



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:31 AM EDT

PDB ID : 3KOY / pdb_00003koy
Title : Crystal Structure of ornithine 4,5 aminomutase in complex with ornithine (Aerobic)
Authors : Wolthers, K.R.; Levy, C.W.; Scrutton, N.S.; Leys, D.
Deposited on : 2009-11-14
Resolution : 2.80 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 ⓘ](#)) 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

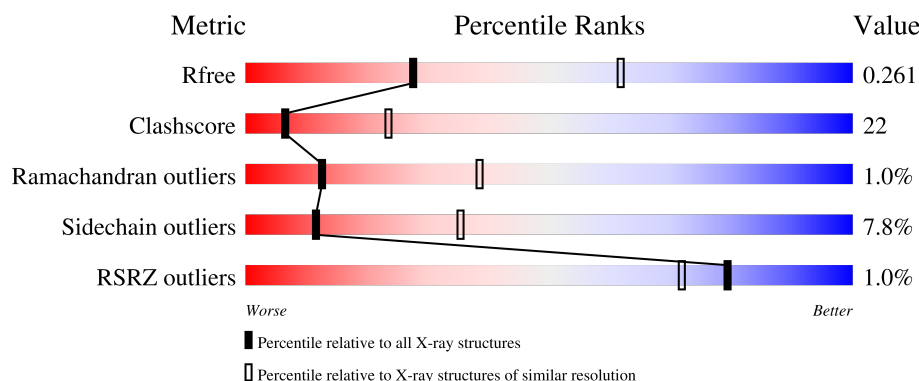
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	A	763	2% 58% 33% 5%
1	B	763	54% 36% 5% 5%
1	C	763	55% 36% 5%
1	D	763	2% 58% 33% 5%
2	E	121	% 52% 36% 9%

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Mol	Chain	Length	Quality of chain
2	F	121	
2	G	121	
2	H	121	

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
3	B12	A	1801	X	-	X	-
3	B12	B	1801	X	-	X	-
3	B12	C	1801	X	-	X	-
3	B12	D	1801	X	-	X	-
5	5AD	A	1500	X	-	-	-
5	5AD	B	1500	X	-	-	-
5	5AD	C	1500	X	-	-	-
5	5AD	D	1500	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26592 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 D-ornithine aminomutase E component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5634	3550	976	1075	33			
1	B	728	Total	C	N	O	S	0	0	0
			5665	3574	983	1074	34			
1	C	728	Total	C	N	O	S	0	0	0
			5654	3570	981	1069	34			
1	D	728	Total	C	N	O	S	0	0	0
			5664	3575	984	1071	34			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
A	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
A	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
A	744	SER	-	expression tag	UNP Q8VPJ5
A	745	GLU	-	expression tag	UNP Q8VPJ5
A	746	ASP	-	expression tag	UNP Q8VPJ5
A	747	PRO	-	expression tag	UNP Q8VPJ5
A	748	ASN	-	expression tag	UNP Q8VPJ5
A	749	SER	-	expression tag	UNP Q8VPJ5
A	750	SER	-	expression tag	UNP Q8VPJ5
A	751	SER	-	expression tag	UNP Q8VPJ5
A	752	VAL	-	expression tag	UNP Q8VPJ5
A	753	ASP	-	expression tag	UNP Q8VPJ5
A	754	LYS	-	expression tag	UNP Q8VPJ5
A	755	LEU	-	expression tag	UNP Q8VPJ5
A	756	ALA	-	expression tag	UNP Q8VPJ5
A	757	ALA	-	expression tag	UNP Q8VPJ5
A	758	ALA	-	expression tag	UNP Q8VPJ5
A	759	LEU	-	expression tag	UNP Q8VPJ5
A	760	GLU	-	expression tag	UNP Q8VPJ5
A	761	HIS	-	expression tag	UNP Q8VPJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	762	HIS	-	expression tag	UNP Q8VPJ5
A	763	HIS	-	expression tag	UNP Q8VPJ5
A	764	HIS	-	expression tag	UNP Q8VPJ5
A	765	HIS	-	expression tag	UNP Q8VPJ5
A	766	HIS	-	expression tag	UNP Q8VPJ5
B	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
B	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
B	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
B	744	SER	-	expression tag	UNP Q8VPJ5
B	745	GLU	-	expression tag	UNP Q8VPJ5
B	746	ASP	-	expression tag	UNP Q8VPJ5
B	747	PRO	-	expression tag	UNP Q8VPJ5
B	748	ASN	-	expression tag	UNP Q8VPJ5
B	749	SER	-	expression tag	UNP Q8VPJ5
B	750	SER	-	expression tag	UNP Q8VPJ5
B	751	SER	-	expression tag	UNP Q8VPJ5
B	752	VAL	-	expression tag	UNP Q8VPJ5
B	753	ASP	-	expression tag	UNP Q8VPJ5
B	754	LYS	-	expression tag	UNP Q8VPJ5
B	755	LEU	-	expression tag	UNP Q8VPJ5
B	756	ALA	-	expression tag	UNP Q8VPJ5
B	757	ALA	-	expression tag	UNP Q8VPJ5
B	758	ALA	-	expression tag	UNP Q8VPJ5
B	759	LEU	-	expression tag	UNP Q8VPJ5
B	760	GLU	-	expression tag	UNP Q8VPJ5
B	761	HIS	-	expression tag	UNP Q8VPJ5
B	762	HIS	-	expression tag	UNP Q8VPJ5
B	763	HIS	-	expression tag	UNP Q8VPJ5
B	764	HIS	-	expression tag	UNP Q8VPJ5
B	765	HIS	-	expression tag	UNP Q8VPJ5
B	766	HIS	-	expression tag	UNP Q8VPJ5
C	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
C	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
C	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
C	744	SER	-	expression tag	UNP Q8VPJ5
C	745	GLU	-	expression tag	UNP Q8VPJ5
C	746	ASP	-	expression tag	UNP Q8VPJ5
C	747	PRO	-	expression tag	UNP Q8VPJ5
C	748	ASN	-	expression tag	UNP Q8VPJ5
C	749	SER	-	expression tag	UNP Q8VPJ5
C	750	SER	-	expression tag	UNP Q8VPJ5
C	751	SER	-	expression tag	UNP Q8VPJ5

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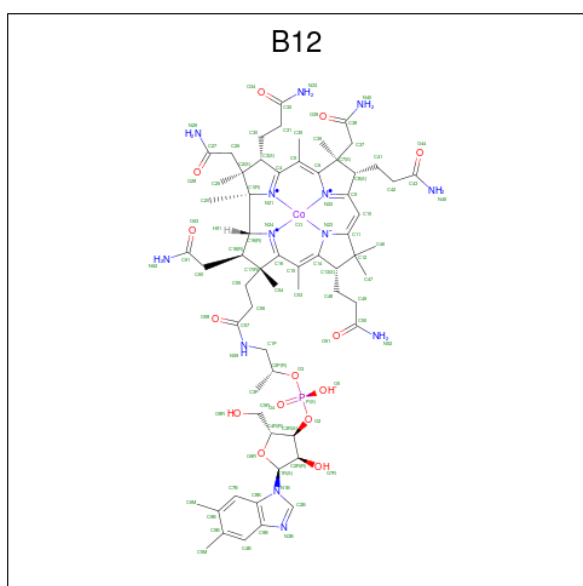
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Chain	Residue	Modelled	Actual	Comment	Reference
C	752	VAL	-	expression tag	UNP Q8VPJ5
C	753	ASP	-	expression tag	UNP Q8VPJ5
C	754	LYS	-	expression tag	UNP Q8VPJ5
C	755	LEU	-	expression tag	UNP Q8VPJ5
C	756	ALA	-	expression tag	UNP Q8VPJ5
C	757	ALA	-	expression tag	UNP Q8VPJ5
C	758	ALA	-	expression tag	UNP Q8VPJ5
C	759	LEU	-	expression tag	UNP Q8VPJ5
C	760	GLU	-	expression tag	UNP Q8VPJ5
C	761	HIS	-	expression tag	UNP Q8VPJ5
C	762	HIS	-	expression tag	UNP Q8VPJ5
C	763	HIS	-	expression tag	UNP Q8VPJ5
C	764	HIS	-	expression tag	UNP Q8VPJ5
C	765	HIS	-	expression tag	UNP Q8VPJ5
C	766	HIS	-	expression tag	UNP Q8VPJ5
D	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
D	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
D	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
D	744	SER	-	expression tag	UNP Q8VPJ5
D	745	GLU	-	expression tag	UNP Q8VPJ5
D	746	ASP	-	expression tag	UNP Q8VPJ5
D	747	PRO	-	expression tag	UNP Q8VPJ5
D	748	ASN	-	expression tag	UNP Q8VPJ5
D	749	SER	-	expression tag	UNP Q8VPJ5
D	750	SER	-	expression tag	UNP Q8VPJ5
D	751	SER	-	expression tag	UNP Q8VPJ5
D	752	VAL	-	expression tag	UNP Q8VPJ5
D	753	ASP	-	expression tag	UNP Q8VPJ5
D	754	LYS	-	expression tag	UNP Q8VPJ5
D	755	LEU	-	expression tag	UNP Q8VPJ5
D	756	ALA	-	expression tag	UNP Q8VPJ5
D	757	ALA	-	expression tag	UNP Q8VPJ5
D	758	ALA	-	expression tag	UNP Q8VPJ5
D	759	LEU	-	expression tag	UNP Q8VPJ5
D	760	GLU	-	expression tag	UNP Q8VPJ5
D	761	HIS	-	expression tag	UNP Q8VPJ5
D	762	HIS	-	expression tag	UNP Q8VPJ5
D	763	HIS	-	expression tag	UNP Q8VPJ5
D	764	HIS	-	expression tag	UNP Q8VPJ5
D	765	HIS	-	expression tag	UNP Q8VPJ5
D	766	HIS	-	expression tag	UNP Q8VPJ5

- Molecule 2 is a protein called D-ornithine aminomutase S component.

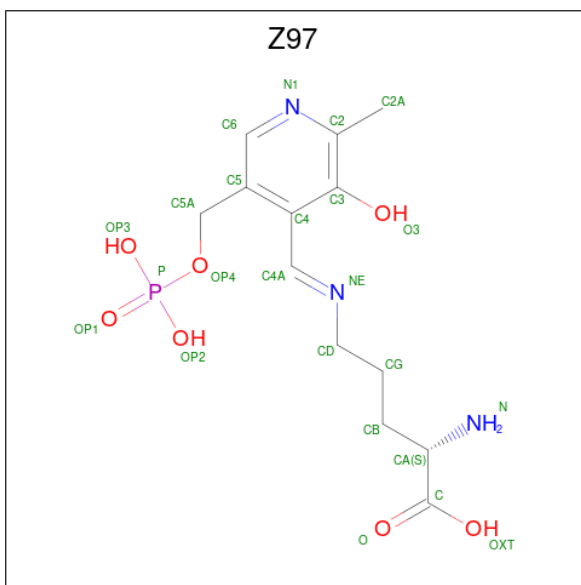
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	110	Total	C	N	O	S	0	0	0
			860	541	153	162	4			
2	F	110	Total	C	N	O	S	0	0	0
			863	542	153	164	4			
2	G	110	Total	C	N	O	S	0	0	0
			860	541	153	162	4			
2	H	110	Total	C	N	O	S	0	0	0
			860	541	153	162	4			

- Molecule 3 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



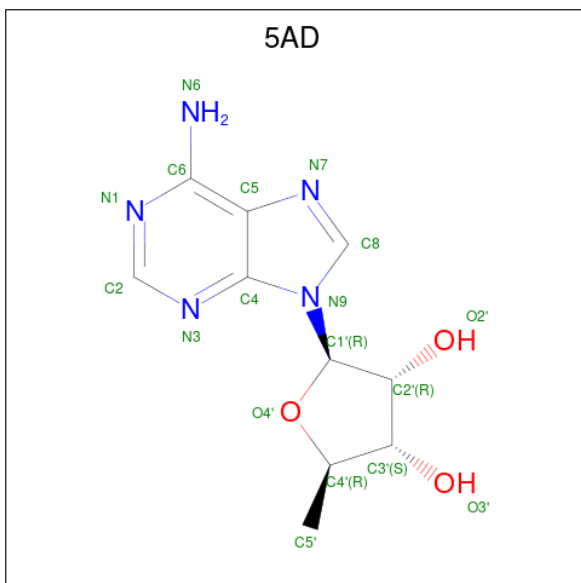
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
3	B	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
3	C	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
3	D	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0

- Molecule 4 is (E)-N 5 -({3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methylidene)-L-ornithine (CCD ID: Z97) (formula: $C_{13}H_{20}N_3O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			24	13	3	7	1		
4	B	1	Total	C	N	O	P	0	0
			24	13	3	7	1		
4	C	1	Total	C	N	O	P	0	0
			24	13	3	7	1		
4	D	1	Total	C	N	O	P	0	0
			24	13	3	7	1		

- Molecule 5 is 5'-DEOXYADENOSINE (CCD ID: 5AD) (formula: $C_{10}H_{13}N_5O_3$).

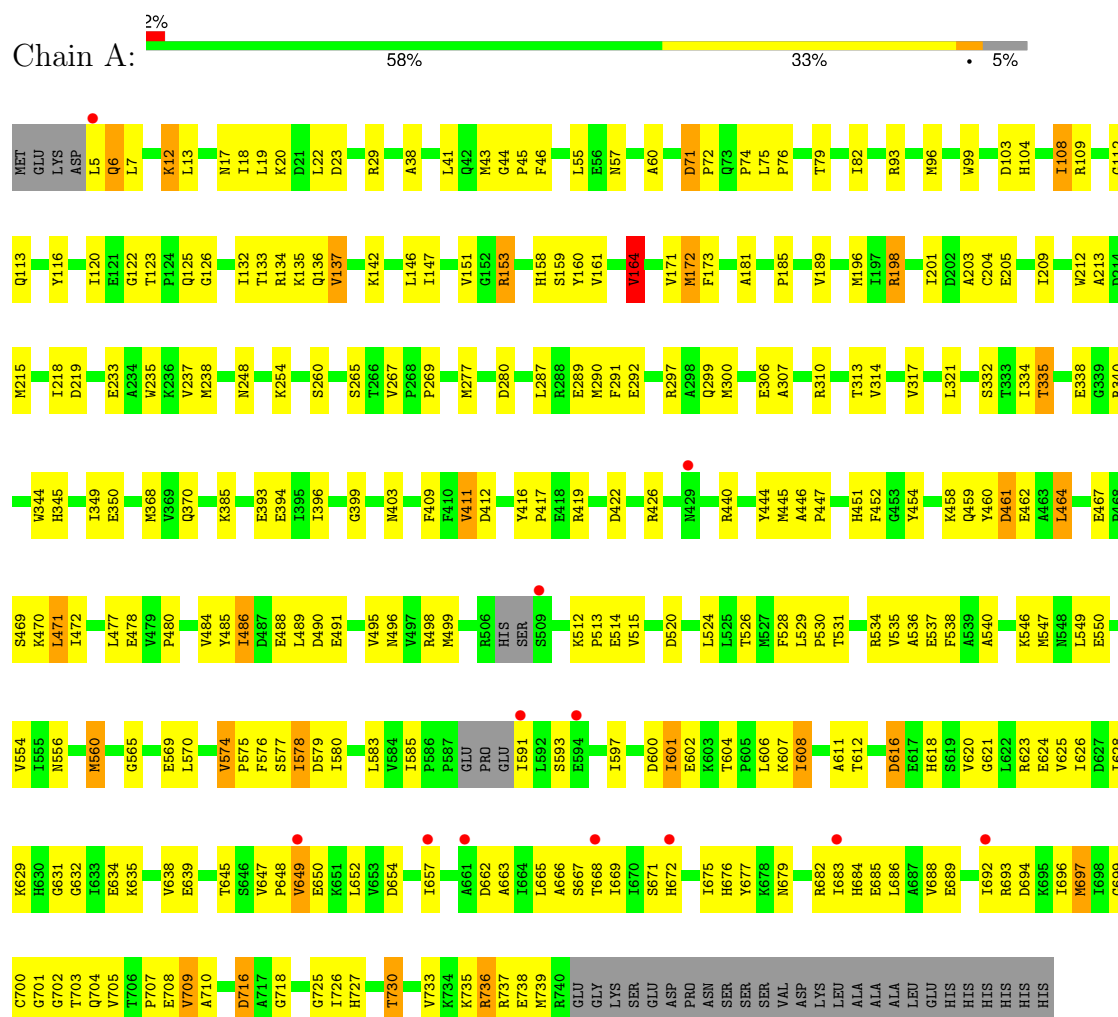


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 18	C 10	N 5	O 3	0	0
5	B	1	Total 18	C 10	N 5	O 3	0	0
5	C	1	Total 18	C 10	N 5	O 3	0	0
5	D	1	Total 18	C 10	N 5	O 3	0	0

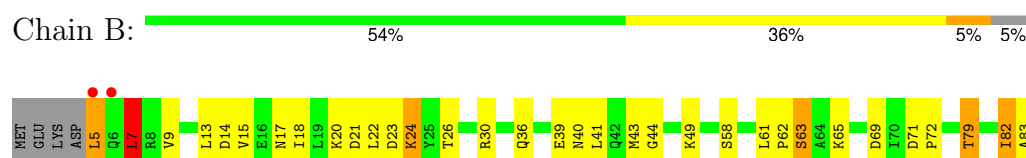
3 Residue-property plots

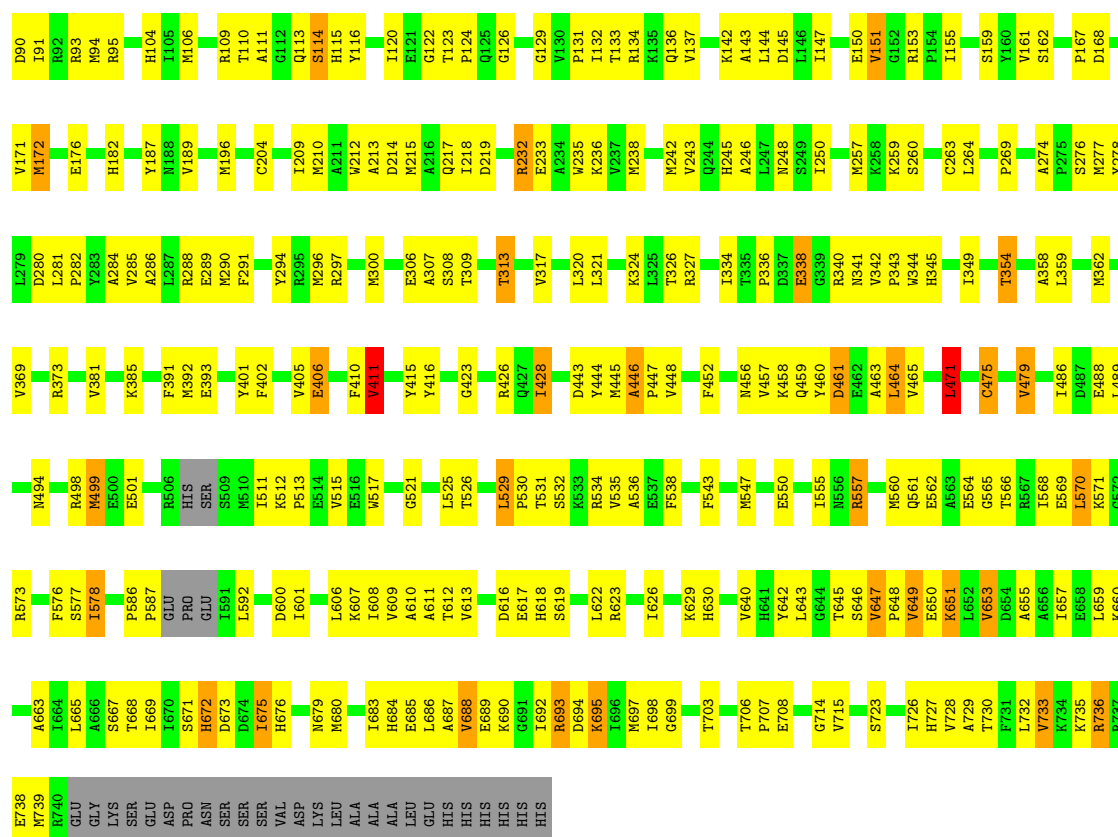
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: D-ornithine aminomutase E component



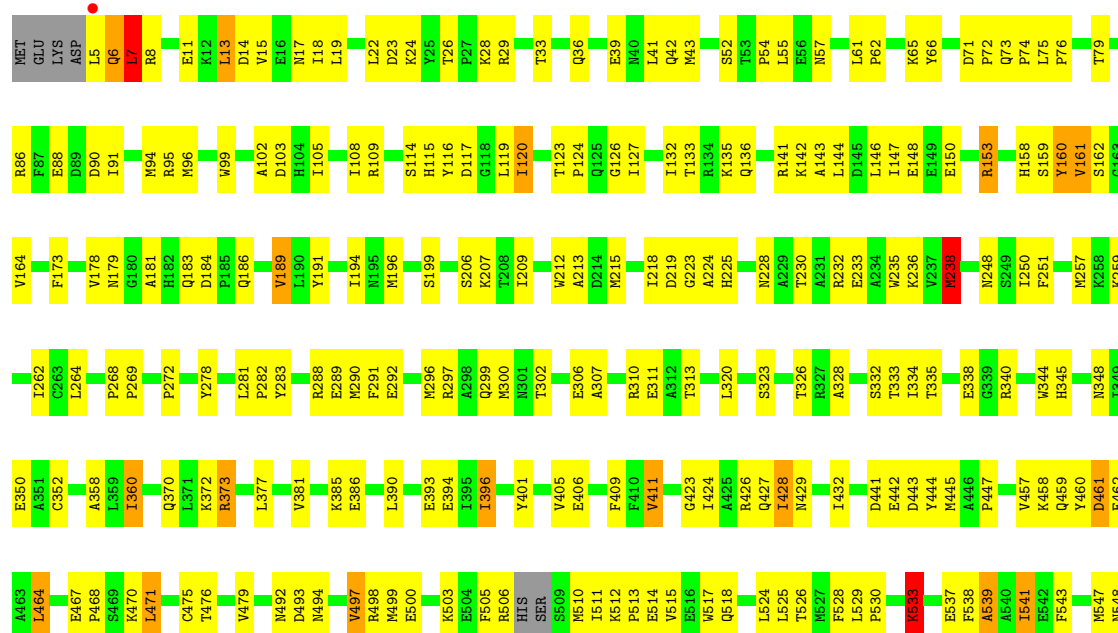
• Molecule 1: D-ornithine aminomutase E component

