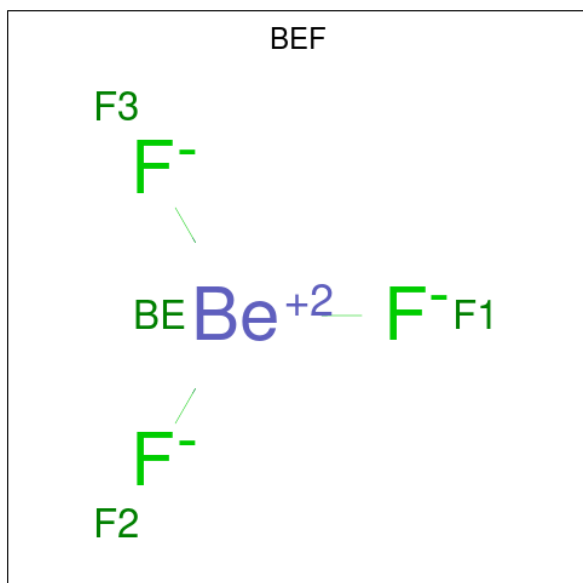
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	H	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	N	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	P	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	O	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	M	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	J	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	L	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	I	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	K	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	f	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	h	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	g	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	e	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	b	1	Total 27	C 10	N 5	O 10	P 2	0	0
10	d	1	Total 27	C 10	N 5	O 10	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	a	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	c	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	n	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	p	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	o	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	m	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	j	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	l	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	i	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	k	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 11 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	F	1	Total	Be	F	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	H	1	Total 4	Be 1	F 3	0	0
11	G	1	Total 4	Be 1	F 3	0	0
11	E	1	Total 4	Be 1	F 3	0	0
11	B	1	Total 4	Be 1	F 3	0	0
11	D	1	Total 4	Be 1	F 3	0	0
11	A	1	Total 4	Be 1	F 3	0	0
11	C	1	Total 4	Be 1	F 3	0	0
11	N	1	Total 4	Be 1	F 3	0	0
11	P	1	Total 4	Be 1	F 3	0	0
11	O	1	Total 4	Be 1	F 3	0	0
11	M	1	Total 4	Be 1	F 3	0	0
11	J	1	Total 4	Be 1	F 3	0	0
11	L	1	Total 4	Be 1	F 3	0	0
11	I	1	Total 4	Be 1	F 3	0	0
11	K	1	Total 4	Be 1	F 3	0	0
11	f	1	Total 4	Be 1	F 3	0	0
11	h	1	Total 4	Be 1	F 3	0	0
11	g	1	Total 4	Be 1	F 3	0	0
11	e	1	Total 4	Be 1	F 3	0	0
11	b	1	Total 4	Be 1	F 3	0	0
11	d	1	Total 4	Be 1	F 3	0	0

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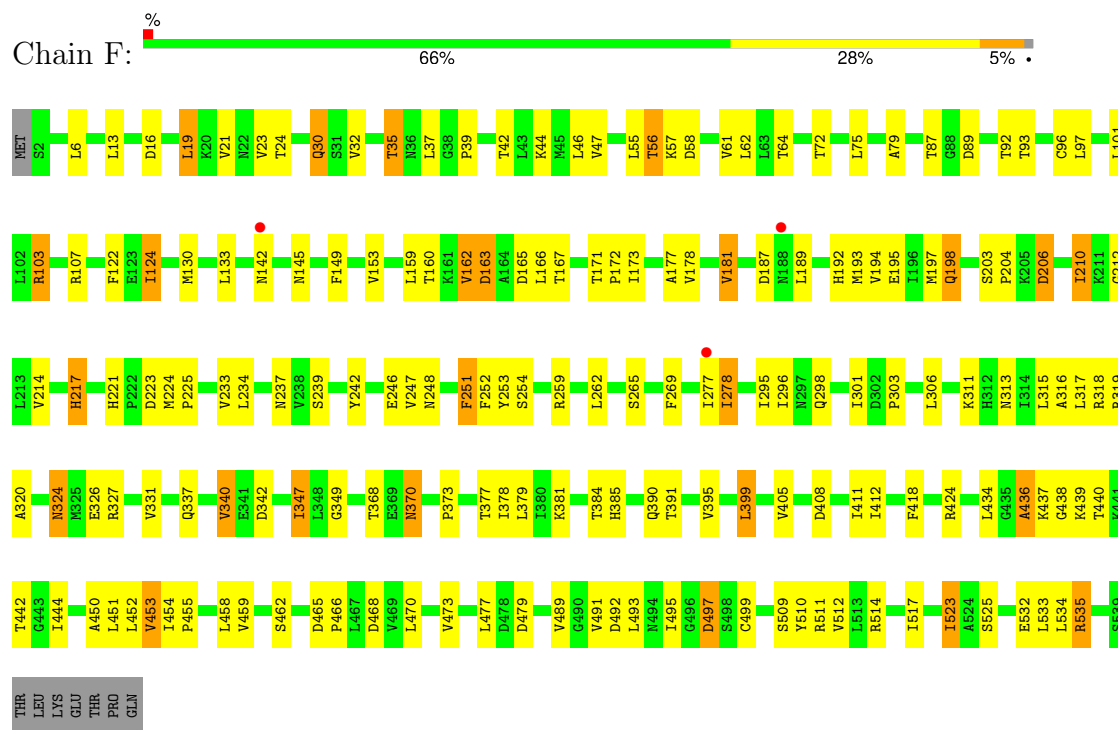
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	a	1	Total 4	Be 1	F 3	0	0
11	c	1	Total 4	Be 1	F 3	0	0
11	n	1	Total 4	Be 1	F 3	0	0
11	p	1	Total 4	Be 1	F 3	0	0
11	o	1	Total 4	Be 1	F 3	0	0
11	m	1	Total 4	Be 1	F 3	0	0
11	j	1	Total 4	Be 1	F 3	0	0
11	l	1	Total 4	Be 1	F 3	0	0
11	i	1	Total 4	Be 1	F 3	0	0
11	k	1	Total 4	Be 1	F 3	0	0

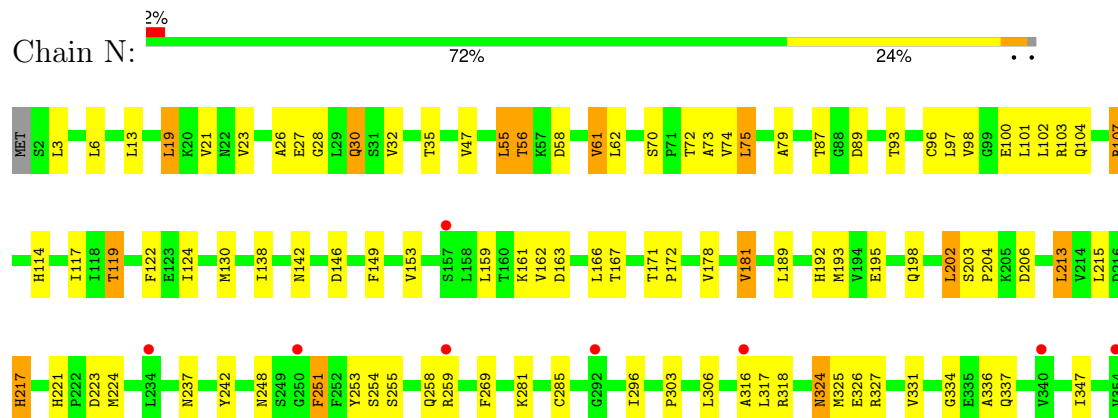
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: T-complex protein 1 subunit zeta

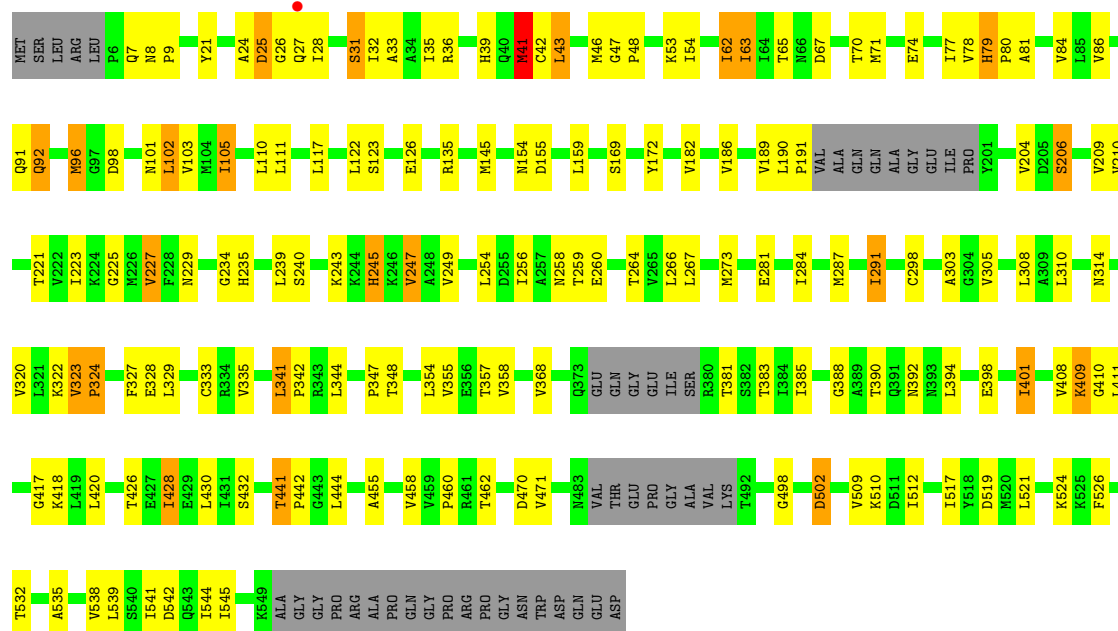


- Molecule 1: T-complex protein 1 subunit zeta



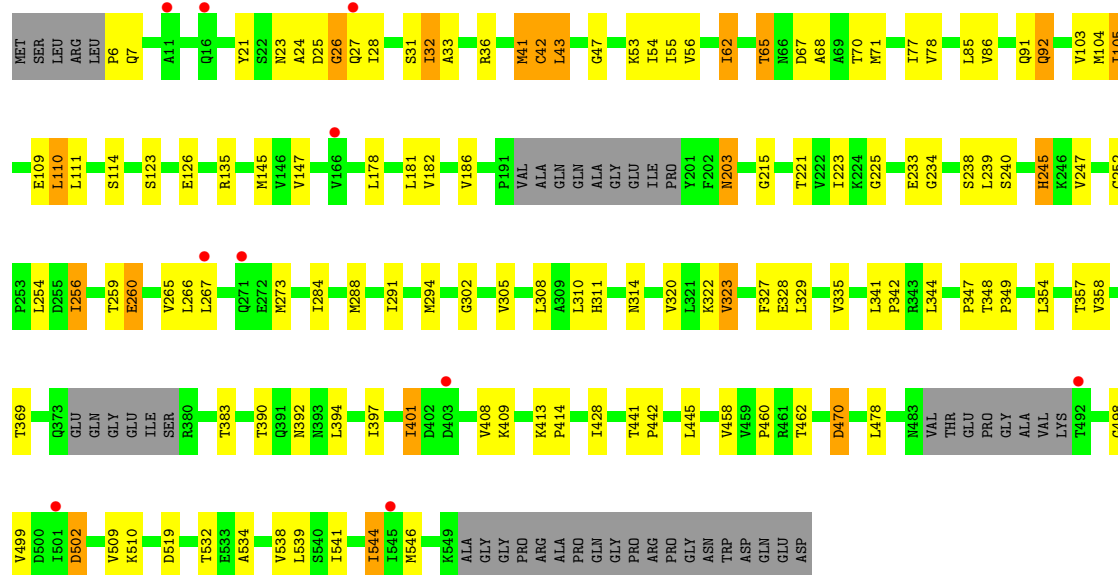


Chain H:  63% 25% 8%



• Molecule 2: T-complex protein 1 subunit theta

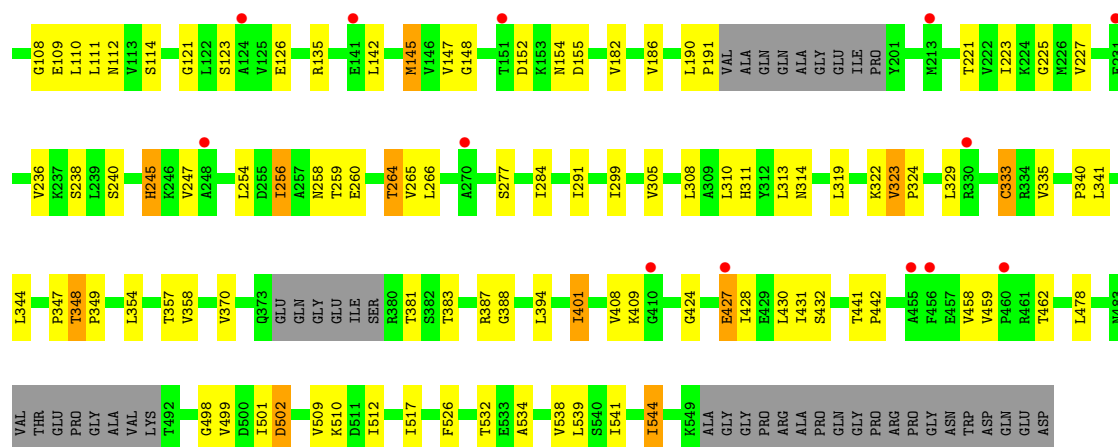
Chain P:  69% 19% 8%



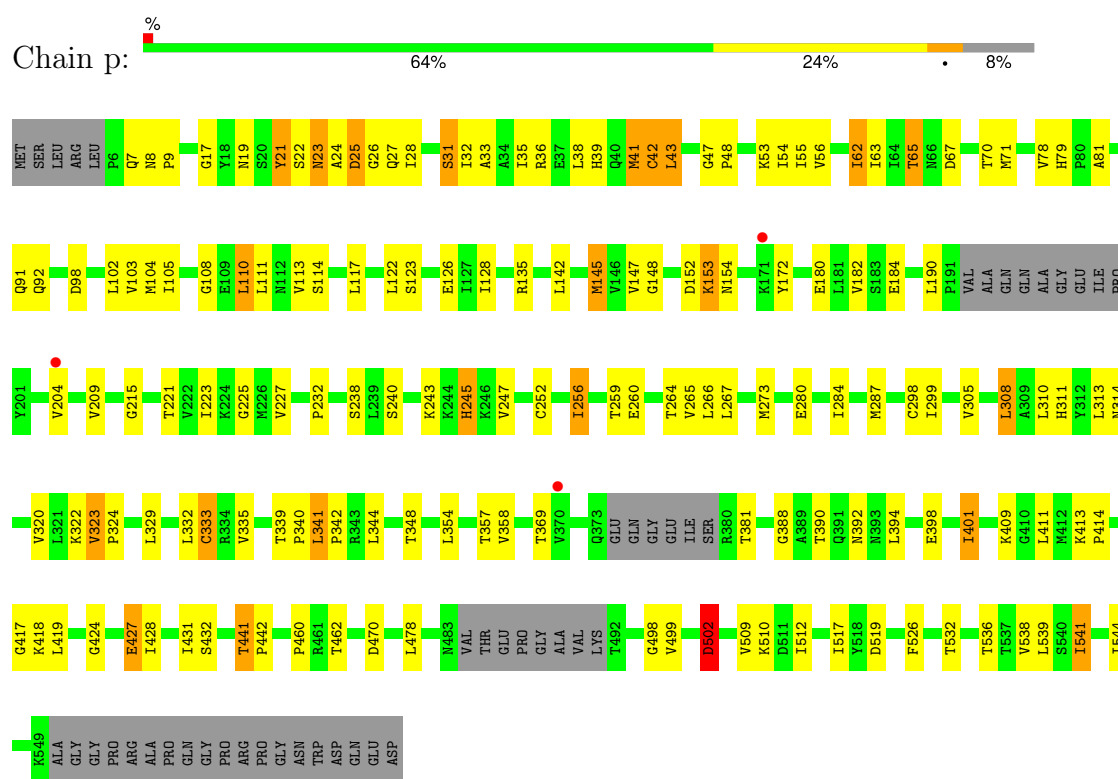
• Molecule 2: T-complex protein 1 subunit theta

Chain h:  68% 21% 8%

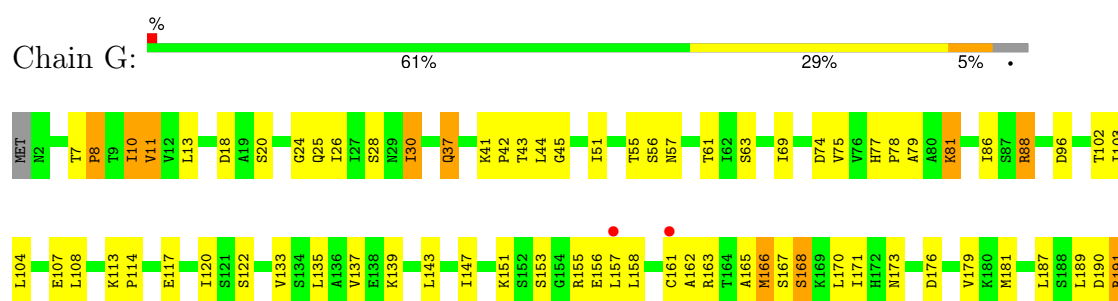


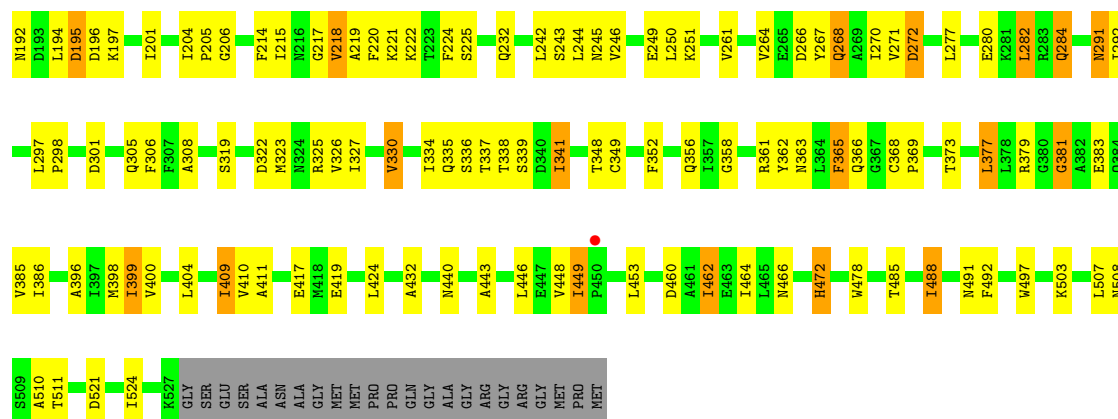


• Molecule 2: T-complex protein 1 subunit theta

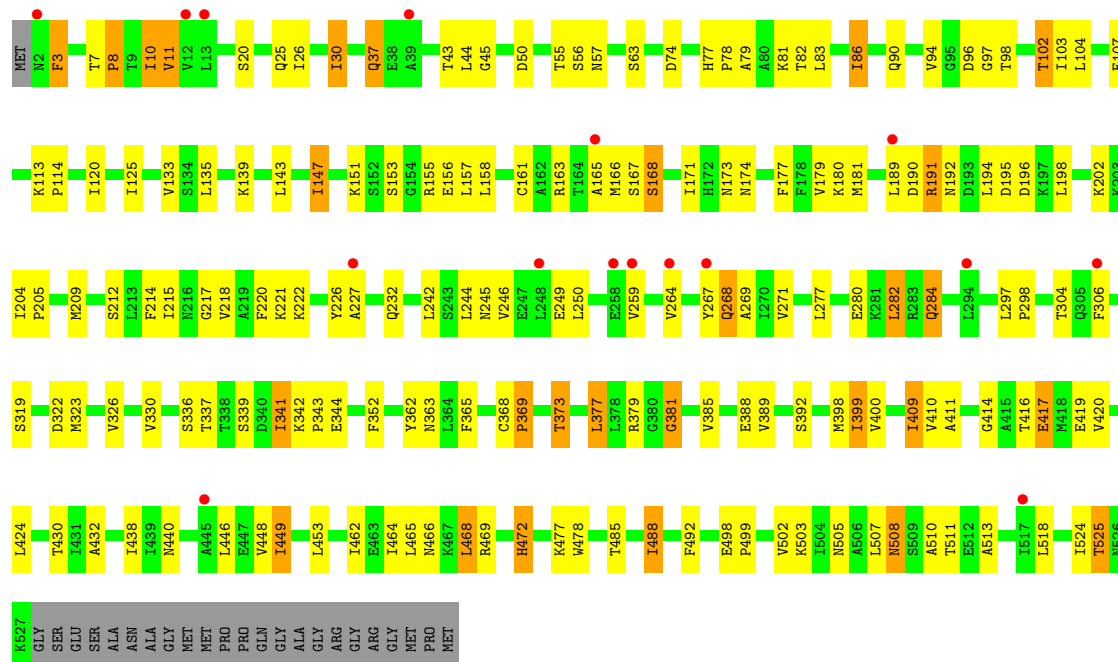


• Molecule 3: T-complex protein 1 subunit eta

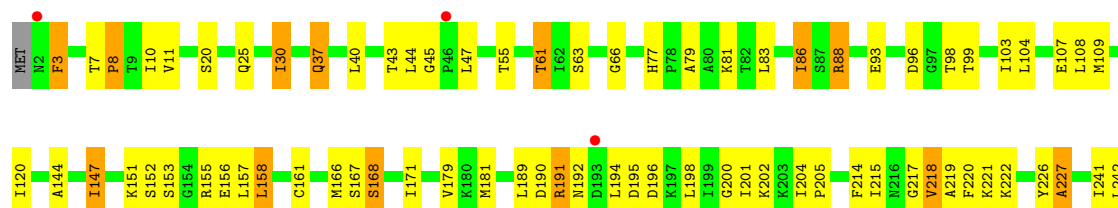


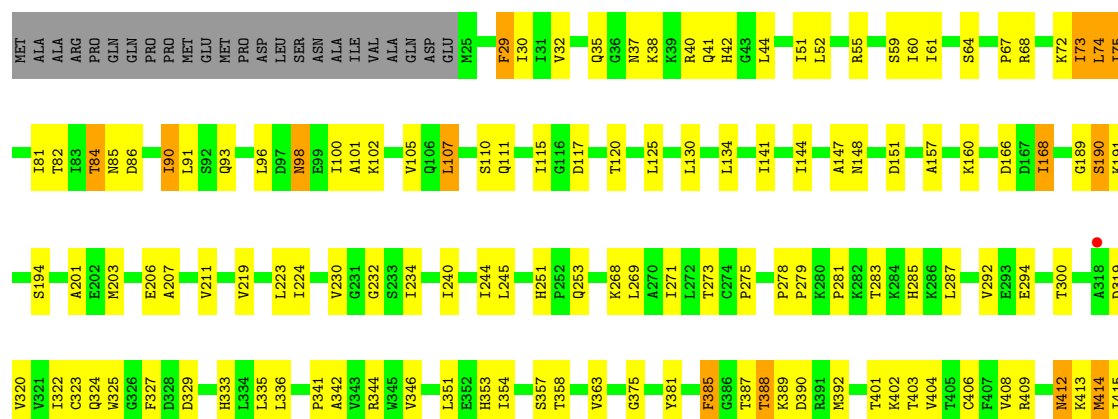


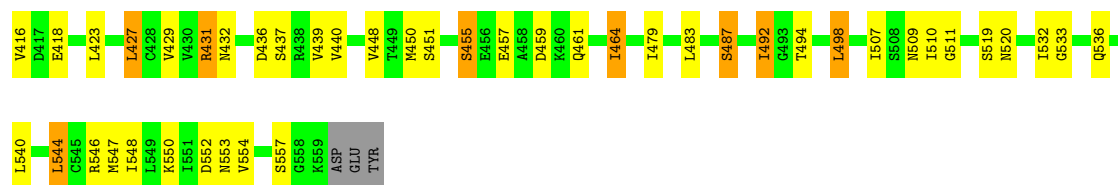
• Molecule 3: T-complex protein 1 subunit eta



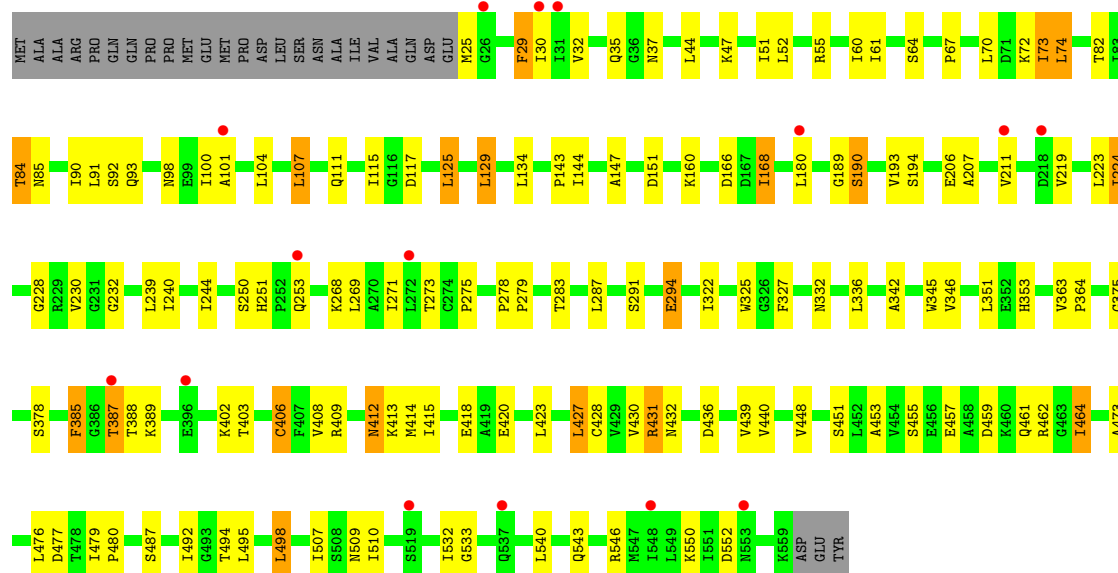
• Molecule 3: T-complex protein 1 subunit eta



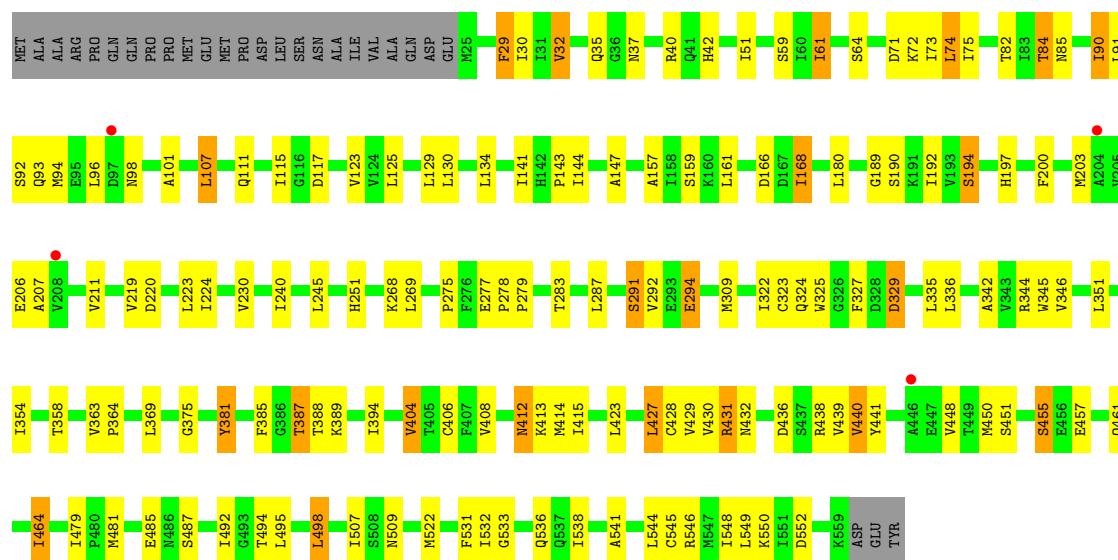




• Molecule 4: T-complex protein 1 subunit epsilon

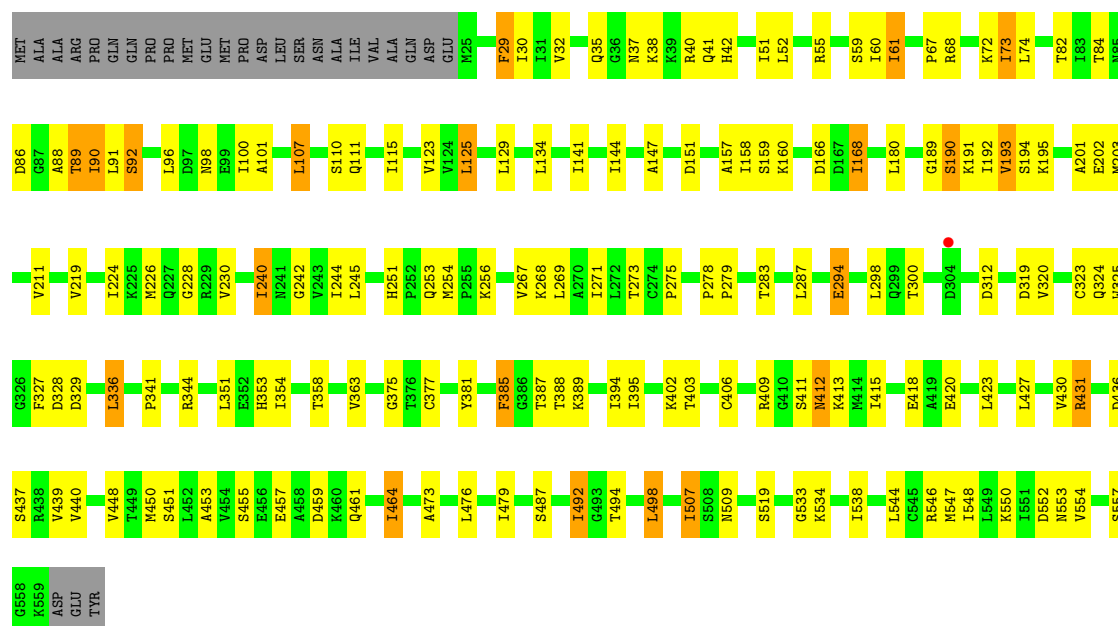


• Molecule 4: T-complex protein 1 subunit epsilon



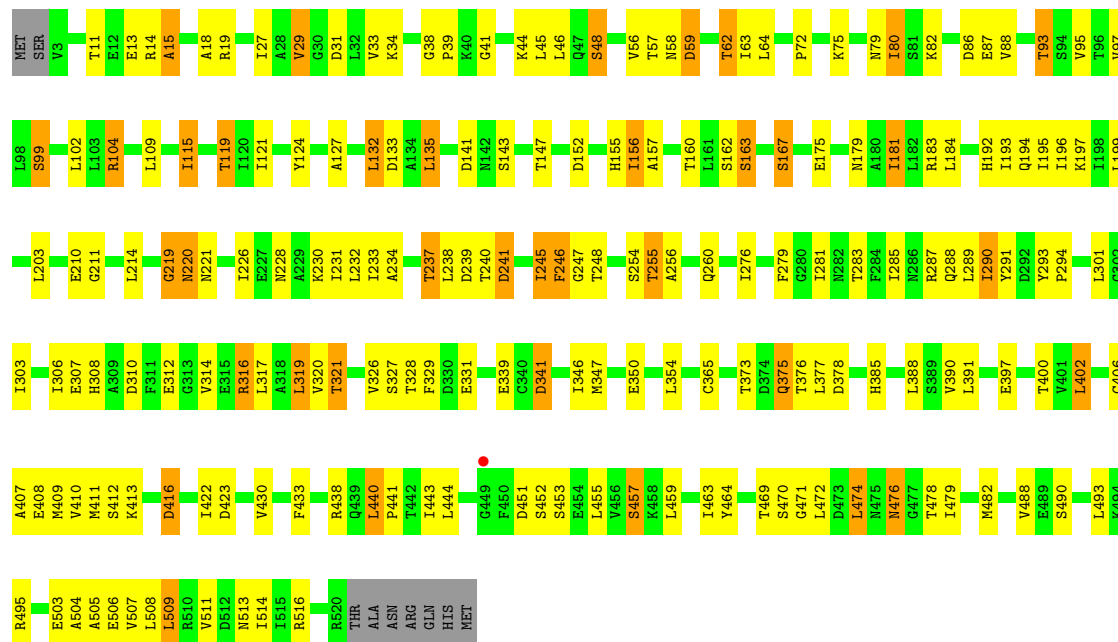
• Molecule 4: T-complex protein 1 subunit epsilon

Chain m: 



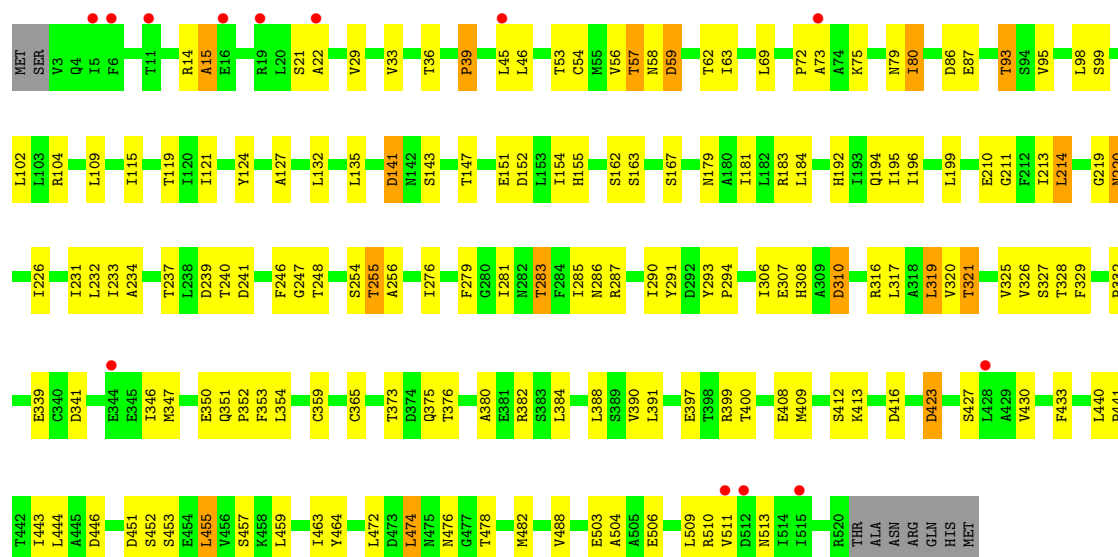
• Molecule 5: T-complex protein 1 subunit beta

Chain B: 



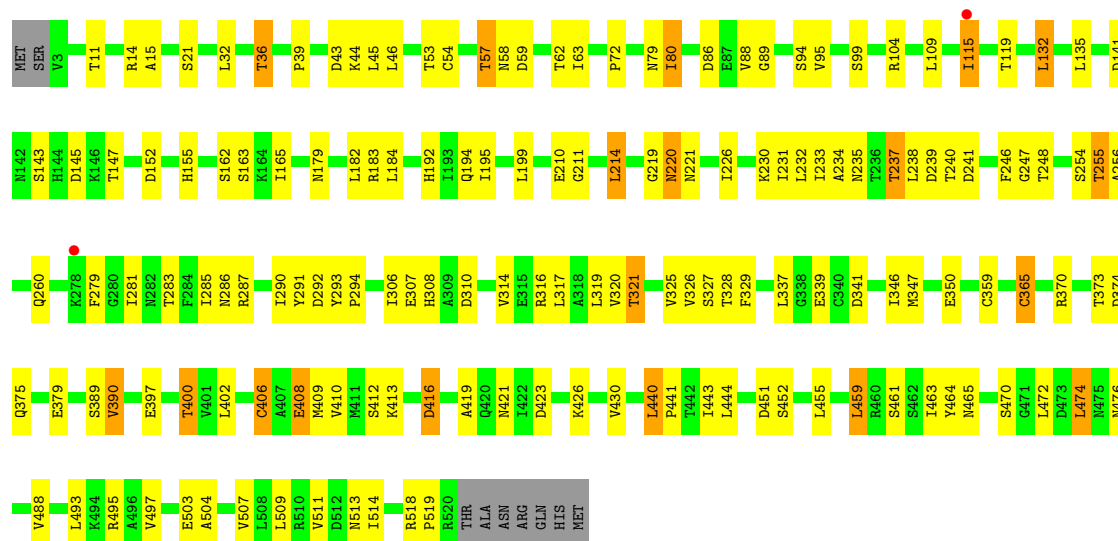
• Molecule 5: T-complex protein 1 subunit beta

Chain J: 



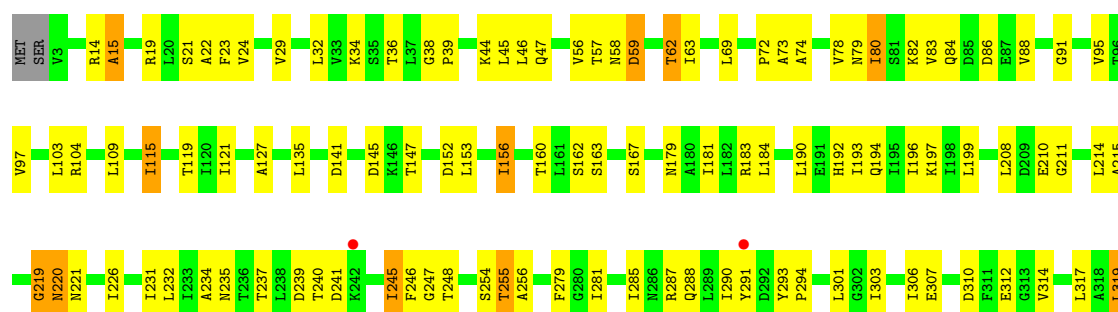
• Molecule 5: T-complex protein 1 subunit beta

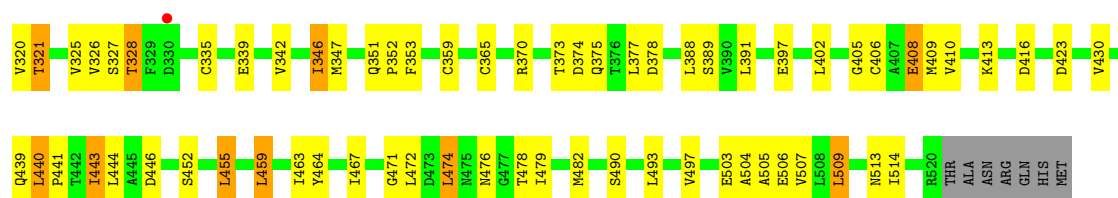
Chain b: 68% 27%



• Molecule 5: T-complex protein 1 subunit beta

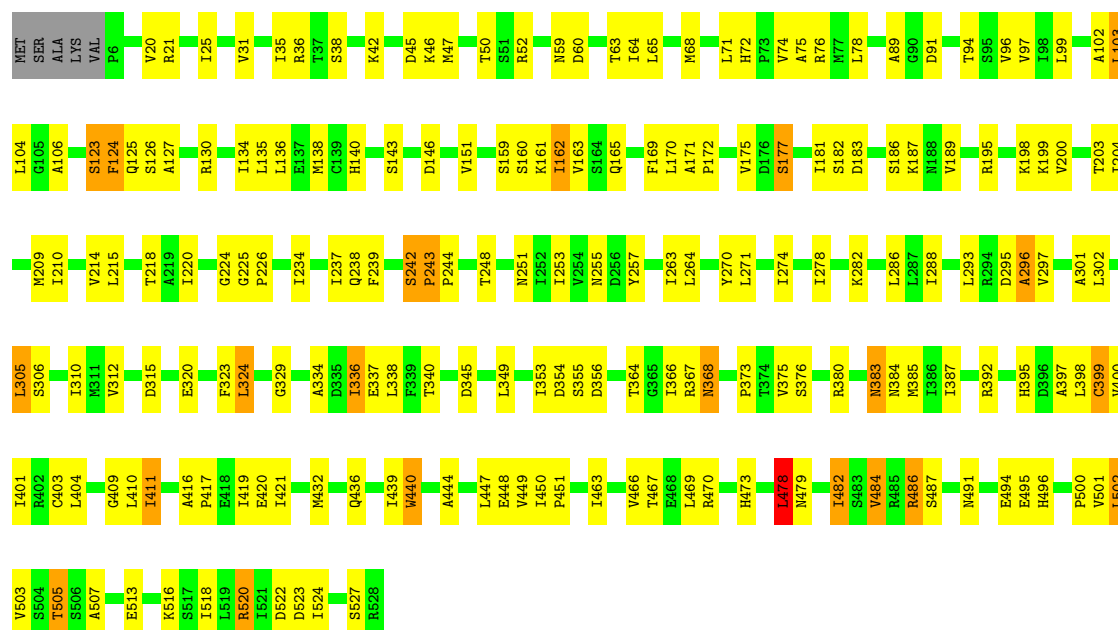
Chain j: 65% 29%





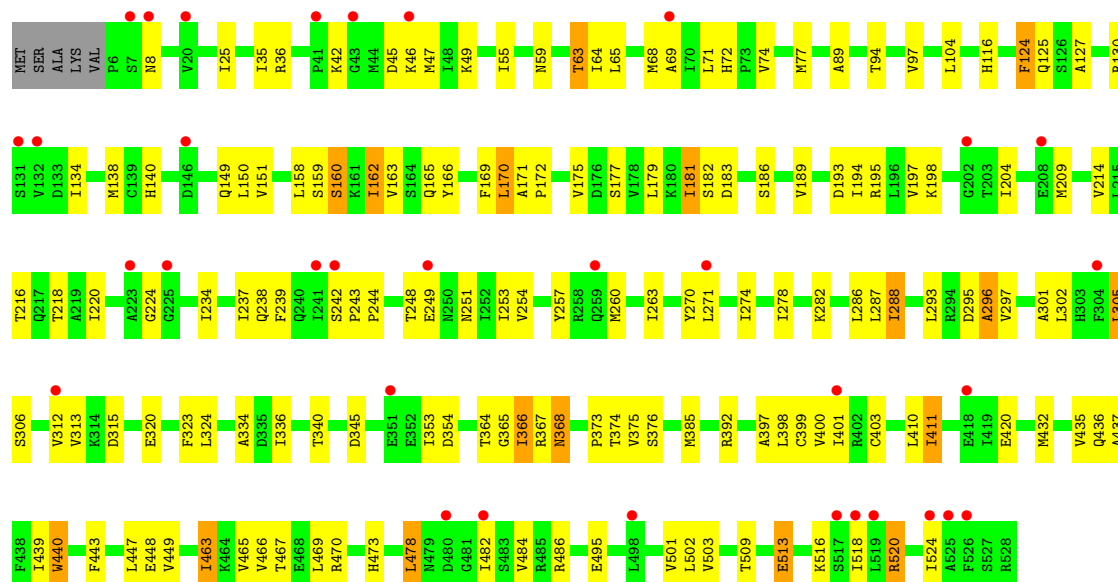
• Molecule 6: T-complex protein 1 subunit delta

Chain D: 62% 33% ..

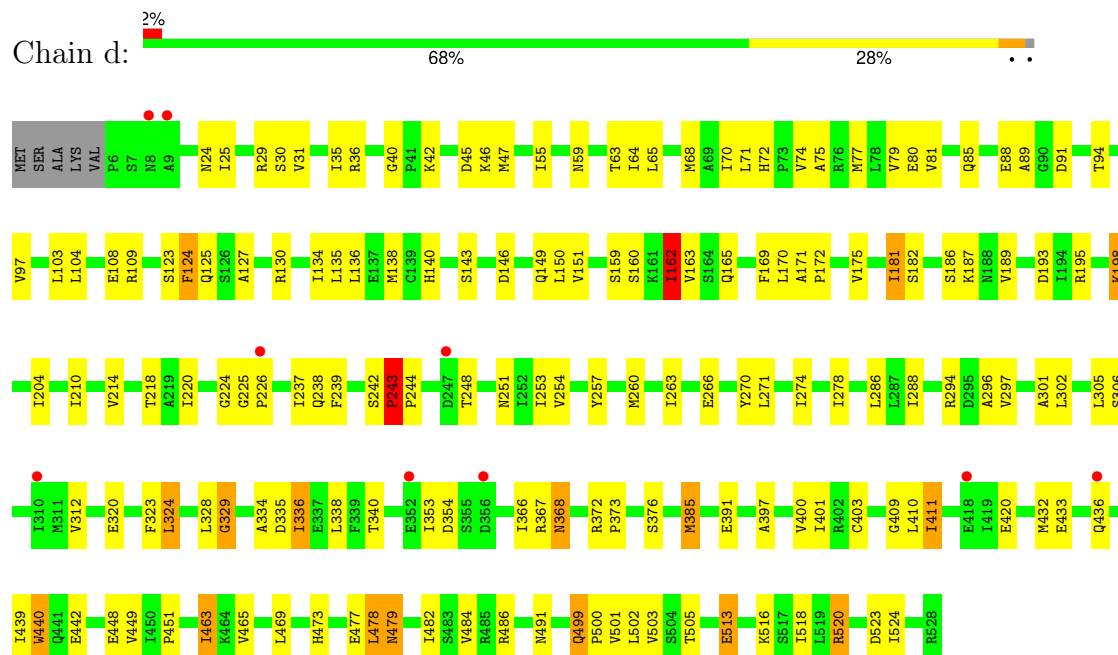


• Molecule 6: T-complex protein 1 subunit delta

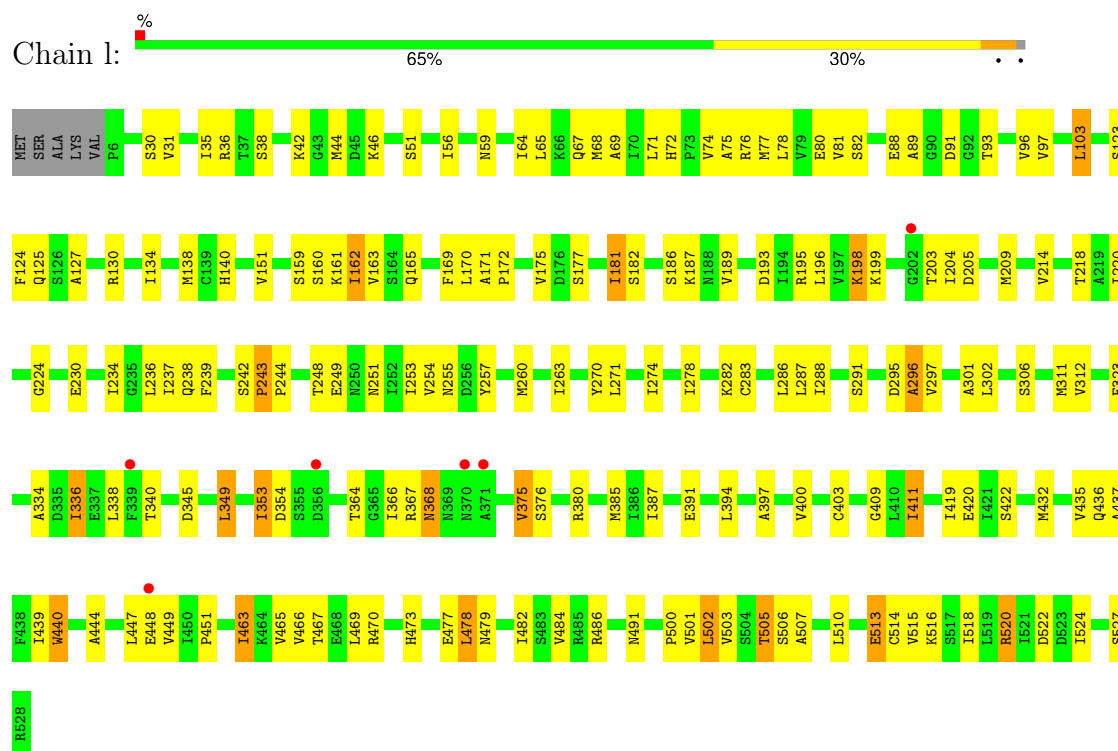
Chain L: 6% 69% 27% ..



- Molecule 6: T-complex protein 1 subunit delta

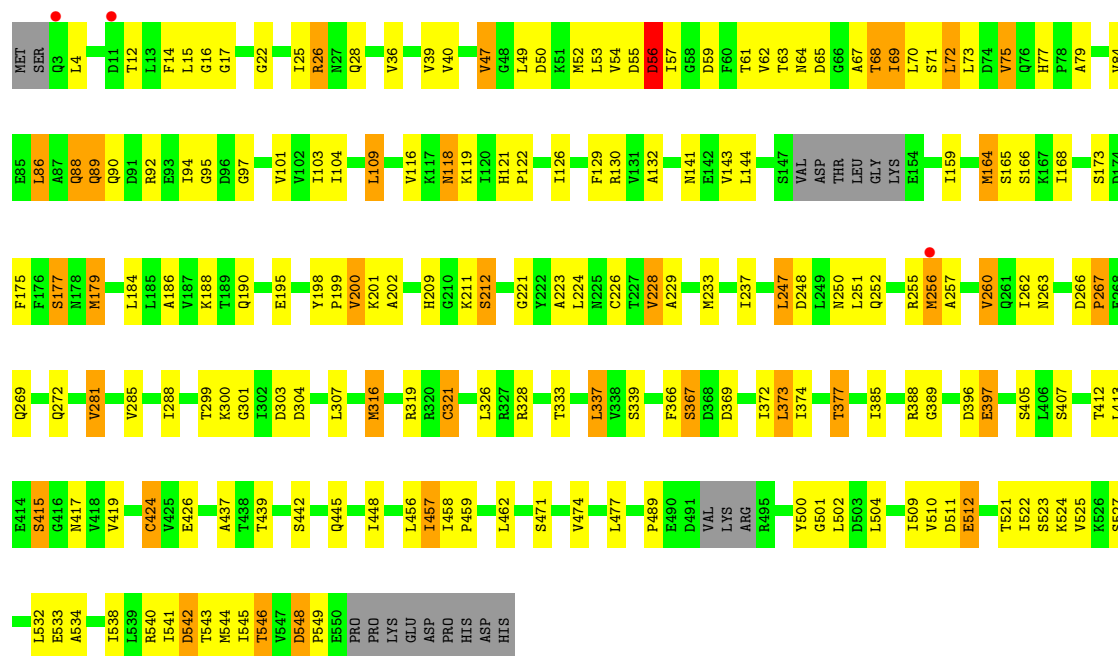


- Molecule 6: T-complex protein 1 subunit delta

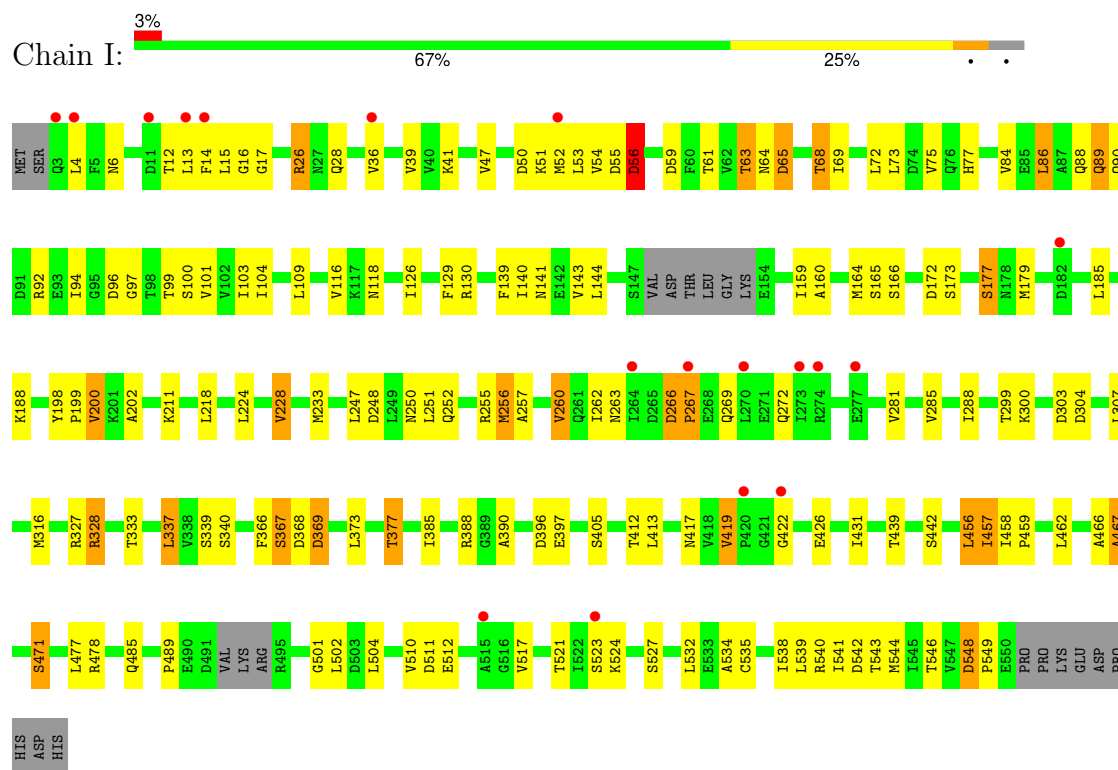


- Molecule 7: T-complex protein 1 subunit alpha

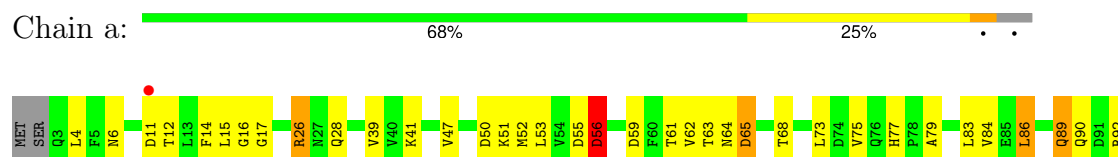


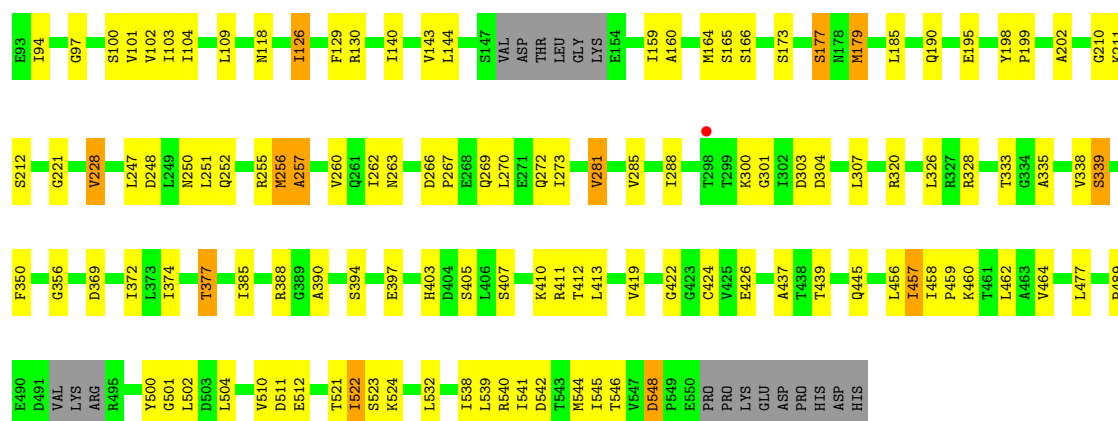


• Molecule 7: T-complex protein 1 subunit alpha

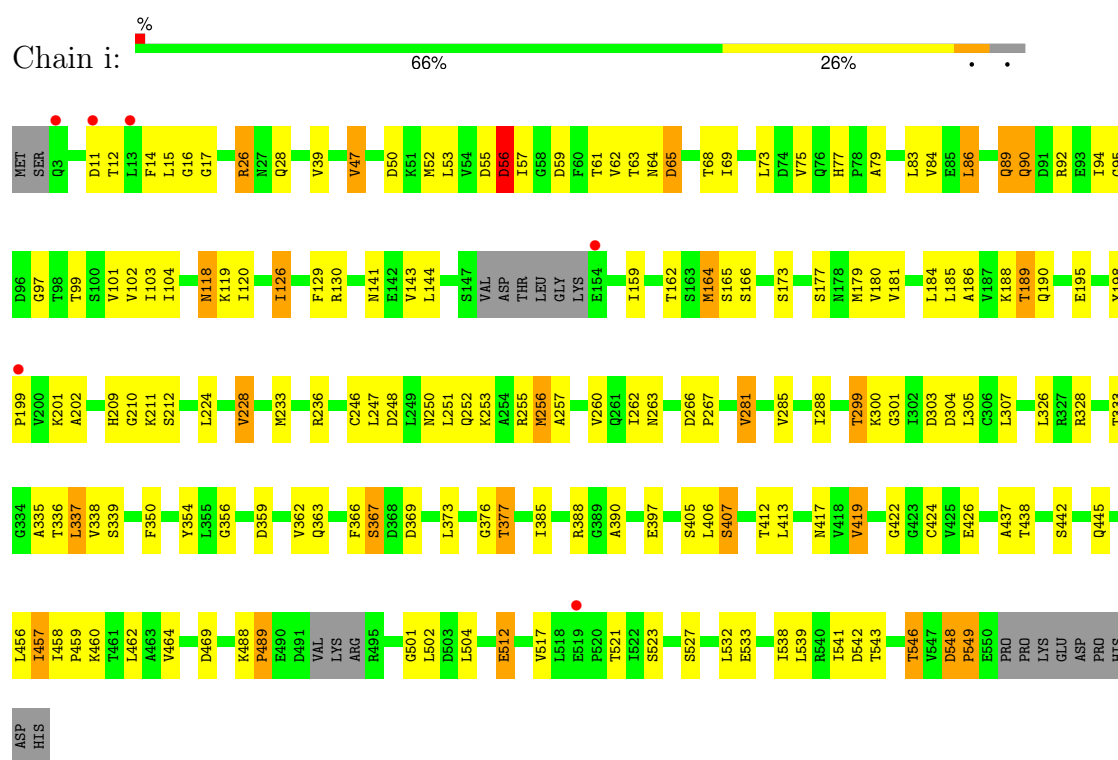


• Molecule 7: T-complex protein 1 subunit alpha



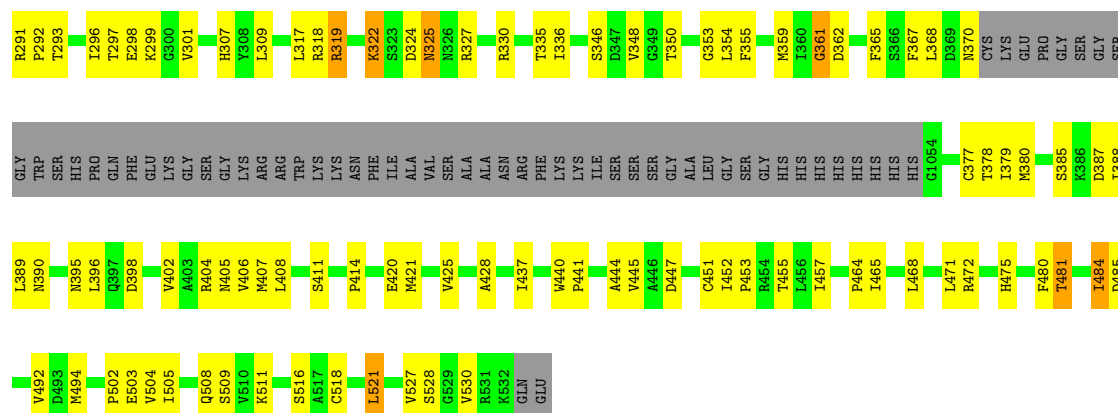


• Molecule 7: T-complex protein 1 subunit alpha

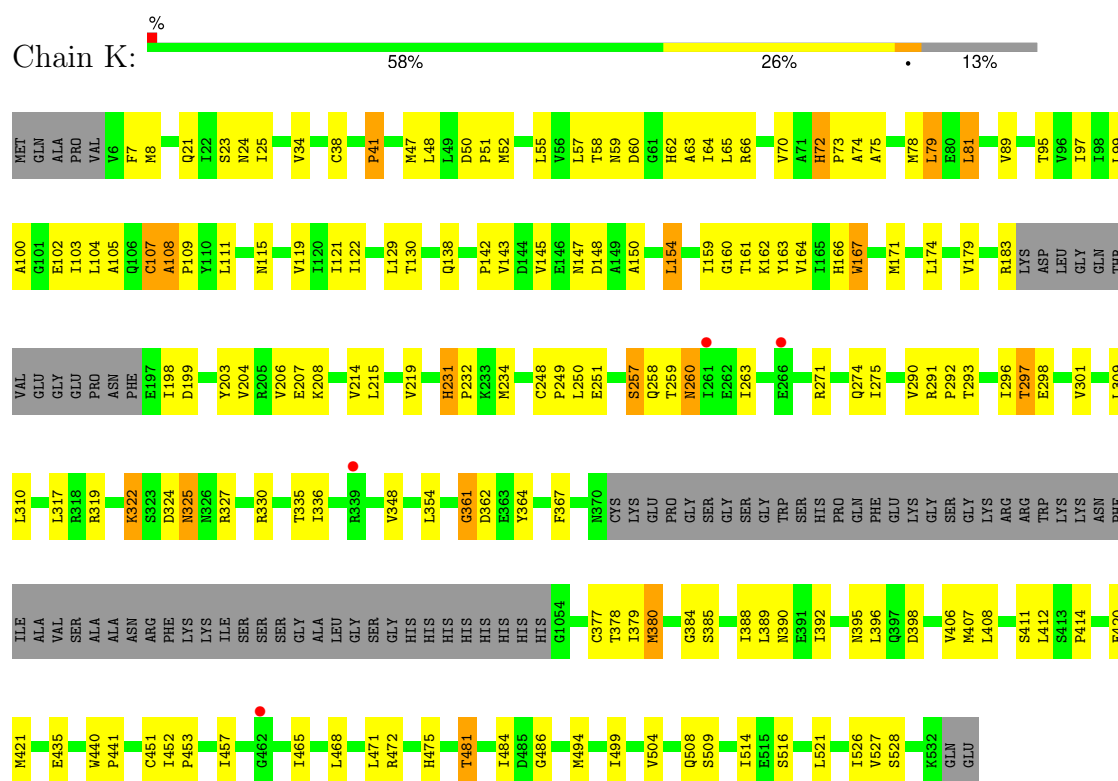


• Molecule 8: T-complex protein 1 subunit gamma

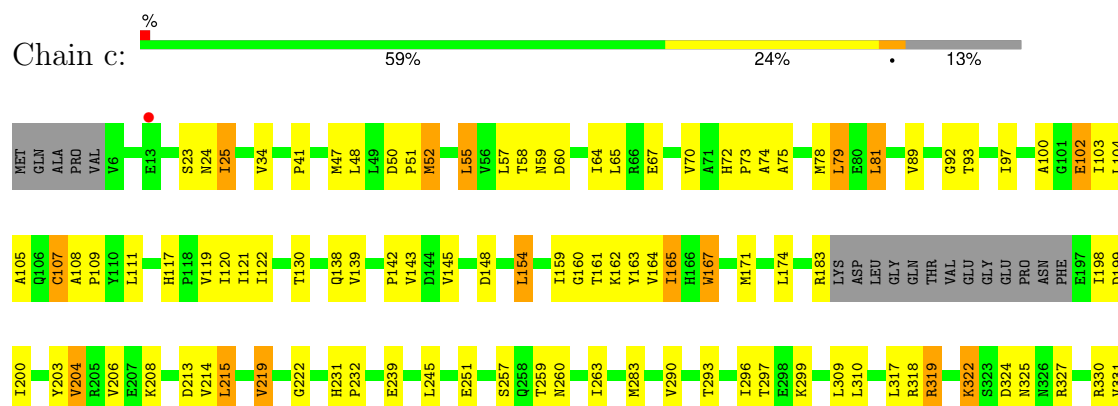


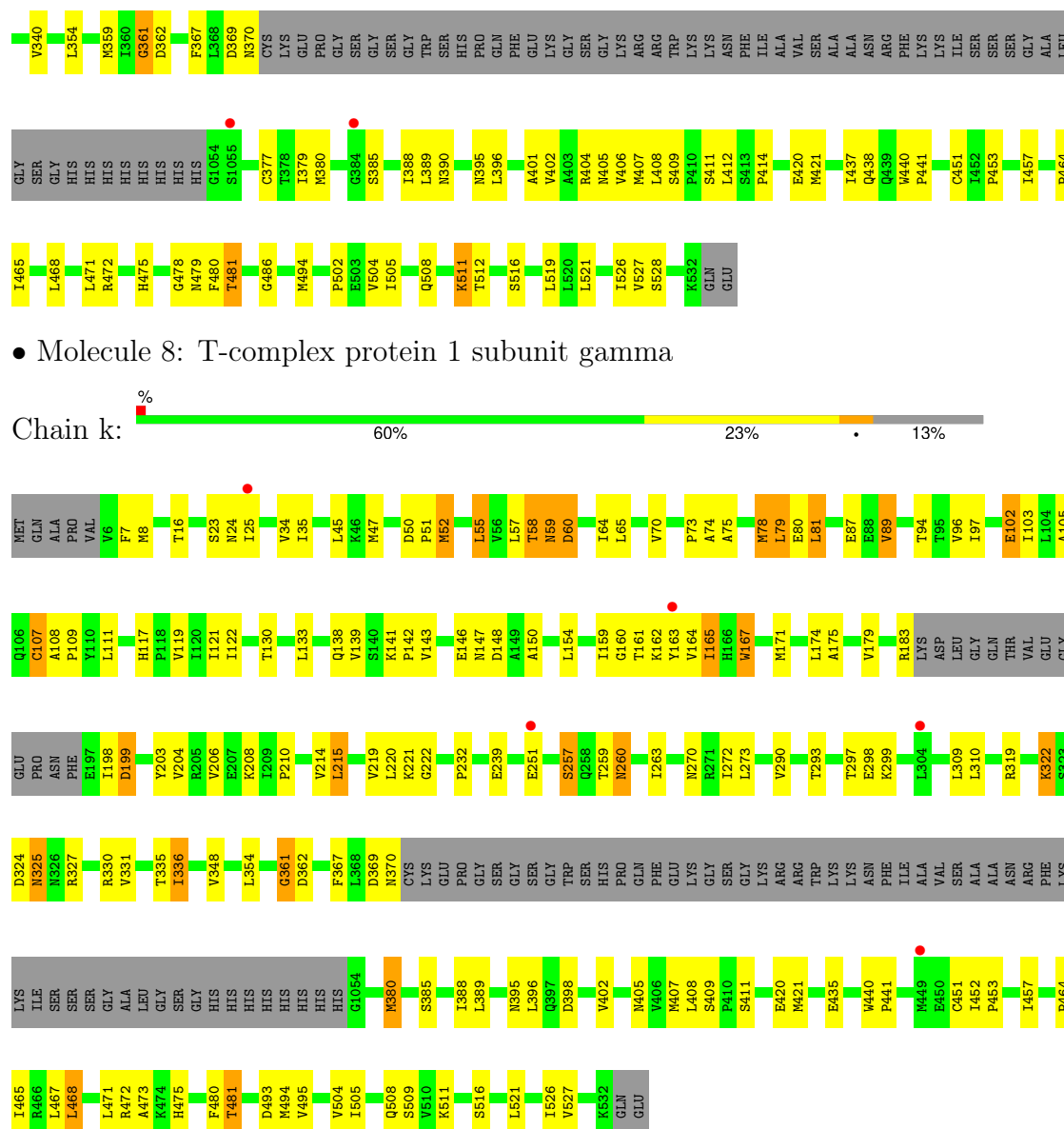


• Molecule 8: T-complex protein 1 subunit gamma



• Molecule 8: T-complex protein 1 subunit gamma





• Molecule 8: T-complex protein 1 subunit gamma

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	159.10Å 162.54Å 268.10Å 85.23° 81.15° 61.17°	Depositor
Resolution (Å)	30.00 – 3.80 30.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	91.6 (30.00-3.80) 91.4 (30.00-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.75Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.257 , 0.305 0.278 , 0.315	Depositor DCC
R_{free} test set	10463 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	116.0	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 119.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.024 for -h,-h+k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	120080	wwPDB-VP
Average B, all atoms (Å ²)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, BEF

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	F	0.49	0/3886	0.88	1/5318 (0.0%)
1	N	0.49	0/3886	0.86	0/5318
1	f	0.48	0/3886	0.85	1/5318 (0.0%)
1	n	0.50	1/3886 (0.0%)	0.87	3/5318 (0.1%)
2	H	0.53	0/3661	0.91	5/5005 (0.1%)
2	P	0.53	0/3661	0.89	3/5005 (0.1%)
2	h	0.53	1/3661 (0.0%)	0.88	2/5005 (0.0%)
2	p	0.53	0/3661	0.88	2/5005 (0.0%)
3	G	0.51	1/3803 (0.0%)	0.89	5/5194 (0.1%)
3	O	0.48	1/3803 (0.0%)	0.89	6/5194 (0.1%)
3	g	0.51	1/3803 (0.0%)	0.90	3/5194 (0.1%)
3	o	0.50	0/3803	0.89	5/5194 (0.1%)
4	E	0.46	0/3849	0.86	2/5252 (0.0%)
4	M	0.47	1/3849 (0.0%)	0.88	3/5252 (0.1%)
4	e	0.49	0/3849	0.88	1/5252 (0.0%)
4	m	0.48	0/3849	0.88	1/5252 (0.0%)
5	B	0.50	0/3726	0.92	5/5077 (0.1%)
5	J	0.49	0/3726	0.87	0/5077
5	b	0.48	0/3726	0.89	0/5077
5	j	0.52	1/3726 (0.0%)	0.90	3/5077 (0.1%)
6	D	0.51	0/3723	0.91	1/5089 (0.0%)
6	L	0.49	0/3723	0.88	3/5089 (0.1%)
6	d	0.50	0/3723	0.89	6/5089 (0.1%)
6	l	0.51	0/3723	0.89	1/5089 (0.0%)
7	A	0.51	0/3805	0.93	9/5196 (0.2%)
7	I	0.49	0/3805	0.89	4/5196 (0.1%)
7	a	0.49	0/3805	0.89	4/5196 (0.1%)
7	i	0.50	0/3805	0.90	5/5196 (0.1%)
8	C	0.54	0/3657	0.92	5/5003 (0.1%)
8	K	0.51	0/3657	0.89	5/5003 (0.1%)
8	c	0.51	0/3657	0.91	7/5003 (0.1%)
8	k	0.50	0/3657	0.91	4/5003 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.50	7/120440 (0.0%)	0.89	105/164536 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
6	d	0	1
6	l	0	1
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	449	ILE	CA-CB	7.91	1.58	1.54
2	h	459	VAL	CA-CB	6.64	1.57	1.54
1	n	454	ILE	CA-CB	5.86	1.57	1.54
3	O	449	ILE	CA-CB	5.36	1.56	1.54
4	M	479	ILE	CA-CB	5.30	1.57	1.54
3	g	449	ILE	CA-CB	5.21	1.57	1.54
5	j	452	SER	CB-OG	5.21	1.52	1.42

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	548	ASP	CA-C-N	7.51	129.22	119.84
7	I	548	ASP	C-N-CA	7.51	129.22	119.84
7	A	548	ASP	CA-C-N	7.21	128.85	119.84
7	A	548	ASP	C-N-CA	7.21	128.85	119.84
8	C	231	HIS	CA-C-N	6.71	126.22	119.24
8	C	231	HIS	C-N-CA	6.71	126.22	119.24
2	H	47	GLY	CA-C-N	6.70	126.32	119.56
2	H	47	GLY	C-N-CA	6.70	126.32	119.56
7	i	266	ASP	CA-C-N	6.58	128.06	119.84
7	i	266	ASP	C-N-CA	6.58	128.06	119.84
1	F	436	ALA	N-CA-C	6.46	118.36	110.41
8	c	199	ASP	N-CA-C	6.36	118.73	110.53
3	O	477	LYS	N-CA-C	6.22	118.06	111.28
3	g	477	LYS	N-CA-C	6.21	117.71	111.07
5	B	38	GLY	CA-C-N	6.14	127.52	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	38	GLY	C-N-CA	6.14	127.52	119.84
8	c	117	HIS	CA-C-N	6.12	125.60	119.24
8	c	117	HIS	C-N-CA	6.12	125.60	119.24
7	i	301	GLY	N-CA-C	6.04	120.28	112.54
2	P	47	GLY	CA-C-N	6.02	125.57	119.19
2	P	47	GLY	C-N-CA	6.02	125.57	119.19
4	E	363	VAL	N-CA-C	5.95	113.97	107.60
3	g	63	SER	N-CA-C	5.94	117.27	108.60
7	I	266	ASP	CA-C-N	5.93	127.26	119.84
7	I	266	ASP	C-N-CA	5.93	127.26	119.84
8	K	199	ASP	N-CA-C	5.91	118.16	110.53
8	C	199	ASP	N-CA-C	5.90	119.15	110.59
7	A	266	ASP	CA-C-N	5.87	127.18	119.84
7	A	266	ASP	C-N-CA	5.87	127.18	119.84
3	g	191	ARG	N-CA-C	-5.86	102.09	110.59
3	o	191	ARG	N-CA-C	-5.86	101.34	110.42
6	D	478	LEU	N-CA-C	5.85	119.77	110.70
7	i	548	ASP	CA-C-N	5.81	127.11	119.84
7	i	548	ASP	C-N-CA	5.81	127.11	119.84
7	a	266	ASP	CA-C-N	5.77	127.06	119.84
7	a	266	ASP	C-N-CA	5.77	127.06	119.84
6	L	478	LEU	N-CA-C	5.72	119.56	110.70
1	f	436	ALA	N-CA-C	5.71	117.69	110.33
8	c	409	SER	CA-C-N	5.70	125.80	119.87
8	c	409	SER	C-N-CA	5.70	125.80	119.87
6	d	478	LEU	N-CA-C	5.68	118.43	109.39
3	G	63	SER	N-CA-C	5.66	117.45	108.79
7	A	168	ILE	N-CA-C	5.65	117.06	110.62
3	G	191	ARG	N-CA-C	-5.60	101.73	110.42
3	O	191	ARG	N-CA-C	-5.57	102.27	110.52
3	o	368	CYS	CA-C-N	5.57	126.80	119.84
3	o	368	CYS	C-N-CA	5.57	126.80	119.84
4	e	84	THR	N-CA-C	5.56	117.43	109.14
7	A	389	GLY	N-CA-C	5.54	118.05	110.69
2	h	47	GLY	CA-C-N	5.53	125.18	119.05
2	h	47	GLY	C-N-CA	5.53	125.18	119.05
5	j	38	GLY	CA-C-N	5.51	126.73	119.84
5	j	38	GLY	C-N-CA	5.51	126.73	119.84
3	O	63	SER	N-CA-C	5.51	116.64	108.60
4	m	363	VAL	N-CA-C	5.50	113.48	107.60
2	H	239	LEU	N-CA-C	-5.46	106.69	113.19
8	C	209	ILE	CA-C-N	5.45	125.45	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	209	ILE	C-N-CA	5.45	125.45	119.90
8	K	72	HIS	CA-C-N	5.44	125.09	119.05
8	K	72	HIS	C-N-CA	5.44	125.09	119.05
2	p	47	GLY	CA-C-N	5.44	125.52	119.32
2	p	47	GLY	C-N-CA	5.44	125.52	119.32
4	M	84	THR	N-CA-C	5.42	116.50	108.86
7	A	301	GLY	N-CA-C	5.41	119.47	112.54
4	E	84	THR	N-CA-C	5.40	116.85	109.18
8	K	231	HIS	CA-C-N	5.39	124.85	119.24
8	K	231	HIS	C-N-CA	5.39	124.85	119.24
3	G	368	CYS	CA-C-N	5.39	126.57	119.84
3	G	368	CYS	C-N-CA	5.39	126.57	119.84
8	c	231	HIS	CA-C-N	5.37	124.83	119.24
8	c	231	HIS	C-N-CA	5.37	124.83	119.24
8	k	199	ASP	N-CA-C	5.36	118.37	110.59
5	B	331	GLU	CA-C-N	5.35	125.02	119.56
5	B	331	GLU	C-N-CA	5.35	125.02	119.56
2	H	79	HIS	CA-C-N	5.34	124.97	119.05
2	H	79	HIS	C-N-CA	5.34	124.97	119.05
6	d	40	GLY	CA-C-N	5.33	125.14	119.28
6	d	40	GLY	C-N-CA	5.33	125.14	119.28
6	L	116	HIS	CA-C-N	5.30	125.11	119.28
6	L	116	HIS	C-N-CA	5.30	125.11	119.28
1	n	153	VAL	N-CA-C	-5.29	107.67	112.96
7	A	474	VAL	N-CA-C	5.25	115.69	110.23
3	O	341	ILE	N-CA-C	5.24	116.17	109.30
5	B	422	ILE	N-CA-C	5.22	115.43	110.53
8	k	409	SER	CA-C-N	5.20	125.89	120.12
8	k	409	SER	C-N-CA	5.20	125.89	120.12
5	j	219	GLY	N-CA-C	5.18	120.62	113.99
6	l	477	GLU	N-CA-C	5.16	115.63	108.00
4	M	85	ASN	N-CA-C	-5.15	108.27	114.75
3	o	45	GLY	CA-C-N	5.14	125.19	119.32
3	o	45	GLY	C-N-CA	5.14	125.19	119.32
1	n	465	ASP	CA-C-N	5.14	124.76	119.05
1	n	465	ASP	C-N-CA	5.14	124.76	119.05
3	O	45	GLY	CA-C-N	5.13	124.75	119.05
3	O	45	GLY	C-N-CA	5.13	124.75	119.05
4	M	363	VAL	N-CA-C	5.13	113.09	107.60
6	d	499	GLN	CA-C-N	5.10	125.03	119.78
6	d	499	GLN	C-N-CA	5.10	125.03	119.78
6	d	477	GLU	N-CA-C	5.09	115.54	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	a	548	ASP	CA-C-N	5.05	126.16	119.84
7	a	548	ASP	C-N-CA	5.05	126.16	119.84
7	A	40	VAL	N-CA-C	5.05	116.41	111.91
2	P	239	LEU	N-CA-C	-5.05	107.18	113.19
8	k	59	ASN	N-CA-C	-5.03	107.22	113.55
3	G	341	ILE	N-CA-C	5.02	115.71	108.93

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	194	VAL	Peptide
6	d	243	PRO	Peptide
6	l	243	PRO	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3836	0	3618	124	0
1	N	3836	0	3618	104	0
1	f	3836	0	3618	98	0
1	n	3836	0	3618	87	0
2	H	3619	0	3425	109	0
2	P	3619	0	3425	85	0
2	h	3619	0	3425	82	0
2	p	3619	0	3425	108	0
3	G	3752	0	3581	129	0
3	O	3752	0	3581	117	0
3	g	3752	0	3581	103	0
3	o	3752	0	3581	113	0
4	E	3798	0	3576	107	0
4	M	3798	0	3576	86	0
4	e	3798	0	3576	94	0
4	m	3798	0	3576	100	0
5	B	3689	0	3546	136	0
5	J	3689	0	3546	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	b	3689	0	3546	104	0
5	j	3689	0	3546	123	0
6	D	3685	0	3540	134	0
6	L	3685	0	3540	102	0
6	d	3685	0	3540	116	0
6	l	3685	0	3540	115	0
7	A	3770	0	3626	132	0
7	I	3770	0	3626	114	0
7	a	3770	0	3626	113	0
7	i	3770	0	3626	121	0
8	C	3615	0	3455	141	0
8	K	3615	0	3455	100	0
8	c	3615	0	3455	101	0
8	k	3615	0	3455	101	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
9	G	1	0	0	0	0
9	H	1	0	0	0	0
9	I	1	0	0	0	0
9	J	1	0	0	0	0
9	K	1	0	0	0	0
9	L	1	0	0	0	0
9	M	1	0	0	0	0
9	N	1	0	0	0	0
9	O	1	0	0	0	0
9	P	1	0	0	0	0
9	a	1	0	0	0	0
9	b	1	0	0	0	0
9	c	1	0	0	0	0
9	d	1	0	0	0	0
9	e	1	0	0	0	0
9	f	1	0	0	0	0
9	g	1	0	0	0	0
9	h	1	0	0	0	0
9	i	1	0	0	0	0
9	j	1	0	0	0	0
9	k	1	0	0	0	0
9	l	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	m	1	0	0	0	0
9	n	1	0	0	0	0
9	o	1	0	0	0	0
9	p	1	0	0	0	0
10	A	27	0	12	0	0
10	B	27	0	12	1	0
10	C	27	0	12	1	0
10	D	27	0	12	1	0
10	E	27	0	12	1	0
10	F	27	0	12	0	0
10	G	27	0	12	0	0
10	H	27	0	12	0	0
10	I	27	0	12	1	0
10	J	27	0	12	1	0
10	K	27	0	12	1	0
10	L	27	0	12	0	0
10	M	27	0	12	1	0
10	N	27	0	12	0	0
10	O	27	0	12	0	0
10	P	27	0	12	0	0
10	a	27	0	12	1	0
10	b	27	0	12	3	0
10	c	27	0	12	4	0
10	d	27	0	12	1	0
10	e	27	0	12	0	0
10	f	27	0	12	0	0
10	g	27	0	12	0	0
10	h	27	0	12	0	0
10	i	27	0	12	0	0
10	j	27	0	12	1	0
10	k	27	0	12	1	0
10	l	27	0	12	0	0
10	m	27	0	12	0	0
10	n	27	0	12	0	0
10	o	27	0	12	0	0
10	p	27	0	12	0	0
11	A	4	0	0	0	0
11	B	4	0	0	0	0
11	C	4	0	0	1	0
11	D	4	0	0	1	0
11	E	4	0	0	1	0
11	F	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	G	4	0	0	0	0
11	H	4	0	0	0	0
11	I	4	0	0	0	0
11	J	4	0	0	1	0
11	K	4	0	0	1	0
11	L	4	0	0	0	0
11	M	4	0	0	1	0
11	N	4	0	0	0	0
11	O	4	0	0	0	0
11	P	4	0	0	0	0
11	a	4	0	0	0	0
11	b	4	0	0	2	0
11	c	4	0	0	1	0
11	d	4	0	0	1	0
11	e	4	0	0	0	0
11	f	4	0	0	0	0
11	g	4	0	0	1	0
11	h	4	0	0	0	0
11	i	4	0	0	0	0
11	j	4	0	0	0	0
11	k	4	0	0	1	0
11	l	4	0	0	0	0
11	m	4	0	0	0	0
11	n	4	0	0	0	0
11	o	4	0	0	1	0
11	p	4	0	0	0	0
All	All	120080	0	113852	3203	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (3203) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:27:GLN:HE21	2:H:544:ILE:HD11	1.02	1.15
3:G:107:GLU:HG2	3:G:448:VAL:HG21	1.24	1.11
3:g:147:ILE:HD11	3:g:409:ILE:HB	1.28	1.11
7:i:26:ARG:HG3	7:i:26:ARG:HH11	1.13	1.09
6:d:520:ARG:HH21	6:d:520:ARG:HG3	1.18	1.08
3:O:107:GLU:HG2	3:O:448:VAL:HG21	1.31	1.07
7:A:26:ARG:HG3	7:A:26:ARG:HH11	1.18	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:26:ARG:HG3	7:I:26:ARG:HH11	1.20	1.05
6:l:353:ILE:HG22	6:l:354:ASP:H	1.20	1.04
2:H:27:GLN:NE2	2:H:544:ILE:HD11	1.72	1.03
6:L:520:ARG:HH21	6:L:520:ARG:HG3	1.20	1.03
5:b:290:ILE:HG12	5:b:307:GLU:HB3	1.39	1.02
1:n:97:LEU:O	1:n:101:LEU:HB2	1.60	1.02
4:m:219:VAL:HG11	4:m:431:ARG:HB2	1.40	1.02
5:b:232:LEU:HB2	5:b:281:ILE:HD13	1.41	1.01
6:d:165:GLN:HG3	7:a:130:ARG:HD3	1.37	1.01
4:e:219:VAL:HG11	4:e:431:ARG:HB2	1.39	1.01
6:l:520:ARG:HH21	6:l:520:ARG:HG3	1.25	1.01
7:a:26:ARG:HG3	7:a:26:ARG:HH11	1.24	1.00
5:J:290:ILE:HG12	5:J:307:GLU:HB3	1.44	0.99
8:K:103:ILE:O	8:K:107:CYS:HB3	1.62	0.98
8:c:183:ARG:HD3	8:c:407:MET:HE3	1.45	0.98
6:D:165:GLN:HG3	7:A:130:ARG:HD3	1.43	0.97
5:j:239:ASP:HA	5:j:291:TYR:HB2	1.47	0.95
6:D:138:MET:HB2	6:D:478:LEU:HD13	1.45	0.95
8:K:59:ASN:HB3	8:K:162:LYS:HG2	1.47	0.95
2:p:62:ILE:HD11	3:o:81:LYS:HD3	1.49	0.94
1:N:97:LEU:O	1:N:101:LEU:HB2	1.65	0.93
8:k:183:ARG:HD3	8:k:407:MET:HE3	1.50	0.93
1:f:97:LEU:O	1:f:101:LEU:HB2	1.68	0.92
3:o:218:VAL:HG21	3:o:326:VAL:HA	1.48	0.92
4:M:219:VAL:HG11	4:M:431:ARG:HB2	1.49	0.92
5:j:183:ARG:HH11	5:j:365:CYS:HB3	1.34	0.92
6:l:165:GLN:HG3	7:i:130:ARG:HD3	1.52	0.92
8:c:103:ILE:O	8:c:107:CYS:HB3	1.71	0.91
6:l:35:ILE:HA	6:l:46:LYS:HZ1	1.35	0.91
6:l:448:GLU:OE2	6:l:466:VAL:HG11	1.71	0.91
6:L:138:MET:HB2	6:L:478:LEU:HD13	1.52	0.90
3:O:218:VAL:HG21	3:O:326:VAL:HA	1.53	0.90
2:p:333:CYS:SG	2:p:340:PRO:HD3	2.12	0.90
1:F:97:LEU:O	1:F:101:LEU:HB2	1.71	0.89
7:A:52:MET:HE3	8:C:73:PRO:HB2	1.52	0.89
2:H:27:GLN:HA	2:H:31:SER:HB2	1.54	0.89
8:C:65:LEU:HB3	8:C:79:LEU:HD13	1.51	0.89
6:l:448:GLU:CD	6:l:470:ARG:HH22	1.79	0.89
1:F:254:SER:HB3	2:H:266:LEU:O	1.73	0.89
8:K:481:THR:HG22	8:K:494:MET:HB2	1.54	0.89
7:A:256:MET:HB3	7:A:260:VAL:HB	1.52	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:195:GLU:HG3	1:f:327:ARG:NH1	1.88	0.88
8:C:103:ILE:O	8:C:107:CYS:HB3	1.73	0.87
5:J:219:GLY:O	5:J:220:ASN:HB2	1.71	0.87
8:k:103:ILE:O	8:k:107:CYS:HB3	1.74	0.87
3:G:218:VAL:HG21	3:G:326:VAL:HA	1.54	0.87
6:l:138:MET:HB2	6:l:478:LEU:HD13	1.55	0.87
3:G:88:ARG:HH11	3:G:88:ARG:HG2	1.37	0.87
4:M:51:ILE:HD13	4:M:134:LEU:HB2	1.57	0.87
3:G:243:SER:HB3	3:G:323:MET:HE1	1.57	0.86
5:b:239:ASP:HA	5:b:291:TYR:HB2	1.58	0.86
2:H:27:GLN:HE21	2:H:544:ILE:CD1	1.87	0.86
1:n:75:LEU:HD12	8:k:55:LEU:HD23	1.55	0.86
3:O:147:ILE:HD11	3:O:409:ILE:HB	1.56	0.86
5:j:413:LYS:HA	5:j:464:TYR:HE1	1.41	0.86
8:C:198:ILE:HG21	8:C:408:LEU:HD21	1.57	0.85
6:D:520:ARG:HH21	6:D:520:ARG:HG3	1.41	0.85
6:l:127:ALA:HA	6:l:440:TRP:HE1	1.41	0.85
3:o:147:ILE:HD11	3:o:409:ILE:HB	1.56	0.85
5:B:219:GLY:O	5:B:220:ASN:HB2	1.76	0.85
5:J:413:LYS:HA	5:J:464:TYR:HE1	1.40	0.85
7:a:55:ASP:HB2	7:a:59:ASP:O	1.75	0.85
6:l:432:MET:SD	6:l:440:TRP:HZ3	2.00	0.85
3:O:107:GLU:CG	3:O:448:VAL:HG21	2.07	0.84
7:I:12:THR:HB	7:I:14:PHE:CE2	2.12	0.84
5:J:239:ASP:HA	5:J:291:TYR:HB2	1.57	0.84
5:b:413:LYS:HA	5:b:464:TYR:HE1	1.43	0.84
3:o:189:LEU:HD11	3:o:195:ASP:O	1.78	0.84
5:j:232:LEU:HB2	5:j:281:ILE:HD13	1.59	0.84
8:c:59:ASN:HB3	8:c:162:LYS:HG2	1.58	0.84
1:f:195:GLU:HG3	1:f:327:ARG:HH11	1.43	0.84
2:P:41:MET:HE1	3:O:524:ILE:HD11	1.60	0.83
3:O:135:LEU:HD23	3:O:424:LEU:HD23	1.61	0.83
3:g:218:VAL:HG21	3:g:326:VAL:HA	1.60	0.83
4:E:107:LEU:HG	4:E:544:LEU:HD13	1.59	0.83
7:a:12:THR:HB	7:a:14:PHE:CE2	2.14	0.83
5:b:183:ARG:HH11	5:b:365:CYS:HB3	1.40	0.83
7:a:256:MET:HG2	8:c:257:SER:HB2	1.59	0.83
5:j:183:ARG:HH22	5:j:211:GLY:H	1.27	0.83
4:E:219:VAL:HG11	4:E:431:ARG:HB2	1.61	0.82
1:N:251:PHE:HB3	8:K:263:ILE:HB	1.61	0.82
4:M:72:LYS:HB2	4:M:90:ILE:HD12	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:448:GLU:OE2	6:D:466:VAL:HG11	1.79	0.82
4:E:115:ILE:HD13	4:E:533:GLY:HA2	1.60	0.82
7:A:16:GLY:O	7:A:548:ASP:N	2.11	0.82
3:O:86:ILE:HD11	3:O:510:ALA:HA	1.62	0.82
3:O:297:LEU:HB3	3:O:298:PRO:HD2	1.58	0.82
5:B:290:ILE:HG12	5:B:307:GLU:HB3	1.60	0.82
7:A:55:ASP:O	7:A:56:ASP:HB3	1.78	0.82
3:g:297:LEU:HB3	3:g:298:PRO:HD2	1.60	0.82
7:A:26:ARG:HH11	7:A:26:ARG:CG	1.92	0.82
3:O:107:GLU:HG2	3:O:448:VAL:CG2	2.09	0.82
5:b:441:PRO:HA	5:b:444:LEU:HD12	1.62	0.82
8:c:453:PRO:O	8:c:457:ILE:HG12	1.80	0.82
6:l:353:ILE:HG22	6:l:354:ASP:N	1.95	0.81
7:I:129:PHE:HB3	7:I:532:LEU:HD11	1.62	0.81
6:l:35:ILE:HA	6:l:46:LYS:NZ	1.95	0.81
6:l:64:ILE:HG22	6:l:68:MET:HE3	1.62	0.81
8:C:481:THR:HG22	8:C:494:MET:HB2	1.63	0.81
3:G:297:LEU:HB3	3:G:298:PRO:HD2	1.60	0.81
6:D:25:ILE:HG23	6:D:104:LEU:HB3	1.62	0.81
3:g:88:ARG:HG2	3:g:88:ARG:HH11	1.45	0.81
6:l:71:LEU:HD21	7:i:15:LEU:HB2	1.63	0.81
6:d:138:MET:HB2	6:d:478:LEU:HD13	1.63	0.81
3:G:107:GLU:CG	3:G:448:VAL:HG21	2.09	0.80
6:D:127:ALA:HA	6:D:440:TRP:HE1	1.46	0.80
5:J:291:TYR:HB3	5:J:294:PRO:HD2	1.63	0.80
7:I:52:MET:HE3	8:K:73:PRO:HB2	1.63	0.80
7:I:94:ILE:HD13	7:I:523:SER:HA	1.64	0.80
5:j:279:PHE:HB3	5:j:281:ILE:HD12	1.62	0.80
8:C:183:ARG:HD3	8:C:407:MET:HE3	1.64	0.80
7:a:212:SER:HB2	8:c:511:LYS:HE3	1.63	0.80
5:j:183:ARG:NH1	5:j:365:CYS:HB3	1.95	0.80
3:G:86:ILE:HD11	3:G:510:ALA:HA	1.64	0.79
3:g:107:GLU:HG2	3:g:448:VAL:HG21	1.64	0.79
7:I:256:MET:HB3	7:I:260:VAL:HB	1.65	0.79
5:j:285:ILE:HG22	5:j:306:ILE:HB	1.64	0.79
2:h:62:ILE:HD11	3:g:81:LYS:HD3	1.65	0.78
7:i:12:THR:HB	7:i:14:PHE:CE2	2.18	0.78
7:i:103:ILE:HG22	7:i:457:ILE:HG21	1.63	0.78
6:L:165:GLN:HG3	7:I:130:ARG:HD3	1.66	0.78
6:d:244:PRO:HD3	6:d:270:TYR:CE2	2.18	0.78
2:h:41:MET:HE2	2:h:53:LYS:HD3	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:c:162:LYS:HB2	8:c:395:ASN:OD1	1.83	0.78
3:G:280:GLU:O	3:G:284:GLN:HB2	1.82	0.78
2:P:225:GLY:HA2	2:P:335:VAL:HG21	1.66	0.78
1:f:254:SER:HB3	2:h:266:LEU:O	1.84	0.78
2:h:46:MET:HE2	2:h:105:ILE:HD13	1.66	0.78
5:b:285:ILE:HD12	5:b:317:LEU:HD13	1.65	0.78
5:J:46:LEU:HD11	5:J:63:ILE:HA	1.66	0.77
5:B:239:ASP:HA	5:B:291:TYR:HB2	1.66	0.77
7:A:164:MET:HA	7:A:164:MET:HE2	1.66	0.77
1:n:439:LYS:O	1:n:442:THR:HG22	1.83	0.77
5:B:232:LEU:HB2	5:B:281:ILE:HD13	1.66	0.77
5:J:232:LEU:HB2	5:J:281:ILE:HD13	1.66	0.77
3:o:297:LEU:HB3	3:o:298:PRO:HD2	1.65	0.77
5:j:285:ILE:HD12	5:j:317:LEU:HD13	1.64	0.77
3:G:107:GLU:HG2	3:G:448:VAL:CG2	2.10	0.77
1:n:254:SER:HB3	2:p:266:LEU:O	1.84	0.77
7:a:55:ASP:O	7:a:56:ASP:HB3	1.81	0.77
5:j:301:LEU:HD23	5:j:303:ILE:HD11	1.65	0.77
1:F:251:PHE:HB3	8:C:263:ILE:HB	1.64	0.77
5:B:46:LEU:HD11	5:B:63:ILE:HA	1.67	0.77
8:C:50:ASP:HB2	8:C:51:PRO:HD3	1.66	0.77
5:J:183:ARG:HH11	5:J:365:CYS:HB3	1.50	0.77
2:h:225:GLY:HA2	2:h:335:VAL:HG21	1.66	0.77
5:b:285:ILE:HG22	5:b:306:ILE:HB	1.64	0.76
3:o:37:GLN:HG3	3:o:103:ILE:HA	1.66	0.76
3:G:147:ILE:HD11	3:G:409:ILE:HB	1.67	0.76
5:j:46:LEU:HD11	5:j:63:ILE:HA	1.66	0.76
6:D:210:ILE:HD12	6:D:214:VAL:HG22	1.67	0.76
7:I:458:ILE:HB	7:I:459:PRO:HD3	1.65	0.76
1:F:93:THR:O	1:F:97:LEU:HB2	1.85	0.76
5:B:285:ILE:HD12	5:B:317:LEU:HD13	1.66	0.76
5:B:291:TYR:HB3	5:B:294:PRO:HD2	1.67	0.76
7:A:17:GLY:HA2	7:A:546:THR:O	1.86	0.76
2:P:546:MET:HE1	3:O:10:ILE:HG23	1.66	0.76
4:M:73:ILE:HD11	5:J:72:PRO:HB2	1.65	0.76
2:H:225:GLY:HA2	2:H:335:VAL:HG21	1.68	0.76
7:A:129:PHE:HB3	7:A:532:LEU:HD11	1.67	0.76
5:B:183:ARG:HH22	5:B:210:GLU:HA	1.50	0.76
6:L:237:ILE:HD11	6:L:286:LEU:HD22	1.67	0.76
4:e:107:LEU:HG	4:e:544:LEU:HD13	1.66	0.76
2:h:284:ILE:HD11	2:h:308:LEU:HB3	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:86:ILE:HD11	3:g:510:ALA:HA	1.67	0.75
6:L:288:ILE:HD13	6:L:297:VAL:HG21	1.67	0.75
7:I:16:GLY:O	7:I:548:ASP:N	2.19	0.75
6:l:35:ILE:HD11	6:l:65:LEU:HD21	1.67	0.75
4:e:180:LEU:HD22	4:e:430:VAL:HG13	1.67	0.75
8:c:198:ILE:HG21	8:c:408:LEU:HD21	1.67	0.75
7:A:262:ILE:HG21	8:C:259:THR:HG23	1.68	0.75
4:m:115:ILE:HD13	4:m:533:GLY:HA2	1.66	0.75
5:B:80:ILE:HD12	5:B:504:ALA:HB2	1.68	0.75
7:i:94:ILE:HD13	7:i:523:SER:HA	1.69	0.75
8:k:89:VAL:HG11	8:k:505:ILE:CG1	2.17	0.75
8:k:162:LYS:HB2	8:k:395:ASN:OD1	1.86	0.75
6:D:448:GLU:CD	6:D:470:ARG:HH22	1.95	0.74
5:b:291:TYR:HB3	5:b:294:PRO:HD2	1.68	0.74
7:i:262:ILE:HG21	8:k:259:THR:HG23	1.69	0.74
4:e:192:ILE:HD11	4:e:415:ILE:HG23	1.69	0.74
6:D:288:ILE:HD13	6:D:297:VAL:HG21	1.68	0.74
7:I:165:SER:O	7:I:166:SER:HB3	1.86	0.74
7:i:458:ILE:HB	7:i:459:PRO:HD3	1.70	0.74
3:O:189:LEU:HD11	3:O:195:ASP:O	1.86	0.74
6:L:448:GLU:CD	6:L:470:ARG:HH22	1.94	0.74
5:b:95:VAL:HG22	5:b:497:VAL:HA	1.67	0.74
7:a:52:MET:HE3	8:c:73:PRO:HB2	1.70	0.74
4:E:211:VAL:HG12	4:E:402:LYS:O	1.87	0.74
7:a:262:ILE:HG21	8:c:259:THR:HG23	1.68	0.74
2:H:78:VAL:HB	3:G:11:VAL:O	1.88	0.74
8:K:162:LYS:HB2	8:K:395:ASN:OD1	1.87	0.74
3:G:478:TRP:CE3	3:G:492:PHE:HB2	2.22	0.74
6:L:71:LEU:HD21	7:I:15:LEU:HB2	1.69	0.74
6:L:420:GLU:HB2	6:L:473:HIS:CE1	2.23	0.74
6:l:288:ILE:HD13	6:l:297:VAL:HG21	1.69	0.74
4:e:64:SER:HB2	4:e:72:LYS:NZ	2.03	0.74
5:b:231:ILE:HD12	5:b:321:THR:HG21	1.69	0.74
5:b:409:MET:HG3	5:b:459:LEU:HD21	1.70	0.74
8:C:59:ASN:HB3	8:C:162:LYS:HG2	1.70	0.73
6:L:274:ILE:O	6:L:278:ILE:HG12	1.88	0.73
5:j:490:SER:HB3	5:j:493:LEU:HB2	1.70	0.73
6:d:274:ILE:O	6:d:278:ILE:HG12	1.87	0.73
7:A:50:ASP:OD1	7:A:64:ASN:HB2	1.89	0.73
8:k:111:LEU:HD22	8:k:440:TRP:HB3	1.70	0.73
1:n:253:TYR:CE1	1:n:259:ARG:HG3	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:204:ILE:HD13	3:g:362:TYR:CE2	2.23	0.73
7:I:26:ARG:HH11	7:I:26:ARG:CG	2.00	0.73
5:B:183:ARG:NH2	5:B:210:GLU:HA	2.03	0.73
8:C:24:ASN:HD22	8:C:74:ALA:HB2	1.54	0.73
7:A:304:ASP:HA	7:A:307:LEU:HD12	1.71	0.73
5:B:231:ILE:HD12	5:B:321:THR:HG21	1.71	0.73
8:C:353:GLY:HA3	8:C:370:ASN:HB2	1.69	0.73
2:P:240:SER:HA	2:P:245:HIS:NE2	2.04	0.73
3:O:77:HIS:CE1	3:O:79:ALA:HB3	2.24	0.73
7:a:16:GLY:O	7:a:548:ASP:N	2.22	0.73
3:o:204:ILE:HD12	3:o:205:PRO:HD2	1.70	0.72
6:l:274:ILE:O	6:l:278:ILE:HG12	1.88	0.72
2:H:65:THR:HG22	2:H:67:ASP:H	1.54	0.72
1:N:195:GLU:HG3	1:N:327:ARG:NH1	2.04	0.72
7:I:103:ILE:HG22	7:I:457:ILE:HG21	1.71	0.72
7:A:94:ILE:HD13	7:A:523:SER:HA	1.70	0.72
5:b:183:ARG:NH1	5:b:365:CYS:HB3	2.03	0.72
6:L:47:MET:HE3	7:I:544:MET:SD	2.29	0.72
5:j:219:GLY:O	5:j:220:ASN:HB2	1.88	0.72
6:l:353:ILE:CG2	6:l:354:ASP:H	1.99	0.72
7:i:55:ASP:HB2	7:i:59:ASP:O	1.89	0.72
1:N:254:SER:HB3	2:P:266:LEU:O	1.89	0.72
3:G:242:LEU:HD22	3:G:244:LEU:HG	1.71	0.72
2:H:62:ILE:HD11	3:G:81:LYS:HD3	1.72	0.72
4:e:51:ILE:HD13	4:e:134:LEU:HB2	1.72	0.72
2:p:225:GLY:HA2	2:p:335:VAL:HG21	1.72	0.72
5:J:373:THR:HG21	6:L:77:MET:HE3	1.70	0.72
3:g:189:LEU:HD11	3:g:195:ASP:O	1.90	0.72
8:C:208:LYS:HE3	8:C:390:ASN:OD1	1.89	0.72
3:O:446:LEU:HD21	3:O:507:LEU:HD21	1.69	0.72
7:I:179:MET:HE1	7:I:385:ILE:HG23	1.71	0.72
6:d:127:ALA:HA	6:d:440:TRP:HE1	1.54	0.72
8:k:481:THR:HG22	8:k:494:MET:HB2	1.71	0.72
8:C:31:VAL:HG11	8:C:78:MET:HG2	1.71	0.71
2:P:62:ILE:HD11	3:O:81:LYS:HD3	1.72	0.71
8:c:481:THR:HG22	8:c:494:MET:HB2	1.71	0.71
3:g:242:LEU:HD22	3:g:244:LEU:HG	1.71	0.71
4:e:387:THR:HB	5:b:86:ASP:O	1.90	0.71
8:k:89:VAL:HG11	8:k:505:ILE:HG12	1.70	0.71
3:g:446:LEU:HD21	3:g:507:LEU:HD21	1.71	0.71
7:A:458:ILE:HB	7:A:459:PRO:HD3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:j:373:THR:HG22	5:j:375:GLN:H	1.55	0.71
5:b:413:LYS:HA	5:b:464:TYR:CE1	2.25	0.71
5:j:290:ILE:HG12	5:j:307:GLU:HB3	1.72	0.71
5:J:413:LYS:HA	5:J:464:TYR:CE1	2.25	0.71
8:k:121:ILE:HG23	8:k:441:PRO:HB3	1.73	0.71
8:K:50:ASP:HB2	8:K:51:PRO:HD3	1.72	0.71
7:I:164:MET:HA	7:I:164:MET:HE2	1.73	0.71
7:i:63:THR:HA	7:i:397:GLU:HG3	1.73	0.71
5:b:80:ILE:HD12	5:b:504:ALA:HB2	1.73	0.70
3:o:88:ARG:HG2	3:o:88:ARG:HH11	1.56	0.70
6:L:520:ARG:HH21	6:L:520:ARG:CG	2.03	0.70
7:I:86:LEU:HD21	7:I:101:VAL:HG12	1.73	0.70
6:D:353:ILE:HG22	6:D:354:ASP:N	2.06	0.70
7:A:26:ARG:HG3	7:A:26:ARG:NH1	2.00	0.70
7:A:55:ASP:HB2	7:A:59:ASP:O	1.91	0.70
6:d:35:ILE:HA	6:d:46:LYS:NZ	2.07	0.70
4:m:411:SER:HB3	5:j:503:GLU:OE1	1.92	0.70
6:D:237:ILE:HD11	6:D:286:LEU:HD22	1.72	0.70
1:N:103:ARG:O	1:N:107:ARG:HD2	1.92	0.70
4:M:494:THR:O	4:M:498:LEU:HB2	1.92	0.70
1:n:159:LEU:HA	1:n:167:THR:HG21	1.73	0.70
3:o:280:GLU:O	3:o:284:GLN:HB2	1.92	0.70
7:i:164:MET:HE2	7:i:164:MET:HA	1.73	0.70
7:i:165:SER:O	7:i:166:SER:HB3	1.89	0.70
2:H:240:SER:HA	2:H:245:HIS:NE2	2.07	0.70
4:m:328:ASP:OD2	5:j:245:ILE:HD11	1.92	0.70
2:H:41:MET:HE2	2:H:53:LYS:HD3	1.73	0.70
7:A:424:CYS:SG	7:A:500:TYR:HB2	2.31	0.70
7:a:104:ILE:HG12	7:a:458:ILE:HD11	1.73	0.70
1:F:253:TYR:CE1	1:F:259:ARG:HG3	2.27	0.70
8:C:50:ASP:HB2	8:C:51:PRO:CD	2.22	0.70
8:C:367:PHE:HE2	8:C:380:MET:HE1	1.57	0.70
7:i:63:THR:HG23	7:i:397:GLU:HG2	1.74	0.70
3:G:147:ILE:HD13	3:G:157:LEU:HD11	1.74	0.69
3:G:220:PHE:C	3:G:222:LYS:H	1.99	0.69
3:g:388:GLU:O	3:g:392:SER:HB2	1.92	0.69
6:d:244:PRO:HD3	6:d:270:TYR:HE2	1.56	0.69
4:m:494:THR:O	4:m:498:LEU:HB2	1.92	0.69
3:O:245:ASN:HB3	3:O:336:SER:HA	1.74	0.69
6:l:448:GLU:CD	6:l:470:ARG:NH2	2.49	0.69
1:F:181:VAL:HG22	1:F:193:MET:CB	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:130:ARG:O	6:D:134:ILE:HG13	1.93	0.69
6:D:74:VAL:HG13	6:D:518:ILE:HD12	1.72	0.69
3:o:264:VAL:HG23	4:m:294:GLU:OE2	1.91	0.69
1:F:159:LEU:HA	1:F:167:THR:HG21	1.75	0.69
5:J:183:ARG:HH22	5:J:211:GLY:H	1.39	0.69
7:A:462:LEU:HB3	7:A:504:LEU:HD11	1.75	0.69
1:n:93:THR:O	1:n:97:LEU:HB2	1.92	0.69
6:D:274:ILE:O	6:D:278:ILE:HG12	1.92	0.69
2:h:240:SER:HA	2:h:245:HIS:NE2	2.08	0.69
7:i:28:GLN:HE21	7:i:77:HIS:HE1	1.40	0.69
5:b:440:LEU:HB3	5:b:441:PRO:HD3	1.74	0.69
6:d:125:GLN:HE21	6:d:513:GLU:HG2	1.58	0.69
6:d:214:VAL:HG23	6:d:376:SER:HB3	1.74	0.69
7:a:256:MET:HB3	7:a:260:VAL:HB	1.75	0.69
2:p:27:GLN:HE21	2:p:544:ILE:HD11	1.58	0.69
3:o:107:GLU:HG2	3:o:448:VAL:HG21	1.75	0.69
4:E:96:LEU:HD13	4:E:101:ALA:HB1	1.74	0.69
6:D:35:ILE:HA	6:D:46:LYS:NZ	2.08	0.69
6:D:238:GLN:HB2	6:D:334:ALA:HA	1.75	0.69
5:b:132:LEU:HD21	5:b:495:ARG:HG3	1.75	0.69
8:K:47:MET:HG3	8:K:57:LEU:HB3	1.75	0.68
7:a:103:ILE:HG22	7:a:457:ILE:HG21	1.76	0.68
1:n:251:PHE:HB3	8:k:263:ILE:HB	1.74	0.68
8:C:162:LYS:HB2	8:C:395:ASN:OD1	1.92	0.68
1:N:181:VAL:HG22	1:N:193:MET:CB	2.23	0.68
6:d:520:ARG:HH21	6:d:520:ARG:CG	2.02	0.68
2:h:333:CYS:SG	2:h:340:PRO:HD3	2.33	0.68
3:g:153:SER:HB3	3:g:156:GLU:CB	2.23	0.68
3:G:163:ARG:HG2	3:G:179:VAL:HG21	1.75	0.68
7:a:164:MET:HE2	7:a:164:MET:HA	1.74	0.68
3:o:167:SER:O	3:o:168:SER:HB3	1.91	0.68
6:l:244:PRO:HD3	6:l:270:TYR:CE2	2.29	0.68
1:f:181:VAL:HG22	1:f:193:MET:CB	2.23	0.68
5:b:132:LEU:CD2	5:b:495:ARG:HG3	2.24	0.68
5:j:80:ILE:HD12	5:j:504:ALA:HB2	1.75	0.68
5:B:285:ILE:HG22	5:B:306:ILE:HB	1.76	0.68
6:l:138:MET:SD	6:l:478:LEU:HD22	2.34	0.68
7:i:256:MET:HB3	7:i:260:VAL:HB	1.76	0.68
4:e:29:PHE:H	4:e:29:PHE:HD2	1.42	0.68
5:j:413:LYS:HA	5:j:464:TYR:CE1	2.25	0.68
6:l:163:VAL:HG23	6:l:204:ILE:HG21	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:421:MET:HE2	8:C:472:ARG:HA	1.75	0.67
5:J:285:ILE:HG22	5:J:306:ILE:HB	1.76	0.67
3:g:419:GLU:HB2	3:g:472:HIS:HE1	1.59	0.67
7:a:501:GLY:HA3	7:a:512:GLU:HG2	1.76	0.67
6:D:253:ILE:CG2	7:A:263:ASN:HB2	2.24	0.67
6:D:432:MET:SD	6:D:440:TRP:HZ3	2.17	0.67
3:O:204:ILE:HD12	3:O:205:PRO:HD2	1.74	0.67
6:d:35:ILE:HD11	6:d:65:LEU:HD21	1.76	0.67
6:d:288:ILE:HD13	6:d:297:VAL:HG21	1.75	0.67
5:j:279:PHE:HB3	5:j:281:ILE:CD1	2.24	0.67
1:N:178:VAL:HG22	1:N:399:LEU:HD23	1.74	0.67
7:i:52:MET:HE3	8:k:73:PRO:HB2	1.75	0.67
3:G:88:ARG:HG2	3:G:88:ARG:NH1	2.09	0.67
3:G:147:ILE:HD13	3:G:157:LEU:CD1	2.25	0.67
6:D:353:ILE:CG2	6:D:354:ASP:H	2.08	0.67
4:e:211:VAL:HB	4:e:223:LEU:HD23	1.74	0.67
7:i:26:ARG:HH11	7:i:26:ARG:CG	1.97	0.67
6:L:127:ALA:HA	6:L:440:TRP:HE1	1.59	0.67
6:l:138:MET:SD	6:l:478:LEU:CD2	2.83	0.67
4:M:98:ASN:HD22	4:M:101:ALA:H	1.42	0.67
6:L:448:GLU:OE2	6:L:466:VAL:HG11	1.95	0.67
1:F:248:ASN:HB2	8:C:260:ASN:HB3	1.75	0.67
2:P:26:GLY:O	2:P:31:SER:HB2	1.94	0.67
7:a:251:LEU:HD23	7:a:285:VAL:HG22	1.76	0.67
1:F:79:ALA:HB2	1:F:523:ILE:HD12	1.76	0.67
6:L:238:GLN:HB2	6:L:334:ALA:HA	1.75	0.67
3:G:419:GLU:HB2	3:G:472:HIS:HE1	1.60	0.67
6:D:520:ARG:HH21	6:D:520:ARG:CG	2.07	0.67
4:M:73:ILE:HG22	5:J:511:VAL:HG13	1.77	0.67
4:M:115:ILE:HD13	4:M:533:GLY:HA2	1.77	0.67
5:j:231:ILE:HD12	5:j:321:THR:HG21	1.76	0.67
3:G:55:THR:HG22	3:G:56:SER:H	1.59	0.66
8:C:162:LYS:O	8:C:164:VAL:N	2.28	0.66
8:C:219:VAL:HG22	8:C:379:ILE:HG12	1.76	0.66
3:G:245:ASN:HB3	3:G:336:SER:HA	1.77	0.66
1:N:75:LEU:HD12	8:K:55:LEU:HD23	1.75	0.66
3:O:77:HIS:HE1	3:O:79:ALA:HB3	1.59	0.66
2:p:509:VAL:CG1	2:p:510:LYS:H	2.08	0.66
4:m:40:ARG:NH1	4:m:42:HIS:ND1	2.43	0.66
7:i:55:ASP:O	7:i:56:ASP:HB3	1.93	0.66
6:D:479:ASN:HB2	6:D:491:ASN:OD1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:50:ASP:OD1	7:a:64:ASN:HB2	1.95	0.66
6:l:520:ARG:HH21	6:l:520:ARG:CG	2.05	0.66
8:C:414:PRO:CB	8:C:481:THR:HG23	2.25	0.66
5:J:231:ILE:HD12	5:J:321:THR:HG21	1.76	0.66
7:I:41:LYS:HE2	7:I:103:ILE:HG23	1.78	0.66
5:b:219:GLY:O	5:b:220:ASN:HB2	1.94	0.66
2:p:27:GLN:HA	2:p:31:SER:HB2	1.76	0.66
2:p:509:VAL:CG1	2:p:510:LYS:N	2.57	0.66
3:o:221:LYS:HA	3:o:362:TYR:CZ	2.31	0.66
6:L:397:ALA:O	6:L:400:VAL:HG22	1.95	0.66
3:g:45:GLY:HA3	3:g:453:LEU:HD22	1.77	0.66
5:B:183:ARG:HH11	5:B:365:CYS:HB3	1.61	0.66
6:D:38:SER:HB2	6:D:46:LYS:HE3	1.78	0.66
7:a:53:LEU:HD23	8:c:527:VAL:HB	1.78	0.66
3:O:362:TYR:CE1	3:O:377:LEU:HD21	2.31	0.66
4:M:61:ILE:HD11	4:M:91:LEU:HD21	1.77	0.66
7:I:17:GLY:HA2	7:I:546:THR:O	1.95	0.66
8:c:65:LEU:HB3	8:c:79:LEU:HD13	1.77	0.66
1:n:181:VAL:HG22	1:n:193:MET:CB	2.26	0.66
4:m:107:LEU:HG	4:m:544:LEU:HD13	1.77	0.66
6:d:64:ILE:HG22	6:d:68:MET:HE3	1.77	0.66
1:n:248:ASN:HB2	8:k:260:ASN:HB3	1.78	0.66
1:N:79:ALA:HB2	1:N:523:ILE:HD12	1.77	0.66
8:c:367:PHE:HE2	8:c:380:MET:HE1	1.61	0.66
7:A:165:SER:O	7:A:166:SER:HB3	1.96	0.65
3:G:204:ILE:HD12	3:G:205:PRO:HD2	1.78	0.65
6:D:421:ILE:HG22	6:D:447:LEU:HD13	1.76	0.65
8:c:208:LYS:HD2	8:c:389:LEU:HB3	1.78	0.65
3:o:282:LEU:HD21	3:o:306:PHE:HB3	1.77	0.65
7:i:26:ARG:HG3	7:i:26:ARG:NH1	1.93	0.65
1:F:75:LEU:HD12	8:C:55:LEU:HD23	1.78	0.65
2:H:25:ASP:C	2:H:27:GLN:H	2.03	0.65
8:K:50:ASP:HB2	8:K:51:PRO:CD	2.26	0.65
4:M:211:VAL:HB	4:M:223:LEU:HD23	1.76	0.65
2:h:42:CYS:HB3	2:h:71:MET:HE1	1.78	0.65
7:A:109:LEU:HD11	7:A:538:ILE:HG21	1.79	0.65
7:A:256:MET:HG2	8:C:257:SER:HB2	1.78	0.65
7:a:462:LEU:HB3	7:a:504:LEU:HD11	1.78	0.65
4:E:144:ILE:HD11	4:E:550:LYS:HA	1.78	0.65
8:C:167:TRP:CE3	8:C:214:VAL:HB	2.31	0.65
7:a:190:GLN:HA	7:a:195:GLU:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:41:MET:HE2	2:p:53:LYS:HD3	1.79	0.65
7:i:458:ILE:O	7:i:462:LEU:HG	1.97	0.65
3:O:352:PHE:CD1	3:O:365:PHE:HB3	2.32	0.65
6:L:214:VAL:HG23	6:L:376:SER:HB3	1.77	0.65
6:L:244:PRO:HD3	6:L:270:TYR:CE2	2.31	0.65
6:l:448:GLU:OE1	6:l:470:ARG:NH2	2.29	0.65
4:E:147:ALA:HB1	4:E:546:ARG:HG3	1.78	0.65
5:B:109:LEU:HB3	5:B:115:ILE:HD12	1.78	0.65
5:B:179:ASN:O	5:B:183:ARG:HB2	1.97	0.65
6:D:71:LEU:HD21	7:A:15:LEU:HB2	1.77	0.65
7:A:63:THR:HA	7:A:397:GLU:HG3	1.79	0.65
3:o:478:TRP:CE3	3:o:492:PHE:HB2	2.32	0.65
3:G:158:LEU:HB3	3:G:400:VAL:HG13	1.78	0.65
5:J:287:ARG:HG3	5:J:310:ASP:HA	1.79	0.65
6:L:411:ILE:HD11	6:L:501:VAL:HA	1.78	0.65
7:I:52:MET:HE2	8:K:526:ILE:HG12	1.79	0.65
10:K:1102:ADP:O3B	11:K:1103:BEF:F2	2.05	0.65
3:o:147:ILE:HD13	3:o:157:LEU:HD11	1.79	0.65
4:m:413:LYS:H	5:j:79:ASN:ND2	1.95	0.65
3:G:352:PHE:CD1	3:G:365:PHE:HB3	2.32	0.65
6:D:244:PRO:HD3	6:D:270:TYR:CE2	2.32	0.65
5:J:233:ILE:HG12	5:J:285:ILE:HD11	1.78	0.65
2:p:509:VAL:HG12	2:p:510:LYS:N	2.12	0.65
2:H:24:ALA:O	2:H:28:ILE:N	2.29	0.64
5:J:181:ILE:HD11	5:J:388:LEU:HA	1.79	0.64
6:d:520:ARG:HG3	6:d:520:ARG:NH2	1.98	0.64
5:j:472:LEU:HB3	5:j:474:LEU:HD13	1.79	0.64
8:k:385:SER:HB3	8:k:388:ILE:HG12	1.78	0.64
8:K:421:MET:HE2	8:K:472:ARG:HA	1.79	0.64
4:E:292:VAL:HG21	5:B:260:GLN:HB3	1.78	0.64
2:P:509:VAL:CG1	2:P:510:LYS:N	2.61	0.64
1:f:326:GLU:HG2	8:c:232:PRO:HB3	1.80	0.64
2:H:42:CYS:HB3	2:H:71:MET:HE1	1.79	0.64
6:D:353:ILE:CG2	6:D:354:ASP:N	2.61	0.64
7:A:250:ASN:HB3	7:A:300:LYS:HB3	1.79	0.64
7:I:63:THR:HG23	7:I:397:GLU:HG2	1.79	0.64
1:f:253:TYR:CE1	1:f:259:ARG:HG3	2.32	0.64
3:o:206:GLY:HA2	4:m:110:SER:HB3	1.78	0.64
1:N:492:ASP:HB2	1:N:499:CYS:HB3	1.79	0.64
8:K:108:ALA:HB3	8:K:109:PRO:HD3	1.79	0.64
4:e:96:LEU:HD13	4:e:101:ALA:HB1	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:182:VAL:HG22	2:p:401:ILE:HG13	1.78	0.64
4:E:494:THR:O	4:E:498:LEU:HB2	1.98	0.64
6:D:138:MET:SD	6:D:478:LEU:HD22	2.37	0.64
6:D:214:VAL:HG23	6:D:376:SER:HB3	1.79	0.64
1:f:509:SER:HB2	1:f:512:VAL:HG23	1.79	0.64
4:e:73:ILE:HD11	5:b:72:PRO:HB2	1.80	0.64
8:k:24:ASN:HD22	8:k:74:ALA:HB2	1.61	0.64
6:d:420:GLU:HB2	6:d:473:HIS:CE1	2.32	0.64
5:J:39:PRO:HD2	5:J:474:LEU:HD23	1.80	0.64
7:I:75:VAL:HG21	7:I:84:VAL:HG21	1.79	0.64
8:k:162:LYS:O	8:k:164:VAL:N	2.31	0.64
1:F:195:GLU:HG3	1:F:327:ARG:NH1	2.13	0.64
3:G:37:GLN:HG3	3:G:103:ILE:HA	1.80	0.64
3:G:323:MET:HA	3:G:326:VAL:HG12	1.79	0.64
4:E:73:ILE:HG23	5:B:514:ILE:HG12	1.79	0.64
5:B:59:ASP:HB3	5:B:62:THR:OG1	1.97	0.64
1:N:251:PHE:CB	8:K:263:ILE:HB	2.28	0.64
4:e:115:ILE:HD13	4:e:533:GLY:HA2	1.79	0.64
3:G:282:LEU:HD21	3:G:306:PHE:HB3	1.79	0.64
7:A:199:PRO:HB2	7:A:202:ALA:HB2	1.80	0.64
4:M:412:ASN:HB2	5:J:80:ILE:HG12	1.80	0.64
5:J:183:ARG:NH2	5:J:210:GLU:HA	2.12	0.64
1:F:535:ARG:NH1	2:P:6:PRO:HB2	2.13	0.63
2:H:509:VAL:CG1	2:H:510:LYS:N	2.61	0.63
8:K:161:THR:HG22	8:K:162:LYS:HG3	1.79	0.63
7:a:165:SER:O	7:a:166:SER:HB3	1.97	0.63
2:H:420:LEU:HD11	2:H:521:LEU:HD12	1.79	0.63
6:D:502:LEU:HA	6:D:505:THR:HB	1.81	0.63
2:p:240:SER:HA	2:p:245:HIS:NE2	2.13	0.63
1:F:153:VAL:HG11	1:F:405:VAL:HG21	1.80	0.63
1:N:221:HIS:HD2	1:N:223:ASP:H	1.47	0.63
6:d:224:GLY:HA3	6:d:306:SER:OG	1.97	0.63
1:N:93:THR:O	1:N:97:LEU:HB2	1.99	0.63
2:P:24:ALA:O	2:P:28:ILE:N	2.21	0.63
1:f:221:HIS:HD2	1:f:223:ASP:H	1.47	0.63
3:g:280:GLU:O	3:g:284:GLN:HB2	1.97	0.63
6:l:242:SER:HB3	6:l:243:PRO:CD	2.29	0.63
7:A:63:THR:HG23	7:A:397:GLU:HG2	1.81	0.63
5:J:285:ILE:HD12	5:J:317:LEU:HD13	1.80	0.63
6:d:237:ILE:HD11	6:d:286:LEU:HD22	1.80	0.63
3:o:460:ASP:O	3:o:464:ILE:HG12	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:221:HIS:HD2	1:F:223:ASP:H	1.44	0.63
3:O:478:TRP:CE3	3:O:492:PHE:HB2	2.32	0.63
1:f:173:ILE:HG23	1:f:209:PHE:HB2	1.81	0.63
3:g:107:GLU:CG	3:g:448:VAL:HG21	2.29	0.63
6:d:31:VAL:HG21	6:d:75:ALA:HB1	1.80	0.63
7:a:75:VAL:HG21	7:a:84:VAL:HG21	1.81	0.63
8:c:121:ILE:HG23	8:c:441:PRO:HB3	1.81	0.63
3:g:204:ILE:HD13	3:g:362:TYR:HE2	1.61	0.63
4:E:168:ILE:HD11	4:E:439:VAL:HG13	1.80	0.63
4:E:412:ASN:HB3	4:E:415:ILE:HD12	1.80	0.63
5:B:441:PRO:HB3	5:B:472:LEU:HD11	1.81	0.63
1:N:325:MET:HE3	1:N:336:ALA:HB1	1.81	0.63
3:g:220:PHE:C	3:g:222:LYS:H	2.05	0.63
5:j:59:ASP:HB3	5:j:62:THR:OG1	1.99	0.63
4:E:73:ILE:CG2	5:B:514:ILE:HG12	2.29	0.63
6:D:138:MET:SD	6:D:478:LEU:CD2	2.87	0.63
4:M:412:ASN:HB3	4:M:415:ILE:CD1	2.29	0.63
1:f:130:MET:HE1	1:f:514:ARG:CG	2.28	0.63
1:N:163:ASP:HB2	1:N:166:LEU:HB3	1.81	0.62
3:O:221:LYS:HA	3:O:362:TYR:CZ	2.34	0.62
3:O:280:GLU:O	3:O:284:GLN:HB2	1.98	0.62
3:g:245:ASN:HB3	3:g:336:SER:HA	1.81	0.62
4:e:494:THR:O	4:e:498:LEU:HB2	1.99	0.62
7:a:28:GLN:HE21	7:a:77:HIS:HE1	1.46	0.62
8:c:421:MET:HG2	8:c:453:PRO:HG2	1.80	0.62
1:n:195:GLU:HG3	1:n:327:ARG:NH1	2.14	0.62
3:o:86:ILE:HD11	3:o:510:ALA:HA	1.81	0.62
5:J:80:ILE:HD12	5:J:504:ALA:HB2	1.81	0.62
5:J:293:TYR:HB3	5:J:294:PRO:HD3	1.80	0.62
8:k:324:ASP:HA	8:k:327:ARG:NH2	2.14	0.62
5:J:441:PRO:HA	5:J:444:LEU:HD12	1.81	0.62
8:c:24:ASN:HD22	8:c:74:ALA:HB2	1.64	0.62
4:m:60:ILE:O	4:m:72:LYS:HE2	2.00	0.62
6:L:162:ILE:HB	7:I:540:ARG:HD3	1.82	0.62
7:I:160:ALA:O	7:I:164:MET:HG2	2.00	0.62
3:o:74:ASP:O	4:m:32:VAL:HA	2.00	0.62
4:m:228:GLY:HA3	4:m:420:GLU:OE2	1.99	0.62
3:G:26:ILE:O	3:G:30:ILE:HD12	2.00	0.62
5:B:238:LEU:HD13	5:B:290:ILE:HG23	1.81	0.62
6:D:35:ILE:HA	6:D:46:LYS:HZ3	1.63	0.62
2:P:509:VAL:HG12	2:P:510:LYS:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:419:GLU:HB2	3:O:472:HIS:HE1	1.63	0.62
7:I:198:TYR:CE2	7:I:413:LEU:HB3	2.35	0.62
5:b:317:LEU:HA	5:b:320:VAL:HG12	1.81	0.62
8:c:111:LEU:HD22	8:c:440:TRP:HB3	1.81	0.62
5:B:82:LYS:NZ	5:B:86:ASP:OD2	2.32	0.62
6:L:42:LYS:HE2	6:L:484:VAL:HG13	1.80	0.62
3:G:166:MET:HE3	3:G:396:ALA:HB2	1.80	0.62
6:D:50:THR:HG22	6:D:52:ARG:H	1.65	0.62
7:i:16:GLY:O	7:i:548:ASP:N	2.29	0.62
6:D:242:SER:HB3	6:D:243:PRO:CD	2.29	0.62
8:C:81:LEU:CD1	8:C:516:SER:HB2	2.30	0.62
1:f:87:THR:CG2	1:f:512:VAL:HG22	2.30	0.62
7:i:75:VAL:HG21	7:i:84:VAL:HG21	1.82	0.62
2:H:284:ILE:HD11	2:H:308:LEU:HB3	1.81	0.62
6:L:239:PHE:HB3	6:L:334:ALA:O	2.00	0.62
4:e:64:SER:HB2	4:e:72:LYS:HZ3	1.64	0.62
1:n:79:ALA:HB2	1:n:523:ILE:HD12	1.82	0.62
8:k:481:THR:HG21	8:k:495:VAL:HG23	1.81	0.62
3:G:326:VAL:HG23	3:G:365:PHE:HE1	1.65	0.61
7:a:458:ILE:O	7:a:462:LEU:HG	1.99	0.61
6:d:220:ILE:HG21	6:d:302:LEU:HD21	1.81	0.61
3:o:446:LEU:HD21	3:o:507:LEU:HD21	1.80	0.61
4:m:86:ASP:HB3	4:m:89:THR:OG1	2.00	0.61
6:l:502:LEU:HA	6:l:505:THR:HB	1.82	0.61
1:F:225:PRO:HG2	1:F:315:LEU:HB2	1.82	0.61
4:E:60:ILE:O	4:E:72:LYS:HE2	2.00	0.61
4:E:412:ASN:HB3	4:E:415:ILE:CD1	2.29	0.61
1:N:56:THR:HB	1:N:61:VAL:HG11	1.82	0.61
1:f:325:MET:HE3	1:f:336:ALA:HB1	1.82	0.61
8:c:167:TRP:HE3	8:c:215:LEU:HD13	1.63	0.61
1:n:221:HIS:HD2	1:n:223:ASP:H	1.47	0.61
4:m:245:LEU:HD11	4:m:354:ILE:HD11	1.81	0.61
8:c:159:ILE:O	8:c:161:THR:N	2.32	0.61
2:p:43:LEU:HG	2:p:462:THR:CG2	2.31	0.61
3:o:26:ILE:O	3:o:30:ILE:HD12	2.01	0.61
5:j:184:LEU:HD11	5:j:192:HIS:HB2	1.81	0.61
2:P:42:CYS:HB3	2:P:71:MET:HE1	1.81	0.61
3:o:20:SER:HB2	3:o:25:GLN:NE2	2.15	0.61
1:f:7:ASN:ND2	1:f:10:ALA:HB2	2.15	0.61
7:a:26:ARG:HH11	7:a:26:ARG:CG	2.07	0.61
5:j:183:ARG:HH22	5:j:211:GLY:N	1.96	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:413:LYS:HA	5:B:464:TYR:HE1	1.66	0.61
7:A:12:THR:HB	7:A:14:PHE:CE2	2.35	0.61
5:J:184:LEU:HD11	5:J:192:HIS:HB2	1.81	0.61
4:e:507:ILE:HG22	4:e:509:ASN:H	1.66	0.61
7:a:501:GLY:CA	7:a:512:GLU:HG2	2.30	0.61
5:j:405:GLY:O	5:j:408:GLU:HG2	2.01	0.61
4:m:240:ILE:HD13	4:m:244:ILE:HD11	1.82	0.61
6:l:244:PRO:HD3	6:l:270:TYR:HE2	1.65	0.61
7:i:52:MET:HE2	8:k:526:ILE:HG12	1.82	0.61
5:B:184:LEU:HD11	5:B:192:HIS:HB2	1.83	0.61
7:I:55:ASP:O	7:I:56:ASP:HB3	2.01	0.61
7:I:304:ASP:HA	7:I:307:LEU:HD12	1.81	0.61
1:f:111:GLU:HG2	1:n:467:LEU:HD13	1.83	0.61
2:H:428:ILE:HD11	2:H:460:PRO:HG3	1.83	0.61
1:N:159:LEU:HA	1:N:167:THR:HG21	1.82	0.61
3:O:242:LEU:HD22	3:O:244:LEU:HG	1.82	0.61
6:L:89:ALA:HA	6:L:403:CYS:SG	2.40	0.61
1:n:251:PHE:HZ	2:p:259:THR:HB	1.66	0.61
1:F:251:PHE:CB	8:C:263:ILE:HB	2.31	0.60
1:N:47:VAL:HB	2:P:546:MET:HG2	1.83	0.60
3:g:221:LYS:HA	3:g:362:TYR:CZ	2.36	0.60
3:o:181:MET:HE2	3:o:214:PHE:HB2	1.83	0.60
8:C:353:GLY:HA3	8:C:370:ASN:CB	2.31	0.60
7:I:126:ILE:HG13	7:I:539:LEU:HD23	1.82	0.60
6:d:130:ARG:O	6:d:134:ILE:HG13	2.00	0.60
7:i:129:PHE:HB3	7:i:532:LEU:HD11	1.82	0.60
1:F:269:PHE:HA	8:C:270:ASN:HD21	1.65	0.60
5:B:476:ASN:HB3	5:B:478:THR:HG22	1.83	0.60
8:C:62:HIS:O	8:C:66:ARG:HB2	2.01	0.60
7:I:26:ARG:HG3	7:I:26:ARG:NH1	2.00	0.60
8:K:41:PRO:HG2	8:K:486:GLY:HA3	1.82	0.60
8:K:164:VAL:CG1	8:K:171:MET:HG3	2.31	0.60
6:d:181:ILE:HD11	6:d:193:ASP:HB3	1.82	0.60
4:E:32:VAL:HG11	7:I:4:LEU:HD21	1.83	0.60
8:C:108:ALA:HB3	8:C:109:PRO:HD3	1.83	0.60
1:N:248:ASN:HB2	8:K:260:ASN:HB3	1.84	0.60
3:g:158:LEU:HB3	3:g:400:VAL:HG13	1.83	0.60
6:d:165:GLN:HG3	7:a:130:ARG:CD	2.22	0.60
4:m:327:PHE:CD2	4:m:344:ARG:HD3	2.35	0.60
1:F:124:ILE:HD11	1:F:434:LEU:HD11	1.81	0.60
2:H:291:ILE:HD13	2:H:347:PRO:HG3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:414:PRO:HB2	8:C:481:THR:HG23	1.82	0.60
4:e:457:GLU:O	4:e:461:GLN:HG2	2.02	0.60
8:c:162:LYS:O	8:c:164:VAL:N	2.34	0.60
4:E:29:PHE:H	4:E:29:PHE:HD2	1.48	0.60
7:A:86:LEU:HD21	7:A:101:VAL:HG12	1.82	0.60
4:M:448:VAL:HG21	4:M:498:LEU:HD22	1.83	0.60
1:n:450:ALA:O	1:n:453:VAL:HG22	2.01	0.60
6:l:59:ASN:HB3	6:l:161:LYS:HG2	1.84	0.60
8:k:50:ASP:HB2	8:k:51:PRO:CD	2.31	0.60
1:F:458:LEU:HD22	1:F:493:LEU:HD11	1.82	0.60
6:d:135:LEU:HA	6:d:138:MET:HG2	1.83	0.60
3:o:419:GLU:HB2	3:o:472:HIS:HE1	1.66	0.60
4:M:275:PRO:HD3	4:M:325:TRP:HE3	1.66	0.60
3:g:88:ARG:HG2	3:g:88:ARG:NH1	2.16	0.60
7:a:63:THR:HA	7:a:397:GLU:HG3	1.83	0.60
7:i:86:LEU:HD21	7:i:101:VAL:HG12	1.83	0.60
1:F:296:ILE:HG12	1:F:317:LEU:HD23	1.83	0.60
8:K:59:ASN:CB	8:K:162:LYS:HG2	2.28	0.60
7:i:538:ILE:HA	7:i:541:ILE:HD12	1.84	0.60
5:B:508:LEU:O	5:B:511:VAL:HB	2.02	0.60
6:L:74:VAL:HG13	6:L:518:ILE:HD12	1.84	0.60
5:b:232:LEU:HB2	5:b:281:ILE:CD1	2.25	0.60
8:k:421:MET:HE2	8:k:472:ARG:HA	1.84	0.60
4:E:327:PHE:CE2	4:E:342:ALA:HB1	2.37	0.59
3:O:464:ILE:O	3:O:468:LEU:HB2	2.02	0.59
5:J:192:HIS:CD2	5:J:319:LEU:HD12	2.37	0.59
6:L:35:ILE:HD11	6:L:65:LEU:HD21	1.83	0.59
1:f:337:GLN:CG	1:f:347:ILE:HG21	2.31	0.59
7:a:63:THR:HG23	7:a:397:GLU:HG2	1.83	0.59
3:G:215:ILE:HG22	3:G:217:GLY:H	1.67	0.59
6:D:220:ILE:HG21	6:D:302:LEU:HD21	1.84	0.59
1:N:19:LEU:O	1:N:23:VAL:HG23	2.02	0.59
8:K:162:LYS:O	8:K:164:VAL:N	2.35	0.59
3:g:204:ILE:HG23	3:g:379:ARG:HD3	1.83	0.59
1:n:153:VAL:HG11	1:n:405:VAL:HG21	1.83	0.59
5:B:181:ILE:HD11	5:B:388:LEU:HA	1.84	0.59
6:D:162:ILE:HB	7:A:540:ARG:HD3	1.84	0.59
3:O:449:ILE:O	3:O:453:LEU:HG	2.03	0.59
5:J:14:ARG:HG2	5:J:15:ALA:H	1.67	0.59
4:E:507:ILE:HG22	4:E:509:ASN:H	1.67	0.59
2:h:478:LEU:HD22	2:h:499:VAL:HG23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:i:17:GLY:CA	7:i:546:THR:O	2.50	0.59
4:E:273:THR:HG23	4:E:324:GLN:OE1	2.01	0.59
6:D:125:GLN:HE21	6:D:513:GLU:HA	1.66	0.59
3:g:107:GLU:HG2	3:g:448:VAL:CG2	2.31	0.59
5:b:109:LEU:HB3	5:b:115:ILE:HD12	1.84	0.59
3:o:449:ILE:O	3:o:453:LEU:HG	2.02	0.59
7:i:83:LEU:HD23	7:i:102:VAL:HG13	1.85	0.59
7:i:190:GLN:HA	7:i:195:GLU:O	2.02	0.59
2:H:498:GLY:O	2:H:509:VAL:HG13	2.03	0.59
5:B:162:SER:HA	5:B:167:SER:OG	2.02	0.59
4:M:64:SER:HB2	4:M:72:LYS:NZ	2.18	0.59
2:h:154:ASN:HB3	2:h:190:LEU:HD13	1.83	0.59
2:h:299:ILE:HD12	2:h:313:LEU:HD21	1.85	0.59
4:m:287:LEU:HD12	5:j:248:THR:HG22	1.84	0.59
3:G:220:PHE:HD2	3:G:363:ASN:HB2	1.67	0.59
6:D:89:ALA:HA	6:D:403:CYS:SG	2.42	0.59
6:D:520:ARG:HG3	6:D:520:ARG:NH2	2.16	0.59
8:C:146:GLU:OE2	8:C:183:ARG:NH1	2.34	0.59
6:l:214:VAL:HG23	6:l:376:SER:HB3	1.85	0.59
7:i:173:SER:O	7:i:177:SER:HB2	2.03	0.59
3:O:20:SER:HB2	3:O:25:GLN:HE21	1.68	0.59
7:I:188:LYS:HG2	7:I:198:TYR:CE1	2.37	0.59
1:f:130:MET:HE1	1:f:514:ARG:HG2	1.82	0.59
7:a:159:ILE:HD13	7:a:412:THR:HG21	1.85	0.59
6:l:238:GLN:HB2	6:l:334:ALA:HA	1.85	0.59
3:O:20:SER:HB2	3:O:25:GLN:NE2	2.18	0.59
3:g:282:LEU:HD21	3:g:306:PHE:HB3	1.84	0.59
8:c:208:LYS:HE3	8:c:390:ASN:OD1	2.02	0.59
4:m:73:ILE:HD11	5:j:72:PRO:HB2	1.84	0.59
4:m:275:PRO:HD3	4:m:325:TRP:HE3	1.66	0.59
6:l:220:ILE:HG21	6:l:302:LEU:HD21	1.84	0.59
7:i:97:GLY:O	7:i:101:VAL:HG23	2.03	0.59
2:H:123:SER:HB3	2:H:126:GLU:HG3	1.84	0.59
4:E:98:ASN:HD22	4:E:101:ALA:H	1.51	0.59
7:A:159:ILE:HD13	7:A:412:THR:HG21	1.85	0.59
8:C:119:VAL:HA	8:C:122:ILE:HD12	1.84	0.59
8:C:385:SER:HB3	8:C:388:ILE:HG12	1.85	0.59
5:j:183:ARG:NH2	5:j:210:GLU:HA	2.16	0.59
8:k:402:VAL:HA	8:k:405:ASN:HD22	1.68	0.59
1:F:439:LYS:O	1:F:442:THR:HG22	2.02	0.58
8:C:125:LEU:HD22	8:C:445:VAL:CG2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:268:GLN:HA	3:O:271:VAL:HG12	1.85	0.58
10:J:602:ADP:O3B	11:J:603:BEF:F3	2.10	0.58
5:b:183:ARG:NH2	5:b:210:GLU:HA	2.17	0.58
2:H:27:GLN:CA	2:H:31:SER:HB2	2.31	0.58
5:B:505:ALA:O	5:B:509:LEU:HB2	2.03	0.58
6:D:234:ILE:H	6:D:345:ASP:HB3	1.69	0.58
7:A:179:MET:HE1	7:A:385:ILE:HG23	1.84	0.58
1:N:337:GLN:CG	1:N:347:ILE:HG21	2.33	0.58
6:d:35:ILE:HA	6:d:46:LYS:HZ1	1.66	0.58
7:a:89:GLN:HA	7:a:92:ARG:HD3	1.86	0.58
3:o:107:GLU:CG	3:o:448:VAL:HG21	2.33	0.58
6:l:503:VAL:O	6:l:507:ALA:HB2	2.03	0.58
2:H:186:VAL:HG11	2:H:408:VAL:HG11	1.84	0.58
3:G:352:PHE:HD1	3:G:365:PHE:HB3	1.68	0.58
6:D:420:GLU:HB2	6:D:473:HIS:CE1	2.38	0.58
1:N:171:THR:HB	1:N:172:PRO:HD3	1.85	0.58
7:I:104:ILE:HG12	7:I:458:ILE:HD11	1.85	0.58
8:K:142:PRO:HA	8:K:411:SER:HA	1.84	0.58
1:f:533:LEU:HD22	8:c:47:MET:HE2	1.84	0.58
2:H:509:VAL:HG12	2:H:510:LYS:N	2.19	0.58
2:P:509:VAL:CG1	2:P:510:LYS:H	2.15	0.58
8:K:111:LEU:HD22	8:K:440:TRP:HB3	1.84	0.58
5:j:317:LEU:HA	5:j:320:VAL:HG12	1.83	0.58
7:I:54:VAL:HG12	7:I:56:ASP:H	1.69	0.58
3:g:352:PHE:CD1	3:g:365:PHE:HB3	2.38	0.58
5:b:406:CYS:O	5:b:410:VAL:HG23	2.03	0.58
2:p:33:ALA:HA	2:p:36:ARG:HD3	1.85	0.58
4:m:73:ILE:HG23	5:j:514:ILE:HG12	1.85	0.58
4:m:219:VAL:CG1	4:m:431:ARG:HB2	2.26	0.58
6:D:397:ALA:O	6:D:400:VAL:HG22	2.04	0.58
3:O:153:SER:HB3	3:O:156:GLU:CB	2.34	0.58
2:h:322:LYS:O	2:h:323:VAL:HB	2.03	0.58
3:g:37:GLN:HG3	3:g:103:ILE:HA	1.84	0.58
3:g:77:HIS:CE1	3:g:79:ALA:HB3	2.39	0.58
7:a:17:GLY:CA	7:a:546:THR:O	2.51	0.58
7:i:63:THR:HG22	7:i:64:ASN:N	2.19	0.58
2:H:39:HIS:O	2:H:43:LEU:HB2	2.04	0.58
8:C:81:LEU:HD13	8:C:516:SER:HB2	1.86	0.58
3:O:147:ILE:HD13	3:O:157:LEU:HD11	1.85	0.58
6:L:177:SER:OG	6:L:375:VAL:HG11	2.03	0.58
2:h:509:VAL:HG12	2:h:510:LYS:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:141:ILE:HD11	6:l:463:ILE:HD12	1.86	0.58
2:p:284:ILE:HD11	2:p:308:LEU:HB3	1.86	0.58
2:p:388:GLY:HA3	2:p:394:LEU:HD21	1.86	0.58
6:l:177:SER:OG	6:l:375:VAL:HG11	2.03	0.58
5:B:194:GLN:HB2	5:B:316:ARG:NH1	2.18	0.58
5:B:490:SER:HB3	5:B:493:LEU:HB2	1.84	0.58
1:N:26:ALA:HB3	1:N:102:LEU:HD12	1.86	0.58
5:J:109:LEU:HB3	5:J:115:ILE:HD12	1.86	0.58
1:N:242:TYR:CZ	2:P:260:GLU:HB3	2.39	0.58
3:O:220:PHE:C	3:O:222:LYS:H	2.11	0.58
5:J:232:LEU:HB2	5:J:281:ILE:CD1	2.34	0.58
3:g:167:SER:O	3:g:168:SER:HB3	2.04	0.58
4:e:327:PHE:CE2	4:e:342:ALA:HB1	2.39	0.58
5:b:179:ASN:O	5:b:183:ARG:HB2	2.04	0.58
6:l:420:GLU:HB2	6:l:473:HIS:CE1	2.38	0.58
8:k:89:VAL:HG11	8:k:505:ILE:HG13	1.85	0.58
3:O:326:VAL:HG23	3:O:365:PHE:HE1	1.69	0.58
2:h:512:ILE:HG23	2:h:517:ILE:HB	1.85	0.58
3:o:163:ARG:HG2	3:o:179:VAL:HG21	1.86	0.58
5:j:197:LYS:NZ	5:j:378:ASP:OD1	2.37	0.58
1:F:210:ILE:HD13	1:F:214:VAL:HG21	1.84	0.57
3:O:167:SER:O	3:O:168:SER:HB3	2.02	0.57
8:K:159:ILE:O	8:K:161:THR:N	2.33	0.57
5:b:155:HIS:CB	5:b:488:VAL:HG22	2.34	0.57
5:B:232:LEU:HB2	5:B:281:ILE:CD1	2.34	0.57
6:D:31:VAL:HG21	6:D:75:ALA:HB1	1.85	0.57
7:a:160:ALA:O	7:a:164:MET:HG2	2.04	0.57
5:J:184:LEU:HD11	5:J:192:HIS:CB	2.34	0.57
7:a:26:ARG:HG3	7:a:26:ARG:NH1	2.02	0.57
2:p:65:THR:HG22	2:p:67:ASP:H	1.69	0.57
8:k:105:ALA:O	8:k:109:PRO:HD2	2.04	0.57
4:E:64:SER:HB2	4:E:72:LYS:NZ	2.20	0.57
7:A:247:LEU:HD11	7:A:288:ILE:HD13	1.87	0.57
4:M:29:PHE:H	4:M:29:PHE:HD2	1.53	0.57
7:i:17:GLY:HA2	7:i:546:THR:O	2.04	0.57
3:G:167:SER:O	3:G:168:SER:HB3	2.04	0.57
1:N:153:VAL:HG11	1:N:405:VAL:HG21	1.87	0.57
2:P:182:VAL:HG22	2:P:401:ILE:HG13	1.87	0.57
4:M:275:PRO:HD3	4:M:325:TRP:CE3	2.39	0.57
6:d:72:HIS:CD2	6:d:74:VAL:HB	2.40	0.57
6:d:244:PRO:CD	6:d:270:TYR:CE2	2.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:m:180:LEU:HD22	4:m:430:VAL:HG13	1.86	0.57
5:B:301:LEU:HD23	5:B:303:ILE:HD11	1.86	0.57
8:C:79:LEU:C	8:C:81:LEU:H	2.12	0.57
2:P:25:ASP:C	2:P:27:GLN:H	2.12	0.57
5:b:46:LEU:HD21	5:b:63:ILE:HG23	1.87	0.57
6:d:89:ALA:HA	6:d:403:CYS:SG	2.45	0.57
8:c:208:LYS:HB3	8:c:389:LEU:HD13	1.87	0.57
8:k:50:ASP:HB2	8:k:51:PRO:HD3	1.84	0.57
1:F:533:LEU:HD22	8:C:47:MET:HE2	1.87	0.57
3:G:232:GLN:HG2	3:G:308:ALA:HA	1.86	0.57
6:D:336:ILE:C	6:D:338:LEU:H	2.12	0.57
7:A:209:HIS:HE1	8:C:83:ARG:HH21	1.52	0.57
3:O:181:MET:HE2	3:O:214:PHE:HB2	1.87	0.57
8:c:198:ILE:CG2	8:c:408:LEU:HD21	2.35	0.57
2:p:215:GLY:H	3:o:505:ASN:HD21	1.53	0.57
5:j:439:GLN:O	5:j:443:ILE:HG13	2.05	0.57
6:l:125:GLN:HE21	6:l:513:GLU:HA	1.68	0.57
4:E:40:ARG:NH1	4:E:42:HIS:ND1	2.52	0.57
4:E:72:LYS:HG3	5:B:513:ASN:HB3	1.87	0.57
7:A:104:ILE:HG12	7:A:458:ILE:HD11	1.87	0.57
8:C:444:ALA:HA	8:C:447:ASP:HB2	1.87	0.57
5:J:183:ARG:HH22	5:J:210:GLU:HA	1.68	0.57
8:c:402:VAL:HA	8:c:405:ASN:ND2	2.20	0.57
3:o:94:VAL:HG11	3:o:502:VAL:HG22	1.87	0.57
8:k:65:LEU:HB3	8:k:79:LEU:HD13	1.85	0.57
5:B:194:GLN:HB2	5:B:316:ARG:HH12	1.69	0.57
5:B:233:ILE:HG12	5:B:285:ILE:HD11	1.86	0.57
6:D:203:THR:HA	7:A:533:GLU:OE2	2.04	0.57
6:D:353:ILE:HG22	6:D:354:ASP:H	1.68	0.57
4:M:412:ASN:HB3	4:M:415:ILE:HD12	1.87	0.57
6:d:64:ILE:CG2	6:d:68:MET:HE3	2.35	0.57
5:j:291:TYR:HB3	5:j:294:PRO:HD2	1.87	0.57
6:l:514:CYS:O	6:l:518:ILE:HG12	2.04	0.57
5:B:406:CYS:O	5:B:410:VAL:HG23	2.05	0.57
8:K:174:LEU:HD22	8:K:219:VAL:HG23	1.85	0.57
3:o:191:ARG:O	3:o:192:ASN:C	2.48	0.57
7:i:251:LEU:HD23	7:i:285:VAL:HG22	1.86	0.57
4:M:413:LYS:H	5:J:79:ASN:ND2	2.02	0.56
6:L:448:GLU:OE1	6:L:470:ARG:NH2	2.37	0.56
7:I:462:LEU:HB3	7:I:504:LEU:HD11	1.87	0.56
7:I:535:CYS:O	7:I:539:LEU:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:293:TYR:HB3	5:B:294:PRO:HD3	1.86	0.56
4:M:507:ILE:HG22	4:M:509:ASN:H	1.70	0.56
5:J:98:LEU:HB2	5:J:440:LEU:HD11	1.87	0.56
4:e:168:ILE:HD11	4:e:439:VAL:HG13	1.86	0.56
8:c:402:VAL:HA	8:c:405:ASN:HD22	1.70	0.56
2:p:56:VAL:HB	3:o:525:THR:HG23	1.87	0.56
8:k:107:CYS:SG	8:k:108:ALA:N	2.78	0.56
1:F:130:MET:HE1	1:F:514:ARG:HG2	1.86	0.56
1:F:262:LEU:HA	1:F:265:SER:HB2	1.86	0.56
6:L:234:ILE:HB	6:L:345:ASP:HB3	1.85	0.56
7:I:250:ASN:HB3	7:I:300:LYS:HB3	1.86	0.56
8:K:81:LEU:HD13	8:K:516:SER:HB2	1.87	0.56
3:g:166:MET:HE3	3:g:396:ALA:HB2	1.87	0.56
4:e:413:LYS:H	5:b:79:ASN:ND2	2.03	0.56
5:b:373:THR:HG22	5:b:375:GLN:H	1.70	0.56
6:d:238:GLN:HB2	6:d:334:ALA:HA	1.87	0.56
8:c:167:TRP:CE3	8:c:215:LEU:HD13	2.39	0.56
8:c:174:LEU:HD22	8:c:219:VAL:HG23	1.87	0.56
4:m:72:LYS:HG3	5:j:513:ASN:HB3	1.87	0.56
5:j:109:LEU:HB3	5:j:115:ILE:HD12	1.86	0.56
6:l:171:ALA:HB3	6:l:172:PRO:HD3	1.87	0.56
2:H:247:VAL:HG22	2:H:298:CYS:HB3	1.87	0.56
3:G:135:LEU:HD23	3:G:424:LEU:HD23	1.87	0.56
4:E:64:SER:HB2	4:E:72:LYS:HZ2	1.70	0.56
5:J:255:THR:CG2	6:L:263:ILE:HA	2.35	0.56
7:I:173:SER:O	7:I:177:SER:HB2	2.06	0.56
4:e:74:LEU:HD13	4:e:93:GLN:HG3	1.88	0.56
4:e:147:ALA:HB1	4:e:546:ARG:HG3	1.88	0.56
1:F:337:GLN:CG	1:F:347:ILE:HG21	2.35	0.56
4:E:211:VAL:HB	4:E:223:LEU:HD23	1.87	0.56
7:A:141:ASN:HA	7:A:144:LEU:HD12	1.87	0.56
6:L:195:ARG:HD3	6:L:323:PHE:CZ	2.41	0.56
8:K:102:GLU:OE1	8:K:451:CYS:HB2	2.06	0.56
2:h:186:VAL:HG11	2:h:408:VAL:HG11	1.88	0.56
4:e:412:ASN:ND2	4:e:414:MET:SD	2.61	0.56
5:b:46:LEU:HD11	5:b:63:ILE:HA	1.85	0.56
2:p:26:GLY:O	2:p:31:SER:HB2	2.06	0.56
3:o:189:LEU:HD13	3:o:199:ILE:HG23	1.88	0.56
6:l:432:MET:SD	6:l:440:TRP:CZ3	2.92	0.56
7:i:73:LEU:HB3	8:k:8:MET:HE1	1.88	0.56
2:P:65:THR:HG22	2:P:67:ASP:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:50:ASP:OD1	7:I:64:ASN:HB2	2.06	0.56
2:p:65:THR:HG21	2:p:70:THR:HB	1.87	0.56
2:p:478:LEU:HD22	2:p:499:VAL:HG23	1.87	0.56
2:H:509:VAL:CG1	2:H:510:LYS:H	2.18	0.56
6:D:76:ARG:HG2	6:D:76:ARG:HH11	1.70	0.56
6:D:239:PHE:HB3	6:D:334:ALA:O	2.05	0.56
6:D:451:PRO:HB3	6:D:482:ILE:HD11	1.86	0.56
8:c:164:VAL:CG1	8:c:171:MET:HG3	2.36	0.56
2:H:54:ILE:HD11	3:G:78:PRO:HB2	1.88	0.56
3:G:173:ASN:HD21	4:E:148:ASN:HA	1.71	0.56
7:I:89:GLN:HA	7:I:92:ARG:HD3	1.88	0.56
4:e:115:ILE:HD11	4:e:536:GLN:HB3	1.88	0.56
8:c:41:PRO:HG2	8:c:486:GLY:HA3	1.88	0.56
1:n:163:ASP:HB2	1:n:166:LEU:HB3	1.87	0.56
5:j:441:PRO:HB3	5:j:472:LEU:HD11	1.88	0.56
1:F:87:THR:CG2	1:F:512:VAL:HG22	2.35	0.56
5:B:293:TYR:HB3	5:B:294:PRO:CD	2.36	0.56
6:L:35:ILE:HA	6:L:46:LYS:HZ1	1.69	0.56
3:g:323:MET:HA	3:g:326:VAL:HG12	1.87	0.56
8:k:164:VAL:CG1	8:k:171:MET:HG3	2.36	0.56
2:H:310:LEU:O	2:H:314:ASN:HB2	2.06	0.56
3:G:45:GLY:HA3	3:G:453:LEU:HD22	1.88	0.56
7:A:71:SER:HB2	7:A:88:GLN:NE2	2.22	0.56
6:L:224:GLY:HA3	6:L:306:SER:OG	2.05	0.56
3:g:166:MET:HA	3:g:166:MET:HE2	1.88	0.56
4:e:220:ASP:HB3	4:e:223:LEU:HB2	1.88	0.56
7:a:179:MET:HE1	7:a:385:ILE:HG23	1.88	0.56
7:i:104:ILE:HG12	7:i:458:ILE:HD11	1.87	0.56
1:F:370:ASN:H	1:F:370:ASN:HD22	1.53	0.55
7:A:15:LEU:C	7:A:17:GLY:N	2.62	0.55
2:P:43:LEU:HG	2:P:462:THR:HG22	1.88	0.55
3:O:337:THR:HG22	3:O:339:SER:H	1.71	0.55
2:h:311:HIS:CD2	3:g:336:SER:H	2.24	0.55
7:a:39:VAL:HG11	7:a:73:LEU:HD11	1.88	0.55
2:p:232:PRO:HG3	2:p:369:THR:OG1	2.05	0.55
3:o:224:PHE:CD2	3:o:225:SER:N	2.73	0.55
7:i:55:ASP:CB	7:i:59:ASP:O	2.54	0.55
7:a:4:LEU:HD21	4:m:32:VAL:HG11	1.86	0.55
4:m:29:PHE:H	4:m:29:PHE:HD2	1.55	0.55
5:j:39:PRO:HD2	5:j:474:LEU:HD23	1.88	0.55
1:F:412:ILE:HD12	1:F:510:TYR:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:33:ALA:HA	2:H:36:ARG:HD3	1.89	0.55
3:G:153:SER:HB3	3:G:156:GLU:CB	2.36	0.55
2:P:284:ILE:HD11	2:P:308:LEU:HB3	1.88	0.55
3:O:411:ALA:HB2	3:O:478:TRP:CD2	2.42	0.55
1:f:171:THR:HB	1:f:172:PRO:HD3	1.89	0.55
4:e:448:VAL:HG21	4:e:498:LEU:HD22	1.87	0.55
6:d:74:VAL:HG13	6:d:518:ILE:HD12	1.89	0.55
6:d:367:ARG:O	6:d:368:ASN:CB	2.55	0.55
7:a:41:LYS:HE2	7:a:103:ILE:HG23	1.88	0.55
6:l:224:GLY:HA3	6:l:306:SER:OG	2.07	0.55
8:k:108:ALA:HB3	8:k:109:PRO:HD3	1.87	0.55
8:k:179:VAL:HG12	8:k:407:MET:HE1	1.88	0.55
8:k:464:PRO:O	8:k:468:LEU:HB2	2.05	0.55
8:C:250:LEU:HD12	8:C:301:VAL:HG22	1.89	0.55
8:C:324:ASP:OD1	8:C:327:ARG:NH2	2.39	0.55
2:P:33:ALA:HA	2:P:36:ARG:HD3	1.87	0.55
5:b:230:LYS:O	5:b:281:ILE:HG23	2.06	0.55
6:d:35:ILE:HD12	6:d:97:VAL:HG11	1.88	0.55
8:c:50:ASP:HB2	8:c:51:PRO:CD	2.37	0.55
4:m:544:LEU:O	4:m:548:ILE:HG12	2.05	0.55
5:j:373:THR:HG21	6:l:77:MET:HE3	1.87	0.55
7:i:228:VAL:HG12	7:i:233:MET:SD	2.47	0.55
1:F:171:THR:HB	1:F:172:PRO:HD3	1.89	0.55
2:H:27:GLN:HE22	2:H:81:ALA:HB2	1.71	0.55
5:B:127:ALA:HB2	5:B:430:VAL:HG13	1.88	0.55
6:D:143:SER:HB2	6:D:146:ASP:HB2	1.89	0.55
8:C:167:TRP:N	8:C:167:TRP:CD1	2.74	0.55
7:I:458:ILE:O	7:I:462:LEU:HG	2.05	0.55
8:c:297:THR:HG22	8:c:299:LYS:H	1.71	0.55
4:m:84:THR:HG22	4:m:418:GLU:OE1	2.05	0.55
5:j:471:GLY:HA3	5:j:482:MET:CG	2.37	0.55
4:E:67:PRO:HA	4:E:190:SER:HA	1.88	0.55
4:E:322:ILE:HG23	4:E:346:VAL:HG21	1.88	0.55
5:B:152:ASP:OD1	5:B:400:THR:HG21	2.07	0.55
4:M:464:ILE:H	4:M:464:ILE:HD12	1.71	0.55
6:L:35:ILE:HA	6:L:46:LYS:NZ	2.22	0.55
7:I:199:PRO:HB2	7:I:202:ALA:HB2	1.89	0.55
2:h:509:VAL:CG1	2:h:510:LYS:N	2.70	0.55
3:g:7:THR:O	3:g:8:PRO:O	2.25	0.55
7:a:28:GLN:HE21	7:a:77:HIS:CE1	2.25	0.55
8:c:369:ASP:HB3	8:c:370:ASN:HD22	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:c:385:SER:HB3	8:c:388:ILE:HG12	1.88	0.55
5:j:184:LEU:HD11	5:j:192:HIS:CB	2.37	0.55
7:i:53:LEU:HD23	8:k:527:VAL:HB	1.88	0.55
3:O:174:ASN:ND2	4:M:546:ARG:HH22	2.04	0.55
4:M:180:LEU:HD22	4:M:430:VAL:HG13	1.89	0.55
1:f:439:LYS:O	1:f:442:THR:HG22	2.05	0.55
2:h:111:LEU:HD11	2:h:538:VAL:HG21	1.88	0.55
3:g:221:LYS:HA	3:g:362:TYR:CE1	2.41	0.55
4:e:322:ILE:HG23	4:e:346:VAL:HG21	1.88	0.55
7:a:394:SER:HB2	8:c:519:LEU:HD22	1.89	0.55
8:c:324:ASP:HA	8:c:327:ARG:NH2	2.22	0.55
1:n:203:SER:O	1:n:206:ASP:HB2	2.07	0.55
1:n:368:THR:HG22	1:n:369:GLU:H	1.71	0.55
6:l:138:MET:SD	6:l:478:LEU:HD21	2.47	0.55
7:i:281:VAL:O	7:i:285:VAL:HG23	2.06	0.55
8:k:96:VAL:HG22	8:k:509:SER:HA	1.89	0.55
4:E:115:ILE:HD11	4:E:536:GLN:HB3	1.89	0.55
6:D:244:PRO:HD3	6:D:270:TYR:HE2	1.70	0.55
7:A:523:SER:O	7:A:527:SER:HB2	2.07	0.55
3:O:319:SER:HB3	3:O:322:ASP:HB2	1.88	0.55
5:b:165:ILE:HG12	6:d:520:ARG:NH2	2.21	0.55
5:j:179:ASN:O	5:j:183:ARG:HB2	2.07	0.55
3:G:383:GLU:HA	3:G:386:ILE:HD12	1.89	0.55
3:G:411:ALA:HB2	3:G:478:TRP:CD2	2.41	0.55
5:B:13:GLU:O	5:B:18:ALA:HB2	2.06	0.55
1:N:337:GLN:HG2	1:N:347:ILE:HG21	1.89	0.55
8:K:179:VAL:HG12	8:K:407:MET:HE1	1.89	0.55
8:K:457:ILE:HD11	8:K:484:ILE:HG12	1.89	0.55
1:f:159:LEU:HA	1:f:167:THR:HG21	1.88	0.55
3:g:167:SER:O	3:g:168:SER:CB	2.54	0.55
5:b:503:GLU:O	5:b:507:VAL:HG23	2.06	0.55
7:i:252:GLN:HA	7:i:303:ASP:HB2	1.88	0.55
7:i:417:ASN:HB3	7:i:521:THR:HB	1.89	0.55
1:F:248:ASN:HD22	8:C:260:ASN:HB3	1.72	0.55
3:G:181:MET:HE2	3:G:214:PHE:HB2	1.88	0.55
6:L:237:ILE:HG22	6:L:239:PHE:H	1.72	0.55
6:L:295:ASP:O	6:L:296:ALA:HB3	2.07	0.55
7:I:164:MET:HE3	7:I:405:SER:HB2	1.89	0.55
3:g:198:LEU:HB3	3:g:373:THR:OG1	2.07	0.55
3:g:200:GLY:HA3	3:g:325:ARG:CZ	2.37	0.55
7:a:129:PHE:HB3	7:a:532:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:j:74:ALA:O	5:j:78:VAL:HG23	2.07	0.55
1:F:153:VAL:HG11	1:F:405:VAL:CG2	2.36	0.54
5:B:281:ILE:HG22	5:B:283:THR:H	1.72	0.54
1:N:56:THR:HG22	1:N:58:ASP:H	1.72	0.54
1:N:430:ASN:HD21	1:N:441:LYS:CB	2.20	0.54
1:N:458:LEU:HD22	1:N:493:LEU:HD11	1.88	0.54
3:O:133:VAL:HB	3:O:511:THR:HG21	1.88	0.54
3:O:352:PHE:HD1	3:O:365:PHE:HB3	1.70	0.54
8:K:322:LYS:H	8:K:322:LYS:HD3	1.71	0.54
5:b:183:ARG:HH22	5:b:211:GLY:H	1.55	0.54
7:a:83:LEU:HD23	7:a:102:VAL:HG13	1.89	0.54
7:i:99:THR:O	7:i:103:ILE:HG13	2.07	0.54
8:k:367:PHE:HE2	8:k:380:MET:HE1	1.72	0.54
2:H:227:VAL:HG13	2:H:368:VAL:CG1	2.37	0.54
4:E:423:LEU:O	4:E:427:LEU:N	2.39	0.54
7:A:333:THR:HG22	7:A:377:THR:HG22	1.89	0.54
1:N:296:ILE:HA	1:N:317:LEU:HB3	1.88	0.54
1:f:178:VAL:HG22	1:f:399:LEU:HD23	1.89	0.54
2:h:123:SER:HB3	2:h:126:GLU:HG3	1.88	0.54
8:c:401:ALA:O	8:c:404:ARG:HG3	2.08	0.54
2:p:43:LEU:HG	2:p:462:THR:HG22	1.89	0.54
2:p:428:ILE:HD11	2:p:460:PRO:HG3	1.89	0.54
8:k:369:ASP:HB3	8:k:370:ASN:HD22	1.72	0.54
2:P:56:VAL:HB	3:O:525:THR:HG23	1.90	0.54
4:M:269:LEU:H	4:M:375:GLY:H	1.54	0.54
8:c:322:LYS:H	8:c:322:LYS:HD3	1.72	0.54
7:A:28:GLN:HE21	7:A:77:HIS:HE1	1.56	0.54
7:A:415:SER:OG	7:A:522:ILE:HD11	2.07	0.54
8:C:161:THR:HG22	8:C:162:LYS:HG3	1.88	0.54
1:f:103:ARG:O	1:f:107:ARG:HD2	2.08	0.54
2:h:24:ALA:O	2:h:28:ILE:N	2.31	0.54
8:c:414:PRO:HB3	8:c:481:THR:HG23	1.88	0.54
1:n:326:GLU:HG2	8:k:232:PRO:HB3	1.88	0.54
5:j:58:ASN:O	5:j:59:ASP:C	2.51	0.54
8:k:222:GLY:HA2	8:k:331:VAL:HG11	1.90	0.54
7:A:63:THR:HG22	7:A:64:ASN:N	2.23	0.54
2:P:109:GLU:HG2	2:P:458:VAL:CG2	2.37	0.54
3:O:242:LEU:HD21	3:O:341:ILE:HD13	1.90	0.54
6:L:181:ILE:HD11	6:L:193:ASP:HB3	1.90	0.54
7:I:53:LEU:HD23	8:K:527:VAL:HB	1.89	0.54
4:m:457:GLU:O	4:m:461:GLN:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:48:PRO:HB3	2:H:172:TYR:CD1	2.42	0.54
3:G:7:THR:O	3:G:8:PRO:O	2.26	0.54
8:C:414:PRO:HB3	8:C:481:THR:HG23	1.89	0.54
1:N:459:VAL:HG22	1:N:491:VAL:HG11	1.89	0.54
2:P:123:SER:HB3	2:P:126:GLU:HG3	1.88	0.54
2:h:65:THR:HG21	2:h:70:THR:HB	1.90	0.54
3:g:261:VAL:HG21	3:g:270:ILE:HD13	1.90	0.54
5:b:374:ASP:HB2	6:d:80:GLU:OE1	2.07	0.54
8:c:81:LEU:CD1	8:c:516:SER:HB2	2.38	0.54
1:n:269:PHE:HA	8:k:270:ASN:HD21	1.73	0.54
2:p:509:VAL:HG13	2:p:510:LYS:H	1.72	0.54
3:o:249:GLU:O	3:o:278:ILE:HG21	2.08	0.54
4:m:275:PRO:HD3	4:m:325:TRP:CE3	2.43	0.54
6:l:31:VAL:HG21	6:l:75:ALA:HB1	1.89	0.54
8:k:159:ILE:O	8:k:161:THR:N	2.41	0.54
2:H:79:HIS:HD2	2:H:81:ALA:H	1.56	0.54
5:B:412:SER:O	5:B:416:ASP:HB2	2.07	0.54
6:D:436:GLN:HA	6:D:439:ILE:HD12	1.88	0.54
7:A:164:MET:HE3	7:A:405:SER:HB2	1.88	0.54
8:C:122:ILE:HG23	8:C:518:CYS:HB3	1.89	0.54
3:O:385:VAL:O	3:O:389:VAL:HG23	2.08	0.54
5:J:22:ALA:HA	5:J:73:ALA:CB	2.38	0.54
5:J:373:THR:HG22	5:J:375:GLN:H	1.73	0.54
7:I:28:GLN:HE21	7:I:77:HIS:HE1	1.55	0.54
4:e:73:ILE:HG23	5:b:514:ILE:HG12	1.90	0.54
10:b:602:ADP:O3B	11:b:603:BEF:F2	2.16	0.54
6:d:353:ILE:HG22	6:d:354:ASP:N	2.23	0.54
7:i:212:SER:HB2	8:k:511:LYS:HE3	1.90	0.54
3:G:113:LYS:O	3:G:117:GLU:HG2	2.08	0.54
3:G:323:MET:O	3:G:326:VAL:HG12	2.07	0.54
5:B:121:ILE:HG12	5:B:506:GLU:HG2	1.90	0.54
4:M:251:HIS:CE1	5:J:325:VAL:HB	2.43	0.54
8:K:219:VAL:HG22	8:K:379:ILE:HG12	1.90	0.54
10:d:602:ADP:O3B	11:d:603:BEF:F2	2.16	0.54
8:c:50:ASP:HB2	8:c:51:PRO:HD3	1.89	0.54
3:o:158:LEU:HB3	3:o:400:VAL:HG13	1.90	0.54
5:B:132:LEU:HD23	5:B:495:ARG:HG3	1.89	0.54
8:C:223:VAL:HA	8:C:378:THR:OG1	2.08	0.54
10:C:1102:ADP:O3B	11:C:1103:BEF:F2	2.15	0.54
5:J:472:LEU:HB3	5:J:474:LEU:HD13	1.89	0.54
4:e:161:LEU:HD11	4:e:440:VAL:HG11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:183:ARG:HH22	5:b:210:GLU:HA	1.73	0.54
5:b:472:LEU:HB3	5:b:474:LEU:HD13	1.90	0.54
7:A:228:VAL:HG12	7:A:233:MET:SD	2.48	0.54
7:A:256:MET:HE3	7:A:260:VAL:HG11	1.90	0.54
5:J:69:LEU:O	5:J:75:LYS:HE3	2.08	0.54
8:K:183:ARG:HD3	8:K:407:MET:HE3	1.88	0.54
4:e:291:SER:HB3	4:e:294:GLU:HB2	1.89	0.54
2:p:329:LEU:O	2:p:333:CYS:HB2	2.08	0.54
4:m:98:ASN:HD22	4:m:101:ALA:H	1.56	0.54
5:B:377:LEU:O	5:B:378:ASP:C	2.51	0.53
7:A:26:ARG:CG	7:A:26:ARG:NH1	2.58	0.53
6:L:253:ILE:CG2	7:I:263:ASN:HB2	2.38	0.53
4:e:451:SER:O	4:e:455:SER:HB2	2.08	0.53
4:e:544:LEU:O	4:e:548:ILE:HG12	2.08	0.53
3:o:362:TYR:CE1	3:o:377:LEU:HD21	2.43	0.53
7:i:141:ASN:HA	7:i:144:LEU:HD12	1.90	0.53
2:H:322:LYS:C	2:H:324:PRO:HD2	2.32	0.53
1:N:189:LEU:HD22	8:K:364:TYR:HE1	1.73	0.53
3:O:297:LEU:HB3	3:O:298:PRO:CD	2.34	0.53
4:M:67:PRO:HA	4:M:190:SER:HA	1.90	0.53
4:M:84:THR:HG22	4:M:418:GLU:OE1	2.08	0.53
1:f:296:ILE:HG12	1:f:317:LEU:HD23	1.91	0.53
5:b:409:MET:HE3	5:b:459:LEU:HD23	1.91	0.53
7:a:94:ILE:HD13	7:a:523:SER:HA	1.89	0.53
8:c:222:GLY:HA2	8:c:331:VAL:HG11	1.89	0.53
3:o:242:LEU:HD22	3:o:244:LEU:HG	1.90	0.53
3:G:297:LEU:HB3	3:G:298:PRO:CD	2.35	0.53
1:N:521:THR:O	1:N:525:SER:HB3	2.09	0.53
2:P:43:LEU:HG	2:P:462:THR:CG2	2.38	0.53
3:O:249:GLU:HG2	3:O:250:LEU:H	1.72	0.53
4:M:253:GLN:HE21	5:J:325:VAL:HG23	1.72	0.53
5:J:179:ASN:O	5:J:183:ARG:HB2	2.08	0.53
8:K:198:ILE:HG21	8:K:408:LEU:HD21	1.89	0.53
7:a:52:MET:HE2	8:c:526:ILE:HG12	1.90	0.53
2:p:247:VAL:HG22	2:p:298:CYS:HB3	1.90	0.53
3:o:113:LYS:O	3:o:117:GLU:HG2	2.08	0.53
4:m:52:LEU:HA	4:m:55:ARG:HB2	1.90	0.53
7:i:39:VAL:HG11	7:i:73:LEU:HD11	1.89	0.53
8:k:324:ASP:HA	8:k:327:ARG:HH21	1.74	0.53
3:G:77:HIS:CE1	3:G:79:ALA:HB3	2.43	0.53
4:E:412:ASN:ND2	4:E:414:MET:SD	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:251:PHE:HB3	8:c:263:ILE:HB	1.90	0.53
8:c:108:ALA:HB3	8:c:109:PRO:HD3	1.90	0.53
3:o:323:MET:HA	3:o:326:VAL:HG12	1.89	0.53
8:k:133:LEU:HD21	8:k:511:LYS:HD2	1.89	0.53
1:N:509:SER:HB2	1:N:512:VAL:HG23	1.91	0.53
3:O:86:ILE:HD11	3:O:510:ALA:CA	2.37	0.53
1:f:75:LEU:HD12	8:c:55:LEU:HD23	1.91	0.53
5:b:155:HIS:HB2	5:b:488:VAL:HG22	1.89	0.53
6:d:432:MET:HG3	6:d:440:TRP:CZ3	2.44	0.53
8:c:324:ASP:HA	8:c:327:ARG:HH21	1.73	0.53
2:p:390:THR:HG21	3:o:82:THR:HG23	1.91	0.53
3:o:220:PHE:HE1	3:o:322:ASP:HB3	1.73	0.53
8:k:102:GLU:HA	8:k:105:ALA:HB3	1.90	0.53
1:F:87:THR:HG21	1:F:512:VAL:HA	1.90	0.53
5:B:194:GLN:HE21	5:B:196:ILE:HD11	1.74	0.53
4:M:60:ILE:O	4:M:72:LYS:HE2	2.08	0.53
6:L:242:SER:HB3	6:L:243:PRO:CD	2.38	0.53
1:f:192:HIS:NE2	1:f:326:GLU:HB2	2.24	0.53
2:h:43:LEU:HG	2:h:462:THR:HG22	1.90	0.53
6:d:260:MET:SD	7:a:273:ILE:HG23	2.49	0.53
7:a:250:ASN:HB3	7:a:300:LYS:HB3	1.89	0.53
3:o:221:LYS:HA	3:o:362:TYR:CE1	2.42	0.53
5:j:239:ASP:OD1	5:j:291:TYR:HD1	1.91	0.53
7:i:180:VAL:HG13	7:i:406:LEU:HD23	1.91	0.53
1:F:509:SER:HB2	1:F:512:VAL:HG23	1.90	0.53
4:E:86:ASP:O	4:E:90:ILE:HG12	2.07	0.53
6:D:305:LEU:HD12	6:D:310:ILE:HD12	1.91	0.53
6:d:71:LEU:HD21	7:a:15:LEU:HB2	1.90	0.53
1:n:465:ASP:HB3	1:n:468:ASP:HB2	1.90	0.53
2:p:48:PRO:HB3	2:p:172:TYR:CD1	2.42	0.53
2:p:512:ILE:HG23	2:p:517:ILE:HB	1.90	0.53
5:j:413:LYS:HG3	5:j:464:TYR:HD1	1.74	0.53
5:B:48:SER:HA	6:D:527:SER:O	2.08	0.53
7:A:143:VAL:O	7:A:143:VAL:HG12	2.07	0.53
8:C:457:ILE:HG21	8:C:464:PRO:HA	1.89	0.53
2:P:291:ILE:HD13	2:P:347:PRO:HG3	1.89	0.53
3:O:163:ARG:HG2	3:O:179:VAL:HG21	1.91	0.53
5:J:95:VAL:O	5:J:99:SER:HB2	2.09	0.53
1:f:163:ASP:HB2	1:f:166:LEU:HB3	1.91	0.53
2:h:65:THR:HG22	2:h:67:ASP:H	1.72	0.53
1:n:204:PRO:HB3	1:n:391:THR:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o:319:SER:HB3	3:o:322:ASP:HB2	1.91	0.53
4:m:329:ASP:OD2	5:j:235:ASN:HB3	2.09	0.53
4:m:507:ILE:HG22	4:m:509:ASN:H	1.72	0.53
6:l:195:ARG:HD3	6:l:323:PHE:CZ	2.43	0.53
3:G:282:LEU:HD21	3:G:306:PHE:CB	2.39	0.53
3:G:319:SER:HB3	3:G:322:ASP:HB2	1.91	0.53
4:E:102:LYS:O	4:E:105:VAL:HB	2.09	0.53
6:D:171:ALA:HB3	6:D:172:PRO:HD3	1.91	0.53
6:D:253:ILE:HG21	7:A:263:ASN:HB2	1.91	0.53
7:A:477:LEU:HD11	7:A:502:LEU:HD13	1.90	0.53
1:N:253:TYR:CE1	1:N:259:ARG:HG3	2.43	0.53
2:P:322:LYS:O	2:P:323:VAL:HB	2.08	0.53
4:M:73:ILE:CG2	5:J:511:VAL:HG13	2.39	0.53
7:I:12:THR:HB	7:I:14:PHE:HE2	1.70	0.53
3:g:352:PHE:HD1	3:g:365:PHE:HB3	1.73	0.53
1:n:192:HIS:NE2	1:n:326:GLU:HB2	2.24	0.53
1:n:197:MET:HE2	1:n:364:PHE:HE2	1.74	0.53
2:p:21:TYR:CD2	2:p:21:TYR:N	2.76	0.53
1:F:203:SER:O	1:F:206:ASP:HB2	2.08	0.53
3:G:163:ARG:NH2	3:G:176:ASP:OD1	2.42	0.53
5:B:413:LYS:HA	5:B:464:TYR:CE1	2.44	0.53
3:O:220:PHE:HE1	3:O:322:ASP:HB3	1.74	0.53
3:o:245:ASN:HB3	3:o:336:SER:HA	1.91	0.53
1:F:424:ARG:HH21	1:F:477:LEU:HD22	1.74	0.52
4:E:85:ASN:HB3	4:E:191:LYS:HG2	1.90	0.52
7:A:188:LYS:HG2	7:A:198:TYR:CE1	2.43	0.52
2:P:327:PHE:CG	2:P:328:GLU:N	2.77	0.52
2:h:27:GLN:HE21	2:h:544:ILE:HD11	1.73	0.52
3:g:478:TRP:CE3	3:g:492:PHE:HB2	2.44	0.52
4:e:440:VAL:HG12	4:e:441:TYR:H	1.74	0.52
7:i:63:THR:HA	7:i:397:GLU:CG	2.38	0.52
8:k:79:LEU:C	8:k:81:LEU:H	2.18	0.52
1:F:492:ASP:HB2	1:F:499:CYS:HB3	1.91	0.52
4:E:207:ALA:HB1	4:E:224:ILE:HD12	1.90	0.52
7:A:164:MET:HE3	7:A:405:SER:CB	2.39	0.52
6:L:353:ILE:HG22	6:L:354:ASP:N	2.24	0.52
7:I:17:GLY:CA	7:I:546:THR:O	2.57	0.52
7:I:144:LEU:CD2	7:I:419:VAL:HG22	2.40	0.52
7:I:262:ILE:HG21	8:K:259:THR:HG23	1.90	0.52
4:e:324:GLN:HB2	4:e:351:LEU:HD11	1.92	0.52
6:d:25:ILE:HG23	6:d:104:LEU:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:173:SER:O	7:a:177:SER:HB2	2.09	0.52
8:c:203:TYR:HE1	8:c:330:ARG:HE	1.57	0.52
8:c:219:VAL:HG22	8:c:379:ILE:HG12	1.91	0.52
1:n:439:LYS:O	1:n:442:THR:CG2	2.55	0.52
2:p:322:LYS:HG3	2:p:323:VAL:HG23	1.90	0.52
3:o:297:LEU:HB3	3:o:298:PRO:CD	2.37	0.52
5:j:254:SER:O	5:j:256:ALA:N	2.43	0.52
8:C:65:LEU:HD11	8:C:97:ILE:HD13	1.90	0.52
5:J:183:ARG:HH22	5:J:211:GLY:N	2.05	0.52
7:I:63:THR:HA	7:I:397:GLU:HG3	1.91	0.52
7:I:256:MET:HG2	8:K:257:SER:HB2	1.90	0.52
2:h:43:LEU:HA	2:h:105:ILE:HD11	1.91	0.52
4:e:412:ASN:HB3	4:e:415:ILE:CD1	2.38	0.52
1:n:221:HIS:CD2	1:n:223:ASP:H	2.25	0.52
2:p:27:GLN:HG3	2:p:541:ILE:HB	1.92	0.52
2:p:92:GLN:OE1	2:p:103:VAL:HG23	2.09	0.52
4:m:298:LEU:HD21	5:j:248:THR:HG21	1.92	0.52
6:l:162:ILE:O	6:l:162:ILE:HG13	2.08	0.52
6:l:239:PHE:HB3	6:l:334:ALA:O	2.09	0.52
2:H:243:LYS:HA	2:H:245:HIS:CE1	2.44	0.52
5:B:181:ILE:HD13	5:B:391:LEU:CB	2.40	0.52
3:O:167:SER:O	3:O:168:SER:CB	2.57	0.52
4:M:385:PHE:O	4:M:409:ARG:NH2	2.42	0.52
8:K:367:PHE:HE2	8:K:380:MET:HE1	1.74	0.52
2:h:33:ALA:HA	2:h:36:ARG:HD3	1.91	0.52
2:h:478:LEU:HD22	2:h:499:VAL:CG2	2.40	0.52
8:c:47:MET:HG3	8:c:57:LEU:HB3	1.90	0.52
7:i:63:THR:HG22	7:i:65:ASP:H	1.75	0.52
7:i:304:ASP:HA	7:i:307:LEU:HD12	1.91	0.52
3:G:409:ILE:HD13	3:G:497:TRP:HE3	1.74	0.52
3:G:478:TRP:HE3	3:G:492:PHE:HB2	1.70	0.52
3:O:83:LEU:O	3:O:86:ILE:HG22	2.09	0.52
3:O:147:ILE:HD13	3:O:157:LEU:CD1	2.39	0.52
4:M:72:LYS:HB2	4:M:90:ILE:CD1	2.37	0.52
6:L:257:TYR:HA	6:L:260:MET:HE2	1.92	0.52
1:f:518:THR:HG21	8:c:213:ASP:HB3	1.90	0.52
3:g:215:ILE:HG22	3:g:217:GLY:H	1.74	0.52
1:n:303:PRO:HA	1:n:306:LEU:HD12	1.92	0.52
1:F:251:PHE:HZ	2:H:259:THR:HB	1.74	0.52
3:G:224:PHE:CD2	3:G:225:SER:N	2.77	0.52
5:B:132:LEU:CD2	5:B:495:ARG:HG3	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:255:ARG:HA	8:K:257:SER:HA	1.91	0.52
1:f:337:GLN:HG2	1:f:347:ILE:HG21	1.91	0.52
3:g:25:GLN:HG2	3:g:521:ASP:C	2.34	0.52
3:g:107:GLU:CD	3:g:448:VAL:HG21	2.34	0.52
3:g:226:TYR:O	3:g:227:ALA:C	2.53	0.52
7:a:248:ASP:HB3	7:a:339:SER:HA	1.91	0.52
7:i:458:ILE:H	7:i:458:ILE:HD12	1.75	0.52
3:G:246:VAL:HA	3:G:297:LEU:HD12	1.90	0.52
4:E:269:LEU:H	4:E:375:GLY:H	1.56	0.52
4:E:324:GLN:HB2	4:E:351:LEU:HD11	1.92	0.52
5:B:438:ARG:O	5:B:441:PRO:HD2	2.09	0.52
6:D:35:ILE:CG2	6:D:94:THR:HG23	2.40	0.52
2:h:85:LEU:HD22	2:h:534:ALA:HB1	1.91	0.52
3:o:462:ILE:O	3:o:466:ASN:HB2	2.10	0.52
1:F:133:LEU:HD11	1:F:412:ILE:CD1	2.40	0.52
7:A:103:ILE:HG22	7:A:457:ILE:HG21	1.91	0.52
1:N:142:ASN:HD22	1:N:409:LYS:HA	1.75	0.52
3:O:44:LEU:HD22	3:O:103:ILE:HD13	1.91	0.52
7:I:165:SER:O	7:I:166:SER:CB	2.57	0.52
2:h:329:LEU:O	2:h:333:CYS:HB2	2.10	0.52
3:g:204:ILE:HD12	3:g:205:PRO:HD2	1.91	0.52
6:d:175:VAL:HA	6:d:401:ILE:HD13	1.91	0.52
4:m:144:ILE:HD11	4:m:550:LYS:HA	1.92	0.52
3:G:167:SER:O	3:G:168:SER:CB	2.58	0.52
3:G:220:PHE:C	3:G:222:LYS:N	2.68	0.52
5:B:472:LEU:HB3	5:B:474:LEU:HD13	1.91	0.52
6:D:367:ARG:O	6:D:368:ASN:CB	2.58	0.52
7:A:417:ASN:HB3	7:A:521:THR:HB	1.92	0.52
4:M:115:ILE:HG22	4:M:117:ASP:H	1.74	0.52
5:J:373:THR:HB	5:J:376:THR:OG1	2.10	0.52
4:e:40:ARG:NH1	4:e:42:HIS:ND1	2.58	0.52
6:d:125:GLN:NE2	6:d:513:GLU:HG2	2.22	0.52
2:p:245:HIS:HD1	2:p:245:HIS:H	1.57	0.52
3:o:107:GLU:CD	3:o:448:VAL:HG21	2.35	0.52
5:j:374:ASP:HB2	6:l:80:GLU:OE1	2.09	0.52
5:j:440:LEU:HB3	5:j:441:PRO:HD3	1.92	0.52
5:j:455:LEU:HD22	5:j:472:LEU:HD23	1.91	0.52
1:F:233:VAL:N	1:F:349:GLY:O	2.42	0.52
3:G:51:ILE:HB	3:G:69:ILE:HD12	1.92	0.52
5:B:444:LEU:HB3	5:B:474:LEU:HD21	1.92	0.52
1:N:255:SER:HB3	1:N:258:GLN:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:520:ARG:HG3	6:L:520:ARG:NH2	2.01	0.52
7:I:417:ASN:HB3	7:I:521:THR:HB	1.90	0.52
5:b:152:ASP:OD1	5:b:400:THR:HG21	2.10	0.52
6:d:432:MET:HG3	6:d:440:TRP:CE3	2.44	0.52
7:a:458:ILE:HB	7:a:459:PRO:HD3	1.92	0.52
3:o:77:HIS:CE1	3:o:79:ALA:HB3	2.44	0.52
6:l:254:VAL:HB	7:i:262:ILE:HD13	1.92	0.52
7:i:164:MET:HE3	7:i:405:SER:HB2	1.92	0.52
8:k:119:VAL:HA	8:k:122:ILE:HD12	1.92	0.52
1:F:303:PRO:HA	1:F:306:LEU:HD12	1.91	0.51
2:H:25:ASP:C	2:H:27:GLN:N	2.68	0.51
5:J:22:ALA:HA	5:J:73:ALA:HB2	1.92	0.51
6:L:367:ARG:O	6:L:368:ASN:CB	2.57	0.51
7:I:247:LEU:HD11	7:I:288:ILE:HD13	1.92	0.51
7:I:538:ILE:HA	7:I:541:ILE:HD12	1.91	0.51
8:K:324:ASP:HA	8:K:327:ARG:NH2	2.25	0.51
2:h:85:LEU:CD2	2:h:534:ALA:HB1	2.40	0.51
3:g:298:PRO:HB3	3:g:317:ARG:CZ	2.40	0.51
6:d:163:VAL:HG23	6:d:204:ILE:HG21	1.91	0.51
5:j:22:ALA:HA	5:j:73:ALA:HB2	1.92	0.51
1:F:327:ARG:O	1:F:331:VAL:HG23	2.10	0.51
4:E:157:ALA:HB1	4:E:450:MET:HE3	1.90	0.51
6:L:234:ILE:HD12	6:L:345:ASP:OD2	2.11	0.51
8:K:48:LEU:HD11	8:K:64:ILE:HA	1.92	0.51
4:e:428:CYS:O	4:e:431:ARG:HG3	2.11	0.51
5:b:408:GLU:HG3	5:b:441:PRO:HD3	1.92	0.51
6:d:254:VAL:HB	7:a:262:ILE:HD13	1.92	0.51
6:d:397:ALA:O	6:d:400:VAL:HG22	2.09	0.51
3:o:215:ILE:HG23	3:o:366:GLN:HB3	1.92	0.51
6:l:432:MET:HG3	6:l:440:TRP:CE3	2.45	0.51
2:H:182:VAL:O	2:H:186:VAL:HG23	2.11	0.51
5:B:409:MET:HB3	5:B:463:ILE:HD13	1.91	0.51
6:D:45:ASP:OD1	6:D:59:ASN:HB2	2.10	0.51
7:A:132:ALA:HB2	7:A:448:ILE:HG23	1.90	0.51
7:A:190:GLN:HA	7:A:195:GLU:O	2.11	0.51
8:C:159:ILE:O	8:C:161:THR:N	2.37	0.51
2:P:55:ILE:HD11	2:P:71:MET:HG3	1.91	0.51
3:O:221:LYS:HA	3:O:362:TYR:CE1	2.45	0.51
4:M:115:ILE:HG23	4:M:432:ASN:ND2	2.26	0.51
6:L:25:ILE:HG23	6:L:104:LEU:HB3	1.91	0.51
1:f:248:ASN:HD22	8:c:260:ASN:HB3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:64:SER:HB2	4:e:72:LYS:HZ2	1.75	0.51
4:e:115:ILE:HG23	4:e:432:ASN:ND2	2.25	0.51
4:e:207:ALA:HB1	4:e:224:ILE:HD12	1.93	0.51
6:d:162:ILE:HB	7:a:540:ARG:HD3	1.92	0.51
6:d:335:ASP:OD1	6:d:336:ILE:N	2.44	0.51
4:m:385:PHE:O	4:m:409:ARG:NH2	2.43	0.51
8:k:452:ILE:HB	8:k:453:PRO:HD3	1.92	0.51
5:B:14:ARG:HG2	5:B:15:ALA:H	1.76	0.51
7:A:71:SER:HB2	7:A:88:GLN:HE22	1.76	0.51
8:C:52:MET:HE3	8:C:52:MET:C	2.36	0.51
8:C:121:ILE:HG23	8:C:441:PRO:HB3	1.93	0.51
8:K:65:LEU:HB3	8:K:79:LEU:HD13	1.92	0.51
3:g:179:VAL:C	3:g:181:MET:H	2.17	0.51
6:d:411:ILE:HD11	6:d:501:VAL:HA	1.93	0.51
3:o:352:PHE:CD1	3:o:365:PHE:HB3	2.45	0.51
4:m:67:PRO:HA	4:m:190:SER:HA	1.91	0.51
4:m:73:ILE:CG2	5:j:514:ILE:HG12	2.40	0.51
6:l:444:ALA:HA	6:l:447:LEU:HD12	1.93	0.51
6:l:479:ASN:HB2	6:l:491:ASN:OD1	2.11	0.51
3:G:173:ASN:ND2	4:E:148:ASN:HA	2.25	0.51
5:B:39:PRO:HG3	10:B:602:ADP:C5	2.45	0.51
4:M:64:SER:HB2	4:M:72:LYS:HZ3	1.75	0.51
6:L:171:ALA:HB3	6:L:172:PRO:HD3	1.91	0.51
7:I:368:ASP:O	7:I:369:ASP:HB2	2.09	0.51
1:f:221:HIS:HB3	1:f:224:MET:HG3	1.92	0.51
1:f:274:LEU:O	1:f:278:ILE:HG13	2.11	0.51
4:e:73:ILE:CG2	5:b:514:ILE:HG12	2.40	0.51
7:a:521:THR:HG23	7:a:522:ILE:HG13	1.93	0.51
3:o:88:ARG:HG2	3:o:88:ARG:NH1	2.25	0.51
4:m:327:PHE:H	4:m:344:ARG:HD2	1.75	0.51
6:l:151:VAL:HA	6:l:175:VAL:HG21	1.91	0.51
1:F:97:LEU:HD11	1:F:451:LEU:HD23	1.92	0.51
3:G:120:ILE:HD11	7:I:471:SER:HB2	1.93	0.51
1:N:130:MET:HE1	1:N:514:ARG:CG	2.41	0.51
2:P:186:VAL:HG11	2:P:408:VAL:HG11	1.93	0.51
3:O:94:VAL:HG11	3:O:502:VAL:HG22	1.91	0.51
5:J:412:SER:O	5:J:416:ASP:HB2	2.11	0.51
1:f:465:ASP:HB3	1:f:468:ASP:HB2	1.92	0.51
1:f:492:ASP:HB2	1:f:499:CYS:HB3	1.92	0.51
2:h:26:GLY:O	2:h:31:SER:HB2	2.11	0.51
6:d:29:ARG:HH12	6:d:108:GLU:CD	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:i:63:THR:HG22	7:i:64:ASN:H	1.75	0.51
4:E:251:HIS:HE1	4:E:253:GLN:HG2	1.75	0.51
10:E:602:ADP:O3B	11:E:603:BEF:F2	2.18	0.51
5:B:234:ALA:HA	5:B:326:VAL:O	2.11	0.51
5:B:301:LEU:HD23	5:B:303:ILE:CD1	2.41	0.51
7:A:75:VAL:HG21	7:A:84:VAL:HG21	1.92	0.51
3:O:215:ILE:HG22	3:O:217:GLY:H	1.75	0.51
1:f:87:THR:HG22	1:f:89:ASP:H	1.75	0.51
2:h:77:ILE:HD13	2:h:86:VAL:HG21	1.93	0.51
3:g:301:ASP:O	3:g:305:GLN:HG2	2.11	0.51
5:b:43:ASP:OD2	6:d:520:ARG:NH2	2.44	0.51
5:b:279:PHE:HB3	5:b:281:ILE:HD12	1.93	0.51
1:n:13:LEU:HD13	1:n:21:VAL:HG21	1.93	0.51
1:n:133:LEU:HD11	1:n:412:ILE:CD1	2.41	0.51
3:o:204:ILE:HG23	3:o:379:ARG:HD3	1.91	0.51
6:D:68:MET:HE2	7:A:545:ILE:HD13	1.93	0.51
6:D:444:ALA:HA	6:D:447:LEU:HD12	1.93	0.51
7:A:252:GLN:HA	7:A:303:ASP:HB2	1.93	0.51
8:C:324:ASP:HA	8:C:327:ARG:NH2	2.25	0.51
1:N:224:MET:HE1	1:N:316:ALA:HB3	1.93	0.51
1:N:534:LEU:HD12	8:K:48:LEU:CD2	2.41	0.51
2:P:68:ALA:HA	2:P:71:MET:HE2	1.93	0.51
7:I:431:ILE:HB	7:I:485:GLN:HE22	1.75	0.51
4:e:412:ASN:HB2	5:b:80:ILE:HG12	1.93	0.51
4:m:226:MET:HE1	4:m:423:LEU:HD13	1.93	0.51
5:j:153:LEU:HD22	5:j:391:LEU:HG	1.93	0.51
6:l:506:SER:O	6:l:510:LEU:HG	2.11	0.51
6:l:520:ARG:HG3	6:l:520:ARG:NH2	2.06	0.51
8:k:361:GLY:O	8:k:362:ASP:HB2	2.11	0.51
1:F:195:GLU:HG3	1:F:327:ARG:HH11	1.75	0.51
4:E:52:LEU:HA	4:E:55:ARG:HB2	1.93	0.51
6:D:419:ILE:HD13	6:D:469:LEU:HG	1.93	0.51
6:D:516:LYS:O	6:D:520:ARG:HG2	2.11	0.51
7:A:70:LEU:HB3	7:A:84:VAL:HG13	1.93	0.51
7:A:501:GLY:HA3	7:A:512:GLU:HG2	1.93	0.51
8:C:105:ALA:O	8:C:109:PRO:HD2	2.11	0.51
8:C:111:LEU:HD22	8:C:440:TRP:HB3	1.92	0.51
2:P:546:MET:HE1	3:O:10:ILE:CG2	2.39	0.51
3:g:45:GLY:CA	3:g:453:LEU:HD22	2.39	0.51
5:b:281:ILE:HD11	5:b:337:LEU:HD11	1.92	0.51
7:a:538:ILE:HA	7:a:541:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:c:41:PRO:HG3	10:c:1102:ADP:C6	2.46	0.51
2:p:79:HIS:HD2	2:p:81:ALA:H	1.58	0.51
3:o:198:LEU:O	3:o:373:THR:HG23	2.10	0.51
6:l:291:SER:CB	6:l:296:ALA:HA	2.41	0.51
7:i:50:ASP:OD1	7:i:64:ASN:HB2	2.10	0.51
8:k:208:LYS:HB3	8:k:389:LEU:HD13	1.92	0.51
2:H:41:MET:HE1	3:G:524:ILE:HD11	1.92	0.51
5:B:239:ASP:OD1	5:B:291:TYR:HD1	1.94	0.51
6:D:494:GLU:C	6:D:496:HIS:H	2.19	0.51
2:P:267:LEU:HD13	2:P:273:MET:HG2	1.93	0.51
6:L:89:ALA:O	6:L:399:CYS:HB3	2.10	0.51
2:h:109:GLU:HG2	2:h:458:VAL:CG2	2.41	0.51
3:g:411:ALA:HB2	3:g:478:TRP:CD2	2.46	0.51
6:d:220:ILE:HD12	6:d:302:LEU:HD11	1.93	0.51
7:a:477:LEU:HD11	7:a:502:LEU:HD22	1.94	0.51
5:j:88:VAL:O	5:j:389:SER:HB3	2.11	0.51
7:i:523:SER:O	7:i:527:SER:HB2	2.11	0.51
1:F:296:ILE:HA	1:F:317:LEU:HB3	1.92	0.50
2:H:43:LEU:HG	2:H:462:THR:CG2	2.41	0.50
2:H:123:SER:HB3	2:H:126:GLU:CG	2.41	0.50
3:G:44:LEU:HD22	3:G:103:ILE:HD13	1.93	0.50
6:D:432:MET:HG3	6:D:440:TRP:CE3	2.46	0.50
7:A:55:ASP:O	7:A:56:ASP:CB	2.56	0.50
8:C:324:ASP:HA	8:C:327:ARG:HH21	1.76	0.50
1:N:98:VAL:HG13	1:N:524:ALA:HB2	1.93	0.50
1:f:509:SER:HB2	1:f:512:VAL:CG2	2.41	0.50
4:e:157:ALA:HB1	4:e:450:MET:HE3	1.94	0.50
7:a:198:TYR:CE2	7:a:413:LEU:HB3	2.46	0.50
8:c:457:ILE:HG21	8:c:464:PRO:HA	1.93	0.50
2:p:322:LYS:O	2:p:323:VAL:HB	2.11	0.50
5:j:409:MET:HB3	5:j:463:ILE:HD13	1.93	0.50
1:F:55:LEU:HD11	2:H:541:ILE:CD1	2.41	0.50
1:F:224:MET:HE1	1:F:316:ALA:HB3	1.93	0.50
2:H:43:LEU:HG	2:H:462:THR:HG22	1.94	0.50
5:B:184:LEU:HD11	5:B:192:HIS:CB	2.41	0.50
7:A:173:SER:O	7:A:177:SER:HB2	2.11	0.50
2:P:267:LEU:HB2	3:O:259:VAL:HG22	1.93	0.50
3:O:282:LEU:HD11	3:O:306:PHE:HB2	1.93	0.50
5:J:155:HIS:CB	5:J:488:VAL:HG22	2.40	0.50
6:L:130:ARG:O	6:L:134:ILE:HG13	2.12	0.50
4:e:277:GLU:O	4:e:309:MET:HE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:c:81:LEU:HD13	8:c:516:SER:HB2	1.93	0.50
4:m:88:ALA:O	4:m:92:SER:HB2	2.11	0.50
6:l:181:ILE:HD11	6:l:193:ASP:HB3	1.93	0.50
1:F:46:LEU:HD23	2:H:545:ILE:HB	1.94	0.50
3:G:51:ILE:HG12	4:E:553:ASN:HB3	1.93	0.50
4:E:51:ILE:HD13	4:E:134:LEU:HB2	1.93	0.50
4:E:141:ILE:HD11	6:L:463:ILE:HD12	1.94	0.50
4:E:385:PHE:O	4:E:409:ARG:NH2	2.45	0.50
6:D:244:PRO:CD	6:D:270:TYR:CE2	2.95	0.50
6:D:411:ILE:HD11	6:D:501:VAL:HA	1.92	0.50
6:L:46:LYS:HB2	6:L:64:ILE:HD12	1.93	0.50
5:b:440:LEU:HB3	5:b:441:PRO:CD	2.41	0.50
2:p:41:MET:HE1	3:o:524:ILE:HD11	1.93	0.50
2:H:227:VAL:HG13	2:H:368:VAL:HG11	1.93	0.50
4:E:333:HIS:CE1	5:B:326:VAL:HG13	2.46	0.50
8:C:65:LEU:HD22	8:C:79:LEU:HB2	1.94	0.50
5:J:380:ALA:O	5:J:384:LEU:HB2	2.11	0.50
6:L:55:ILE:HB	6:L:385:MET:HE2	1.93	0.50
1:f:217:HIS:NE2	1:f:320:ALA:HA	2.26	0.50
3:g:3:PHE:CD2	3:g:3:PHE:N	2.76	0.50
3:o:220:PHE:C	3:o:222:LYS:H	2.17	0.50
2:H:210:VAL:O	2:H:385:ILE:HA	2.11	0.50
3:G:157:LEU:O	3:G:161:CYS:HB2	2.12	0.50
5:B:162:SER:O	5:B:163:SER:HB3	2.11	0.50
5:B:346:ILE:HG22	5:B:347:MET:H	1.76	0.50
1:N:198:GLN:HB2	1:N:388:LEU:HD13	1.94	0.50
4:M:211:VAL:HG12	4:M:402:LYS:O	2.11	0.50
8:K:453:PRO:O	8:K:457:ILE:HG12	2.12	0.50
1:f:458:LEU:HB3	1:f:493:LEU:HD21	1.93	0.50
3:g:337:THR:HG22	3:g:339:SER:H	1.76	0.50
6:d:198:LYS:HE2	6:d:391:GLU:OE1	2.12	0.50
7:a:143:VAL:O	7:a:143:VAL:HG12	2.10	0.50
8:c:167:TRP:CE3	8:c:214:VAL:HB	2.47	0.50
2:p:25:ASP:C	2:p:27:GLN:H	2.18	0.50
3:o:385:VAL:O	3:o:389:VAL:HG23	2.12	0.50
3:o:482:VAL:HG22	3:o:491:ASN:HD21	1.77	0.50
8:C:179:VAL:HG12	8:C:407:MET:HE1	1.94	0.50
1:N:58:ASP:HA	1:N:161:LYS:HE2	1.93	0.50
7:I:139:PHE:CE2	7:I:143:VAL:HG21	2.47	0.50
8:K:203:TYR:HE1	8:K:330:ARG:HE	1.59	0.50
4:e:287:LEU:HD12	5:b:248:THR:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:d:257:TYR:HA	6:d:260:MET:HE2	1.93	0.50
8:c:48:LEU:HD11	8:c:64:ILE:HA	1.93	0.50
7:i:52:MET:HG3	7:i:62:VAL:HG22	1.94	0.50
8:k:70:VAL:HG11	8:k:75:ALA:CB	2.42	0.50
1:F:163:ASP:HB2	1:F:166:LEU:HB3	1.93	0.50
1:F:337:GLN:HG2	1:F:347:ILE:HG21	1.92	0.50
4:E:287:LEU:HD12	5:B:248:THR:HG22	1.94	0.50
5:B:193:ILE:HA	5:B:365:CYS:O	2.11	0.50
7:A:62:VAL:O	7:A:397:GLU:HG3	2.12	0.50
1:N:23:VAL:HG13	1:N:102:LEU:HB3	1.93	0.50
3:O:462:ILE:O	3:O:466:ASN:HB2	2.11	0.50
5:J:476:ASN:HB3	5:J:478:THR:HG22	1.94	0.50
3:g:44:LEU:HD22	3:g:103:ILE:HD13	1.93	0.50
5:b:44:LYS:HD3	6:d:523:ASP:HB3	1.93	0.50
5:b:255:THR:CG2	6:d:263:ILE:HA	2.42	0.50
7:a:17:GLY:HA3	7:a:546:THR:O	2.11	0.50
1:n:255:SER:HB3	1:n:258:GLN:HB2	1.94	0.50
2:p:310:LEU:O	2:p:314:ASN:HB2	2.12	0.50
6:l:130:ARG:O	6:l:134:ILE:HG13	2.11	0.50
1:F:252:PHE:HD1	2:H:264:THR:HB	1.76	0.50
1:N:130:MET:HE1	1:N:514:ARG:HG2	1.94	0.50
3:g:98:THR:OG1	11:g:603:BEF:F2	2.20	0.50
6:d:432:MET:SD	6:d:440:TRP:HZ3	2.35	0.50
2:H:65:THR:HG21	2:H:70:THR:HB	1.94	0.50
3:G:449:ILE:O	3:G:453:LEU:HG	2.12	0.50
8:C:164:VAL:CG1	8:C:171:MET:HG3	2.42	0.50
4:M:151:ASP:OD2	4:M:546:ARG:HD3	2.12	0.50
5:J:234:ALA:C	5:J:286:ASN:HD22	2.20	0.50
5:J:254:SER:O	5:J:256:ALA:N	2.44	0.50
6:L:138:MET:SD	6:L:478:LEU:HD22	2.52	0.50
1:f:251:PHE:HZ	2:h:259:THR:HB	1.76	0.50
2:h:311:HIS:HB2	3:g:336:SER:HB2	1.94	0.50
4:e:438:ARG:HH21	4:e:531:PHE:HE2	1.60	0.50
2:H:96:MET:HE1	2:H:410:GLY:HA3	1.94	0.49
4:E:251:HIS:CE1	4:E:253:GLN:HG2	2.46	0.49
6:L:323:PHE:C	6:L:323:PHE:CD1	2.90	0.49
8:K:385:SER:HB3	8:K:388:ILE:HG12	1.93	0.49
2:h:109:GLU:HG2	2:h:458:VAL:HG21	1.93	0.49
8:c:119:VAL:HA	8:c:122:ILE:HD12	1.93	0.49
1:n:242:TYR:CZ	2:p:260:GLU:HB3	2.47	0.49
5:j:279:PHE:HE1	5:j:335:CYS:SG	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:i:255:ARG:HA	8:k:257:SER:HA	1.93	0.49
2:H:135:ARG:HB2	2:H:532:THR:HG21	1.93	0.49
8:C:160:GLY:HA2	8:C:165:ILE:HG12	1.93	0.49
7:I:86:LEU:HD13	7:I:534:ALA:HB2	1.93	0.49
8:K:62:HIS:O	8:K:66:ARG:HB2	2.12	0.49
8:K:231:HIS:HB3	8:K:234:MET:HG3	1.93	0.49
4:e:450:MET:HE1	4:e:538:ILE:CD1	2.42	0.49
6:d:138:MET:SD	6:d:478:LEU:CD2	3.00	0.49
2:p:238:SER:C	2:p:240:SER:N	2.69	0.49
2:p:323:VAL:O	2:p:324:PRO:C	2.54	0.49
7:i:199:PRO:HB2	7:i:202:ALA:HB2	1.94	0.49
1:F:440:THR:O	1:F:444:ILE:HD12	2.11	0.49
2:H:444:LEU:HD12	2:H:444:LEU:H	1.77	0.49
6:D:46:LYS:HB2	6:D:64:ILE:HD12	1.93	0.49
8:C:78:MET:O	8:C:81:LEU:HB3	2.12	0.49
1:N:6:LEU:HB3	8:K:70:VAL:HG13	1.93	0.49
7:I:97:GLY:O	7:I:101:VAL:HG23	2.12	0.49
2:h:25:ASP:C	2:h:27:GLN:H	2.20	0.49
5:b:214:LEU:HD11	5:b:317:LEU:HD11	1.93	0.49
7:a:12:THR:CB	7:a:14:PHE:CE2	2.93	0.49
7:a:437:ALA:HB1	7:a:445:GLN:HG3	1.95	0.49
1:n:245:THR:HG21	8:k:272:ILE:HD12	1.94	0.49
1:n:296:ILE:HG12	1:n:317:LEU:HD23	1.92	0.49
3:o:383:GLU:HA	3:o:386:ILE:HD12	1.94	0.49
4:m:242:GLY:HA3	4:m:395:ILE:O	2.11	0.49
5:j:103:LEU:HD21	5:j:505:ALA:HA	1.94	0.49
6:l:244:PRO:CD	6:l:270:TYR:CE2	2.95	0.49
7:i:228:VAL:HG23	7:i:363:GLN:OE1	2.11	0.49
1:F:242:TYR:CZ	2:H:260:GLU:HB3	2.48	0.49
1:N:87:THR:CG2	1:N:512:VAL:HG22	2.43	0.49
1:f:87:THR:HG21	1:f:512:VAL:HG22	1.93	0.49
1:f:199:MET:HG3	1:f:379:LEU:HD21	1.94	0.49
4:e:292:VAL:HG21	5:b:260:GLN:HB3	1.93	0.49
5:b:254:SER:O	5:b:256:ALA:N	2.46	0.49
6:d:134:ILE:HG22	6:d:138:MET:HE2	1.94	0.49
2:p:238:SER:C	2:p:240:SER:H	2.19	0.49
2:p:332:LEU:O	2:p:335:VAL:HG12	2.12	0.49
7:i:55:ASP:O	7:i:56:ASP:CB	2.60	0.49
10:k:1102:ADP:O3B	11:k:1103:BEF:F2	2.20	0.49
2:H:323:VAL:O	2:H:324:PRO:C	2.56	0.49
2:P:111:LEU:HD11	2:P:538:VAL:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:226:TYR:O	3:O:227:ALA:C	2.55	0.49
8:K:121:ILE:HG23	8:K:441:PRO:HB3	1.93	0.49
1:f:119:THR:HG23	1:f:525:SER:OG	2.13	0.49
6:d:45:ASP:OD1	6:d:59:ASN:HB2	2.13	0.49
6:d:242:SER:HB3	6:d:243:PRO:CD	2.42	0.49
2:p:498:GLY:O	2:p:509:VAL:HG13	2.13	0.49
8:k:167:TRP:CE3	8:k:214:VAL:HB	2.47	0.49
5:B:156:ILE:HD13	5:B:488:VAL:HG23	1.95	0.49
5:B:238:LEU:HB2	5:B:289:LEU:O	2.13	0.49
2:P:310:LEU:O	2:P:314:ASN:HB2	2.13	0.49
5:J:45:LEU:HD23	6:L:524:ILE:HG12	1.93	0.49
5:J:192:HIS:HD2	5:J:319:LEU:HD12	1.75	0.49
5:J:255:THR:HG22	6:L:263:ILE:HA	1.93	0.49
6:d:72:HIS:HD2	6:d:74:VAL:HB	1.76	0.49
7:a:26:ARG:CG	7:a:26:ARG:NH1	2.71	0.49
7:a:62:VAL:O	7:a:397:GLU:HG3	2.13	0.49
3:o:90:GLN:HE21	3:o:97:GLY:HA3	1.78	0.49
4:m:168:ILE:HD11	4:m:439:VAL:HG13	1.93	0.49
2:H:80:PRO:O	2:H:84:VAL:HG23	2.13	0.49