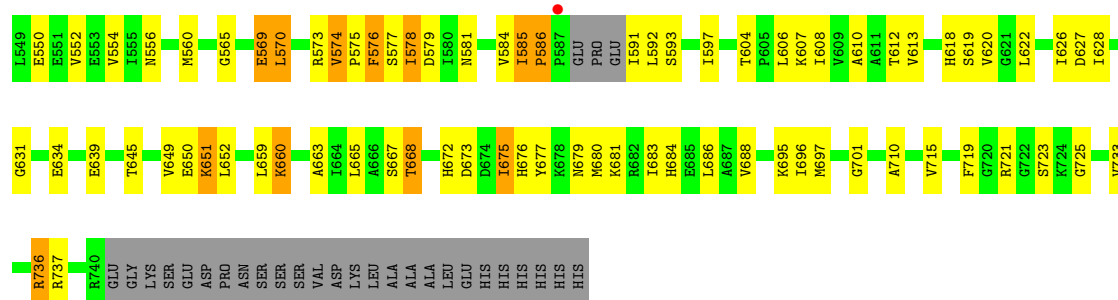




• Molecule 1: D-ornithine aminomutase E component

Chain C: 55% 36% 5%

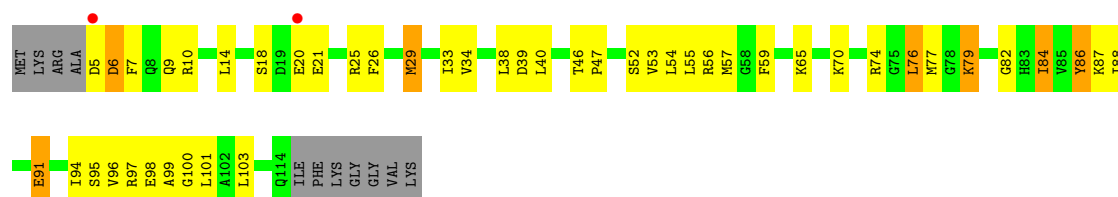




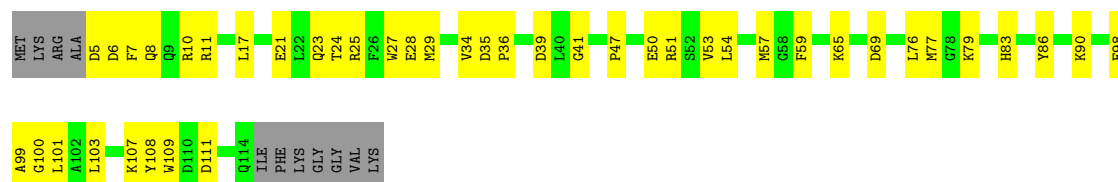
● Molecule 2: D-ornithine aminomutase S component



● Molecule 2: D-ornithine aminomutase S component



● Molecule 2: D-ornithine aminomutase S component



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.52Å 233.22Å 124.14Å 90.00° 103.43° 90.00°	Depositor
Resolution (Å)	60.37 – 2.80 60.37 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.8 (60.37-2.80) 93.8 (60.37-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.5_2, REFMAC 5.5.0066	Depositor
R, R_{free}	0.183 , 0.263 0.181 , 0.261	Depositor DCC
R_{free} test set	4265 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26592	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.10% 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: 5AD, Z97, B12

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	A	0.57	0/5739	0.94	12/7776 (0.2%)
1	B	0.57	0/5770	0.94	11/7809 (0.1%)
1	C	0.56	0/5759	0.94	15/7796 (0.2%)
1	D	0.58	0/5769	0.93	10/7808 (0.1%)
2	E	0.55	0/872	0.89	0/1170
2	F	0.59	0/875	0.91	0/1174
2	G	0.52	0/872	0.85	1/1170 (0.1%)
2	H	0.58	0/872	0.88	1/1170 (0.1%)
All	All	0.57	0/26528	0.93	50/35873 (0.1%)

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	585	ILE	CA-C-N	8.59	129.22	120.38
1	C	585	ILE	C-N-CA	8.59	129.22	120.38
1	D	272	PRO	CA-C-O	-7.30	115.64	120.90
1	C	73	GLN	CA-C-N	6.45	126.82	119.92
1	C	73	GLN	C-N-CA	6.45	126.82	119.92
1	B	479	VAL	CA-C-N	6.40	126.89	119.47
1	B	479	VAL	C-N-CA	6.40	126.89	119.47
1	D	276	SER	N-CA-C	6.32	118.97	111.33
1	A	560	MET	N-CA-C	-6.28	103.00	112.04
1	D	272	PRO	O-C-N	6.14	124.13	121.31
1	C	539	ALA	N-CA-C	-6.06	104.67	111.28
1	A	335	THR	CA-C-N	6.05	125.73	119.56
1	A	335	THR	C-N-CA	6.05	125.73	119.56
1	A	529	LEU	CA-C-N	6.02	127.36	119.84
1	A	529	LEU	C-N-CA	6.02	127.36	119.84
2	G	33	ILE	N-CA-C	5.95	116.73	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	113	GLN	N-CA-C	-5.91	105.33	112.54
1	C	71	ASP	CA-C-N	5.88	125.89	119.90
1	C	71	ASP	C-N-CA	5.88	125.89	119.90
1	A	716	ASP	N-CA-C	5.87	117.35	111.07
1	A	71	ASP	CA-C-N	5.87	125.62	119.76
1	A	71	ASP	C-N-CA	5.87	125.62	119.76
1	B	647	VAL	N-CA-C	5.63	113.44	107.76
2	H	99	ALA	N-CA-C	-5.53	105.15	111.07
1	C	272	PRO	CA-C-O	-5.49	116.94	120.90
1	B	564	GLU	N-CA-C	5.45	117.98	111.71
1	C	160	TYR	N-CA-C	5.45	117.29	108.41
1	B	475	CYS	N-CA-C	-5.39	102.00	110.36
1	C	533	LYS	N-CA-C	5.38	116.95	111.14
1	C	238	MET	CA-C-N	-5.35	113.11	119.05
1	C	238	MET	C-N-CA	-5.35	113.11	119.05
1	D	84	SER	N-CA-C	-5.35	107.41	114.31
1	A	161	VAL	N-CA-C	-5.33	107.78	112.90
1	A	164	VAL	CB-CA-C	-5.33	102.55	111.29
1	C	585	ILE	N-CA-C	5.33	113.42	108.15
1	B	529	LEU	CA-C-N	5.32	126.50	119.84
1	B	529	LEU	C-N-CA	5.32	126.50	119.84
1	A	82	ILE	N-CA-C	5.31	116.16	107.24
1	D	693	ARG	N-CA-C	5.30	116.91	111.03
1	D	189	VAL	N-CA-C	5.28	115.94	110.82
1	D	479	VAL	CA-C-N	5.20	124.87	119.56
1	D	479	VAL	C-N-CA	5.20	124.87	119.56
1	B	446	ALA	CA-C-N	5.16	126.28	119.84
1	B	446	ALA	C-N-CA	5.16	126.28	119.84
1	D	574	VAL	CA-C-N	5.10	124.71	119.56
1	D	574	VAL	C-N-CA	5.10	124.71	119.56
1	C	479	VAL	CA-C-N	5.04	126.14	119.84
1	C	479	VAL	C-N-CA	5.04	126.14	119.84
1	B	69	ASP	N-CA-C	5.02	118.69	112.47
1	A	593	SER	N-CA-C	5.00	116.56	110.41

There are no chirality outliers.

There are no planarity outliers.

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	A	5634	0	5544	252	0
1	B	5665	0	5629	256	0
1	C	5654	0	5621	248	0
1	D	5664	0	5636	252	0
2	E	860	0	865	40	0
2	F	863	0	867	34	0
2	G	860	0	865	45	0
2	H	860	0	865	37	0
3	A	91	0	87	22	0
3	B	91	0	87	25	0
3	C	91	0	87	26	0
3	D	91	0	87	33	0
4	A	24	0	18	0	0
4	B	24	0	18	4	0
4	C	24	0	18	2	0
4	D	24	0	18	2	0
5	A	18	0	8	3	0
5	B	18	0	8	4	0
5	C	18	0	9	0	0
5	D	18	0	8	4	0
All	All	26592	0	26345	1152	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 22.