7:A:17:GLY:CA	7:A:546:THR:O	2.56	0.49
7:A:267:PRO:HB3	8:C:272:ILE:HG23	1.94	0.49
8:C:355:PHE:HD2	8:C:368:LEU:CD1	2.26	0.49
1:N:93:THR:HG23	1:N:454:ILE:HD11	1.95	0.49
8:c:167:TRP:N	8:c:167:TRP:CD1	2.81	0.49
8:c:204:VAL:HA	8:c:377:CYS:O	2.12	0.49
4:m:91:LEU:HD11	4:m:123:VAL:HG21	1.93	0.49
1:F:130:MET:HE1	1:F:514:ARG:CG	2.42	0.49
1:F:217:HIS:HD1	1:F:317:LEU:HD11	1.77	0.49
1:F:221:HIS:CD2	1:F:223:ASP:H	2.28	0.49
2:H:254:LEU:HB2	2:H:305:VAL:HG22	1.95	0.49
4:E:269:LEU:CD1	4:E:358:THR:HG21	2.42	0.49
4:E:385:PHE:HD2	4:E:390:ASP:O	1.95	0.49
5:B:27:ILE:HG12	5:B:104:ARG:HG2	1.94	0.49
8:C:139:VAL:HG12	8:C:480:PHE:CD1	2.48	0.49
3:O:323:MET:HA	3:O:326:VAL:HG12	1.94	0.49
5:J:346:ILE:HG22	5:J:347:MET:N	2.28	0.49
6:L:150:LEU:HD23	6:L:179:LEU:HD11	1.94	0.49
7:I:99:THR:O	7:I:103:ILE:HG13	2.13	0.49
1:f:252:PHE:HD1	2:h:264:THR:HB	1.78	0.49
3:g:242:LEU:HD21	3:g:341:ILE:HD13	1.95	0.49
4:e:251:HIS:CE1	5:b:325:VAL:HB	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:d:138:MET:HB2	6:d:478:LEU:CD1	2.40	0.49
1:n:325:MET:HE3	1:n:336:ALA:HB1	1.94	0.49
8:k:175:ALA:O	8:k:179:VAL:HG23	2.13	0.49
1:F:35:THR:HG22	1:F:42:THR:OG1	2.13	0.49
1:F:133:LEU:HD11	1:F:412:ILE:HD11	1.95	0.49
2:H:182:VAL:HG22	2:H:401:ILE:HG13	1.95	0.49
3:G:215:ILE:HD13	3:G:219:ALA:HB2	1.95	0.49
3:G:462:ILE:O	3:G:466:ASN:HB2	2.13	0.49
4:E:234:ILE:HA	4:E:409:ARG:O	2.13	0.49
4:E:511:GLY:O	4:E:520:ASN:HB3	2.11	0.49
7:a:97:GLY:O	7:a:101:VAL:HG23	2.13	0.49
7:a:100:SER:O	7:a:104:ILE:HG13	2.12	0.49
7:a:126:ILE:HG13	7:a:539:LEU:HD23	1.95	0.49
7:a:333:THR:HG22	7:a:377:THR:HG22	1.95	0.49
2:p:209:VAL:HG11	2:p:398:GLU:HG3	1.93	0.49
3:G:25:GLN:HG2	3:G:521:ASP:C	2.38	0.49
4:E:115:ILE:HG23	4:E:432:ASN:ND2	2.28	0.49
5:B:56:VAL:HG23	5:B:375:GLN:HG2	1.93	0.49
6:D:42:LYS:HE2	6:D:484:VAL:HG13	1.94	0.49
7:A:28:GLN:HE21	7:A:77:HIS:CE1	2.30	0.49
7:A:77:HIS:CD2	7:A:79:ALA:H	2.31	0.49
1:N:221:HIS:HB3	1:N:224:MET:HG3	1.95	0.49
7:I:26:ARG:CG	7:I:26:ARG:NH1	2.65	0.49
8:K:129:LEU:HD13	8:K:514:ILE:HD12	1.95	0.49
1:f:6:LEU:HB3	8:c:70:VAL:HG13	1.95	0.49
3:g:297:LEU:HB3	3:g:298:PRO:CD	2.36	0.49
2:p:135:ARG:HB2	2:p:532:THR:HG21	1.94	0.49
2:p:284:ILE:CD1	2:p:308:LEU:HB3	2.42	0.49
4:m:320:VAL:HG22	4:m:341:PRO:HB2	1.95	0.49
8:k:297:THR:HG22	8:k:299:LYS:H	1.77	0.49
1:F:534:LEU:HB2	8:C:48:LEU:HD23	1.94	0.48
5:B:58:ASN:O	5:B:59:ASP:C	2.56	0.48
6:D:199:LYS:O	6:D:380:ARG:NH1	2.46	0.48
8:C:269:TRP:NE1	8:C:273:LEU:HD22	2.28	0.48
2:P:413:LYS:CB	2:P:414:PRO:HD3	2.43	0.48
7:I:251:LEU:HD23	7:I:285:VAL:HG22	1.95	0.48
1:f:234:LEU:HD11	1:f:343:LEU:HD11	1.94	0.48
1:f:459:VAL:HG22	1:f:491:VAL:HG11	1.95	0.48
3:g:362:TYR:CE1	3:g:377:LEU:HD21	2.48	0.48
6:d:35:ILE:HA	6:d:46:LYS:HZ3	1.77	0.48
1:n:133:LEU:HD11	1:n:412:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:509:SER:HB2	1:n:512:VAL:HG23	1.94	0.48
2:p:43:LEU:HG	2:p:462:THR:HG21	1.95	0.48
3:o:157:LEU:O	3:o:161:CYS:HB2	2.12	0.48
7:i:28:GLN:HE21	7:i:77:HIS:CE1	2.27	0.48
8:k:322:LYS:HD3	8:k:322:LYS:H	1.77	0.48
7:A:211:LYS:H	8:C:508:GLN:HE22	1.61	0.48
3:O:55:THR:HG22	3:O:56:SER:H	1.78	0.48
3:O:157:LEU:O	3:O:161:CYS:HB2	2.14	0.48
3:O:204:ILE:HG23	3:O:379:ARG:HD3	1.95	0.48
4:M:160:LYS:HG3	4:M:453:ALA:HB1	1.95	0.48
1:f:111:GLU:CG	1:n:467:LEU:HD13	2.42	0.48
5:b:293:TYR:HA	6:d:334:ALA:HB1	1.94	0.48
5:b:419:ALA:C	5:b:421:ASN:H	2.21	0.48
6:d:436:GLN:HA	6:d:439:ILE:HD12	1.95	0.48
3:o:167:SER:O	3:o:168:SER:CB	2.61	0.48
4:m:157:ALA:HB1	4:m:450:MET:HE3	1.94	0.48
7:i:198:TYR:CE2	7:i:413:LEU:HB3	2.48	0.48
5:B:255:THR:CG2	6:D:263:ILE:HA	2.44	0.48
6:D:135:LEU:HA	6:D:138:MET:HG2	1.94	0.48
1:N:146:ASP:HB3	1:N:149:PHE:HB3	1.94	0.48
3:O:113:LYS:HB3	3:O:114:PRO:HD3	1.95	0.48
3:O:381:GLY:HA2	4:M:540:LEU:HD22	1.95	0.48
4:e:143:PRO:O	4:e:549:LEU:HD23	2.13	0.48
5:b:233:ILE:HG12	5:b:285:ILE:HD11	1.94	0.48
6:d:271:LEU:HD23	6:d:301:ALA:HB2	1.94	0.48
1:n:455:PRO:O	1:n:459:VAL:HG23	2.14	0.48
2:p:27:GLN:HA	2:p:31:SER:CB	2.43	0.48
4:m:254:MET:SD	4:m:341:PRO:HA	2.53	0.48
2:H:27:GLN:HA	2:H:31:SER:CB	2.35	0.48
5:B:95:VAL:O	5:B:99:SER:HB2	2.13	0.48
6:L:163:VAL:HG23	6:L:204:ILE:HG21	1.96	0.48
1:f:189:LEU:HA	8:c:359:MET:SD	2.53	0.48
2:h:123:SER:HB3	2:h:126:GLU:CG	2.43	0.48
2:h:142:LEU:HA	2:h:145:MET:HG3	1.95	0.48
2:p:267:LEU:HD13	2:p:273:MET:HG2	1.94	0.48
1:F:107:ARG:HG3	1:N:107:ARG:CZ	2.43	0.48
2:H:509:VAL:HG13	2:H:510:LYS:H	1.77	0.48
3:G:139:LYS:O	3:G:143:LEU:HB2	2.13	0.48
6:D:295:ASP:O	6:D:296:ALA:HB3	2.14	0.48
6:D:323:PHE:C	6:D:323:PHE:CD1	2.91	0.48
6:D:421:ILE:CG2	6:D:447:LEU:HD13	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:165:SER:O	7:A:166:SER:CB	2.61	0.48
8:C:453:PRO:O	8:C:457:ILE:HG12	2.14	0.48
1:N:450:ALA:O	1:N:453:VAL:HG22	2.13	0.48
2:P:27:GLN:HE21	2:P:544:ILE:HG12	1.79	0.48
6:L:271:LEU:HD23	6:L:301:ALA:HB2	1.94	0.48
1:f:248:ASN:HB2	8:c:260:ASN:HB3	1.95	0.48
8:c:183:ARG:HD3	8:c:407:MET:CE	2.29	0.48
5:j:121:ILE:HG12	5:j:506:GLU:HG2	1.96	0.48
6:l:203:THR:HG22	6:l:205:ASP:H	1.79	0.48
1:F:217:HIS:NE2	1:F:320:ALA:HA	2.29	0.48
4:E:275:PRO:HD3	4:E:325:TRP:HE3	1.77	0.48
6:D:175:VAL:HA	6:D:401:ILE:HD13	1.95	0.48
7:A:56:ASP:OD1	7:A:56:ASP:C	2.56	0.48
1:N:248:ASN:HD22	8:K:260:ASN:HB3	1.79	0.48
1:N:452:LEU:HD22	1:N:470:LEU:HD21	1.94	0.48
3:O:37:GLN:HG3	3:O:103:ILE:HA	1.96	0.48
5:J:33:VAL:HB	5:J:93:THR:HG23	1.96	0.48
5:J:183:ARG:NH1	5:J:365:CYS:HB3	2.23	0.48
5:J:327:SER:O	5:J:329:PHE:N	2.47	0.48
2:h:92:GLN:HG3	2:h:526:PHE:HB3	1.94	0.48
3:g:157:LEU:O	3:g:161:CYS:HB2	2.13	0.48
7:a:199:PRO:HB2	7:a:202:ALA:HB2	1.96	0.48
1:n:237:ASN:HB3	1:n:325:MET:HE2	1.96	0.48
5:j:181:ILE:HD11	5:j:388:LEU:HA	1.95	0.48
6:l:74:VAL:HG13	6:l:518:ILE:HD12	1.95	0.48
7:i:462:LEU:HB3	7:i:504:LEU:HD11	1.94	0.48
5:B:157:ALA:HB2	5:B:391:LEU:HD11	1.95	0.48
8:C:48:LEU:HD11	8:C:64:ILE:HA	1.94	0.48
8:C:173:GLU:O	8:C:177:ASP:HB2	2.14	0.48
2:h:509:VAL:CG1	2:h:510:LYS:H	2.26	0.48
6:d:465:VAL:O	6:d:469:LEU:HB2	2.13	0.48
7:a:55:ASP:O	7:a:56:ASP:CB	2.56	0.48
2:p:154:ASN:HB3	2:p:190:LEU:HD13	1.95	0.48
7:i:501:GLY:CA	7:i:512:GLU:HG2	2.43	0.48
8:k:7:PHE:CG	8:k:8:MET:N	2.81	0.48
8:k:324:ASP:OD1	8:k:327:ARG:NH2	2.47	0.48
1:F:13:LEU:HD13	1:F:21:VAL:HG21	1.96	0.48
5:B:45:LEU:HD13	5:B:56:VAL:HG22	1.95	0.48
5:B:155:HIS:HB3	5:B:488:VAL:HG22	1.95	0.48
7:A:538:ILE:HA	7:A:541:ILE:HD12	1.95	0.48
4:e:29:PHE:N	4:e:29:PHE:CD2	2.80	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:269:LEU:HD13	4:e:322:ILE:HD12	1.94	0.48
6:d:35:ILE:CG2	6:d:94:THR:HG23	2.43	0.48
8:c:471:LEU:O	8:c:475:HIS:HB2	2.14	0.48
4:m:211:VAL:HG12	4:m:402:LYS:O	2.14	0.48
6:l:465:VAL:O	6:l:469:LEU:HB2	2.13	0.48
3:G:242:LEU:HD21	3:G:341:ILE:HD13	1.95	0.48
7:A:209:HIS:CE1	8:C:83:ARG:HH21	2.30	0.48
7:A:228:VAL:HG22	7:A:372:ILE:HD11	1.96	0.48
3:O:220:PHE:C	3:O:222:LYS:N	2.70	0.48
3:O:342:LYS:C	3:O:344:GLU:H	2.22	0.48
4:M:228:GLY:HA3	4:M:420:GLU:OE2	2.13	0.48
6:L:420:GLU:HB2	6:L:473:HIS:HE1	1.73	0.48
8:K:291:ARG:N	8:K:292:PRO:HD3	2.29	0.48
3:g:166:MET:HE1	3:g:171:ILE:HD11	1.95	0.48
4:e:335:LEU:HD23	4:e:342:ALA:HB2	1.95	0.48
5:b:231:ILE:HG12	5:b:283:THR:HB	1.96	0.48
7:a:269:GLN:HA	7:a:272:GLN:HB2	1.95	0.48
5:j:459:LEU:HD13	5:j:472:LEU:HG	1.96	0.48
7:i:17:GLY:HA3	7:i:546:THR:O	2.14	0.48
7:i:181:VAL:O	7:i:185:LEU:HB2	2.14	0.48
8:k:220:LEU:O	8:k:222:GLY:N	2.46	0.48
5:B:230:LYS:O	5:B:281:ILE:HG23	2.14	0.48
6:D:138:MET:SD	6:D:478:LEU:HD21	2.54	0.48
5:J:279:PHE:CE2	5:J:332:PRO:HG3	2.48	0.48
6:L:465:VAL:O	6:L:469:LEU:HB2	2.13	0.48
7:I:248:ASP:HB3	7:I:339:SER:HA	1.95	0.48
2:h:310:LEU:O	2:h:314:ASN:HB2	2.14	0.48
3:g:20:SER:HB2	3:g:25:GLN:NE2	2.29	0.48
3:g:202:LYS:HE2	3:g:221:LYS:H	1.79	0.48
6:d:409:GLY:C	6:d:501:VAL:HG23	2.38	0.48
6:l:96:VAL:HG23	6:l:507:ALA:O	2.14	0.48
3:G:282:LEU:HD11	3:G:306:PHE:HB2	1.96	0.47
8:C:57:LEU:HG	8:C:57:LEU:O	2.14	0.47
8:C:102:GLU:HA	8:C:105:ALA:HB3	1.95	0.47
3:O:191:ARG:O	3:O:192:ASN:C	2.58	0.47
4:M:273:THR:O	4:M:273:THR:HG22	2.13	0.47
1:f:56:THR:HG22	1:f:58:ASP:H	1.79	0.47
8:c:142:PRO:HA	8:c:411:SER:HA	1.96	0.47
1:n:28:GLY:O	1:n:32:VAL:HG23	2.12	0.47
3:o:51:ILE:HG12	4:m:553:ASN:HB3	1.96	0.47
3:o:301:ASP:O	3:o:305:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:l:271:LEU:HD23	6:l:301:ALA:HB2	1.95	0.47
6:l:411:ILE:HD11	6:l:501:VAL:HA	1.94	0.47
1:F:450:ALA:O	1:F:453:VAL:HG22	2.14	0.47
7:A:248:ASP:HB3	7:A:339:SER:HA	1.97	0.47
8:C:35:ILE:HB	8:C:97:ILE:HD11	1.96	0.47
1:N:100:GLU:OE1	1:N:103:ARG:NH1	2.47	0.47
1:N:418:PHE:HE2	1:N:517:ILE:HD11	1.79	0.47
3:O:74:ASP:O	4:M:32:VAL:HA	2.14	0.47
2:h:387:ARG:HH22	3:g:93:GLU:CD	2.22	0.47
3:g:202:LYS:HB3	3:g:377:LEU:HD23	1.96	0.47
4:e:275:PRO:HD3	4:e:325:TRP:HE3	1.79	0.47
6:d:210:ILE:HD12	6:d:214:VAL:HG22	1.96	0.47
5:j:459:LEU:HG	5:j:463:ILE:HD12	1.96	0.47
8:k:47:MET:HG3	8:k:57:LEU:HB3	1.96	0.47
3:G:191:ARG:O	3:G:192:ASN:C	2.57	0.47
5:J:409:MET:HB3	5:J:463:ILE:HD13	1.96	0.47
8:K:79:LEU:C	8:K:81:LEU:H	2.22	0.47
7:a:210:GLY:O	7:a:388:ARG:HB3	2.13	0.47
1:n:296:ILE:HA	1:n:317:LEU:HB3	1.96	0.47
5:j:190:LEU:N	5:j:190:LEU:HD12	2.28	0.47
7:i:250:ASN:HB3	7:i:300:LYS:HB3	1.97	0.47
3:G:189:LEU:HD11	3:G:195:ASP:O	2.14	0.47
3:G:220:PHE:HE1	3:G:322:ASP:HB3	1.79	0.47
2:P:182:VAL:O	2:P:186:VAL:HG23	2.14	0.47
5:J:482:MET:HE2	5:J:482:MET:HA	1.96	0.47
6:L:149:GLN:HE21	6:L:410:LEU:HD23	1.79	0.47
8:K:145:VAL:HG12	8:K:406:VAL:HG12	1.95	0.47
4:e:322:ILE:HG21	4:e:354:ILE:HD13	1.96	0.47
7:a:211:LYS:H	8:c:508:GLN:HE22	1.62	0.47
1:n:337:GLN:CG	1:n:347:ILE:HG21	2.44	0.47
5:j:215:ALA:HA	5:j:353:PHE:HD1	1.79	0.47
7:i:179:MET:HE1	7:i:385:ILE:HG23	1.95	0.47
2:H:27:GLN:HG3	2:H:541:ILE:HB	1.97	0.47
4:E:61:ILE:HD11	4:E:91:LEU:HD21	1.96	0.47
5:B:34:LYS:HD2	5:B:443:ILE:HD13	1.96	0.47
7:A:94:ILE:CD1	7:A:523:SER:HA	2.42	0.47
5:J:320:VAL:O	5:J:359:CYS:HB3	2.14	0.47
2:h:27:GLN:HA	2:h:31:SER:HB3	1.95	0.47
5:b:36:THR:HG23	5:b:58:ASN:CG	2.40	0.47
6:d:124:PHE:O	6:d:127:ALA:HB3	2.14	0.47
6:d:320:GLU:O	6:d:324:LEU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:l:42:LYS:HE2	6:l:484:VAL:HG13	1.96	0.47
6:l:253:ILE:CG2	7:i:263:ASN:HB2	2.44	0.47
2:H:267:LEU:HD13	2:H:273:MET:HG2	1.96	0.47
2:H:512:ILE:HG23	2:H:517:ILE:HB	1.95	0.47
3:G:326:VAL:HG23	3:G:365:PHE:CE1	2.49	0.47
6:D:432:MET:SD	6:D:440:TRP:CZ3	3.04	0.47
7:A:251:LEU:HD23	7:A:285:VAL:HG22	1.97	0.47
3:O:173:ASN:HB2	4:M:546:ARG:NH1	2.29	0.47
7:I:179:MET:HE3	7:I:218:LEU:HB2	1.95	0.47
8:K:119:VAL:HA	8:K:122:ILE:HD12	1.96	0.47
4:e:115:ILE:HG22	4:e:117:ASP:H	1.80	0.47
4:e:541:ALA:O	4:e:545:CYS:HB2	2.14	0.47
6:d:195:ARG:HD3	6:d:323:PHE:CZ	2.50	0.47
2:p:123:SER:HB3	2:p:126:GLU:HG3	1.96	0.47
1:F:454:ILE:H	1:F:454:ILE:HD12	1.79	0.47
2:H:54:ILE:CD1	3:G:78:PRO:HB2	2.44	0.47
3:G:356:GLN:HB2	3:G:361:ARG:CZ	2.45	0.47
4:E:151:ASP:OD2	4:E:546:ARG:HD3	2.15	0.47
4:E:281:PRO:HD2	4:E:285:HIS:CE1	2.49	0.47
5:B:15:ALA:HB1	5:B:19:ARG:HH12	1.80	0.47
6:D:78:LEU:HD22	6:D:97:VAL:HG13	1.96	0.47
7:A:47:VAL:HG12	8:C:117:HIS:NE2	2.30	0.47
7:A:198:TYR:CE2	7:A:413:LEU:HB3	2.49	0.47
1:N:30:GLN:HB2	1:N:96:CYS:HA	1.97	0.47
1:N:75:LEU:HD12	8:K:55:LEU:CD2	2.45	0.47
2:P:109:GLU:HG2	2:P:458:VAL:HG21	1.96	0.47
2:P:111:LEU:HD21	2:P:538:VAL:HG23	1.96	0.47
4:M:207:ALA:HB1	4:M:224:ILE:HD12	1.97	0.47
4:M:322:ILE:HG23	4:M:346:VAL:HG21	1.95	0.47
5:J:14:ARG:HG2	5:J:15:ALA:N	2.28	0.47
5:J:194:GLN:HE21	5:J:196:ILE:HD11	1.79	0.47
8:K:21:GLN:O	8:K:25:ILE:HD12	2.15	0.47
8:K:24:ASN:HD22	8:K:74:ALA:HB2	1.78	0.47
8:K:102:GLU:HA	8:K:105:ALA:HB3	1.97	0.47
2:h:6:PRO:HB2	1:n:535:ARG:HH12	1.79	0.47
2:h:182:VAL:HG22	2:h:401:ILE:HG13	1.96	0.47
3:g:20:SER:HB2	3:g:25:GLN:HE21	1.80	0.47
3:g:30:ILE:HG13	3:g:109:MET:HB3	1.97	0.47
4:e:90:ILE:HG22	4:e:94:MET:HE3	1.95	0.47
6:d:149:GLN:HE21	6:d:410:LEU:HD23	1.80	0.47
2:p:38:LEU:O	2:p:41:MET:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:m:125:LEU:HD22	4:m:129:LEU:HD13	1.96	0.47
6:l:409:GLY:C	6:l:501:VAL:HG23	2.40	0.47
7:i:188:LYS:HG2	7:i:198:TYR:CE1	2.49	0.47
8:k:78:MET:HE2	8:k:81:LEU:HD22	1.96	0.47
8:k:167:TRP:HE3	8:k:215:LEU:HD13	1.79	0.47
8:k:457:ILE:HG21	8:k:464:PRO:HA	1.95	0.47
1:F:56:THR:HB	1:F:61:VAL:HG11	1.97	0.47
1:F:326:GLU:HG2	8:C:232:PRO:HG3	1.97	0.47
3:G:337:THR:HG22	3:G:339:SER:H	1.78	0.47
4:E:41:GLN:HB2	4:E:554:VAL:HB	1.96	0.47
5:B:102:LEU:HD21	5:B:433:PHE:CD2	2.50	0.47
8:C:361:GLY:O	8:C:362:ASP:HB2	2.13	0.47
1:N:26:ALA:CB	1:N:102:LEU:HD12	2.45	0.47
2:P:65:THR:HG21	2:P:70:THR:HB	1.97	0.47
5:J:155:HIS:HB3	5:J:488:VAL:HG22	1.96	0.47
6:L:69:ALA:O	7:I:14:PHE:HA	2.14	0.47
7:I:211:LYS:H	8:K:508:GLN:HE22	1.60	0.47
8:K:65:LEU:HD11	8:K:97:ILE:HD13	1.96	0.47
7:a:403:HIS:O	7:a:407:SER:HB2	2.15	0.47
8:c:102:GLU:OE1	8:c:451:CYS:HB2	2.15	0.47
3:o:166:MET:HE3	3:o:396:ALA:HB2	1.97	0.47
4:m:32:VAL:HG12	4:m:35:GLN:HG3	1.96	0.47
4:m:201:ALA:C	4:m:203:MET:H	2.23	0.47
5:j:444:LEU:HB3	5:j:474:LEU:HD21	1.97	0.47
7:i:118:ASN:O	7:i:119:LYS:HG2	2.15	0.47
7:i:210:GLY:O	7:i:388:ARG:HB3	2.14	0.47
1:F:149:PHE:HZ	1:F:411:ILE:HG21	1.80	0.47
2:H:77:ILE:HD13	2:H:86:VAL:HG21	1.97	0.47
4:E:32:VAL:HG12	4:E:35:GLN:HG3	1.97	0.47
8:C:248:CYS:O	8:C:297:THR:CG2	2.63	0.47
8:C:296:ILE:HG12	8:C:317:LEU:HB2	1.97	0.47
1:N:248:ASN:HB2	8:K:260:ASN:CB	2.45	0.47
1:N:334:GLY:HA3	1:N:347:ILE:O	2.15	0.47
2:P:254:LEU:HB2	2:P:305:VAL:HG22	1.97	0.47
5:J:57:THR:HG23	5:J:382:ARG:HE	1.79	0.47
7:I:55:ASP:HB2	7:I:59:ASP:O	2.15	0.47
6:d:55:ILE:HB	6:d:385:MET:HE2	1.97	0.47
1:n:337:GLN:HG2	1:n:347:ILE:HG21	1.97	0.47
2:p:92:GLN:HG3	2:p:526:PHE:HB3	1.96	0.47
2:p:111:LEU:HD21	2:p:538:VAL:CG2	2.45	0.47
2:p:424:GLY:HA2	2:p:427:GLU:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o:478:TRP:HE3	3:o:492:PHE:HB2	1.79	0.47
5:j:192:HIS:CD2	5:j:319:LEU:CD1	2.98	0.47
6:l:295:ASP:O	6:l:296:ALA:HB3	2.15	0.47
7:i:159:ILE:HD13	7:i:412:THR:HG21	1.96	0.47
1:F:248:ASN:HB2	8:C:260:ASN:CB	2.44	0.47
4:E:271:ILE:HG23	4:E:351:LEU:HD22	1.97	0.47
6:D:138:MET:HB2	6:D:478:LEU:CD1	2.32	0.47
7:A:143:VAL:O	7:A:143:VAL:CG1	2.62	0.47
8:C:298:GLU:HG3	8:C:325:ASN:OD1	2.14	0.47
8:C:402:VAL:HA	8:C:405:ASN:HD22	1.80	0.47
1:N:104:GLN:HG3	1:N:450:ALA:HA	1.97	0.47
1:N:269:PHE:HE1	8:K:274:GLN:HG3	1.80	0.47
2:P:25:ASP:C	2:P:27:GLN:N	2.73	0.47
2:P:123:SER:HB3	2:P:126:GLU:CG	2.45	0.47
4:M:73:ILE:HG21	5:J:511:VAL:HG11	1.97	0.47
4:M:291:SER:HB3	4:M:294:GLU:HB2	1.95	0.47
4:M:451:SER:O	4:M:455:SER:HB2	2.15	0.47
5:J:453:SER:O	5:J:457:SER:HB2	2.14	0.47
6:L:287:LEU:HD23	6:L:313:VAL:HB	1.97	0.47
1:f:458:LEU:HD22	1:f:493:LEU:HD11	1.97	0.47
2:h:79:HIS:HD2	2:h:81:ALA:H	1.61	0.47
2:h:428:ILE:HD11	2:h:478:LEU:HD21	1.97	0.47
3:g:77:HIS:HE1	3:g:79:ALA:HB3	1.76	0.47
7:a:458:ILE:H	7:a:458:ILE:HD12	1.80	0.47
1:n:86:ILE:HD11	8:k:210:PRO:HG2	1.96	0.47
1:n:533:LEU:HD22	8:k:47:MET:HE2	1.96	0.47
2:p:411:LEU:HD12	2:p:417:GLY:HA3	1.97	0.47
3:o:108:LEU:HB3	3:o:514:THR:HG21	1.97	0.47
5:j:408:GLU:HG3	5:j:441:PRO:HD3	1.96	0.47
6:l:44:MET:HE2	6:l:44:MET:HA	1.97	0.47
6:l:230:GLU:HG2	6:l:349:LEU:HD12	1.97	0.47
7:i:437:ALA:HB1	7:i:445:GLN:HG3	1.97	0.47
2:H:229:ASN:HA	2:H:368:VAL:HG22	1.96	0.46
3:G:221:LYS:HA	3:G:362:TYR:CZ	2.49	0.46
4:E:498:LEU:HD21	4:E:510:ILE:O	2.15	0.46
6:D:65:LEU:HD11	6:D:97:VAL:HG21	1.97	0.46
6:D:177:SER:OG	6:D:375:VAL:HG11	2.15	0.46
6:D:224:GLY:HA3	6:D:306:SER:OG	2.15	0.46
6:D:448:GLU:O	6:D:451:PRO:HD2	2.15	0.46
6:D:495:GLU:O	6:D:495:GLU:HG3	2.15	0.46
7:A:458:ILE:O	7:A:462:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:98:ASN:HD21	4:M:100:ILE:HB	1.80	0.46
4:M:271:ILE:HG23	4:M:351:LEU:HD22	1.96	0.46
6:L:47:MET:O	7:I:544:MET:HA	2.14	0.46
7:I:458:ILE:H	7:I:458:ILE:HD12	1.80	0.46
4:e:74:LEU:HD22	4:e:93:GLN:HB2	1.96	0.46
5:b:463:ILE:HD11	5:b:470:SER:O	2.15	0.46
2:p:31:SER:OG	2:p:81:ALA:CB	2.63	0.46
5:j:192:HIS:CD2	5:j:319:LEU:HD12	2.49	0.46
6:l:237:ILE:HD11	6:l:286:LEU:HD22	1.97	0.46
8:k:59:ASN:O	8:k:60:ASP:C	2.58	0.46
8:k:139:VAL:HG12	8:k:480:PHE:CD1	2.50	0.46
3:G:267:TYR:O	3:G:270:ILE:HG12	2.15	0.46
3:G:268:GLN:HA	3:G:271:VAL:HG12	1.98	0.46
4:E:81:ILE:HD11	5:B:75:LYS:HD2	1.97	0.46
5:B:135:LEU:HG	5:B:411:MET:HE2	1.98	0.46
5:B:503:GLU:O	5:B:507:VAL:HG23	2.15	0.46
6:D:102:ALA:CB	6:D:449:VAL:HG21	2.45	0.46
7:A:229:ALA:HB2	7:A:319:ARG:HG2	1.97	0.46
8:C:297:THR:HG22	8:C:299:LYS:H	1.80	0.46
4:M:287:LEU:HD12	5:J:248:THR:HG22	1.96	0.46
7:I:366:PHE:O	7:I:367:SER:C	2.58	0.46
8:K:219:VAL:HG13	8:K:377:CYS:SG	2.55	0.46
1:f:79:ALA:HB2	1:f:523:ILE:HD12	1.97	0.46
2:h:388:GLY:HA3	2:h:394:LEU:HD21	1.95	0.46
3:g:86:ILE:HD11	3:g:510:ALA:CA	2.41	0.46
3:g:449:ILE:O	3:g:453:LEU:HG	2.15	0.46
6:d:77:MET:O	6:d:81:VAL:HG23	2.15	0.46
8:c:93:THR:OG1	11:c:1103:BEF:F2	2.21	0.46
3:o:242:LEU:HD13	3:o:285:VAL:HG13	1.96	0.46
7:i:460:LYS:O	7:i:464:VAL:HG23	2.14	0.46
2:H:53:LYS:HD2	2:H:71:MET:SD	2.55	0.46
2:H:102:LEU:HD13	2:H:524:LYS:HE2	1.97	0.46
4:E:451:SER:O	4:E:455:SER:HB2	2.15	0.46
2:P:135:ARG:HB2	2:P:532:THR:HG21	1.98	0.46
2:P:509:VAL:HG13	2:P:510:LYS:H	1.79	0.46
4:M:477:ASP:C	4:M:480:PRO:HD2	2.41	0.46
7:I:252:GLN:HA	7:I:303:ASP:HB2	1.97	0.46
3:g:108:LEU:HB3	3:g:514:THR:HG21	1.98	0.46
4:e:51:ILE:HG12	4:e:130:LEU:HB3	1.96	0.46
7:a:17:GLY:HA2	7:a:546:THR:O	2.15	0.46
1:n:225:PRO:HG2	1:n:315:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o:20:SER:HB2	3:o:25:GLN:HE21	1.78	0.46
5:j:45:LEU:HD23	6:l:524:ILE:HG12	1.97	0.46
5:j:69:LEU:HD13	5:j:74:ALA:HB1	1.96	0.46
2:H:35:ILE:HD13	2:H:111:LEU:HD13	1.98	0.46
2:H:117:LEU:HB3	2:H:122:LEU:HD12	1.98	0.46
4:E:73:ILE:HD11	5:B:72:PRO:HB2	1.96	0.46
5:B:321:THR:HG22	5:B:339:GLU:N	2.31	0.46
6:D:63:THR:HG21	6:D:392:ARG:CD	2.45	0.46
8:C:58:THR:O	8:C:64:ILE:HD11	2.14	0.46
8:C:96:VAL:HG22	8:C:509:SER:HA	1.97	0.46
5:J:219:GLY:O	5:J:220:ASN:CB	2.54	0.46
6:L:125:GLN:HE21	6:L:513:GLU:HG2	1.80	0.46
8:K:164:VAL:O	8:K:164:VAL:HG12	2.14	0.46
1:f:450:ALA:O	1:f:453:VAL:HG22	2.15	0.46
1:f:454:ILE:HB	1:f:455:PRO:HD3	1.97	0.46
4:e:72:LYS:HB2	4:e:90:ILE:HD12	1.97	0.46
5:b:412:SER:O	5:b:416:ASP:HB2	2.15	0.46
7:a:221:GLY:HA3	7:a:374:ILE:O	2.16	0.46
3:o:77:HIS:HE1	3:o:79:ALA:HB3	1.81	0.46
4:m:86:ASP:O	4:m:90:ILE:HG12	2.16	0.46
5:j:279:PHE:CB	5:j:281:ILE:HD12	2.39	0.46
6:l:64:ILE:O	6:l:68:MET:HG2	2.15	0.46
7:i:15:LEU:C	7:i:17:GLY:N	2.71	0.46
3:G:162:ALA:HB3	3:G:179:VAL:HG23	1.97	0.46
5:B:31:ASP:HA	5:B:34:LYS:HG3	1.98	0.46
5:B:254:SER:O	5:B:256:ALA:N	2.49	0.46
5:B:255:THR:HG22	6:D:263:ILE:HA	1.97	0.46
7:A:15:LEU:O	7:A:17:GLY:N	2.49	0.46
2:P:43:LEU:HA	2:P:105:ILE:HD11	1.98	0.46
4:M:269:LEU:HD13	4:M:322:ILE:HD12	1.97	0.46
5:J:455:LEU:HD22	5:J:472:LEU:HD23	1.97	0.46
6:L:166:TYR:O	6:L:170:LEU:HB2	2.15	0.46
5:b:183:ARG:HH22	5:b:211:GLY:N	2.13	0.46
10:c:1102:ADP:H5'2	10:c:1102:ADP:H8	1.81	0.46
2:p:245:HIS:ND1	2:p:245:HIS:N	2.64	0.46
1:F:269:PHE:CG	8:C:273:LEU:HD23	2.51	0.46
4:E:269:LEU:H	4:E:375:GLY:N	2.13	0.46
8:C:203:TYR:HE1	8:C:330:ARG:HE	1.62	0.46
2:P:110:LEU:O	2:P:114:SER:HB2	2.14	0.46
3:O:86:ILE:CD1	3:O:510:ALA:HA	2.40	0.46
3:O:478:TRP:HE3	3:O:492:PHE:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:327:PHE:CE2	4:M:342:ALA:HB1	2.50	0.46
6:L:398:LEU:HA	6:L:401:ILE:HD12	1.97	0.46
5:b:255:THR:HG22	6:d:263:ILE:HA	1.98	0.46
6:d:143:SER:HB2	6:d:146:ASP:HB2	1.98	0.46
2:p:27:GLN:NE2	2:p:544:ILE:HD11	2.29	0.46
3:o:83:LEU:HA	3:o:86:ILE:HG22	1.97	0.46
4:m:147:ALA:HB1	4:m:546:ARG:HG3	1.98	0.46
4:m:451:SER:O	4:m:455:SER:HB2	2.16	0.46
7:i:77:HIS:CD2	7:i:79:ALA:HB3	2.51	0.46
7:i:95:GLY:HA3	7:i:407:SER:OG	2.15	0.46
2:H:329:LEU:O	2:H:333:CYS:HB2	2.16	0.46
2:H:390:THR:C	2:H:392:ASN:H	2.23	0.46
3:G:264:VAL:O	3:G:267:TYR:HB2	2.15	0.46
3:G:449:ILE:H	3:G:449:ILE:HD12	1.80	0.46
7:A:54:VAL:HG12	7:A:56:ASP:H	1.80	0.46
2:P:85:LEU:CD2	2:P:534:ALA:HB1	2.46	0.46
2:P:428:ILE:HD11	2:P:478:LEU:HD21	1.98	0.46
3:O:158:LEU:HB3	3:O:400:VAL:HG13	1.98	0.46
7:I:159:ILE:HD13	7:I:412:THR:HG21	1.98	0.46
1:f:242:TYR:CZ	2:h:260:GLU:HB3	2.50	0.46
4:m:51:ILE:HD13	4:m:134:LEU:HB2	1.98	0.46
4:m:464:ILE:HD12	4:m:464:ILE:H	1.81	0.46
5:j:409:MET:CB	5:j:463:ILE:HD13	2.45	0.46
7:i:101:VAL:HG22	7:i:527:SER:OG	2.16	0.46
2:H:281:GLU:OE1	3:G:337:THR:HG21	2.16	0.46
3:G:55:THR:HG22	3:G:56:SER:N	2.30	0.46
3:G:327:ILE:HA	3:G:330:VAL:HG12	1.97	0.46
5:B:317:LEU:HA	5:B:320:VAL:HG12	1.98	0.46
6:D:271:LEU:HD23	6:D:301:ALA:HB2	1.97	0.46
7:I:39:VAL:HG11	7:I:73:LEU:HD11	1.97	0.46
1:f:177:ALA:O	1:f:181:VAL:HG23	2.16	0.46
2:h:43:LEU:HG	2:h:462:THR:CG2	2.45	0.46
2:h:512:ILE:CG2	2:h:517:ILE:O	2.64	0.46
4:e:72:LYS:HG3	5:b:513:ASN:HB3	1.98	0.46
6:l:30:SER:OG	7:i:11:ASP:HB3	2.16	0.46
6:l:78:LEU:HD22	6:l:97:VAL:HG13	1.98	0.46
6:l:500:PRO:HB2	6:l:503:VAL:HG23	1.98	0.46
7:i:77:HIS:HD2	7:i:79:ALA:HB3	1.80	0.46
4:E:168:ILE:HD11	4:E:439:VAL:CG1	2.44	0.46
5:B:183:ARG:HH22	5:B:211:GLY:H	1.64	0.46
6:D:450:ILE:HB	6:D:451:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:52:MET:HG3	7:A:62:VAL:HG22	1.97	0.46
7:A:198:TYR:N	7:A:198:TYR:CD2	2.84	0.46
8:C:142:PRO:HA	8:C:411:SER:HA	1.98	0.46
8:C:246:LEU:HD13	8:C:250:LEU:HD21	1.97	0.46
1:N:195:GLU:HG3	1:N:327:ARG:HH11	1.77	0.46
2:P:92:GLN:OE1	2:P:103:VAL:HG23	2.16	0.46
4:M:415:ILE:HD13	5:J:503:GLU:OE1	2.15	0.46
6:L:63:THR:HG21	6:L:392:ARG:HD3	1.98	0.46
6:L:244:PRO:HD3	6:L:270:TYR:HE2	1.75	0.46
6:L:286:LEU:HD12	6:L:305:LEU:HD21	1.96	0.46
8:K:208:LYS:HE3	8:K:390:ASN:OD1	2.16	0.46
4:e:224:ILE:HD13	4:e:404:VAL:HG12	1.97	0.46
6:d:479:ASN:HB2	6:d:491:ASN:OD1	2.15	0.46
7:a:281:VAL:O	7:a:285:VAL:HG23	2.15	0.46
2:p:252:CYS:HB2	2:p:342:PRO:O	2.16	0.46
3:o:288:THR:HG22	3:o:346:LEU:HD11	1.98	0.46
4:m:269:LEU:H	4:m:375:GLY:H	1.62	0.46
4:m:323:CYS:HB3	4:m:327:PHE:CE1	2.51	0.46
7:i:488:LYS:CB	7:i:489:PRO:HD2	2.46	0.46
8:k:142:PRO:HA	8:k:411:SER:HA	1.98	0.46
3:G:446:LEU:HD21	3:G:507:LEU:HD21	1.97	0.46
4:E:275:PRO:HD3	4:E:325:TRP:CE3	2.51	0.46
4:E:322:ILE:HD13	4:E:354:ILE:HD13	1.97	0.46
5:B:441:PRO:HB3	5:B:472:LEU:CD1	2.45	0.46
6:D:103:LEU:O	6:D:106:ALA:HB3	2.15	0.46
8:C:204:VAL:HA	8:C:377:CYS:O	2.16	0.46
4:M:98:ASN:ND2	4:M:101:ALA:H	2.12	0.46
4:M:168:ILE:HD11	4:M:439:VAL:HG13	1.97	0.46
6:L:469:LEU:O	6:L:473:HIS:HB2	2.16	0.46
7:I:501:GLY:HA3	7:I:512:GLU:HG2	1.98	0.46
7:I:523:SER:O	7:I:527:SER:HB2	2.16	0.46
8:K:147:ASN:HB3	8:K:150:ALA:HB3	1.98	0.46
1:f:225:PRO:HG2	1:f:315:LEU:HB2	1.98	0.46
5:j:234:ALA:HA	5:j:326:VAL:O	2.16	0.46
5:j:320:VAL:O	5:j:359:CYS:HB3	2.16	0.46
5:j:321:THR:HG22	5:j:339:GLU:N	2.31	0.46
5:j:440:LEU:CB	5:j:441:PRO:HD3	2.45	0.46
7:i:366:PHE:O	7:i:367:SER:C	2.58	0.46
2:H:155:ASP:O	2:H:159:LEU:HG	2.17	0.45
5:B:438:ARG:C	5:B:440:LEU:H	2.23	0.45
5:B:440:LEU:HB3	5:B:441:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:267:TYR:C	3:O:269:ALA:H	2.24	0.45
4:M:240:ILE:HD12	4:M:244:ILE:HD11	1.98	0.45
6:L:520:ARG:CG	6:L:520:ARG:NH2	2.71	0.45
1:f:153:VAL:HG11	1:f:405:VAL:HG21	1.98	0.45
1:f:251:PHE:HZ	2:h:259:THR:CB	2.29	0.45
3:g:249:GLU:O	3:g:278:ILE:HG21	2.16	0.45
3:o:368:CYS:HA	3:o:369:PRO:HD2	1.70	0.45
1:F:103:ARG:O	1:F:107:ARG:HD2	2.17	0.45
1:F:178:VAL:HG22	1:F:399:LEU:HD23	1.98	0.45
1:F:509:SER:HB2	1:F:512:VAL:CG2	2.46	0.45
3:G:424:LEU:HB2	3:G:443:ALA:HB2	1.98	0.45
8:C:99:LEU:O	8:C:103:ILE:HG13	2.16	0.45
8:C:252:TYR:H	8:C:252:TYR:HD2	1.62	0.45
2:h:291:ILE:HD13	2:h:347:PRO:HG3	1.97	0.45
6:d:24:ASN:CG	6:d:74:VAL:HG21	2.41	0.45
1:n:509:SER:HB2	1:n:512:VAL:CG2	2.46	0.45
5:j:346:ILE:HG22	5:j:347:MET:H	1.81	0.45
6:l:103:LEU:HB3	6:l:515:VAL:HG21	1.98	0.45
6:l:236:LEU:HD12	6:l:287:LEU:HB2	1.98	0.45
8:k:167:TRP:CD1	8:k:167:TRP:N	2.84	0.45
8:k:198:ILE:CG2	8:k:408:LEU:HD21	2.46	0.45
8:k:298:GLU:HG3	8:k:325:ASN:OD1	2.17	0.45
1:F:197:MET:HE3	1:F:198:GLN:O	2.15	0.45
1:F:301:ILE:CG1	1:F:318:ARG:HB3	2.46	0.45
2:H:21:TYR:CE1	3:G:10:ILE:HG13	2.51	0.45
2:H:322:LYS:O	2:H:323:VAL:HB	2.15	0.45
6:D:195:ARG:HD3	6:D:323:PHE:CZ	2.51	0.45
1:N:221:HIS:CD2	1:N:223:ASP:H	2.32	0.45
5:J:443:ILE:HA	5:J:446:ASP:HB2	1.98	0.45
2:h:238:SER:C	2:h:240:SER:H	2.24	0.45
3:g:40:LEU:HG	3:g:99:THR:HG23	1.98	0.45
3:g:342:LYS:C	3:g:344:GLU:H	2.25	0.45
4:e:278:PRO:HA	4:e:279:PRO:HD3	1.83	0.45
5:b:184:LEU:HD11	5:b:192:HIS:HB2	1.99	0.45
1:n:473:VAL:HG13	1:n:489:VAL:HG22	1.99	0.45
2:p:79:HIS:HD2	2:p:81:ALA:N	2.15	0.45
2:p:128:ILE:HG12	2:p:536:THR:HG23	1.98	0.45
7:i:52:MET:HE1	8:k:24:ASN:HD21	1.80	0.45
7:i:164:MET:HE3	7:i:405:SER:CB	2.47	0.45
8:k:102:GLU:OE1	8:k:451:CYS:HB2	2.15	0.45
3:G:77:HIS:HE1	3:G:79:ALA:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:86:ILE:HD11	3:G:510:ALA:CA	2.40	0.45
4:E:327:PHE:H	4:E:344:ARG:HD2	1.80	0.45
5:B:181:ILE:HD13	5:B:391:LEU:HB3	1.99	0.45
7:A:221:GLY:HA3	7:A:374:ILE:O	2.16	0.45
1:N:281:LYS:O	1:N:285:CYS:HB2	2.17	0.45
1:N:439:LYS:O	1:N:442:THR:CG2	2.64	0.45
5:J:214:LEU:HD11	5:J:317:LEU:HD11	1.99	0.45
8:K:298:GLU:HG3	8:K:325:ASN:OD1	2.17	0.45
1:f:457:THR:HA	1:f:460:LYS:HB2	1.98	0.45
4:e:61:ILE:HD11	4:e:91:LEU:HD21	1.98	0.45
4:e:481:MET:O	4:e:485:GLU:HB2	2.17	0.45
5:b:320:VAL:O	5:b:359:CYS:HB3	2.15	0.45
1:n:57:LYS:O	1:n:57:LYS:HG2	2.15	0.45
1:n:130:MET:HE1	1:n:514:ARG:HG2	1.98	0.45
1:n:195:GLU:HG3	1:n:327:ARG:HH11	1.81	0.45
4:m:267:VAL:HB	4:m:377:CYS:HB2	1.99	0.45
6:l:257:TYR:HA	6:l:260:MET:HE2	1.99	0.45
7:i:501:GLY:HA3	7:i:512:GLU:HG2	1.99	0.45
1:F:30:GLN:HB2	1:F:96:CYS:HA	1.97	0.45
1:F:79:ALA:HB2	1:F:523:ILE:CD1	2.45	0.45
3:G:88:ARG:NH1	3:G:88:ARG:CG	2.79	0.45
6:D:162:ILE:O	6:D:162:ILE:CG1	2.64	0.45
1:N:102:LEU:HD11	1:N:527:LEU:HD13	1.98	0.45
1:N:153:VAL:HG11	1:N:405:VAL:CG2	2.46	0.45
1:N:327:ARG:O	1:N:331:VAL:HG23	2.16	0.45
4:M:413:LYS:H	5:J:79:ASN:HD21	1.65	0.45
5:J:213:ILE:HG22	5:J:353:PHE:HB3	1.98	0.45
7:I:164:MET:HE3	7:I:405:SER:CB	2.45	0.45
7:I:466:ALA:O	7:I:467:ALA:HB3	2.17	0.45
6:d:42:LYS:HE2	6:d:484:VAL:HG13	1.97	0.45
6:d:237:ILE:HG23	6:d:239:PHE:CE2	2.52	0.45
7:a:250:ASN:HB3	7:a:300:LYS:CB	2.47	0.45
7:a:262:ILE:CG2	8:c:259:THR:HG23	2.43	0.45
8:c:23:SER:HB3	8:c:72:HIS:CE1	2.51	0.45
1:n:252:PHE:HD1	2:p:264:THR:HB	1.81	0.45
3:o:7:THR:O	3:o:8:PRO:O	2.35	0.45
5:j:23:PHE:O	5:j:24:VAL:C	2.59	0.45
1:F:465:ASP:HB3	1:F:468:ASP:HB2	1.98	0.45
4:E:232:GLY:H	5:B:87:GLU:HG3	1.81	0.45
4:E:492:ILE:H	4:E:492:ILE:HG13	1.46	0.45
1:N:13:LEU:HD13	1:N:21:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:119:THR:HG21	1:N:529:LEU:HD11	1.99	0.45
3:O:264:VAL:O	3:O:267:TYR:HB2	2.16	0.45
5:J:255:THR:HG21	6:L:263:ILE:HA	1.98	0.45
7:I:366:PHE:HB3	7:I:388:ARG:NH1	2.32	0.45
1:f:30:GLN:HB2	1:f:96:CYS:HA	1.98	0.45
1:f:296:ILE:HA	1:f:317:LEU:HB3	1.99	0.45
3:g:282:LEU:HD21	3:g:306:PHE:CB	2.47	0.45
4:e:32:VAL:HG12	4:e:35:GLN:HG3	1.98	0.45
5:b:293:TYR:HB3	5:b:294:PRO:HD3	1.99	0.45
6:d:353:ILE:CG2	6:d:354:ASP:N	2.79	0.45
8:c:25:ILE:HG21	8:c:109:PRO:HG3	1.99	0.45
2:p:428:ILE:HA	2:p:431:ILE:HD12	1.99	0.45
4:m:273:THR:O	4:m:273:THR:HG22	2.16	0.45
4:m:324:GLN:HB2	4:m:351:LEU:HD11	1.99	0.45
5:j:14:ARG:O	5:j:15:ALA:C	2.59	0.45
6:l:134:ILE:HG22	6:l:138:MET:HE2	1.99	0.45
6:l:198:LYS:HE2	6:l:391:GLU:OE1	2.16	0.45
3:G:204:ILE:HB	3:G:362:TYR:OH	2.17	0.45
5:B:181:ILE:HD13	5:B:391:LEU:HB2	1.98	0.45
5:B:293:TYR:HA	6:D:334:ALA:HB1	1.98	0.45
2:P:109:GLU:CG	2:P:458:VAL:HG21	2.46	0.45
2:P:428:ILE:HD11	2:P:460:PRO:HG3	1.98	0.45
3:O:488:ILE:H	3:O:488:ILE:HG13	1.47	0.45
8:K:70:VAL:HG11	8:K:75:ALA:CB	2.47	0.45
1:f:221:HIS:CD2	1:f:223:ASP:H	2.30	0.45
3:g:147:ILE:HG22	3:g:152:SER:HB3	1.98	0.45
6:d:138:MET:SD	6:d:478:LEU:HD22	2.56	0.45
3:o:108:LEU:HD21	3:o:442:PHE:CE2	2.52	0.45
3:o:179:VAL:C	3:o:181:MET:H	2.24	0.45
4:m:448:VAL:HG21	4:m:498:LEU:HD22	1.99	0.45
1:F:192:HIS:NE2	1:F:326:GLU:HB2	2.32	0.45
1:F:324:ASN:ND2	1:F:327:ARG:HD2	2.32	0.45
1:F:370:ASN:H	1:F:370:ASN:ND2	2.14	0.45
4:E:74:LEU:HD13	4:E:93:GLN:HG3	1.99	0.45
10:D:602:ADP:O3B	11:D:603:BEF:F2	2.24	0.45
8:C:59:ASN:CB	8:C:162:LYS:HG2	2.44	0.45
5:J:53:THR:HG22	5:J:54:CYS:N	2.32	0.45
5:J:317:LEU:HA	5:J:320:VAL:HG12	1.98	0.45
1:f:45:MET:HB2	2:h:541:ILE:HD12	1.97	0.45
4:e:73:ILE:HG22	5:b:511:VAL:HG13	1.99	0.45
6:d:46:LYS:HB2	6:d:64:ILE:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:422:GLY:HA2	10:a:602:ADP:N3	2.32	0.45
2:p:39:HIS:ND1	2:p:108:GLY:HA3	2.32	0.45
7:i:248:ASP:HB3	7:i:339:SER:HA	1.98	0.45
1:F:122:PHE:HD1	1:F:525:SER:HB2	1.82	0.45
3:G:348:THR:HG22	3:G:349:CYS:H	1.81	0.45
5:B:192:HIS:CD2	5:B:319:LEU:CD1	3.00	0.45
7:A:4:LEU:HD21	4:M:32:VAL:HG11	1.99	0.45
3:O:465:LEU:HD12	3:O:469:ARG:HH21	1.82	0.45
4:M:250:SER:HB3	4:M:332:ASN:OD1	2.17	0.45
7:I:28:GLN:HE21	7:I:77:HIS:CE1	2.34	0.45
1:f:35:THR:HG22	1:f:42:THR:OG1	2.16	0.45
1:f:237:ASN:HB3	1:f:325:MET:HE2	1.98	0.45
7:a:335:ALA:HB2	7:a:356:GLY:N	2.32	0.45
8:c:154:LEU:HG	8:c:412:LEU:HD21	1.98	0.45
8:c:164:VAL:O	8:c:164:VAL:HG12	2.17	0.45
2:p:22:SER:OG	2:p:23:ASN:N	2.50	0.45
6:D:336:ILE:C	6:D:338:LEU:N	2.75	0.45
6:D:469:LEU:O	6:D:473:HIS:HB2	2.17	0.45
8:C:118:PRO:O	8:C:122:ILE:HG13	2.17	0.45
8:C:208:LYS:HB3	8:C:389:LEU:HD13	1.99	0.45
2:P:32:ILE:HG13	2:P:111:LEU:HB3	1.99	0.45
5:J:152:ASP:OD1	5:J:400:THR:HG21	2.16	0.45
3:g:220:PHE:HE1	3:g:322:ASP:HB3	1.80	0.45
4:e:323:CYS:HB3	4:e:327:PHE:CE1	2.52	0.45
4:e:363:VAL:HA	4:e:364:PRO:HD3	1.84	0.45
4:e:464:ILE:H	4:e:464:ILE:HD12	1.81	0.45
5:b:14:ARG:HG3	5:b:513:ASN:ND2	2.32	0.45
6:d:162:ILE:O	6:d:162:ILE:HG13	2.17	0.45
7:A:212:SER:HB2	8:C:511:LYS:HE3	2.00	0.44
7:A:366:PHE:O	7:A:367:SER:C	2.59	0.44
8:C:198:ILE:CG2	8:C:199:ASP:N	2.80	0.44
1:N:114:HIS:O	1:N:117:ILE:HB	2.17	0.44
2:P:77:ILE:HD13	2:P:86:VAL:HG21	2.00	0.44
3:O:416:THR:O	3:O:420:VAL:HG23	2.17	0.44
7:I:68:THR:O	7:I:72:LEU:HG	2.17	0.44
8:K:414:PRO:HB3	8:K:481:THR:HG23	2.00	0.44
2:h:6:PRO:HB2	1:n:535:ARG:NH1	2.32	0.44
6:d:469:LEU:O	6:d:473:HIS:HB2	2.17	0.44
7:a:86:LEU:HD21	7:a:101:VAL:HG12	1.99	0.44
4:m:41:GLN:HB2	4:m:554:VAL:HB	1.99	0.44
7:i:336:THR:HB	7:i:354:TYR:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:k:35:ILE:HB	8:k:97:ILE:HD11	1.99	0.44
1:F:39:PRO:HD3	1:F:160:THR:HG22	2.00	0.44
1:F:47:VAL:HG21	2:H:80:PRO:HG3	2.00	0.44
1:F:455:PRO:O	1:F:459:VAL:HG23	2.17	0.44
6:L:516:LYS:O	6:L:520:ARG:HG2	2.17	0.44
6:d:253:ILE:CG2	7:a:263:ASN:HB2	2.47	0.44
7:a:165:SER:O	7:a:166:SER:CB	2.65	0.44
8:c:219:VAL:HG13	8:c:377:CYS:SG	2.57	0.44
8:c:361:GLY:O	8:c:362:ASP:HB2	2.16	0.44
2:p:21:TYR:N	2:p:21:TYR:HD2	2.15	0.44
3:o:488:ILE:H	3:o:488:ILE:HG13	1.64	0.44
5:j:192:HIS:HD2	5:j:319:LEU:HD12	1.82	0.44
5:j:197:LYS:HB2	5:j:377:LEU:HD22	1.99	0.44
1:F:37:LEU:HD23	1:F:458:LEU:HG	1.98	0.44
1:F:452:LEU:HD22	1:F:470:LEU:HD21	1.99	0.44
5:B:474:LEU:HD12	5:B:474:LEU:HA	1.85	0.44
7:A:175:PHE:C	7:A:177:SER:H	2.25	0.44
3:O:3:PHE:CD2	3:O:3:PHE:N	2.81	0.44
3:O:232:GLN:NE2	3:O:304:THR:HG23	2.32	0.44
7:I:512:GLU:OE1	7:I:517:VAL:HG21	2.18	0.44
1:f:465:ASP:HA	1:f:466:PRO:HD3	1.86	0.44
3:g:40:LEU:HD11	3:g:66:GLY:HA2	1.99	0.44
5:b:321:THR:HG22	5:b:339:GLU:N	2.32	0.44
10:b:602:ADP:O3B	11:b:603:BEF:F3	2.26	0.44
7:a:12:THR:HB	7:a:14:PHE:HE2	1.77	0.44
7:a:228:VAL:HG22	7:a:372:ILE:HD11	2.00	0.44
4:m:211:VAL:HG11	4:m:224:ILE:CD1	2.48	0.44
4:m:319:ASP:O	4:m:341:PRO:HD2	2.17	0.44
4:m:413:LYS:H	5:j:79:ASN:HD21	1.64	0.44
5:j:293:TYR:HB3	5:j:294:PRO:CD	2.47	0.44
6:l:89:ALA:C	6:l:91:ASP:H	2.26	0.44
5:B:287:ARG:HG3	5:B:310:ASP:HA	1.98	0.44
6:D:163:VAL:HG23	6:D:204:ILE:HG21	1.99	0.44
7:A:316:MET:O	7:A:316:MET:HG2	2.16	0.44
7:A:477:LEU:CD2	7:A:509:ILE:HG12	2.47	0.44
8:C:353:GLY:CA	8:C:370:ASN:HB2	2.43	0.44
1:N:87:THR:HG22	1:N:89:ASP:H	1.83	0.44
5:J:234:ALA:HA	5:J:326:VAL:O	2.17	0.44
5:b:88:VAL:O	5:b:389:SER:HB3	2.17	0.44
1:n:196:ILE:HG21	1:n:392:LYS:HG3	1.99	0.44
4:m:61:ILE:HD11	4:m:91:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:l:336:ILE:C	6:l:338:LEU:H	2.25	0.44
6:l:367:ARG:O	6:l:368:ASN:CB	2.65	0.44
7:i:247:LEU:HD11	7:i:288:ILE:HD13	1.99	0.44
1:F:436:ALA:C	1:F:438:GLY:H	2.26	0.44
3:G:74:ASP:O	4:E:32:VAL:HA	2.16	0.44
4:E:115:ILE:CD1	4:E:536:GLN:HB3	2.48	0.44
4:E:323:CYS:HB3	4:E:327:PHE:CE1	2.52	0.44
8:C:209:ILE:HA	8:C:210:PRO:HD2	1.78	0.44
5:J:102:LEU:HD21	5:J:433:PHE:CD2	2.53	0.44
7:I:327:ARG:HH22	7:I:328:ARG:NH2	2.16	0.44
8:K:377:CYS:SG	8:K:378:THR:N	2.90	0.44
1:f:324:ASN:ND2	1:f:327:ARG:HD2	2.32	0.44
4:e:98:ASN:HD22	4:e:101:ALA:H	1.65	0.44
1:n:241:GLU:HA	1:n:302:ASP:HB2	1.98	0.44
2:p:42:CYS:SG	2:p:104:MET:HG2	2.58	0.44
3:o:107:GLU:HG2	3:o:448:VAL:CG2	2.47	0.44
4:m:38:LYS:HG2	4:m:557:SER:HA	1.99	0.44
7:i:198:TYR:CD2	7:i:198:TYR:N	2.84	0.44
7:i:253:LYS:HE2	7:i:305:LEU:HD22	2.00	0.44
1:F:189:LEU:HA	8:C:359:MET:SD	2.57	0.44
2:H:92:GLN:OE1	2:H:103:VAL:HG23	2.17	0.44
4:E:38:LYS:HG2	4:E:557:SER:HA	1.99	0.44
4:E:413:LYS:H	5:B:79:ASN:ND2	2.15	0.44
6:D:96:VAL:HG23	6:D:507:ALA:O	2.17	0.44
7:A:255:ARG:HA	8:C:257:SER:HA	1.98	0.44
7:A:366:PHE:HB3	7:A:388:ARG:NH1	2.33	0.44
7:A:525:VAL:C	7:A:527:SER:H	2.25	0.44
1:N:534:LEU:HD12	8:K:48:LEU:HD23	1.99	0.44
2:P:233:GLU:HB2	2:P:320:VAL:HB	1.99	0.44
3:O:179:VAL:HG13	3:O:180:LYS:N	2.32	0.44
4:M:428:CYS:O	4:M:431:ARG:HG3	2.17	0.44
8:K:389:LEU:HA	8:K:392:ILE:HD12	1.99	0.44
5:b:287:ARG:HG3	5:b:310:ASP:HA	2.00	0.44
5:b:346:ILE:HG22	5:b:347:MET:N	2.33	0.44
7:a:103:ILE:HG22	7:a:457:ILE:CG2	2.46	0.44
7:a:338:VAL:HG21	7:a:350:PHE:HE1	1.82	0.44
8:c:92:GLY:HA2	10:c:1102:ADP:O2B	2.17	0.44
8:c:478:GLY:O	8:c:479:ASN:HB2	2.17	0.44
2:p:413:LYS:CB	2:p:414:PRO:HD3	2.48	0.44
4:m:450:MET:HE1	4:m:538:ILE:HD11	2.00	0.44
7:i:335:ALA:HB2	7:i:356:GLY:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:298:GLN:O	1:F:319:ARG:HA	2.17	0.44
4:E:84:THR:HG22	4:E:418:GLU:OE1	2.18	0.44
5:B:33:VAL:HB	5:B:93:THR:HG23	2.00	0.44
6:D:124:PHE:O	6:D:127:ALA:HB3	2.17	0.44
6:D:420:GLU:HB2	6:D:473:HIS:HE1	1.81	0.44
7:A:53:LEU:HD11	7:A:69:ILE:HG23	1.99	0.44
8:C:291:ARG:N	8:C:292:PRO:HD3	2.33	0.44
1:N:27:GLU:HG2	1:N:103:ARG:HE	1.83	0.44
4:M:387:THR:HB	5:J:86:ASP:O	2.17	0.44
5:J:57:THR:HG21	5:J:62:THR:HB	2.00	0.44
7:I:55:ASP:O	7:I:56:ASP:CB	2.66	0.44
8:K:257:SER:O	8:K:258:GLN:HG2	2.17	0.44
8:K:389:LEU:HD23	8:K:392:ILE:HD12	1.99	0.44
8:K:457:ILE:CD1	8:K:484:ILE:HG12	2.48	0.44
2:h:135:ARG:HB2	2:h:532:THR:HG21	2.00	0.44
3:g:242:LEU:HD13	3:g:285:VAL:HG13	1.98	0.44
3:g:424:LEU:HB2	3:g:443:ALA:HB2	2.00	0.44
4:e:324:GLN:HB2	4:e:351:LEU:CD1	2.48	0.44
5:b:155:HIS:HB3	5:b:488:VAL:HG22	1.99	0.44
7:a:410:LYS:HD3	7:a:411:ARG:NE	2.33	0.44
2:p:78:VAL:HB	3:o:11:VAL:O	2.18	0.44
2:p:341:LEU:HD23	2:p:342:PRO:HD2	2.00	0.44
5:j:46:LEU:HD21	5:j:63:ILE:HG23	1.99	0.44
5:j:193:ILE:HA	5:j:365:CYS:O	2.17	0.44
5:j:370:ARG:NH2	6:l:88:GLU:OE2	2.50	0.44
6:l:520:ARG:CG	6:l:520:ARG:NH2	2.73	0.44
7:i:236:ARG:HG3	7:i:362:VAL:HG22	1.98	0.44
1:F:210:ILE:C	1:F:212:GLY:H	2.26	0.44
2:H:154:ASN:HB3	2:H:190:LEU:HD13	1.99	0.44
2:H:409:LYS:HD2	2:H:409:LYS:O	2.17	0.44
3:G:348:THR:HG22	3:G:349:CYS:N	2.33	0.44
3:G:385:VAL:HA	4:E:547:MET:HE1	2.00	0.44
4:E:320:VAL:HG22	4:E:341:PRO:HB2	2.00	0.44
5:B:119:THR:OG1	6:L:8:ASN:OD1	2.25	0.44
6:D:161:LYS:O	6:D:163:VAL:N	2.50	0.44
7:A:68:THR:O	7:A:72:LEU:HG	2.18	0.44
1:N:533:LEU:HD22	8:K:47:MET:HE2	1.98	0.44
2:P:42:CYS:SG	2:P:104:MET:HG2	2.57	0.44
2:h:428:ILE:HA	2:h:431:ILE:HD12	2.00	0.44
5:b:518:ARG:HA	5:b:519:PRO:HD2	1.87	0.44
6:d:138:MET:SD	6:d:478:LEU:HD21	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:252:GLN:HA	7:a:303:ASP:HB2	2.00	0.44
1:n:459:VAL:HG22	1:n:491:VAL:HG11	2.00	0.44
5:j:32:LEU:O	5:j:44:LYS:HE3	2.18	0.44
8:k:473:ALA:C	8:k:475:HIS:H	2.25	0.44
1:F:6:LEU:HB3	8:C:70:VAL:HG13	1.99	0.44
2:H:471:VAL:HG21	8:K:115:ASN:HD22	1.82	0.44
4:E:388:THR:HG21	5:B:385:HIS:HE1	1.83	0.44
7:A:501:GLY:CA	7:A:512:GLU:HG2	2.48	0.44
2:P:302:GLY:HA3	2:P:329:LEU:HD11	1.99	0.44
5:J:346:ILE:HG22	5:J:347:MET:H	1.83	0.44
7:I:144:LEU:HD23	7:I:419:VAL:HG13	1.99	0.44
1:f:133:LEU:HD11	1:f:412:ILE:HD11	2.00	0.44
8:c:79:LEU:C	8:c:81:LEU:H	2.25	0.44
1:n:253:TYR:O	2:p:265:VAL:HA	2.18	0.44
2:p:147:VAL:O	2:p:419:LEU:HB2	2.18	0.44
4:m:251:HIS:CE1	5:j:325:VAL:HB	2.52	0.44
4:m:324:GLN:HB2	4:m:351:LEU:CD1	2.47	0.44
4:m:381:TYR:CE1	4:m:394:ILE:HD12	2.52	0.44
6:l:432:MET:HG3	6:l:440:TRP:HE3	1.83	0.44
7:i:338:VAL:HG21	7:i:350:PHE:HE1	1.83	0.44
1:F:473:VAL:HG13	1:F:489:VAL:HG22	1.99	0.43
3:G:204:ILE:HG23	3:G:379:ARG:HD3	1.99	0.43
5:B:402:LEU:H	5:B:402:LEU:HD12	1.83	0.43
5:B:407:ALA:O	5:B:411:MET:HG3	2.17	0.43
6:D:242:SER:HB3	6:D:243:PRO:HD2	2.00	0.43
6:D:448:GLU:OE1	6:D:470:ARG:NH2	2.51	0.43
7:A:25:ILE:HG21	7:A:542:ASP:O	2.18	0.43
7:A:53:LEU:HD23	8:C:527:VAL:HB	2.00	0.43
8:C:485:ASP:HB2	8:C:492:VAL:HG21	1.98	0.43
2:P:78:VAL:HB	3:O:11:VAL:O	2.17	0.43
2:P:305:VAL:HG11	2:P:310:LEU:HD12	2.00	0.43
3:O:83:LEU:HB3	3:O:102:THR:HG23	2.00	0.43
4:M:47:LYS:NZ	4:M:143:PRO:HG3	2.32	0.43
4:M:498:LEU:HD21	4:M:510:ILE:O	2.18	0.43
6:L:49:LYS:HD3	7:I:546:THR:HG23	1.99	0.43
8:K:81:LEU:CD1	8:K:516:SER:HB2	2.47	0.43
8:K:271:ARG:O	8:K:275:ILE:HG13	2.16	0.43
2:h:27:GLN:NE2	2:h:544:ILE:HD11	2.32	0.43
5:b:426:LYS:O	5:b:430:VAL:HG23	2.18	0.43
6:d:336:ILE:C	6:d:338:LEU:H	2.25	0.43
8:c:102:GLU:HA	8:c:105:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:m:96:LEU:HD13	4:m:101:ALA:HB1	1.99	0.43
4:E:353:HIS:HB3	4:E:403:THR:HG21	1.99	0.43
6:D:102:ALA:HB2	6:D:449:VAL:HG21	1.99	0.43
8:C:78:MET:HE2	8:C:81:LEU:HD22	2.00	0.43
8:C:425:VAL:HA	8:C:428:ALA:HB3	1.99	0.43
8:C:440:TRP:HB2	8:C:441:PRO:HD3	1.99	0.43
1:N:30:GLN:HB2	1:N:96:CYS:HB3	2.00	0.43
2:P:311:HIS:CD2	3:O:336:SER:H	2.36	0.43
4:M:52:LEU:HA	4:M:55:ARG:HB2	1.99	0.43
4:M:457:GLU:O	4:M:461:GLN:HG2	2.17	0.43
5:J:162:SER:HA	5:J:167:SER:OG	2.18	0.43
6:L:72:HIS:HB2	7:I:13:LEU:HD12	1.99	0.43
6:L:436:GLN:HA	6:L:439:ILE:HD12	1.99	0.43
7:I:53:LEU:HD11	7:I:69:ILE:HG23	2.00	0.43
7:I:266:ASP:HA	7:I:267:PRO:HD2	1.84	0.43
7:I:269:GLN:HA	7:I:272:GLN:HB2	2.00	0.43
1:n:269:PHE:CG	8:k:273:LEU:HD23	2.53	0.43
2:p:8:ASN:HA	2:p:9:PRO:HD3	1.87	0.43
3:o:395:ASP:OD2	11:o:603:BEF:F2	2.26	0.43
4:m:158:ILE:HG13	4:m:159:SER:N	2.33	0.43
8:k:78:MET:O	8:k:81:LEU:HB3	2.18	0.43
8:k:147:ASN:HB3	8:k:150:ALA:HB3	1.99	0.43
1:F:269:PHE:HE1	8:C:274:GLN:HG3	1.83	0.43
2:H:411:LEU:HD12	2:H:417:GLY:HA3	2.01	0.43
1:N:101:LEU:HG	1:N:122:PHE:CE1	2.53	0.43
1:N:192:HIS:NE2	1:N:326:GLU:HB2	2.33	0.43
3:O:165:ALA:HB2	3:O:399:ILE:HD12	1.99	0.43
5:J:281:ILE:HG22	5:J:283:THR:H	1.83	0.43
2:h:121:GLY:HA3	8:k:464:PRO:HG2	2.00	0.43
3:g:478:TRP:HE3	3:g:492:PHE:HB2	1.82	0.43
4:e:200:PHE:HA	4:e:203:MET:HE2	2.00	0.43
4:e:245:LEU:HD11	4:e:354:ILE:HD11	2.00	0.43
4:e:381:TYR:CE1	4:e:394:ILE:HD12	2.54	0.43
7:a:143:VAL:O	7:a:143:VAL:CG1	2.66	0.43
7:a:247:LEU:HD11	7:a:288:ILE:HD13	2.00	0.43
8:c:296:ILE:HG12	8:c:317:LEU:HB2	2.00	0.43
1:n:457:THR:HA	1:n:460:LYS:HB2	2.00	0.43
3:o:385:VAL:HA	4:m:547:MET:HE1	2.00	0.43
4:m:160:LYS:HG3	4:m:453:ALA:HB1	1.99	0.43
3:G:301:ASP:O	3:G:305:GLN:HG2	2.18	0.43
5:B:203:LEU:N	6:D:513:GLU:OE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:47:MET:O	7:A:544:MET:HA	2.18	0.43
1:N:55:LEU:HD11	2:P:541:ILE:HD11	1.99	0.43
1:N:296:ILE:HG12	1:N:317:LEU:HD23	2.00	0.43
1:N:458:LEU:HB3	1:N:493:LEU:HD21	1.99	0.43
2:P:21:TYR:CD2	2:P:21:TYR:N	2.86	0.43
6:L:158:LEU:O	6:L:160:SER:N	2.51	0.43
8:K:99:LEU:HG	8:K:452:ILE:HD11	1.98	0.43
1:f:84:ASP:HB2	1:f:91:THR:HG21	2.00	0.43
1:f:418:PHE:HE2	1:f:517:ILE:HD11	1.82	0.43
5:b:234:ALA:HA	5:b:326:VAL:O	2.19	0.43
6:d:420:GLU:HB2	6:d:473:HIS:HE1	1.81	0.43
6:d:516:LYS:O	6:d:520:ARG:HG2	2.19	0.43
7:a:424:CYS:SG	7:a:500:TYR:HB2	2.57	0.43
2:p:280:GLU:O	2:p:284:ILE:HG12	2.17	0.43
3:o:51:ILE:HB	3:o:69:ILE:HD12	2.00	0.43
3:o:247:GLU:HB3	3:o:298:PRO:HD2	2.00	0.43
5:j:82:LYS:NZ	5:j:86:ASP:OD2	2.50	0.43
5:j:503:GLU:O	5:j:507:VAL:HG23	2.19	0.43
6:l:397:ALA:O	6:l:400:VAL:HG22	2.18	0.43
7:i:47:VAL:HG12	8:k:117:HIS:NE2	2.34	0.43
1:F:177:ALA:O	1:F:181:VAL:HG23	2.18	0.43
1:F:277:ILE:HG13	1:F:340:VAL:HG11	2.01	0.43
1:F:459:VAL:HA	1:F:462:SER:HB3	1.99	0.43
2:H:25:ASP:O	2:H:27:GLN:N	2.52	0.43
2:H:189:VAL:HG11	2:H:206:SER:HB3	2.01	0.43
4:E:322:ILE:CG2	4:E:346:VAL:HG21	2.48	0.43
1:N:203:SER:O	1:N:206:ASP:HB2	2.17	0.43
1:N:303:PRO:HA	1:N:306:LEU:HD12	2.01	0.43
1:N:420:ILE:O	1:N:424:ARG:HG3	2.19	0.43
5:J:151:GLU:HA	5:J:154:ILE:HD12	2.01	0.43
5:J:181:ILE:HD13	5:J:391:LEU:HB3	2.01	0.43
6:L:151:VAL:HA	6:L:175:VAL:HG21	2.00	0.43
1:f:22:ASN:HA	1:f:72:THR:HG21	2.00	0.43
1:f:70:SER:HB3	1:f:73:ALA:HB3	2.01	0.43
2:h:256:ILE:H	2:h:256:ILE:HG13	1.59	0.43
3:g:83:LEU:HA	3:g:86:ILE:HG22	1.99	0.43
5:b:370:ARG:NH2	6:d:88:GLU:OE2	2.51	0.43
8:c:100:ALA:O	8:c:104:LEU:HD12	2.18	0.43
1:n:121:GLY:HA3	1:n:443:GLY:HA3	2.00	0.43
2:p:62:ILE:H	2:p:62:ILE:HG13	1.67	0.43
2:p:117:LEU:HD22	2:p:122:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o:337:THR:HG22	3:o:339:SER:H	1.83	0.43
6:l:138:MET:HB2	6:l:478:LEU:CD1	2.39	0.43
1:F:342:ASP:HB3	8:C:307:HIS:CE1	2.53	0.43
7:A:55:ASP:CB	7:A:59:ASP:O	2.62	0.43
6:L:295:ASP:O	6:L:296:ALA:CB	2.67	0.43
6:L:320:GLU:O	6:L:324:LEU:HB2	2.19	0.43
7:I:333:THR:HA	7:I:377:THR:HG22	1.99	0.43
8:K:471:LEU:O	8:K:475:HIS:HB2	2.18	0.43
3:g:86:ILE:CD1	3:g:510:ALA:HA	2.43	0.43
6:d:500:PRO:HB2	6:d:503:VAL:HG23	2.00	0.43
6:d:520:ARG:CG	6:d:520:ARG:NH2	2.70	0.43
8:c:502:PRO:HD2	8:c:505:ILE:HD12	2.01	0.43
3:o:45:GLY:HA3	3:o:453:LEU:HD22	2.01	0.43
5:j:440:LEU:CB	5:j:441:PRO:CD	2.96	0.43
7:i:162:THR:HG23	7:i:517:VAL:HG13	2.01	0.43
7:i:209:HIS:NE2	8:k:87:GLU:OE1	2.50	0.43
8:k:59:ASN:HB3	8:k:162:LYS:HG2	2.00	0.43
2:H:79:HIS:HA	2:H:80:PRO:HD3	1.83	0.43
4:E:245:LEU:HD11	4:E:354:ILE:HD11	1.99	0.43
7:A:56:ASP:OD1	7:A:57:ILE:N	2.52	0.43
8:C:144:ASP:CG	8:C:147:ASN:HB2	2.44	0.43
1:N:465:ASP:HB3	1:N:468:ASP:HB2	2.00	0.43
3:O:94:VAL:CG1	3:O:502:VAL:HG22	2.49	0.43
3:O:209:MET:HG2	4:M:543:GLN:NE2	2.34	0.43
6:L:45:ASP:OD1	6:L:59:ASN:HB2	2.19	0.43
6:L:242:SER:HB3	6:L:243:PRO:HD2	1.99	0.43
7:I:179:MET:CE	7:I:385:ILE:HG23	2.45	0.43
8:K:250:LEU:HD12	8:K:301:VAL:HG22	2.00	0.43
7:a:411:ARG:HB3	7:a:522:ILE:HD12	1.99	0.43
7:a:522:ILE:HG13	7:a:522:ILE:H	1.63	0.43
2:p:311:HIS:HB2	3:o:336:SER:HB2	2.00	0.43
4:m:412:ASN:OD1	4:m:415:ILE:HG13	2.18	0.43
6:l:77:MET:O	6:l:81:VAL:HG23	2.18	0.43
8:k:58:THR:O	8:k:64:ILE:HD11	2.18	0.43
2:H:512:ILE:CG2	2:H:517:ILE:O	2.67	0.43
3:G:206:GLY:HA2	4:E:110:SER:HB3	2.01	0.43
4:E:269:LEU:HD12	4:E:358:THR:HG21	2.01	0.43
6:D:404:LEU:HD11	6:D:410:LEU:HD13	2.00	0.43
7:A:121:HIS:CG	7:A:122:PRO:HD2	2.53	0.43
2:P:478:LEU:HD22	2:P:499:VAL:CG2	2.49	0.43
3:O:202:LYS:HB3	3:O:377:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:473:ALA:HA	4:M:476:LEU:HD12	2.01	0.43
6:L:220:ILE:HG21	6:L:302:LEU:HD21	2.01	0.43
6:L:244:PRO:CD	6:L:270:TYR:CE2	3.00	0.43
8:K:167:TRP:N	8:K:167:TRP:CD1	2.86	0.43
1:f:255:SER:HB3	1:f:258:GLN:HB2	2.01	0.43
2:h:323:VAL:O	2:h:324:PRO:C	2.61	0.43
4:e:91:LEU:HD11	4:e:123:VAL:HG21	2.01	0.43
8:c:145:VAL:HG12	8:c:406:VAL:HG12	2.01	0.43
1:n:210:ILE:C	1:n:212:GLY:H	2.26	0.43
1:n:251:PHE:HZ	2:p:259:THR:CB	2.29	0.43
3:o:153:SER:HB3	3:o:156:GLU:CB	2.49	0.43
3:o:162:ALA:O	3:o:166:MET:HG2	2.19	0.43
7:i:56:ASP:OD1	7:i:57:ILE:N	2.51	0.43
7:i:126:ILE:HG13	7:i:539:LEU:HD23	1.99	0.43
2:H:122:LEU:HD22	2:H:126:GLU:HB3	2.00	0.43
5:B:46:LEU:HD21	5:B:63:ILE:HG23	2.01	0.43
5:B:326:VAL:HG12	5:B:327:SER:O	2.19	0.43
6:D:161:LYS:C	6:D:163:VAL:H	2.26	0.43
8:C:102:GLU:OE1	8:C:451:CYS:HB2	2.19	0.43
1:N:492:ASP:HB2	1:N:499:CYS:CB	2.48	0.43
2:P:252:CYS:HB2	2:P:342:PRO:O	2.19	0.43
3:O:26:ILE:O	3:O:30:ILE:HD12	2.18	0.43
8:K:154:LEU:HG	8:K:412:LEU:HD21	2.01	0.43
1:f:79:ALA:HB2	1:f:523:ILE:CD1	2.48	0.43
2:h:424:GLY:HA2	2:h:427:GLU:HG2	1.99	0.43
7:a:164:MET:HE3	7:a:405:SER:CB	2.49	0.43
7:a:255:ARG:O	7:a:257:ALA:N	2.52	0.43
7:a:510:VAL:HG12	7:a:511:ASP:N	2.33	0.43
2:p:24:ALA:O	2:p:28:ILE:N	2.30	0.43
2:p:55:ILE:HD11	2:p:71:MET:HG3	2.00	0.43
2:p:322:LYS:O	2:p:324:PRO:HD3	2.18	0.43
2:p:478:LEU:HD22	2:p:499:VAL:CG2	2.48	0.43
4:m:271:ILE:HG23	4:m:351:LEU:HD22	2.00	0.43
8:k:35:ILE:O	8:k:35:ILE:CG2	2.66	0.43
1:F:301:ILE:HG12	1:F:318:ARG:HB3	2.00	0.43
2:H:63:ILE:HG21	2:H:74:GLU:HG3	1.99	0.43
3:G:18:ASP:O	3:G:524:ILE:HA	2.19	0.43
5:B:279:PHE:HB3	5:B:281:ILE:CD1	2.49	0.43
6:D:64:ILE:O	6:D:68:MET:HG2	2.19	0.43
8:C:457:ILE:HD13	8:C:484:ILE:HG21	2.01	0.43
4:M:74:LEU:HD13	4:M:93:GLN:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:254:VAL:HB	7:I:262:ILE:HD13	2.00	0.43
1:f:454:ILE:H	1:f:454:ILE:HD12	1.84	0.43
5:b:409:MET:HG3	5:b:459:LEU:CD2	2.46	0.43
7:a:63:THR:HG22	7:a:65:ASP:H	1.84	0.43
8:c:283:MET:HE3	8:c:340:VAL:HG21	2.01	0.43
1:n:178:VAL:HG22	1:n:399:LEU:HD23	2.00	0.43
1:n:418:PHE:HE2	1:n:517:ILE:HD11	1.83	0.43
3:o:220:PHE:C	3:o:222:LYS:N	2.72	0.43
5:j:56:VAL:HG23	5:j:375:GLN:HG2	2.00	0.43
6:l:436:GLN:HA	6:l:439:ILE:HD12	2.01	0.43
1:F:57:LYS:O	1:F:57:LYS:HG2	2.19	0.42
1:F:221:HIS:HB3	1:F:224:MET:HG3	2.01	0.42
1:F:278:ILE:H	1:F:278:ILE:HG13	1.67	0.42
3:G:218:VAL:HG12	3:G:219:ALA:H	1.83	0.42
3:G:322:ASP:HA	3:G:325:ARG:HB2	2.01	0.42
5:B:220:ASN:HB3	5:B:221:ASN:H	1.59	0.42
6:D:225:GLY:N	6:D:226:PRO:HD3	2.34	0.42
6:D:253:ILE:HG22	7:A:263:ASN:HB2	2.01	0.42
7:A:53:LEU:HB3	8:C:530:VAL:HG21	2.01	0.42
8:C:471:LEU:O	8:C:475:HIS:HB2	2.19	0.42
3:O:220:PHE:HD2	3:O:363:ASN:HB2	1.83	0.42
3:O:297:LEU:CB	3:O:298:PRO:HD2	2.40	0.42
4:M:72:LYS:HG3	5:J:513:ASN:HB3	2.01	0.42
5:J:293:TYR:HB3	5:J:294:PRO:CD	2.49	0.42
4:e:275:PRO:HD3	4:e:325:TRP:CE3	2.55	0.42
2:p:39:HIS:O	2:p:43:LEU:HB2	2.18	0.42
3:o:25:GLN:HG2	3:o:521:ASP:C	2.44	0.42
3:o:411:ALA:HB2	3:o:478:TRP:CD2	2.54	0.42
4:m:507:ILE:H	4:m:507:ILE:HG13	1.62	0.42
8:k:203:TYR:HE1	8:k:330:ARG:HE	1.67	0.42
2:H:327:PHE:CG	2:H:328:GLU:N	2.86	0.42
5:B:175:GLU:O	5:B:179:ASN:HB2	2.19	0.42
5:B:197:LYS:HB2	5:B:377:LEU:HD13	2.01	0.42
8:C:206:VAL:HG13	8:C:379:ILE:HB	2.01	0.42
1:N:202:LEU:O	1:N:383:SER:HB3	2.18	0.42
1:N:253:TYR:O	2:P:265:VAL:HA	2.19	0.42
3:O:498:GLU:HA	3:O:499:PRO:HD3	1.90	0.42
10:M:602:ADP:O3B	11:M:603:BEF:F2	2.27	0.42
5:J:321:THR:HG22	5:J:339:GLU:N	2.33	0.42
7:I:126:ILE:HD11	7:I:539:LEU:HB3	2.01	0.42
8:K:70:VAL:HG11	8:K:75:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:248:CYS:O	8:K:297:THR:CG2	2.67	0.42
3:g:263:HIS:HA	4:e:294:GLU:OE2	2.19	0.42
5:b:32:LEU:O	5:b:44:LYS:HE3	2.19	0.42
7:a:77:HIS:CD2	7:a:79:ALA:HB3	2.54	0.42
8:c:161:THR:HG21	10:c:1102:ADP:O2A	2.19	0.42
1:n:285:CYS:SG	1:n:293:PHE:HB2	2.59	0.42
3:o:220:PHE:HD2	3:o:363:ASN:HB2	1.83	0.42
3:o:226:TYR:O	3:o:227:ALA:C	2.63	0.42
5:j:22:ALA:HA	5:j:73:ALA:CB	2.49	0.42
5:j:255:THR:CG2	6:l:263:ILE:HA	2.49	0.42
6:l:242:SER:O	6:l:244:PRO:HD3	2.19	0.42
7:i:12:THR:CB	7:i:14:PHE:CE2	2.98	0.42
7:i:422:GLY:O	7:i:502:LEU:HB3	2.19	0.42
8:k:467:LEU:O	8:k:471:LEU:HB2	2.18	0.42
2:H:92:GLN:HG3	2:H:526:PHE:HB3	2.01	0.42
3:G:488:ILE:H	3:G:488:ILE:HG13	1.58	0.42
4:E:100:ILE:HG23	4:E:548:ILE:HD12	2.02	0.42
5:B:327:SER:O	5:B:329:PHE:N	2.53	0.42
5:B:438:ARG:C	5:B:440:LEU:N	2.77	0.42
6:D:398:LEU:HA	6:D:401:ILE:HD12	2.00	0.42
7:A:97:GLY:O	7:A:101:VAL:HG23	2.20	0.42
6:L:366:ILE:HD13	6:L:366:ILE:N	2.34	0.42
7:I:143:VAL:O	7:I:143:VAL:CG1	2.67	0.42
8:K:494:MET:SD	8:K:499:ILE:HB	2.59	0.42
1:f:329:GLN:HG2	1:f:334:GLY:O	2.19	0.42
1:f:467:LEU:HD13	1:n:111:GLU:HG2	2.01	0.42
3:g:120:ILE:HD13	7:i:469:ASP:OD2	2.20	0.42
3:g:181:MET:HE2	3:g:214:PHE:HB2	2.01	0.42
5:b:239:ASP:CA	5:b:291:TYR:HB2	2.38	0.42
5:b:390:VAL:CG1	5:b:493:LEU:HD12	2.49	0.42
6:d:225:GLY:N	6:d:226:PRO:HD3	2.35	0.42
6:d:463:ILE:HD12	4:m:141:ILE:HD11	2.00	0.42
1:n:202:LEU:O	1:n:383:SER:HB3	2.20	0.42
3:o:55:THR:HG22	3:o:56:SER:H	1.84	0.42
6:l:419:ILE:O	6:l:422:SER:HB3	2.18	0.42
7:i:89:GLN:HA	7:i:92:ARG:HD3	2.01	0.42
7:i:333:THR:HG22	7:i:377:THR:HG22	2.00	0.42
3:G:113:LYS:HB3	3:G:114:PRO:HD3	2.00	0.42
3:G:133:VAL:O	3:G:137:VAL:HG23	2.19	0.42
3:G:491:ASN:HD22	3:G:491:ASN:HA	1.73	0.42
4:E:357:SER:HA	4:E:401:THR:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:70:SER:HB3	1:N:73:ALA:HB3	2.01	0.42
4:M:144:ILE:HD11	4:M:550:LYS:HA	2.01	0.42
6:L:509:THR:O	6:L:513:GLU:HB2	2.20	0.42
7:I:422:GLY:O	7:I:502:LEU:HB3	2.19	0.42
8:K:322:LYS:H	8:K:322:LYS:CD	2.32	0.42
1:f:202:LEU:O	1:f:383:SER:HB3	2.19	0.42
3:g:191:ARG:O	3:g:192:ASN:C	2.61	0.42
5:b:234:ALA:C	5:b:286:ASN:HD22	2.26	0.42
6:d:448:GLU:O	6:d:451:PRO:HD2	2.20	0.42
1:n:521:THR:O	1:n:525:SER:HB3	2.19	0.42
2:p:54:ILE:O	2:p:54:ILE:HG23	2.20	0.42
2:p:123:SER:HB3	2:p:126:GLU:CG	2.48	0.42
4:m:191:LYS:C	4:m:193:VAL:H	2.27	0.42
4:m:269:LEU:CD1	4:m:358:THR:HG21	2.49	0.42
4:m:473:ALA:O	4:m:476:LEU:HB2	2.19	0.42
5:j:287:ARG:HG3	5:j:310:ASP:HA	2.01	0.42
5:j:314:VAL:HG11	5:j:325:VAL:HG13	2.02	0.42
5:j:374:ASP:HB2	6:l:80:GLU:CD	2.45	0.42
6:l:323:PHE:CD1	6:l:323:PHE:C	2.98	0.42
7:i:359:ASP:HB2	7:i:376:GLY:HA3	2.02	0.42
1:F:204:PRO:HA	1:F:381:LYS:O	2.19	0.42
1:F:234:LEU:HD23	1:F:295:ILE:HG12	2.02	0.42
6:D:59:ASN:HB3	6:D:161:LYS:HG2	2.02	0.42
7:A:63:THR:HG22	7:A:64:ASN:H	1.85	0.42
7:A:437:ALA:HB1	7:A:445:GLN:HG3	2.01	0.42
8:C:402:VAL:HA	8:C:405:ASN:ND2	2.35	0.42
1:N:455:PRO:O	1:N:459:VAL:HG23	2.19	0.42
1:f:424:ARG:HH21	1:f:477:LEU:HD22	1.85	0.42
4:e:71:ASP:OD1	4:e:85:ASN:HB2	2.19	0.42
4:e:329:ASP:OD2	5:b:235:ASN:HB3	2.20	0.42
7:a:63:THR:HG22	7:a:64:ASN:N	2.34	0.42
8:c:70:VAL:HG11	8:c:75:ALA:CB	2.49	0.42
3:o:243:SER:HB3	3:o:323:MET:HE1	2.01	0.42
5:j:47:GLN:O	6:l:527:SER:N	2.45	0.42
5:j:220:ASN:HB3	5:j:221:ASN:H	1.61	0.42
6:l:198:LYS:HB3	6:l:387:ILE:HG21	2.01	0.42
7:i:248:ASP:HA	7:i:299:THR:HB	2.01	0.42
8:k:165:ILE:H	8:k:165:ILE:HG13	1.63	0.42
2:H:8:ASN:HA	2:H:9:PRO:HD3	1.86	0.42
2:H:455:ALA:O	2:H:458:VAL:HG23	2.19	0.42
3:G:75:VAL:O	3:G:81:LYS:HE3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:352:PHE:C	3:G:352:PHE:CD2	2.97	0.42
3:G:460:ASP:O	3:G:464:ILE:HG12	2.19	0.42
7:A:15:LEU:O	7:A:16:GLY:C	2.62	0.42
8:C:7:PHE:CG	8:C:8:MET:N	2.87	0.42
8:C:133:LEU:HD21	8:C:511:LYS:HD2	2.01	0.42
8:C:140:SER:HA	8:C:414:PRO:HD3	2.02	0.42
1:N:204:PRO:HA	1:N:381:LYS:O	2.19	0.42
1:N:326:GLU:HG2	8:K:232:PRO:HB3	2.02	0.42
3:O:86:ILE:HD12	3:O:513:ALA:CB	2.50	0.42
4:M:73:ILE:CG2	5:J:511:VAL:CG1	2.97	0.42
4:M:423:LEU:O	4:M:427:LEU:N	2.43	0.42
5:J:58:ASN:O	5:J:59:ASP:C	2.62	0.42
5:J:141:ASP:HA	5:J:399:ARG:HA	2.00	0.42
7:I:422:GLY:HA2	10:I:602:ADP:N3	2.34	0.42
7:I:510:VAL:HG12	7:I:511:ASP:N	2.35	0.42
4:e:90:ILE:H	4:e:90:ILE:HG12	1.68	0.42
5:b:155:HIS:HB2	5:b:488:VAL:CG2	2.49	0.42
5:b:292:ASP:HB3	6:d:238:GLN:OE1	2.20	0.42
7:a:256:MET:CG	8:c:257:SER:HB2	2.41	0.42
3:o:282:LEU:C	3:o:284:GLN:N	2.78	0.42
5:j:80:ILE:HG22	5:j:95:VAL:HG11	2.01	0.42
7:i:120:ILE:HD13	7:i:120:ILE:HA	1.87	0.42
8:k:336:ILE:H	8:k:336:ILE:HG13	1.72	0.42
8:k:440:TRP:HB2	8:k:441:PRO:HD3	2.01	0.42
1:F:459:VAL:HG22	1:F:491:VAL:HG11	2.01	0.42
2:H:35:ILE:HD13	2:H:111:LEU:CD1	2.50	0.42
3:G:409:ILE:HD13	3:G:497:TRP:CE3	2.53	0.42
4:E:115:ILE:HG22	4:E:117:ASP:H	1.84	0.42
4:E:464:ILE:H	4:E:464:ILE:HD12	1.84	0.42
7:A:471:SER:HB2	3:O:120:ILE:HD11	2.01	0.42
8:C:208:LYS:HD2	8:C:389:LEU:HB3	2.01	0.42
8:C:255:GLY:C	8:C:257:SER:H	2.26	0.42
3:O:326:VAL:HG23	3:O:365:PHE:CE1	2.52	0.42
8:K:60:ASP:HB3	8:K:63:ALA:HB3	2.00	0.42
1:f:100:GLU:HA	1:f:103:ARG:HB3	2.00	0.42
2:h:56:VAL:HB	3:g:525:THR:HG23	2.02	0.42
2:h:142:LEU:HG	2:h:430:LEU:HD21	2.01	0.42
3:g:419:GLU:HB2	3:g:472:HIS:CE1	2.46	0.42
4:e:72:LYS:N	4:e:72:LYS:HD2	2.35	0.42
3:o:133:VAL:HB	3:o:511:THR:HG21	2.01	0.42
5:j:95:VAL:HG22	5:j:497:VAL:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:j:476:ASN:HB3	5:j:478:THR:HG22	2.01	0.42
7:i:144:LEU:CD2	7:i:419:VAL:HG22	2.50	0.42
8:k:171:MET:HE2	8:k:174:LEU:HD12	2.01	0.42
5:B:453:SER:O	5:B:457:SER:HB2	2.20	0.42
7:A:522:ILE:H	7:A:522:ILE:HG13	1.69	0.42
1:N:87:THR:HG21	1:N:512:VAL:HA	2.02	0.42
1:N:215:LEU:HD22	1:N:217:HIS:HE1	1.85	0.42
3:O:179:VAL:C	3:O:181:MET:H	2.27	0.42
5:J:121:ILE:HG23	5:J:506:GLU:CD	2.45	0.42
5:J:351:GLN:HA	5:J:352:PRO:HD3	1.79	0.42
7:I:269:GLN:HE21	7:I:269:GLN:HB2	1.66	0.42
1:f:253:TYR:O	2:h:265:VAL:HA	2.20	0.42
3:g:482:VAL:HG22	3:g:491:ASN:HD21	1.85	0.42
1:n:221:HIS:HB3	1:n:224:MET:HG3	2.01	0.42
2:p:299:ILE:HD12	2:p:313:LEU:HD21	2.02	0.42
4:m:269:LEU:HG	4:m:375:GLY:O	2.18	0.42
4:m:278:PRO:HA	4:m:279:PRO:HD3	1.93	0.42
5:j:327:SER:O	5:j:328:THR:C	2.62	0.42
6:l:72:HIS:CD2	6:l:74:VAL:HB	2.55	0.42
2:H:234:GLY:O	2:H:235:HIS:CG	2.73	0.42
5:B:121:ILE:HG23	5:B:506:GLU:CD	2.45	0.42
5:B:228:ASN:N	5:B:341:ASP:O	2.46	0.42
6:D:99:LEU:O	6:D:103:LEU:HB2	2.20	0.42
7:A:250:ASN:HB3	7:A:300:LYS:CB	2.49	0.42
2:P:41:MET:HE2	2:P:53:LYS:HD3	2.02	0.42
4:M:168:ILE:HD11	4:M:439:VAL:CG1	2.50	0.42
5:J:455:LEU:HD22	5:J:472:LEU:CD2	2.50	0.42
6:L:35:ILE:CG2	6:L:94:THR:HG23	2.50	0.42
7:I:65:ASP:HB3	7:I:68:THR:OG1	2.19	0.42
7:I:140:ILE:O	7:I:144:LEU:HG	2.19	0.42
1:f:518:THR:HG21	8:c:213:ASP:CB	2.50	0.42
3:g:424:LEU:HD13	3:g:442:PHE:HD1	1.84	0.42
5:b:165:ILE:HG12	6:d:520:ARG:HH22	1.84	0.42
6:d:448:GLU:C	6:d:451:PRO:HD2	2.45	0.42
8:c:65:LEU:HD11	8:c:97:ILE:HD13	2.02	0.42
1:n:153:VAL:HG11	1:n:405:VAL:CG2	2.49	0.42
1:n:162:VAL:HB	1:n:166:LEU:HD23	2.02	0.42
4:m:253:GLN:HB2	4:m:336:LEU:HD11	2.01	0.42
5:j:219:GLY:O	5:j:220:ASN:CB	2.64	0.42
6:l:199:LYS:O	6:l:380:ARG:NH1	2.53	0.42
6:l:448:GLU:C	6:l:451:PRO:HD2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:i:90:GLN:NE2	7:i:94:ILE:HD12	2.35	0.42
4:E:201:ALA:C	4:E:203:MET:H	2.27	0.42
5:B:471:GLY:HA3	5:B:482:MET:CG	2.50	0.42
6:D:200:VAL:HG13	6:D:387:ILE:HD11	2.00	0.42
6:D:420:GLU:HG2	6:D:478:LEU:HD11	2.02	0.42
7:A:67:ALA:HB1	7:A:88:GLN:HG3	2.01	0.42
8:C:252:TYR:CD2	8:C:252:TYR:N	2.88	0.42
4:M:147:ALA:HB1	4:M:546:ARG:HG3	2.01	0.42
5:J:155:HIS:HB2	5:J:488:VAL:HG22	2.02	0.42
6:L:65:LEU:HD11	6:L:97:VAL:HG21	2.02	0.42
7:I:15:LEU:C	7:I:17:GLY:N	2.77	0.42
7:I:337:LEU:HD23	7:I:337:LEU:HA	1.88	0.42
1:f:173:ILE:HG12	1:f:209:PHE:HB2	2.01	0.42
2:h:152:ASP:HB3	2:h:155:ASP:HB2	2.01	0.42
2:h:348:THR:HA	2:h:349:PRO:HD3	1.88	0.42
3:g:327:ILE:HA	3:g:330:VAL:HG12	2.02	0.42
1:n:529:LEU:HB3	8:k:45:LEU:HD13	2.01	0.42
2:p:35:ILE:HD11	2:p:81:ALA:O	2.20	0.42
1:F:173:ILE:HG22	1:F:378:ILE:HG12	2.01	0.41
1:F:459:VAL:HB	1:F:466:PRO:HA	2.02	0.41
3:G:41:LYS:N	3:G:42:PRO:CD	2.83	0.41
3:G:158:LEU:HD21	3:G:404:LEU:HG	2.02	0.41
3:G:268:GLN:O	3:G:272:ASP:HB2	2.19	0.41
4:E:278:PRO:HA	4:E:279:PRO:HD3	1.92	0.41
4:E:292:VAL:CG2	5:B:260:GLN:HB3	2.47	0.41
4:E:448:VAL:HG21	4:E:498:LEU:HD22	2.01	0.41
6:D:384:ASN:HA	6:D:387:ILE:HD12	2.02	0.41
7:A:184:LEU:C	7:A:186:ALA:H	2.28	0.41
1:N:213:LEU:HD21	1:N:324:ASN:ND2	2.35	0.41
1:N:251:PHE:HZ	2:P:259:THR:HB	1.85	0.41
2:P:238:SER:C	2:P:240:SER:H	2.27	0.41
2:P:256:ILE:H	2:P:256:ILE:HG13	1.67	0.41
4:M:70:LEU:HB3	5:J:510:ARG:O	2.20	0.41
7:I:15:LEU:O	7:I:16:GLY:C	2.62	0.41
8:K:361:GLY:O	8:K:362:ASP:HB2	2.18	0.41
2:h:190:LEU:HA	2:h:191:PRO:HD3	1.87	0.41
5:b:409:MET:CG	5:b:459:LEU:HD21	2.47	0.41
7:a:15:LEU:C	7:a:17:GLY:N	2.76	0.41
8:c:52:MET:H	8:c:52:MET:HG3	1.74	0.41
2:p:305:VAL:HG11	2:p:310:LEU:HD12	2.02	0.41
4:m:251:HIS:CE1	4:m:253:GLN:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:l:56:ILE:HD13	6:l:67:GLN:HG3	2.01	0.41
6:l:234:ILE:H	6:l:345:ASP:HB3	1.85	0.41
6:l:435:VAL:C	6:l:437:ALA:H	2.27	0.41
7:i:189:THR:CG2	7:i:190:GLN:N	2.83	0.41
1:F:204:PRO:HB3	1:F:391:THR:HG21	2.01	0.41
1:F:454:ILE:HB	1:F:455:PRO:HD3	2.02	0.41
3:G:24:GLY:O	3:G:28:SER:HB2	2.20	0.41
4:E:51:ILE:HG12	4:E:130:LEU:HB3	2.03	0.41
7:A:510:VAL:HG12	7:A:511:ASP:N	2.35	0.41
2:P:390:THR:HG21	3:O:82:THR:HG23	2.02	0.41
4:M:73:ILE:HG21	5:J:511:VAL:CG1	2.50	0.41
5:J:239:ASP:CA	5:J:291:TYR:HB2	2.40	0.41
7:I:12:THR:CB	7:I:14:PHE:HE2	2.33	0.41
3:g:61:THR:HG23	3:g:384:GLN:HE22	1.85	0.41
4:e:269:LEU:H	4:e:375:GLY:H	1.67	0.41
6:d:151:VAL:HA	6:d:175:VAL:HG21	2.02	0.41
7:a:460:LYS:O	7:a:464:VAL:HG23	2.20	0.41
1:n:124:ILE:HD11	1:n:434:LEU:HD11	2.02	0.41
1:n:130:MET:HE1	1:n:514:ARG:CG	2.49	0.41
4:m:324:GLN:HG2	4:m:325:TRP:CD1	2.56	0.41
4:m:353:HIS:HB3	4:m:403:THR:HG21	2.02	0.41
6:l:69:ALA:O	7:i:14:PHE:HA	2.20	0.41
8:k:141:LYS:HA	8:k:142:PRO:HD2	1.92	0.41
8:k:198:ILE:CG2	8:k:199:ASP:N	2.82	0.41
3:G:165:ALA:HB2	3:G:399:ILE:HD12	2.03	0.41
3:G:291:ASN:O	3:G:292:ILE:HG13	2.21	0.41
4:E:29:PHE:N	4:E:29:PHE:CD2	2.83	0.41
4:E:483:LEU:O	4:E:487:SER:HB2	2.20	0.41
5:B:183:ARG:NH1	5:B:365:CYS:HB3	2.31	0.41
7:A:39:VAL:HG11	7:A:73:LEU:HD11	2.02	0.41
8:C:59:ASN:O	8:C:60:ASP:C	2.62	0.41
3:O:198:LEU:O	3:O:373:THR:HG23	2.20	0.41
8:K:167:TRP:CE3	8:K:214:VAL:HB	2.55	0.41
1:f:47:VAL:HG22	1:f:53:ILE:HG12	2.02	0.41
1:f:149:PHE:HZ	1:f:411:ILE:HG21	1.85	0.41
2:h:109:GLU:CG	2:h:458:VAL:HG21	2.49	0.41
4:e:144:ILE:HD11	4:e:550:LYS:HA	2.02	0.41
6:d:89:ALA:C	6:d:91:ASP:H	2.28	0.41
7:a:262:ILE:HB	8:c:259:THR:HA	2.02	0.41
7:a:458:ILE:HD12	7:a:458:ILE:N	2.36	0.41
8:c:139:VAL:HG12	8:c:480:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:247:VAL:O	1:n:248:ASN:C	2.61	0.41
3:o:113:LYS:HB3	3:o:114:PRO:HD3	2.01	0.41
4:m:411:SER:CB	5:j:503:GLU:OE1	2.64	0.41
8:k:121:ILE:HG12	8:k:441:PRO:HG3	2.02	0.41
1:F:87:THR:HG22	1:F:89:ASP:H	1.85	0.41
8:C:198:ILE:CG2	8:C:199:ASP:H	2.33	0.41
2:P:62:ILE:H	2:P:62:ILE:HG13	1.61	0.41
2:P:498:GLY:O	2:P:509:VAL:HG13	2.21	0.41
8:K:72:HIS:HA	8:K:73:PRO:HD3	1.86	0.41
8:K:100:ALA:O	8:K:104:LEU:HD12	2.21	0.41
3:g:47:LEU:HD12	3:g:457:ALA:HB1	2.03	0.41
5:b:256:ALA:HA	6:d:266:GLU:CD	2.45	0.41
1:n:100:GLU:HA	1:n:103:ARG:HB3	2.03	0.41
2:p:142:LEU:HA	2:p:145:MET:HG3	2.03	0.41
2:p:502:ASP:C	2:p:502:ASP:OD1	2.62	0.41
5:j:14:ARG:HG2	5:j:15:ALA:N	2.35	0.41
5:j:194:GLN:HE21	5:j:196:ILE:HD11	1.84	0.41
2:H:247:VAL:HG21	2:H:355:VAL:CG2	2.50	0.41
4:E:319:ASP:O	4:E:341:PRO:HD2	2.21	0.41
4:E:423:LEU:O	4:E:427:LEU:HB2	2.19	0.41
6:D:123:SER:HA	6:D:126:SER:HB2	2.02	0.41
6:D:355:SER:O	6:D:356:ASP:HB3	2.20	0.41
6:D:500:PRO:HB2	6:D:503:VAL:HG23	2.01	0.41
2:P:54:ILE:HD11	3:O:78:PRO:HB2	2.02	0.41
2:P:178:LEU:HA	2:P:181:LEU:HD12	2.01	0.41
4:M:412:ASN:OD1	4:M:415:ILE:HG13	2.21	0.41
5:J:36:THR:HG23	5:J:58:ASN:CG	2.45	0.41
5:J:59:ASP:HB3	5:J:62:THR:OG1	2.20	0.41
6:L:64:ILE:HG22	6:L:68:MET:HE3	2.02	0.41
6:L:323:PHE:CZ	6:L:374:THR:HG21	2.56	0.41
6:L:495:GLU:HG3	6:L:495:GLU:O	2.20	0.41
8:K:7:PHE:CG	8:K:8:MET:N	2.88	0.41
1:f:285:CYS:O	1:f:286:GLY:C	2.63	0.41
5:b:57:THR:HA	5:b:379:GLU:OE1	2.21	0.41
5:b:89:GLY:HA3	5:b:389:SER:HB3	2.02	0.41
2:p:152:ASP:O	2:p:153:LYS:C	2.64	0.41
3:o:334:ILE:H	3:o:334:ILE:HG13	1.72	0.41
4:m:29:PHE:CD2	4:m:29:PHE:N	2.88	0.41
5:j:79:ASN:O	5:j:83:VAL:HG23	2.21	0.41
5:j:287:ARG:HH21	5:j:288:GLN:CD	2.28	0.41
6:l:65:LEU:HD11	6:l:97:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:162:VAL:HB	1:F:163:ASP:H	1.75	0.41
1:F:311:LYS:C	1:F:313:ASN:H	2.28	0.41
6:D:89:ALA:HB1	6:D:503:VAL:HG22	2.02	0.41
6:D:395:HIS:O	6:D:399:CYS:HB2	2.20	0.41
7:A:223:ALA:HA	7:A:373:LEU:HD12	2.01	0.41
7:A:226:CYS:SG	7:A:321:CYS:HB3	2.61	0.41
8:C:269:TRP:O	8:C:272:ILE:HG13	2.20	0.41
3:O:107:GLU:CD	3:O:448:VAL:HG21	2.45	0.41
3:O:419:GLU:HB2	3:O:472:HIS:CE1	2.51	0.41
4:M:239:LEU:HD13	4:M:406:CYS:SG	2.60	0.41
6:L:89:ALA:HB1	6:L:503:VAL:HG22	2.01	0.41
7:I:94:ILE:HG22	7:I:96:ASP:H	1.86	0.41
4:e:269:LEU:HD12	4:e:358:THR:HG21	2.02	0.41
5:b:53:THR:HG22	5:b:54:CYS:N	2.36	0.41
5:b:239:ASP:HA	5:b:291:TYR:CB	2.39	0.41
1:n:458:LEU:HD22	1:n:493:LEU:HD11	2.02	0.41
2:p:110:LEU:O	2:p:114:SER:HB2	2.20	0.41
1:F:246:GLU:CB	8:C:252:TYR:HE1	2.34	0.41
2:H:21:TYR:CD2	2:H:21:TYR:N	2.88	0.41
3:G:327:ILE:HG21	3:G:334:ILE:HG13	2.03	0.41
3:G:381:GLY:HA2	4:E:540:LEU:HD22	2.02	0.41
6:D:72:HIS:CD2	6:D:74:VAL:HB	2.55	0.41
6:D:75:ALA:O	6:D:78:LEU:HB2	2.20	0.41
7:A:281:VAL:O	7:A:285:VAL:HG23	2.21	0.41
7:A:337:LEU:HD23	7:A:337:LEU:HA	1.94	0.41
8:C:367:PHE:CE2	8:C:380:MET:HE1	2.47	0.41
3:O:90:GLN:HE21	3:O:97:GLY:HA3	1.85	0.41
3:O:508:ASN:HD22	3:O:508:ASN:HA	1.64	0.41
6:L:435:VAL:C	6:L:437:ALA:H	2.28	0.41
1:f:57:LYS:O	1:f:57:LYS:HG2	2.21	0.41
1:f:440:THR:O	1:f:444:ILE:HD12	2.20	0.41
3:g:218:VAL:HG12	3:g:219:ALA:H	1.85	0.41
5:b:39:PRO:HG3	10:b:602:ADP:C5	2.56	0.41
6:d:70:ILE:HD12	6:d:79:VAL:CG2	2.51	0.41
6:d:171:ALA:HB3	6:d:172:PRO:HD3	2.02	0.41
8:c:318:ARG:O	8:c:319:ARG:C	2.63	0.41
2:p:390:THR:C	2:p:392:ASN:H	2.29	0.41
3:o:418:MET:HG3	3:o:468:LEU:HD22	2.03	0.41
7:i:211:LYS:H	8:k:508:GLN:HE22	1.68	0.41
7:i:246:CYS:HB3	7:i:337:LEU:HD23	2.03	0.41
1:F:124:ILE:CG2	1:F:444:ILE:HD11	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:535:ARG:HH12	2:P:6:PRO:HB2	1.82	0.41
2:H:111:LEU:HD11	2:H:538:VAL:HG21	2.03	0.41
2:H:341:LEU:HD23	2:H:342:PRO:HD2	2.02	0.41
5:B:39:PRO:C	5:B:41:GLY:H	2.29	0.41
8:C:50:ASP:CB	8:C:51:PRO:CD	2.94	0.41
8:C:72:HIS:HA	8:C:73:PRO:HD3	1.96	0.41
8:C:81:LEU:HD11	8:C:516:SER:HB2	2.03	0.41
1:N:473:VAL:HG13	1:N:489:VAL:HG22	2.02	0.41
3:O:246:VAL:HA	3:O:297:LEU:HD12	2.03	0.41
4:M:278:PRO:HA	4:M:279:PRO:HD3	1.92	0.41
5:J:409:MET:CB	5:J:463:ILE:HD13	2.51	0.41
6:L:162:ILE:O	6:L:162:ILE:HG13	2.19	0.41
6:L:432:MET:HG3	6:L:440:TRP:CE3	2.55	0.41
6:L:432:MET:SD	6:L:440:TRP:HZ3	2.43	0.41
7:I:141:ASN:HA	7:I:144:LEU:HD12	2.02	0.41
8:K:440:TRP:HB2	8:K:441:PRO:HD3	2.03	0.41
1:f:93:THR:O	1:f:97:LEU:HB2	2.21	0.41
2:h:498:GLY:O	2:h:509:VAL:HG13	2.21	0.41
3:g:144:ALA:HB1	3:g:408:LEU:HG	2.03	0.41
4:e:335:LEU:HD12	4:e:335:LEU:HA	1.96	0.41
2:p:256:ILE:H	2:p:256:ILE:HG13	1.67	0.41
3:o:108:LEU:HD21	3:o:442:PHE:HE2	1.85	0.41
3:o:174:ASN:ND2	4:m:546:ARG:HH22	2.19	0.41
3:o:202:LYS:HB3	3:o:377:LEU:HD23	2.03	0.41
5:j:39:PRO:HG3	10:j:602:ADP:C5	2.56	0.41
5:j:162:SER:HA	5:j:167:SER:OG	2.20	0.41
6:l:51:SER:O	7:i:549:PRO:HA	2.21	0.41
8:k:52:MET:H	8:k:52:MET:HG3	1.65	0.41
1:F:418:PHE:HE2	1:F:517:ILE:HD11	1.86	0.41
2:H:46:MET:HE2	2:H:105:ILE:HD12	2.03	0.41
2:H:111:LEU:HD21	2:H:535:ALA:O	2.21	0.41
2:H:190:LEU:HA	2:H:191:PRO:HD3	1.88	0.41
2:H:209:VAL:HG11	2:H:398:GLU:HG3	2.03	0.41
2:H:388:GLY:HA3	2:H:394:LEU:HD21	2.03	0.41
2:H:390:THR:C	2:H:392:ASN:N	2.79	0.41
3:G:358:GLY:HA3	3:G:379:ARG:HH22	1.84	0.41
5:B:44:LYS:HD3	6:D:523:ASP:HB3	2.02	0.41
5:B:287:ARG:HH21	5:B:288:GLN:CD	2.29	0.41
6:D:383:ASN:O	6:D:384:ASN:C	2.64	0.41
6:D:409:GLY:C	6:D:501:VAL:HG23	2.45	0.41
7:A:25:ILE:HG21	7:A:542:ASP:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:145:VAL:HG12	8:C:406:VAL:HG12	2.02	0.41
8:C:502:PRO:HD2	8:C:505:ILE:HD12	2.02	0.41
2:P:85:LEU:HD22	2:P:534:ALA:HB1	2.01	0.41
3:O:7:THR:O	3:O:8:PRO:O	2.38	0.41
3:O:177:PHE:HE2	3:O:212:SER:HB2	1.85	0.41
3:O:414:GLY:O	3:O:417:GLU:HG2	2.21	0.41
5:J:127:ALA:HB2	5:J:430:VAL:HG13	2.03	0.41
5:J:276:ILE:O	5:J:279:PHE:HB2	2.21	0.41
6:L:124:PHE:O	6:L:127:ALA:HB3	2.21	0.41
7:I:228:VAL:HG12	7:I:233:MET:SD	2.60	0.41
8:K:248:CYS:HB2	8:K:249:PRO:HD2	2.03	0.41
8:K:296:ILE:HG12	8:K:317:LEU:HB2	2.02	0.41
1:f:162:VAL:HB	1:f:163:ASP:H	1.62	0.41
1:f:327:ARG:O	1:f:331:VAL:HG23	2.21	0.41
4:e:292:VAL:CG2	5:b:260:GLN:HB3	2.50	0.41
5:b:220:ASN:HB3	5:b:221:ASN:H	1.66	0.41
7:a:304:ASP:HA	7:a:307:LEU:HD12	2.03	0.41
1:n:178:VAL:HG21	1:n:402:VAL:HB	2.03	0.41
2:p:19:ASN:HB3	2:p:21:TYR:CE2	2.56	0.41
3:o:424:LEU:HD13	3:o:442:PHE:HD1	1.86	0.41
3:o:503:LYS:HD3	3:o:503:LYS:HA	1.87	0.41
5:j:84:GLN:HG2	5:j:91:GLY:O	2.21	0.41
7:i:26:ARG:CG	7:i:26:ARG:NH1	2.64	0.41
8:k:146:GLU:OE2	8:k:183:ARG:NH1	2.54	0.41
2:H:79:HIS:HD2	2:H:81:ALA:N	2.19	0.41
3:G:249:GLU:HG2	3:G:250:LEU:H	1.86	0.41
5:B:237:THR:O	5:B:238:LEU:HG	2.21	0.41
5:B:409:MET:CB	5:B:463:ILE:HD13	2.51	0.41
6:D:60:ASP:O	6:D:64:ILE:HG12	2.21	0.41
1:N:521:THR:O	1:N:525:SER:CB	2.68	0.41
3:O:368:CYS:HA	3:O:369:PRO:HD2	1.73	0.41
6:L:138:MET:SD	6:L:478:LEU:CD2	3.09	0.41
6:d:328:LEU:O	6:d:329:GLY:C	2.64	0.41
6:d:372:ARG:HA	6:d:373:PRO:HD3	1.94	0.41
5:j:34:LYS:HD2	5:j:443:ILE:HD13	2.03	0.41
5:j:406:CYS:O	5:j:410:VAL:HG23	2.20	0.41
5:j:443:ILE:HA	5:j:446:ASP:HB2	2.03	0.41
5:j:509:LEU:HD12	5:j:509:LEU:HA	1.93	0.41
8:k:70:VAL:HG11	8:k:75:ALA:HB3	2.03	0.41
1:F:395:VAL:O	1:F:399:LEU:HB2	2.21	0.40
2:H:426:THR:O	2:H:430:LEU:HG	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:107:GLU:O	3:G:107:GLU:HG3	2.21	0.40
3:G:349:CYS:HB2	3:G:366:GLN:O	2.22	0.40
3:G:503:LYS:HD3	3:G:503:LYS:HA	1.85	0.40
4:E:415:ILE:HG12	5:B:507:VAL:HG21	2.03	0.40
5:B:45:LEU:HD23	6:D:524:ILE:HG12	2.03	0.40
5:B:192:HIS:CD2	5:B:319:LEU:HD12	2.56	0.40
7:A:95:GLY:HA3	7:A:407:SER:OG	2.21	0.40
7:A:532:LEU:C	7:A:534:ALA:N	2.79	0.40
8:C:167:TRP:HE3	8:C:215:LEU:HD13	1.86	0.40
8:C:322:LYS:HE2	8:C:322:LYS:HB2	1.86	0.40
8:C:521:LEU:HD12	8:C:521:LEU:HA	1.92	0.40
1:N:28:GLY:O	1:N:32:VAL:HG23	2.22	0.40
1:N:509:SER:HB2	1:N:512:VAL:CG2	2.50	0.40
2:P:55:ILE:HG12	3:O:524:ILE:HD12	2.02	0.40
2:P:288:MET:HE2	2:P:288:MET:HA	2.03	0.40
3:O:86:ILE:HD12	3:O:513:ALA:HB2	2.03	0.40
4:M:232:GLY:H	5:J:87:GLU:HG3	1.86	0.40
6:L:443:PHE:CE1	6:L:447:LEU:HD11	2.56	0.40
1:f:87:THR:HG21	1:f:512:VAL:HA	2.02	0.40
1:f:107:ARG:CZ	1:n:107:ARG:HG3	2.51	0.40
1:f:203:SER:O	1:f:206:ASP:HB2	2.21	0.40
2:h:284:ILE:CD1	2:h:308:LEU:HB3	2.43	0.40
3:g:352:PHE:CD2	3:g:352:PHE:C	2.99	0.40
7:a:140:ILE:O	7:a:144:LEU:HG	2.21	0.40
7:a:301:GLY:HA2	7:a:320:ARG:HD2	2.01	0.40
2:p:428:ILE:HD11	2:p:478:LEU:HD21	2.03	0.40
3:o:147:ILE:CD1	3:o:409:ILE:HB	2.38	0.40
3:o:282:LEU:C	3:o:284:GLN:H	2.28	0.40
4:m:193:VAL:O	4:m:195:LYS:N	2.54	0.40
4:m:492:ILE:H	4:m:492:ILE:HG13	1.63	0.40
6:l:76:ARG:HH11	6:l:76:ARG:HG2	1.85	0.40
1:F:42:THR:HB	2:H:542:ASP:OD1	2.21	0.40
1:F:465:ASP:HA	1:F:466:PRO:HD3	1.78	0.40
2:H:31:SER:OG	2:H:81:ALA:HB3	2.20	0.40
3:G:266:ASP:O	3:G:270:ILE:HG12	2.21	0.40
4:E:144:ILE:CD1	4:E:550:LYS:HA	2.49	0.40
5:B:276:ILE:O	5:B:279:PHE:HB2	2.21	0.40
5:B:293:TYR:CB	5:B:294:PRO:CD	2.98	0.40
7:A:118:ASN:HB3	7:A:119:LYS:H	1.71	0.40
8:C:166:HIS:HB2	8:C:167:TRP:CD1	2.56	0.40
1:N:204:PRO:HB3	1:N:391:THR:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:240:SER:HA	2:P:245:HIS:CE1	2.56	0.40
2:P:394:LEU:HD23	2:P:397:ILE:HD11	2.03	0.40
4:M:32:VAL:HG12	4:M:35:GLN:HG3	2.04	0.40
4:M:104:LEU:HD23	4:M:107:LEU:HD12	2.03	0.40
4:M:125:LEU:HD22	4:M:129:LEU:HD13	2.03	0.40
4:M:353:HIS:HB3	4:M:403:THR:HG21	2.03	0.40
7:I:501:GLY:CA	7:I:512:GLU:HG2	2.51	0.40
2:h:79:HIS:HA	2:h:80:PRO:HD3	1.91	0.40
3:g:297:LEU:CB	3:g:298:PRO:HD2	2.40	0.40
3:g:352:PHE:CE1	3:g:365:PHE:CD2	3.10	0.40
4:e:522:MET:HA	4:e:522:MET:HE2	2.02	0.40
5:b:45:LEU:HD23	6:d:524:ILE:HG12	2.04	0.40
5:b:194:GLN:HB2	5:b:316:ARG:NH1	2.36	0.40
6:d:109:ARG:NH2	6:d:442:GLU:OE1	2.50	0.40
8:c:52:MET:HE3	8:c:52:MET:C	2.46	0.40
8:c:165:ILE:H	8:c:165:ILE:HG13	1.68	0.40
8:c:421:MET:HE2	8:c:472:ARG:HA	2.03	0.40
1:n:327:ARG:O	1:n:331:VAL:HG23	2.22	0.40
2:p:79:HIS:CE1	3:o:10:ILE:HD13	2.56	0.40
2:p:243:LYS:HA	2:p:245:HIS:CE1	2.56	0.40
3:o:83:LEU:HB3	3:o:102:THR:HG23	2.03	0.40
4:m:256:LYS:O	4:m:381:TYR:HA	2.21	0.40
7:i:184:LEU:C	7:i:186:ALA:H	2.29	0.40
8:k:174:LEU:HD22	8:k:219:VAL:HG23	2.03	0.40
1:F:142:ASN:O	1:F:145:ASN:ND2	2.54	0.40
3:G:362:TYR:CE1	3:G:377:LEU:HD21	2.56	0.40
5:B:29:VAL:HG13	5:B:64:LEU:HD21	2.03	0.40
5:B:245:ILE:H	5:B:245:ILE:HG13	1.59	0.40
2:P:203:ASN:HD22	2:P:203:ASN:HA	1.66	0.40
2:P:294:MET:SD	2:P:349:PRO:HG3	2.61	0.40
5:J:36:THR:HG23	5:J:58:ASN:OD1	2.22	0.40
5:J:46:LEU:HD21	5:J:63:ILE:HG23	2.03	0.40
1:f:253:TYR:CE1	1:f:259:ARG:CG	3.04	0.40
2:h:110:LEU:O	2:h:114:SER:HB2	2.20	0.40
2:h:254:LEU:HB2	2:h:305:VAL:HG22	2.03	0.40
3:g:264:VAL:HG23	4:e:294:GLU:OE2	2.21	0.40
5:b:237:THR:O	5:b:238:LEU:HG	2.22	0.40
6:d:323:PHE:CD1	6:d:323:PHE:C	2.99	0.40
1:n:162:VAL:HB	1:n:163:ASP:H	1.74	0.40
2:p:19:ASN:HB3	2:p:21:TYR:HE2	1.86	0.40
2:p:25:ASP:C	2:p:27:GLN:N	2.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:79:HIS:ND1	3:o:10:ILE:HB	2.36	0.40
3:o:352:PHE:HD1	3:o:365:PHE:HB3	1.86	0.40
4:m:98:ASN:HD21	4:m:100:ILE:HB	1.85	0.40
4:m:534:LYS:O	4:m:538:ILE:HD12	2.21	0.40
6:l:82:SER:OG	6:l:93:THR:HB	2.21	0.40
6:l:89:ALA:HA	6:l:403:CYS:SG	2.61	0.40
6:l:203:THR:HG23	7:i:533:GLU:CD	2.46	0.40
6:l:237:ILE:HD11	6:l:286:LEU:HD13	2.03	0.40
6:l:237:ILE:HG23	6:l:239:PHE:CE2	2.57	0.40
6:l:516:LYS:O	6:l:520:ARG:HG2	2.21	0.40
7:i:99:THR:HG22	7:i:103:ILE:HD11	2.03	0.40
1:F:19:LEU:O	1:F:23:VAL:HG23	2.21	0.40
1:F:56:THR:HG22	1:F:58:ASP:H	1.87	0.40
1:F:384:THR:HB	1:F:385:HIS:H	1.67	0.40
1:F:495:ILE:HG13	1:F:497:ASP:HB2	2.04	0.40
2:H:234:GLY:O	2:H:235:HIS:ND1	2.55	0.40
4:E:75:ILE:HD12	5:B:516:ARG:HG3	2.03	0.40
6:D:89:ALA:C	6:D:91:ASP:H	2.28	0.40
6:D:320:GLU:O	6:D:324:LEU:HB2	2.21	0.40
7:A:89:GLN:HA	7:A:92:ARG:HD3	2.02	0.40
8:C:318:ARG:O	8:C:319:ARG:C	2.64	0.40
1:N:326:GLU:HG2	8:K:232:PRO:HG3	2.02	0.40
3:O:139:LYS:O	3:O:143:LEU:HB2	2.22	0.40
3:O:388:GLU:O	3:O:392:SER:HB2	2.22	0.40
5:J:56:VAL:HG23	5:J:375:GLN:HG2	2.02	0.40
6:L:35:ILE:HD12	6:L:97:VAL:HG11	2.02	0.40
7:I:456:LEU:HD11	7:I:478:ARG:HH11	1.86	0.40
1:f:452:LEU:HD22	1:f:470:LEU:HD21	2.03	0.40
2:h:27:GLN:HE21	2:h:544:ILE:CD1	2.33	0.40
3:g:244:LEU:HD13	3:g:248:LEU:HD11	2.03	0.40
4:e:194:SER:HA	4:e:197:HIS:HB3	2.02	0.40
4:e:412:ASN:OD1	4:e:415:ILE:HG13	2.21	0.40
5:b:327:SER:O	5:b:329:PHE:N	2.54	0.40
6:d:30:SER:OG	7:a:11:ASP:HB3	2.21	0.40
6:d:47:MET:HE3	7:a:544:MET:SD	2.61	0.40
6:d:68:MET:HE2	7:a:545:ILE:HD13	2.04	0.40
6:d:499:GLN:HA	6:d:500:PRO:HD3	1.93	0.40
1:n:457:THR:HG22	1:n:460:LYS:HD2	2.03	0.40
3:o:94:VAL:CG1	3:o:502:VAL:HG22	2.50	0.40
4:m:151:ASP:OD2	4:m:546:ARG:HD3	2.21	0.40
5:j:127:ALA:HB2	5:j:430:VAL:HG13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:j:152:ASP:O	5:j:156:ILE:HG12	2.22	0.40
5:j:293:TYR:HB3	5:j:294:PRO:HD3	2.04	0.40
6:l:196:LEU:HD22	6:l:394:LEU:HD13	2.03	0.40
7:i:56:ASP:OD1	7:i:56:ASP:C	2.64	0.40
7:i:337:LEU:HD23	7:i:337:LEU:HA	1.94	0.40
8:k:35:ILE:CG2	8:k:94:THR:HG23	2.50	0.40
1:F:532:GLU:O	1:F:533:LEU:HD23	2.21	0.40
2:H:240:SER:HA	2:H:245:HIS:CE1	2.57	0.40
3:G:335:GLN:HG3	3:G:341:ILE:HG12	2.04	0.40
4:E:72:LYS:HD2	4:E:72:LYS:N	2.37	0.40
4:E:244:ILE:HG22	4:E:392:MET:HE2	2.04	0.40
4:E:457:GLU:O	4:E:461:GLN:HG2	2.22	0.40
5:B:14:ARG:HG2	5:B:15:ALA:N	2.37	0.40
6:D:20:VAL:O	6:D:21:ARG:C	2.64	0.40
6:D:257:TYR:HB3	7:A:272:GLN:HB3	2.03	0.40
6:D:416:ALA:HB3	6:D:417:PRO:HD3	2.03	0.40
6:D:486:ARG:O	6:D:487:SER:HB3	2.21	0.40
7:A:269:GLN:HA	7:A:272:GLN:HB2	2.04	0.40
8:C:224:LEU:HD11	8:C:365:PHE:HB3	2.02	0.40
2:P:215:GLY:H	3:O:505:ASN:HD21	1.68	0.40
3:O:125:ILE:O	3:O:438:ILE:HG21	2.21	0.40
7:I:109:LEU:HG	7:I:535:CYS:HB2	2.03	0.40
7:I:477:LEU:HD11	7:I:502:LEU:HD13	2.04	0.40
2:h:108:GLY:O	2:h:112:ASN:HB2	2.22	0.40
2:h:236:VAL:HA	2:h:319:LEU:HD13	2.02	0.40
2:h:238:SER:C	2:h:240:SER:N	2.79	0.40
3:g:243:SER:HB3	3:g:323:MET:HE1	2.03	0.40
4:e:363:VAL:HG21	4:e:369:LEU:HD12	2.03	0.40
4:e:423:LEU:O	4:e:427:LEU:N	2.41	0.40
5:b:461:SER:O	5:b:465:ASN:HB2	2.22	0.40
7:a:12:THR:CB	7:a:14:PHE:HE2	2.33	0.40
7:a:390:ALA:HA	8:c:512:THR:HG22	2.03	0.40
1:n:114:HIS:O	1:n:117:ILE:HB	2.22	0.40
1:n:173:ILE:HG23	1:n:209:PHE:HB2	2.02	0.40
2:p:180:GLU:O	2:p:184:GLU:HB2	2.22	0.40
3:o:292:ILE:HD13	3:o:352:PHE:CD1	2.57	0.40
5:j:15:ALA:HB1	5:j:19:ARG:HH12	1.86	0.40
5:j:351:GLN:HA	5:j:352:PRO:HD3	1.86	0.40
8:k:481:THR:HB	8:k:493:ASP:OD1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	536/546 (98%)	477 (89%)	56 (10%)	3 (1%)	21	54
1	N	536/546 (98%)	483 (90%)	51 (10%)	2 (0%)	30	62
1	f	536/546 (98%)	484 (90%)	49 (9%)	3 (1%)	21	54
1	n	536/546 (98%)	486 (91%)	48 (9%)	2 (0%)	30	62
2	H	513/568 (90%)	445 (87%)	57 (11%)	11 (2%)	5	31
2	P	513/568 (90%)	458 (89%)	47 (9%)	8 (2%)	7	35
2	h	513/568 (90%)	460 (90%)	46 (9%)	7 (1%)	9	37
2	p	513/568 (90%)	450 (88%)	53 (10%)	10 (2%)	6	32
3	G	524/550 (95%)	467 (89%)	48 (9%)	9 (2%)	7	34
3	O	524/550 (95%)	479 (91%)	36 (7%)	9 (2%)	7	34
3	g	524/550 (95%)	477 (91%)	38 (7%)	9 (2%)	7	34
3	o	524/550 (95%)	472 (90%)	41 (8%)	11 (2%)	5	31
4	E	533/562 (95%)	482 (90%)	45 (8%)	6 (1%)	11	41
4	M	533/562 (95%)	494 (93%)	31 (6%)	8 (2%)	8	36
4	e	533/562 (95%)	500 (94%)	27 (5%)	6 (1%)	11	41
4	m	533/562 (95%)	492 (92%)	33 (6%)	8 (2%)	8	36
5	B	516/527 (98%)	452 (88%)	48 (9%)	16 (3%)	3	25
5	J	516/527 (98%)	460 (89%)	42 (8%)	14 (3%)	4	27
5	b	516/527 (98%)	461 (89%)	41 (8%)	14 (3%)	4	27
5	j	516/527 (98%)	459 (89%)	47 (9%)	10 (2%)	6	32
6	D	521/528 (99%)	457 (88%)	46 (9%)	18 (4%)	3	23
6	L	521/528 (99%)	474 (91%)	33 (6%)	14 (3%)	4	27
6	d	521/528 (99%)	473 (91%)	34 (6%)	14 (3%)	4	27
6	l	521/528 (99%)	469 (90%)	41 (8%)	11 (2%)	5	31
7	A	533/559 (95%)	470 (88%)	50 (9%)	13 (2%)	4	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	I	533/559 (95%)	483 (91%)	36 (7%)	14 (3%)	4	27
7	a	533/559 (95%)	482 (90%)	43 (8%)	8 (2%)	8	36
7	i	533/559 (95%)	484 (91%)	37 (7%)	12 (2%)	5	30
8	C	507/590 (86%)	445 (88%)	54 (11%)	8 (2%)	7	35
8	K	507/590 (86%)	454 (90%)	43 (8%)	10 (2%)	6	32
8	c	507/590 (86%)	456 (90%)	44 (9%)	7 (1%)	9	37
8	k	507/590 (86%)	448 (88%)	50 (10%)	9 (2%)	6	33
All	All	16732/17720 (94%)	15033 (90%)	1395 (8%)	304 (2%)	6	33

All (304) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	323	VAL
2	H	442	PRO
2	H	502	ASP
3	G	8	PRO
4	E	389	LYS
5	B	15	ALA
5	B	163	SER
5	B	220	ASN
5	B	255	THR
6	D	159	SER
6	D	160	SER
6	D	368	ASN
7	A	257	ALA
8	C	163	TYR
8	C	239	GLU
2	P	323	VAL
2	P	442	PRO
2	P	502	ASP
3	O	8	PRO
4	M	190	SER
4	M	389	LYS
5	J	15	ALA
5	J	163	SER
5	J	220	ASN
5	J	255	THR
5	J	328	THR
6	L	160	SER
6	L	182	SER

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Mol	Chain	Res	Type
6	L	368	ASN
7	I	257	ALA
8	K	163	TYR
2	h	323	VAL
2	h	442	PRO
2	h	502	ASP
3	g	8	PRO
4	e	389	LYS
5	b	15	ALA
5	b	163	SER
5	b	220	ASN
5	b	255	THR
5	b	328	THR
6	d	368	ASN
8	c	163	TYR
2	p	323	VAL
2	p	442	PRO
2	p	502	ASP
3	o	8	PRO
4	m	190	SER
4	m	389	LYS
5	j	15	ALA
5	j	163	SER
5	j	220	ASN
5	j	255	THR
5	j	328	THR
6	l	282	LYS
6	l	368	ASN
8	k	163	TYR
2	H	26	GLY
3	G	151	LYS
3	G	168	SER
3	G	381	GLY
3	G	432	ALA
4	E	189	GLY
4	E	190	SER
4	E	194	SER
5	B	246	PHE
5	B	328	THR
5	B	451	ASP
6	D	183	ASP
6	D	189	VAL