All (1152) 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:E:5:ASP:HA	2:E:7:PHE:N	1.53	1.22
2:F:5:ASP:HA	2:F:7:PHE:N	1.61	1.13
1:D:537:GLU:HG3	1:D:554:VAL:HG21	1.36	1.07
1:B:393:GLU:HG3	2:F:29:MET:HE1	1.32	1.06
1:A:306:GLU:HG3	1:A:307:ALA:H	0.87	1.03
1:C:458:LYS:HG3	1:C:462:GLU:HG3	1.41	1.01
1:A:526:THR:HG22	1:A:569:GLU:HG2	1.39	1.01
2:G:5:ASP:HA	2:G:7:PHE:N	1.76	0.99
2:F:5:ASP:HA	2:F:7:PHE:H	0.84	0.98
5:B:1500:5AD:H5'3	3:D:1801:B12:C16	1.93	0.98
1:A:306:GLU:HG3	1:A:307:ALA:N	1.67	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:MET:HE2	1:B:321:LEU:HD23	1.47	0.96
3:C:1801:B12:H401	3:C:1801:B12:H8	1.30	0.95
1:D:459:GLN:HG3	1:D:460:TYR:CD2	2.03	0.94
1:C:458:LYS:HE3	1:C:462:GLU:HG2	1.52	0.92
1:C:668:THR:HG23	1:C:676:HIS:HB2	1.49	0.92
1:C:96:MET:HE1	1:C:345:HIS:HB3	1.50	0.92
1:A:306:GLU:CG	1:A:307:ALA:H	1.80	0.91
2:E:5:ASP:HA	2:E:7:PHE:H	1.22	0.90
3:B:1801:B12:C16	5:D:1500:5AD:H5'2	2.00	0.89
1:C:373:ARG:HH11	1:C:373:ARG:HG3	1.37	0.88
2:F:5:ASP:CA	2:F:7:PHE:H	1.81	0.88
3:D:1801:B12:H601	3:D:1801:B12:H262	1.55	0.88
2:H:5:ASP:HA	2:H:7:PHE:N	1.89	0.88
1:A:43:MET:HE1	1:A:72:PRO:HA	1.56	0.87
2:G:57:MET:HE1	2:G:82:GLY:HA2	1.57	0.86
1:D:394:GLU:HG2	1:D:409:PHE:CE2	2.11	0.86
1:B:526:THR:HG23	1:B:569:GLU:HG2	1.56	0.86
1:A:277:MET:HE2	1:A:321:LEU:HD23	1.59	0.84
1:A:96:MET:HG2	1:C:560:MET:HB3	1.59	0.84
1:D:394:GLU:HG2	1:D:409:PHE:HE2	1.38	0.84
1:B:23:ASP:OD2	1:B:24:LYS:HE3	1.78	0.83
3:B:1801:B12:H8	3:B:1801:B12:H401	1.43	0.83
2:G:87:LYS:O	2:G:91:GLU:HB2	1.79	0.83
2:H:5:ASP:HA	2:H:7:PHE:H	1.44	0.82
3:A:1801:B12:H262	3:A:1801:B12:H601	1.62	0.81
1:A:396:ILE:HD12	2:E:29:MET:HE2	1.63	0.81
1:A:41:LEU:HD21	1:A:43:MET:HE2	1.60	0.81
1:A:577:SER:O	1:A:578:ILE:HD12	1.79	0.81
1:B:232:ARG:HH21	1:D:598:ARG:HH22	1.28	0.81
1:A:682:ARG:HG2	1:A:686:LEU:HD13	1.63	0.81
1:B:577:SER:O	1:B:578:ILE:HD12	1.82	0.80
1:C:218:ILE:HD13	1:C:297:ARG:HD2	1.62	0.80
1:A:96:MET:HE1	1:A:345:HIS:HB3	1.63	0.80
1:C:668:THR:CG2	1:C:676:HIS:HB2	2.11	0.80
1:A:233:GLU:HG2	1:A:235:TRP:CH2	2.16	0.79
1:C:43:MET:HE1	1:C:72:PRO:HA	1.63	0.79
3:C:1801:B12:H362	3:C:1801:B12:H351	1.63	0.79
5:B:1500:5AD:H5'2	3:D:1801:B12:H261	1.64	0.79
1:D:459:GLN:HG3	1:D:460:TYR:HD2	1.46	0.79
1:B:393:GLU:HG3	2:F:29:MET:CE	2.12	0.79
1:A:618:HIS:HB2	1:A:669:ILE:HG13	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:GLU:HG2	1:D:235:TRP:CZ2	2.19	0.78
1:D:406:GLU:OE2	1:D:428:ILE:HG23	1.83	0.78
1:A:606:LEU:HD12	1:A:607:LYS:H	1.48	0.78
1:D:41:LEU:HD23	1:D:43:MET:HE2	1.64	0.78
3:D:1801:B12:N40	3:D:1801:B12:H8	1.99	0.78
1:D:649:VAL:HG11	1:D:682:ARG:HB3	1.64	0.77
2:F:6:ASP:O	2:F:10:ARG:HG3	1.84	0.77
1:B:137:VAL:HG21	1:B:172:MET:HE1	1.66	0.77
1:A:464:LEU:HD23	1:A:471:LEU:HD23	1.67	0.77
1:B:525:LEU:HD23	1:B:570:LEU:HD13	1.65	0.77
1:B:14:ASP:OD2	1:B:17:ASN:HB2	1.85	0.76
1:A:134:ARG:HA	1:A:172:MET:HE3	1.68	0.76
1:A:738:GLU:HG3	1:A:739:MET:N	1.99	0.76
1:D:611:ALA:HB2	1:D:643:LEU:HB2	1.67	0.76
1:D:88:GLU:OE2	1:D:498:ARG:HD2	1.86	0.76
1:A:459:GLN:HG3	1:A:460:TYR:HD2	1.50	0.75
1:D:123:THR:HG23	1:D:135:LYS:HD3	1.67	0.75
1:C:577:SER:O	1:C:578:ILE:HD12	1.87	0.75
1:A:123:THR:HG23	1:A:135:LYS:HD3	1.69	0.75
3:B:1801:B12:H8	3:B:1801:B12:N40	1.98	0.75
2:E:54:LEU:HD23	2:E:57:MET:HE2	1.69	0.74
1:B:82:ILE:HD13	1:B:93:ARG:HD2	1.69	0.74
1:C:459:GLN:HG3	1:C:460:TYR:CD2	2.22	0.74
1:B:534:ARG:HG3	1:B:534:ARG:HH11	1.52	0.74
1:B:488:GLU:O	1:B:489:LEU:HD23	1.88	0.73
1:B:623:ARG:HD3	1:D:115:HIS:CE1	2.24	0.73
1:C:259:LYS:HA	1:C:262:ILE:HD12	1.70	0.73
1:C:225:HIS:O	1:C:228:ASN:HB2	1.89	0.73
1:C:290:MET:HE3	2:G:26:PHE:CD2	2.24	0.72
1:A:18:ILE:HG23	1:A:142:LYS:HD3	1.70	0.72
1:A:459:GLN:HG3	1:A:460:TYR:CD2	2.24	0.72
1:B:196:MET:SD	1:B:402:PHE:CD1	2.83	0.72
1:A:668:THR:HG21	1:A:676:HIS:HA	1.71	0.72
1:B:109:ARG:HG2	1:B:132:ILE:HG13	1.72	0.72
1:C:189:VAL:HG11	1:C:196:MET:HB3	1.68	0.72
1:C:512:LYS:HB2	1:C:513:PRO:HD2	1.70	0.72
2:F:109:TRP:O	2:F:113:ILE:HG13	1.90	0.71
1:A:393:GLU:HA	2:E:29:MET:HE1	1.72	0.71
1:B:88:GLU:OE2	1:B:498:ARG:HD2	1.90	0.71
1:C:233:GLU:HB3	1:C:235:TRP:CZ3	2.24	0.71
1:C:575:PRO:HD2	1:C:576:PHE:CE2	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:5:ASP:HA	2:G:6:ASP:C	2.14	0.71
3:A:1801:B12:H5R1	3:A:1801:B12:H3P1	1.71	0.71
1:D:219:ASP:HB3	1:D:248:ASN:ND2	2.06	0.71
3:D:1801:B12:H262	3:D:1801:B12:C60	2.21	0.71
2:F:54:LEU:HD23	2:F:57:MET:HE2	1.73	0.71
1:A:528:PHE:CE1	1:A:565:GLY:HA3	2.25	0.70
2:F:57:MET:HE1	2:F:82:GLY:HA2	1.74	0.70
1:C:213:ALA:HB3	1:C:215:MET:HG3	1.73	0.70
1:B:232:ARG:HE	1:D:598:ARG:CZ	2.04	0.70
1:B:120:ILE:HG13	1:B:133:THR:HG22	1.73	0.70
1:A:396:ILE:HD12	2:E:29:MET:CE	2.21	0.70
3:A:1801:B12:H2B	3:A:1801:B12:O7R	1.91	0.70
1:D:510:MET:CE	1:D:577:SER:HB2	2.21	0.70
1:A:120:ILE:HG13	1:A:133:THR:HG22	1.73	0.70
1:C:610:ALA:HB1	1:C:622:LEU:HD21	1.74	0.70
1:C:460:TYR:O	1:C:461:ASP:HB2	1.92	0.69
3:D:1801:B12:H362	3:D:1801:B12:H351	1.75	0.69
1:A:612:THR:HG22	1:A:616:ASP:HB3	1.75	0.69
1:A:550:GLU:HG3	1:A:575:PRO:HG3	1.76	0.68
1:A:671:SER:HB2	1:A:676:HIS:CE1	2.27	0.68
2:F:74:ARG:O	2:F:76:LEU:HD13	1.94	0.68
1:A:277:MET:CE	1:A:321:LEU:HD23	2.24	0.68
3:A:1801:B12:H401	3:A:1801:B12:H8	1.57	0.67
1:B:278:TYR:CD1	1:D:368:MET:HE3	2.27	0.67
1:B:606:LEU:HD21	1:B:732:LEU:HB3	1.76	0.67
1:A:677:TYR:CE1	1:A:709:VAL:HB	2.29	0.67
3:A:1801:B12:H362	3:A:1801:B12:H351	1.74	0.67
3:A:1801:B12:H8	3:A:1801:B12:N40	2.08	0.67
1:B:134:ARG:HA	1:B:172:MET:HE3	1.74	0.67
2:H:5:ASP:HA	2:H:6:ASP:HB3	1.76	0.67
1:A:103:ASP:HB3	1:A:153:ARG:NH1	2.09	0.67
1:C:250:ILE:HG23	2:G:34:VAL:HG21	1.75	0.67
1:A:445:MET:CE	1:A:471:LEU:HD12	2.25	0.67
1:B:243:VAL:HG22	1:B:392:MET:HG3	1.76	0.67
2:H:59:PHE:CE1	2:H:100:GLY:HA3	2.30	0.67
1:D:526:THR:HG23	1:D:569:GLU:HG2	1.77	0.66
2:F:63:GLU:O	2:F:67:ILE:HG13	1.95	0.66
1:D:649:VAL:HG13	1:D:683:ILE:HG13	1.78	0.66
1:D:120:ILE:HG13	1:D:133:THR:HG22	1.76	0.66
1:A:385:LYS:HE2	2:E:23:GLN:HE21	1.60	0.66
1:C:74:PRO:HB2	1:C:76:PRO:HD2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:MET:CE	1:A:72:PRO:HA	2.24	0.66
1:A:560:MET:HB3	1:C:96:MET:HE3	1.76	0.66
1:C:579:ASP:OD1	1:C:581:ASN:HB2	1.95	0.66
1:C:593:SER:O	1:C:597:ILE:HG12	1.96	0.66
1:D:649:VAL:CG1	1:D:683:ILE:HG13	2.25	0.66
1:A:738:GLU:HG3	1:A:739:MET:H	1.60	0.66
2:E:5:ASP:CA	2:E:7:PHE:H	2.01	0.66
3:B:1801:B12:H362	3:B:1801:B12:H351	1.76	0.65
2:G:97:ARG:O	2:G:101:LEU:HB2	1.95	0.65
1:D:632:GLY:HA2	1:D:725:GLY:HA3	1.78	0.65
1:A:440:ARG:NH1	1:A:444:TYR:CE2	2.65	0.65
1:A:484:VAL:HG11	2:E:60:SER:HB3	1.77	0.65
1:B:115:HIS:CE1	1:D:623:ARG:HD3	2.31	0.65
1:C:238:MET:HE3	1:C:283:TYR:HB2	1.78	0.65
2:F:88:ILE:HG13	2:F:103:LEU:HD11	1.79	0.65
1:A:486:ILE:N	1:A:486:ILE:HD12	2.11	0.65
1:D:512:LYS:HB2	1:D:513:PRO:HD2	1.79	0.65
3:D:1801:B12:H421	3:D:1801:B12:H10	1.79	0.65
1:B:79:THR:HG23	1:B:104:HIS:CG	2.32	0.65
1:C:458:LYS:HE3	1:C:462:GLU:CG	2.26	0.64
1:D:460:TYR:CE1	2:H:86:TYR:HE2	2.15	0.64
1:C:649:VAL:HG12	1:C:686:LEU:HD12	1.78	0.64
2:G:95:SER:OG	2:G:98:GLU:HG2	1.98	0.64
1:B:86:ARG:HG3	1:B:517:TRP:CE2	2.33	0.64
2:E:5:ASP:HA	2:E:6:ASP:C	2.22	0.64
1:C:543:PHE:O	1:C:547:MET:HG3	1.97	0.64
1:D:109:ARG:HG2	1:D:132:ILE:HG12	1.80	0.64
1:C:124:PRO:HA	1:C:493:ASP:OD1	1.98	0.64
1:C:475:CYS:HB2	2:G:56:ARG:O	1.98	0.64
3:D:1801:B12:H311	3:D:1801:B12:H353	1.80	0.64
1:A:580:ILE:HA	1:A:583:LEU:HD12	1.80	0.64
1:B:671:SER:HA	1:B:676:HIS:ND1	2.13	0.64
1:B:689:GLU:O	1:B:689:GLU:HG2	1.97	0.64
1:C:612:THR:HB	1:C:645:THR:HG22	1.80	0.64
1:B:162:SER:HB2	4:B:767:Z97:H6	1.80	0.63
2:F:54:LEU:HD23	2:F:57:MET:CE	2.27	0.63
3:C:1801:B12:H262	3:C:1801:B12:H601	1.79	0.63
1:C:550:GLU:HG3	1:C:573:ARG:NH2	2.13	0.63
1:C:668:THR:HG21	1:C:680:MET:HE2	1.80	0.63
1:A:335:THR:O	1:A:338:GLU:HB2	1.98	0.63
3:A:1801:B12:O7R	3:A:1801:B12:C2B	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:LYS:HE2	2:E:31:GLU:HG3	1.81	0.63
1:A:526:THR:OG1	1:C:524:LEU:HB3	1.98	0.63
1:A:606:LEU:HD12	1:A:607:LYS:N	2.14	0.63
1:C:394:GLU:HG2	1:C:409:PHE:CE2	2.34	0.63
1:B:608:ILE:HG21	1:B:665:LEU:HD12	1.81	0.63
1:A:537:GLU:HG3	1:A:554:VAL:HG21	1.81	0.63
1:A:238:MET:HE2	1:A:269:PRO:HG2	1.81	0.63
3:B:1801:B12:H203	3:B:1801:B12:H301	1.81	0.63
1:D:619:SER:HB2	1:D:623:ARG:CZ	2.29	0.62
1:C:550:GLU:HB2	1:C:573:ARG:HB3	1.81	0.62
1:D:724:LYS:HB2	1:D:726:ILE:HG22	1.81	0.62
2:G:52:SER:HA	2:G:55:LEU:HD12	1.80	0.62
2:E:47:PRO:O	2:E:51:ARG:HG3	2.00	0.62
1:D:277:MET:HE1	1:D:321:LEU:HG	1.82	0.62
1:A:218:ILE:HD13	1:A:297:ARG:HD2	1.80	0.62
1:A:205:GLU:O	1:A:209:ILE:HD12	1.99	0.62
1:B:79:THR:HA	1:B:104:HIS:HB3	1.81	0.62
1:A:628:ILE:HG13	1:A:635:LYS:HB2	1.82	0.62
2:H:47:PRO:O	2:H:51:ARG:HG3	2.00	0.62
1:B:426:ARG:NH1	1:D:634:GLU:OE2	2.25	0.61
1:C:677:TYR:HA	1:C:680:MET:HE3	1.82	0.61
1:D:196:MET:SD	1:D:402:PHE:CD1	2.93	0.61
1:D:219:ASP:HB3	1:D:248:ASN:HD22	1.63	0.61
2:F:97:ARG:O	2:F:101:LEU:HB2	2.00	0.61
2:G:18:SER:OG	2:G:21:GLU:HG3	1.99	0.61
1:B:668:THR:O	1:B:668:THR:HG23	2.00	0.61
1:A:514:GLU:HA	1:A:520:ASP:OD1	2.01	0.61
2:E:74:ARG:HB2	2:E:76:LEU:HD12	1.82	0.61
1:C:649:VAL:HG12	1:C:686:LEU:CD1	2.31	0.61
3:D:1801:B12:H421	3:D:1801:B12:C10	2.31	0.61
1:B:391:PHE:HA	1:B:416:TYR:CZ	2.36	0.61
2:F:112:ALA:C	2:F:114:GLN:H	2.09	0.61
1:C:560:MET:HE2	1:C:560:MET:HA	1.83	0.61
2:E:49:ILE:O	2:E:53:VAL:HG23	2.00	0.61
1:B:15:VAL:HG12	1:B:499:MET:HE1	1.81	0.61
1:B:445:MET:HE1	1:B:447:PRO:HB3	1.83	0.60
1:B:653:VAL:O	1:B:657:ILE:HG13	2.01	0.60
1:C:514:GLU:OE2	1:C:518:GLN:HA	2.01	0.60
3:C:1801:B12:H8	3:C:1801:B12:N40	2.05	0.60
1:A:547:MET:HE2	1:C:574:VAL:HG22	1.83	0.60
1:C:233:GLU:HB3	1:C:235:TRP:CH2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LEU:HD12	1:C:499:MET:HE2	1.83	0.60
1:D:224:ALA:HB3	1:D:245:HIS:CE1	2.36	0.60
1:A:667:SER:HB2	3:A:1801:B12:H4B	1.83	0.60
1:C:126:GLY:O	1:C:127:ILE:HD13	2.02	0.60
1:B:459:GLN:HG3	1:B:460:TYR:CD2	2.36	0.60
1:B:204:CYS:HB3	1:B:452:PHE:CD2	2.37	0.60
1:C:29:ARG:NH2	1:C:148:GLU:OE2	2.32	0.60
2:G:88:ILE:HG13	2:G:103:LEU:HD11	1.84	0.60
1:D:79:THR:HG23	1:D:104:HIS:CG	2.36	0.60
1:A:547:MET:HE2	1:C:574:VAL:CG2	2.31	0.60
3:D:1801:B12:H601	3:D:1801:B12:C26	2.32	0.60
1:A:574:VAL:CG2	1:C:547:MET:HE2	2.32	0.60
1:A:685:GLU:O	1:A:689:GLU:HB2	2.01	0.60
2:E:107:LYS:O	2:E:108:TYR:HB2	2.00	0.60
1:B:532:SER:OG	1:B:535:VAL:HG23	2.02	0.60
1:A:604:THR:HB	1:A:736:ARG:HH12	1.66	0.59
1:A:684:HIS:O	1:A:688:VAL:HG23	2.02	0.59
3:A:1801:B12:H351	3:A:1801:B12:H372	1.84	0.59
2:E:81:ALA:O	2:E:85:VAL:HG23	2.01	0.59
1:B:324:LYS:HE2	1:B:362:MET:O	2.02	0.59
1:C:428:ILE:HG12	1:C:428:ILE:O	2.01	0.59
1:C:445:MET:HE1	1:C:447:PRO:HB3	1.84	0.59
1:D:358:ALA:O	1:D:362:MET:HG3	2.03	0.59
1:D:668:THR:HG23	1:D:668:THR:O	2.02	0.59
1:A:546:LYS:NZ	1:C:578:ILE:HD11	2.17	0.59
1:D:109:ARG:HG2	1:D:132:ILE:CG1	2.32	0.59
1:D:172:MET:HE3	1:D:176:GLU:HG3	1.84	0.59
1:D:464:LEU:HD23	1:D:471:LEU:HD13	1.84	0.59
1:A:267:VAL:HG22	1:A:299:GLN:HB3	1.83	0.59
1:C:659:LEU:O	1:C:660:LYS:HG2	2.02	0.59
1:D:250:ILE:HG23	2:H:34:VAL:HG21	1.84	0.59
1:D:416:TYR:CG	1:D:417:PRO:HA	2.37	0.59
1:A:606:LEU:HB2	1:A:736:ARG:NH2	2.18	0.59
1:B:109:ARG:HG2	1:B:132:ILE:CG1	2.33	0.58
1:B:111:ALA:O	1:D:620:VAL:HG11	2.03	0.58
1:B:281:LEU:O	1:B:285:VAL:HG23	2.03	0.58
1:B:300:MET:HB2	1:B:334:ILE:HG12	1.85	0.58
2:F:5:ASP:N	2:F:6:ASP:HB3	2.18	0.58
1:A:585:ILE:HG12	1:C:538:PHE:CD2	2.38	0.58
1:C:158:HIS:CD2	1:C:159:SER:N	2.71	0.58
1:C:109:ARG:HH21	4:C:767:Z97:P	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:GLN:O	1:B:263:CYS:HB2	2.03	0.58
3:C:1801:B12:H203	3:C:1801:B12:H302	1.84	0.58
1:C:307:ALA:O	1:C:340:ARG:HD3	2.03	0.58
1:C:373:ARG:HH11	1:C:373:ARG:CG	2.15	0.58
1:D:669:ILE:HG22	3:D:1801:B12:H202	1.85	0.58
2:G:54:LEU:HD23	2:G:57:MET:CE	2.33	0.58
1:B:687:ALA:C	1:B:693:ARG:HB2	2.28	0.58
1:C:109:ARG:HG2	1:C:132:ILE:HG12	1.84	0.58
1:B:264:LEU:HD21	1:B:291:PHE:CD1	2.39	0.57
1:D:6:GLN:HG2	1:D:7:LEU:N	2.19	0.57
1:D:653:VAL:O	1:D:657:ILE:HG12	2.04	0.57
2:E:109:TRP:O	2:E:113:ILE:HG13	2.04	0.57
1:A:708:GLU:C	1:A:710:ALA:H	2.13	0.57
1:B:120:ILE:HG13	1:B:133:THR:CG2	2.33	0.57
1:B:461:ASP:OD1	1:B:463:ALA:HB3	2.04	0.57
1:D:290:MET:HE2	1:D:385:LYS:HG2	1.85	0.57
1:A:370:GLN:HG2	1:C:372:LYS:HG3	1.86	0.57
1:B:660:LYS:HG3	1:B:660:LYS:O	2.02	0.57
1:C:427:GLN:C	1:C:429:ASN:H	2.13	0.57
1:B:464:LEU:HD23	1:B:471:LEU:CD1	2.34	0.57
1:C:218:ILE:HD13	1:C:297:ARG:CD	2.32	0.57
1:D:124:PRO:O	1:D:131:PRO:HG2	2.03	0.57
1:A:445:MET:HE3	1:A:471:LEU:CD1	2.35	0.57
1:C:335:THR:HG22	1:C:348:ASN:HA	1.86	0.57
1:A:41:LEU:CD2	1:A:43:MET:HE2	2.30	0.57
1:A:60:ALA:HB2	1:A:71:ASP:HB2	1.86	0.57
1:A:79:THR:HB	1:A:332:SER:HA	1.86	0.57
1:A:560:MET:CB	1:C:96:MET:HE3	2.35	0.57
1:B:286:ALA:HB2	1:B:381:VAL:HG13	1.87	0.57
1:C:443:ASP:OD1	2:G:79:LYS:HE2	2.05	0.57
1:B:464:LEU:HD23	1:B:471:LEU:HD13	1.87	0.57
3:C:1801:B12:O7R	3:C:1801:B12:H2B	2.04	0.57
1:D:197:ILE:HD11	1:D:428:ILE:CD1	2.34	0.57
1:C:109:ARG:HG2	1:C:132:ILE:CG1	2.35	0.57
1:D:526:THR:HG23	1:D:569:GLU:CG	2.35	0.57
1:A:631:GLY:O	1:A:725:GLY:HA3	2.05	0.56
1:B:232:ARG:HH21	1:D:598:ARG:NH2	1.99	0.56
1:B:277:MET:CE	1:B:321:LEU:HD23	2.29	0.56
3:C:1801:B12:H531	3:C:1801:B12:H543	1.87	0.56
2:F:49:ILE:O	2:F:53:VAL:HG23	2.04	0.56
5:A:1500:5AD:C4'	3:C:1801:B12:N23	2.67	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:VAL:HG12	1:B:686:LEU:CD1	2.36	0.56
1:D:6:GLN:HG2	1:D:7:LEU:H	1.69	0.56
1:D:454:TYR:C	1:D:454:TYR:CD2	2.84	0.56
2:H:5:ASP:HA	2:H:6:ASP:CB	2.32	0.56
1:B:63:SER:HB2	1:D:311:GLU:OE2	2.06	0.56
3:C:1801:B12:O7R	3:C:1801:B12:C2B	2.53	0.56
2:H:54:LEU:HD23	2:H:57:MET:HE2	1.87	0.56
1:D:467:GLU:HA	1:D:467:GLU:OE1	2.04	0.56
1:B:313:THR:O	1:B:317:VAL:HG23	2.06	0.56
1:D:25:TYR:HD2	1:D:138:ARG:HG2	1.71	0.56
1:B:557:ARG:HG3	1:B:557:ARG:HH11	1.69	0.56
3:B:1801:B12:H291	3:B:1801:B12:H251	1.70	0.56
1:B:534:ARG:HG3	1:B:534:ARG:NH1	2.18	0.56
1:B:86:ARG:HG3	1:B:517:TRP:NE1	2.20	0.56
1:B:672:HIS:O	1:B:673:ASP:HB2	2.06	0.56
1:A:57:ASN:HB3	1:A:99:TRP:CH2	2.41	0.55
1:B:246:ALA:O	1:B:250:ILE:HG22	2.05	0.55
1:C:36:GLN:O	1:C:52:SER:HB2	2.04	0.55
3:D:1801:B12:H531	3:D:1801:B12:H543	1.87	0.55
1:C:290:MET:HE3	2:G:26:PHE:CG	2.40	0.55
1:D:618:HIS:HB2	1:D:669:ILE:HG13	1.87	0.55
1:A:540:ALA:HB1	1:A:570:LEU:HD11	1.88	0.55
1:B:619:SER:HB2	1:B:623:ARG:CZ	2.36	0.55
2:F:92:LYS:HG3	2:F:108:TYR:CE1	2.40	0.55
1:D:608:ILE:HG13	1:D:663:ALA:HB3	1.88	0.55
1:D:626:ILE:O	1:D:634:GLU:HB2	2.06	0.55
1:A:445:MET:HE3	1:A:471:LEU:HD12	1.87	0.55
1:B:612:THR:HG22	1:B:616:ASP:HB3	1.88	0.55
1:D:468:PRO:O	1:D:471:LEU:HB2	2.06	0.55
1:A:693:ARG:HH22	1:A:716:ASP:CG	2.14	0.55
1:C:43:MET:CE	1:C:72:PRO:HA	2.32	0.55
1:D:541:ILE:HD11	1:D:554:VAL:HG23	1.89	0.55
1:A:7:LEU:HD12	1:A:146:LEU:HB3	1.88	0.55
1:A:707:PRO:HA	1:A:718:GLY:HA3	1.89	0.55
1:D:561:GLN:HB3	1:D:564:GLU:HB2	1.88	0.55
1:A:290:MET:SD	2:E:23:GLN:HG2	2.47	0.55
1:A:458:LYS:HG3	1:A:462:GLU:HA	1.88	0.55
1:D:79:THR:HG23	1:D:104:HIS:ND1	2.22	0.55
3:A:1801:B12:H601	3:A:1801:B12:C26	2.36	0.55
1:B:7:LEU:HD13	1:B:150:GLU:HB2	1.88	0.55
3:B:1801:B12:H261	5:D:1500:5AD:C5'	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ILE:O	1:B:151:VAL:HG13	2.07	0.55
1:C:123:THR:HG23	1:C:135:LYS:HD3	1.89	0.55
1:D:26:THR:HG22	1:D:27:PRO:HD2	1.89	0.55
1:D:109:ARG:HH21	4:D:767:Z97:P	2.30	0.55
1:D:737:ARG:C	1:D:739:MET:H	2.15	0.55
1:A:368:MET:HE3	1:C:278:TYR:CE1	2.41	0.55
2:E:5:ASP:CA	2:E:7:PHE:N	2.47	0.55
1:C:411:VAL:O	1:C:423:GLY:HA2	2.06	0.55
1:B:649:VAL:HG12	1:B:686:LEU:HD12	1.89	0.54
3:C:1801:B12:H362	3:C:1801:B12:C35	2.34	0.54
1:D:137:VAL:HG21	1:D:172:MET:HE1	1.89	0.54
1:D:441:ASP:OD2	2:H:79:LYS:NZ	2.39	0.54
1:D:663:ALA:HB2	1:D:697:MET:HE3	1.89	0.54
1:D:706:THR:HB	1:D:709:VAL:HG23	1.88	0.54
1:D:719:PHE:HB3	1:D:723:SER:OG	2.07	0.54
1:C:467:GLU:HB3	1:C:470:LYS:HG2	1.88	0.54
1:A:137:VAL:HB	1:A:172:MET:HE1	1.88	0.54
1:B:344:TRP:CG	1:B:515:VAL:HB	2.42	0.54
1:C:510:MET:HE3	1:C:577:SER:HB2	1.90	0.54
1:D:205:GLU:OE2	1:D:451:HIS:HA	2.07	0.54
1:C:411:VAL:HB	1:C:424:ILE:H	1.73	0.54
2:E:54:LEU:HD23	2:E:57:MET:CE	2.38	0.54
1:C:103:ASP:HB3	1:C:153:ARG:NH1	2.23	0.54
1:C:219:ASP:O	1:C:225:HIS:HE1	1.90	0.54
1:A:185:PRO:HG3	1:A:203:ALA:CB	2.38	0.54
1:B:137:VAL:CG2	1:B:172:MET:HE1	2.35	0.54
2:F:113:ILE:HG22	2:F:113:ILE:O	2.06	0.54
2:G:86:TYR:O	2:G:87:LYS:C	2.51	0.54
1:D:116:TYR:CE2	1:D:120:ILE:HD13	2.43	0.54
1:D:622:LEU:HG	1:D:626:ILE:HD12	1.90	0.54
1:A:307:ALA:HB1	1:A:556:ASN:HB2	1.89	0.54
1:A:447:PRO:HG2	2:E:57:MET:SD	2.48	0.54
1:B:167:PRO:HD2	2:F:48:SER:OG	2.08	0.54
1:C:132:ILE:HA	1:C:136:GLN:OE1	2.08	0.54
1:C:649:VAL:CG1	1:C:686:LEU:HD12	2.38	0.54
1:C:719:PHE:HB3	1:C:723:SER:OG	2.08	0.54
1:A:464:LEU:HD23	1:A:471:LEU:CD2	2.36	0.54
1:B:410:PHE:C	1:B:411:VAL:HG23	2.33	0.54
1:D:373:ARG:NH1	1:D:378:GLY:HA2	2.23	0.54
1:D:510:MET:HE2	1:D:577:SER:HB2	1.88	0.54
1:A:123:THR:O	1:A:498:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:GLU:OE2	2:F:25:ARG:NH1	2.39	0.53
1:D:19:LEU:HD23	1:D:22:LEU:HD11	1.91	0.53
1:D:591:ILE:HD12	1:D:591:ILE:N	2.23	0.53
1:A:607:LYS:HG3	1:A:639:GLU:HB3	1.89	0.53
1:C:6:GLN:HG2	1:C:8:ARG:HG3	1.89	0.53
1:C:631:GLY:O	1:C:725:GLY:HA3	2.08	0.53
3:C:1801:B12:H251	3:C:1801:B12:N29	2.22	0.53
2:G:59:PHE:CZ	2:G:100:GLY:HA3	2.43	0.53
1:A:416:TYR:CD1	1:A:417:PRO:HA	2.43	0.53
2:F:20:GLU:H	2:F:20:GLU:CD	2.17	0.53
1:C:461:ASP:HB3	1:C:464:LEU:HD22	1.89	0.53
2:H:5:ASP:HA	2:H:6:ASP:C	2.29	0.53
1:D:123:THR:O	1:D:498:ARG:NH2	2.42	0.53
1:A:585:ILE:HG23	1:C:538:PHE:CE2	2.43	0.53
1:B:162:SER:OG	4:B:767:Z97:N1	2.40	0.53
1:C:444:TYR:C	1:C:444:TYR:CD2	2.87	0.53
1:A:604:THR:HB	1:A:736:ARG:NH1	2.24	0.53
1:C:75:LEU:N	1:C:76:PRO:CD	2.71	0.53
1:D:6:GLN:CG	1:D:7:LEU:H	2.20	0.53
1:D:607:LYS:C	1:D:608:ILE:HD12	2.33	0.53
3:B:1801:B12:H351	3:B:1801:B12:H372	1.91	0.53
1:D:204:CYS:HB3	1:D:452:PHE:CD2	2.44	0.53
1:D:438:PHE:CD2	2:H:77:MET:HG3	2.43	0.53
3:D:1801:B12:H302	3:D:1801:B12:H203	1.91	0.53
1:B:13:LEU:HD13	1:B:91:ILE:HG22	1.91	0.53
1:B:79:THR:HG23	1:B:104:HIS:ND1	2.24	0.53
1:B:278:TYR:CE1	1:D:368:MET:HE3	2.43	0.53
1:D:671:SER:OG	1:D:704:GLN:HG3	2.09	0.53
1:D:233:GLU:HG2	1:D:235:TRP:CH2	2.44	0.53
1:D:411:VAL:HG12	1:D:411:VAL:O	2.10	0.53
2:H:5:ASP:CB	2:H:8:GLN:HG2	2.39	0.53
1:A:13:LEU:HD22	1:A:18:ILE:HD11	1.90	0.52
1:B:683:ILE:HG22	1:B:698:ILE:HD13	1.91	0.52
1:C:651:LYS:O	1:C:652:LEU:C	2.52	0.52
3:A:1801:B12:H353	3:A:1801:B12:H311	1.92	0.52
1:B:512:LYS:HB2	1:B:513:PRO:CD	2.39	0.52
1:B:557:ARG:HH11	1:B:557:ARG:CG	2.22	0.52
1:C:86:ARG:HG3	1:C:517:TRP:NE1	2.23	0.52
1:C:471:LEU:HD12	2:G:86:TYR:OH	2.09	0.52
1:D:161:VAL:HG12	1:D:161:VAL:O	2.10	0.52
1:A:716:ASP:OD2	1:A:735:LYS:HE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:CYS:HB2	2:F:56:ARG:O	2.09	0.52
1:C:14:ASP:CG	1:C:17:ASN:HB2	2.34	0.52
2:E:25:ARG:O	2:E:29:MET:HG3	2.08	0.52
3:C:1801:B12:H251	3:C:1801:B12:H291	1.75	0.52
2:G:57:MET:HE1	2:G:82:GLY:CA	2.35	0.52
1:B:606:LEU:HD21	1:B:732:LEU:HD22	1.91	0.52
1:B:671:SER:HB2	1:B:676:HIS:CE1	2.44	0.52
1:C:123:THR:O	1:C:494:ASN:HA	2.09	0.52
1:D:671:SER:HB2	1:D:676:HIS:ND1	2.24	0.52
3:D:1801:B12:H601	3:D:1801:B12:H252	1.92	0.52
1:A:549:LEU:HD21	1:A:574:VAL:HG23	1.92	0.52
1:B:550:GLU:HG3	1:B:573:ARG:NH2	2.24	0.52
2:G:76:LEU:O	2:G:77:MET:C	2.52	0.52
1:D:688:VAL:HG22	1:D:693:ARG:HG2	1.91	0.52
2:H:65:LYS:HG2	2:H:69:ASP:OD2	2.09	0.52
1:B:695:LYS:HB2	1:B:695:LYS:NZ	2.25	0.52
1:C:189:VAL:HG11	1:C:196:MET:CB	2.38	0.52
1:A:445:MET:HE1	1:A:447:PRO:HA	1.92	0.52
1:C:18:ILE:HG23	1:C:142:LYS:HD3	1.91	0.52
1:C:373:ARG:HD2	1:C:373:ARG:O	2.09	0.52
1:D:7:LEU:HD13	1:D:150:GLU:CD	2.35	0.52
1:A:147:ILE:O	1:A:151:VAL:HG22	2.10	0.52
1:A:440:ARG:HH22	1:A:451:HIS:CE1	2.28	0.52
1:B:320:LEU:HD13	1:B:358:ALA:HB3	1.91	0.52
1:D:235:TRP:O	1:D:238:MET:HE3	2.10	0.52
1:D:510:MET:HE3	1:D:577:SER:HB2	1.92	0.52
1:D:537:GLU:O	1:D:541:ILE:HG12	2.10	0.52
1:A:666:ALA:O	1:A:700:CYS:HA	2.10	0.52
1:B:651:LYS:HA	1:B:651:LYS:NZ	2.24	0.52
1:C:610:ALA:HA	1:C:665:LEU:O	2.10	0.52
1:A:688:VAL:HG22	1:A:693:ARG:CB	2.40	0.51
1:B:607:LYS:C	1:B:608:ILE:HD12	2.35	0.51
1:C:406:GLU:HG2	1:C:426:ARG:O	2.10	0.51
1:D:189:VAL:CG2	1:D:196:MET:HA	2.40	0.51
1:A:738:GLU:CG	1:A:739:MET:N	2.70	0.51
1:C:320:LEU:HD13	1:C:358:ALA:HB3	1.91	0.51
1:C:541:ILE:HG23	1:C:552:VAL:HG11	1.92	0.51
1:C:668:THR:CG2	1:C:668:THR:O	2.58	0.51
1:A:116:TYR:CE2	1:A:120:ILE:HD13	2.46	0.51
1:B:39:GLU:O	1:B:40:ASN:C	2.53	0.51
1:D:684:HIS:O	1:D:687:ALA:HB3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:N	1:A:76:PRO:CD	2.73	0.51
1:A:618:HIS:ND1	1:A:669:ILE:HB	2.26	0.51
1:C:55:LEU:CD2	1:C:153:ARG:HB2	2.40	0.51
1:C:460:TYR:CE1	2:G:86:TYR:HE2	2.29	0.51
2:G:88:ILE:HG22	2:G:99:ALA:HB1	1.91	0.51
1:A:96:MET:HG2	1:C:560:MET:CB	2.37	0.51
1:B:126:GLY:HA3	1:B:129:GLY:O	2.11	0.51
1:B:460:TYR:O	1:B:461:ASP:HB2	2.09	0.51
1:B:219:ASP:HB3	1:B:248:ASN:HD22	1.76	0.51
1:B:735:LYS:O	1:B:735:LYS:HG3	2.09	0.51
2:H:50:GLU:HG2	2:H:77:MET:HE1	1.93	0.51
2:G:70:LYS:O	2:G:74:ARG:HG2	2.10	0.51
1:D:461:ASP:OD1	1:D:463:ALA:HB3	2.11	0.51
1:A:601:ILE:HG22	1:A:601:ILE:O	2.10	0.51
1:A:738:GLU:CG	1:A:739:MET:H	2.22	0.51
1:B:120:ILE:C	1:B:133:THR:HG22	2.35	0.51
1:B:274:ALA:O	1:B:276:SER:N	2.44	0.51
3:B:1801:B12:H362	3:B:1801:B12:C35	2.41	0.51
3:B:1801:B12:C15	5:D:1500:5AD:H5'2	2.31	0.51
1:C:90:ASP:O	1:C:94:MET:HG3	2.11	0.51
1:D:541:ILE:HG22	1:D:545:LYS:HE3	1.93	0.51
1:A:74:PRO:HB2	1:A:76:PRO:HD2	1.91	0.51
3:B:1801:B12:H252	3:B:1801:B12:H601	1.93	0.51
1:A:164:VAL:O	1:A:198:ARG:NH2	2.43	0.51
1:A:579:ASP:O	1:A:583:LEU:HG	2.11	0.51
1:B:684:HIS:CG	1:B:714:GLY:HA3	2.45	0.51
1:C:556:ASN:HB3	1:C:569:GLU:HB2	1.93	0.51
2:H:50:GLU:CG	2:H:77:MET:HE1	2.41	0.51
1:B:686:LEU:O	1:B:690:LYS:HG2	2.10	0.50
1:C:476:THR:OG1	2:G:56:ARG:HA	2.11	0.50
1:D:285:VAL:O	1:D:289:GLU:HG3	2.11	0.50
1:A:445:MET:HE1	1:A:471:LEU:HD12	1.94	0.50
1:C:547:MET:O	1:C:548:ASN:HB2	2.12	0.50
1:D:616:ASP:HA	1:D:670:ILE:HD12	1.92	0.50
1:A:688:VAL:HG22	1:A:693:ARG:HG2	1.92	0.50
2:F:66:ALA:O	2:F:70:LYS:HG3	2.10	0.50
1:D:575:PRO:HD2	1:D:576:PHE:CE2	2.46	0.50
1:A:287:LEU:HD12	1:A:291:PHE:CD2	2.47	0.50
1:A:528:PHE:CZ	1:A:565:GLY:HA3	2.46	0.50
1:A:575:PRO:HD2	1:A:576:PHE:CE2	2.46	0.50
1:A:626:ILE:O	1:A:634:GLU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:ARG:HG2	1:A:686:LEU:CD1	2.39	0.50
1:A:697:MET:HE1	1:A:736:ARG:HB2	1.93	0.50
1:B:143:ALA:O	1:B:147:ILE:HG13	2.10	0.50
1:B:406:GLU:HG3	1:B:428:ILE:HG22	1.93	0.50
1:B:512:LYS:HB2	1:B:513:PRO:HD2	1.93	0.50
1:B:115:HIS:HB3	1:D:623:ARG:HH11	1.76	0.50
3:B:1801:B12:H531	3:B:1801:B12:C55	2.42	0.50
3:C:1801:B12:H203	3:C:1801:B12:C30	2.41	0.50
1:D:31:GLY:O	1:D:179:ASN:HB3	2.11	0.50
1:D:416:TYR:CD1	1:D:417:PRO:HA	2.46	0.50
1:B:210:MET:HE2	1:B:257:MET:HE1	1.92	0.50
1:C:194:ILE:HG12	1:C:432:ILE:HB	1.94	0.50
1:A:29:ARG:HG3	1:A:29:ARG:HH11	1.77	0.50
1:A:300:MET:HB2	1:A:334:ILE:HG12	1.92	0.50
1:B:232:ARG:HE	1:D:598:ARG:NH1	2.10	0.50
1:D:737:ARG:C	1:D:739:MET:N	2.68	0.50
1:C:158:HIS:HD2	1:C:159:SER:N	2.09	0.50
1:D:653:VAL:O	1:D:653:VAL:HG12	2.10	0.50
1:B:655:ALA:O	1:B:659:LEU:HG	2.12	0.50
2:F:59:PHE:CE1	2:F:100:GLY:HA3	2.47	0.50
1:D:135:LYS:HG3	1:D:485:TYR:OH	2.12	0.50
1:D:406:GLU:CD	1:D:428:ILE:HG23	2.36	0.50
1:B:167:PRO:O	1:B:171:VAL:HG23	2.11	0.49
1:C:467:GLU:N	1:C:468:PRO:HD3	2.27	0.49
1:C:528:PHE:CE1	1:C:565:GLY:HA3	2.47	0.49
1:C:710:ALA:O	1:C:715:VAL:HG22	2.12	0.49
1:D:164:VAL:HG12	1:D:194:ILE:HG23	1.94	0.49
1:D:668:THR:O	1:D:668:THR:CG2	2.60	0.49
1:D:671:SER:HB2	1:D:676:HIS:CE1	2.46	0.49
1:D:688:VAL:HG22	1:D:693:ARG:CG	2.42	0.49
1:A:313:THR:O	1:A:317:VAL:HG23	2.12	0.49
1:A:495:VAL:HG13	1:A:496:ASN:N	2.27	0.49
1:B:284:ALA:O	1:B:288:ARG:HD3	2.12	0.49
1:C:373:ARG:HG3	1:C:373:ARG:NH1	2.16	0.49
1:D:336:PRO:HD2	1:D:347:TYR:HB3	1.93	0.49
1:A:399:GLY:HA3	1:A:403:ASN:HD22	1.76	0.49
1:A:416:TYR:CG	1:A:417:PRO:HA	2.47	0.49
1:D:668:THR:HG23	1:D:676:HIS:HB2	1.94	0.49
1:A:113:GLN:HG3	1:A:116:TYR:CD2	2.47	0.49
1:B:570:LEU:HD12	1:B:570:LEU:H	1.78	0.49
1:C:290:MET:HB3	1:C:291:PHE:CD2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:THR:CG2	1:A:135:LYS:HD3	2.41	0.49
1:A:290:MET:HE3	2:E:26:PHE:CG	2.48	0.49
2:E:70:LYS:O	2:E:74:ARG:HG2	2.13	0.49
1:C:5:LEU:O	1:C:6:GLN:CB	2.61	0.49
1:D:234:ALA:O	1:D:237:VAL:HG12	2.13	0.49
1:A:45:PRO:HD2	1:A:46:PHE:CD2	2.47	0.49
1:A:618:HIS:CB	1:A:669:ILE:HG13	2.37	0.49
1:B:693:ARG:HG3	1:B:693:ARG:O	2.12	0.49
2:G:6:ASP:O	2:G:10:ARG:HG3	2.12	0.49
1:D:631:GLY:HA2	1:D:635:LYS:HD2	1.95	0.49
1:A:5:LEU:O	1:A:6:GLN:HB2	2.13	0.49
1:A:159:SER:HB3	1:A:173:PHE:CZ	2.47	0.49
3:B:1801:B12:H251	3:B:1801:B12:N29	2.27	0.49
1:C:144:LEU:HD23	1:C:147:ILE:HD12	1.94	0.49
1:D:579:ASP:HB3	1:D:582:SER:OG	2.13	0.49
1:A:531:THR:CG2	1:A:536:ALA:HB2	2.43	0.49
1:B:116:TYR:CE1	3:D:1801:B12:H491	2.48	0.49
3:B:1801:B12:H601	3:B:1801:B12:H262	1.94	0.49
2:G:53:VAL:HG12	2:G:57:MET:HE2	1.94	0.49
1:A:237:VAL:HG22	1:A:237:VAL:O	2.13	0.49
1:B:212:TRP:C	1:B:214:ASP:H	2.21	0.49
2:F:74:ARG:HG3	2:F:74:ARG:HH11	1.78	0.49
1:D:42:GLN:HG3	1:D:47:ILE:HG13	1.95	0.49
1:A:538:PHE:CD2	1:C:585:ILE:HG12	2.48	0.48
1:B:543:PHE:O	1:B:547:MET:HG3	2.14	0.48
1:C:618:HIS:CE1	3:C:1801:B12:N22	2.81	0.48
1:A:38:ALA:HB1	1:A:41:LEU:HB2	1.94	0.48
1:C:541:ILE:HG23	1:C:552:VAL:CG1	2.43	0.48
3:D:1801:B12:H362	3:D:1801:B12:C35	2.43	0.48
1:B:232:ARG:HH11	1:B:232:ARG:HA	1.78	0.48
1:B:411:VAL:O	1:B:423:GLY:HA2	2.13	0.48
3:B:1801:B12:C16	5:D:1500:5AD:C5'	2.83	0.48
1:C:161:VAL:HG23	1:C:181:ALA:HB1	1.94	0.48
1:C:386:GLU:O	1:C:390:LEU:HG	2.13	0.48
3:D:1801:B12:H492	3:D:1801:B12:H471	1.95	0.48
1:A:679:ASN:O	1:A:683:ILE:HG13	2.14	0.48
1:B:570:LEU:HD12	1:B:570:LEU:N	2.27	0.48
1:C:405:VAL:CG1	1:C:426:ARG:HB2	2.43	0.48
1:C:668:THR:HG23	1:C:676:HIS:CB	2.34	0.48
1:D:700:CYS:O	1:D:718:GLY:HA2	2.13	0.48
3:D:1801:B12:O7R	3:D:1801:B12:C2B	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:VAL:CB	1:A:172:MET:HE1	2.43	0.48
1:C:61:LEU:O	1:C:62:PRO:C	2.54	0.48
1:D:723:SER:H	3:D:1801:B12:H5R2	1.77	0.48
1:A:344:TRP:CG	1:A:515:VAL:HB	2.49	0.48
1:A:445:MET:HE1	1:A:447:PRO:CA	2.44	0.48
1:A:478:GLU:O	1:A:480:PRO:HD3	2.14	0.48
2:H:5:ASP:CA	2:H:6:ASP:CB	2.91	0.48
1:A:422:ASP:OD1	1:A:422:ASP:N	2.46	0.48
1:B:629:LYS:O	1:B:630:HIS:HD2	1.97	0.48
3:D:1801:B12:H253	3:D:1801:B12:H301	1.52	0.48
1:A:5:LEU:O	1:A:6:GLN:CB	2.62	0.48
1:B:58:SER:HB2	1:B:71:ASP:OD2	2.13	0.48
1:B:161:VAL:HG12	1:B:161:VAL:O	2.14	0.48
2:G:76:LEU:HB3	2:G:84:ILE:HD11	1.95	0.48
1:D:622:LEU:HD23	1:D:642:TYR:HE1	1.79	0.48
1:A:6:GLN:O	1:A:7:LEU:HB2	2.13	0.48
3:A:1801:B12:H362	3:A:1801:B12:C35	2.41	0.48
1:B:618:HIS:CE1	3:B:1801:B12:N21	2.81	0.48
1:C:13:LEU:HD13	1:C:91:ILE:HG22	1.96	0.48
1:C:164:VAL:HG13	1:C:194:ILE:HD13	1.95	0.48
1:D:288:ARG:HG3	1:D:288:ARG:HH11	1.79	0.48
1:A:394:GLU:HG2	1:A:409:PHE:CE2	2.48	0.47
1:A:470:LYS:O	1:A:472:ILE:N	2.47	0.47
1:A:606:LEU:HB2	1:A:736:ARG:HH21	1.78	0.47
2:E:59:PHE:CE1	2:E:100:GLY:HA3	2.48	0.47
1:C:22:LEU:C	1:C:24:LYS:H	2.22	0.47
1:C:79:THR:HB	1:C:332:SER:HA	1.96	0.47
1:C:492:ASN:O	1:C:497:VAL:HG11	2.13	0.47
1:C:607:LYS:HE2	1:C:639:GLU:OE2	2.14	0.47
1:D:25:TYR:CD2	1:D:138:ARG:HG2	2.48	0.47
1:A:267:VAL:CG2	1:A:299:GLN:HB3	2.44	0.47
1:B:132:ILE:HA	1:B:136:GLN:OE1	2.14	0.47
1:B:189:VAL:HG22	1:B:196:MET:HA	1.96	0.47
1:B:650:GLU:O	1:B:651:LYS:C	2.55	0.47
1:C:264:LEU:HD22	1:C:296:MET:HE1	1.96	0.47
1:D:5:LEU:O	1:D:6:GLN:HB2	2.13	0.47
3:D:1801:B12:O28	3:D:1801:B12:H3	2.15	0.47
1:A:462:GLU:CD	1:A:462:GLU:H	2.22	0.47
2:E:23:GLN:O	2:E:26:PHE:HB3	2.15	0.47
1:B:95:ARG:HD3	1:D:564:GLU:HG2	1.96	0.47
1:C:344:TRP:CG	1:C:515:VAL:HB	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:59:PHE:CE1	2:G:100:GLY:HA3	2.49	0.47
2:G:95:SER:O	2:G:96:VAL:C	2.56	0.47
1:D:561:GLN:O	1:D:562:GLU:C	2.56	0.47
2:H:6:ASP:O	2:H:10:ARG:HG3	2.13	0.47
1:A:122:GLY:O	1:A:133:THR:HG21	2.14	0.47
1:B:5:LEU:HD23	1:B:5:LEU:O	2.14	0.47
1:B:123:THR:O	1:B:498:ARG:NH2	2.44	0.47
1:C:672:HIS:O	1:C:673:ASP:CB	2.62	0.47
1:B:290:MET:HE3	1:B:385:LYS:HG2	1.97	0.47
1:C:299:GLN:HG3	1:C:300:MET:N	2.29	0.47
1:A:467:GLU:O	1:A:469:SER:N	2.47	0.47
1:B:326:THR:OG1	1:B:327:ARG:N	2.46	0.47
1:B:622:LEU:HB2	1:B:667:SER:HB2	1.96	0.47
1:B:651:LYS:HA	1:B:651:LYS:CE	2.45	0.47
1:C:373:ARG:HA	1:C:377:LEU:HD23	1.97	0.47
1:D:81:GLU:CD	4:D:767:Z97:HN	2.21	0.47
1:D:305:MET:HE1	1:D:316:HIS:NE2	2.30	0.47
1:D:445:MET:HE1	1:D:447:PRO:HG3	1.95	0.47
3:D:1801:B12:H351	3:D:1801:B12:H372	1.95	0.47
2:H:25:ARG:HA	2:H:28:GLU:HB2	1.97	0.47
1:A:735:LYS:O	1:A:735:LYS:HG3	2.14	0.47
1:C:377:LEU:O	1:C:381:VAL:HG23	2.14	0.47
1:D:387:ARG:NH1	1:D:416:TYR:O	2.48	0.47
1:D:688:VAL:HG22	1:D:693:ARG:CB	2.44	0.47
1:B:297:ARG:O	1:B:297:ARG:HD3	2.15	0.47
1:B:359:LEU:HD23	1:B:359:LEU:HA	1.73	0.47
1:C:41:LEU:HD21	1:C:43:MET:HE2	1.97	0.47
2:G:20:GLU:CD	2:G:20:GLU:H	2.22	0.47
2:G:54:LEU:HD23	2:G:57:MET:HE1	1.96	0.47
3:D:1801:B12:O2	3:D:1801:B12:H2B	2.15	0.47
2:H:35:ASP:HB2	2:H:36:PRO:HD3	1.97	0.47
1:A:75:LEU:N	1:A:76:PRO:HD3	2.30	0.47
1:A:112:GLY:HA3	1:C:620:VAL:HG13	1.96	0.47
1:C:612:THR:CB	1:C:645:THR:HG22	2.44	0.47
1:B:511:ILE:CG1	1:D:530:PRO:HD2	2.45	0.46
1:B:606:LEU:CD2	1:B:732:LEU:HB3	2.44	0.46
1:C:219:ASP:HB3	1:C:248:ASN:ND2	2.31	0.46
1:C:289:GLU:OE2	1:C:385:LYS:NZ	2.44	0.46
1:C:444:TYR:HA	2:G:79:LYS:O	2.15	0.46
1:C:612:THR:HG21	1:C:618:HIS:O	2.14	0.46
1:A:672:HIS:O	1:A:675:ILE:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:MET:CG	1:C:96:MET:HE3	2.45	0.46
1:A:621:GLY:O	1:A:624:GLU:HB2	2.15	0.46
1:B:600:ASP:OD2	1:B:733:VAL:HG23	2.16	0.46
1:C:209:ILE:O	1:C:212:TRP:HB3	2.14	0.46
1:A:125:GLN:HG3	1:A:126:GLY:N	2.30	0.46
1:A:344:TRP:CD1	1:A:515:VAL:HB	2.50	0.46
1:C:233:GLU:OE1	1:C:236:LYS:HD2	2.16	0.46
1:C:394:GLU:HG2	1:C:409:PHE:HE2	1.80	0.46
1:C:396:ILE:CD1	2:G:29:MET:HG3	2.45	0.46
1:D:5:LEU:HD23	1:D:5:LEU:C	2.40	0.46
1:D:197:ILE:HD11	1:D:428:ILE:HD11	1.97	0.46
1:D:342:VAL:O	1:D:343:PRO:C	2.58	0.46
1:A:79:THR:HA	1:A:104:HIS:HB3	1.97	0.46
1:A:109:ARG:HG2	1:A:132:ILE:HG12	1.98	0.46
1:A:310:ARG:O	1:A:314:VAL:HG23	2.15	0.46
1:A:692:ILE:O	1:A:696:ILE:HG22	2.15	0.46
1:B:20:LYS:O	1:B:21:ASP:HB2	2.16	0.46
1:C:143:ALA:O	1:C:146:LEU:HB2	2.15	0.46
1:C:393:GLU:OE2	2:G:25:ARG:NH1	2.49	0.46
1:D:611:ALA:HB1	1:D:647:VAL:HG21	1.97	0.46
1:D:652:LEU:HD23	1:D:683:ILE:HD13	1.96	0.46
3:B:1801:B12:H492	3:B:1801:B12:C47	2.46	0.46
1:C:539:ALA:O	1:C:543:PHE:HD2	1.99	0.46
1:D:8:ARG:HG3	1:D:11:GLU:CD	2.41	0.46
1:D:711:VAL:O	1:D:711:VAL:CG1	2.63	0.46
1:B:124:PRO:O	1:B:131:PRO:HG2	2.16	0.46
1:B:560:MET:HB2	1:B:565:GLY:O	2.16	0.46
1:B:576:PHE:CZ	1:D:546:LYS:HB3	2.50	0.46
1:B:647:VAL:HG12	1:B:648:PRO:O	2.16	0.46
1:B:663:ALA:HB2	1:B:697:MET:HE3	1.97	0.46
3:B:1801:B12:H531	3:B:1801:B12:H543	1.98	0.46
1:C:701:GLY:HA2	1:C:719:PHE:O	2.16	0.46
1:D:8:ARG:HG3	1:D:11:GLU:OE1	2.14	0.46
1:D:390:LEU:HD21	2:H:10:ARG:O	2.14	0.46
1:D:478:GLU:O	1:D:480:PRO:HD3	2.16	0.46
1:D:505:PHE:C	1:D:506:ARG:HG2	2.40	0.46
1:A:709:VAL:HG12	1:A:709:VAL:O	2.16	0.46
1:B:106:MET:CE	1:B:218:ILE:HD12	2.46	0.46
1:B:144:LEU:HD22	1:B:155:ILE:HG21	1.97	0.46
1:B:245:HIS:CG	1:B:264:LEU:HD23	2.51	0.46
1:B:611:ALA:HB2	1:B:643:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:LEU:HB3	1:C:282:PRO:HD3	1.97	0.46
1:C:684:HIS:O	1:C:688:VAL:HG23	2.16	0.46
1:B:182:HIS:HA	1:B:218:ILE:O	2.16	0.46
1:B:649:VAL:CG1	1:B:686:LEU:HD12	2.45	0.46
1:A:218:ILE:HD13	1:A:297:ARG:CD	2.45	0.45
1:B:126:GLY:HA3	1:B:131:PRO:HD3	1.98	0.45
3:B:1801:B12:H2B	3:B:1801:B12:O2	2.15	0.45
1:D:42:GLN:HG2	1:D:46:PHE:O	2.16	0.45
1:A:612:THR:CG2	1:A:616:ASP:HB3	2.43	0.45
3:A:1801:B12:H18	3:A:1801:B12:H561	1.55	0.45
1:B:7:LEU:HD23	1:B:7:LEU:HA	1.44	0.45
1:B:530:PRO:HD2	1:D:511:ILE:HD11	1.98	0.45
1:B:612:THR:HB	1:B:645:THR:HA	1.99	0.45
1:B:729:ALA:O	1:B:733:VAL:HG12	2.15	0.45
1:B:735:LYS:HD2	1:B:738:GLU:OE1	2.16	0.45
2:F:7:PHE:O	2:F:11:ARG:HG2	2.16	0.45
1:D:688:VAL:HG22	1:D:693:ARG:HB2	1.97	0.45
3:D:1801:B12:H8	3:D:1801:B12:H401	1.78	0.45
1:A:726:ILE:HG23	1:A:727:HIS:N	2.31	0.45
1:B:354:THR:OG1	1:D:310:ARG:HD2	2.16	0.45
1:B:529:LEU:HA	1:B:530:PRO:HD3	1.64	0.45
1:B:608:ILE:HG23	1:B:609:VAL:O	2.15	0.45
1:B:668:THR:HG21	1:B:680:MET:HE2	1.98	0.45
1:C:373:ARG:CG	1:C:373:ARG:NH1	2.78	0.45
1:C:695:LYS:HB2	1:C:695:LYS:HE3	1.71	0.45
1:D:373:ARG:HD2	1:D:373:ARG:O	2.16	0.45
1:D:674:ASP:HA	1:D:676:HIS:CE1	2.51	0.45
2:H:53:VAL:O	2:H:57:MET:HG3	2.16	0.45
1:A:109:ARG:HG2	1:A:132:ILE:CG1	2.46	0.45
1:A:349:ILE:HD12	1:A:349:ILE:N	2.31	0.45
2:E:57:MET:HE1	2:E:82:GLY:HA2	1.99	0.45
1:C:184:ASP:OD1	1:C:186:GLN:HB2	2.16	0.45
1:D:7:LEU:HD23	1:D:7:LEU:HA	1.60	0.45
1:D:178:VAL:O	1:D:215:MET:HE3	2.16	0.45
1:D:648:PRO:HD2	1:D:651:LYS:HE3	1.98	0.45
3:A:1801:B12:H301	3:A:1801:B12:H253	1.51	0.45
2:E:72:MET:HG2	2:E:77:MET:HG3	1.99	0.45
1:B:547:MET:HE2	1:D:574:VAL:CG2	2.47	0.45
2:F:112:ALA:O	2:F:114:GLN:N	2.50	0.45
1:C:6:GLN:HG2	1:C:7:LEU:N	2.31	0.45
1:C:41:LEU:HG	1:C:42:GLN:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:723:SER:O	3:D:1801:B12:H5R1	2.16	0.45
1:A:607:LYS:O	1:A:608:ILE:HD12	2.17	0.45
1:B:393:GLU:CG	2:F:29:MET:HE1	2.24	0.45
2:G:29:MET:HB2	2:G:29:MET:HE2	1.40	0.45
1:D:264:LEU:HD21	1:D:291:PHE:CD1	2.52	0.45
1:A:213:ALA:HB3	1:A:215:MET:HG3	1.98	0.45
1:A:289:GLU:O	1:A:292:GLU:HG3	2.17	0.45
1:A:733:VAL:O	1:A:737:ARG:HD2	2.17	0.45
2:E:64:ALA:O	2:E:68:VAL:HG23	2.16	0.45
1:B:65:LYS:HE2	1:D:306:GLU:CG	2.47	0.45
1:B:626:ILE:HD13	1:B:640:VAL:HG11	1.98	0.45
1:B:672:HIS:O	1:B:673:ASP:CB	2.64	0.45
1:B:692:ILE:O	1:B:694:ASP:N	2.50	0.45
1:C:191:TYR:CE1	1:C:230:THR:HG21	2.51	0.45
1:C:592:LEU:HD23	1:C:592:LEU:HA	1.86	0.45
1:D:197:ILE:HD11	1:D:428:ILE:HD12	1.99	0.45
1:D:710:ALA:O	1:D:715:VAL:HG22	2.16	0.45
2:H:7:PHE:O	2:H:11:ARG:HG2	2.17	0.45
1:A:137:VAL:HB	1:A:172:MET:CE	2.47	0.45
1:A:460:TYR:O	1:A:461:ASP:HB2	2.16	0.45
1:B:15:VAL:HG12	1:B:499:MET:CE	2.47	0.45
1:B:309:THR:HG22	1:B:336:PRO:O	2.16	0.45
1:B:415:TYR:O	1:B:416:TYR:C	2.60	0.45
1:C:302:THR:HG22	1:C:334:ILE:HG13	1.99	0.45
1:D:86:ARG:HD3	1:D:498:ARG:HD3	1.99	0.45