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Mol	Chain	Res	Type
6	D	282	LYS
6	D	296	ALA
7	A	56	ASP
7	A	65	ASP
7	A	200	VAL
7	A	201	LYS
7	A	256	MET
8	C	60	ASP
8	C	319	ARG
8	C	361	GLY
3	O	151	LYS
3	O	168	SER
3	O	432	ALA
4	M	345	TRP
6	L	186	SER
6	L	296	ALA
7	I	56	ASP
7	I	65	ASP
7	I	256	MET
7	I	367	SER
7	I	369	ASP
8	K	160	GLY
8	K	166	HIS
8	K	319	ARG
8	K	361	GLY
3	g	168	SER
3	g	381	GLY
4	e	189	GLY
4	e	190	SER
5	b	59	ASP
5	b	145	ASP
5	b	246	PHE
6	d	182	SER
6	d	189	VAL
7	a	56	ASP
7	a	65	ASP
7	a	256	MET
7	a	257	ALA
8	c	160	GLY
8	c	239	GLU
3	o	168	SER
3	o	381	GLY

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Mol	Chain	Res	Type
4	m	194	SER
5	j	247	GLY
6	l	160	SER
6	l	182	SER
6	l	189	VAL
6	l	296	ALA
7	i	56	ASP
7	i	201	LYS
7	i	256	MET
7	i	257	ALA
8	k	160	GLY
1	F	437	LYS
2	H	7	GLN
2	H	303	ALA
4	E	268	LYS
5	B	219	GLY
5	B	350	GLU
6	D	182	SER
6	D	186	SER
6	D	187	LYS
6	D	337	GLU
7	A	369	ASP
1	N	202	LEU
1	N	436	ALA
3	O	190	ASP
3	O	381	GLY
4	M	364	PRO
5	J	143	SER
5	J	310	ASP
5	J	451	ASP
6	L	159	SER
6	L	189	VAL
6	L	282	LYS
6	L	293	LEU
6	L	315	ASP
7	I	549	PRO
1	f	437	LYS
2	h	23	ASN
3	g	151	LYS
3	g	227	ALA
5	b	162	SER
5	b	451	ASP

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Mol	Chain	Res	Type
6	d	160	SER
6	d	186	SER
6	d	433	GLU
8	c	319	ARG
8	c	361	GLY
2	p	7	GLN
2	p	23	ASN
3	o	190	ASP
3	o	432	ALA
4	m	189	GLY
4	m	437	SER
5	j	59	ASP
6	l	187	LYS
6	l	249	GLU
7	i	65	ASP
7	i	118	ASN
7	i	367	SER
7	i	390	ALA
7	i	549	PRO
8	k	60	ASP
8	k	221	LYS
8	k	239	GLU
8	k	319	ARG
8	k	361	GLY
1	F	163	ASP
2	H	41	MET
2	H	96	MET
3	G	369	PRO
5	B	59	ASP
5	B	133	ASP
5	B	143	SER
6	D	293	LEU
6	D	329	GLY
7	A	118	ASN
7	A	367	SER
8	C	160	GLY
2	P	23	ASN
3	O	171	ILE
4	M	189	GLY
5	J	59	ASP
5	J	247	GLY
5	J	423	ASP

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Mol	Chain	Res	Type
6	L	183	ASP
7	I	340	SER
7	I	390	ALA
7	I	467	ALA
1	f	202	LEU
2	h	7	GLN
2	h	148	GLY
3	g	190	ASP
3	g	432	ALA
4	e	194	SER
4	e	345	TRP
5	b	143	SER
6	d	159	SER
6	d	162	ILE
6	d	187	LYS
6	d	296	ALA
6	d	479	ASN
7	a	369	ASP
8	c	60	ASP
8	c	511	LYS
1	n	201	HIS
2	p	148	GLY
4	m	202	GLU
4	m	268	LYS
6	l	186	SER
7	i	267	PRO
7	i	369	ASP
8	k	80	GLU
1	F	373	PRO
2	H	418	LYS
3	G	251	LYS
4	E	437	SER
5	B	312	GLU
6	D	162	ILE
6	D	315	ASP
8	C	41	PRO
8	C	80	GLU
2	P	7	GLN
2	P	470	ASP
4	M	194	SER
4	M	268	LYS
4	M	462	ARG

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Mol	Chain	Res	Type
5	J	350	GLU
6	L	249	GLU
7	I	118	ASN
4	e	268	LYS
5	b	241	ASP
5	b	350	GLU
6	d	294	ARG
7	a	267	PRO
2	p	153	LYS
3	o	151	LYS
3	o	249	GLU
5	j	145	ASP
5	j	312	GLU
3	G	171	ILE
3	G	190	ASP
5	B	241	ASP
5	B	470	SER
6	D	243	PRO
7	A	489	PRO
5	J	241	ASP
8	K	41	PRO
8	K	108	ALA
8	K	207	GLU
8	K	435	GLU
3	g	343	PRO
5	b	247	GLY
7	a	118	ASN
7	a	489	PRO
1	n	437	LYS
2	p	418	LYS
3	o	343	PRO
5	j	241	ASP
6	l	159	SER
8	k	435	GLU
7	A	267	PRO
7	A	549	PRO
2	P	26	GLY
5	J	39	PRO
6	L	373	PRO
3	g	369	PRO
7	i	489	PRO
6	D	373	PRO

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Mol	Chain	Res	Type
3	O	369	PRO
6	L	365	GLY
1	f	162	VAL
3	o	431	ILE
2	H	324	PRO
5	B	247	GLY
7	A	22	GLY
7	I	489	PRO
2	h	17	GLY
6	d	329	GLY
3	o	239	PRO
2	H	441	THR
6	D	242	SER
2	P	234	GLY
3	O	343	PRO
7	I	200	VAL
7	I	267	PRO
8	K	384	GLY
2	p	17	GLY
2	p	441	THR
3	o	369	PRO
6	l	353	ILE
6	d	243	PRO
4	m	192	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	380/463 (82%)	337 (89%)	43 (11%)	5	23
1	N	380/463 (82%)	348 (92%)	32 (8%)	10	34
1	f	380/463 (82%)	355 (93%)	25 (7%)	15	41
1	n	380/463 (82%)	348 (92%)	32 (8%)	10	34
2	H	352/473 (74%)	306 (87%)	46 (13%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	352/473 (74%)	315 (90%)	37 (10%)	6	26
2	h	352/473 (74%)	312 (89%)	40 (11%)	5	23
2	p	352/473 (74%)	307 (87%)	45 (13%)	4	21
3	G	373/454 (82%)	323 (87%)	50 (13%)	4	19
3	O	373/454 (82%)	333 (89%)	40 (11%)	6	25
3	g	373/454 (82%)	330 (88%)	43 (12%)	5	23
3	o	373/454 (82%)	333 (89%)	40 (11%)	6	25
4	E	382/483 (79%)	328 (86%)	54 (14%)	3	18
4	M	382/483 (79%)	340 (89%)	42 (11%)	6	24
4	e	382/483 (79%)	332 (87%)	50 (13%)	4	20
4	m	382/483 (79%)	339 (89%)	43 (11%)	5	23
5	B	374/441 (85%)	316 (84%)	58 (16%)	2	15
5	J	374/441 (85%)	338 (90%)	36 (10%)	8	29
5	b	374/441 (85%)	330 (88%)	44 (12%)	5	22
5	j	374/441 (85%)	334 (89%)	40 (11%)	6	25
6	D	374/454 (82%)	332 (89%)	42 (11%)	6	24
6	L	374/454 (82%)	341 (91%)	33 (9%)	9	33
6	d	374/454 (82%)	340 (91%)	34 (9%)	9	32
6	l	374/454 (82%)	335 (90%)	39 (10%)	7	26
7	A	375/471 (80%)	324 (86%)	51 (14%)	3	18
7	I	375/471 (80%)	335 (89%)	40 (11%)	6	25
7	a	375/471 (80%)	345 (92%)	30 (8%)	11	36
7	i	375/471 (80%)	341 (91%)	34 (9%)	9	32
8	C	359/497 (72%)	308 (86%)	51 (14%)	3	17
8	K	359/497 (72%)	314 (88%)	45 (12%)	4	21
8	c	359/497 (72%)	315 (88%)	44 (12%)	4	21
8	k	359/497 (72%)	313 (87%)	46 (13%)	4	21
All	All	11876/14944 (80%)	10547 (89%)	1329 (11%)	6	24

All (1329) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	16	ASP

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Mol	Chain	Res	Type
1	F	19	LEU
1	F	24	THR
1	F	30	GLN
1	F	32	VAL
1	F	35	THR
1	F	44	LYS
1	F	56	THR
1	F	62	LEU
1	F	64	THR
1	F	72	THR
1	F	92	THR
1	F	103	ARG
1	F	124	ILE
1	F	162	VAL
1	F	165	ASP
1	F	181	VAL
1	F	187	ASP
1	F	198	GLN
1	F	206	ASP
1	F	210	ILE
1	F	217	HIS
1	F	237	ASN
1	F	239	SER
1	F	247	VAL
1	F	251	PHE
1	F	278	ILE
1	F	324	ASN
1	F	340	VAL
1	F	347	ILE
1	F	368	THR
1	F	370	ASN
1	F	377	THR
1	F	379	LEU
1	F	390	GLN
1	F	399	LEU
1	F	408	ASP
1	F	453	VAL
1	F	479	ASP
1	F	497	ASP
1	F	511	ARG
1	F	523	ILE
1	F	535	ARG

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Mol	Chain	Res	Type
2	H	25	ASP
2	H	31	SER
2	H	32	ILE
2	H	41	MET
2	H	43	LEU
2	H	62	ILE
2	H	63	ILE
2	H	91	GLN
2	H	92	GLN
2	H	98	ASP
2	H	101	ASN
2	H	102	LEU
2	H	105	ILE
2	H	110	LEU
2	H	145	MET
2	H	169	SER
2	H	204	VAL
2	H	206	SER
2	H	221	THR
2	H	223	ILE
2	H	227	VAL
2	H	245	HIS
2	H	247	VAL
2	H	249	VAL
2	H	256	ILE
2	H	258	ASN
2	H	287	MET
2	H	291	ILE
2	H	320	VAL
2	H	341	LEU
2	H	344	LEU
2	H	348	THR
2	H	354	LEU
2	H	357	THR
2	H	358	VAL
2	H	381	THR
2	H	383	THR
2	H	401	ILE
2	H	409	LYS
2	H	428	ILE
2	H	432	SER
2	H	441	THR

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Mol	Chain	Res	Type
2	H	470	ASP
2	H	502	ASP
2	H	519	ASP
2	H	539	LEU
3	G	10	ILE
3	G	11	VAL
3	G	13	LEU
3	G	20	SER
3	G	30	ILE
3	G	37	GLN
3	G	43	THR
3	G	57	ASN
3	G	61	THR
3	G	81	LYS
3	G	88	ARG
3	G	96	ASP
3	G	102	THR
3	G	104	LEU
3	G	108	LEU
3	G	122	SER
3	G	155	ARG
3	G	166	MET
3	G	170	LEU
3	G	187	LEU
3	G	194	LEU
3	G	195	ASP
3	G	196	ASP
3	G	197	LYS
3	G	201	ILE
3	G	218	VAL
3	G	261	VAL
3	G	268	GLN
3	G	272	ASP
3	G	277	LEU
3	G	282	LEU
3	G	284	GLN
3	G	291	ASN
3	G	330	VAL
3	G	338	THR
3	G	365	PHE
3	G	373	THR
3	G	377	LEU

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Mol	Chain	Res	Type
3	G	398	MET
3	G	399	ILE
3	G	409	ILE
3	G	410	VAL
3	G	417	GLU
3	G	440	ASN
3	G	462	ILE
3	G	472	HIS
3	G	485	THR
3	G	488	ILE
3	G	508	ASN
3	G	511	THR
4	E	29	PHE
4	E	30	ILE
4	E	37	ASN
4	E	44	LEU
4	E	59	SER
4	E	68	ARG
4	E	73	ILE
4	E	74	LEU
4	E	75	ILE
4	E	82	THR
4	E	90	ILE
4	E	98	ASN
4	E	107	LEU
4	E	111	GLN
4	E	120	THR
4	E	125	LEU
4	E	160	LYS
4	E	166	ASP
4	E	168	ILE
4	E	206	GLU
4	E	230	VAL
4	E	240	ILE
4	E	283	THR
4	E	294	GLU
4	E	300	THR
4	E	329	ASP
4	E	335	LEU
4	E	336	LEU
4	E	381	TYR
4	E	385	PHE

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Mol	Chain	Res	Type
4	E	387	THR
4	E	388	THR
4	E	404	VAL
4	E	406	CYS
4	E	408	VAL
4	E	412	ASN
4	E	414	MET
4	E	416	VAL
4	E	427	LEU
4	E	429	VAL
4	E	431	ARG
4	E	436	ASP
4	E	440	VAL
4	E	455	SER
4	E	459	ASP
4	E	464	ILE
4	E	479	ILE
4	E	487	SER
4	E	492	ILE
4	E	498	LEU
4	E	519	SER
4	E	532	ILE
4	E	544	LEU
4	E	552	ASP
5	B	11	THR
5	B	29	VAL
5	B	48	SER
5	B	57	THR
5	B	62	THR
5	B	80	ILE
5	B	88	VAL
5	B	93	THR
5	B	97	VAL
5	B	99	SER
5	B	104	ARG
5	B	115	ILE
5	B	119	THR
5	B	124	TYR
5	B	132	LEU
5	B	135	LEU
5	B	141	ASP
5	B	147	THR

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Mol	Chain	Res	Type
5	B	156	ILE
5	B	160	THR
5	B	167	SER
5	B	181	ILE
5	B	195	ILE
5	B	199	LEU
5	B	214	LEU
5	B	226	ILE
5	B	237	THR
5	B	240	THR
5	B	241	ASP
5	B	245	ILE
5	B	246	PHE
5	B	290	ILE
5	B	308	HIS
5	B	314	VAL
5	B	316	ARG
5	B	319	LEU
5	B	321	THR
5	B	341	ASP
5	B	354	LEU
5	B	373	THR
5	B	375	GLN
5	B	376	THR
5	B	390	VAL
5	B	397	GLU
5	B	402	LEU
5	B	408	GLU
5	B	416	ASP
5	B	423	ASP
5	B	440	LEU
5	B	452	SER
5	B	455	LEU
5	B	457	SER
5	B	459	LEU
5	B	469	THR
5	B	474	LEU
5	B	476	ASN
5	B	479	ILE
5	B	509	LEU
6	D	36	ARG
6	D	103	LEU

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Mol	Chain	Res	Type
6	D	123	SER
6	D	124	PHE
6	D	136	LEU
6	D	140	HIS
6	D	151	VAL
6	D	169	PHE
6	D	170	LEU
6	D	177	SER
6	D	181	ILE
6	D	198	LYS
6	D	209	MET
6	D	215	LEU
6	D	218	THR
6	D	248	THR
6	D	251	ASN
6	D	255	ASN
6	D	264	LEU
6	D	305	LEU
6	D	312	VAL
6	D	324	LEU
6	D	336	ILE
6	D	340	THR
6	D	349	LEU
6	D	364	THR
6	D	366	ILE
6	D	383	ASN
6	D	385	MET
6	D	399	CYS
6	D	411	ILE
6	D	440	TRP
6	D	463	ILE
6	D	467	THR
6	D	478	LEU
6	D	482	ILE
6	D	484	VAL
6	D	486	ARG
6	D	502	LEU
6	D	505	THR
6	D	520	ARG
6	D	522	ASP
7	A	26	ARG
7	A	36	VAL

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Mol	Chain	Res	Type
7	A	47	VAL
7	A	49	LEU
7	A	56	ASP
7	A	61	THR
7	A	68	THR
7	A	69	ILE
7	A	72	LEU
7	A	75	VAL
7	A	86	LEU
7	A	88	GLN
7	A	89	GLN
7	A	90	GLN
7	A	109	LEU
7	A	116	VAL
7	A	126	ILE
7	A	164	MET
7	A	177	SER
7	A	179	MET
7	A	200	VAL
7	A	212	SER
7	A	224	LEU
7	A	228	VAL
7	A	237	ILE
7	A	247	LEU
7	A	260	VAL
7	A	281	VAL
7	A	299	THR
7	A	316	MET
7	A	321	CYS
7	A	326	LEU
7	A	328	ARG
7	A	337	LEU
7	A	373	LEU
7	A	377	THR
7	A	396	ASP
7	A	397	GLU
7	A	415	SER
7	A	419	VAL
7	A	424	CYS
7	A	426	GLU
7	A	439	THR
7	A	442	SER

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Mol	Chain	Res	Type
7	A	456	LEU
7	A	457	ILE
7	A	512	GLU
7	A	524	LYS
7	A	542	ASP
7	A	543	THR
7	A	546	THR
8	C	23	SER
8	C	31	VAL
8	C	34	VAL
8	C	52	MET
8	C	55	LEU
8	C	58	THR
8	C	78	MET
8	C	79	LEU
8	C	81	LEU
8	C	89	VAL
8	C	95	THR
8	C	102	GLU
8	C	107	CYS
8	C	130	THR
8	C	138	GLN
8	C	143	VAL
8	C	151	MET
8	C	167	TRP
8	C	204	VAL
8	C	206	VAL
8	C	215	LEU
8	C	251	GLU
8	C	257	SER
8	C	260	ASN
8	C	290	VAL
8	C	293	THR
8	C	309	LEU
8	C	322	LYS
8	C	325	ASN
8	C	335	THR
8	C	336	ILE
8	C	346	SER
8	C	348	VAL
8	C	350	THR
8	C	354	LEU

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Mol	Chain	Res	Type
8	C	387	ASP
8	C	396	LEU
8	C	398	ASP
8	C	404	ARG
8	C	420	GLU
8	C	437	ILE
8	C	452	ILE
8	C	455	THR
8	C	465	ILE
8	C	468	LEU
8	C	481	THR
8	C	484	ILE
8	C	503	GLU
8	C	504	VAL
8	C	521	LEU
8	C	528	SER
1	N	3	LEU
1	N	19	LEU
1	N	30	GLN
1	N	35	THR
1	N	55	LEU
1	N	56	THR
1	N	61	VAL
1	N	62	LEU
1	N	72	THR
1	N	74	VAL
1	N	75	LEU
1	N	107	ARG
1	N	119	THR
1	N	124	ILE
1	N	138	ILE
1	N	162	VAL
1	N	181	VAL
1	N	213	LEU
1	N	217	HIS
1	N	237	ASN
1	N	251	PHE
1	N	318	ARG
1	N	324	ASN
1	N	368	THR
1	N	379	LEU
1	N	390	GLN

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Mol	Chain	Res	Type
1	N	399	LEU
1	N	408	ASP
1	N	442	THR
1	N	453	VAL
1	N	497	ASP
1	N	499	CYS
2	P	32	ILE
2	P	41	MET
2	P	42	CYS
2	P	43	LEU
2	P	62	ILE
2	P	65	THR
2	P	91	GLN
2	P	92	GLN
2	P	105	ILE
2	P	110	LEU
2	P	145	MET
2	P	147	VAL
2	P	203	ASN
2	P	221	THR
2	P	223	ILE
2	P	245	HIS
2	P	247	VAL
2	P	256	ILE
2	P	260	GLU
2	P	341	LEU
2	P	344	LEU
2	P	348	THR
2	P	354	LEU
2	P	357	THR
2	P	358	VAL
2	P	369	THR
2	P	383	THR
2	P	392	ASN
2	P	401	ILE
2	P	409	LYS
2	P	441	THR
2	P	445	LEU
2	P	470	ASP
2	P	502	ASP
2	P	519	ASP
2	P	539	LEU

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Mol	Chain	Res	Type
2	P	544	ILE
3	O	3	PHE
3	O	10	ILE
3	O	11	VAL
3	O	30	ILE
3	O	37	GLN
3	O	43	THR
3	O	50	ASP
3	O	57	ASN
3	O	86	ILE
3	O	96	ASP
3	O	98	THR
3	O	102	THR
3	O	104	LEU
3	O	147	ILE
3	O	155	ARG
3	O	166	MET
3	O	194	LEU
3	O	196	ASP
3	O	268	GLN
3	O	277	LEU
3	O	282	LEU
3	O	284	GLN
3	O	330	VAL
3	O	373	THR
3	O	377	LEU
3	O	398	MET
3	O	399	ILE
3	O	409	ILE
3	O	410	VAL
3	O	417	GLU
3	O	430	THR
3	O	440	ASN
3	O	468	LEU
3	O	472	HIS
3	O	485	THR
3	O	488	ILE
3	O	503	LYS
3	O	508	ASN
3	O	518	LEU
3	O	525	THR
4	M	25	MET

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Mol	Chain	Res	Type
4	M	29	PHE
4	M	30	ILE
4	M	37	ASN
4	M	44	LEU
4	M	73	ILE
4	M	74	LEU
4	M	82	THR
4	M	92	SER
4	M	107	LEU
4	M	111	GLN
4	M	125	LEU
4	M	129	LEU
4	M	166	ASP
4	M	168	ILE
4	M	193	VAL
4	M	206	GLU
4	M	224	ILE
4	M	230	VAL
4	M	283	THR
4	M	294	GLU
4	M	336	LEU
4	M	378	SER
4	M	385	PHE
4	M	387	THR
4	M	388	THR
4	M	406	CYS
4	M	408	VAL
4	M	412	ASN
4	M	414	MET
4	M	427	LEU
4	M	431	ARG
4	M	436	ASP
4	M	440	VAL
4	M	459	ASP
4	M	464	ILE
4	M	487	SER
4	M	492	ILE
4	M	495	LEU
4	M	498	LEU
4	M	532	ILE
4	M	552	ASP
5	J	21	SER

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Mol	Chain	Res	Type
5	J	29	VAL
5	J	57	THR
5	J	80	ILE
5	J	93	THR
5	J	104	ARG
5	J	119	THR
5	J	124	TYR
5	J	132	LEU
5	J	135	LEU
5	J	141	ASP
5	J	147	THR
5	J	195	ILE
5	J	199	LEU
5	J	214	LEU
5	J	226	ILE
5	J	237	THR
5	J	240	THR
5	J	246	PHE
5	J	283	THR
5	J	308	HIS
5	J	316	ARG
5	J	319	LEU
5	J	321	THR
5	J	341	ASP
5	J	354	LEU
5	J	390	VAL
5	J	397	GLU
5	J	408	GLU
5	J	423	ASP
5	J	427	SER
5	J	452	SER
5	J	455	LEU
5	J	459	LEU
5	J	474	LEU
5	J	509	LEU
6	L	36	ARG
6	L	63	THR
6	L	124	PHE
6	L	140	HIS
6	L	162	ILE
6	L	169	PHE
6	L	170	LEU

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Mol	Chain	Res	Type
6	L	181	ILE
6	L	194	ILE
6	L	197	VAL
6	L	198	LYS
6	L	209	MET
6	L	216	THR
6	L	218	THR
6	L	248	THR
6	L	251	ASN
6	L	288	ILE
6	L	305	LEU
6	L	312	VAL
6	L	336	ILE
6	L	340	THR
6	L	364	THR
6	L	366	ILE
6	L	411	ILE
6	L	440	TRP
6	L	449	VAL
6	L	463	ILE
6	L	467	THR
6	L	482	ILE
6	L	486	ARG
6	L	502	LEU
6	L	513	GLU
6	L	520	ARG
7	I	6	ASN
7	I	26	ARG
7	I	36	VAL
7	I	47	VAL
7	I	51	LYS
7	I	56	ASP
7	I	61	THR
7	I	63	THR
7	I	68	THR
7	I	86	LEU
7	I	88	GLN
7	I	89	GLN
7	I	90	GLN
7	I	100	SER
7	I	116	VAL
7	I	172	ASP

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Mol	Chain	Res	Type
7	I	177	SER
7	I	185	LEU
7	I	200	VAL
7	I	224	LEU
7	I	228	VAL
7	I	260	VAL
7	I	281	VAL
7	I	299	THR
7	I	316	MET
7	I	328	ARG
7	I	337	LEU
7	I	373	LEU
7	I	377	THR
7	I	396	ASP
7	I	419	VAL
7	I	426	GLU
7	I	439	THR
7	I	442	SER
7	I	456	LEU
7	I	457	ILE
7	I	471	SER
7	I	524	LYS
7	I	542	ASP
7	I	543	THR
8	K	23	SER
8	K	34	VAL
8	K	38	CYS
8	K	52	MET
8	K	58	THR
8	K	78	MET
8	K	79	LEU
8	K	81	LEU
8	K	89	VAL
8	K	95	THR
8	K	107	CYS
8	K	130	THR
8	K	138	GLN
8	K	143	VAL
8	K	148	ASP
8	K	154	LEU
8	K	167	TRP
8	K	204	VAL

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Mol	Chain	Res	Type
8	K	206	VAL
8	K	215	LEU
8	K	251	GLU
8	K	257	SER
8	K	260	ASN
8	K	290	VAL
8	K	293	THR
8	K	297	THR
8	K	309	LEU
8	K	310	LEU
8	K	322	LYS
8	K	325	ASN
8	K	335	THR
8	K	336	ILE
8	K	348	VAL
8	K	354	LEU
8	K	380	MET
8	K	396	LEU
8	K	398	ASP
8	K	420	GLU
8	K	465	ILE
8	K	468	LEU
8	K	481	THR
8	K	504	VAL
8	K	509	SER
8	K	521	LEU
8	K	528	SER
1	f	3	LEU
1	f	19	LEU
1	f	30	GLN
1	f	35	THR
1	f	55	LEU
1	f	56	THR
1	f	72	THR
1	f	75	LEU
1	f	96	CYS
1	f	107	ARG
1	f	124	ILE
1	f	162	VAL
1	f	187	ASP
1	f	198	GLN
1	f	217	HIS

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Mol	Chain	Res	Type
1	f	237	ASN
1	f	251	PHE
1	f	368	THR
1	f	379	LEU
1	f	390	GLN
1	f	399	LEU
1	f	453	VAL
1	f	497	ASP
1	f	499	CYS
1	f	523	ILE
2	h	32	ILE
2	h	41	MET
2	h	42	CYS
2	h	43	LEU
2	h	62	ILE
2	h	65	THR
2	h	91	GLN
2	h	98	ASP
2	h	102	LEU
2	h	105	ILE
2	h	145	MET
2	h	147	VAL
2	h	221	THR
2	h	223	ILE
2	h	227	VAL
2	h	245	HIS
2	h	247	VAL
2	h	256	ILE
2	h	258	ASN
2	h	264	THR
2	h	277	SER
2	h	333	CYS
2	h	341	LEU
2	h	344	LEU
2	h	348	THR
2	h	354	LEU
2	h	357	THR
2	h	358	VAL
2	h	370	VAL
2	h	381	THR
2	h	383	THR
2	h	401	ILE

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Mol	Chain	Res	Type
2	h	409	LYS
2	h	427	GLU
2	h	432	SER
2	h	441	THR
2	h	501	ILE
2	h	502	ASP
2	h	539	LEU
2	h	544	ILE
3	g	3	PHE
3	g	10	ILE
3	g	11	VAL
3	g	30	ILE
3	g	37	GLN
3	g	43	THR
3	g	55	THR
3	g	61	THR
3	g	86	ILE
3	g	88	ARG
3	g	96	ASP
3	g	104	LEU
3	g	147	ILE
3	g	155	ARG
3	g	158	LEU
3	g	194	LEU
3	g	196	ASP
3	g	201	ILE
3	g	218	VAL
3	g	241	ILE
3	g	277	LEU
3	g	282	LEU
3	g	284	GLN
3	g	291	ASN
3	g	330	VAL
3	g	373	THR
3	g	374	CYS
3	g	376	LEU
3	g	377	LEU
3	g	398	MET
3	g	399	ILE
3	g	409	ILE
3	g	410	VAL
3	g	417	GLU

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Mol	Chain	Res	Type
3	g	423	CYS
3	g	430	THR
3	g	462	ILE
3	g	468	LEU
3	g	472	HIS
3	g	485	THR
3	g	488	ILE
3	g	508	ASN
3	g	511	THR
4	e	29	PHE
4	e	30	ILE
4	e	32	VAL
4	e	37	ASN
4	e	59	SER
4	e	61	ILE
4	e	74	LEU
4	e	75	ILE
4	e	82	THR
4	e	84	THR
4	e	90	ILE
4	e	92	SER
4	e	107	LEU
4	e	111	GLN
4	e	125	LEU
4	e	129	LEU
4	e	159	SER
4	e	166	ASP
4	e	168	ILE
4	e	206	GLU
4	e	230	VAL
4	e	240	ILE
4	e	283	THR
4	e	291	SER
4	e	294	GLU
4	e	329	ASP
4	e	336	LEU
4	e	344	ARG
4	e	381	TYR
4	e	385	PHE
4	e	387	THR
4	e	388	THR
4	e	404	VAL

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Mol	Chain	Res	Type
4	e	406	CYS
4	e	408	VAL
4	e	412	ASN
4	e	427	LEU
4	e	429	VAL
4	e	431	ARG
4	e	436	ASP
4	e	440	VAL
4	e	455	SER
4	e	464	ILE
4	e	479	ILE
4	e	487	SER
4	e	492	ILE
4	e	495	LEU
4	e	498	LEU
4	e	532	ILE
4	e	552	ASP
5	b	11	THR
5	b	21	SER
5	b	36	THR
5	b	57	THR
5	b	62	THR
5	b	80	ILE
5	b	94	SER
5	b	99	SER
5	b	104	ARG
5	b	115	ILE
5	b	119	THR
5	b	132	LEU
5	b	135	LEU
5	b	141	ASP
5	b	147	THR
5	b	182	LEU
5	b	195	ILE
5	b	199	LEU
5	b	214	LEU
5	b	226	ILE
5	b	237	THR
5	b	240	THR
5	b	308	HIS
5	b	314	VAL
5	b	319	LEU

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Mol	Chain	Res	Type
5	b	321	THR
5	b	341	ASP
5	b	365	CYS
5	b	390	VAL
5	b	397	GLU
5	b	400	THR
5	b	402	LEU
5	b	406	CYS
5	b	408	GLU
5	b	416	ASP
5	b	423	ASP
5	b	440	LEU
5	b	443	ILE
5	b	452	SER
5	b	455	LEU
5	b	459	LEU
5	b	474	LEU
5	b	476	ASN
5	b	509	LEU
6	d	36	ARG
6	d	63	THR
6	d	85	GLN
6	d	103	LEU
6	d	123	SER
6	d	124	PHE
6	d	136	LEU
6	d	140	HIS
6	d	150	LEU
6	d	162	ILE
6	d	169	PHE
6	d	170	LEU
6	d	181	ILE
6	d	198	LYS
6	d	218	THR
6	d	248	THR
6	d	251	ASN
6	d	305	LEU
6	d	312	VAL
6	d	324	LEU
6	d	336	ILE
6	d	340	THR
6	d	366	ILE

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Mol	Chain	Res	Type
6	d	385	MET
6	d	411	ILE
6	d	440	TRP
6	d	449	VAL
6	d	463	ILE
6	d	482	ILE
6	d	486	ARG
6	d	502	LEU
6	d	505	THR
6	d	513	GLU
6	d	520	ARG
7	a	6	ASN
7	a	26	ARG
7	a	47	VAL
7	a	51	LYS
7	a	56	ASP
7	a	61	THR
7	a	68	THR
7	a	86	LEU
7	a	89	GLN
7	a	90	GLN
7	a	109	LEU
7	a	126	ILE
7	a	177	SER
7	a	179	MET
7	a	185	LEU
7	a	228	VAL
7	a	270	LEU
7	a	281	VAL
7	a	326	LEU
7	a	328	ARG
7	a	339	SER
7	a	377	THR
7	a	419	VAL
7	a	426	GLU
7	a	439	THR
7	a	456	LEU
7	a	457	ILE
7	a	522	ILE
7	a	524	LYS
7	a	542	ASP
8	c	25	ILE