2:H:17:LEU:HD22	2:H:21:GLU:HB3	1.98	0.45
1:B:232:ARG:NH2	1:D:635:LYS:HE2	2.31	0.45
1:B:550:GLU:HA	1:B:550:GLU:OE1	2.17	0.45
1:B:609:VAL:HG12	1:B:659:LEU:HD12	1.99	0.45
1:B:687:ALA:HB3	1:B:693:ARG:HD3	1.97	0.45
1:C:207:LYS:HG2	1:C:257:MET:HE1	1.98	0.45
1:D:123:THR:O	1:D:494:ASN:HA	2.15	0.45
1:D:257:MET:HB3	1:D:262:ILE:HD11	1.99	0.45
1:C:186:GLN:HG2	1:C:401:TYR:OH	2.17	0.45
1:C:344:TRP:O	1:C:345:HIS:C	2.60	0.45
1:C:427:GLN:C	1:C:429:ASN:N	2.75	0.45
1:C:606:LEU:HB2	1:C:736:ARG:NH2	2.32	0.45
3:C:1801:B12:H471	3:C:1801:B12:H492	1.98	0.45
1:D:618:HIS:NE2	3:D:1801:B12:N22	2.64	0.45
2:E:5:ASP:CB	2:E:8:GLN:HG2	2.47	0.44
1:B:49:LYS:HE2	1:D:278:TYR:OH	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ASP:O	1:B:94:MET:HG3	2.17	0.44
1:B:162:SER:CB	4:B:767:Z97:H6	2.47	0.44
1:B:167:PRO:O	1:B:168:ASP:C	2.60	0.44
1:B:629:LYS:HE3	1:B:630:HIS:NE2	2.32	0.44
3:B:1801:B12:H412	3:B:1801:B12:H363	1.52	0.44
1:C:607:LYS:NZ	1:C:660:LYS:HD3	2.32	0.44
1:D:127:ILE:HD12	1:D:128:GLY:N	2.32	0.44
1:D:212:TRP:CH2	1:D:477:LEU:HB3	2.52	0.44
1:D:416:TYR:CD2	1:D:417:PRO:HA	2.52	0.44
1:D:457:VAL:O	1:D:458:LYS:C	2.60	0.44
1:A:17:ASN:HA	1:A:20:LYS:HE2	1.99	0.44
1:A:55:LEU:HD21	1:A:153:ARG:CZ	2.47	0.44
1:A:467:GLU:C	1:A:469:SER:H	2.25	0.44
1:A:574:VAL:HG21	1:C:547:MET:HE2	2.00	0.44
1:B:187:TYR:OH	1:D:629:LYS:HD3	2.18	0.44
1:B:657:ILE:HG12	1:B:692:ILE:HD13	1.99	0.44
1:C:18:ILE:HD13	1:C:143:ALA:HB2	1.98	0.44
1:D:445:MET:O	2:H:83:HIS:HB2	2.16	0.44
1:D:525:LEU:O	1:D:569:GLU:HA	2.17	0.44
1:D:553:GLU:O	1:D:555:ILE:HG23	2.16	0.44
1:D:622:LEU:HD23	1:D:642:TYR:CE1	2.52	0.44
1:D:628:ILE:HG12	1:D:628:ILE:O	2.17	0.44
1:C:75:LEU:N	1:C:76:PRO:HD3	2.31	0.44
1:C:345:HIS:ND1	1:C:515:VAL:O	2.43	0.44
3:C:1801:B12:H531	3:C:1801:B12:C55	2.47	0.44
1:D:164:VAL:HG12	1:D:194:ILE:CG2	2.47	0.44
1:D:459:GLN:CG	1:D:460:TYR:HD2	2.24	0.44
1:A:310:ARG:HD3	1:C:350:GLU:CG	2.48	0.44
1:A:647:VAL:HA	1:A:648:PRO:HD3	1.81	0.44
1:B:232:ARG:HA	1:B:232:ARG:NH1	2.32	0.44
3:B:1801:B12:HM63	3:B:1801:B12:HM51	1.83	0.44
1:C:360:ILE:HD13	1:C:360:ILE:HA	1.77	0.44
1:C:411:VAL:O	1:C:411:VAL:HG12	2.17	0.44
1:C:679:ASN:O	1:C:683:ILE:HG13	2.18	0.44
1:C:733:VAL:O	1:C:737:ARG:HG3	2.16	0.44
1:D:288:ARG:HG3	1:D:288:ARG:NH1	2.32	0.44
1:A:620:VAL:HG21	1:C:116:TYR:HE1	1.82	0.44
1:B:538:PHE:CD2	1:D:585:ILE:HG23	2.53	0.44
1:C:88:GLU:OE1	1:C:498:ARG:NH1	2.50	0.44
1:C:663:ALA:HB2	1:C:697:MET:HB2	2.00	0.44
1:D:444:TYR:CD2	1:D:444:TYR:C	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:MET:SD	1:C:105:ILE:HG21	2.57	0.44
1:C:109:ARG:NH2	1:C:114:SER:OG	2.48	0.44
1:C:396:ILE:HD11	2:G:29:MET:HG3	1.99	0.44
3:C:1801:B12:C53	3:C:1801:B12:H552	2.47	0.44
1:A:628:ILE:O	1:A:629:LYS:C	2.60	0.44
1:A:669:ILE:HG22	3:A:1801:B12:H202	1.99	0.44
1:B:446:ALA:HA	1:B:447:PRO:HD3	1.67	0.44
1:C:584:VAL:O	1:C:586:PRO:HD3	2.17	0.44
1:D:43:MET:HE1	1:D:72:PRO:HA	1.99	0.44
1:D:250:ILE:HD12	1:D:250:ILE:HA	1.65	0.44
1:B:445:MET:HE3	1:B:457:VAL:HG22	2.00	0.44
1:C:291:PHE:O	1:C:292:GLU:C	2.59	0.44
1:C:622:LEU:HB2	1:C:667:SER:HB2	1.98	0.44
2:G:46:THR:HB	2:G:47:PRO:HD2	1.99	0.44
1:D:696:ILE:HG12	1:D:697:MET:H	1.81	0.44
1:A:350:GLU:CG	1:C:310:ARG:HD3	2.48	0.44
1:A:470:LYS:O	1:A:471:LEU:C	2.60	0.44
1:A:618:HIS:HD2	3:A:1801:B12:C48	2.31	0.44
1:B:110:THR:HG22	1:B:131:PRO:HA	2.00	0.44
1:B:116:TYR:HE1	1:D:620:VAL:HG21	1.83	0.44
1:C:335:THR:O	1:C:338:GLU:HB2	2.17	0.44
2:H:25:ARG:O	2:H:29:MET:HG3	2.18	0.44
1:A:708:GLU:C	1:A:710:ALA:N	2.76	0.43
3:A:1801:B12:H451	3:A:1801:B12:H411	1.54	0.43
3:A:1801:B12:H531	3:A:1801:B12:H543	2.00	0.43
1:B:18:ILE:HG23	1:B:142:LYS:HD3	2.00	0.43
1:B:607:LYS:O	1:B:608:ILE:HD12	2.18	0.43
1:B:617:GLU:HA	1:B:645:THR:HB	2.00	0.43
1:B:618:HIS:HD2	3:B:1801:B12:H482	1.83	0.43
1:B:675:ILE:HD11	1:B:679:ASN:HD21	1.81	0.43
1:C:457:VAL:HG13	1:C:471:LEU:HD21	1.99	0.43
1:D:664:ILE:O	1:D:665:LEU:HD23	2.18	0.43
1:A:12:LYS:CE	1:C:530:PRO:O	2.66	0.43
1:B:142:LYS:O	1:B:145:ASP:HB2	2.17	0.43
3:C:1801:B12:H363	3:C:1801:B12:H412	1.48	0.43
1:D:291:PHE:CE1	2:H:27:TRP:CH2	3.06	0.43
1:D:471:LEU:HD12	1:D:471:LEU:HA	1.60	0.43
1:A:310:ARG:HD3	1:C:350:GLU:HG2	1.99	0.43
1:B:93:ARG:HD3	1:B:345:HIS:HA	2.00	0.43
1:C:517:TRP:O	1:C:518:GLN:C	2.60	0.43
1:A:349:ILE:N	1:A:349:ILE:CD1	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:LEU:HA	1:A:699:GLY:O	2.18	0.43
1:B:443:ASP:HA	1:B:456:ASN:HD22	1.84	0.43
1:C:43:MET:HE2	1:C:54:PRO:HG3	2.00	0.43
3:C:1801:B12:H351	3:C:1801:B12:H372	1.99	0.43
3:C:1801:B12:H301	3:C:1801:B12:H253	1.54	0.43
1:D:668:THR:CG2	1:D:676:HIS:HB2	2.48	0.43
2:H:5:ASP:CA	2:H:6:ASP:HB3	2.46	0.43
1:A:7:LEU:HA	1:A:7:LEU:HD23	1.72	0.43
1:A:212:TRP:CZ2	1:A:477:LEU:HB3	2.54	0.43
1:A:307:ALA:O	1:A:340:ARG:HD3	2.18	0.43
1:B:43:MET:O	1:B:44:GLY:C	2.62	0.43
1:B:122:GLY:C	1:B:123:THR:HG23	2.43	0.43
1:B:445:MET:HE3	1:B:471:LEU:HD23	2.01	0.43
1:C:189:VAL:CG1	1:C:196:MET:HB3	2.44	0.43
1:D:574:VAL:HA	1:D:575:PRO:HD3	1.77	0.43
2:E:100:GLY:O	2:E:101:LEU:C	2.62	0.43
1:B:561:GLN:O	1:B:562:GLU:C	2.62	0.43
1:C:23:ASP:OD2	1:C:24:LYS:HG2	2.18	0.43
1:D:94:MET:HE2	1:D:105:ILE:HG21	2.01	0.43
1:A:485:TYR:C	1:A:486:ILE:HD12	2.43	0.43
1:B:236:LYS:HB3	1:B:415:TYR:HB2	2.01	0.43
1:D:243:VAL:O	1:D:247:LEU:HG	2.19	0.43
1:D:266:THR:O	1:D:266:THR:HG23	2.17	0.43
1:D:389:VAL:HG13	2:H:29:MET:HE1	2.01	0.43
1:D:617:GLU:HB2	3:D:1801:B12:C43	2.49	0.43
1:B:126:GLY:CA	1:B:131:PRO:HD3	2.48	0.43
1:B:233:GLU:HB3	1:B:235:TRP:CH2	2.54	0.43
1:B:521:GLY:O	1:B:573:ARG:HA	2.18	0.43
1:B:612:THR:CG2	1:B:616:ASP:HB3	2.48	0.43
1:C:65:LYS:HE2	1:C:66:TYR:CZ	2.54	0.43
1:C:268:PRO:HA	1:C:269:PRO:HD3	1.71	0.43
1:D:57:ASN:HB3	1:D:99:TRP:CH2	2.53	0.43
1:D:116:TYR:CD1	1:D:116:TYR:N	2.86	0.43
1:D:204:CYS:SG	2:H:41:GLY:HA3	2.59	0.43
1:A:189:VAL:CG2	1:A:196:MET:HA	2.49	0.43
1:A:412:ASP:OD1	1:A:419:ARG:HG3	2.19	0.43
1:A:601:ILE:HD13	1:A:638:VAL:HG22	2.01	0.43
1:B:665:LEU:HA	1:B:699:GLY:O	2.19	0.43
1:C:7:LEU:HD23	1:C:7:LEU:HA	1.49	0.43
1:C:537:GLU:HG3	1:C:554:VAL:HG11	2.01	0.43
1:A:43:MET:HE3	1:A:72:PRO:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:ARG:HH12	1:C:634:GLU:CD	2.22	0.43
1:A:702:GLY:O	1:A:703:THR:C	2.61	0.43
3:A:1801:B12:H541	3:A:1801:B12:H602	1.76	0.43
2:F:74:ARG:HG3	2:F:74:ARG:NH1	2.33	0.43
2:F:112:ALA:C	2:F:114:GLN:N	2.73	0.43
1:C:6:GLN:CG	1:C:7:LEU:N	2.82	0.43
1:C:223:GLY:O	1:C:224:ALA:C	2.60	0.43
1:A:470:LYS:C	1:A:472:ILE:N	2.77	0.42
1:A:649:VAL:HG12	1:A:686:LEU:HD22	2.00	0.42
3:A:1801:B12:H601	3:A:1801:B12:H252	2.00	0.42
1:C:116:TYR:HE2	1:C:120:ILE:HD13	1.83	0.42
1:C:464:LEU:HG	1:C:470:LYS:HB2	2.00	0.42
1:D:20:LYS:O	1:D:21:ASP:HB2	2.18	0.42
1:A:93:ARG:HG3	1:A:345:HIS:ND1	2.33	0.42
1:A:534:ARG:O	1:A:535:VAL:C	2.61	0.42
1:D:82:ILE:O	1:D:107:VAL:HG22	2.20	0.42
1:D:360:ILE:HD13	1:D:360:ILE:HA	1.87	0.42
1:A:524:LEU:HB3	1:C:526:THR:HB	2.01	0.42
1:A:574:VAL:HA	1:A:575:PRO:HD3	1.79	0.42
1:B:342:VAL:HG12	1:B:343:PRO:HD2	2.01	0.42
1:B:586:PRO:HA	1:B:587:PRO:HD3	1.87	0.42
1:B:706:THR:HA	1:B:707:PRO:HD3	1.92	0.42
3:C:1801:B12:H562	3:C:1801:B12:H18	1.85	0.42
1:D:138:ARG:HE	1:D:176:GLU:CD	2.26	0.42
1:D:706:THR:O	1:D:707:PRO:C	2.62	0.42
2:E:36:PRO:O	2:E:40:LEU:HG	2.19	0.42
1:B:448:VAL:HB	2:F:56:ARG:HD2	2.01	0.42
1:B:693:ARG:O	1:B:693:ARG:CG	2.67	0.42
2:G:14:LEU:HD23	2:G:14:LEU:HA	1.86	0.42
1:D:613:VAL:HG11	1:D:679:ASN:HB3	2.02	0.42
1:A:446:ALA:HA	1:A:447:PRO:HD3	1.82	0.42
1:A:467:GLU:C	1:A:469:SER:N	2.77	0.42
3:A:1801:B12:H203	3:A:1801:B12:H302	2.02	0.42
1:B:115:HIS:ND1	1:D:623:ARG:HD3	2.34	0.42
1:B:526:THR:HB	1:D:524:LEU:HB3	2.01	0.42
1:C:57:ASN:HB3	1:C:99:TRP:CH2	2.54	0.42
1:D:5:LEU:O	1:D:5:LEU:HD23	2.20	0.42
1:D:116:TYR:N	1:D:116:TYR:HD1	2.17	0.42
1:D:529:LEU:HA	1:D:530:PRO:HD3	1.84	0.42
3:D:1801:B12:C49	3:D:1801:B12:C47	2.88	0.42
1:A:623:ARG:HD3	1:C:115:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:THR:C	1:A:647:VAL:H	2.28	0.42
1:B:86:ARG:O	1:B:87:PHE:C	2.61	0.42
1:B:114:SER:HB2	4:B:767:Z97:OP2	2.19	0.42
1:B:461:ASP:C	1:B:463:ALA:H	2.27	0.42
1:B:479:VAL:HG12	1:B:479:VAL:O	2.18	0.42
1:D:120:ILE:HG13	1:D:133:THR:CG2	2.47	0.42
1:D:373:ARG:HH11	1:D:378:GLY:HA2	1.85	0.42
1:D:456:ASN:OD1	1:D:456:ASN:C	2.63	0.42
1:A:12:LYS:HE2	1:C:530:PRO:O	2.20	0.42
1:A:22:LEU:HD23	1:A:22:LEU:HA	1.88	0.42
1:B:137:VAL:CB	1:B:172:MET:HE1	2.49	0.42
1:B:171:VAL:HG22	1:B:209:ILE:HD13	2.02	0.42
1:B:471:LEU:HD12	1:B:471:LEU:HA	1.83	0.42
1:B:706:THR:HG22	1:B:708:GLU:H	1.85	0.42
5:B:1500:5AD:H5'3	3:D:1801:B12:C15	2.29	0.42
1:C:117:ASP:HA	1:C:164:VAL:HG23	2.01	0.42
1:C:120:ILE:HG13	1:C:133:THR:HG22	2.02	0.42
1:C:493:ASP:OD1	1:C:493:ASP:C	2.63	0.42
1:C:675:ILE:O	1:C:675:ILE:HD12	2.20	0.42
3:C:1801:B12:H492	3:C:1801:B12:C47	2.49	0.42
2:G:40:LEU:HA	2:G:40:LEU:HD23	1.76	0.42
1:D:5:LEU:HD23	1:D:6:GLN:HB2	2.00	0.42
1:D:212:TRP:CZ2	1:D:477:LEU:HB3	2.55	0.42
1:D:540:ALA:HB1	1:D:570:LEU:HD11	2.01	0.42
2:H:5:ASP:CB	2:H:8:GLN:H	2.33	0.42
2:H:59:PHE:CZ	2:H:100:GLY:HA3	2.53	0.42
1:A:662:ASP:O	1:A:663:ALA:HB2	2.20	0.42
1:B:123:THR:O	1:B:494:ASN:HA	2.19	0.42
1:B:242:MET:HE2	1:B:242:MET:HB3	1.67	0.42
1:C:160:TYR:HD1	4:C:767:Z97:C6	2.33	0.42
1:C:406:GLU:OE1	1:C:428:ILE:HB	2.19	0.42
1:C:411:VAL:HB	1:C:424:ILE:HG12	2.00	0.42
1:C:441:ASP:O	1:C:442:GLU:C	2.63	0.42
2:G:38:LEU:HA	2:G:38:LEU:HD23	1.82	0.42
1:D:26:THR:CG2	1:D:27:PRO:HD2	2.49	0.42
1:D:238:MET:O	1:D:239:PRO:C	2.63	0.42
1:D:512:LYS:HE3	1:D:576:PHE:O	2.19	0.42
1:D:711:VAL:O	1:D:711:VAL:HG13	2.20	0.42
1:A:137:VAL:HG21	1:A:172:MET:HE1	2.02	0.42
1:A:204:CYS:HB3	1:A:452:PHE:CD2	2.55	0.42
1:A:597:ILE:HD11	1:A:730:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:HIS:HD2	3:A:1801:B12:H482	1.84	0.42
1:B:14:ASP:O	1:B:18:ILE:HG13	2.20	0.42
1:B:176:GLU:OE1	1:B:176:GLU:HA	2.19	0.42
1:B:445:MET:CE	1:B:471:LEU:HD23	2.49	0.42
1:B:555:ILE:HG21	1:B:571:LYS:HG2	2.02	0.42
1:C:183:GLN:OE1	1:C:207:LYS:HE2	2.19	0.42
1:C:592:LEU:HD13	1:C:597:ILE:HD13	2.02	0.42
1:D:406:GLU:HG3	1:D:428:ILE:HG22	2.01	0.42
1:D:628:ILE:HG13	1:D:635:LYS:HB2	2.01	0.42
1:A:108:ILE:HA	1:A:160:TYR:CE2	2.55	0.42
1:A:600:ASP:C	1:A:602:GLU:H	2.28	0.42
1:B:618:HIS:HD2	3:B:1801:B12:C48	2.33	0.42
1:C:626:ILE:O	1:C:627:ASP:C	2.63	0.42
1:A:19:LEU:HD11	1:A:499:MET:HE2	2.02	0.41
1:A:546:LYS:NZ	1:C:578:ILE:CD1	2.83	0.41
1:A:648:PRO:O	1:A:649:VAL:C	2.62	0.41
1:A:704:GLN:O	1:A:705:VAL:HG23	2.20	0.41
1:B:281:LEU:HB3	1:B:282:PRO:HD3	2.02	0.41
1:B:688:VAL:N	1:B:693:ARG:HB2	2.35	0.41
1:B:689:GLU:O	1:B:689:GLU:CG	2.67	0.41
1:C:116:TYR:CE2	1:C:120:ILE:HD13	2.55	0.41
1:C:250:ILE:HD12	1:C:250:ILE:HA	1.96	0.41
2:G:5:ASP:CA	2:G:7:PHE:N	2.66	0.41
1:D:696:ILE:HG23	1:D:697:MET:N	2.35	0.41
1:A:7:LEU:CD1	1:A:146:LEU:HB3	2.50	0.41
1:A:688:VAL:HG22	1:A:693:ARG:CG	2.49	0.41
2:E:62:LEU:HA	2:E:62:LEU:HD23	1.73	0.41
1:B:13:LEU:CD1	1:B:91:ILE:HG22	2.50	0.41
1:C:554:VAL:HA	1:C:570:LEU:HB3	2.01	0.41
1:D:467:GLU:N	1:D:468:PRO:HD3	2.35	0.41
1:D:618:HIS:HD2	3:D:1801:B12:H481	1.84	0.41
3:D:1801:B12:H351	3:D:1801:B12:C37	2.50	0.41
1:A:488:GLU:O	1:A:489:LEU:HD23	2.20	0.41
1:A:512:LYS:HB2	1:A:513:PRO:CD	2.50	0.41
1:A:546:LYS:HZ2	1:C:578:ILE:HD11	1.83	0.41
1:B:41:LEU:HD23	1:B:43:MET:CE	2.51	0.41
1:B:320:LEU:HD22	1:B:359:LEU:HG	2.03	0.41
1:B:606:LEU:HD13	1:B:736:ARG:CZ	2.50	0.41
1:B:610:ALA:O	1:B:611:ALA:HB2	2.20	0.41
1:C:250:ILE:HG23	1:C:251:PHE:N	2.35	0.41
1:C:533:LYS:HB2	1:C:533:LYS:NZ	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:645:THR:O	1:D:646:SER:HB2	2.20	0.41
5:A:1500:5AD:H5'3	3:C:1801:B12:C16	2.50	0.41
1:C:119:LEU:HD23	1:C:119:LEU:HA	1.84	0.41
1:D:189:VAL:HG21	1:D:196:MET:HA	2.02	0.41
1:A:137:VAL:CG2	1:A:172:MET:HE1	2.50	0.41
1:A:269:PRO:HD2	1:A:280:ASP:CG	2.46	0.41
1:A:393:GLU:OE2	2:E:25:ARG:NH1	2.53	0.41
1:A:600:ASP:OD2	1:A:736:ARG:NH1	2.53	0.41
2:F:57:MET:CE	2:F:82:GLY:HA2	2.49	0.41
1:C:300:MET:CE	1:C:333:THR:HG22	2.50	0.41
1:D:460:TYR:CE1	2:H:86:TYR:CE2	3.04	0.41
1:A:575:PRO:HD2	1:A:576:PHE:CD2	2.55	0.41
1:A:611:ALA:HB3	1:A:652:LEU:HD13	2.01	0.41
2:E:22:LEU:HD12	2:E:22:LEU:HA	1.89	0.41
2:E:39:ASP:HA	2:E:42:LYS:HD2	2.02	0.41
1:B:61:LEU:O	1:B:62:PRO:C	2.63	0.41
1:B:238:MET:O	1:B:242:MET:HG3	2.19	0.41
1:B:264:LEU:HD13	1:B:296:MET:CE	2.49	0.41
5:B:1500:5AD:C4'	3:D:1801:B12:N23	2.79	0.41
1:A:650:GLU:HG2	1:A:654:ASP:OD2	2.21	0.41
1:B:334:ILE:HG23	1:B:338:GLU:HG3	2.02	0.41
1:B:531:THR:HG23	1:B:532:SER:O	2.21	0.41
1:C:173:PHE:CD1	1:C:178:VAL:HG21	2.55	0.41
1:D:447:PRO:HG2	2:H:57:MET:SD	2.60	0.41
1:D:461:ASP:C	1:D:463:ALA:N	2.78	0.41
1:D:534:ARG:O	1:D:538:PHE:HD2	2.03	0.41
1:D:574:VAL:HG13	1:D:576:PHE:CE1	2.55	0.41
1:D:723:SER:N	3:D:1801:B12:H5R2	2.35	0.41
5:A:1500:5AD:H5'2	3:C:1801:B12:H261	2.02	0.41
1:B:172:MET:O	1:B:172:MET:HE2	2.21	0.41
1:B:369:VAL:HG13	1:D:369:VAL:HG13	2.03	0.41
1:C:7:LEU:C	1:C:8:ARG:HG3	2.46	0.41
1:C:102:ALA:HB2	1:C:352:CYS:SG	2.61	0.41
3:C:1801:B12:H601	3:C:1801:B12:H252	2.02	0.41
1:D:445:MET:HE3	1:D:447:PRO:N	2.36	0.41
2:H:103:LEU:HD22	2:H:109:TRP:CZ2	2.56	0.41
1:A:440:ARG:NH1	1:A:454:TYR:O	2.53	0.41
1:A:688:VAL:HG22	1:A:693:ARG:HB3	2.03	0.41
1:A:697:MET:CE	1:A:736:ARG:HB2	2.50	0.41
2:E:91:GLU:C	2:E:92:LYS:HE2	2.46	0.41
1:B:232:ARG:NE	1:D:598:ARG:NH1	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ALA:O	1:B:340:ARG:HD3	2.20	0.41
1:B:547:MET:HE2	1:D:574:VAL:HG22	2.02	0.41
1:B:623:ARG:HH21	1:B:642:TYR:HE2	1.69	0.41
1:C:5:LEU:HD23	1:C:5:LEU:C	2.46	0.41
1:C:141:ARG:NH1	1:C:179:ASN:OD1	2.54	0.41
1:C:264:LEU:HD12	1:C:264:LEU:N	2.35	0.41
3:C:1801:B12:H531	3:C:1801:B12:H552	2.03	0.41
1:D:116:TYR:HE2	1:D:120:ILE:HD13	1.84	0.41
1:D:189:VAL:HG22	1:D:196:MET:HA	2.03	0.41
1:D:320:LEU:HD13	1:D:358:ALA:HB3	2.02	0.41
1:D:580:ILE:HD13	1:D:580:ILE:HA	1.91	0.41
1:A:96:MET:HE1	1:A:345:HIS:CB	2.44	0.41
1:A:735:LYS:HD2	1:A:738:GLU:OE2	2.21	0.41
2:E:88:ILE:HD13	2:E:88:ILE:HA	1.80	0.41
1:B:444:TYR:CD2	1:B:444:TYR:C	2.98	0.41
1:B:566:THR:HG22	1:B:568:ILE:HG12	2.03	0.41
2:F:6:ASP:CG	2:F:10:ARG:HD2	2.46	0.41
1:C:529:LEU:HA	1:C:530:PRO:HD3	1.73	0.41
1:C:619:SER:HB3	1:C:645:THR:HG21	2.02	0.41
1:D:401:TYR:O	1:D:402:PHE:C	2.63	0.41
1:A:201:ILE:HG23	2:E:41:GLY:HA2	2.02	0.40
1:A:297:ARG:HH21	1:A:332:SER:CB	2.34	0.40
1:B:259:LYS:HE2	1:B:294:TYR:CZ	2.55	0.40
1:B:269:PRO:HD2	1:B:280:ASP:OD1	2.21	0.40
1:B:401:TYR:O	1:B:405:VAL:HG23	2.20	0.40
1:B:463:ALA:C	1:B:464:LEU:HD13	2.46	0.40
1:B:531:THR:CG2	1:B:536:ALA:HB2	2.51	0.40
1:B:695:LYS:HB2	1:B:695:LYS:HZ2	1.85	0.40
1:C:6:GLN:HG3	1:C:8:ARG:HD2	2.03	0.40
1:C:310:ARG:O	1:C:311:GLU:C	2.64	0.40
1:D:344:TRP:CD1	1:D:515:VAL:HB	2.56	0.40
1:A:44:GLY:HA3	1:A:45:PRO:HD3	1.84	0.40
1:A:600:ASP:C	1:A:600:ASP:OD2	2.63	0.40
1:A:632:GLY:O	1:A:634:GLU:N	2.54	0.40
1:B:213:ALA:HB3	1:B:215:MET:HG3	2.02	0.40
1:B:669:ILE:HG22	3:B:1801:B12:H202	2.03	0.40
1:B:726:ILE:HG23	1:B:727:HIS:N	2.36	0.40
1:C:161:VAL:HG12	1:C:161:VAL:O	2.21	0.40
1:C:300:MET:HE2	1:C:320:LEU:HD21	2.03	0.40
1:C:460:TYR:CD1	2:G:86:TYR:HE2	2.38	0.40
1:C:503:LYS:C	1:C:505:PHE:H	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:574:VAL:O	1:C:574:VAL:HG12	2.20	0.40
2:G:54:LEU:HA	2:G:57:MET:CE	2.52	0.40
2:G:76:LEU:HD12	2:G:76:LEU:HA	1.86	0.40
1:D:281:LEU:HB3	1:D:282:PRO:HD3	2.01	0.40
1:D:445:MET:HE3	1:D:446:ALA:C	2.46	0.40
1:D:685:GLU:C	1:D:687:ALA:N	2.79	0.40
1:A:635:LYS:HG3	1:C:232:ARG:HH22	1.86	0.40
1:A:701:GLY:HA2	1:A:705:VAL:HG11	2.01	0.40
1:B:685:GLU:O	1:B:688:VAL:HG12	2.20	0.40
3:B:1801:B12:H301	3:B:1801:B12:H253	1.82	0.40
1:C:144:LEU:O	1:C:148:GLU:HG2	2.21	0.40
2:G:54:LEU:HA	2:G:57:MET:HE2	2.03	0.40
1:D:29:ARG:C	1:D:30:ARG:HG2	2.45	0.40
1:D:116:TYR:CD2	1:D:120:ILE:HD13	2.55	0.40
1:D:478:GLU:C	1:D:480:PRO:HD3	2.46	0.40
1:D:528:PHE:CE1	1:D:560:MET:HG3	2.56	0.40
1:A:158:HIS:NE2	1:A:181:ALA:HA	2.36	0.40
1:C:95:ARG:HH21	1:C:150:GLU:CD	2.30	0.40
1:C:323:SER:HB3	1:C:328:ALA:HB2	2.03	0.40
1:C:411:VAL:CB	1:C:424:ILE:HG12	2.51	0.40
1:D:213:ALA:HB3	1:D:215:MET:HG3	2.02	0.40
1:D:238:MET:O	1:D:241:LEU:HB2	2.20	0.40
2:H:10:ARG:HE	2:H:10:ARG:HB3	1.42	0.40
2:H:98:GLU:H	2:H:98:GLU:HG2	1.72	0.40
1:A:189:VAL:HG22	1:A:196:MET:HA	2.04	0.40
1:A:219:ASP:HB3	1:A:248:ASN:ND2	2.35	0.40
1:A:393:GLU:CG	2:E:29:MET:HE1	2.52	0.40
1:A:531:THR:HG22	1:A:536:ALA:HB2	2.03	0.40
1:A:654:ASP:O	1:A:657:ILE:HB	2.22	0.40
1:B:22:LEU:HA	1:B:22:LEU:HD23	1.87	0.40
1:B:43:MET:HE1	1:B:72:PRO:HA	2.03	0.40
1:B:289:GLU:CD	1:B:373:ARG:HH21	2.29	0.40
1:C:288:ARG:HD2	1:C:326:THR:HB	2.02	0.40
1:D:88:GLU:CD	1:D:498:ARG:HH11	2.29	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	A	722/763 (95%)	651 (90%)	61 (8%)	10 (1%)	9	30
1	B	722/763 (95%)	659 (91%)	56 (8%)	7 (1%)	12	38
1	C	722/763 (95%)	658 (91%)	58 (8%)	6 (1%)	16	44
1	D	722/763 (95%)	670 (93%)	49 (7%)	3 (0%)	30	60
2	E	108/121 (89%)	102 (94%)	5 (5%)	1 (1%)	14	41
2	F	108/121 (89%)	100 (93%)	6 (6%)	2 (2%)	6	22
2	G	108/121 (89%)	98 (91%)	8 (7%)	2 (2%)	6	22
2	H	108/121 (89%)	95 (88%)	12 (11%)	1 (1%)	14	41
All	All	3320/3536 (94%)	3033 (91%)	255 (8%)	32 (1%)	12	38

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
2	E	6	ASP
1	C	6	GLN
1	C	461	ASP
2	G	6	ASP
1	A	471	LEU
1	B	461	ASP
1	B	693	ARG
1	D	6	GLN
2	H	108	TYR
1	A	12	LYS
1	A	461	ASP
1	A	601	ILE
1	A	649	VAL
1	B	458	LYS
2	F	6	ASP
2	F	113	ILE

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Mol	Chain	Res	Type
1	C	7	LEU
2	G	86	TYR
1	A	694	ASP
1	B	471	LEU
1	A	411	VAL
1	B	83	ALA
1	B	7	LEU
1	D	411	VAL
1	A	530	PRO
1	A	709	VAL
1	C	586	PRO
1	D	467	GLU
1	B	411	VAL
1	C	161	VAL
1	C	411	VAL

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	A	594/644 (92%)	569 (96%)	25 (4%)	26	61
1	B	602/644 (94%)	547 (91%)	55 (9%)	9	28
1	C	600/644 (93%)	549 (92%)	51 (8%)	10	31
1	D	602/644 (94%)	547 (91%)	55 (9%)	9	28
2	E	89/100 (89%)	82 (92%)	7 (8%)	11	35
2	F	90/100 (90%)	84 (93%)	6 (7%)	15	42
2	G	89/100 (89%)	80 (90%)	9 (10%)	7	23
2	H	89/100 (89%)	81 (91%)	8 (9%)	9	28
All	All	2755/2976 (93%)	2539 (92%)	216 (8%)	11	35

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	108	ILE
1	A	136	GLN
1	A	137	VAL
1	A	153	ARG
1	A	164	VAL
1	A	171	VAL
1	A	172	MET
1	A	198	ARG
1	A	260	SER
1	A	265	SER
1	A	411	VAL
1	A	464	LEU
1	A	486	ILE
1	A	490	ASP
1	A	491	GLU
1	A	574	VAL
1	A	578	ILE
1	A	591	ILE
1	A	608	ILE
1	A	616	ASP
1	A	625	VAL
1	A	697	MET
1	A	730	THR
1	A	736	ARG
2	E	9	GLN
2	E	21	GLU
2	E	88	ILE
2	E	93	ASN
2	E	94	ILE
2	E	101	LEU
2	E	107	LYS
1	B	5	LEU
1	B	7	LEU
1	B	9	VAL
1	B	24	LYS
1	B	26	THR
1	B	30	ARG
1	B	36	GLN
1	B	63	SER
1	B	79	THR
1	B	82	ILE
1	B	114	SER

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Mol	Chain	Res	Type
1	B	151	VAL
1	B	153	ARG
1	B	159	SER
1	B	172	MET
1	B	232	ARG
1	B	260	SER
1	B	306	GLU
1	B	308	SER
1	B	313	THR
1	B	338	GLU
1	B	341	ASN
1	B	349	ILE
1	B	354	THR
1	B	406	GLU
1	B	411	VAL
1	B	428	ILE
1	B	464	LEU
1	B	465	VAL
1	B	471	LEU
1	B	486	ILE
1	B	499	MET
1	B	501	GLU
1	B	557	ARG
1	B	570	LEU
1	B	578	ILE
1	B	592	LEU
1	B	601	ILE
1	B	613	VAL
1	B	646	SER
1	B	649	VAL
1	B	651	LYS
1	B	653	VAL
1	B	672	HIS
1	B	675	ILE
1	B	688	VAL
1	B	695	LYS
1	B	703	THR
1	B	715	VAL
1	B	723	SER
1	B	728	VAL
1	B	730	THR
1	B	733	VAL