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Mol	Chain	Res	Type
8	c	34	VAL
8	c	52	MET
8	c	55	LEU
8	c	58	THR
8	c	67	GLU
8	c	78	MET
8	c	79	LEU
8	c	81	LEU
8	c	89	VAL
8	c	102	GLU
8	c	107	CYS
8	c	120	ILE
8	c	130	THR
8	c	138	GLN
8	c	143	VAL
8	c	148	ASP
8	c	154	LEU
8	c	165	ILE
8	c	167	TRP
8	c	200	ILE
8	c	204	VAL
8	c	206	VAL
8	c	215	LEU
8	c	219	VAL
8	c	245	LEU
8	c	251	GLU
8	c	290	VAL
8	c	293	THR
8	c	309	LEU
8	c	310	LEU
8	c	322	LYS
8	c	325	ASN
8	c	354	LEU
8	c	396	LEU
8	c	420	GLU
8	c	437	ILE
8	c	438	GLN
8	c	465	ILE
8	c	468	LEU
8	c	481	THR
8	c	504	VAL
8	c	521	LEU

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Mol	Chain	Res	Type
8	c	528	SER
1	n	19	LEU
1	n	24	THR
1	n	30	GLN
1	n	35	THR
1	n	55	LEU
1	n	56	THR
1	n	62	LEU
1	n	72	THR
1	n	75	LEU
1	n	96	CYS
1	n	124	ILE
1	n	162	VAL
1	n	181	VAL
1	n	187	ASP
1	n	198	GLN
1	n	210	ILE
1	n	213	LEU
1	n	217	HIS
1	n	237	ASN
1	n	251	PHE
1	n	340	VAL
1	n	347	ILE
1	n	368	THR
1	n	371	THR
1	n	379	LEU
1	n	390	GLN
1	n	399	LEU
1	n	453	VAL
1	n	479	ASP
1	n	497	ASP
1	n	499	CYS
1	n	511	ARG
2	p	21	TYR
2	p	25	ASP
2	p	31	SER
2	p	32	ILE
2	p	41	MET
2	p	42	CYS
2	p	43	LEU
2	p	62	ILE
2	p	63	ILE

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Mol	Chain	Res	Type
2	p	65	THR
2	p	91	GLN
2	p	98	ASP
2	p	102	LEU
2	p	105	ILE
2	p	110	LEU
2	p	113	VAL
2	p	145	MET
2	p	204	VAL
2	p	221	THR
2	p	223	ILE
2	p	227	VAL
2	p	245	HIS
2	p	256	ILE
2	p	287	MET
2	p	308	LEU
2	p	320	VAL
2	p	333	CYS
2	p	339	THR
2	p	341	LEU
2	p	344	LEU
2	p	348	THR
2	p	354	LEU
2	p	357	THR
2	p	358	VAL
2	p	381	THR
2	p	401	ILE
2	p	409	LYS
2	p	427	GLU
2	p	432	SER
2	p	441	THR
2	p	470	ASP
2	p	502	ASP
2	p	519	ASP
2	p	539	LEU
2	p	541	ILE
3	o	10	ILE
3	o	11	VAL
3	o	30	ILE
3	o	37	GLN
3	o	43	THR
3	o	55	THR

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Mol	Chain	Res	Type
3	o	61	THR
3	o	86	ILE
3	o	96	ASP
3	o	102	THR
3	o	104	LEU
3	o	147	ILE
3	o	155	ARG
3	o	161	CYS
3	o	166	MET
3	o	173	ASN
3	o	194	LEU
3	o	195	ASP
3	o	196	ASP
3	o	246	VAL
3	o	268	GLN
3	o	277	LEU
3	o	282	LEU
3	o	284	GLN
3	o	302	LEU
3	o	330	VAL
3	o	334	ILE
3	o	377	LEU
3	o	398	MET
3	o	399	ILE
3	o	409	ILE
3	o	410	VAL
3	o	417	GLU
3	o	430	THR
3	o	440	ASN
3	o	472	HIS
3	o	485	THR
3	o	488	ILE
3	o	511	THR
3	o	518	LEU
4	m	29	PHE
4	m	30	ILE
4	m	37	ASN
4	m	59	SER
4	m	61	ILE
4	m	68	ARG
4	m	73	ILE
4	m	74	LEU

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Mol	Chain	Res	Type
4	m	82	THR
4	m	89	THR
4	m	90	ILE
4	m	92	SER
4	m	107	LEU
4	m	111	GLN
4	m	125	LEU
4	m	166	ASP
4	m	168	ILE
4	m	193	VAL
4	m	230	VAL
4	m	240	ILE
4	m	283	THR
4	m	294	GLU
4	m	300	THR
4	m	312	ASP
4	m	336	LEU
4	m	385	PHE
4	m	387	THR
4	m	388	THR
4	m	406	CYS
4	m	412	ASN
4	m	427	LEU
4	m	431	ARG
4	m	436	ASP
4	m	440	VAL
4	m	459	ASP
4	m	464	ILE
4	m	479	ILE
4	m	487	SER
4	m	492	ILE
4	m	498	LEU
4	m	507	ILE
4	m	519	SER
4	m	552	ASP
5	j	21	SER
5	j	29	VAL
5	j	36	THR
5	j	57	THR
5	j	62	THR
5	j	80	ILE
5	j	97	VAL

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Mol	Chain	Res	Type
5	j	104	ARG
5	j	115	ILE
5	j	119	THR
5	j	135	LEU
5	j	141	ASP
5	j	147	THR
5	j	156	ILE
5	j	160	THR
5	j	199	LEU
5	j	208	LEU
5	j	214	LEU
5	j	226	ILE
5	j	237	THR
5	j	240	THR
5	j	245	ILE
5	j	246	PHE
5	j	319	LEU
5	j	321	THR
5	j	342	VAL
5	j	346	ILE
5	j	397	GLU
5	j	402	LEU
5	j	408	GLU
5	j	416	ASP
5	j	423	ASP
5	j	440	LEU
5	j	443	ILE
5	j	455	LEU
5	j	459	LEU
5	j	467	ILE
5	j	474	LEU
5	j	479	ILE
5	j	509	LEU
6	l	36	ARG
6	l	38	SER
6	l	103	LEU
6	l	123	SER
6	l	124	PHE
6	l	140	HIS
6	l	162	ILE
6	l	169	PHE
6	l	170	LEU

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Mol	Chain	Res	Type
6	l	181	ILE
6	l	198	LYS
6	l	209	MET
6	l	218	THR
6	l	248	THR
6	l	251	ASN
6	l	255	ASN
6	l	283	CYS
6	l	311	MET
6	l	312	VAL
6	l	336	ILE
6	l	340	THR
6	l	349	LEU
6	l	364	THR
6	l	366	ILE
6	l	375	VAL
6	l	385	MET
6	l	411	ILE
6	l	440	TRP
6	l	449	VAL
6	l	463	ILE
6	l	467	THR
6	l	478	LEU
6	l	482	ILE
6	l	486	ARG
6	l	502	LEU
6	l	505	THR
6	l	513	GLU
6	l	520	ARG
6	l	522	ASP
7	i	26	ARG
7	i	47	VAL
7	i	56	ASP
7	i	61	THR
7	i	68	THR
7	i	69	ILE
7	i	86	LEU
7	i	89	GLN
7	i	90	GLN
7	i	126	ILE
7	i	143	VAL
7	i	164	MET

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Mol	Chain	Res	Type
7	i	189	THR
7	i	224	LEU
7	i	228	VAL
7	i	281	VAL
7	i	299	THR
7	i	326	LEU
7	i	328	ARG
7	i	337	LEU
7	i	373	LEU
7	i	377	THR
7	i	407	SER
7	i	419	VAL
7	i	424	CYS
7	i	426	GLU
7	i	438	THR
7	i	442	SER
7	i	456	LEU
7	i	457	ILE
7	i	512	GLU
7	i	542	ASP
7	i	543	THR
7	i	546	THR
8	k	16	THR
8	k	23	SER
8	k	25	ILE
8	k	34	VAL
8	k	52	MET
8	k	55	LEU
8	k	58	THR
8	k	78	MET
8	k	79	LEU
8	k	81	LEU
8	k	89	VAL
8	k	102	GLU
8	k	107	CYS
8	k	130	THR
8	k	138	GLN
8	k	143	VAL
8	k	148	ASP
8	k	154	LEU
8	k	165	ILE
8	k	167	TRP

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Mol	Chain	Res	Type
8	k	204	VAL
8	k	206	VAL
8	k	215	LEU
8	k	251	GLU
8	k	257	SER
8	k	260	ASN
8	k	290	VAL
8	k	293	THR
8	k	309	LEU
8	k	310	LEU
8	k	322	LYS
8	k	325	ASN
8	k	335	THR
8	k	336	ILE
8	k	348	VAL
8	k	354	LEU
8	k	380	MET
8	k	396	LEU
8	k	398	ASP
8	k	420	GLU
8	k	465	ILE
8	k	468	LEU
8	k	481	THR
8	k	504	VAL
8	k	516	SER
8	k	521	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (305) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	30	GLN
1	F	83	GLN
1	F	104	GLN
1	F	145	ASN
1	F	198	GLN
1	F	221	HIS
1	F	248	ASN
1	F	324	ASN
1	F	338	ASN
1	F	430	ASN
1	F	461	ASN
1	F	515	ASN

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Mol	Chain	Res	Type
2	H	19	ASN
2	H	27	GLN
2	H	229	ASN
2	H	311	HIS
2	H	392	ASN
2	H	483	ASN
3	G	21	GLN
3	G	37	GLN
3	G	141	ASN
3	G	172	HIS
3	G	174	ASN
3	G	231	GLN
3	G	238	ASN
3	G	268	GLN
3	G	305	GLN
3	G	394	HIS
3	G	406	ASN
3	G	491	ASN
3	G	505	ASN
3	G	508	ASN
4	E	35	GLN
4	E	41	GLN
4	E	85	ASN
4	E	93	GLN
4	E	98	ASN
4	E	111	GLN
4	E	210	ASN
4	E	333	HIS
4	E	337	GLN
4	E	383	GLN
4	E	432	ASN
4	E	502	GLN
4	E	520	ASN
5	B	52	ASN
5	B	79	ASN
5	B	192	HIS
5	B	385	HIS
6	D	24	ASN
6	D	59	ASN
6	D	85	GLN
6	D	125	GLN
6	D	255	ASN

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Mol	Chain	Res	Type
7	A	6	ASN
7	A	28	GLN
7	A	29	ASN
7	A	64	ASN
7	A	90	GLN
7	A	209	HIS
7	A	231	GLN
7	A	269	GLN
7	A	435	ASN
8	C	19	GLN
8	C	24	ASN
8	C	72	HIS
8	C	85	GLN
8	C	231	HIS
8	C	270	ASN
8	C	370	ASN
8	C	405	ASN
8	C	458	GLN
1	N	22	ASN
1	N	69	GLN
1	N	83	GLN
1	N	104	GLN
1	N	142	ASN
1	N	221	HIS
1	N	248	ASN
1	N	324	ASN
1	N	338	ASN
1	N	390	GLN
1	N	430	ASN
2	P	23	ASN
2	P	203	ASN
2	P	229	ASN
2	P	311	HIS
3	O	37	GLN
3	O	174	ASN
3	O	394	HIS
3	O	406	ASN
3	O	440	ASN
3	O	466	ASN
3	O	491	ASN
3	O	505	ASN
3	O	508	ASN

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Mol	Chain	Res	Type
3	O	515	ASN
4	M	35	GLN
4	M	85	ASN
4	M	98	ASN
4	M	148	ASN
4	M	210	ASN
4	M	227	GLN
4	M	253	GLN
4	M	383	GLN
4	M	424	HIS
4	M	432	ASN
4	M	486	ASN
4	M	502	GLN
4	M	509	ASN
4	M	520	ASN
5	J	52	ASN
5	J	79	ASN
5	J	118	GLN
5	J	192	HIS
5	J	260	GLN
5	J	286	ASN
5	J	288	GLN
5	J	308	HIS
5	J	385	HIS
6	L	24	ASN
6	L	59	ASN
6	L	85	GLN
6	L	125	GLN
6	L	251	ASN
6	L	255	ASN
6	L	303	HIS
7	I	6	ASN
7	I	28	GLN
7	I	29	ASN
7	I	64	ASN
7	I	77	HIS
7	I	90	GLN
7	I	231	GLN
7	I	263	ASN
7	I	269	GLN
7	I	435	ASN
8	K	24	ASN

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Mol	Chain	Res	Type
8	K	115	ASN
8	K	138	GLN
8	K	166	HIS
8	K	226	ASN
8	K	231	HIS
8	K	237	HIS
8	K	270	ASN
8	K	370	ASN
8	K	405	ASN
1	f	22	ASN
1	f	83	GLN
1	f	104	GLN
1	f	142	ASN
1	f	145	ASN
1	f	221	HIS
1	f	248	ASN
1	f	324	ASN
1	f	338	ASN
1	f	390	GLN
1	f	430	ASN
2	h	19	ASN
2	h	27	GLN
2	h	66	ASN
2	h	79	HIS
2	h	229	ASN
2	h	311	HIS
2	h	392	ASN
3	g	57	ASN
3	g	64	ASN
3	g	384	GLN
3	g	440	ASN
3	g	491	ASN
3	g	505	ASN
3	g	508	ASN
4	e	98	ASN
4	e	148	ASN
4	e	296	GLN
4	e	424	HIS
4	e	432	ASN
4	e	502	GLN
4	e	509	ASN
5	b	52	ASN

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Mol	Chain	Res	Type
5	b	79	ASN
5	b	84	GLN
5	b	260	GLN
5	b	288	GLN
5	b	308	HIS
5	b	375	GLN
5	b	385	HIS
5	b	513	ASN
6	d	24	ASN
6	d	59	ASN
6	d	125	GLN
6	d	149	GLN
6	d	240	GLN
6	d	250	ASN
6	d	251	ASN
6	d	255	ASN
6	d	303	HIS
6	d	384	ASN
6	d	473	HIS
7	a	6	ASN
7	a	28	GLN
7	a	29	ASN
7	a	38	ASN
7	a	76	GLN
7	a	90	GLN
7	a	231	GLN
7	a	263	ASN
7	a	269	GLN
7	a	435	ASN
7	a	485	GLN
8	c	12	GLN
8	c	24	ASN
8	c	72	HIS
8	c	85	GLN
8	c	138	GLN
8	c	166	HIS
8	c	237	HIS
8	c	270	ASN
8	c	274	GLN
8	c	279	GLN
8	c	351	ASN
8	c	370	ASN

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Mol	Chain	Res	Type
8	c	405	ASN
1	n	22	ASN
1	n	83	GLN
1	n	104	GLN
1	n	106	HIS
1	n	142	ASN
1	n	145	ASN
1	n	152	GLN
1	n	221	HIS
1	n	248	ASN
1	n	324	ASN
1	n	338	ASN
1	n	390	GLN
1	n	430	ASN
2	p	19	ASN
2	p	27	GLN
2	p	79	HIS
2	p	311	HIS
3	o	21	GLN
3	o	37	GLN
3	o	57	ASN
3	o	64	ASN
3	o	123	HIS
3	o	174	ASN
3	o	231	GLN
3	o	238	ASN
3	o	284	GLN
3	o	394	HIS
3	o	405	GLN
3	o	406	ASN
3	o	472	HIS
3	o	491	ASN
3	o	505	ASN
3	o	508	ASN
4	m	85	ASN
4	m	93	GLN
4	m	98	ASN
4	m	111	GLN
4	m	227	GLN
4	m	296	GLN
4	m	337	GLN
4	m	383	GLN

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Mol	Chain	Res	Type
4	m	432	ASN
4	m	502	GLN
4	m	520	ASN
5	j	52	ASN
5	j	79	ASN
5	j	271	ASN
5	j	286	ASN
5	j	288	GLN
5	j	385	HIS
5	j	513	ASN
6	l	24	ASN
6	l	59	ASN
6	l	72	HIS
6	l	85	GLN
6	l	125	GLN
6	l	255	ASN
6	l	303	HIS
6	l	309	ASN
6	l	441	GLN
6	l	473	HIS
7	i	6	ASN
7	i	28	GLN
7	i	29	ASN
7	i	64	ASN
7	i	76	GLN
7	i	77	HIS
7	i	90	GLN
7	i	158	ASN
7	i	178	ASN
7	i	263	ASN
7	i	269	GLN
7	i	435	ASN
7	i	485	GLN
8	k	9	ASN
8	k	24	ASN
8	k	85	GLN
8	k	138	GLN
8	k	166	HIS
8	k	270	ASN
8	k	370	ASN
8	k	405	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 96 ligands modelled in this entry, 32 are monoatomic - leaving 64 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	ADP	J	602	11,9	28,29,29	1.50	5 (17%)	43,45,45	1.90	9 (20%)
10	ADP	K	1102	11,9	28,29,29	1.44	5 (17%)	43,45,45	1.78	9 (20%)
11	BEF	m	603	10	0,3,3	-	-	-		
11	BEF	F	603	10	0,3,3	-	-	-		
10	ADP	h	602	9	28,29,29	1.45	5 (17%)	43,45,45	1.86	9 (20%)
11	BEF	H	603	-	0,3,3	-	-	-		
10	ADP	p	602	9	28,29,29	1.44	5 (17%)	43,45,45	1.93	10 (23%)
11	BEF	I	603	10	0,3,3	-	-	-		
10	ADP	A	602	11,9	28,29,29	1.49	4 (14%)	43,45,45	1.88	9 (20%)
10	ADP	g	602	9	28,29,29	1.50	5 (17%)	43,45,45	1.83	7 (16%)
11	BEF	n	603	10	0,3,3	-	-	-		
11	BEF	j	603	10	0,3,3	-	-	-		
10	ADP	I	602	11,9	28,29,29	1.42	4 (14%)	43,45,45	1.83	8 (18%)
11	BEF	B	603	10	0,3,3	-	-	-		
11	BEF	K	1103	10	0,3,3	-	-	-		
10	ADP	E	602	11,9	28,29,29	1.41	4 (14%)	43,45,45	1.88	10 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	BEF	O	603	-	0,3,3	-	-	-		
11	BEF	f	603	10	0,3,3	-	-	-		
11	BEF	g	603	-	0,3,3	-	-	-		
11	BEF	a	603	10	0,3,3	-	-	-		
11	BEF	e	603	10	0,3,3	-	-	-		
10	ADP	a	602	11,9	28,29,29	1.48	5 (17%)	43,45,45	1.86	8 (18%)
11	BEF	h	603	-	0,3,3	-	-	-		
11	BEF	J	603	10	0,3,3	-	-	-		
10	ADP	j	602	11,9	28,29,29	1.59	6 (21%)	43,45,45	1.79	7 (16%)
10	ADP	C	1102	11,9	28,29,29	1.44	4 (14%)	43,45,45	1.80	9 (20%)
11	BEF	A	603	10	0,3,3	-	-	-		
11	BEF	b	603	10	0,3,3	-	-	-		
10	ADP	L	602	11,9	28,29,29	1.46	4 (14%)	43,45,45	1.86	9 (20%)
10	ADP	O	602	9	28,29,29	1.51	5 (17%)	43,45,45	1.88	9 (20%)
10	ADP	D	602	11,9	28,29,29	1.43	4 (14%)	43,45,45	1.89	9 (20%)
10	ADP	l	602	11,9	28,29,29	1.47	4 (14%)	43,45,45	1.85	9 (20%)
10	ADP	e	602	11,9	28,29,29	1.43	4 (14%)	43,45,45	1.86	9 (20%)
10	ADP	i	602	11,9	28,29,29	1.45	4 (14%)	43,45,45	1.87	8 (18%)
11	BEF	E	603	10	0,3,3	-	-	-		
10	ADP	B	602	11,9	28,29,29	1.48	5 (17%)	43,45,45	1.80	9 (20%)
10	ADP	F	602	11,9	28,29,29	1.51	5 (17%)	43,45,45	1.75	8 (18%)
10	ADP	N	602	11,9	28,29,29	1.48	5 (17%)	43,45,45	1.82	8 (18%)
10	ADP	P	602	9	28,29,29	1.45	5 (17%)	43,45,45	1.88	10 (23%)
10	ADP	c	1102	11,9	28,29,29	1.43	4 (14%)	43,45,45	1.76	7 (16%)
11	BEF	G	603	-	0,3,3	-	-	-		
10	ADP	M	602	11,9	28,29,29	1.45	5 (17%)	43,45,45	1.87	10 (23%)
11	BEF	P	603	-	0,3,3	-	-	-		
11	BEF	L	603	10	0,3,3	-	-	-		
10	ADP	o	602	9	28,29,29	1.51	5 (17%)	43,45,45	1.90	10 (23%)
10	ADP	k	1102	11,9	28,29,29	1.45	4 (14%)	43,45,45	1.83	8 (18%)
10	ADP	H	602	9	28,29,29	1.45	5 (17%)	43,45,45	1.81	9 (20%)
11	BEF	M	603	10	0,3,3	-	-	-		
11	BEF	c	1103	10	0,3,3	-	-	-		
11	BEF	d	603	10	0,3,3	-	-	-		
11	BEF	i	603	10	0,3,3	-	-	-		
10	ADP	d	602	11,9	28,29,29	1.44	6 (21%)	43,45,45	1.82	9 (20%)
10	ADP	m	602	11,9	28,29,29	1.54	5 (17%)	43,45,45	1.91	9 (20%)
10	ADP	b	602	11,9	28,29,29	1.54	5 (17%)	43,45,45	1.76	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	BEF	o	603	-	0,3,3	-	-	-	-	-
10	ADP	n	602	11,9	28,29,29	1.54	5 (17%)	43,45,45	1.81	8 (18%)
11	BEF	D	603	10	0,3,3	-	-	-	-	-
11	BEF	C	1103	10	0,3,3	-	-	-	-	-
11	BEF	l	603	10	0,3,3	-	-	-	-	-
11	BEF	N	603	10	0,3,3	-	-	-	-	-
11	BEF	p	603	-	0,3,3	-	-	-	-	-
10	ADP	G	602	9	28,29,29	1.44	4 (14%)	43,45,45	1.93	10 (23%)
11	BEF	k	1103	10	0,3,3	-	-	-	-	-
10	ADP	f	602	11,9	28,29,29	1.53	5 (17%)	43,45,45	1.87	9 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	ADP	J	602	11,9	-	2/16/32/32	0/3/3/3
10	ADP	K	1102	11,9	-	1/16/32/32	0/3/3/3
10	ADP	h	602	9	-	1/16/32/32	0/3/3/3
10	ADP	p	602	9	-	1/16/32/32	0/3/3/3
10	ADP	A	602	11,9	-	5/16/32/32	0/3/3/3
10	ADP	g	602	9	-	5/16/32/32	0/3/3/3
10	ADP	I	602	11,9	-	5/16/32/32	0/3/3/3
10	ADP	E	602	11,9	-	7/16/32/32	0/3/3/3
10	ADP	a	602	11,9	-	5/16/32/32	0/3/3/3
10	ADP	j	602	11,9	-	2/16/32/32	0/3/3/3
10	ADP	C	1102	11,9	-	2/16/32/32	0/3/3/3
10	ADP	L	602	11,9	-	7/16/32/32	0/3/3/3
10	ADP	O	602	9	-	4/16/32/32	0/3/3/3
10	ADP	D	602	11,9	-	6/16/32/32	0/3/3/3
10	ADP	l	602	11,9	-	6/16/32/32	0/3/3/3
10	ADP	e	602	11,9	-	8/16/32/32	0/3/3/3
10	ADP	i	602	11,9	-	6/16/32/32	0/3/3/3
10	ADP	B	602	11,9	-	3/16/32/32	0/3/3/3
10	ADP	F	602	11,9	-	8/16/32/32	0/3/3/3
10	ADP	N	602	11,9	-	8/16/32/32	0/3/3/3
10	ADP	P	602	9	-	1/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	ADP	c	1102	11,9	-	2/16/32/32	0/3/3/3
10	ADP	M	602	11,9	-	8/16/32/32	0/3/3/3
10	ADP	o	602	9	-	5/16/32/32	0/3/3/3
10	ADP	k	1102	11,9	-	2/16/32/32	0/3/3/3
10	ADP	H	602	9	-	1/16/32/32	0/3/3/3
10	ADP	d	602	11,9	-	6/16/32/32	0/3/3/3
10	ADP	m	602	11,9	-	7/16/32/32	0/3/3/3
10	ADP	b	602	11,9	-	2/16/32/32	0/3/3/3
10	ADP	n	602	11,9	-	8/16/32/32	0/3/3/3
10	ADP	G	602	9	-	5/16/32/32	0/3/3/3
10	ADP	f	602	11,9	-	7/16/32/32	0/3/3/3

All (150) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	f	602	ADP	C5-C4	5.11	1.48	1.39
10	m	602	ADP	C5-C4	5.07	1.48	1.39
10	n	602	ADP	C5-C4	5.06	1.48	1.39
10	b	602	ADP	C5-C4	5.00	1.48	1.39
10	k	1102	ADP	C5-C4	4.97	1.47	1.39
10	A	602	ADP	C5-C4	4.95	1.47	1.39
10	j	602	ADP	C5-C4	4.93	1.47	1.39
10	l	602	ADP	C5-C4	4.91	1.47	1.39
10	C	1102	ADP	C5-C4	4.90	1.47	1.39
10	c	1102	ADP	C5-C4	4.88	1.47	1.39
10	N	602	ADP	C5-C4	4.87	1.47	1.39
10	G	602	ADP	C5-C4	4.87	1.47	1.39
10	g	602	ADP	C5-C4	4.86	1.47	1.39
10	L	602	ADP	C5-C4	4.80	1.47	1.39
10	i	602	ADP	C5-C4	4.80	1.47	1.39
10	P	602	ADP	C5-C4	4.79	1.47	1.39
10	H	602	ADP	C5-C4	4.79	1.47	1.39
10	o	602	ADP	C5-C4	4.78	1.47	1.39
10	O	602	ADP	C5-C4	4.78	1.47	1.39
10	F	602	ADP	C5-C4	4.77	1.47	1.39
10	e	602	ADP	C5-C4	4.77	1.47	1.39
10	J	602	ADP	C5-C4	4.77	1.47	1.39
10	E	602	ADP	C5-C4	4.74	1.47	1.39
10	a	602	ADP	C5-C4	4.74	1.47	1.39
10	M	602	ADP	C5-C4	4.71	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	1102	ADP	C5-C4	4.70	1.47	1.39
10	p	602	ADP	C5-C4	4.70	1.47	1.39
10	I	602	ADP	C5-C4	4.66	1.47	1.39
10	d	602	ADP	C5-C4	4.65	1.47	1.39
10	h	602	ADP	C5-C4	4.65	1.47	1.39
10	D	602	ADP	C5-C4	4.60	1.47	1.39
10	B	602	ADP	C5-C4	4.58	1.47	1.39
10	j	602	ADP	PA-O3A	3.38	1.63	1.59
10	A	602	ADP	C5-C6	3.22	1.50	1.41
10	n	602	ADP	C5-C6	3.04	1.49	1.41
10	f	602	ADP	C5-C6	3.01	1.49	1.41
10	L	602	ADP	C5-C6	3.00	1.49	1.41
10	m	602	ADP	C5-C6	3.00	1.49	1.41
10	O	602	ADP	PA-O3A	2.99	1.62	1.59
10	F	602	ADP	PA-O3A	2.96	1.62	1.59
10	a	602	ADP	C5-C6	2.96	1.49	1.41
10	b	602	ADP	C5-C6	2.96	1.49	1.41
10	e	602	ADP	C5-C6	2.96	1.49	1.41
10	P	602	ADP	C5-C6	2.95	1.49	1.41
10	p	602	ADP	C5-C6	2.93	1.49	1.41
10	G	602	ADP	C5-C6	2.93	1.49	1.41
10	o	602	ADP	PA-O3A	2.92	1.62	1.59
10	m	602	ADP	PA-O3A	2.91	1.62	1.59
10	M	602	ADP	C5-C6	2.90	1.49	1.41
10	k	1102	ADP	C5-C6	2.90	1.49	1.41
10	B	602	ADP	PA-O3A	2.89	1.62	1.59
10	J	602	ADP	C5-C6	2.89	1.49	1.41
10	F	602	ADP	C5-C6	2.89	1.49	1.41
10	l	602	ADP	C5-C6	2.89	1.49	1.41
10	D	602	ADP	C5-C6	2.88	1.49	1.41
10	C	1102	ADP	C5-C6	2.87	1.49	1.41
10	N	602	ADP	C5-C6	2.87	1.49	1.41
10	d	602	ADP	C5-C6	2.87	1.49	1.41
10	O	602	ADP	C5-C6	2.84	1.48	1.41
10	i	602	ADP	C5-C6	2.84	1.48	1.41
10	H	602	ADP	C5-C6	2.83	1.48	1.41
10	o	602	ADP	C5-C6	2.83	1.48	1.41
10	h	602	ADP	C5-C6	2.82	1.48	1.41
10	c	1102	ADP	C5-C6	2.80	1.48	1.41
10	I	602	ADP	C5-C6	2.78	1.48	1.41
10	K	1102	ADP	C5-C6	2.78	1.48	1.41
10	B	602	ADP	C5-C6	2.71	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	E	602	ADP	C5-C6	2.71	1.48	1.41
10	g	602	ADP	PA-O3A	2.69	1.62	1.59
10	j	602	ADP	C5-C6	2.69	1.48	1.41
10	g	602	ADP	C5-C6	2.68	1.48	1.41
10	J	602	ADP	PA-O3A	2.68	1.62	1.59
10	b	602	ADP	PA-O3A	2.64	1.62	1.59
10	n	602	ADP	PA-O3A	2.60	1.62	1.59
10	g	602	ADP	C5-N7	-2.53	1.34	1.39
10	N	602	ADP	C8-N7	2.53	1.36	1.31
10	h	602	ADP	PA-O3A	2.52	1.62	1.59
10	f	602	ADP	C8-N7	2.52	1.36	1.31
10	n	602	ADP	C8-N7	2.51	1.36	1.31
10	j	602	ADP	C5-N7	-2.50	1.34	1.39
10	A	602	ADP	C8-N7	2.46	1.36	1.31
10	m	602	ADP	C8-N7	2.46	1.36	1.31
10	o	602	ADP	C8-N7	2.45	1.36	1.31
10	l	602	ADP	C8-N7	2.43	1.36	1.31
10	O	602	ADP	C8-N7	2.43	1.36	1.31
10	E	602	ADP	C5-N7	-2.42	1.34	1.39
10	C	1102	ADP	C5-N7	-2.42	1.34	1.39
10	i	602	ADP	C8-N7	2.42	1.36	1.31
10	L	602	ADP	C8-N7	2.41	1.36	1.31
10	c	1102	ADP	C5-N7	-2.41	1.34	1.39
10	a	602	ADP	C8-N7	2.40	1.36	1.31
10	i	602	ADP	C5-N7	-2.39	1.34	1.39
10	F	602	ADP	C8-N7	2.39	1.36	1.31
10	o	602	ADP	C5-N7	-2.39	1.34	1.39
10	B	602	ADP	C5-N7	-2.38	1.34	1.39
10	G	602	ADP	C8-N7	2.38	1.36	1.31
10	I	602	ADP	C5-N7	-2.38	1.34	1.39
10	b	602	ADP	C5-N7	-2.37	1.34	1.39
10	k	1102	ADP	C8-N7	2.37	1.36	1.31
10	e	602	ADP	C8-N7	2.37	1.36	1.31
10	a	602	ADP	PA-O3A	2.36	1.62	1.59
10	J	602	ADP	C8-N7	2.36	1.36	1.31
10	I	602	ADP	C8-N7	2.36	1.36	1.31
10	h	602	ADP	C8-N7	2.36	1.36	1.31
10	b	602	ADP	C8-N7	2.35	1.36	1.31
10	D	602	ADP	C8-N7	2.34	1.36	1.31
10	J	602	ADP	C5-N7	-2.34	1.34	1.39
10	K	1102	ADP	C5-N7	-2.34	1.34	1.39
10	g	602	ADP	C8-N7	2.33	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	602	ADP	C8-N7	2.33	1.36	1.31
10	P	602	ADP	C8-N7	2.32	1.36	1.31
10	O	602	ADP	C5-N7	-2.32	1.34	1.39
10	H	602	ADP	C5-N7	-2.32	1.34	1.39
10	f	602	ADP	C5-N7	-2.31	1.34	1.39
10	D	602	ADP	C5-N7	-2.30	1.34	1.39
10	k	1102	ADP	C5-N7	-2.29	1.34	1.39
10	j	602	ADP	C8-N7	2.29	1.36	1.31
10	H	602	ADP	C8-N7	2.29	1.36	1.31
10	e	602	ADP	C5-N7	-2.28	1.34	1.39
10	l	602	ADP	C5-N7	-2.27	1.34	1.39
10	d	602	ADP	C5-N7	-2.26	1.35	1.39
10	f	602	ADP	PA-O3A	2.26	1.61	1.59
10	M	602	ADP	C5-N7	-2.26	1.35	1.39
10	p	602	ADP	C8-N7	2.25	1.36	1.31
10	p	602	ADP	C5-N7	-2.24	1.35	1.39
10	K	1102	ADP	C4-N9	-2.24	1.33	1.37
10	a	602	ADP	C5-N7	-2.24	1.35	1.39
10	M	602	ADP	C8-N7	2.23	1.36	1.31
10	F	602	ADP	C5-N7	-2.23	1.35	1.39
10	P	602	ADP	C5-N7	-2.22	1.35	1.39
10	L	602	ADP	C5-N7	-2.22	1.35	1.39
10	K	1102	ADP	C8-N7	2.21	1.35	1.31
10	N	602	ADP	C5-N7	-2.21	1.35	1.39
10	h	602	ADP	C5-N7	-2.20	1.35	1.39
10	d	602	ADP	C8-N7	2.19	1.35	1.31
10	n	602	ADP	C5-N7	-2.17	1.35	1.39
10	d	602	ADP	PA-O3A	2.16	1.61	1.59
10	C	1102	ADP	C8-N7	2.15	1.35	1.31
10	G	602	ADP	C5-N7	-2.14	1.35	1.39
10	c	1102	ADP	C8-N7	2.14	1.35	1.31
10	E	602	ADP	C8-N7	2.13	1.35	1.31
10	M	602	ADP	PA-O3A	2.13	1.61	1.59
10	m	602	ADP	C5-N7	-2.12	1.35	1.39
10	N	602	ADP	PA-O3A	2.12	1.61	1.59
10	p	602	ADP	PA-O3A	2.09	1.61	1.59
10	H	602	ADP	PA-O3A	2.06	1.61	1.59
10	A	602	ADP	C5-N7	-2.06	1.35	1.39
10	P	602	ADP	PA-O3A	2.03	1.61	1.59
10	j	602	ADP	C4-N9	-2.02	1.33	1.37
10	d	602	ADP	C4-N9	-2.02	1.33	1.37

All (280) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	i	602	ADP	C5-C4-N3	-6.35	117.97	126.72
10	f	602	ADP	C5-C4-N3	-6.31	118.03	126.72
10	p	602	ADP	C5-C4-N3	-6.29	118.05	126.72
10	m	602	ADP	C5-C4-N3	-6.29	118.06	126.72
10	J	602	ADP	C5-C4-N3	-6.28	118.07	126.72
10	G	602	ADP	C5-C4-N3	-6.25	118.11	126.72
10	o	602	ADP	C5-C4-N3	-6.25	118.11	126.72
10	O	602	ADP	C5-C4-N3	-6.22	118.15	126.72
10	D	602	ADP	C5-C4-N3	-6.16	118.23	126.72
10	h	602	ADP	C5-C4-N3	-6.10	118.31	126.72
10	P	602	ADP	C5-C4-N3	-6.10	118.32	126.72
10	e	602	ADP	C5-C4-N3	-6.04	118.40	126.72
10	g	602	ADP	C5-C4-N3	-6.01	118.44	126.72
10	A	602	ADP	C5-C4-N3	-5.97	118.49	126.72
10	k	1102	ADP	C5-C4-N3	-5.94	118.53	126.72
10	a	602	ADP	C5-C4-N3	-5.93	118.55	126.72
10	n	602	ADP	C5-C4-N3	-5.90	118.59	126.72
10	c	1102	ADP	C5-C4-N3	-5.89	118.61	126.72
10	C	1102	ADP	C5-C4-N3	-5.88	118.62	126.72
10	B	602	ADP	C5-C4-N3	-5.83	118.69	126.72
10	l	602	ADP	C5-C4-N3	-5.83	118.69	126.72
10	L	602	ADP	C5-C4-N3	-5.83	118.69	126.72
10	N	602	ADP	C5-C4-N3	-5.82	118.70	126.72
10	I	602	ADP	C5-C4-N3	-5.81	118.71	126.72
10	b	602	ADP	C5-C4-N3	-5.81	118.71	126.72
10	E	602	ADP	C5-C4-N3	-5.76	118.78	126.72
10	H	602	ADP	C5-C4-N3	-5.76	118.78	126.72
10	M	602	ADP	C5-C4-N3	-5.76	118.78	126.72
10	F	602	ADP	C5-C4-N3	-5.66	118.92	126.72
10	j	602	ADP	C5-C4-N3	-5.57	119.05	126.72
10	d	602	ADP	C5-C4-N3	-5.56	119.06	126.72
10	K	1102	ADP	C5-C4-N3	-5.46	119.20	126.72
10	m	602	ADP	N3-C4-N9	5.04	135.73	127.17
10	G	602	ADP	N3-C4-N9	5.03	135.73	127.17
10	p	602	ADP	N3-C4-N9	4.95	135.59	127.17
10	P	602	ADP	N3-C4-N9	4.80	135.33	127.17
10	h	602	ADP	N3-C4-N9	4.80	135.33	127.17
10	f	602	ADP	N3-C4-N9	4.75	135.25	127.17
10	E	602	ADP	N3-C4-N9	4.72	135.19	127.17
10	D	602	ADP	N3-C4-N9	4.71	135.18	127.17
10	J	602	ADP	N3-C4-N9	4.71	135.17	127.17
10	j	602	ADP	N3-C4-N9	4.69	135.15	127.17
10	g	602	ADP	N3-C4-N9	4.67	135.10	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	o	602	ADP	N3-C4-N9	4.66	135.10	127.17
10	e	602	ADP	N3-C4-N9	4.64	135.06	127.17
10	O	602	ADP	N3-C4-N9	4.64	135.05	127.17
10	B	602	ADP	N3-C4-N9	4.63	135.04	127.17
10	i	602	ADP	N3-C4-N9	4.62	135.03	127.17
10	C	1102	ADP	N3-C4-N9	4.58	134.96	127.17
10	H	602	ADP	N3-C4-N9	4.58	134.96	127.17
10	d	602	ADP	N3-C4-N9	4.57	134.94	127.17
10	M	602	ADP	N3-C4-N9	4.57	134.94	127.17
10	l	602	ADP	N3-C4-N9	4.54	134.89	127.17
10	c	1102	ADP	N3-C4-N9	4.53	134.87	127.17
10	k	1102	ADP	N3-C4-N9	4.52	134.86	127.17
10	b	602	ADP	N3-C4-N9	4.51	134.83	127.17
10	F	602	ADP	N3-C4-N9	4.50	134.81	127.17
10	a	602	ADP	N3-C4-N9	4.48	134.79	127.17
10	n	602	ADP	N3-C4-N9	4.46	134.76	127.17
10	L	602	ADP	N3-C4-N9	4.44	134.72	127.17
10	A	602	ADP	N3-C4-N9	4.43	134.70	127.17
10	I	602	ADP	N3-C4-N9	4.43	134.69	127.17
10	N	602	ADP	N3-C4-N9	4.40	134.64	127.17
10	K	1102	ADP	N3-C4-N9	4.26	134.41	127.17
10	p	602	ADP	C2-N3-C4	4.09	121.82	111.83
10	i	602	ADP	C2-N3-C4	4.08	121.79	111.83
10	o	602	ADP	C2-N3-C4	4.06	121.74	111.83
10	h	602	ADP	C2-N3-C4	4.03	121.67	111.83
10	G	602	ADP	C2-N3-C4	4.02	121.65	111.83
10	O	602	ADP	C2-N3-C4	4.02	121.64	111.83
10	J	602	ADP	C2-N3-C4	4.00	121.60	111.83
10	m	602	ADP	C2-N3-C4	3.99	121.58	111.83
10	D	602	ADP	C2-N3-C4	3.98	121.56	111.83
10	a	602	ADP	C2-N3-C4	3.97	121.53	111.83
10	P	602	ADP	C2-N3-C4	3.96	121.51	111.83
10	A	602	ADP	C4-C5-N7	-3.95	106.06	110.58
10	M	602	ADP	C2-N3-C4	3.94	121.47	111.83
10	f	602	ADP	C2-N3-C4	3.94	121.45	111.83
10	A	602	ADP	C2-N3-C4	3.93	121.43	111.83
10	I	602	ADP	C2-N3-C4	3.91	121.38	111.83
10	e	602	ADP	C2-N3-C4	3.87	121.28	111.83
10	l	602	ADP	C2-N3-C4	3.86	121.26	111.83
10	n	602	ADP	C2-N3-C4	3.85	121.24	111.83
10	E	602	ADP	C2-N3-C4	3.84	121.20	111.83
10	g	602	ADP	C2-N3-C4	3.84	121.20	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	N	602	ADP	C2-N3-C4	3.82	121.16	111.83
10	H	602	ADP	C2-N3-C4	3.81	121.15	111.83
10	L	602	ADP	C2-N3-C4	3.81	121.14	111.83
10	B	602	ADP	C2-N3-C4	3.80	121.12	111.83
10	k	1102	ADP	C2-N3-C4	3.79	121.08	111.83
10	F	602	ADP	C2-N3-C4	3.78	121.07	111.83
10	J	602	ADP	C4-C5-N7	-3.78	106.26	110.58
10	C	1102	ADP	C2-N3-C4	3.76	121.01	111.83
10	O	602	ADP	C4-C5-N7	-3.73	106.31	110.58
10	d	602	ADP	C2-N3-C4	3.72	120.92	111.83
10	L	602	ADP	C4-C5-N7	-3.71	106.34	110.58
10	P	602	ADP	C4-C5-N7	-3.69	106.36	110.58
10	K	1102	ADP	C2-N3-C4	3.69	120.85	111.83
10	D	602	ADP	C4-C5-N7	-3.68	106.37	110.58
10	N	602	ADP	C4-C5-N7	-3.68	106.37	110.58
10	e	602	ADP	C4-C5-N7	-3.68	106.38	110.58
10	a	602	ADP	C4-C5-N7	-3.67	106.38	110.58
10	b	602	ADP	C2-N3-C4	3.67	120.79	111.83
10	M	602	ADP	N3-C2-N1	-3.65	123.06	128.58
10	n	602	ADP	C4-C5-N7	-3.65	106.41	110.58
10	p	602	ADP	C4-C5-N7	-3.65	106.41	110.58
10	j	602	ADP	C2-N3-C4	3.61	120.66	111.83
10	c	1102	ADP	C2-N3-C4	3.60	120.63	111.83
10	f	602	ADP	C4-C5-N7	-3.60	106.47	110.58
10	E	602	ADP	N3-C2-N1	-3.59	123.14	128.58
10	G	602	ADP	C4-C5-N7	-3.59	106.48	110.58
10	h	602	ADP	N3-C2-N1	-3.59	123.15	128.58
10	b	602	ADP	C4-C5-N7	-3.58	106.49	110.58
10	p	602	ADP	N3-C2-N1	-3.58	123.17	128.58
10	i	602	ADP	C4-C5-N7	-3.57	106.50	110.58
10	o	602	ADP	C4-C5-N7	-3.57	106.50	110.58
10	I	602	ADP	N3-C2-N1	-3.55	123.21	128.58
10	c	1102	ADP	C4-C5-N7	-3.54	106.53	110.58
10	I	602	ADP	C4-C5-N7	-3.53	106.54	110.58
10	M	602	ADP	C4-C5-N7	-3.53	106.55	110.58
10	o	602	ADP	N3-C2-N1	-3.52	123.25	128.58
10	m	602	ADP	C4-C5-N7	-3.51	106.57	110.58
10	a	602	ADP	N3-C2-N1	-3.51	123.27	128.58
10	h	602	ADP	C4-C5-N7	-3.51	106.57	110.58
10	l	602	ADP	N3-C2-N1	-3.50	123.28	128.58
10	O	602	ADP	N3-C2-N1	-3.48	123.31	128.58
10	H	602	ADP	N3-C2-N1	-3.48	123.31	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	k	1102	ADP	C4-C5-N7	-3.47	106.61	110.58
10	P	602	ADP	N3-C2-N1	-3.47	123.33	128.58
10	i	602	ADP	N3-C2-N1	-3.46	123.34	128.58
10	g	602	ADP	N3-C2-N1	-3.44	123.38	128.58
10	H	602	ADP	C4-C5-N7	-3.44	106.65	110.58
10	G	602	ADP	N3-C2-N1	-3.43	123.39	128.58
10	d	602	ADP	C4-C5-N7	-3.42	106.67	110.58
10	l	602	ADP	C4-C5-N7	-3.42	106.67	110.58
10	N	602	ADP	N3-C2-N1	-3.41	123.42	128.58
10	n	602	ADP	N3-C2-N1	-3.40	123.43	128.58
10	K	1102	ADP	C4-C5-N7	-3.40	106.70	110.58
10	m	602	ADP	N3-C2-N1	-3.38	123.46	128.58
10	F	602	ADP	N3-C2-N1	-3.38	123.47	128.58
10	d	602	ADP	N3-C2-N1	-3.38	123.47	128.58
10	F	602	ADP	C4-C5-N7	-3.37	106.73	110.58
10	B	602	ADP	C4-C5-N7	-3.35	106.75	110.58
10	K	1102	ADP	N3-C2-N1	-3.34	123.53	128.58
10	f	602	ADP	N3-C2-N1	-3.34	123.53	128.58
10	D	602	ADP	N3-C2-N1	-3.33	123.55	128.58
10	L	602	ADP	N3-C2-N1	-3.32	123.56	128.58
10	C	1102	ADP	C4-C5-N7	-3.31	106.80	110.58
10	k	1102	ADP	N3-C2-N1	-3.29	123.60	128.58
10	A	602	ADP	N3-C2-N1	-3.29	123.60	128.58
10	j	602	ADP	N3-C2-N1	-3.29	123.60	128.58
10	B	602	ADP	N3-C2-N1	-3.28	123.61	128.58
10	J	602	ADP	N3-C2-N1	-3.27	123.62	128.58
10	E	602	ADP	C4-C5-N7	-3.26	106.86	110.58
10	e	602	ADP	N3-C2-N1	-3.25	123.66	128.58
10	g	602	ADP	C4-C5-N7	-3.23	106.89	110.58
10	C	1102	ADP	N3-C2-N1	-3.21	123.72	128.58
10	b	602	ADP	N3-C2-N1	-3.13	123.85	128.58
10	d	602	ADP	C4-N9-C8	3.09	108.99	105.74
10	c	1102	ADP	N3-C2-N1	-3.06	123.96	128.58
10	j	602	ADP	C4-C5-N7	-2.94	107.23	110.58
10	A	602	ADP	C5-N7-C8	2.79	107.84	103.45
10	j	602	ADP	C4-N9-C8	2.76	108.63	105.74
10	P	602	ADP	C5-N7-C8	2.76	107.78	103.45
10	p	602	ADP	C5-N7-C8	2.76	107.78	103.45
10	M	602	ADP	C4-N9-C8	2.74	108.62	105.74
10	G	602	ADP	C5-N7-C8	2.74	107.76	103.45
10	G	602	ADP	C4-N9-C8	2.72	108.60	105.74
10	D	602	ADP	C5-N7-C8	2.71	107.70	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	O	602	ADP	C5-N7-C8	2.69	107.69	103.45
10	J	602	ADP	C5-N7-C8	2.69	107.67	103.45
10	B	602	ADP	C4-N9-C8	2.67	108.55	105.74
10	L	602	ADP	C5-N7-C8	2.66	107.63	103.45
10	e	602	ADP	C5-N7-C8	2.65	107.61	103.45
10	E	602	ADP	C4-N9-C8	2.64	108.52	105.74
10	P	602	ADP	C4-N9-C8	2.64	108.52	105.74
10	h	602	ADP	C5-N7-C8	2.64	107.59	103.45
10	g	602	ADP	C3'-C2'-C1'	2.64	106.45	101.46
10	H	602	ADP	C4-N9-C8	2.62	108.49	105.74
10	m	602	ADP	C5-N7-C8	2.62	107.57	103.45
10	F	602	ADP	C4-N9-C8	2.62	108.49	105.74
10	K	1102	ADP	C4-N9-C8	2.62	108.48	105.74
10	d	602	ADP	C5-N7-C8	2.61	107.55	103.45
10	M	602	ADP	C5-N7-C8	2.59	107.53	103.45
10	N	602	ADP	C5-N7-C8	2.59	107.52	103.45
10	a	602	ADP	C5-N7-C8	2.58	107.51	103.45
10	o	602	ADP	C5-N7-C8	2.58	107.51	103.45
10	J	602	ADP	C3'-C2'-C1'	2.57	106.33	101.46
10	G	602	ADP	C3'-C2'-C1'	2.57	106.33	101.46
10	i	602	ADP	C3'-C2'-C1'	2.57	106.32	101.46
10	A	602	ADP	C6-C5-N7	2.56	137.03	132.09
10	h	602	ADP	C4-N9-C8	2.56	108.42	105.74
10	n	602	ADP	C5-N7-C8	2.55	107.46	103.45
10	o	602	ADP	C3'-C2'-C1'	2.54	106.26	101.46
10	f	602	ADP	C5-N7-C8	2.53	107.43	103.45
10	I	602	ADP	C5-N7-C8	2.52	107.41	103.45
10	B	602	ADP	C5-N7-C8	2.52	107.40	103.45
10	O	602	ADP	C3'-C2'-C1'	2.51	106.21	101.46
10	m	602	ADP	C4-N9-C8	2.50	108.37	105.74
10	H	602	ADP	C5-N7-C8	2.50	107.38	103.45
10	c	1102	ADP	C5-N7-C8	2.50	107.38	103.45
10	l	602	ADP	C5-N7-C8	2.49	107.36	103.45
10	b	602	ADP	C5-N7-C8	2.48	107.35	103.45
10	f	602	ADP	O4'-C1'-N9	2.48	112.84	108.09
10	l	602	ADP	C3'-C2'-C1'	2.47	106.14	101.46
10	p	602	ADP	C4-N9-C8	2.46	108.33	105.74
10	F	602	ADP	C5-N7-C8	2.46	107.31	103.45
10	L	602	ADP	C4-N9-C8	2.46	108.32	105.74
10	E	602	ADP	C5-N7-C8	2.45	107.30	103.45
10	N	602	ADP	C4-N9-C8	2.44	108.30	105.74
10	e	602	ADP	C4-N9-C8	2.44	108.30	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	i	602	ADP	C5-N7-C8	2.44	107.28	103.45
10	I	602	ADP	C4-N9-C8	2.40	108.25	105.74
10	k	1102	ADP	C5-N7-C8	2.38	107.20	103.45
10	D	602	ADP	C4-N9-C8	2.38	108.24	105.74
10	a	602	ADP	C6-C5-N7	2.38	136.68	132.09
10	K	1102	ADP	C5-N7-C8	2.38	107.19	103.45
10	L	602	ADP	C6-C5-N7	2.36	136.63	132.09
10	L	602	ADP	C3'-C2'-C1'	2.35	105.91	101.46
10	J	602	ADP	C6-C5-N7	2.34	136.60	132.09
10	a	602	ADP	C4-N9-C8	2.34	108.19	105.74
10	b	602	ADP	C4-N9-C8	2.34	108.19	105.74
10	I	602	ADP	C6-C5-N7	2.33	136.59	132.09
10	M	602	ADP	C6-C5-N7	2.33	136.59	132.09
10	N	602	ADP	C6-C5-N7	2.33	136.58	132.09
10	g	602	ADP	C5-N7-C8	2.32	107.09	103.45
10	A	602	ADP	C3'-C2'-C1'	2.32	105.85	101.46
10	D	602	ADP	C6-C5-N7	2.31	136.55	132.09
10	m	602	ADP	C3'-C2'-C1'	2.30	105.82	101.46
10	l	602	ADP	C4-N9-C8	2.30	108.15	105.74
10	K	1102	ADP	C6-C5-N7	2.30	136.52	132.09
10	d	602	ADP	C6-C5-N7	2.29	136.51	132.09
10	O	602	ADP	C6-C5-N7	2.28	136.50	132.09
10	n	602	ADP	C6-C5-N7	2.28	136.49	132.09
10	e	602	ADP	C3'-C2'-C1'	2.28	105.77	101.46
10	H	602	ADP	C3'-C2'-C1'	2.27	105.75	101.46
10	P	602	ADP	C6-C5-N7	2.26	136.46	132.09
10	h	602	ADP	C6-C5-N7	2.26	136.46	132.09
10	F	602	ADP	C6-C5-N7	2.26	136.44	132.09
10	i	602	ADP	C6-C5-N7	2.25	136.43	132.09
10	C	1102	ADP	C5-N7-C8	2.25	106.99	103.45
10	e	602	ADP	C6-C5-N7	2.24	136.41	132.09
10	G	602	ADP	C6-C5-N7	2.24	136.40	132.09
10	E	602	ADP	C2'-C3'-C4'	2.23	106.93	102.61
10	k	1102	ADP	C3'-C2'-C1'	2.23	105.69	101.46
10	l	602	ADP	C6-C5-N7	2.23	136.39	132.09
10	p	602	ADP	C6-C5-N7	2.22	136.37	132.09
10	A	602	ADP	C4-N9-C8	2.22	108.07	105.74
10	d	602	ADP	N9-C8-N7	-2.22	110.79	113.94
10	o	602	ADP	C6-C5-N7	2.21	136.36	132.09
10	P	602	ADP	C3'-C2'-C1'	2.21	105.65	101.46
10	j	602	ADP	C5-N7-C8	2.20	106.91	103.45
10	p	602	ADP	C3'-C2'-C1'	2.20	105.62	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	602	ADP	C3'-C2'-C1'	2.19	105.60	101.46
10	H	602	ADP	C6-C5-N7	2.17	136.28	132.09
10	f	602	ADP	C3'-C2'-C1'	2.17	105.57	101.46
10	M	602	ADP	C3'-C2'-C1'	2.15	105.53	101.46
10	p	602	ADP	O4'-C1'-N9	2.15	112.22	108.09
10	K	1102	ADP	C2'-C3'-C4'	2.13	106.73	102.61
10	B	602	ADP	C6-C5-N7	2.12	136.18	132.09
10	b	602	ADP	C6-C5-N7	2.12	136.18	132.09
10	n	602	ADP	C4-N9-C8	2.12	107.96	105.74
10	o	602	ADP	O4'-C1'-N9	2.11	112.14	108.09
10	J	602	ADP	C4-N9-C8	2.11	107.95	105.74
10	m	602	ADP	C6-C5-N7	2.09	136.12	132.09
10	k	1102	ADP	C6-C5-N7	2.08	136.11	132.09
10	C	1102	ADP	C4-N9-C8	2.08	107.92	105.74
10	c	1102	ADP	C4-N9-C8	2.08	107.92	105.74
10	C	1102	ADP	C3'-C2'-C1'	2.07	105.39	101.46
10	P	602	ADP	N9-C8-N7	-2.07	111.00	113.94
10	G	602	ADP	N9-C8-N7	-2.07	111.01	113.94
10	B	602	ADP	N9-C8-N7	-2.06	111.02	113.94
10	M	602	ADP	N9-C8-N7	-2.05	111.03	113.94
10	o	602	ADP	C2'-C3'-C4'	2.04	106.56	102.61
10	f	602	ADP	C6-C5-N7	2.04	136.03	132.09
10	E	602	ADP	C6-C5-N7	2.04	136.02	132.09
10	h	602	ADP	N9-C8-N7	-2.03	111.05	113.94
10	O	602	ADP	C4-N9-C8	2.03	107.87	105.74
10	C	1102	ADP	C6-C5-N7	2.03	135.99	132.09
10	D	602	ADP	N9-C8-N7	-2.00	111.10	113.94

There are no chirality outliers.

All (146) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	F	602	ADP	C5'-O5'-PA-O1A
10	F	602	ADP	C5'-O5'-PA-O2A
10	F	602	ADP	C5'-O5'-PA-O3A
10	G	602	ADP	C5'-O5'-PA-O1A
10	E	602	ADP	C5'-O5'-PA-O3A
10	D	602	ADP	C5'-O5'-PA-O2A
10	D	602	ADP	C5'-O5'-PA-O3A
10	A	602	ADP	C5'-O5'-PA-O3A
10	N	602	ADP	C5'-O5'-PA-O1A
10	N	602	ADP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
10	N	602	ADP	C5'-O5'-PA-O3A
10	O	602	ADP	C5'-O5'-PA-O1A
10	M	602	ADP	C5'-O5'-PA-O1A
10	M	602	ADP	C5'-O5'-PA-O2A
10	M	602	ADP	C5'-O5'-PA-O3A
10	M	602	ADP	C3'-C4'-C5'-O5'
10	L	602	ADP	C5'-O5'-PA-O1A
10	L	602	ADP	C5'-O5'-PA-O2A
10	L	602	ADP	C5'-O5'-PA-O3A
10	I	602	ADP	PB-O3A-PA-O5'
10	I	602	ADP	C5'-O5'-PA-O3A
10	I	602	ADP	O4'-C4'-C5'-O5'
10	I	602	ADP	C3'-C4'-C5'-O5'
10	f	602	ADP	C5'-O5'-PA-O3A
10	f	602	ADP	C3'-C4'-C5'-O5'
10	g	602	ADP	PB-O3A-PA-O5'
10	g	602	ADP	C5'-O5'-PA-O3A
10	g	602	ADP	O4'-C4'-C5'-O5'
10	g	602	ADP	C3'-C4'-C5'-O5'
10	e	602	ADP	C5'-O5'-PA-O1A
10	e	602	ADP	C5'-O5'-PA-O3A
10	e	602	ADP	O4'-C4'-C5'-O5'
10	d	602	ADP	PB-O3A-PA-O5'
10	d	602	ADP	C5'-O5'-PA-O1A
10	d	602	ADP	C5'-O5'-PA-O2A
10	d	602	ADP	C5'-O5'-PA-O3A
10	a	602	ADP	C5'-O5'-PA-O3A
10	a	602	ADP	O4'-C4'-C5'-O5'
10	a	602	ADP	C3'-C4'-C5'-O5'
10	n	602	ADP	C5'-O5'-PA-O1A
10	n	602	ADP	C5'-O5'-PA-O2A
10	n	602	ADP	C5'-O5'-PA-O3A
10	p	602	ADP	PA-O3A-PB-O3B
10	o	602	ADP	PB-O3A-PA-O5'
10	o	602	ADP	C5'-O5'-PA-O1A
10	m	602	ADP	C5'-O5'-PA-O1A
10	m	602	ADP	C5'-O5'-PA-O2A
10	m	602	ADP	C5'-O5'-PA-O3A
10	m	602	ADP	O4'-C4'-C5'-O5'
10	m	602	ADP	C3'-C4'-C5'-O5'
10	l	602	ADP	PA-O3A-PB-O3B
10	l	602	ADP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
10	l	602	ADP	C5'-O5'-PA-O3A
10	i	602	ADP	C5'-O5'-PA-O1A
10	i	602	ADP	C5'-O5'-PA-O2A
10	i	602	ADP	C5'-O5'-PA-O3A
10	G	602	ADP	O4'-C4'-C5'-O5'
10	E	602	ADP	O4'-C4'-C5'-O5'
10	E	602	ADP	C3'-C4'-C5'-O5'
10	D	602	ADP	C3'-C4'-C5'-O5'
10	A	602	ADP	C3'-C4'-C5'-O5'
10	N	602	ADP	C3'-C4'-C5'-O5'
10	L	602	ADP	C3'-C4'-C5'-O5'
10	e	602	ADP	C3'-C4'-C5'-O5'
10	d	602	ADP	C3'-C4'-C5'-O5'
10	n	602	ADP	C3'-C4'-C5'-O5'
10	l	602	ADP	C3'-C4'-C5'-O5'
10	i	602	ADP	C3'-C4'-C5'-O5'
10	F	602	ADP	C3'-C4'-C5'-O5'
10	G	602	ADP	C3'-C4'-C5'-O5'
10	A	602	ADP	O4'-C4'-C5'-O5'
10	N	602	ADP	O4'-C4'-C5'-O5'
10	O	602	ADP	O4'-C4'-C5'-O5'
10	M	602	ADP	O4'-C4'-C5'-O5'
10	L	602	ADP	O4'-C4'-C5'-O5'
10	f	602	ADP	O4'-C4'-C5'-O5'
10	d	602	ADP	O4'-C4'-C5'-O5'
10	n	602	ADP	O4'-C4'-C5'-O5'
10	o	602	ADP	O4'-C4'-C5'-O5'
10	i	602	ADP	O4'-C4'-C5'-O5'
10	O	602	ADP	C3'-C4'-C5'-O5'
10	o	602	ADP	C3'-C4'-C5'-O5'
10	D	602	ADP	O4'-C4'-C5'-O5'
10	l	602	ADP	O4'-C4'-C5'-O5'
10	F	602	ADP	O4'-C4'-C5'-O5'
10	G	602	ADP	PB-O3A-PA-O5'
10	D	602	ADP	PB-O3A-PA-O5'
10	A	602	ADP	PB-O3A-PA-O5'
10	O	602	ADP	PB-O3A-PA-O5'
10	a	602	ADP	PB-O3A-PA-O5'
10	i	602	ADP	PB-O3A-PA-O5'
10	M	602	ADP	PA-O3A-PB-O1B
10	f	602	ADP	PA-O3A-PB-O1B
10	e	602	ADP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
10	n	602	ADP	PA-O3A-PB-O1B
10	J	602	ADP	C3'-C4'-C5'-O5'
10	c	1102	ADP	PB-O3A-PA-O2A
10	j	602	ADP	PB-O3A-PA-O2A
10	E	602	ADP	C5'-O5'-PA-O1A
10	D	602	ADP	C5'-O5'-PA-O1A
10	A	602	ADP	C5'-O5'-PA-O1A
10	I	602	ADP	C5'-O5'-PA-O1A
10	f	602	ADP	C5'-O5'-PA-O1A
10	g	602	ADP	C5'-O5'-PA-O1A
10	e	602	ADP	C5'-O5'-PA-O2A
10	a	602	ADP	C5'-O5'-PA-O1A
10	l	602	ADP	C5'-O5'-PA-O1A
10	N	602	ADP	PA-O3A-PB-O1B
10	G	602	ADP	PB-O3A-PA-O1A
10	B	602	ADP	PB-O3A-PA-O2A
10	C	1102	ADP	PB-O3A-PA-O2A
10	K	1102	ADP	PB-O3A-PA-O2A
10	b	602	ADP	PB-O3A-PA-O2A
10	k	1102	ADP	PB-O3A-PA-O2A
10	b	602	ADP	C3'-C4'-C5'-O5'
10	F	602	ADP	PA-O3A-PB-O1B
10	E	602	ADP	PA-O3A-PB-O1B
10	m	602	ADP	PA-O3A-PB-O1B
10	J	602	ADP	PB-O3A-PA-O2A
10	L	602	ADP	PB-O3A-PA-O5'
10	B	602	ADP	C3'-C4'-C5'-O5'
10	F	602	ADP	PA-O3A-PB-O2B
10	F	602	ADP	PA-O3A-PB-O3B
10	H	602	ADP	PA-O3A-PB-O3B
10	E	602	ADP	PA-O3A-PB-O2B
10	E	602	ADP	PA-O3A-PB-O3B
10	N	602	ADP	PA-O3A-PB-O2B
10	N	602	ADP	PA-O3A-PB-O3B
10	P	602	ADP	PA-O3A-PB-O3B
10	M	602	ADP	PA-O3A-PB-O2B
10	M	602	ADP	PA-O3A-PB-O3B
10	L	602	ADP	PA-O3A-PB-O3B
10	f	602	ADP	PA-O3A-PB-O2B
10	f	602	ADP	PA-O3A-PB-O3B
10	h	602	ADP	PA-O3A-PB-O3B
10	e	602	ADP	PA-O3A-PB-O2B

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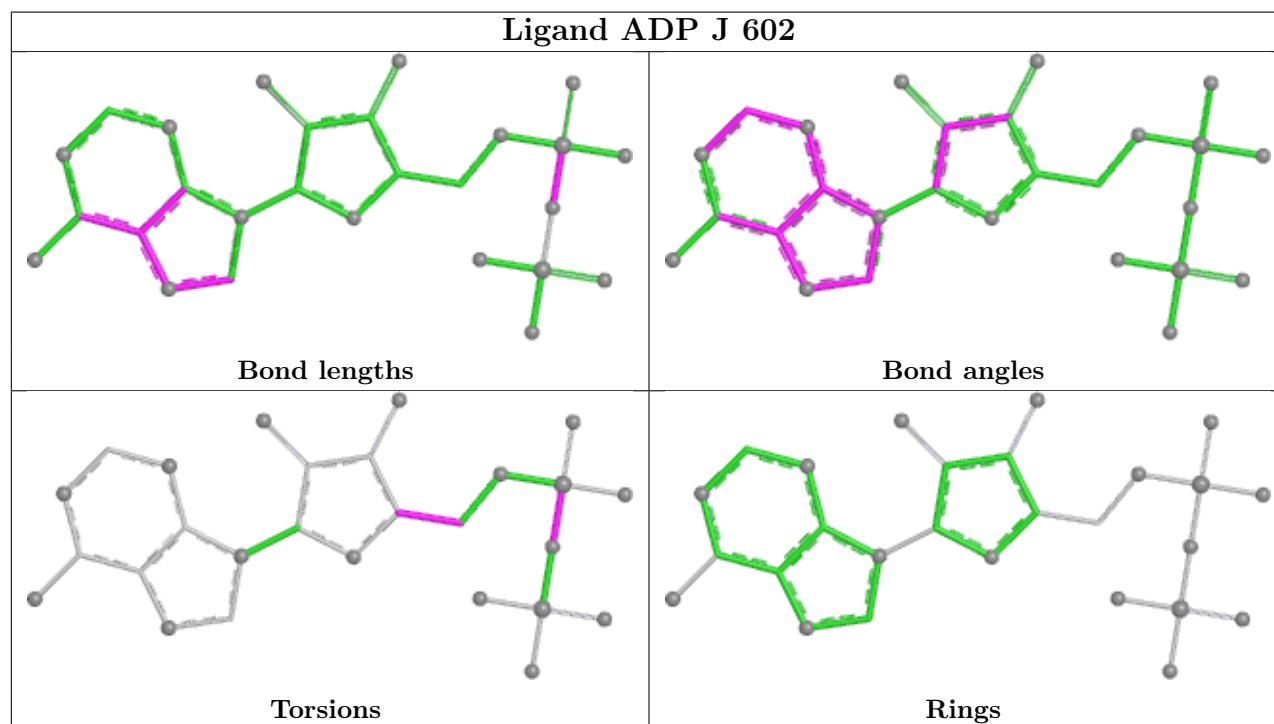
Mol	Chain	Res	Type	Atoms
10	e	602	ADP	PA-O3A-PB-O3B
10	n	602	ADP	PA-O3A-PB-O2B
10	n	602	ADP	PA-O3A-PB-O3B
10	o	602	ADP	PA-O3A-PB-O3B
10	m	602	ADP	PA-O3A-PB-O2B
10	B	602	ADP	PB-O3A-PA-O1A
10	C	1102	ADP	PB-O3A-PA-O1A
10	c	1102	ADP	PB-O3A-PA-O1A
10	j	602	ADP	PB-O3A-PA-O1A
10	k	1102	ADP	PB-O3A-PA-O1A

There are no ring outliers.

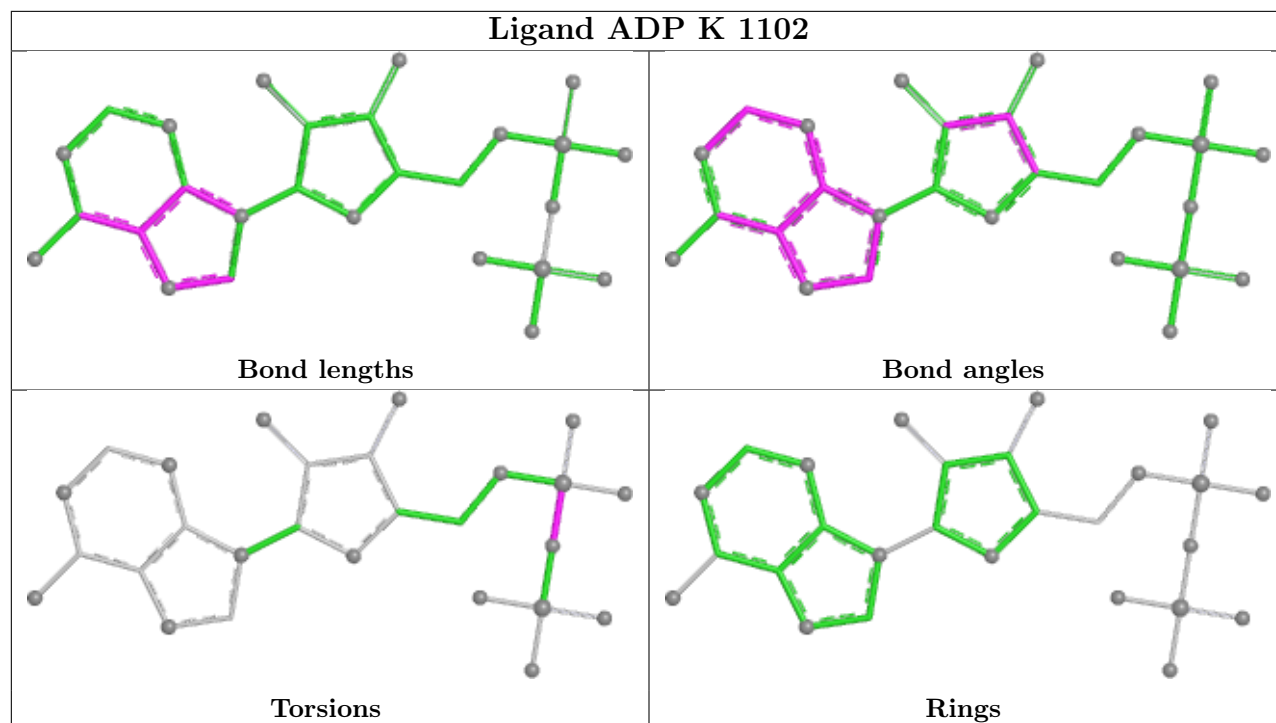
26 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	J	602	ADP	1	0
10	K	1102	ADP	1	0
10	I	602	ADP	1	0
11	K	1103	BEF	1	0
10	E	602	ADP	1	0
11	g	603	BEF	1	0
10	a	602	ADP	1	0
11	J	603	BEF	1	0
10	j	602	ADP	1	0
10	C	1102	ADP	1	0
11	b	603	BEF	2	0
10	D	602	ADP	1	0
11	E	603	BEF	1	0
10	B	602	ADP	1	0
10	c	1102	ADP	4	0
10	M	602	ADP	1	0
10	k	1102	ADP	1	0
11	M	603	BEF	1	0
11	c	1103	BEF	1	0
11	d	603	BEF	1	0
10	d	602	ADP	1	0
10	b	602	ADP	3	0
11	o	603	BEF	1	0
11	D	603	BEF	1	0
11	C	1103	BEF	1	0
11	k	1103	BEF	1	0

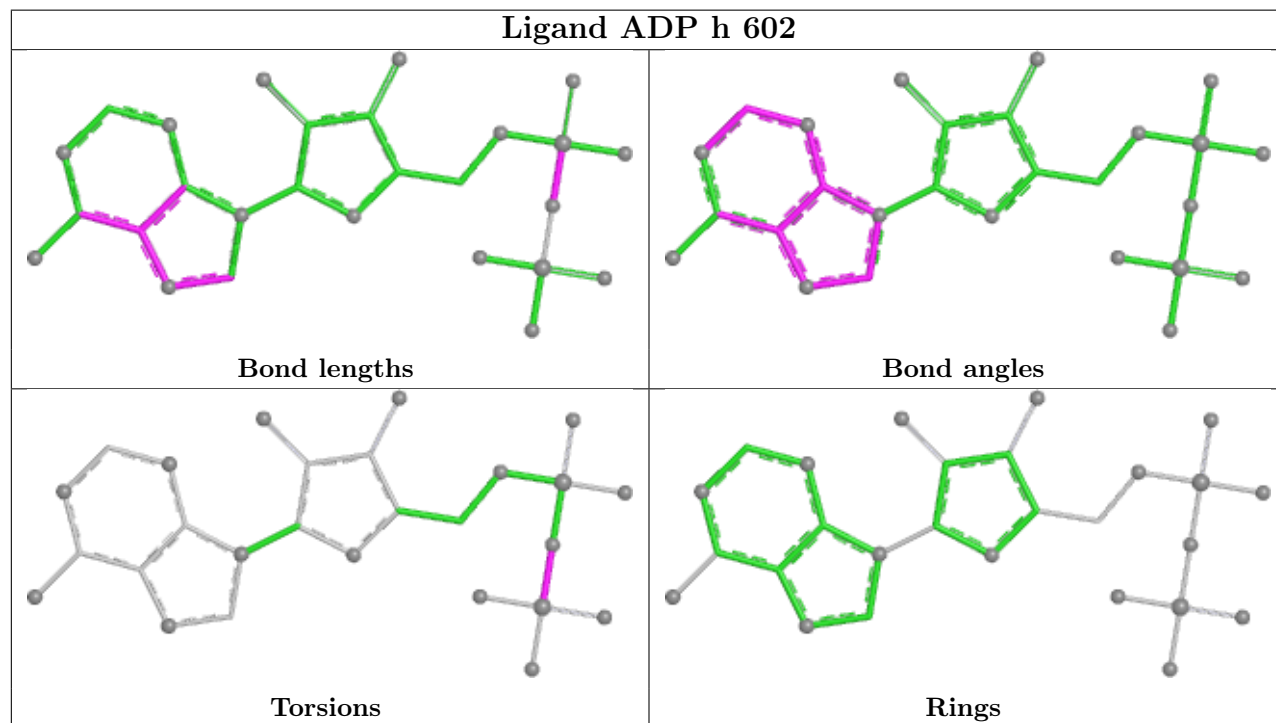
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

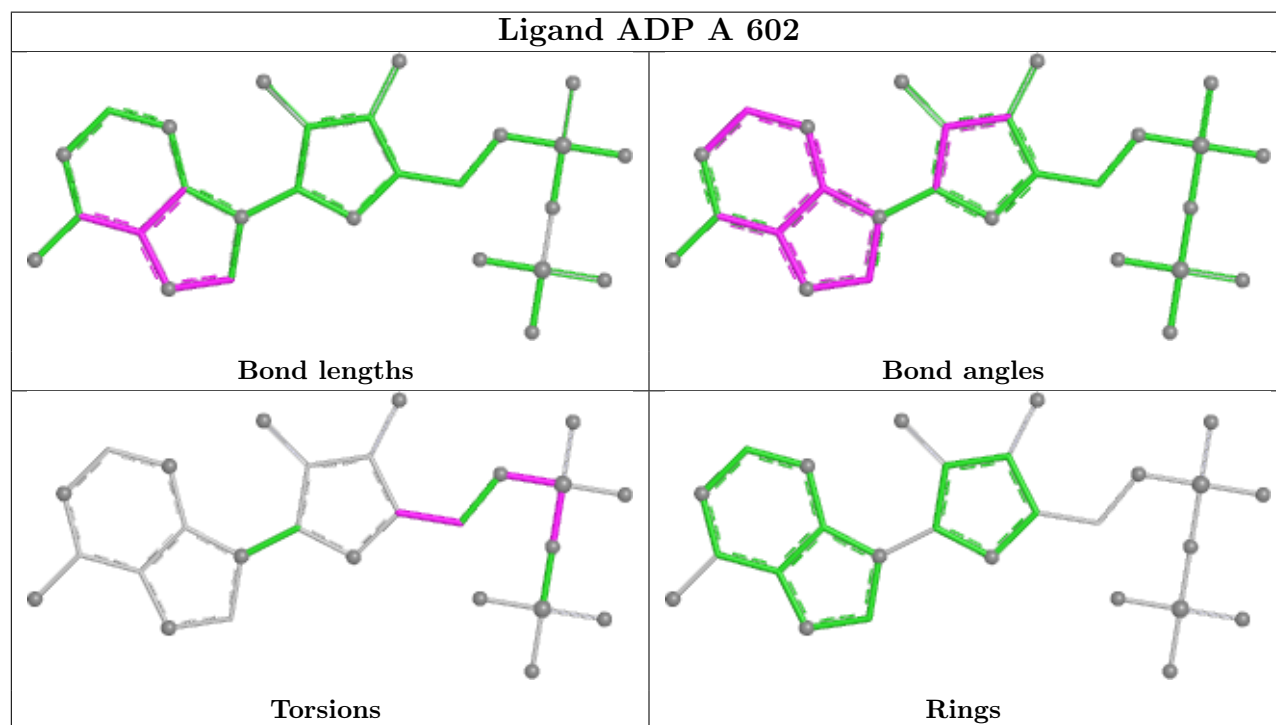
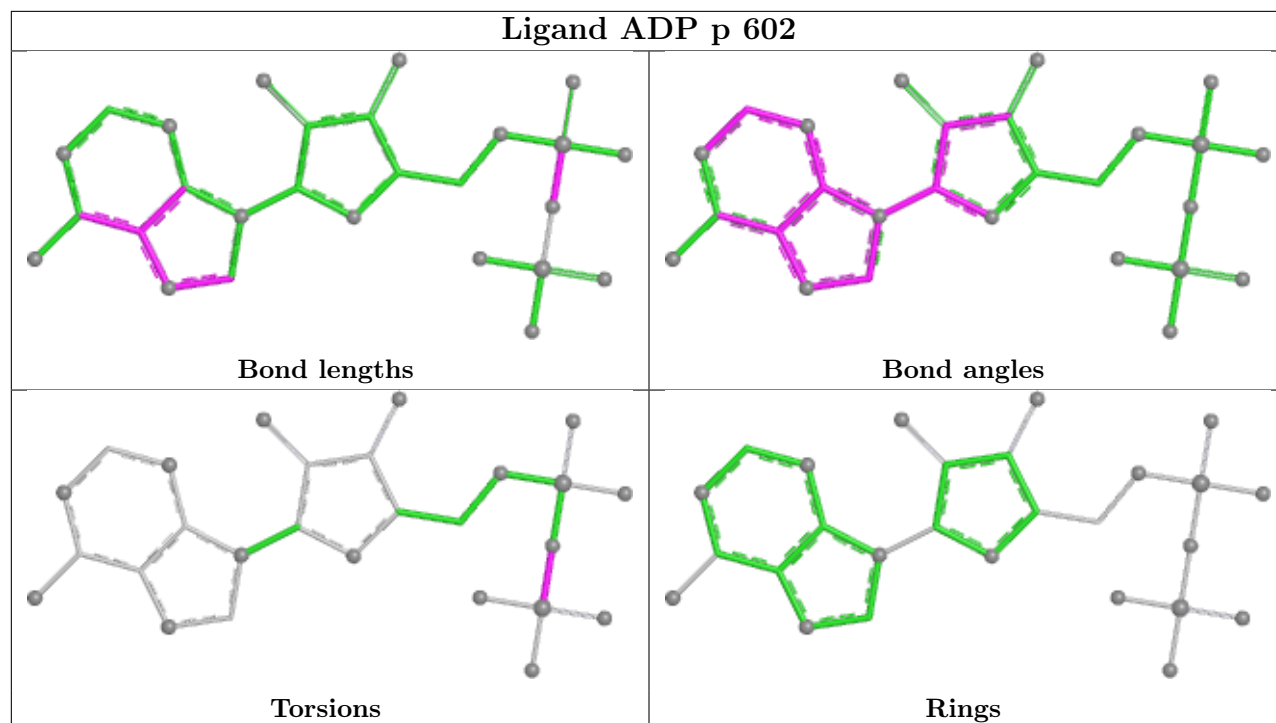


Ligand ADP K 1102

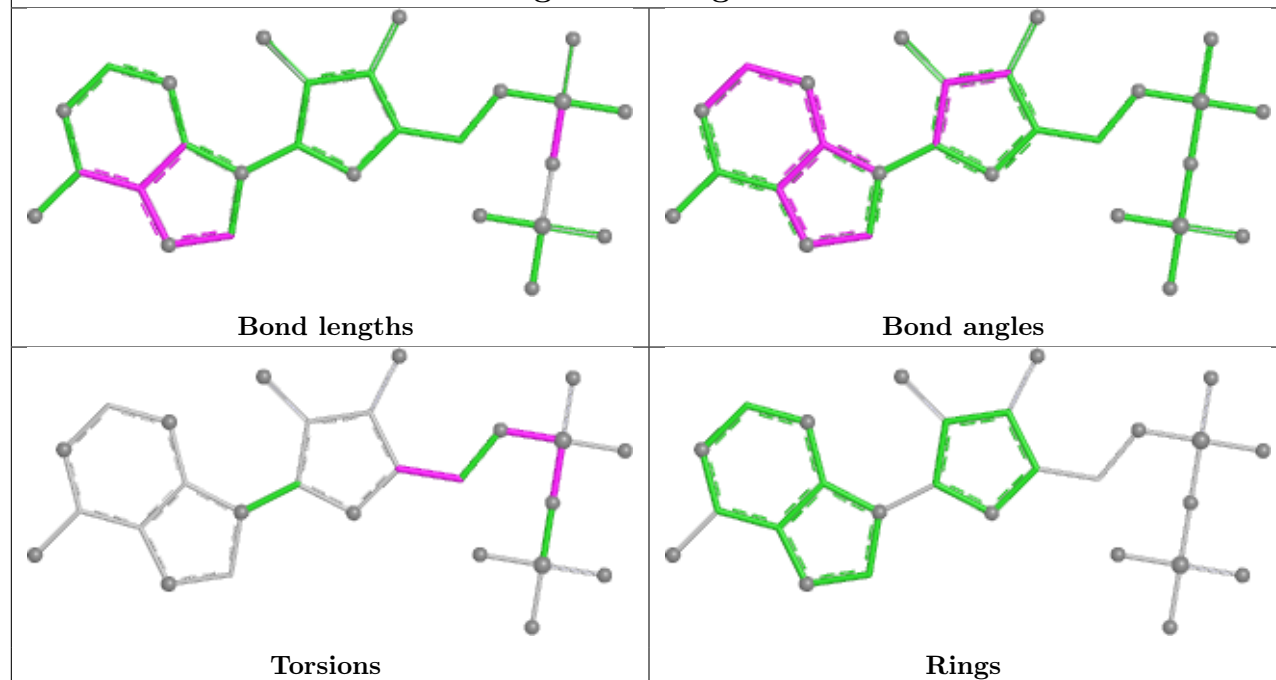


Ligand ADP h 602

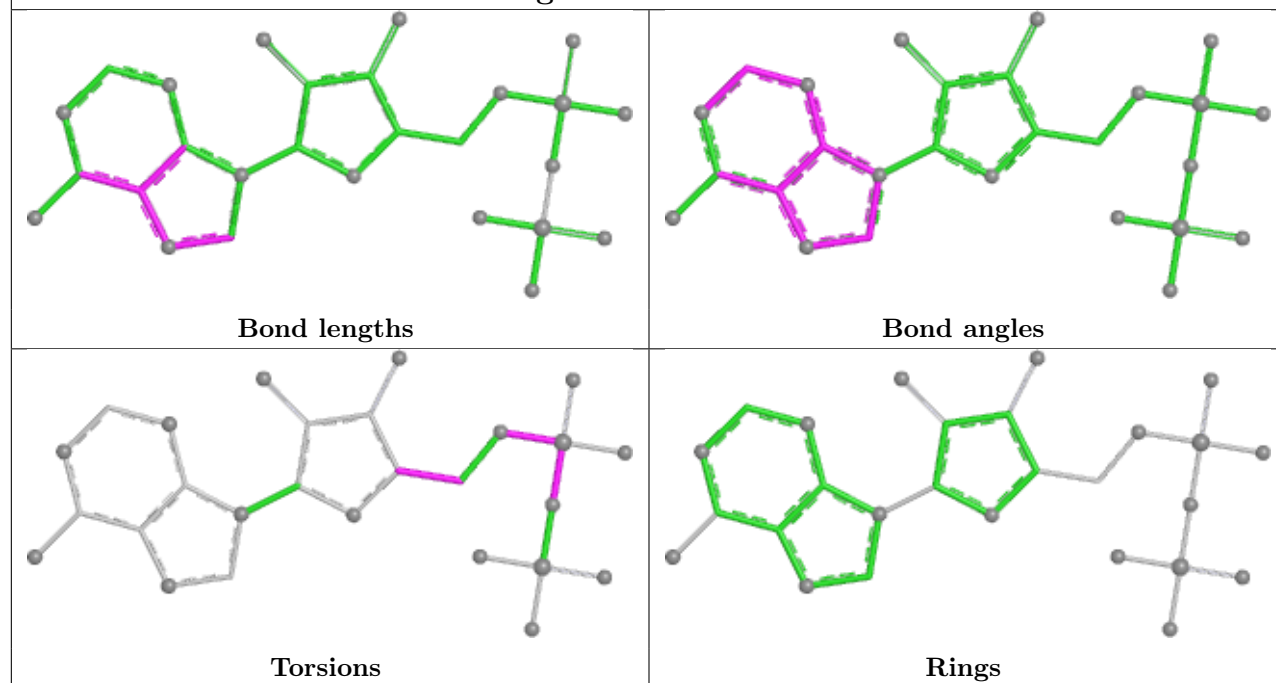




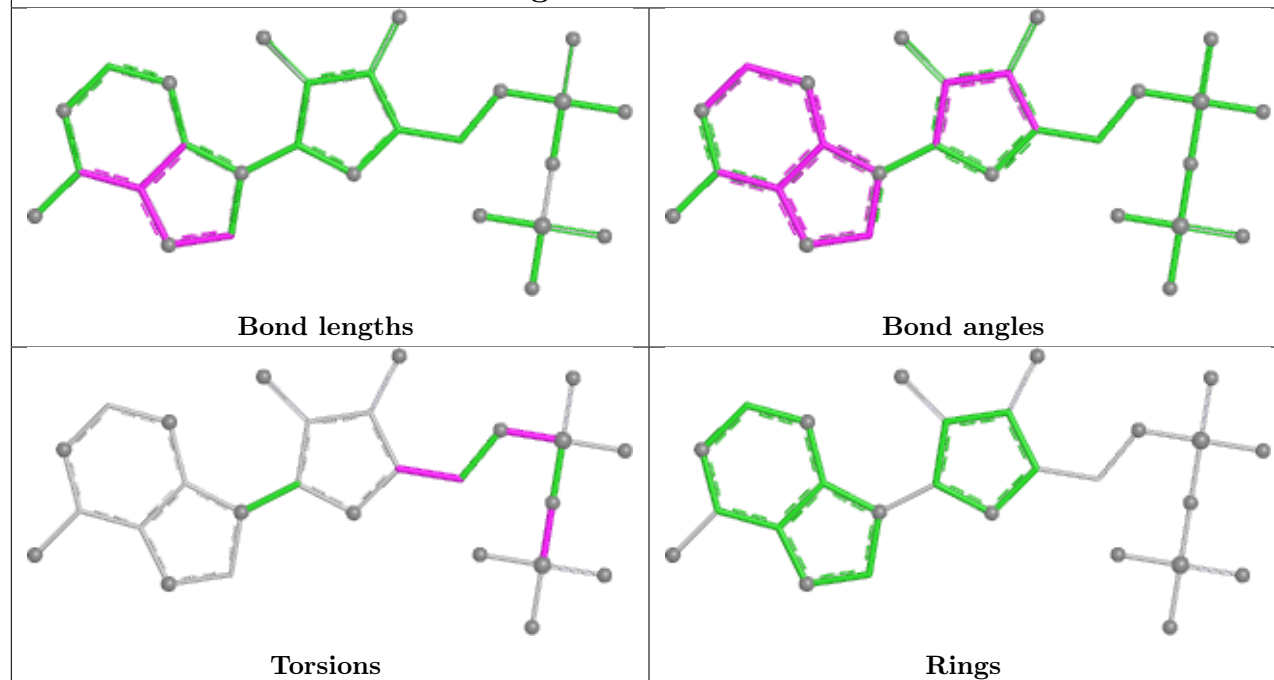
Ligand ADP g 602



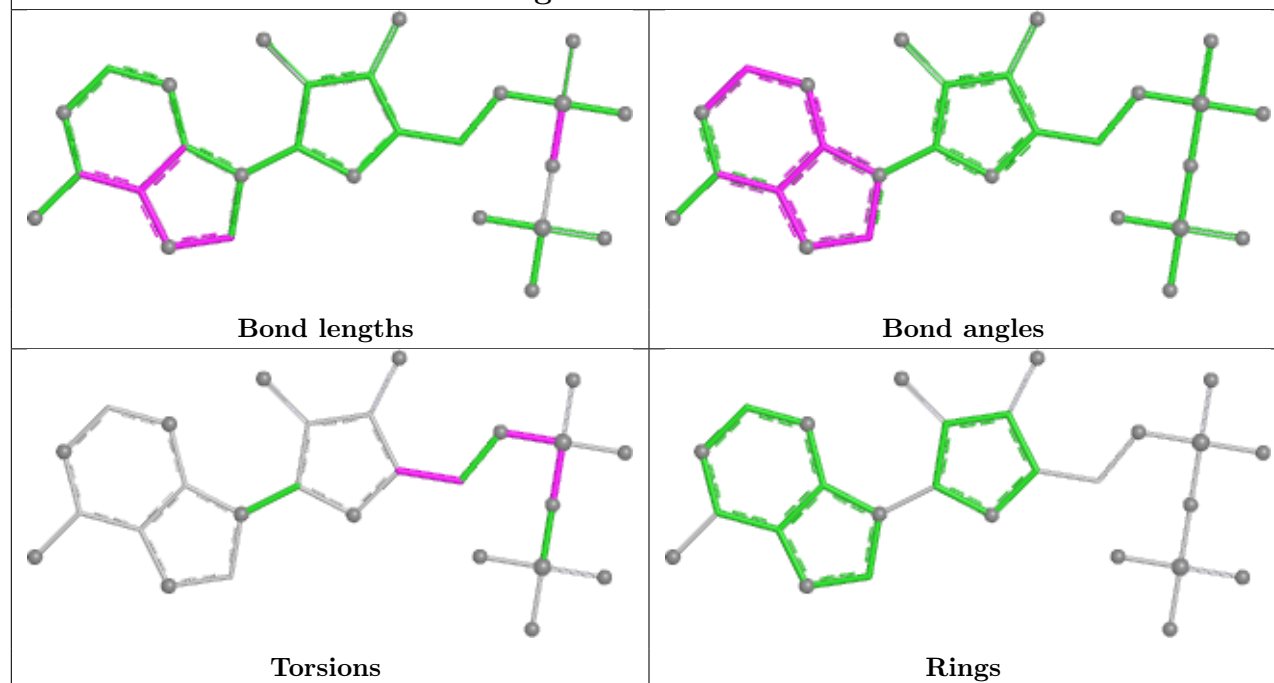
Ligand ADP I 602



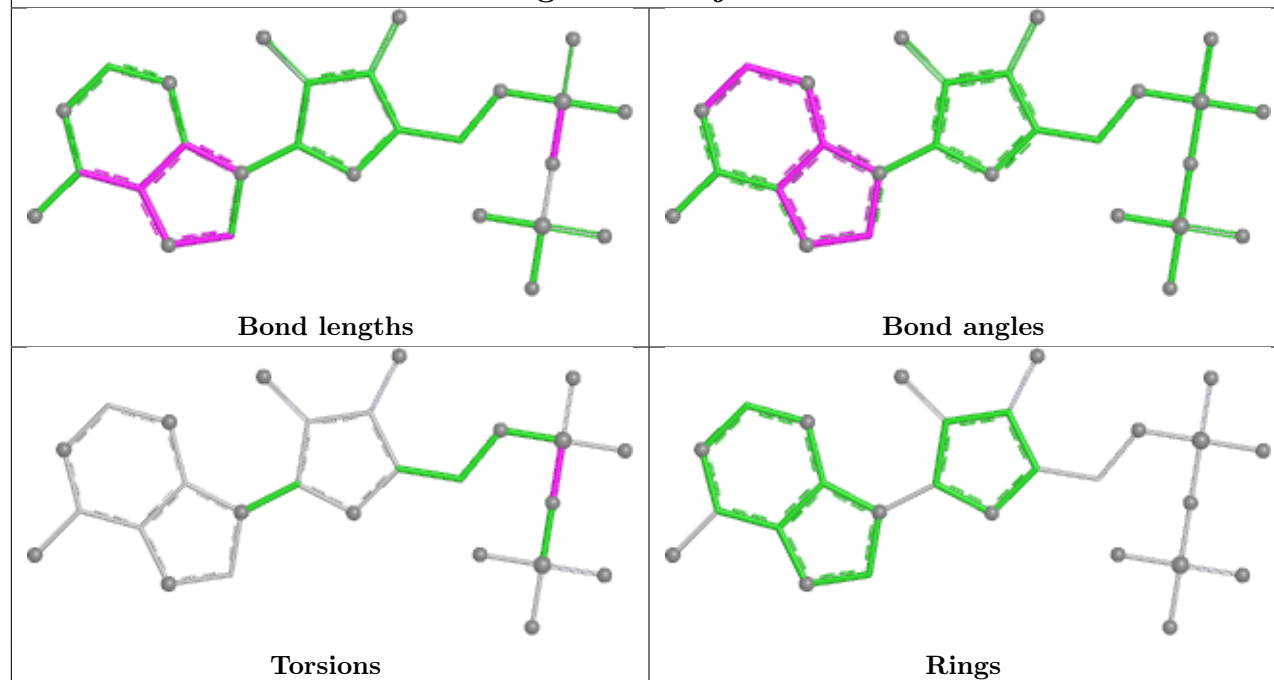
Ligand ADP E 602



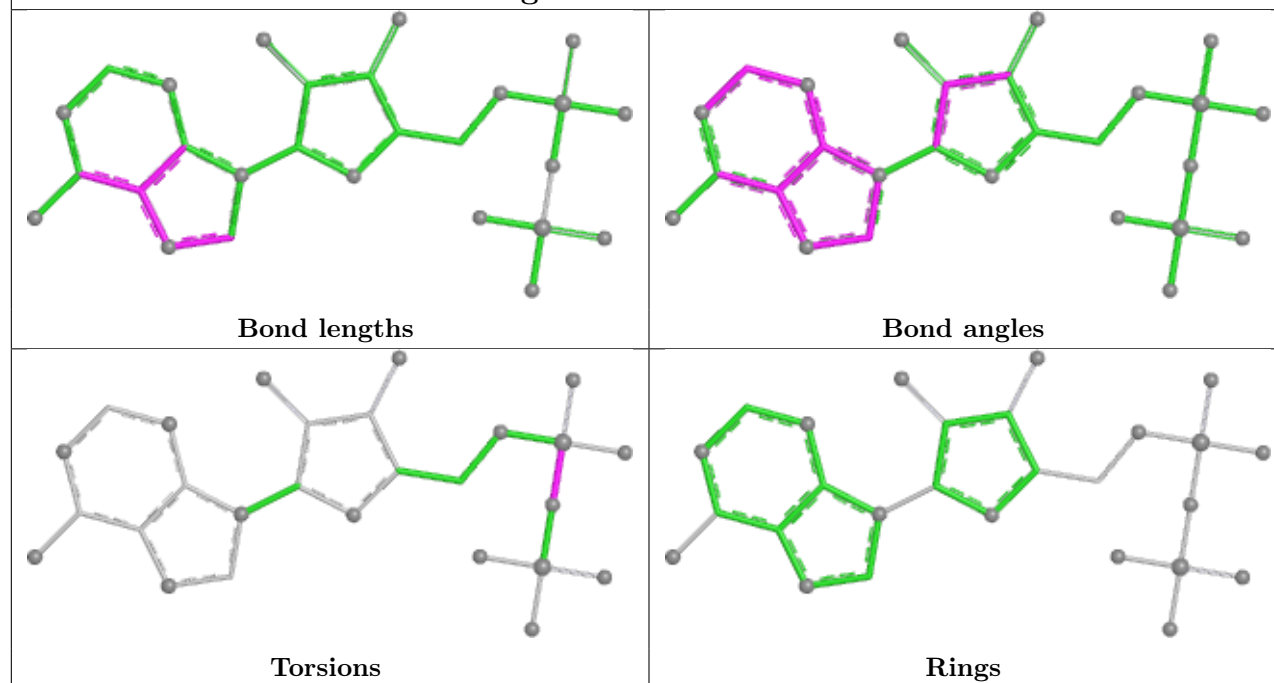
Ligand ADP a 602



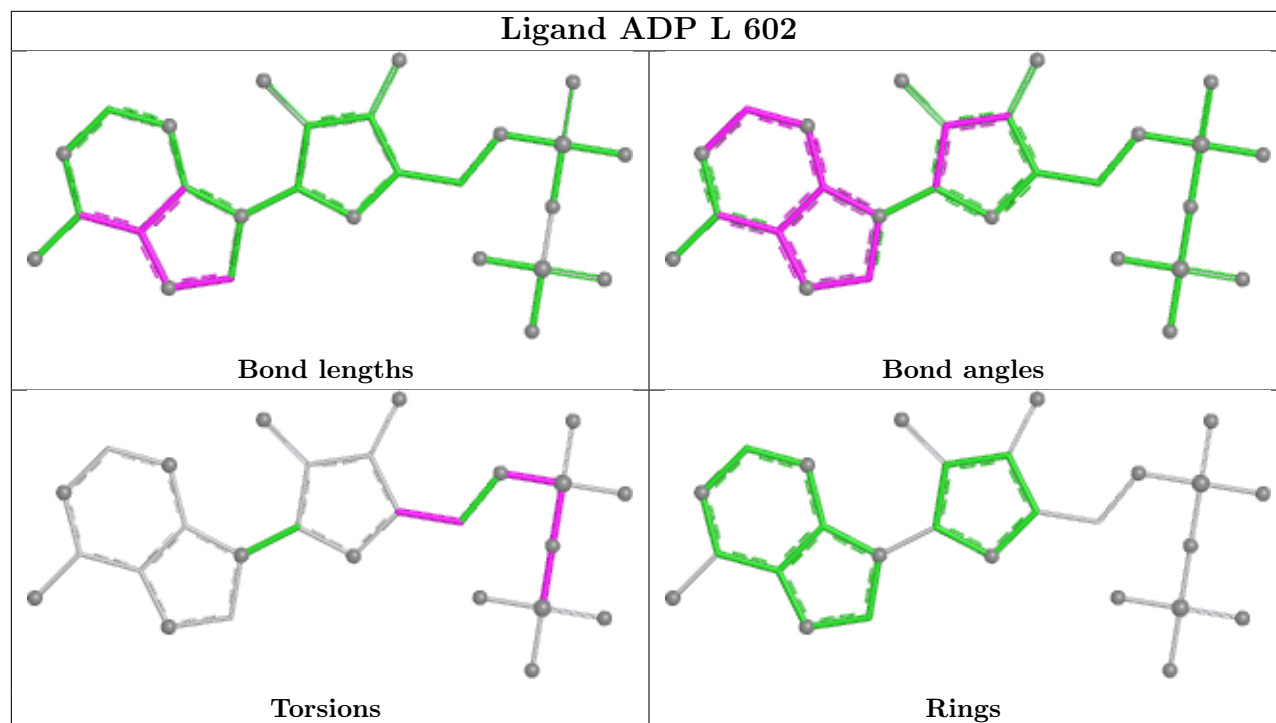
Ligand ADP j 602



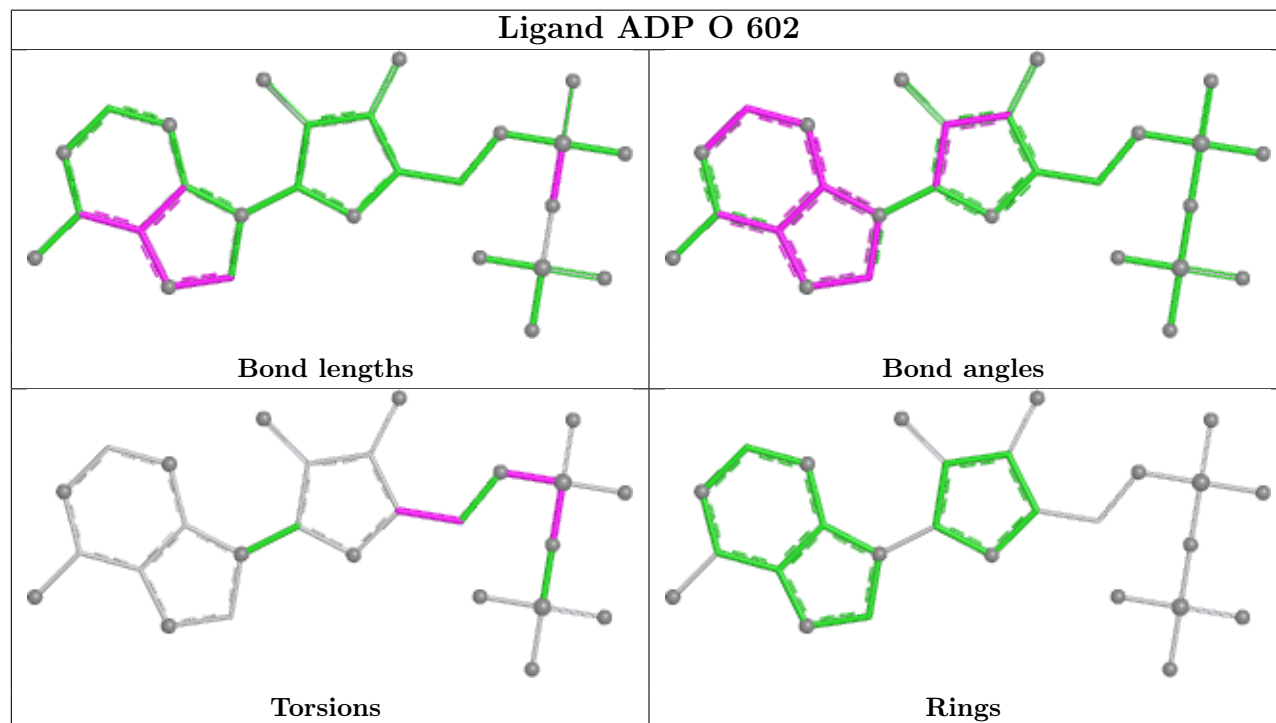
Ligand ADP C 1102

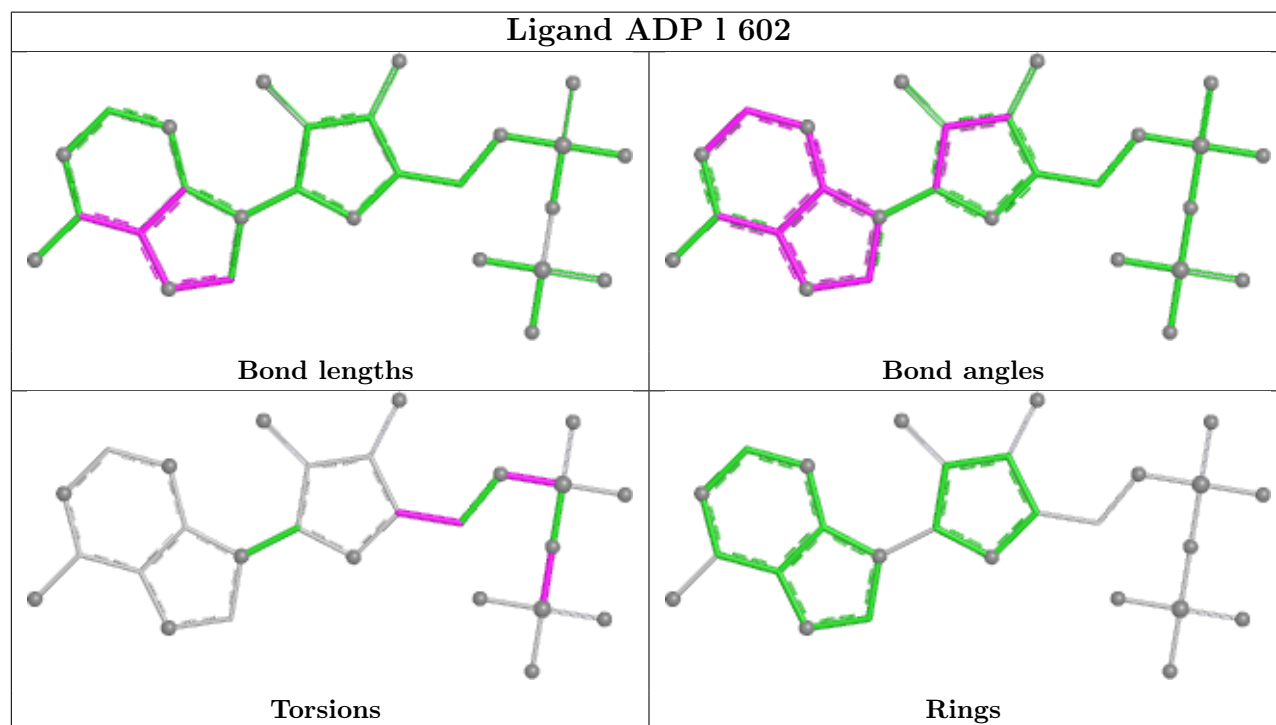
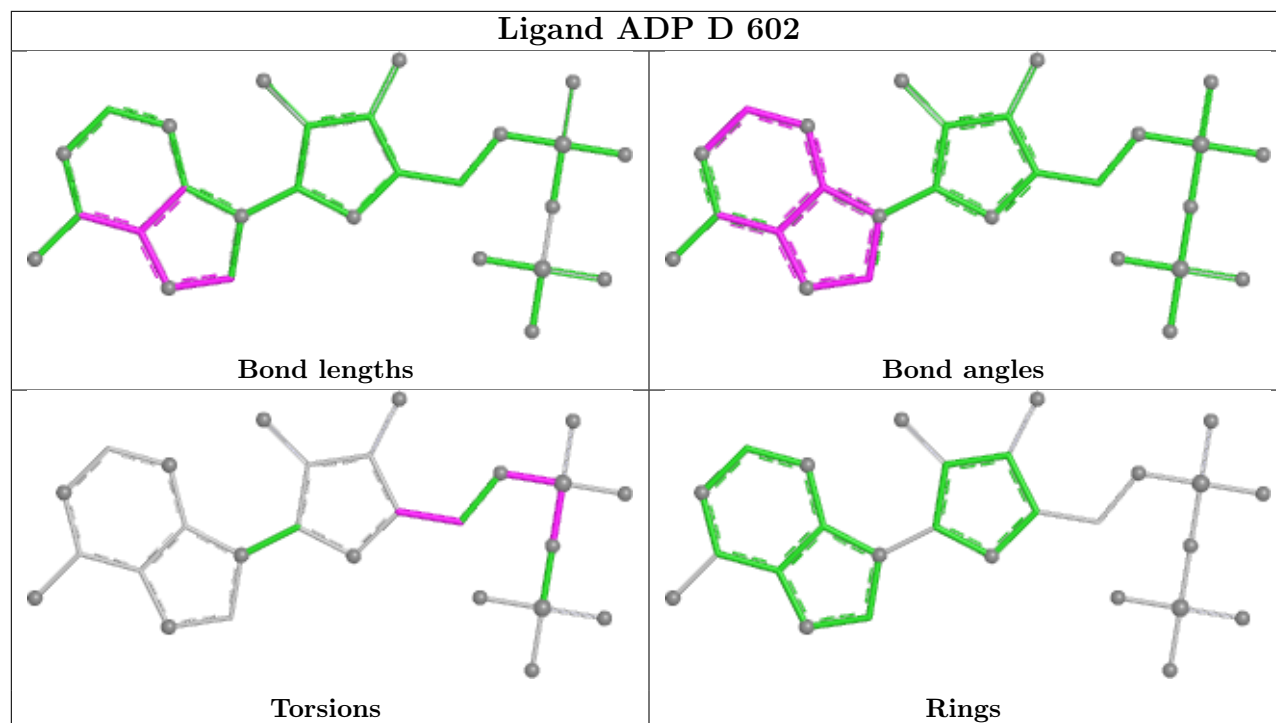


Ligand ADP L 602

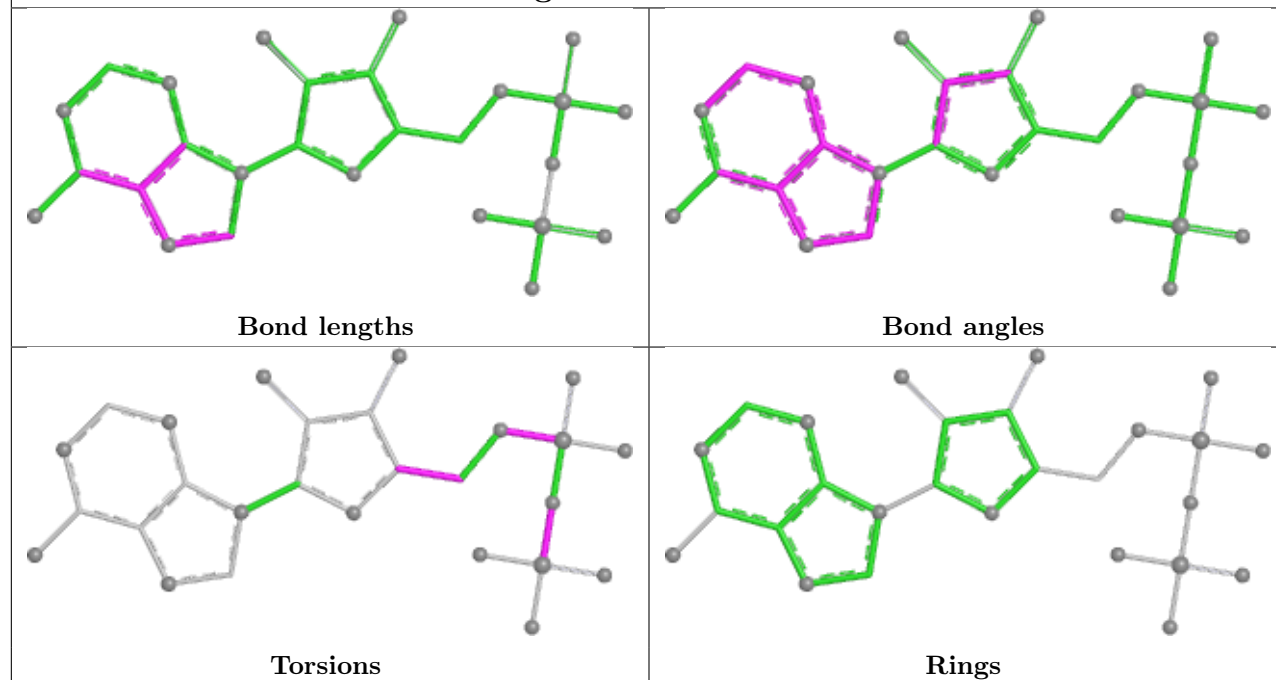


Ligand ADP O 602

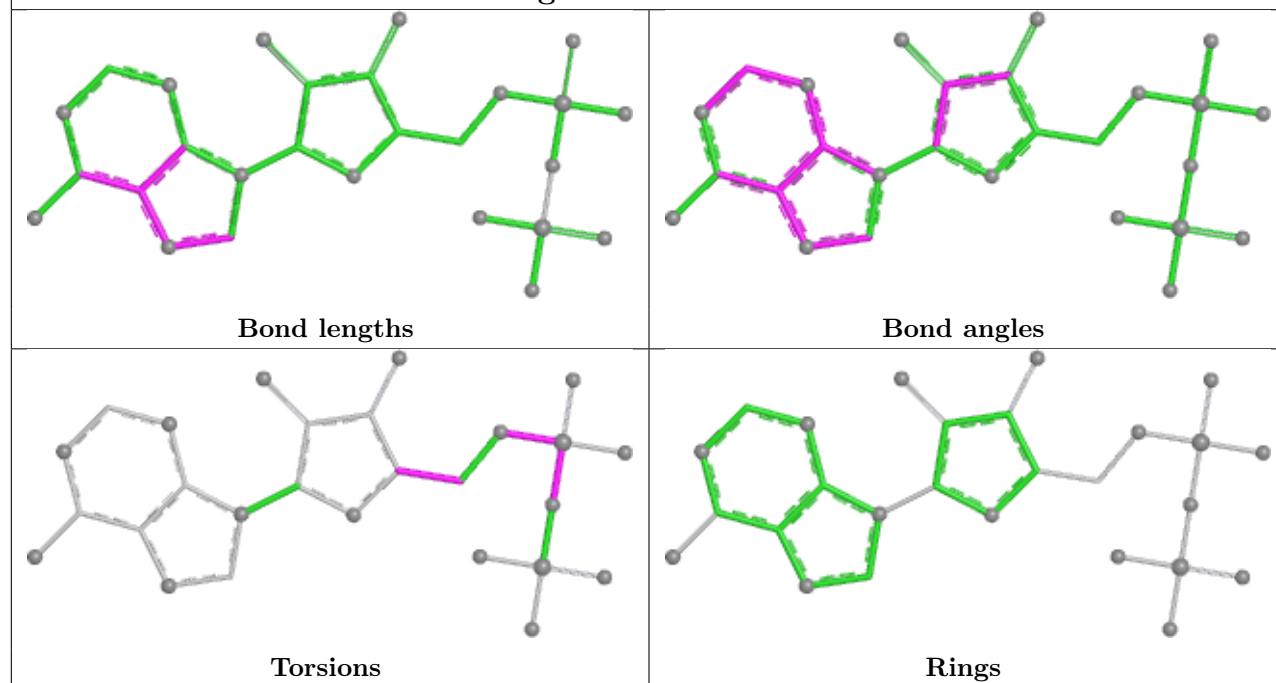


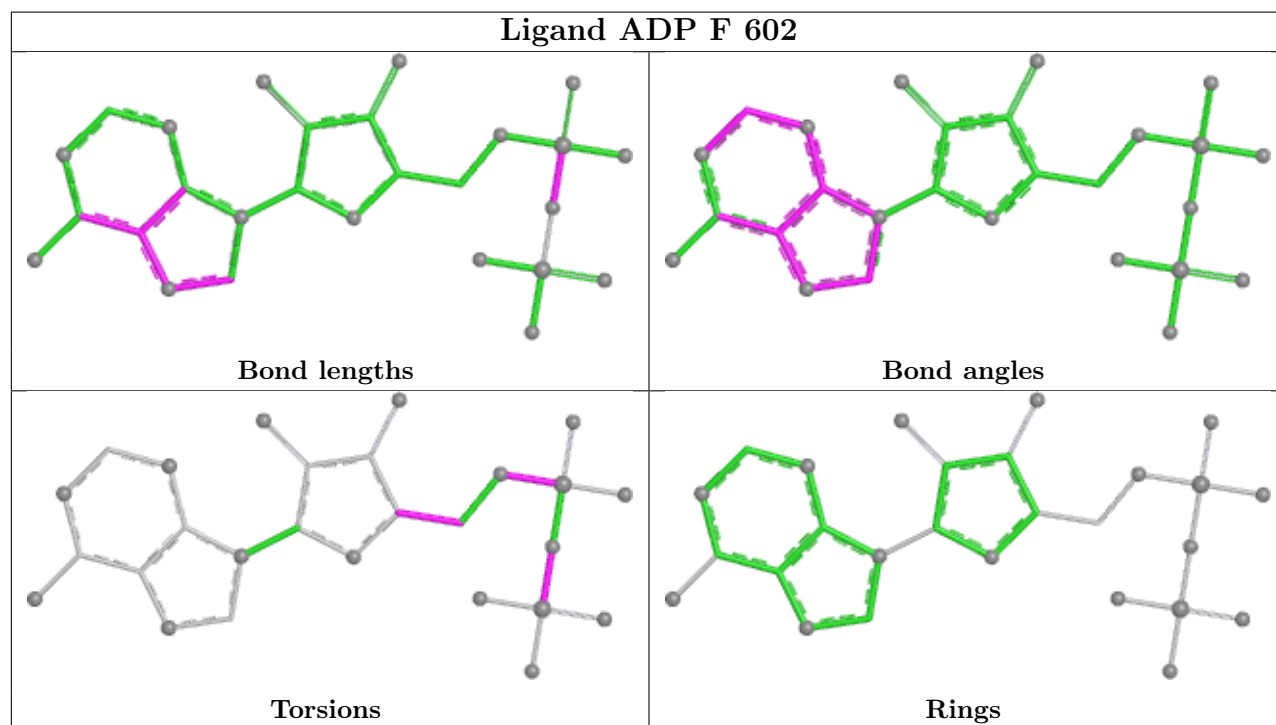
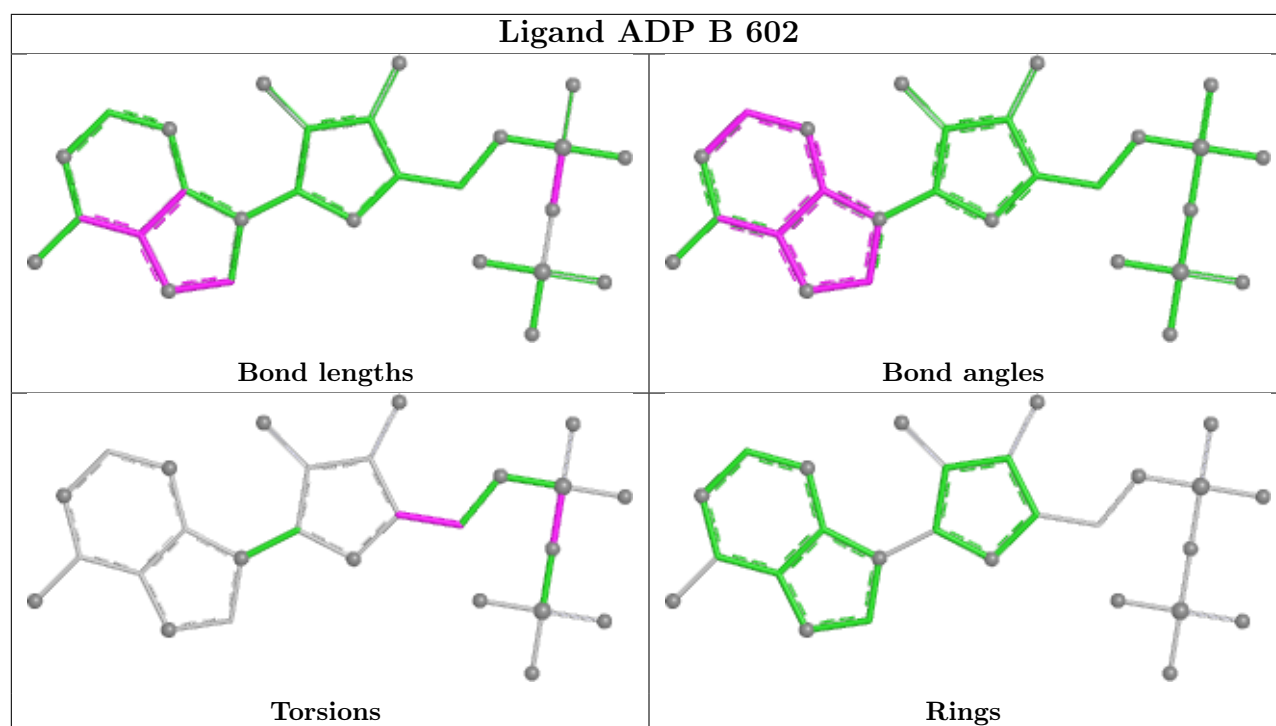


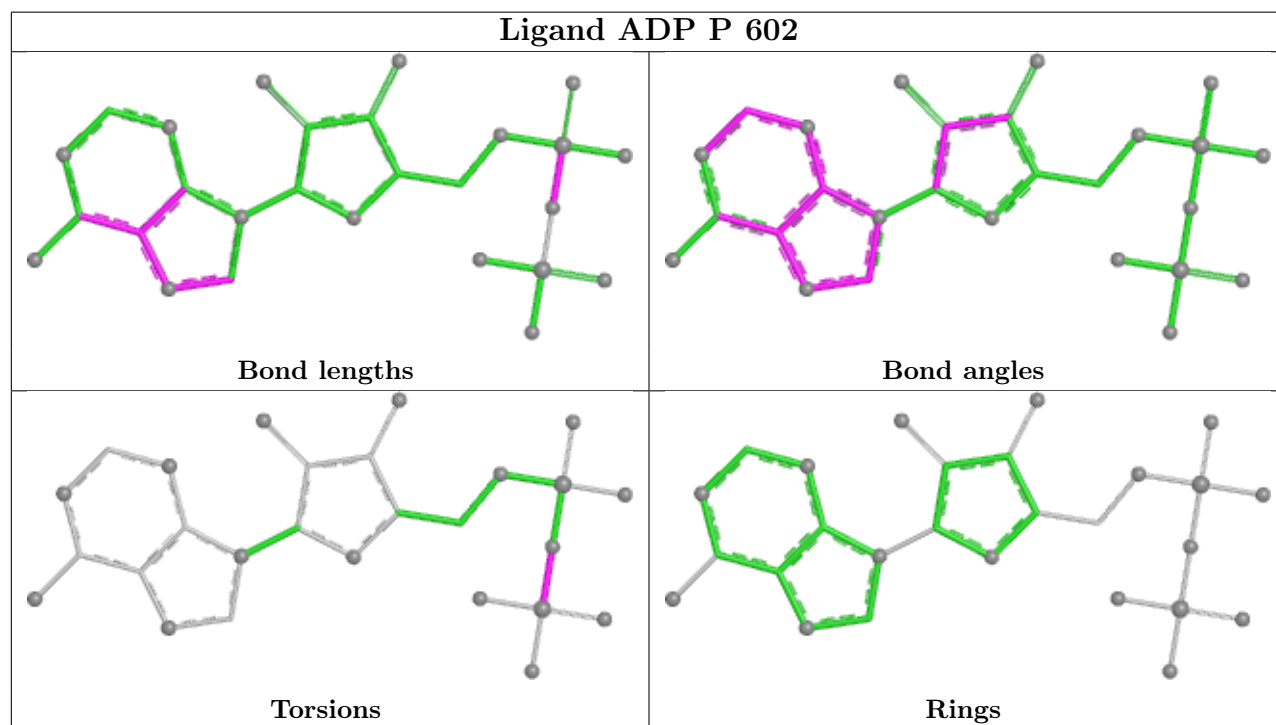
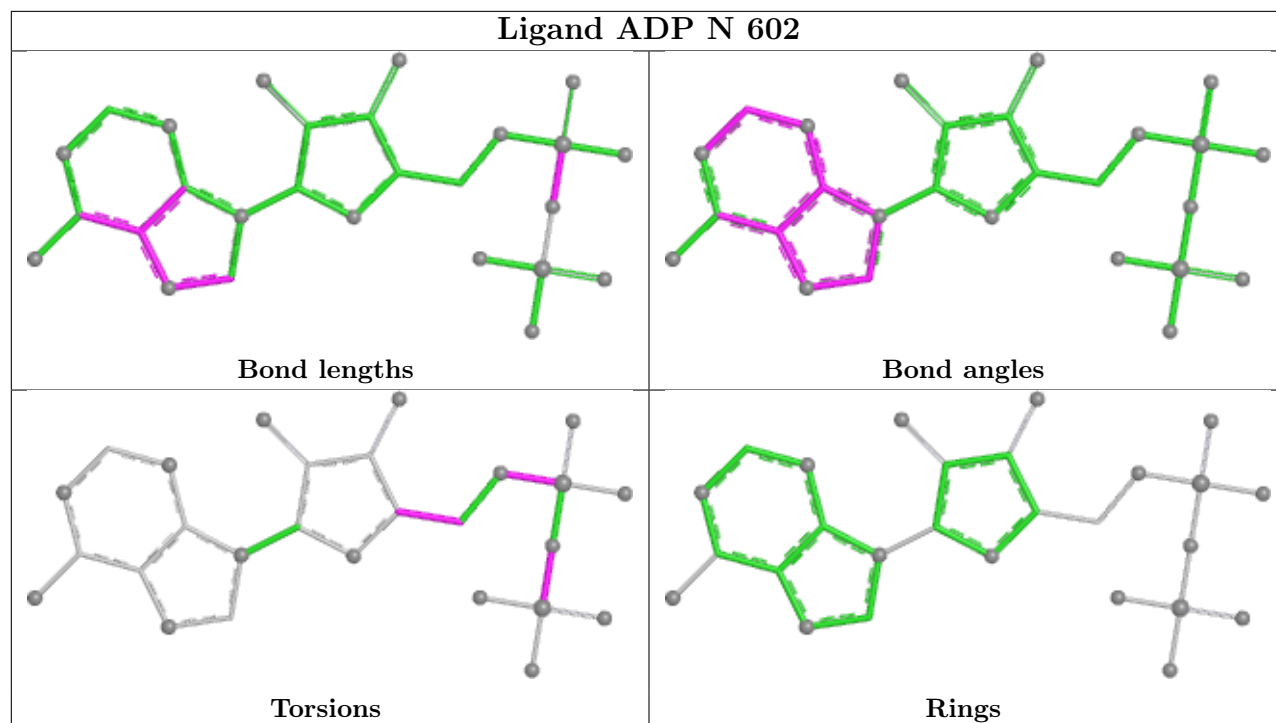
Ligand ADP e 602

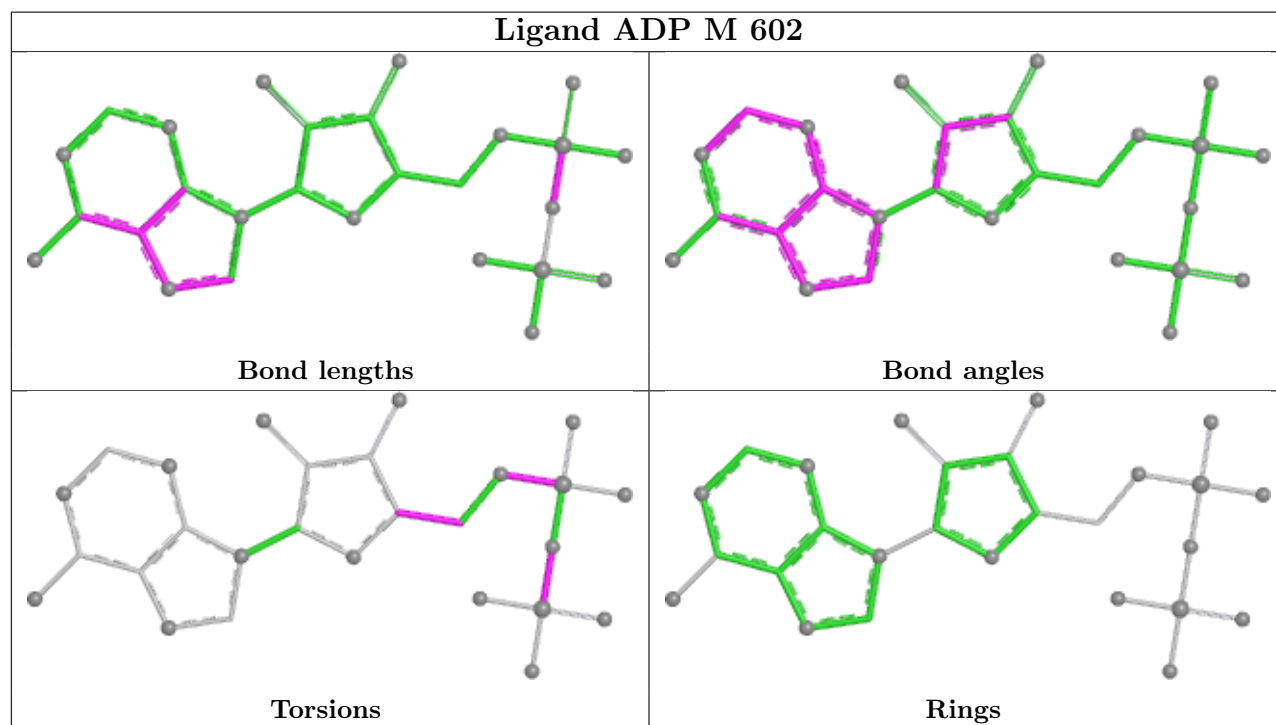
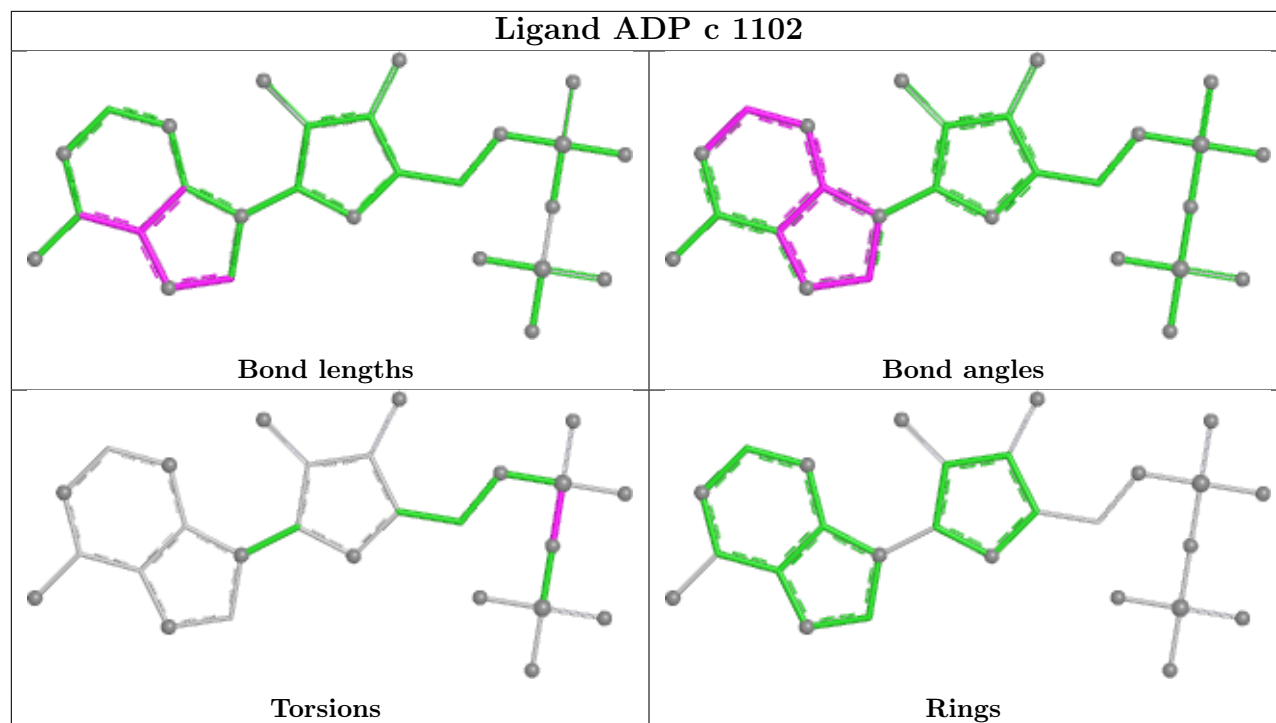


Ligand ADP i 602

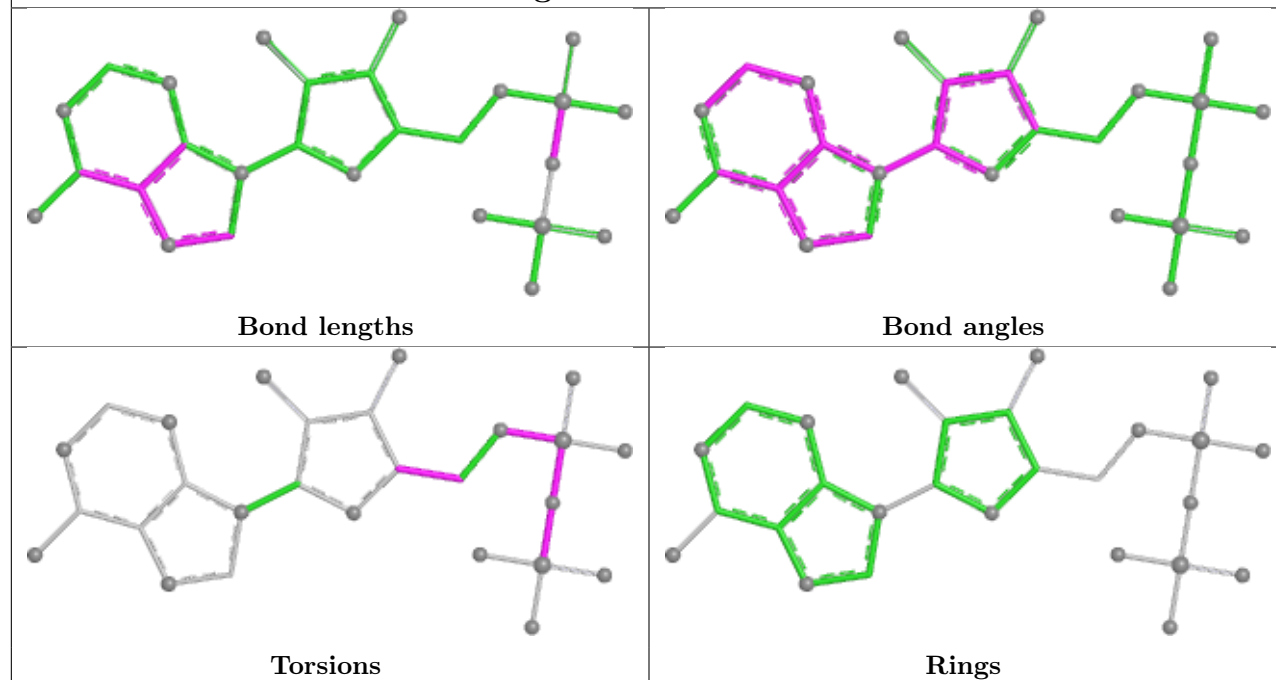




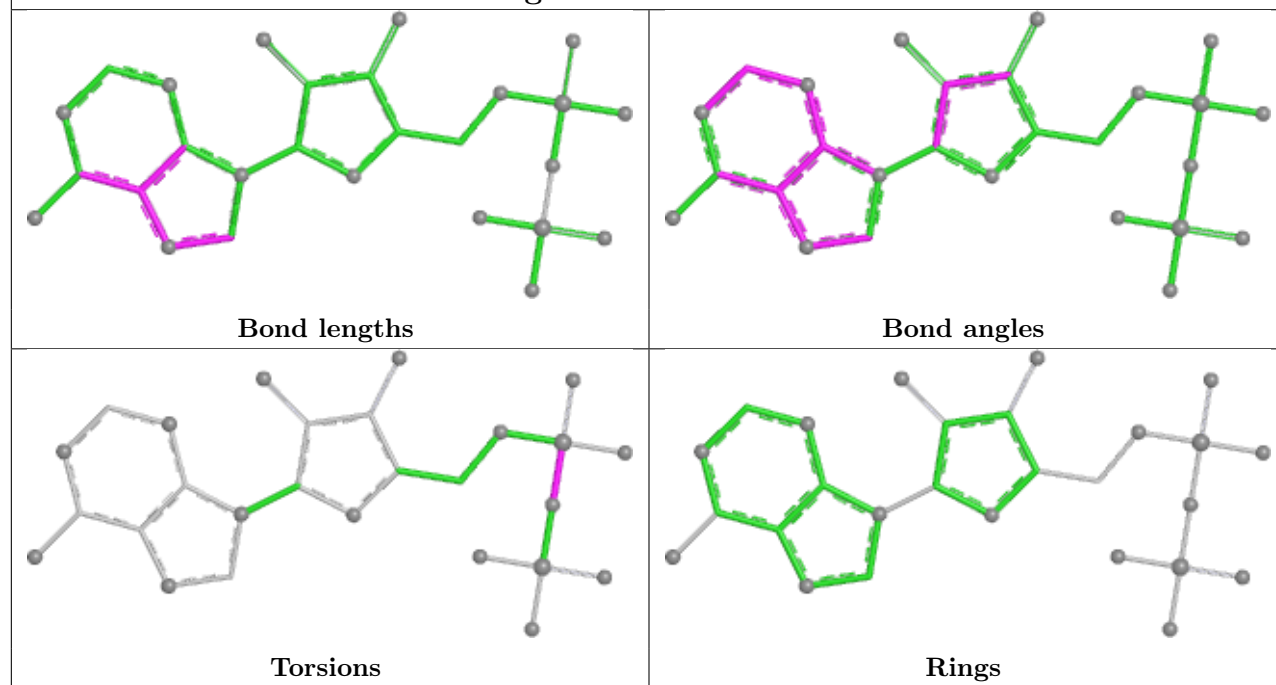


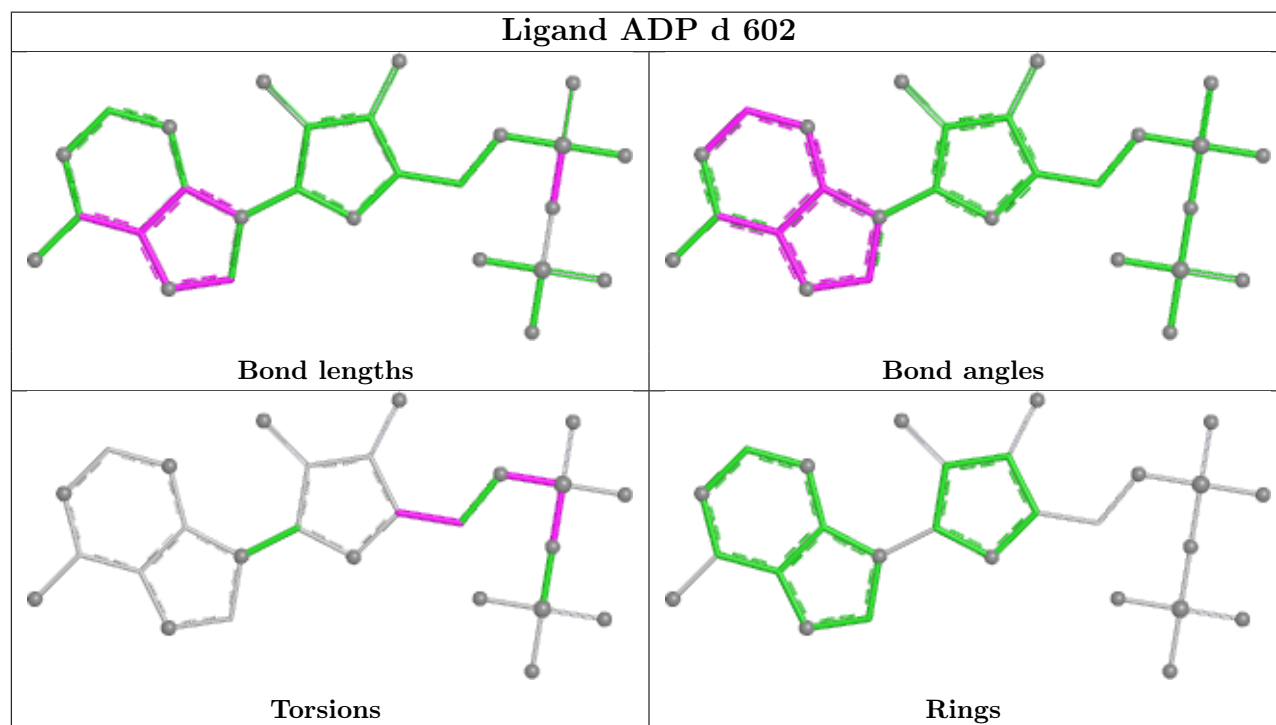
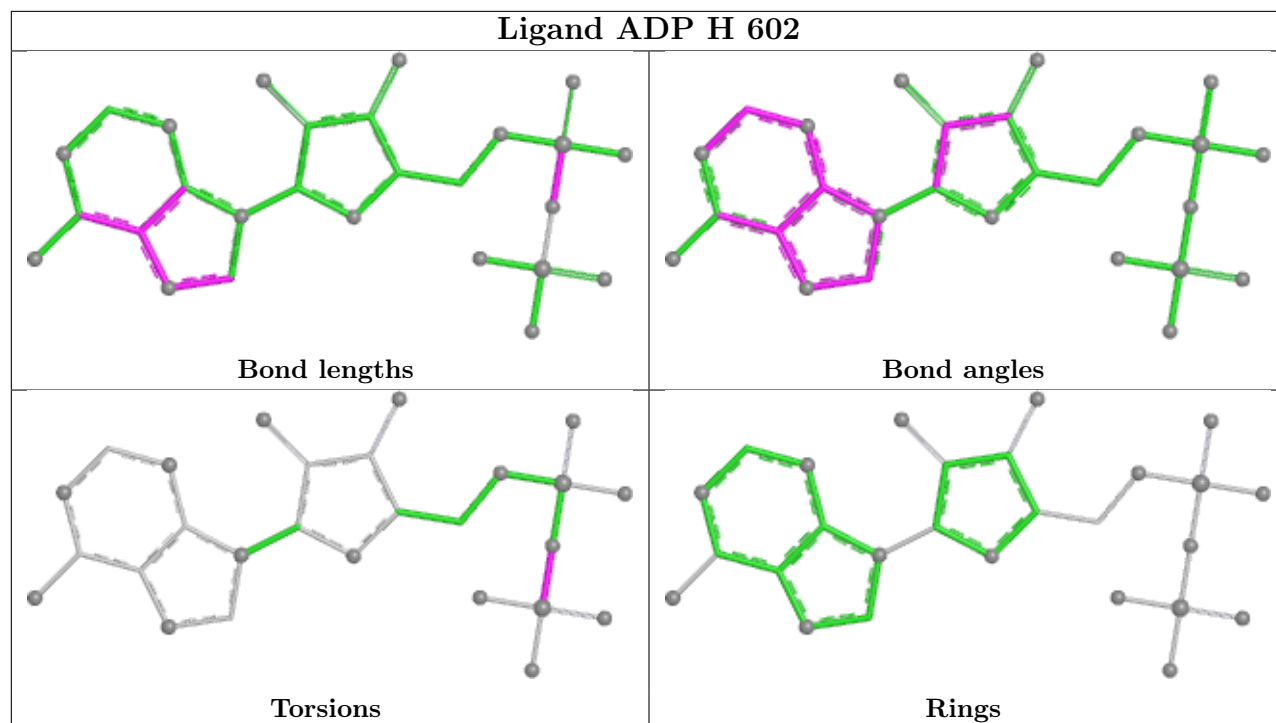


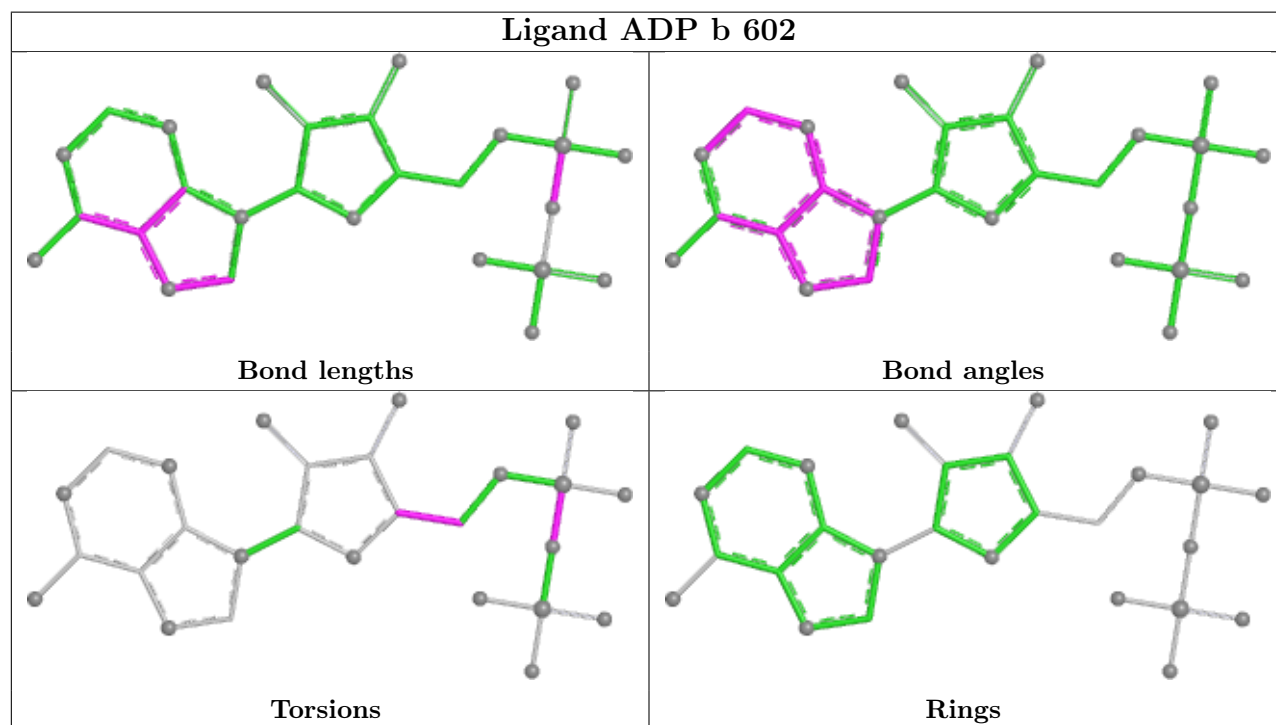
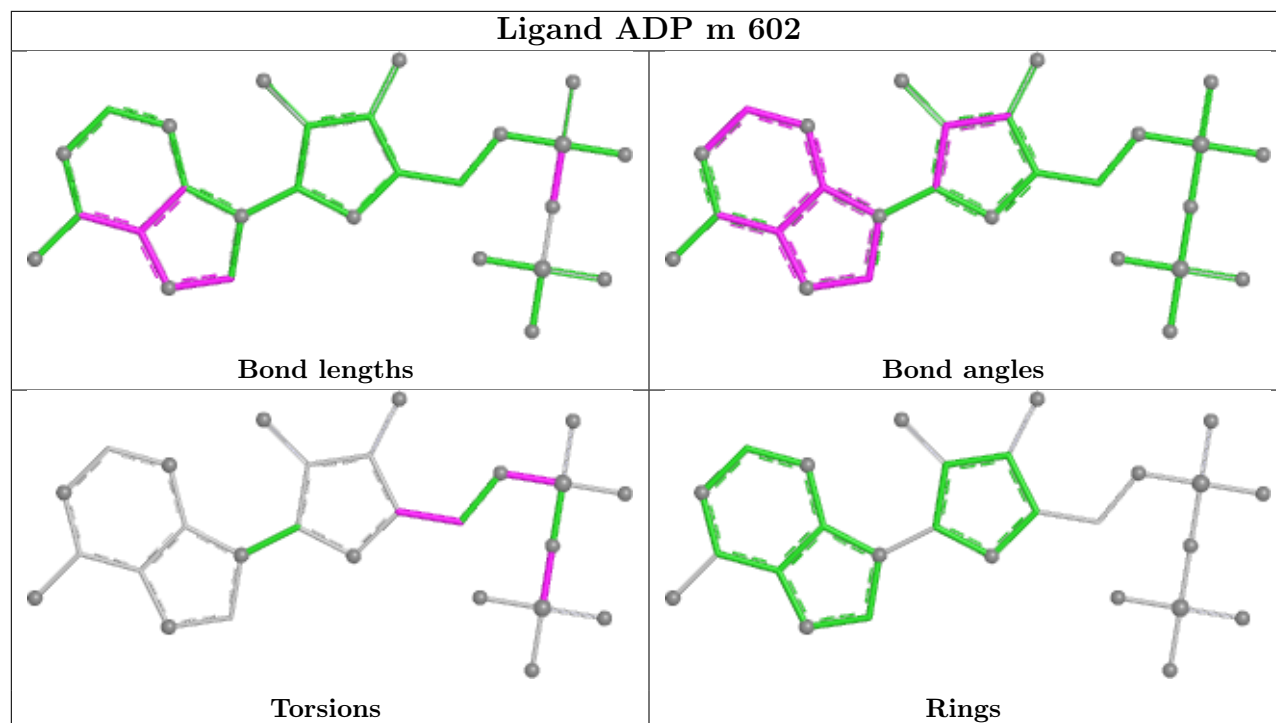
Ligand ADP o 602