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Mol	Chain	Res	Type
1	B	736	ARG
1	B	739	MET
2	F	23	GLN
2	F	65	LYS
2	F	76	LEU
2	F	93	ASN
2	F	94	ILE
2	F	101	LEU
1	C	7	LEU
1	C	11	GLU
1	C	13	LEU
1	C	15	VAL
1	C	26	THR
1	C	28	LYS
1	C	33	THR
1	C	39	GLU
1	C	108	ILE
1	C	120	ILE
1	C	153	ARG
1	C	162	SER
1	C	189	VAL
1	C	199	SER
1	C	206	SER
1	C	238	MET
1	C	306	GLU
1	C	313	THR
1	C	360	ILE
1	C	370	GLN
1	C	373	ARG
1	C	396	ILE
1	C	428	ILE
1	C	464	LEU
1	C	471	LEU
1	C	497	VAL
1	C	500	GLU
1	C	506	ARG
1	C	511	ILE
1	C	525	LEU
1	C	533	LYS
1	C	541	ILE
1	C	569	GLU
1	C	570	LEU

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Mol	Chain	Res	Type
1	C	574	VAL
1	C	576	PHE
1	C	578	ILE
1	C	591	ILE
1	C	604	THR
1	C	608	ILE
1	C	613	VAL
1	C	628	ILE
1	C	650	GLU
1	C	651	LYS
1	C	660	LYS
1	C	668	THR
1	C	675	ILE
1	C	681	LYS
1	C	696	ILE
1	C	721	ARG
1	C	736	ARG
2	G	9	GLN
2	G	29	MET
2	G	39	ASP
2	G	65	LYS
2	G	76	LEU
2	G	79	LYS
2	G	84	ILE
2	G	91	GLU
2	G	94	ILE
1	D	7	LEU
1	D	8	ARG
1	D	9	VAL
1	D	15	VAL
1	D	18	ILE
1	D	29	ARG
1	D	42	GLN
1	D	43	MET
1	D	47	ILE
1	D	50	ASP
1	D	77	VAL
1	D	79	THR
1	D	80	THR
1	D	91	ILE
1	D	108	ILE
1	D	110	THR

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Mol	Chain	Res	Type
1	D	127	ILE
1	D	151	VAL
1	D	153	ARG
1	D	172	MET
1	D	179	ASN
1	D	225	HIS
1	D	232	ARG
1	D	250	ILE
1	D	301	ASN
1	D	306	GLU
1	D	338	GLU
1	D	397	GLU
1	D	427	GLN
1	D	428	ILE
1	D	445	MET
1	D	465	VAL
1	D	467	GLU
1	D	469	SER
1	D	471	LEU
1	D	491	GLU
1	D	499	MET
1	D	502	THR
1	D	506	ARG
1	D	557	ARG
1	D	577	SER
1	D	585	ILE
1	D	608	ILE
1	D	625	VAL
1	D	657	ILE
1	D	668	THR
1	D	682	ARG
1	D	686	LEU
1	D	688	VAL
1	D	690	LYS
1	D	695	LYS
1	D	703	THR
1	D	711	VAL
1	D	730	THR
1	D	736	ARG
2	H	23	GLN
2	H	24	THR
2	H	39	ASP

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Mol	Chain	Res	Type
2	H	76	LEU
2	H	90	LYS
2	H	101	LEU
2	H	107	LYS
2	H	111	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	348	ASN
1	A	403	ASN
2	E	23	GLN
1	B	186	GLN
1	B	348	ASN
1	B	403	ASN
1	B	630	HIS
1	C	40	ASN
1	C	125	GLN
1	C	226	ASN
1	C	228	ASN
1	C	319	ASN
1	C	429	ASN
2	G	8	GLN
1	D	115	HIS
1	D	245	HIS
1	D	248	ASN
1	D	319	ASN
1	D	407	GLN
2	H	9	GLN

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 ⓘ

12 ligands are modelled in this entry.

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$
4	Z97	A	767	-	23,24,24	2.54	9 (39%)	27,33,33	1.79	8 (29%)
3	B12	B	1801	1	94,101,101	1.50	11 (11%)	149,166,166	2.25	35 (23%)
5	5AD	C	1500	-	20,20,20	2.19	8 (40%)	28,30,30	3.98	18 (64%)
3	B12	C	1801	1	94,101,101	1.58	12 (12%)	149,166,166	2.41	37 (24%)
4	Z97	C	767	-	23,24,24	2.54	7 (30%)	27,33,33	1.65	5 (18%)
3	B12	A	1801	1	94,101,101	1.48	11 (11%)	149,166,166	2.30	40 (26%)
5	5AD	B	1500	-	20,20,20	2.23	8 (40%)	28,30,30	4.19	16 (57%)
3	B12	D	1801	1	94,101,101	1.53	12 (12%)	149,166,166	2.27	31 (20%)
5	5AD	D	1500	-	20,20,20	2.22	9 (45%)	28,30,30	4.01	18 (64%)
4	Z97	B	767	-	23,24,24	2.35	7 (30%)	27,33,33	1.60	4 (14%)
4	Z97	D	767	-	23,24,24	2.51	8 (34%)	27,33,33	1.89	6 (22%)
5	5AD	A	1500	-	20,20,20	2.09	6 (30%)	28,30,30	3.96	17 (60%)

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
3	B12	B	1801	1	1/1/36/38	20/56/223/223	0/3/11/11
5	5AD	C	1500	-	3/3/4/4	0/4/20/20	0/3/3/3
4	Z97	A	767	-	-	7/18/18/18	0/1/1/1
3	B12	C	1801	1	1/1/36/38	13/56/223/223	0/3/11/11

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	Z97	C	767	-	-	10/18/18/18	0/1/1/1
3	B12	A	1801	1	1/1/36/38	26/56/223/223	0/3/11/11
5	5AD	B	1500	-	2/2/4/4	0/4/20/20	0/3/3/3
3	B12	D	1801	1	1/1/36/38	21/56/223/223	0/3/11/11
5	5AD	D	1500	-	3/3/4/4	1/4/20/20	0/3/3/3
4	Z97	B	767	-	-	11/18/18/18	0/1/1/1
4	Z97	D	767	-	-	9/18/18/18	0/1/1/1
5	5AD	A	1500	-	2/2/4/4	1/4/20/20	0/3/3/3

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1801	B12	C19-N24	-6.87	1.40	1.49
4	C	767	Z97	C4-C5	6.30	1.50	1.42
4	D	767	Z97	C4-C5	6.16	1.50	1.42
4	A	767	Z97	C4-C5	6.03	1.50	1.42
3	D	1801	B12	C19-N24	-5.93	1.41	1.49
3	B	1801	B12	C19-N24	-5.89	1.41	1.49
3	A	1801	B12	C19-N24	-5.84	1.41	1.49
4	B	767	Z97	C4-C5	5.81	1.50	1.42
3	C	1801	B12	C8B-C9B	5.69	1.49	1.40
3	D	1801	B12	C14-N23	5.62	1.42	1.35
3	B	1801	B12	C14-N23	5.54	1.42	1.35
4	C	767	Z97	C4A-NE	5.42	1.45	1.27
4	B	767	Z97	C4A-NE	5.40	1.45	1.27
4	D	767	Z97	C4A-NE	5.29	1.44	1.27
3	C	1801	B12	C14-N23	5.28	1.42	1.35
3	A	1801	B12	C14-N23	5.22	1.42	1.35
3	B	1801	B12	C8B-C9B	5.20	1.48	1.40
4	C	767	Z97	C2-N1	5.20	1.43	1.33
4	A	767	Z97	C4A-NE	5.17	1.44	1.27
3	A	1801	B12	C8B-C9B	5.16	1.48	1.40
3	D	1801	B12	C8B-C9B	5.11	1.48	1.40
4	A	767	Z97	C2-N1	5.05	1.42	1.33
4	D	767	Z97	C2-N1	4.82	1.42	1.33
3	D	1801	B12	C9-N22	4.74	1.42	1.30
3	A	1801	B12	C9-N22	4.70	1.42	1.30
3	B	1801	B12	C9-N22	4.69	1.42	1.30
3	C	1801	B12	C9-N22	4.52	1.41	1.30
4	C	767	Z97	C6-N1	4.39	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1500	5AD	C8-N7	4.36	1.40	1.31
5	B	1500	5AD	C8-N7	4.35	1.40	1.31
4	B	767	Z97	C2-N1	4.29	1.41	1.33
5	D	1500	5AD	C8-N7	4.24	1.39	1.31
4	D	767	Z97	C6-N1	4.19	1.43	1.34
5	C	1500	5AD	C8-N7	4.15	1.39	1.31
3	C	1801	B12	C16-C15	-3.94	1.33	1.44
4	A	767	Z97	C6-N1	3.89	1.42	1.34
5	C	1500	5AD	C2-N3	3.84	1.40	1.33
3	D	1801	B12	C16-C15	-3.80	1.33	1.44
5	B	1500	5AD	C2-N3	3.77	1.40	1.33
3	B	1801	B12	C16-C15	-3.67	1.34	1.44
5	D	1500	5AD	C2-N3	3.65	1.40	1.33
3	A	1801	B12	C16-C15	-3.62	1.34	1.44
3	B	1801	B12	C11-N23	3.58	1.43	1.36
5	A	1500	5AD	C2-N3	3.56	1.40	1.33
3	D	1801	B12	C11-N23	3.51	1.43	1.36
5	D	1500	5AD	C6-N6	3.49	1.43	1.34
4	B	767	Z97	C6-N1	3.46	1.41	1.34
3	A	1801	B12	C11-N23	3.46	1.43	1.36
3	C	1801	B12	C6B-C5B	3.45	1.49	1.40
3	D	1801	B12	C6B-C5B	3.44	1.49	1.40
5	D	1500	5AD	C5-N7	-3.42	1.32	1.39
5	B	1500	5AD	C5-N7	-3.41	1.32	1.39
5	A	1500	5AD	C6-N6	3.40	1.42	1.34
5	C	1500	5AD	C5-N7	-3.38	1.32	1.39
3	A	1801	B12	C6B-C5B	3.35	1.49	1.40
5	C	1500	5AD	C6-N6	3.31	1.42	1.34
5	B	1500	5AD	C6-N6	3.28	1.42	1.34
4	A	767	Z97	C3-C2	3.21	1.44	1.41
3	B	1801	B12	C6B-C5B	3.14	1.48	1.40
3	C	1801	B12	C11-N23	3.07	1.42	1.36
5	A	1500	5AD	C5-N7	-2.99	1.33	1.39
4	D	767	Z97	C4-C3	-2.97	1.36	1.41
3	D	1801	B12	C10-C9	2.95	1.47	1.39
5	D	1500	5AD	C6-N1	2.92	1.43	1.35
3	A	1801	B12	C10-C9	2.90	1.47	1.39
3	C	1801	B12	C8B-N1B	-2.88	1.33	1.39
5	B	1500	5AD	C6-N1	2.86	1.43	1.35
4	A	767	Z97	C4-C4A	2.79	1.52	1.46
5	C	1500	5AD	C6-N1	2.76	1.43	1.35
3	D	1801	B12	C8B-N1B	-2.71	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1801	B12	C9B-N3B	-2.71	1.34	1.39
5	A	1500	5AD	C6-N1	2.67	1.43	1.35
4	B	767	Z97	C4-C3	-2.65	1.36	1.41
3	C	1801	B12	C2B-N3B	2.59	1.36	1.31
3	C	1801	B12	C10-C9	2.59	1.46	1.39
4	D	767	Z97	OXT-C	2.57	1.38	1.30
5	B	1500	5AD	C5-C4	2.56	1.43	1.39
4	B	767	Z97	C4-C4A	2.54	1.52	1.46
4	C	767	Z97	OXT-C	2.53	1.38	1.30
4	A	767	Z97	OXT-C	2.52	1.38	1.30
3	A	1801	B12	C9B-N3B	-2.48	1.35	1.39
4	C	767	Z97	C4-C3	-2.46	1.37	1.41
3	D	1801	B12	C9B-N3B	-2.44	1.35	1.39
3	B	1801	B12	C8B-N1B	-2.44	1.34	1.39
3	B	1801	B12	C10-C9	2.42	1.46	1.39
4	C	767	Z97	C4-C4A	2.41	1.51	1.46
5	C	1500	5AD	C5-C4	2.41	1.43	1.39
5	A	1500	5AD	C5-C4	2.41	1.43	1.39
4	D	767	Z97	C4-C4A	2.37	1.51	1.46
3	D	1801	B12	C2B-N3B	2.35	1.36	1.31
3	B	1801	B12	C2B-N3B	2.30	1.36	1.31
5	D	1500	5AD	C5-C4	2.28	1.43	1.39
5	B	1500	5AD	O4'-C1'	2.25	1.47	1.42
4	B	767	Z97	OXT-C	2.24	1.37	1.30
5	D	1500	5AD	O4'-C1'	2.21	1.47	1.42
3	A	1801	B12	C2B-N3B	2.16	1.35	1.31
4	A	767	Z97	C2A-C2	2.16	1.53	1.50
3	C	1801	B12	C9B-N3B	-2.15	1.35	1.39
3	C	1801	B12	C1-C19	-2.11	1.50	1.55
5	D	1500	5AD	O2'-C2'	-2.10	1.37	1.43
5	B	1500	5AD	C4-N3	2.10	1.38	1.34
5	D	1500	5AD	C5-C6	-2.09	1.35	1.41
3	D	1801	B12	C14-C15	2.08	1.47	1.38
3	A	1801	B12	C8B-N1B	-2.08	1.35	1.39
5	C	1500	5AD	O4'-C1'	2.07	1.46	1.42
4	D	767	Z97	C3-C2	2.04	1.43	1.41
5	C	1500	5AD	C4-N9	-2.04	1.33	1.37
4	A	767	Z97	C4-C3	-2.00	1.37	1.41