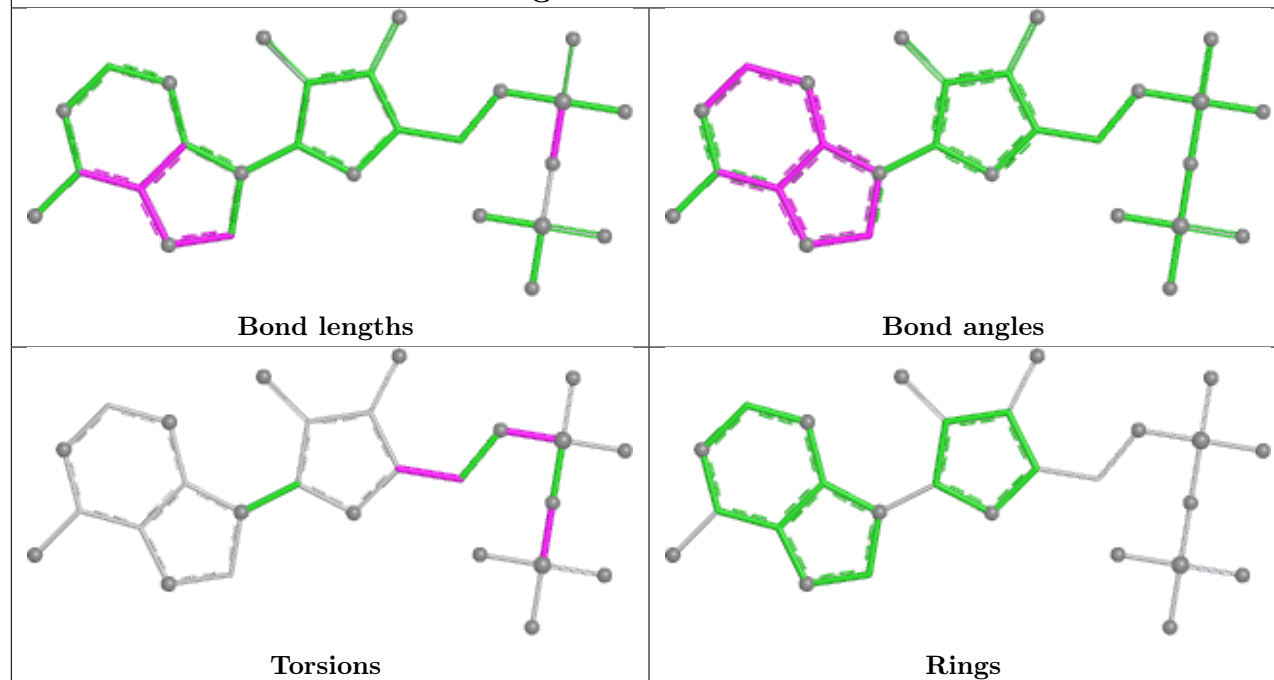
Ligand ADP k 1102



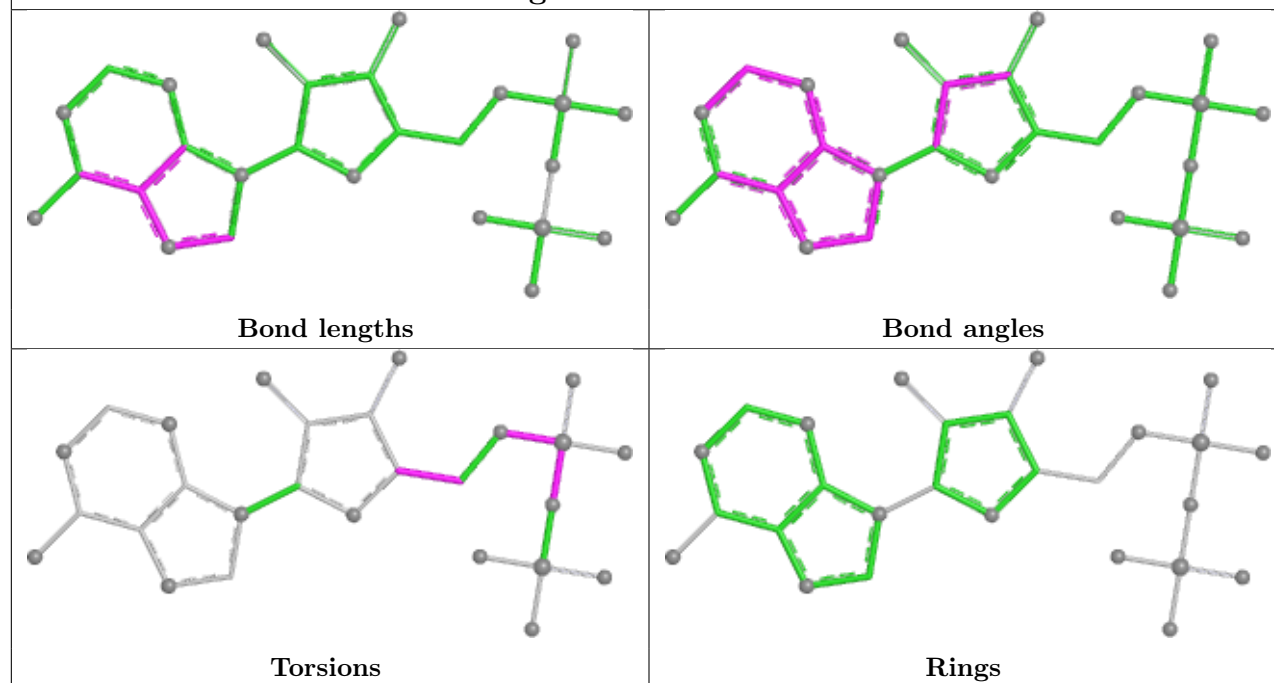


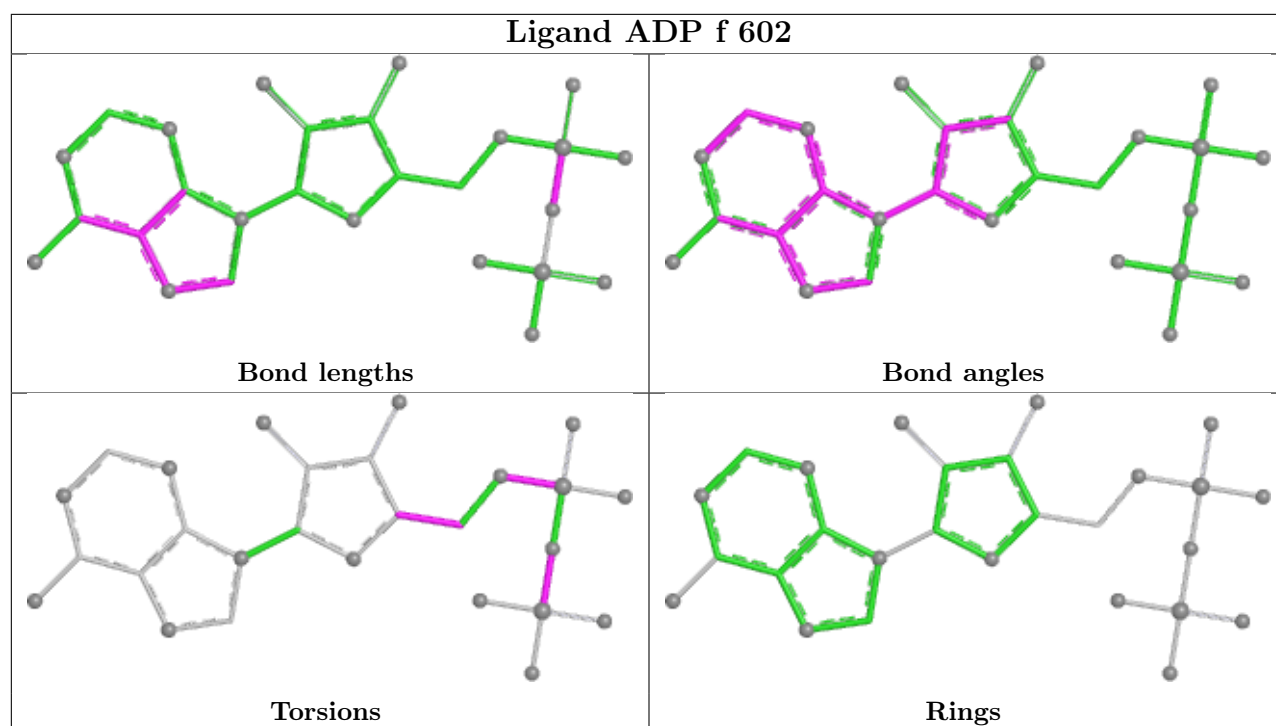


Ligand ADP n 602



Ligand ADP G 602





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	F	538/546 (98%)	-0.22	3 (0%) 85 68	94, 122, 163, 189	0
1	N	538/546 (98%)	0.17	9 (1%) 69 47	111, 164, 220, 255	0
1	f	538/546 (98%)	0.24	11 (2%) 65 44	132, 160, 198, 229	0
1	n	538/546 (98%)	0.04	2 (0%) 88 74	112, 129, 161, 201	0
2	H	521/568 (91%)	-0.13	1 (0%) 91 81	94, 131, 172, 189	0
2	P	521/568 (91%)	0.27	10 (1%) 66 45	119, 171, 234, 265	0
2	h	521/568 (91%)	0.36	17 (3%) 49 34	133, 160, 194, 273	0
2	p	521/568 (91%)	0.15	3 (0%) 85 68	101, 140, 177, 203	0
3	G	526/550 (95%)	-0.09	3 (0%) 85 68	95, 137, 174, 196	0
3	O	526/550 (95%)	0.48	16 (3%) 52 36	106, 157, 253, 338	0
3	g	526/550 (95%)	0.27	8 (1%) 72 50	115, 141, 180, 238	0
3	o	526/550 (95%)	0.07	5 (0%) 79 58	99, 128, 174, 247	0
4	E	535/562 (95%)	-0.15	1 (0%) 91 81	88, 130, 172, 188	0
4	M	535/562 (95%)	0.43	15 (2%) 55 38	106, 140, 233, 319	0
4	e	535/562 (95%)	0.15	4 (0%) 84 65	100, 124, 173, 249	0
4	m	535/562 (95%)	0.02	1 (0%) 91 81	94, 113, 161, 235	0
5	B	518/527 (98%)	-0.28	1 (0%) 91 81	75, 100, 146, 172	0
5	J	518/527 (98%)	0.30	13 (2%) 58 40	101, 127, 198, 249	0
5	b	518/527 (98%)	0.04	2 (0%) 88 74	100, 116, 141, 176	0
5	j	518/527 (98%)	-0.06	3 (0%) 85 68	90, 110, 131, 155	0
6	D	523/528 (99%)	-0.22	0 100 100	78, 119, 153, 183	0
6	L	523/528 (99%)	0.65	33 (6%) 26 21	118, 160, 239, 313	0
6	d	523/528 (99%)	0.10	9 (1%) 69 47	112, 136, 166, 182	0
6	l	523/528 (99%)	0.07	6 (1%) 78 56	103, 129, 170, 196	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
7	A	539/559 (96%)	-0.22	3 (0%) 85 68	88, 120, 160, 203	0
7	I	539/559 (96%)	0.32	18 (3%) 49 34	107, 144, 223, 317	0
7	a	539/559 (96%)	0.06	2 (0%) 88 74	112, 135, 177, 208	0
7	i	539/559 (96%)	0.11	6 (1%) 78 56	101, 132, 185, 212	0
8	C	513/590 (86%)	-0.19	0 100 100	91, 121, 154, 181	0
8	K	513/590 (86%)	0.11	4 (0%) 82 62	103, 150, 238, 312	0
8	c	513/590 (86%)	0.23	3 (0%) 85 68	121, 143, 186, 223	0
8	k	513/590 (86%)	0.10	5 (0%) 79 58	114, 131, 176, 246	0
All	All	16852/17720 (95%)	0.10	217 (1%) 75 53	75, 134, 194, 338	0

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	267	TYR	5.6
1	f	142	ASN	5.3
6	L	351	GLU	4.8
4	e	204	ALA	4.5
2	h	455	ALA	4.1
7	I	264	ILE	4.1
3	O	39	ALA	4.0
3	O	12	VAL	3.9
7	I	11	ASP	3.8
6	L	41	PRO	3.8
1	f	234	LEU	3.7
6	L	524	ILE	3.7
3	o	2	ASN	3.6
7	i	11	ASP	3.5
6	l	356	ASP	3.5
6	L	482	ILE	3.5
6	l	370	ASN	3.5
6	L	43	GLY	3.4
6	L	8	ASN	3.4
7	I	3	GLN	3.3
3	O	165	ALA	3.3
1	f	23	VAL	3.2
2	h	456	PHE	3.2
1	N	157	SER	3.2
7	I	14	PHE	3.1
1	f	436	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	h	6	PRO	3.1
8	c	384	GLY	3.1
5	J	5	ILE	3.1
2	H	27	GLN	3.0
6	L	418	GLU	3.0
5	J	512	ASP	3.0
7	i	154	GLU	3.0
7	I	4	LEU	2.9
5	J	511	VAL	2.9
7	I	182	ASP	2.8
5	J	515	ILE	2.8
6	L	20	VAL	2.8
6	d	247	ASP	2.8
8	k	163	TYR	2.8
4	M	548	ILE	2.8
6	L	241	ILE	2.8
6	d	418	GLU	2.8
8	k	449	MET	2.8
4	M	396	GLU	2.8
4	M	387	THR	2.8
6	L	46	LYS	2.8
6	L	271	LEU	2.8
1	N	292	GLY	2.8
7	I	36	VAL	2.7
1	n	527	LEU	2.7
4	M	272	LEU	2.7
2	P	11	ALA	2.7
6	L	223	ALA	2.7
3	g	2	ASN	2.7
4	e	208	VAL	2.7
6	L	208	GLU	2.7
1	f	316	ALA	2.6
8	K	339	ARG	2.6
6	d	356	ASP	2.6
1	N	250	GLY	2.6
6	L	526	PHE	2.6
7	i	519	GLU	2.6
5	j	242	LYS	2.6
3	o	148	THR	2.6
3	O	189	LEU	2.6
8	k	304	LEU	2.6
3	o	12	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
3	O	2	ASN	2.5
1	N	436	ALA	2.5
1	n	250	GLY	2.5
6	L	7	SER	2.5
6	L	517	SER	2.5
7	a	11	ASP	2.5
6	l	339	PHE	2.5
7	I	420	PRO	2.5
3	O	517	ILE	2.5
3	O	294	LEU	2.5
2	h	231	GLU	2.5
4	M	180	LEU	2.5
6	L	480	ASP	2.5
3	o	39	ALA	2.4
6	d	226	PRO	2.4
7	I	422	GLY	2.4
1	f	508	ASP	2.4
2	P	403	ASP	2.4
2	P	492	THR	2.4
2	p	204	VAL	2.4
3	o	252	ALA	2.4
5	J	73	ALA	2.4
3	g	193	ASP	2.4
2	P	501	ILE	2.4
1	N	259	ARG	2.4
2	h	410	GLY	2.4
2	p	370	VAL	2.4
3	g	483	PHE	2.4
3	g	417	GLU	2.4
5	J	16	GLU	2.4
2	P	166	VAL	2.4
1	f	426	LEU	2.4
4	e	446	ALA	2.4
2	P	271	GLN	2.3
3	O	306	PHE	2.3
3	g	381	GLY	2.3
3	O	248	LEU	2.3
4	M	31	ILE	2.3
7	i	13	LEU	2.3
2	h	248	ALA	2.3
6	L	69	ALA	2.3
8	K	266	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
3	O	13	LEU	2.3
1	f	430	ASN	2.3
1	N	340	VAL	2.3
1	f	294	VAL	2.3
7	a	298	THR	2.3
6	d	9	ALA	2.3
6	l	371	ALA	2.3
7	I	515	ALA	2.3
2	h	330	ARG	2.3
5	b	278	LYS	2.3
6	L	304	PHE	2.3
6	L	132	VAL	2.3
6	L	525	ALA	2.3
7	i	199	PRO	2.3
5	J	45	LEU	2.3
5	j	330	ASP	2.3
1	F	188	ASN	2.2
1	f	158	LEU	2.2
6	L	401	ILE	2.2
6	d	310	ILE	2.2
2	h	81	ALA	2.2
7	I	267	PRO	2.2
4	m	304	ASP	2.2
2	h	28	ILE	2.2
6	d	436	GLN	2.2
7	A	3	GLN	2.2
6	L	131	SER	2.2
2	h	141	GLU	2.2
3	O	264	VAL	2.2
5	J	344	GLU	2.2
3	G	157	LEU	2.2
3	O	259	VAL	2.2
6	d	352	GLU	2.2
8	k	251	GLU	2.2
4	M	218	ASP	2.2
4	M	537	GLN	2.2
6	L	519	LEU	2.2
7	I	523	SER	2.2
4	M	211	VAL	2.2
2	h	460	PRO	2.2
6	L	202	GLY	2.2
6	l	202	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
7	I	273	ILE	2.2
5	J	6	PHE	2.2
6	d	8	ASN	2.2
5	J	22	ALA	2.2
6	L	146	ASP	2.2
2	P	27	GLN	2.2
7	I	13	LEU	2.2
4	M	26	GLY	2.2
6	L	225	GLY	2.2
8	K	462	GLY	2.2
2	h	151	THR	2.2
2	h	213	MET	2.2
4	M	553	ASN	2.2
4	M	101	ALA	2.1
2	P	545	ILE	2.1
3	g	258	GLU	2.1
2	h	270	ALA	2.1
3	O	445	ALA	2.1
8	K	261	ILE	2.1
1	f	493	LEU	2.1
7	I	270	LEU	2.1
4	E	318	ALA	2.1
5	J	19	ARG	2.1
3	g	46	PRO	2.1
2	P	267	LEU	2.1
7	A	256	MET	2.1
1	N	316	ALA	2.1
1	F	142	ASN	2.1
6	L	498	LEU	2.1
7	I	52	MET	2.1
3	G	161	CYS	2.1
7	I	277	GLU	2.1
8	k	25	ILE	2.1
1	N	354	VAL	2.1
5	J	11	THR	2.1
6	l	448	GLU	2.1
1	F	277	ILE	2.1
2	h	124	ALA	2.1
8	c	1055	SER	2.1
2	P	16	GLN	2.1
4	M	253	GLN	2.1
6	L	259	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
7	i	3	GLN	2.1
5	J	428	LEU	2.1
5	B	449	GLY	2.0
5	j	291	TYR	2.0
3	G	450	PRO	2.0
4	e	97	ASP	2.0
2	h	427	GLU	2.0
6	L	249	GLU	2.0
7	I	274	ARG	2.0
4	M	30	ILE	2.0
8	c	13	GLU	2.0
2	h	27	GLN	2.0
5	b	115	ILE	2.0
3	g	354	GLU	2.0
7	A	11	ASP	2.0
4	M	519	SER	2.0
6	L	312	VAL	2.0
2	p	171	LYS	2.0
6	L	518	ILE	2.0
1	N	234	LEU	2.0
3	O	258	GLU	2.0
3	O	227	ALA	2.0
6	L	242	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	MG	L	601	1/1	0.68	0.15	124,124,124,124	0
9	MG	c	1101	1/1	0.71	0.09	129,129,129,129	0
11	BEF	N	603	4/4	0.77	0.12	132,135,135,137	0
11	BEF	h	603	4/4	0.81	0.15	55,55,55,55	0
11	BEF	k	1103	4/4	0.85	0.09	110,111,111,112	0
11	BEF	p	603	4/4	0.86	0.09	130,132,133,133	0
9	MG	d	601	1/1	0.87	0.12	115,115,115,115	0
10	ADP	N	602	27/27	0.87	0.11	133,145,153,154	0
9	MG	h	601	1/1	0.88	0.08	151,151,151,151	0
11	BEF	f	603	4/4	0.89	0.08	152,152,154,156	0
10	ADP	f	602	27/27	0.89	0.11	149,154,159,160	0
9	MG	o	601	1/1	0.89	0.09	115,115,115,115	0
11	BEF	o	603	4/4	0.89	0.07	116,118,119,119	0
11	BEF	L	603	4/4	0.89	0.08	135,138,138,141	0
11	BEF	J	603	4/4	0.90	0.10	110,112,113,114	0
9	MG	N	601	1/1	0.90	0.12	132,132,132,132	0
10	ADP	p	602	27/27	0.90	0.11	133,145,154,156	0
11	BEF	G	603	4/4	0.90	0.10	110,110,112,116	0
11	BEF	c	1103	4/4	0.90	0.07	126,127,127,129	0
11	BEF	D	603	4/4	0.90	0.09	89,89,91,94	0
10	ADP	L	602	27/27	0.90	0.10	135,138,144,147	0
11	BEF	O	603	4/4	0.90	0.08	117,118,119,120	0
9	MG	a	601	1/1	0.91	0.12	126,126,126,126	0
11	BEF	n	603	4/4	0.91	0.06	115,115,116,118	0
11	BEF	K	1103	4/4	0.91	0.06	118,120,120,123	0
10	ADP	c	1102	27/27	0.91	0.09	134,138,142,143	0
10	ADP	n	602	27/27	0.91	0.09	112,116,123,124	0
10	ADP	O	602	27/27	0.92	0.11	109,115,120,121	0
10	ADP	m	602	27/27	0.92	0.11	102,106,108,109	0
10	ADP	i	602	27/27	0.92	0.10	113,121,126,127	0
10	ADP	h	602	27/27	0.92	0.14	152,159,166,167	0
11	BEF	e	603	4/4	0.92	0.11	114,114,116,118	0
10	ADP	P	602	27/27	0.93	0.09	136,143,148,149	0
9	MG	l	601	1/1	0.93	0.12	107,107,107,107	0
10	ADP	o	602	27/27	0.93	0.09	119,128,133,134	0
9	MG	k	1101	1/1	0.93	0.11	111,111,111,111	0
10	ADP	F	602	27/27	0.93	0.07	97,105,112,113	0
11	BEF	g	603	4/4	0.93	0.07	128,132,132,134	0
10	ADP	k	1102	27/27	0.93	0.10	115,117,120,121	0
11	BEF	d	603	4/4	0.93	0.07	116,120,121,121	0
11	BEF	a	603	4/4	0.93	0.09	118,120,121,121	0

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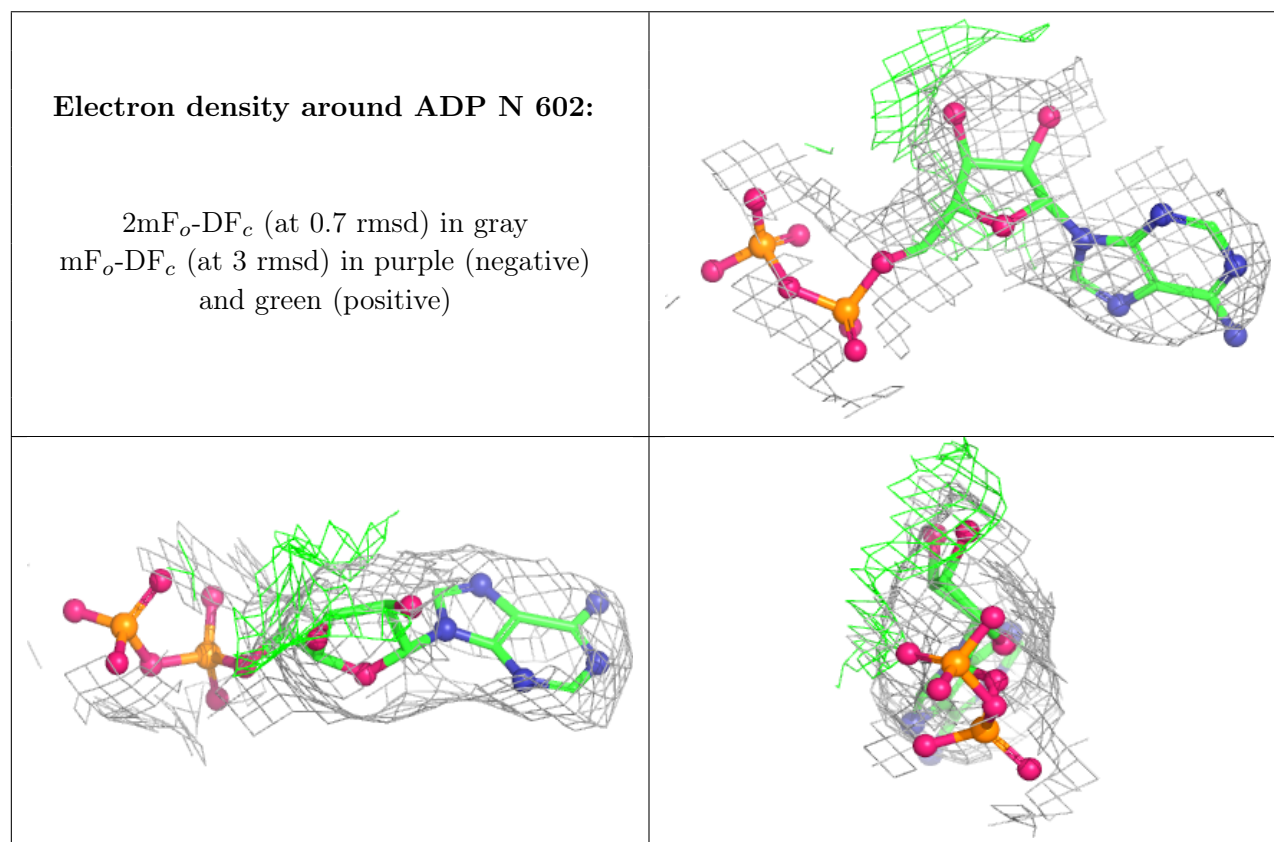
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	ADP	A	602	27/27	0.93	0.10	98,113,126,127	0
11	BEF	B	603	4/4	0.93	0.10	76,77,77,78	0
10	ADP	g	602	27/27	0.93	0.10	132,141,149,150	0
10	ADP	d	602	27/27	0.93	0.10	125,135,149,151	0
11	BEF	i	603	4/4	0.93	0.07	104,105,105,106	0
9	MG	j	601	1/1	0.93	0.13	88,88,88,88	0
11	BEF	b	603	4/4	0.94	0.07	103,105,105,107	0
11	BEF	l	603	4/4	0.94	0.09	107,110,111,111	0
11	BEF	C	1103	4/4	0.94	0.09	91,92,93,94	0
10	ADP	M	602	27/27	0.94	0.09	104,111,114,115	0
10	ADP	b	602	27/27	0.95	0.10	104,109,115,115	0
11	BEF	E	603	4/4	0.95	0.09	98,98,100,102	0
10	ADP	H	602	27/27	0.95	0.07	106,117,128,130	0
10	ADP	a	602	27/27	0.95	0.09	126,139,146,148	0
10	ADP	B	602	27/27	0.95	0.08	78,83,86,87	0
10	ADP	D	602	27/27	0.95	0.09	95,106,120,123	0
10	ADP	I	602	27/27	0.95	0.09	121,126,133,135	0
10	ADP	K	1102	27/27	0.95	0.08	122,131,144,147	0
9	MG	I	601	1/1	0.95	0.11	121,121,121,121	0
10	ADP	j	602	27/27	0.95	0.12	94,100,106,107	0
9	MG	m	601	1/1	0.95	0.06	84,84,84,84	0
9	MG	n	601	1/1	0.95	0.07	108,108,108,108	0
9	MG	K	1101	1/1	0.96	0.07	126,126,126,126	0
10	ADP	l	602	27/27	0.96	0.08	117,129,144,145	0
11	BEF	P	603	4/4	0.96	0.04	140,141,142,145	0
10	ADP	G	602	27/27	0.96	0.09	111,127,140,142	0
11	BEF	M	603	4/4	0.96	0.06	111,113,114,116	0
9	MG	O	601	1/1	0.96	0.06	113,113,113,113	0
11	BEF	H	603	4/4	0.96	0.05	105,106,106,108	0
9	MG	C	1101	1/1	0.96	0.08	99,99,99,99	0
11	BEF	m	603	4/4	0.96	0.08	99,100,101,103	0
10	ADP	J	602	27/27	0.96	0.08	104,108,113,113	0
10	ADP	e	602	27/27	0.96	0.09	117,124,127,128	0
9	MG	D	601	1/1	0.96	0.09	89,89,89,89	0
11	BEF	A	603	4/4	0.97	0.06	91,91,92,95	0
9	MG	A	601	1/1	0.97	0.13	102,102,102,102	0
10	ADP	E	602	27/27	0.97	0.07	102,115,123,124	0
9	MG	E	601	1/1	0.97	0.07	91,91,91,91	0
9	MG	g	601	1/1	0.97	0.08	129,129,129,129	0
9	MG	e	601	1/1	0.97	0.07	102,102,102,102	0
10	ADP	C	1102	27/27	0.97	0.06	100,111,118,119	0
9	MG	G	601	1/1	0.97	0.09	113,113,113,113	0

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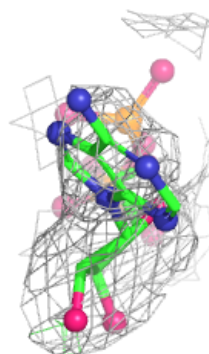
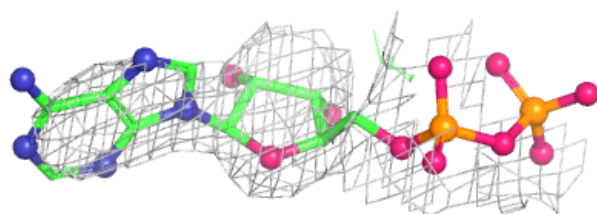
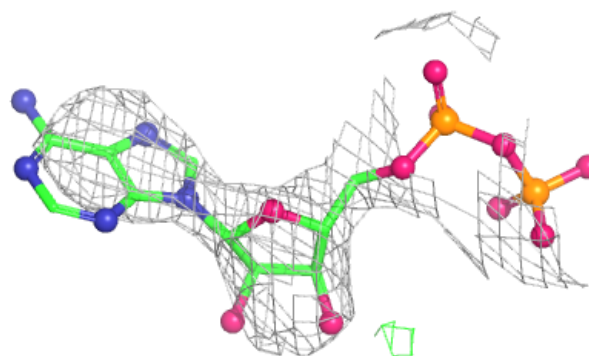
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	BEF	F	603	4/4	0.98	0.04	99,101,101,102	0
9	MG	f	601	1/1	0.98	0.05	143,143,143,143	0
9	MG	b	601	1/1	0.98	0.12	97,97,97,97	0
9	MG	i	601	1/1	0.98	0.06	111,111,111,111	0
9	MG	p	601	1/1	0.98	0.05	131,131,131,131	0
11	BEF	j	603	4/4	0.98	0.11	93,94,94,96	0
9	MG	F	601	1/1	0.98	0.03	94,94,94,94	0
9	MG	P	601	1/1	0.98	0.04	140,140,140,140	0
11	BEF	I	603	4/4	0.98	0.05	119,119,120,122	0
9	MG	J	601	1/1	0.99	0.06	101,101,101,101	0
9	MG	H	601	1/1	0.99	0.02	109,109,109,109	0
9	MG	B	601	1/1	0.99	0.04	70,70,70,70	0
9	MG	M	601	1/1	0.99	0.07	96,96,96,96	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

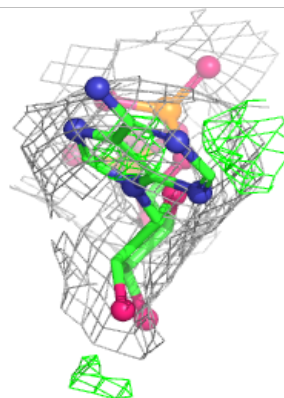
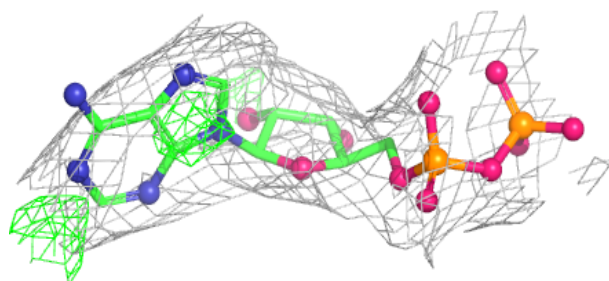
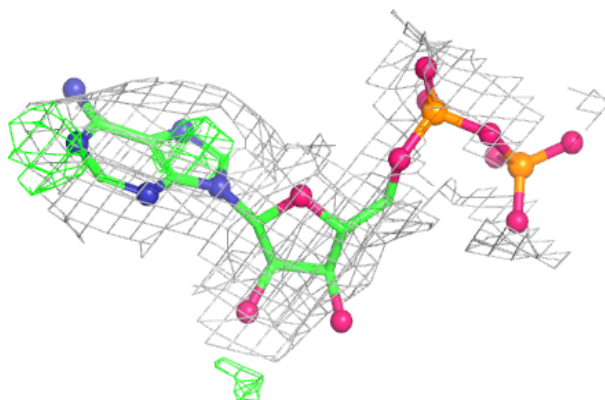


Electron density around ADP f 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

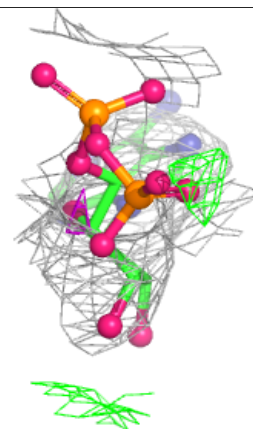
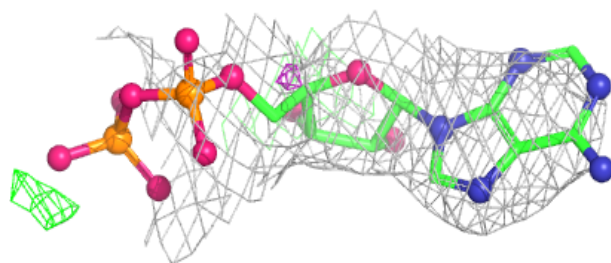
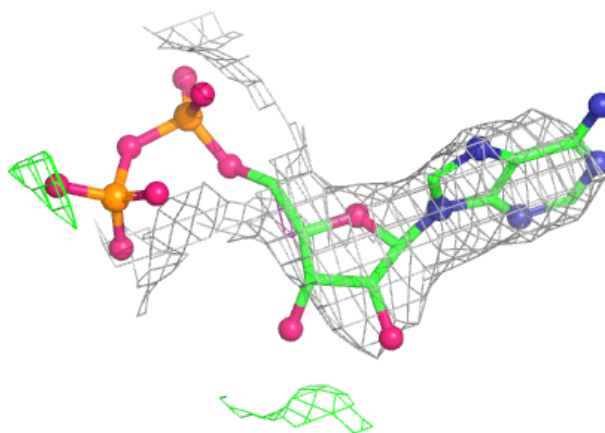
**Electron density around ADP p 602:**

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and green (positive)

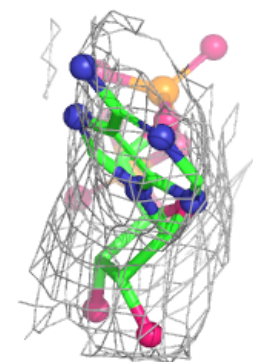
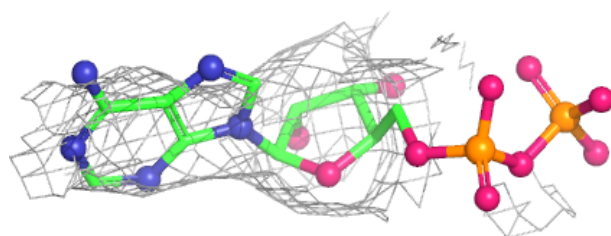
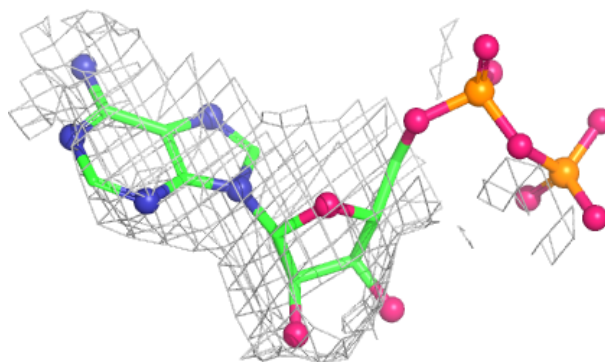


Electron density around ADP L 602:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

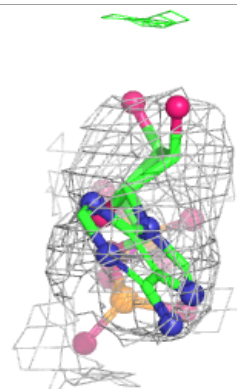
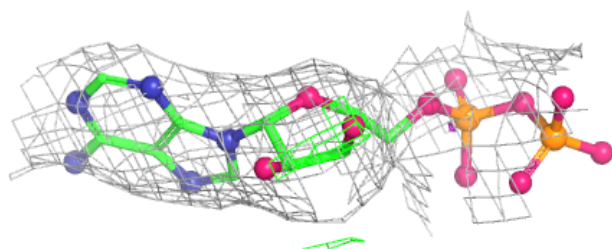
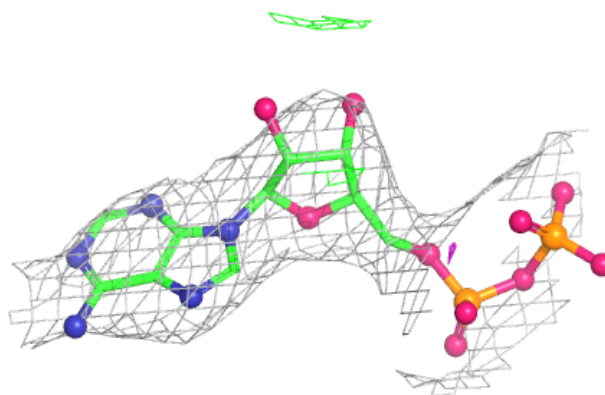
**Electron density around ADP c 1102:**

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 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

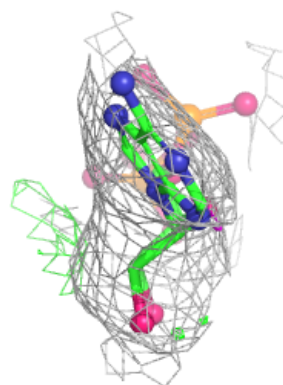
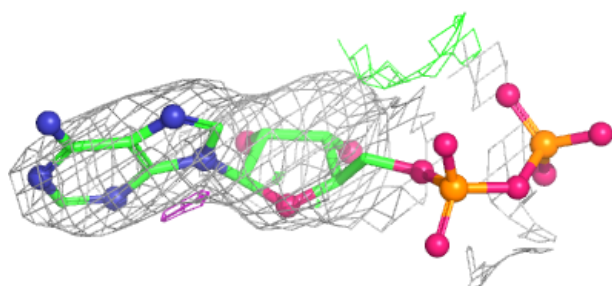
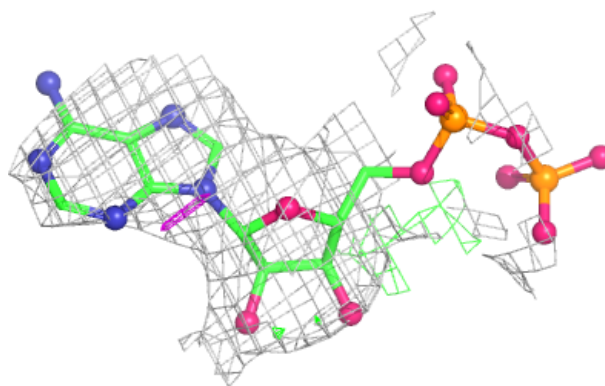


Electron density around ADP n 602:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

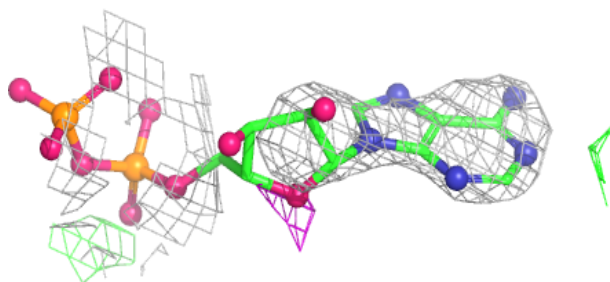
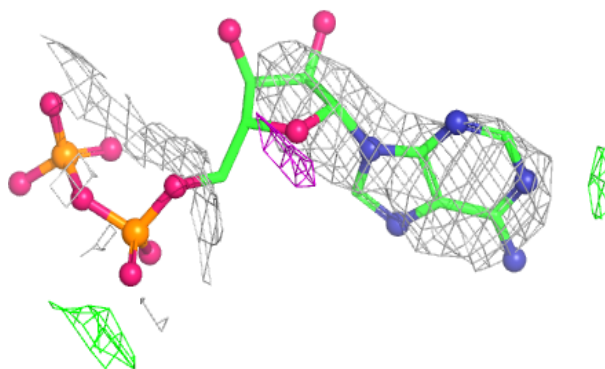
**Electron density around ADP O 602:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

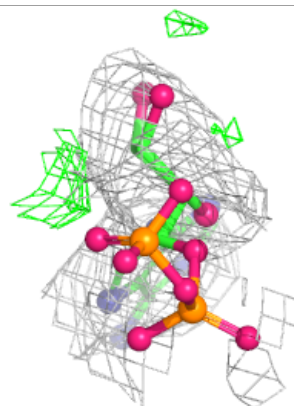
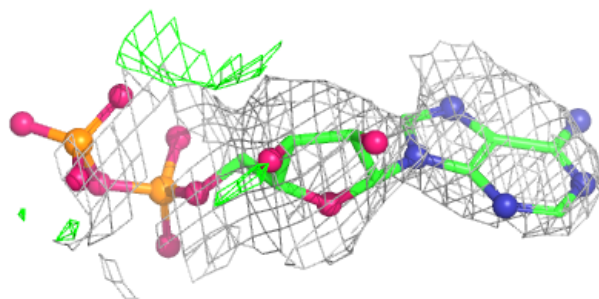
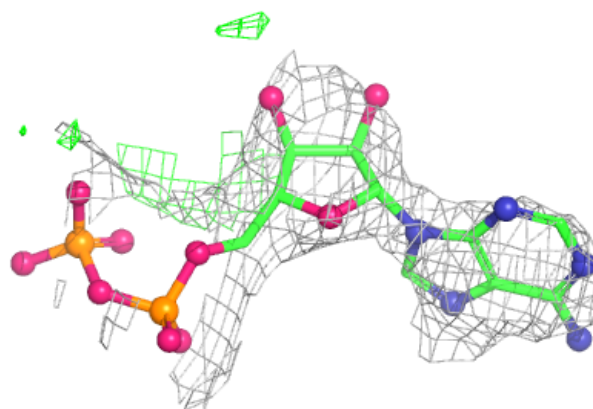


Electron density around ADP m 602:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

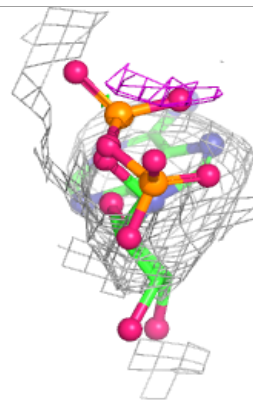
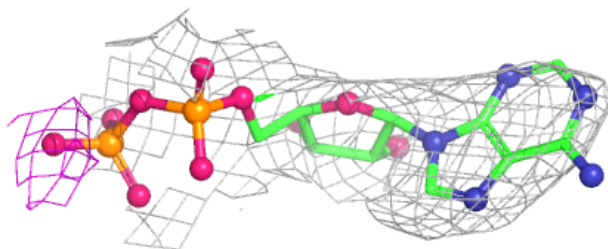
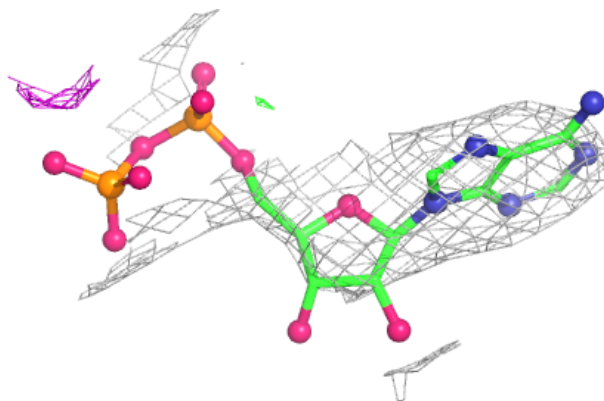
**Electron density around ADP i 602:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

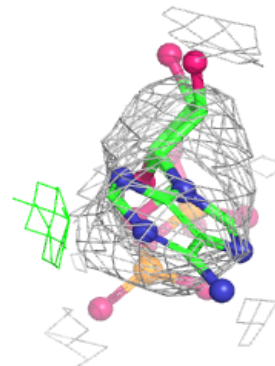
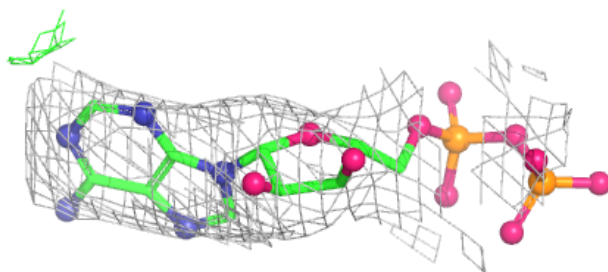
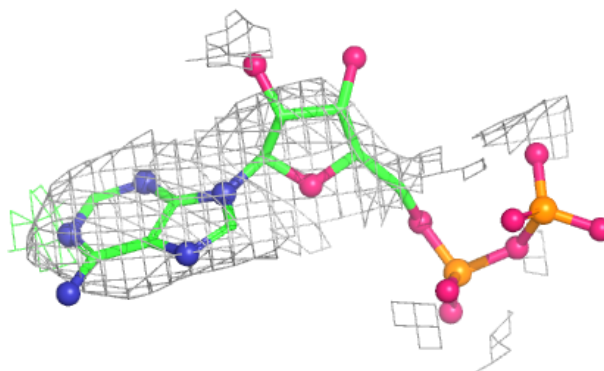


Electron density around ADP h 602:

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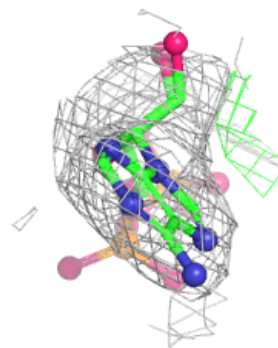
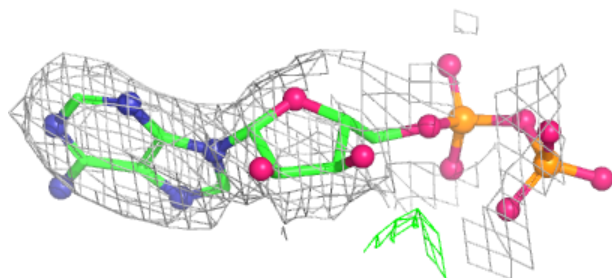
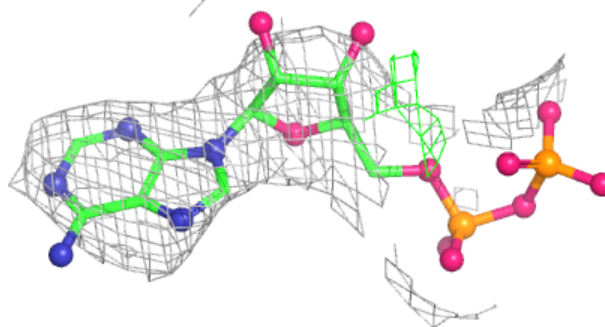
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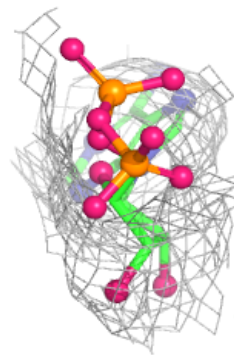
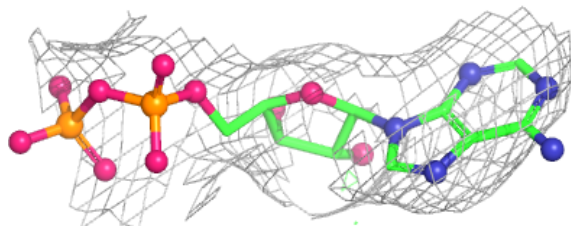
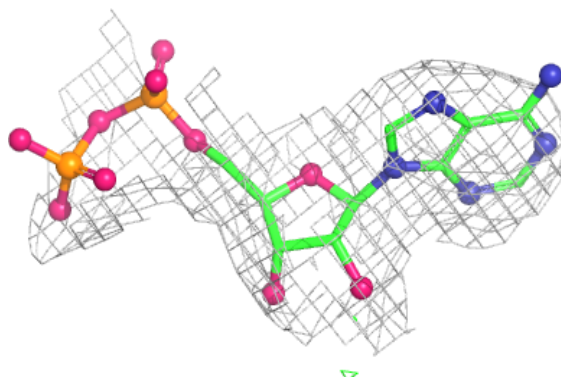


Electron density around ADP o 602:

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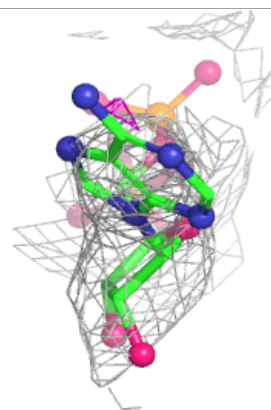
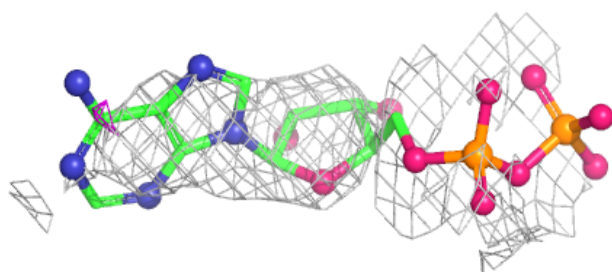
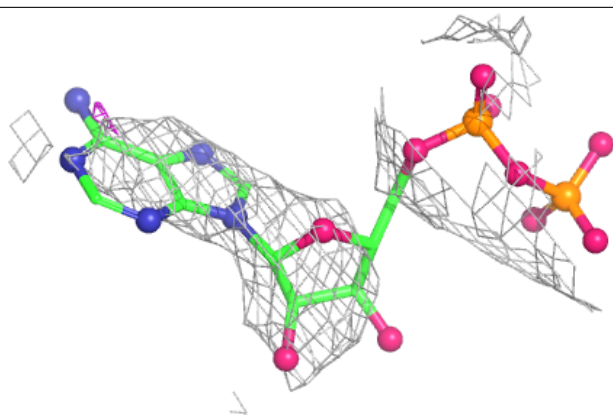
**Electron density around ADP F 602:**

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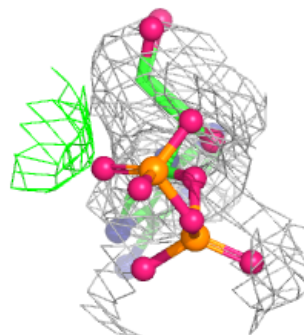
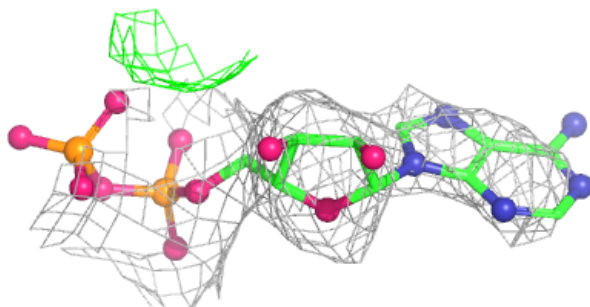
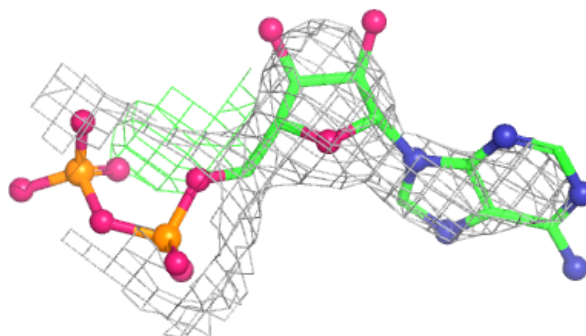


Electron density around ADP k 1102:

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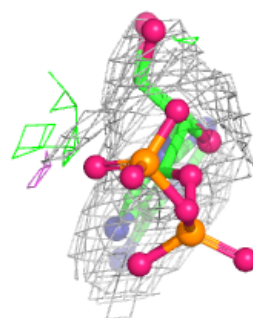
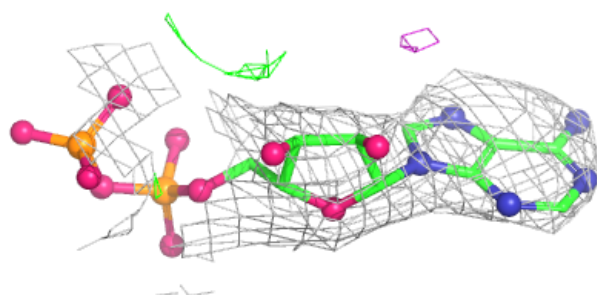
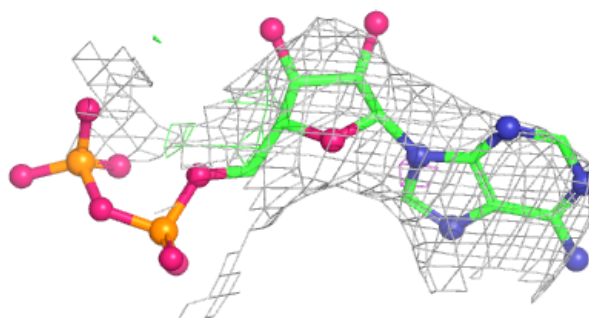
**Electron density around ADP A 602:**

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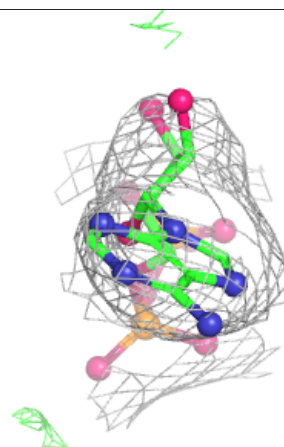
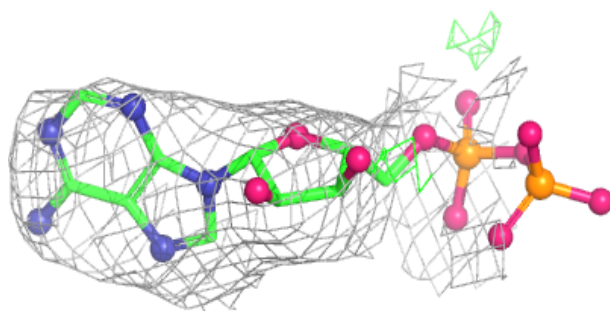
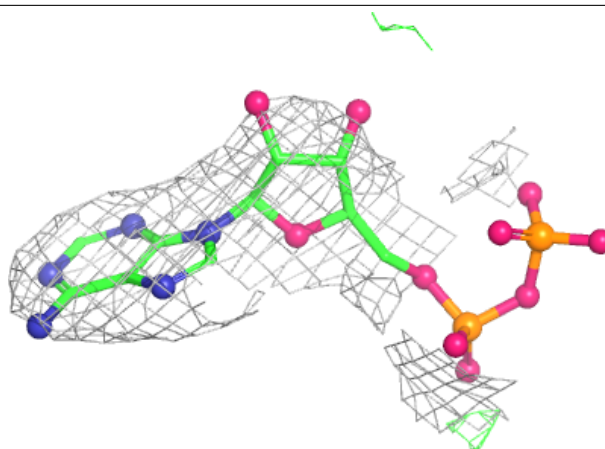
Electron density around ADP g 602:

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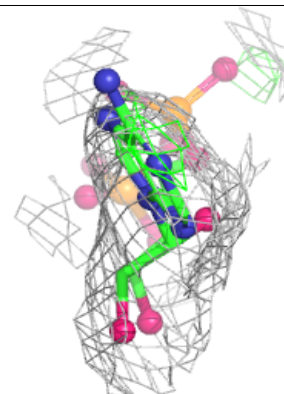
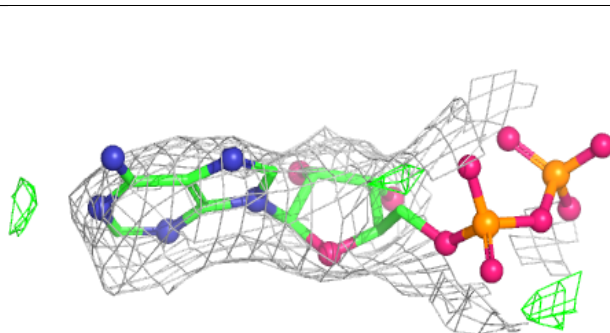
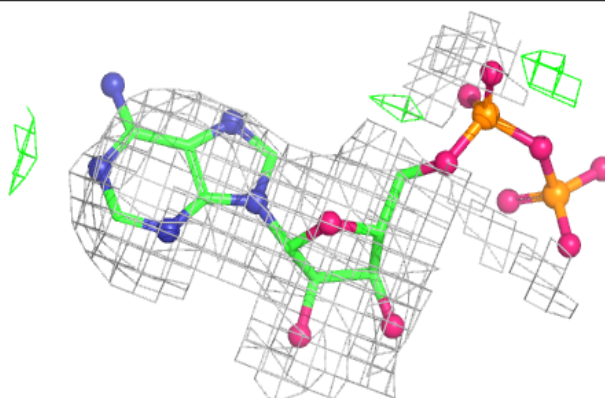


Electron density around ADP d 602:

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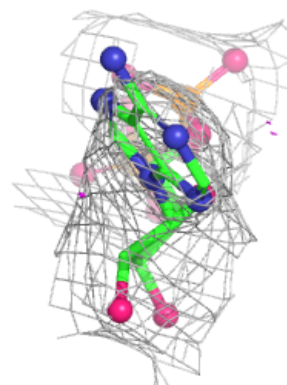
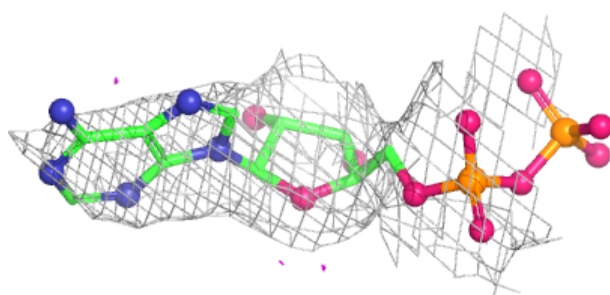
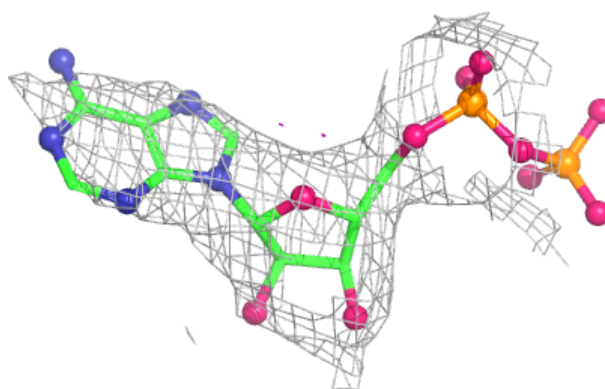
**Electron density around ADP M 602:**

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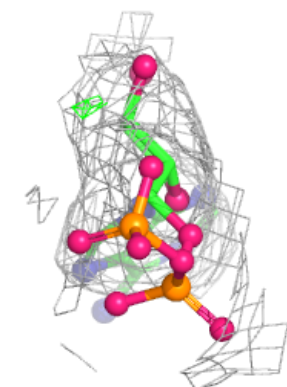
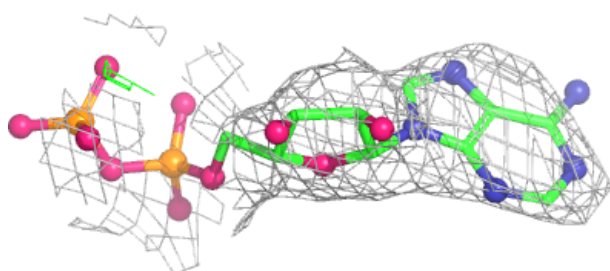
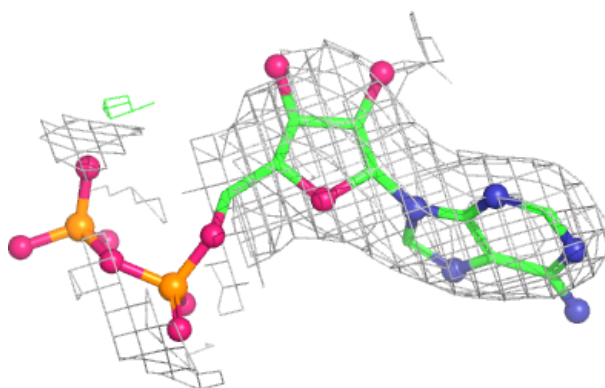


Electron density around ADP b 602:

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and green (positive)

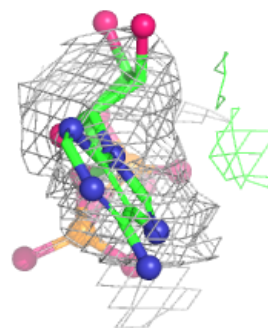
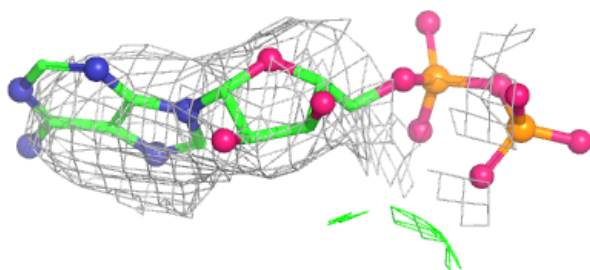
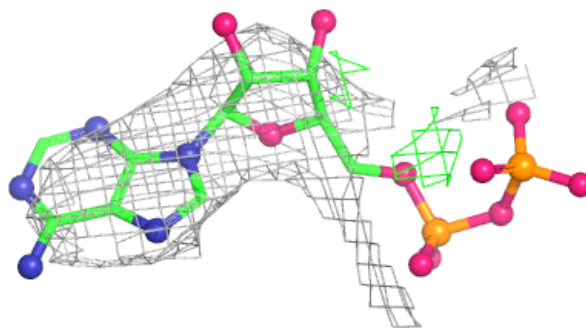
**Electron density around ADP H 602:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

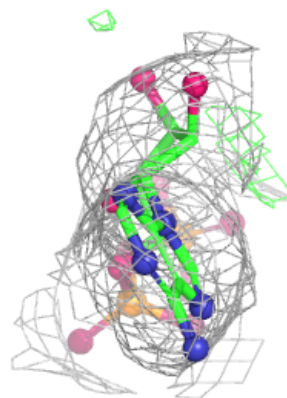
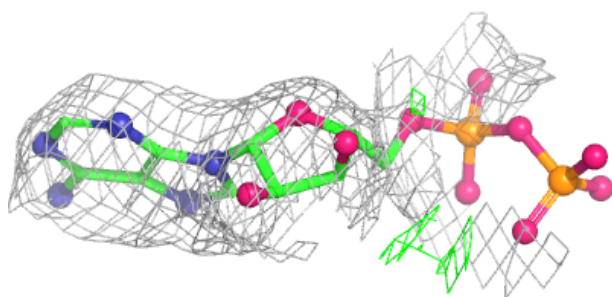
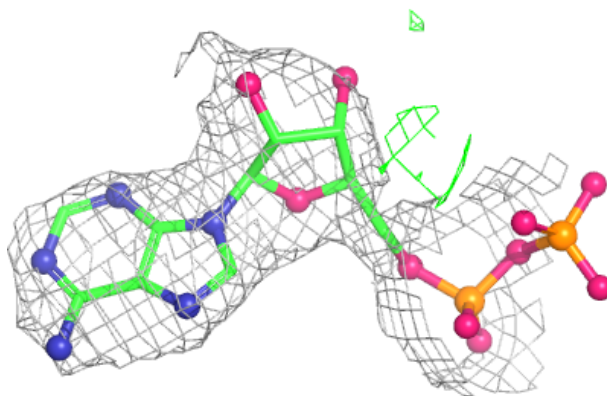


Electron density around ADP a 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

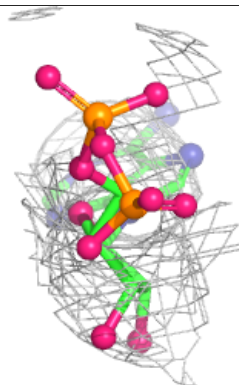
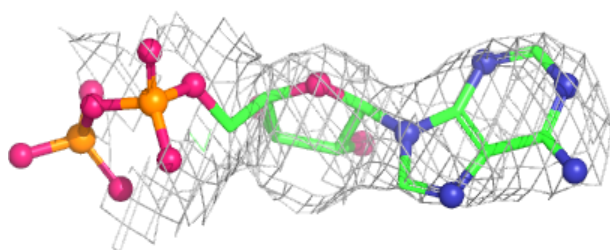
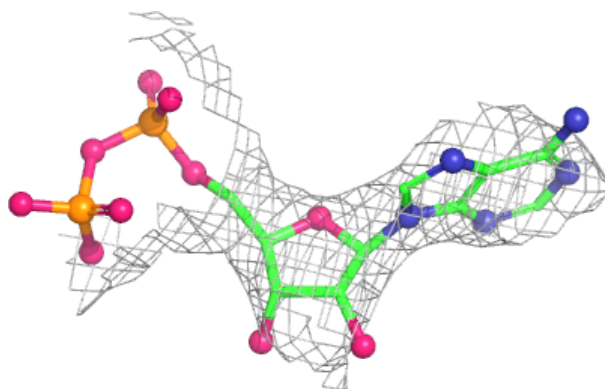
**Electron density around ADP B 602:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

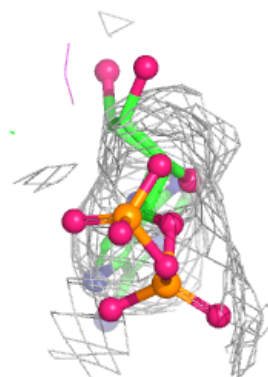
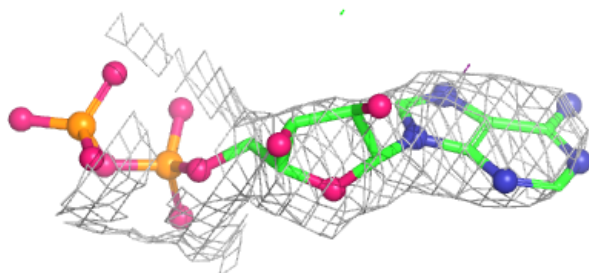
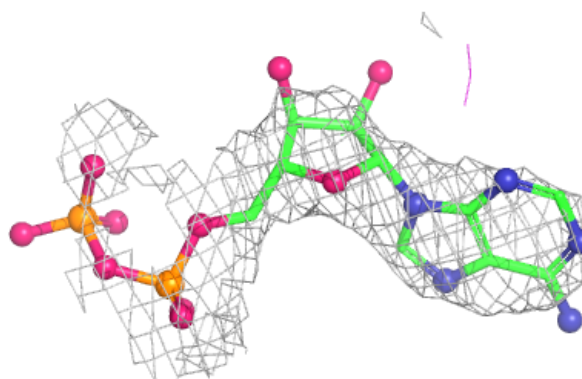


Electron density around ADP D 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

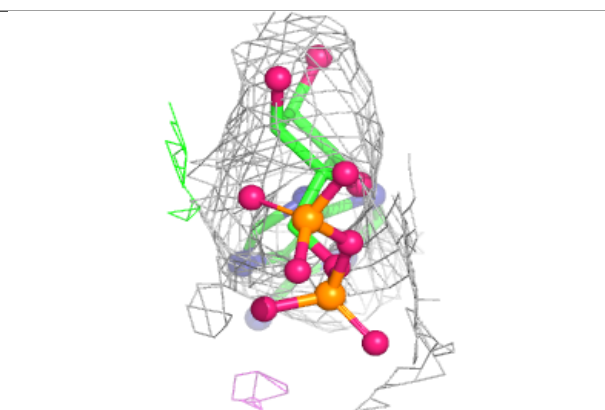
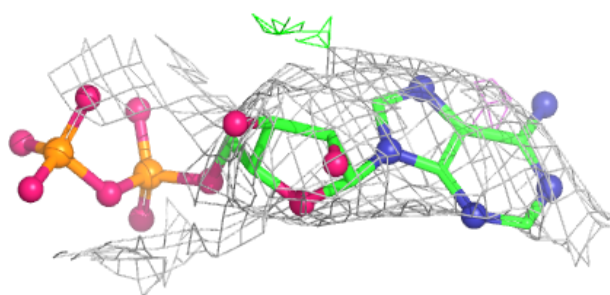
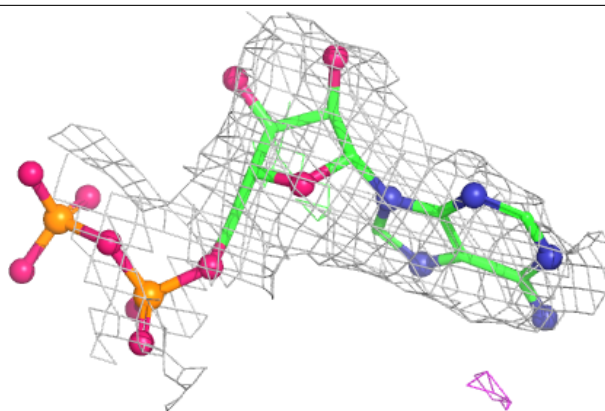
**Electron density around ADP I 602:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

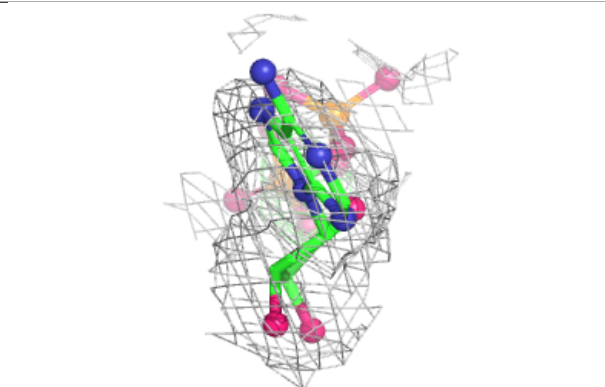
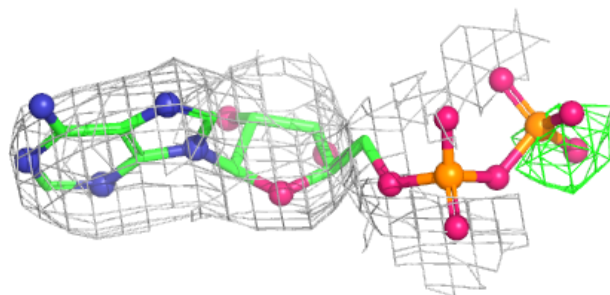
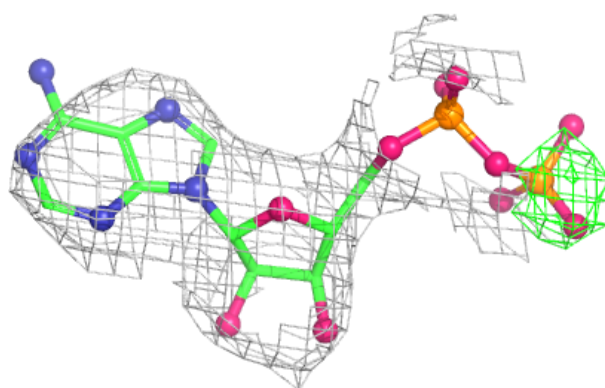


Electron density around ADP K 1102:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

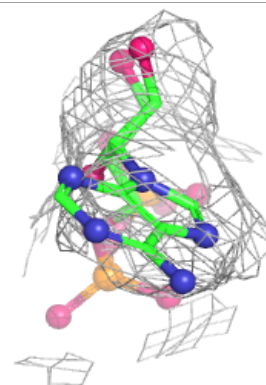
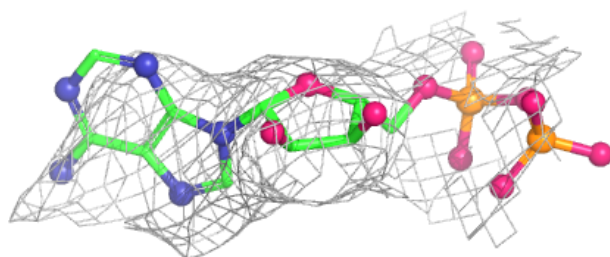
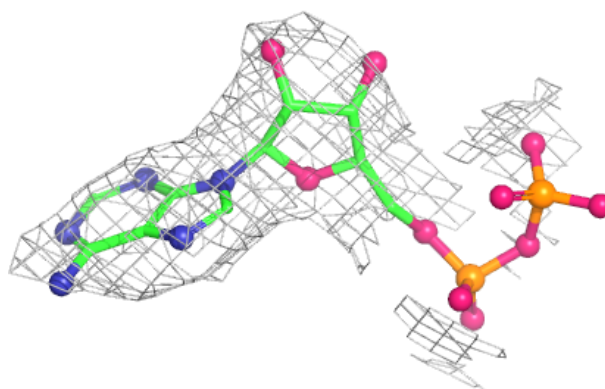
**Electron density around ADP j 602:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

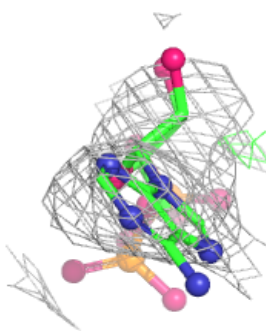
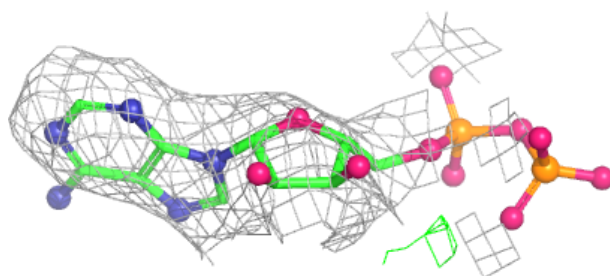
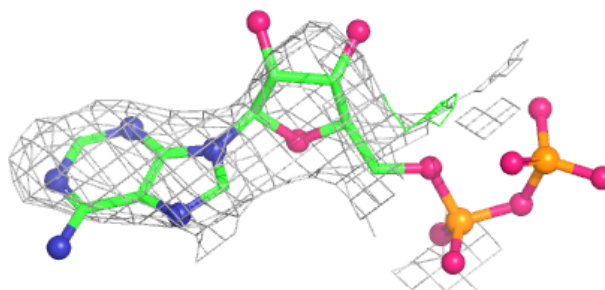


Electron density around ADP 1 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

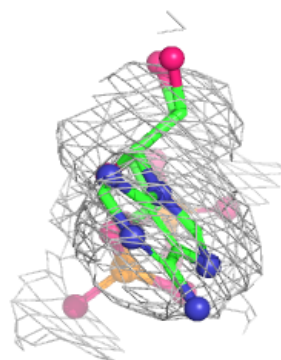
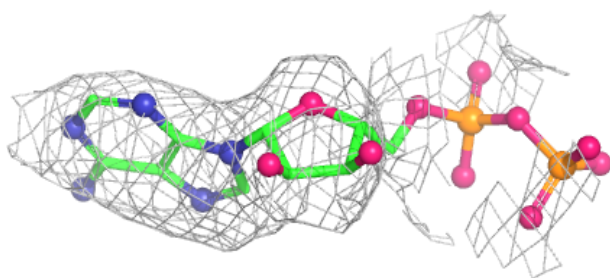
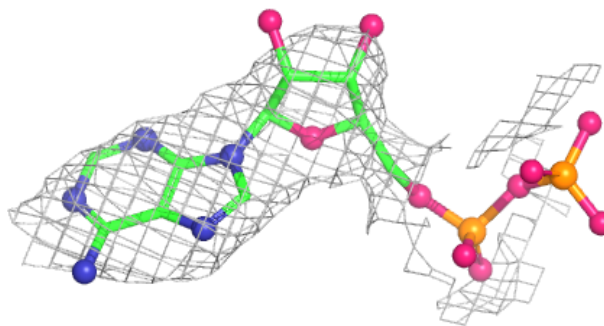
**Electron density around ADP G 602:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

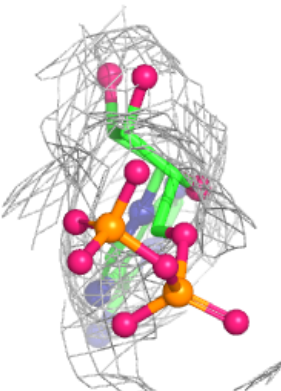
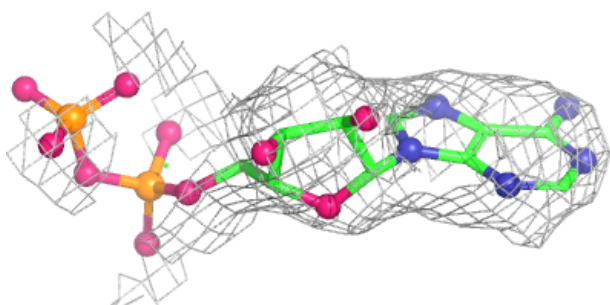
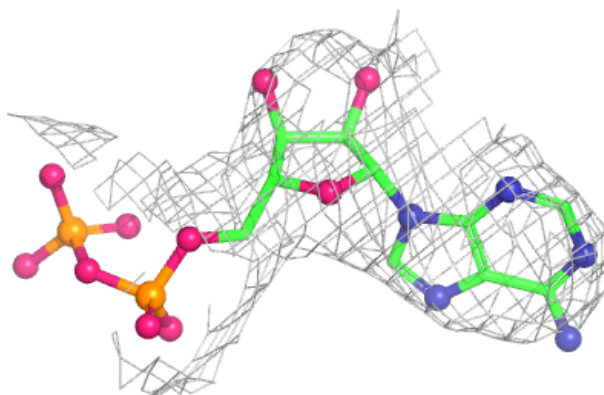


Electron density around ADP J 602:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

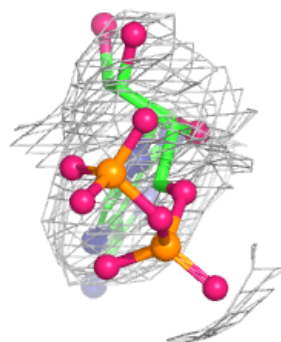
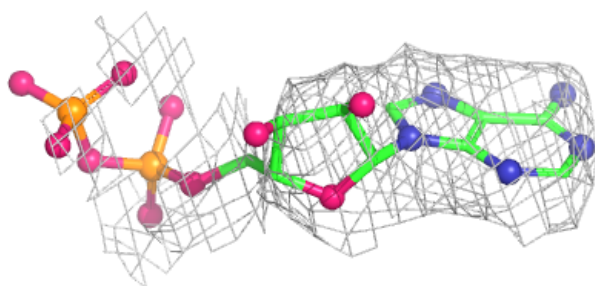
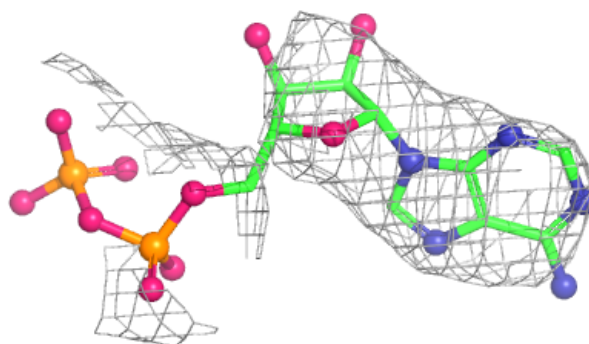
**Electron density around ADP e 602:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

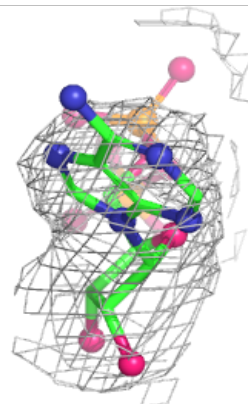
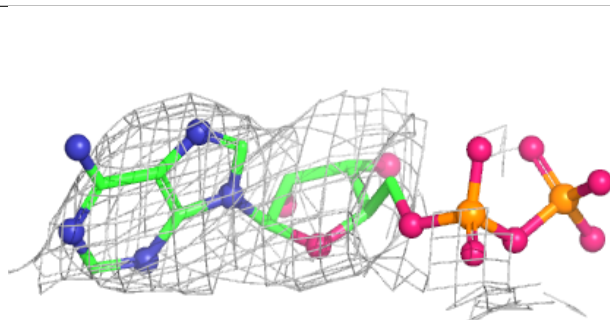
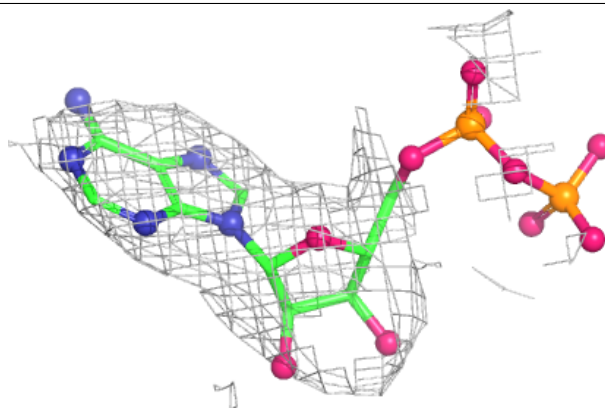


Electron density around ADP E 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP C 1102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.