All (235) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1500	5AD	C5'-C4'-C3'	12.46	128.78	115.70
5	C	1500	5AD	C5'-C4'-C3'	10.53	126.75	115.70
5	D	1500	5AD	C5'-C4'-C3'	10.12	126.33	115.70
5	A	1500	5AD	C5'-C4'-C3'	9.85	126.04	115.70
3	A	1801	B12	C1-C19-N24	9.49	116.81	106.25
5	A	1500	5AD	C2'-C1'-N9	9.45	136.78	113.30
3	C	1801	B12	C20-C1-C19	-9.34	100.35	109.35
5	B	1500	5AD	C2'-C1'-N9	9.05	135.78	113.30
5	D	1500	5AD	C2'-C1'-N9	9.00	135.67	113.30
3	D	1801	B12	C1-C19-N24	8.93	116.18	106.25
5	C	1500	5AD	C2'-C1'-N9	8.82	135.23	113.30
3	B	1801	B12	C1-C19-N24	8.65	115.87	106.25
3	B	1801	B12	C13-C12-C11	-8.53	91.44	100.97
3	C	1801	B12	C1-C19-N24	8.11	115.27	106.25
3	C	1801	B12	C46-C12-C13	-7.86	80.89	112.74
3	D	1801	B12	C46-C12-C13	-7.85	80.92	112.74
3	A	1801	B12	C13-C12-C11	-7.65	92.42	100.97
3	C	1801	B12	C47-C12-C46	7.61	122.01	109.41
3	D	1801	B12	C47-C12-C46	7.53	121.88	109.41
3	C	1801	B12	C13-C12-C11	-7.53	92.56	100.97
3	A	1801	B12	C46-C12-C13	-7.51	82.29	112.74
3	A	1801	B12	C47-C12-C46	7.36	121.60	109.41
3	B	1801	B12	C1-C19-C18	7.34	133.80	121.90
3	D	1801	B12	C13-C12-C11	-7.24	92.87	100.97
3	B	1801	B12	C47-C12-C46	6.83	120.72	109.41
3	D	1801	B12	C12-C11-N23	6.79	121.18	111.83
3	A	1801	B12	C12-C11-N23	6.68	121.03	111.83
3	B	1801	B12	C46-C12-C13	-6.65	85.80	112.74
5	B	1500	5AD	O3'-C3'-C4'	6.63	126.72	110.47
3	C	1801	B12	C1-C19-C18	6.61	132.62	121.90
3	D	1801	B12	C18-C19-N24	6.22	111.68	102.33
5	D	1500	5AD	O3'-C3'-C4'	6.16	125.56	110.47
3	D	1801	B12	C1-C19-C18	6.15	131.87	121.90
5	C	1500	5AD	O3'-C3'-C4'	6.08	125.37	110.47
3	B	1801	B12	C12-C11-N23	6.03	120.14	111.83
3	A	1801	B12	C1-C19-C18	6.03	131.68	121.90
5	A	1500	5AD	O3'-C3'-C4'	6.01	125.20	110.47
3	C	1801	B12	C26-C2-C1	6.00	119.27	110.00
5	D	1500	5AD	N3-C2-N1	-5.95	119.58	128.58
3	C	1801	B12	C18-C19-N24	5.93	111.24	102.33
3	A	1801	B12	C18-C19-N24	5.92	111.22	102.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1801	B12	C47-C12-C13	-5.84	89.06	112.74
3	D	1801	B12	C12-C11-C10	-5.82	115.89	123.40
3	B	1801	B12	C12-C11-C10	-5.75	115.98	123.40
5	B	1500	5AD	N3-C2-N1	-5.72	119.92	128.58
5	C	1500	5AD	N3-C2-N1	-5.68	119.99	128.58
3	B	1801	B12	C47-C12-C13	-5.68	89.74	112.74
3	A	1801	B12	C12-C11-C10	-5.44	116.39	123.40
5	A	1500	5AD	N3-C2-N1	-5.39	120.43	128.58
4	D	767	Z97	OP4-C5A-C5	5.38	119.43	109.36
3	C	1801	B12	C12-C11-N23	5.25	119.06	111.83
3	C	1801	B12	C12-C11-C10	-5.23	116.66	123.40
3	A	1801	B12	C20-C1-C19	-5.22	104.33	109.35
3	C	1801	B12	C55-C17-C16	-5.17	106.49	116.59
3	D	1801	B12	C47-C12-C13	-5.12	91.99	112.74
5	A	1500	5AD	O3'-C3'-C2'	5.08	128.09	111.82
3	B	1801	B12	C18-C19-N24	5.04	109.90	102.33
3	C	1801	B12	C47-C12-C13	-5.02	92.40	112.74
4	C	767	Z97	OP4-C5A-C5	5.02	118.76	109.36
5	B	1500	5AD	O2'-C2'-C3'	5.00	127.84	111.82
3	B	1801	B12	C55-C17-C16	-4.97	106.88	116.59
3	C	1801	B12	C30-C3-C2	-4.95	108.09	119.00
5	A	1500	5AD	O2'-C2'-C3'	4.95	127.68	111.82
5	D	1500	5AD	C5-C4-N3	-4.95	119.91	126.72
5	A	1500	5AD	O2'-C2'-C1'	4.93	127.07	110.10
5	B	1500	5AD	O2'-C2'-C1'	4.92	127.05	110.10
5	C	1500	5AD	O2'-C2'-C1'	4.86	126.86	110.10
5	B	1500	5AD	O3'-C3'-C2'	4.82	127.28	111.82
3	D	1801	B12	C19-C1-N21	4.82	107.10	102.14
3	D	1801	B12	C30-C3-C2	-4.79	108.43	119.00
5	A	1500	5AD	C5-C4-N3	-4.78	120.14	126.72
5	D	1500	5AD	O2'-C2'-C1'	4.67	126.18	110.10
3	D	1801	B12	C55-C17-C16	-4.66	107.47	116.59
5	C	1500	5AD	C5-C4-N3	-4.63	120.34	126.72
5	C	1500	5AD	O2'-C2'-C3'	4.58	126.49	111.82
5	B	1500	5AD	C5-C4-N3	-4.51	120.50	126.72
3	C	1801	B12	C8B-C9B-N3B	-4.47	105.17	110.00
5	D	1500	5AD	O2'-C2'-C3'	4.44	126.06	111.82
3	D	1801	B12	C20-C1-C19	-4.39	105.13	109.35
3	B	1801	B12	C19-C1-N21	4.32	106.59	102.14
3	B	1801	B12	C2P-C1P-N59	-4.27	106.64	112.92
4	D	767	Z97	CD-NE-C4A	-4.25	105.11	118.72
5	D	1500	5AD	O3'-C3'-C2'	4.24	125.40	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1500	5AD	N9-C8-N7	-4.21	107.96	113.94
5	D	1500	5AD	N9-C8-N7	-4.19	107.99	113.94
3	A	1801	B12	C19-C1-N21	4.17	106.43	102.14
5	B	1500	5AD	N9-C8-N7	-4.15	108.06	113.94
5	C	1500	5AD	N9-C8-N7	-4.13	108.08	113.94
3	C	1801	B12	C19-C1-N21	4.07	106.33	102.14
5	C	1500	5AD	O3'-C3'-C2'	4.07	124.85	111.82
3	C	1801	B12	C2-C1-C19	4.06	124.93	118.61
3	C	1801	B12	C2-C1-N21	4.04	107.40	101.78
3	A	1801	B12	C30-C3-C2	-4.00	110.18	119.00
4	A	767	Z97	OP4-C5A-C5	3.96	116.78	109.36
4	B	767	Z97	OP4-C5A-C5	3.93	116.72	109.36
4	A	767	Z97	CG-CD-NE	3.86	121.05	110.83
3	B	1801	B12	C20-C1-C19	-3.82	105.67	109.35
3	C	1801	B12	C13-C14-N23	3.82	114.27	109.09
3	D	1801	B12	C2-C1-N21	3.81	107.08	101.78
3	B	1801	B12	C2-C1-N21	3.72	106.94	101.78
3	C	1801	B12	C15-C14-N23	-3.72	121.78	126.26
3	A	1801	B12	C55-C17-C16	-3.71	109.34	116.59
3	D	1801	B12	C12-C13-C14	3.69	108.33	102.26
3	A	1801	B12	C26-C2-C1	3.67	115.67	110.00
5	C	1500	5AD	C2'-C3'-C4'	3.65	107.75	102.36
3	A	1801	B12	C8B-C9B-N3B	-3.58	106.13	110.00
3	B	1801	B12	C47-C12-C11	3.57	122.82	110.08
5	D	1500	5AD	C2-N3-C4	3.53	120.46	111.83
3	C	1801	B12	C9B-C8B-N1B	3.51	106.86	105.30
3	A	1801	B12	C13-C14-N23	3.51	113.85	109.09
3	D	1801	B12	C8B-C9B-N3B	-3.50	106.21	110.00
3	A	1801	B12	C2-C1-N21	3.50	106.64	101.78
3	B	1801	B12	C8B-C9B-N3B	-3.45	106.26	110.00
5	A	1500	5AD	C2-N3-C4	3.40	120.13	111.83
3	A	1801	B12	C12-C13-C14	3.36	107.78	102.26
5	C	1500	5AD	C2-N3-C4	3.34	119.98	111.83
3	C	1801	B12	C18-C60-C61	-3.32	105.61	114.04
5	D	1500	5AD	O4'-C1'-N9	3.31	114.45	108.09
3	B	1801	B12	C15-C14-N23	-3.31	122.27	126.26
5	B	1500	5AD	C2-N3-C4	3.27	119.81	111.83
3	C	1801	B12	C9B-N3B-C2B	3.25	108.39	104.40
3	D	1801	B12	C13-C14-N23	3.24	113.48	109.09
5	D	1500	5AD	N3-C4-N9	3.19	132.59	127.17
3	D	1801	B12	C25-C2-C1	-3.17	109.01	113.75
5	A	1500	5AD	O4'-C1'-N9	3.17	114.18	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1801	B12	C15-C14-N23	-3.13	122.49	126.26
3	C	1801	B12	C25-C2-C1	-3.12	109.09	113.75
4	D	767	Z97	CG-CD-NE	3.08	118.97	110.83
5	A	1500	5AD	C5-N7-C8	3.04	108.23	103.45
3	A	1801	B12	C7-C6-N22	3.02	113.44	107.94
3	D	1801	B12	C26-C2-C1	3.01	114.66	110.00
5	C	1500	5AD	O4'-C1'-N9	3.00	113.86	108.09
5	C	1500	5AD	C5-N7-C8	2.99	108.15	103.45
4	D	767	Z97	C3-C4-C5	2.99	120.67	118.28
3	D	1801	B12	C46-C12-C11	2.98	120.74	110.08
5	B	1500	5AD	C5-N7-C8	2.96	108.11	103.45
5	D	1500	5AD	C5-N7-C8	2.95	108.09	103.45
3	B	1801	B12	C12-C13-C14	2.95	107.11	102.26
3	B	1801	B12	C13-C14-N23	2.95	113.08	109.09
3	D	1801	B12	C18-C17-C16	2.94	104.24	100.69
5	B	1500	5AD	O4'-C4'-C5'	2.93	124.58	110.28
3	D	1801	B12	C7-C6-N22	2.93	113.27	107.94
3	A	1801	B12	C9B-N3B-C2B	2.93	108.00	104.40
5	B	1500	5AD	O4'-C1'-N9	2.93	113.71	108.09
3	B	1801	B12	C26-C2-C1	2.92	114.52	110.00
5	A	1500	5AD	O4'-C4'-C5'	2.90	124.42	110.28
5	D	1500	5AD	C2'-C3'-C4'	2.89	106.62	102.36
3	B	1801	B12	C20-C1-C2	-2.89	108.52	113.28
4	B	767	Z97	CD-NE-C4A	-2.87	109.52	118.72
5	C	1500	5AD	O4'-C4'-C5'	2.87	124.25	110.28
5	D	1500	5AD	C3'-C2'-C1'	2.85	106.85	101.46
3	B	1801	B12	C9-N22-C6	-2.84	101.86	105.28
5	D	1500	5AD	O4'-C4'-C5'	2.83	124.08	110.28
4	A	767	Z97	C5-C4-C4A	-2.83	117.11	121.47
4	A	767	Z97	CD-NE-C4A	-2.80	109.75	118.72
3	D	1801	B12	C9B-C8B-N1B	2.79	106.54	105.30
3	A	1801	B12	C7B-C8B-C9B	-2.77	119.15	122.47
4	B	767	Z97	OXT-C-O	-2.77	117.79	124.08
3	D	1801	B12	C15-C14-N23	-2.77	122.92	126.26
4	B	767	Z97	C5-C6-N1	-2.74	119.37	123.83
5	A	1500	5AD	N3-C4-N9	2.72	131.79	127.17
3	B	1801	B12	C30-C3-C2	-2.71	113.01	119.00
3	A	1801	B12	C46-C12-C11	2.71	119.76	110.08
5	B	1500	5AD	N3-C4-N9	2.69	131.75	127.17
3	C	1801	B12	C47-C12-C11	2.68	119.66	110.08
3	C	1801	B12	C8B-N1B-C2B	2.66	108.68	106.26
4	C	767	Z97	CD-NE-C4A	-2.66	110.20	118.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1500	5AD	N3-C4-N9	2.65	131.67	127.17
3	A	1801	B12	C3R-C2R-C1R	2.61	105.62	99.89
3	B	1801	B12	C9B-C8B-N1B	2.60	106.46	105.30
3	D	1801	B12	C20-C1-C2	-2.60	108.99	113.28
3	A	1801	B12	C16-C15-C14	-2.59	117.31	121.26
3	B	1801	B12	C9B-N3B-C2B	2.58	107.57	104.40
3	D	1801	B12	C9B-N3B-C2B	2.56	107.55	104.40
5	A	1500	5AD	C4-C5-N7	-2.56	107.66	110.58
5	C	1500	5AD	C4-C5-N7	-2.55	107.67	110.58
3	C	1801	B12	C7-C6-N22	2.55	112.58	107.94
4	A	767	Z97	OXT-C-O	-2.55	118.31	124.08
3	A	1801	B12	C20-C1-C2	-2.53	109.11	113.28
3	B	1801	B12	C2-C26-C27	-2.52	108.19	115.19
3	C	1801	B12	C30-C31-C32	-2.51	104.02	112.55
3	A	1801	B12	C9-C10-C11	-2.51	122.38	125.97
3	C	1801	B12	C20-C1-C2	-2.45	109.24	113.28
5	D	1500	5AD	C4-N9-C8	2.45	108.31	105.74
3	B	1801	B12	C9-C10-C11	-2.44	122.48	125.97
4	D	767	Z97	O3-C3-C2	2.41	122.58	117.58
3	A	1801	B12	C18-C17-C16	2.41	103.59	100.69
3	B	1801	B12	C7-C6-N22	2.39	112.29	107.94
3	A	1801	B12	C7-C6-C5	-2.38	124.35	128.07
3	B	1801	B12	C18-C17-C16	2.38	103.56	100.69
3	D	1801	B12	C30-C31-C32	-2.38	104.48	112.55
3	B	1801	B12	C3R-C2R-C1R	2.36	105.09	99.89
3	C	1801	B12	C4B-C9B-N3B	2.35	134.47	130.51
3	B	1801	B12	C1-C2-C3	2.33	104.53	101.60
5	B	1500	5AD	C4-C5-N7	-2.32	107.92	110.58
5	B	1500	5AD	C4-N9-C8	2.31	108.16	105.74
3	B	1801	B12	C25-C2-C1	-2.31	110.30	113.75
4	D	767	Z97	C5-C6-N1	-2.30	120.09	123.83
3	B	1801	B12	C7B-C8B-C9B	-2.30	119.72	122.47
4	C	767	Z97	OXT-C-O	-2.28	118.90	124.08
3	A	1801	B12	C47-C12-C11	2.28	118.23	110.08
3	A	1801	B12	C18-C60-C61	-2.28	108.25	114.04
3	C	1801	B12	C48-C13-C14	2.27	114.15	108.51
5	C	1500	5AD	C4-N9-C8	2.26	108.12	105.74
3	C	1801	B12	C46-C12-C11	2.26	118.16	110.08
3	A	1801	B12	C9B-C8B-N1B	2.25	106.30	105.30
4	C	767	Z97	CG-CD-NE	2.24	116.76	110.83
4	A	767	Z97	CB-CA-N	2.24	115.95	110.12
5	A	1500	5AD	C4-N9-C8	2.23	108.08	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	767	Z97	C3-C4-C4A	2.23	124.42	120.40
3	A	1801	B12	C25-C2-C1	-2.22	110.43	113.75
3	A	1801	B12	C1-C2-C3	2.21	104.38	101.60
3	D	1801	B12	C7-C6-C5	-2.20	124.63	128.07
4	A	767	Z97	OP2-P-OP4	2.20	112.40	106.67
3	C	1801	B12	C9-N22-C6	-2.20	102.63	105.28
5	C	1500	5AD	C3'-C2'-C1'	2.20	105.62	101.46
3	A	1801	B12	C30-C31-C32	-2.19	105.10	112.55
3	A	1801	B12	C54-C17-C18	-2.18	109.86	112.99
4	C	767	Z97	C3-C4-C5	2.17	120.02	118.28
3	A	1801	B12	C2P-C1P-N59	-2.17	109.73	112.92
3	C	1801	B12	C18-C17-C16	2.16	103.30	100.69
5	D	1500	5AD	C4-C5-N7	-2.16	108.11	110.58
3	C	1801	B12	N1B-C2B-N3B	-2.14	110.89	113.94
3	A	1801	B12	C2-C1-C19	2.14	121.94	118.61
3	C	1801	B12	C12-C13-C14	2.12	105.75	102.26
3	D	1801	B12	C2P-C1P-N59	-2.12	109.80	112.92
3	D	1801	B12	C9-N22-C6	-2.11	102.73	105.28
3	A	1801	B12	C53-C15-C16	2.08	123.89	120.36
5	A	1500	5AD	C5-C4-N9	2.07	108.07	105.81
3	C	1801	B12	C7-C6-C5	-2.06	124.85	128.07
3	D	1801	B12	C8B-N1B-C2B	2.06	108.13	106.26
3	C	1801	B12	C54-C17-C18	-2.05	110.05	112.99
3	B	1801	B12	C54-C17-C18	-2.05	110.05	112.99
3	B	1801	B12	C18-C60-C61	-2.03	108.89	114.04
3	A	1801	B12	C9-N22-C6	-2.01	102.86	105.28

All (14) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1801	B12	C19
3	B	1801	B12	C19
3	C	1801	B12	C19
3	D	1801	B12	C19
5	A	1500	5AD	C3'
5	A	1500	5AD	C2'
5	B	1500	5AD	C3'
5	B	1500	5AD	C2'
5	C	1500	5AD	C3'
5	C	1500	5AD	C4'
5	C	1500	5AD	C2'
5	D	1500	5AD	C3'

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Mol	Chain	Res	Type	Atom
5	D	1500	5AD	C4'
5	D	1500	5AD	C2'

All (119) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1801	B12	C14-C13-C48-C49
3	A	1801	B12	C16-C17-C55-C56
3	A	1801	B12	C54-C17-C55-C56
3	A	1801	B12	C18-C17-C55-C56
3	A	1801	B12	C56-C57-N59-C1P
3	A	1801	B12	C1P-C2P-O3-P
3	A	1801	B12	C3P-C2P-O3-P
3	B	1801	B12	C42-C41-C8-C9
3	B	1801	B12	C16-C17-C55-C56
3	B	1801	B12	C54-C17-C55-C56
3	B	1801	B12	C18-C17-C55-C56
3	C	1801	B12	C42-C41-C8-C9
3	C	1801	B12	C16-C17-C55-C56
3	C	1801	B12	C54-C17-C55-C56
3	C	1801	B12	C18-C17-C55-C56
3	D	1801	B12	C38-C37-C7-C6
3	D	1801	B12	C38-C37-C7-C8
3	D	1801	B12	C16-C17-C55-C56
3	D	1801	B12	C54-C17-C55-C56
3	D	1801	B12	C18-C17-C55-C56
4	A	767	Z97	C-CA-CB-CG
4	A	767	Z97	N-CA-CB-CG
4	A	767	Z97	CA-CB-CG-CD
4	A	767	Z97	C4-C4A-NE-CD
4	B	767	Z97	C5A-OP4-P-OP1
4	B	767	Z97	C5A-OP4-P-OP2
4	B	767	Z97	C5A-OP4-P-OP3
4	C	767	Z97	C5A-OP4-P-OP2
4	D	767	Z97	C-CA-CB-CG
3	A	1801	B12	O58-C57-N59-C1P
3	C	1801	B12	C42-C41-C8-C7
3	A	1801	B12	C4-C3-C30-C31
3	C	1801	B12	C7-C37-C38-N40
3	A	1801	B12	C42-C41-C8-C9
3	C	1801	B12	C2R-C1R-N1B-C2B
3	A	1801	B12	C12-C13-C48-C49

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Mol	Chain	Res	Type	Atoms
3	B	1801	B12	C42-C41-C8-C7
3	C	1801	B12	C4-C3-C30-C31
4	D	767	Z97	OXT-C-CA-N
4	C	767	Z97	NE-CD-CG-CB
3	B	1801	B12	C7-C37-C38-N40
3	C	1801	B12	C7-C37-C38-O39
3	C	1801	B12	C2R-C1R-N1B-C8B
4	B	767	Z97	NE-CD-CG-CB
4	D	767	Z97	NE-CD-CG-CB
3	A	1801	B12	C7-C37-C38-N40
3	B	1801	B12	C7-C37-C38-O39
4	A	767	Z97	CG-CD-NE-C4A
4	B	767	Z97	OXT-C-CA-N
3	D	1801	B12	C4-C3-C30-C31
3	A	1801	B12	C8-C41-C42-C43
4	C	767	Z97	C5A-OP4-P-OP1
4	D	767	Z97	C5A-OP4-P-OP1
3	D	1801	B12	C7-C37-C38-N40
3	A	1801	B12	C2R-C1R-N1B-C2B
3	B	1801	B12	C2R-C1R-N1B-C2B
3	A	1801	B12	C2R-C1R-N1B-C8B
3	B	1801	B12	C2R-C1R-N1B-C8B
3	A	1801	B12	C13-C48-C49-C50
4	A	767	Z97	O-C-CA-CB
3	D	1801	B12	O58-C57-N59-C1P
4	C	767	Z97	CA-CB-CG-CD
3	A	1801	B12	C7-C37-C38-O39
3	D	1801	B12	C7-C37-C38-O39
4	D	767	Z97	O-C-CA-N
3	B	1801	B12	C41-C42-C43-O44
3	B	1801	B12	C41-C42-C43-N45
4	C	767	Z97	OXT-C-CA-N
3	B	1801	B12	O6R-C4R-C5R-O8R
3	D	1801	B12	C18-C60-C61-N62
4	C	767	Z97	C5A-OP4-P-OP3
3	C	1801	B12	O6R-C1R-N1B-C8B
3	D	1801	B12	C2R-C1R-N1B-C2B
3	D	1801	B12	C56-C57-N59-C1P
4	B	767	Z97	N-CA-CB-CG
3	B	1801	B12	O58-C57-N59-C1P
3	D	1801	B12	C18-C60-C61-O63
3	B	1801	B12	C2-C26-C27-N29

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Mol	Chain	Res	Type	Atoms
3	A	1801	B12	C17-C18-C60-C61
3	A	1801	B12	O6R-C1R-N1B-C8B
3	B	1801	B12	O6R-C1R-N1B-C8B
3	D	1801	B12	C2R-C1R-N1B-C8B
3	D	1801	B12	O6R-C1R-N1B-C8B
3	D	1801	B12	C1P-C2P-O3-P
4	D	767	Z97	O-C-CA-CB
4	C	767	Z97	C3-C4-C4A-NE
3	A	1801	B12	C30-C31-C32-N33
3	A	1801	B12	C2-C3-C30-C31
4	B	767	Z97	CG-CD-NE-C4A
3	B	1801	B12	C2-C26-C27-O28
4	C	767	Z97	O-C-CA-N
3	A	1801	B12	C19-C18-C60-C61
3	A	1801	B12	C30-C31-C32-O34
3	B	1801	B12	C56-C57-N59-C1P
4	C	767	Z97	OXT-C-CA-CB
3	D	1801	B12	O6R-C1R-N1B-C2B
4	C	767	Z97	O-C-CA-CB
3	A	1801	B12	C3-C2-C26-C27
3	B	1801	B12	C3-C2-C26-C27
4	D	767	Z97	C5A-OP4-P-OP2
5	A	1500	5AD	O4'-C1'-N9-C8
4	B	767	Z97	O-C-CA-CB
3	D	1801	B12	C17-C18-C60-C61
4	B	767	Z97	OXT-C-CA-CB
3	A	1801	B12	O6R-C1R-N1B-C2B
5	D	1500	5AD	O4'-C1'-N9-C8
3	C	1801	B12	C2P-O3-P-O5
3	D	1801	B12	N59-C1P-C2P-O3
3	D	1801	B12	C2P-O3-P-O5
4	A	767	Z97	OXT-C-CA-CB
4	D	767	Z97	OXT-C-CA-CB
3	A	1801	B12	C41-C42-C43-N45
3	B	1801	B12	O6R-C1R-N1B-C2B
3	C	1801	B12	O6R-C1R-N1B-C2B
4	B	767	Z97	CA-CB-CG-CD
4	D	767	Z97	CA-CB-CG-CD
3	B	1801	B12	C19-C18-C60-C61
3	D	1801	B12	C19-C18-C60-C61
4	B	767	Z97	O-C-CA-N

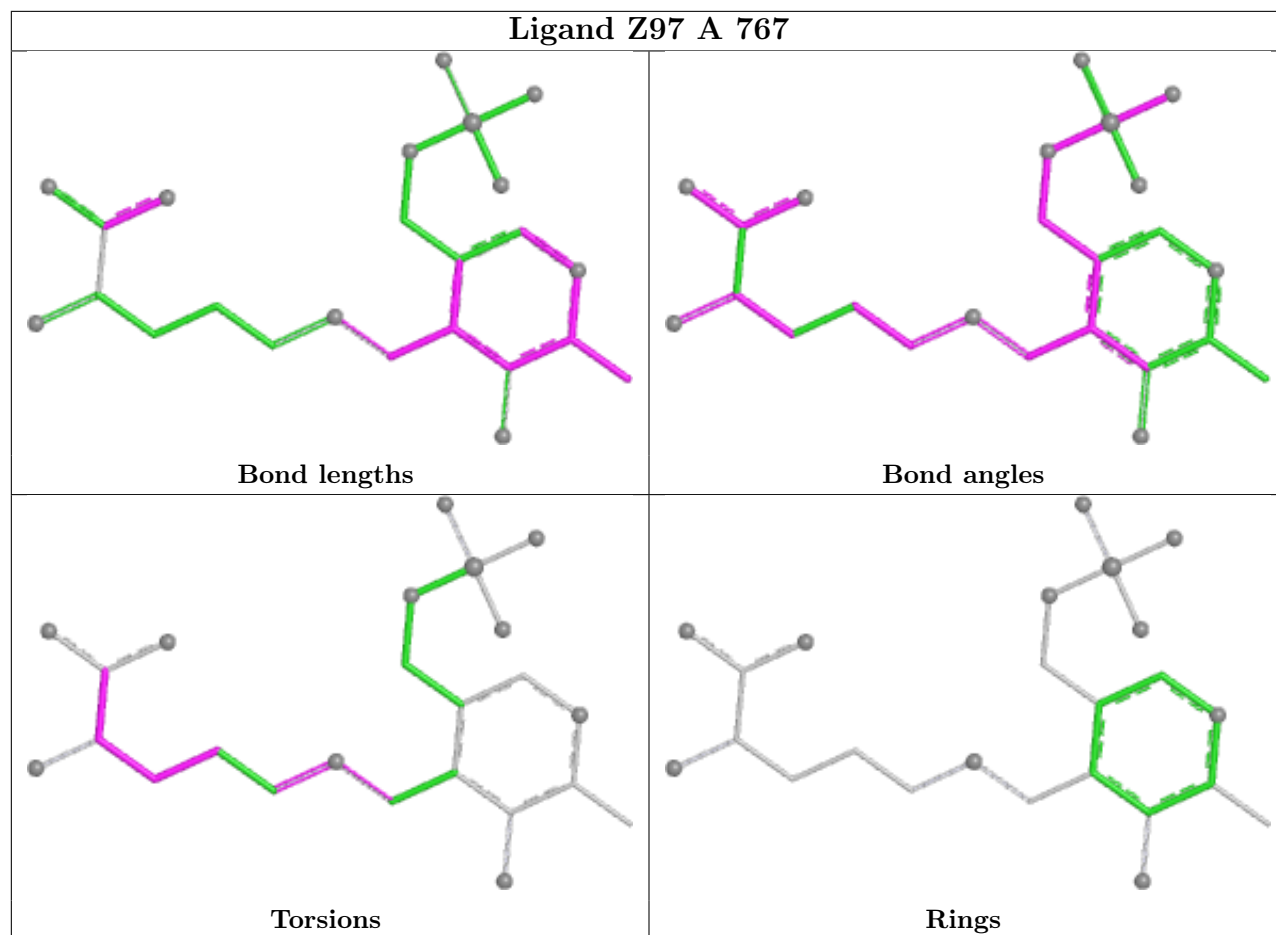
There are no ring outliers.

10 monomers are involved in 114 short contacts:

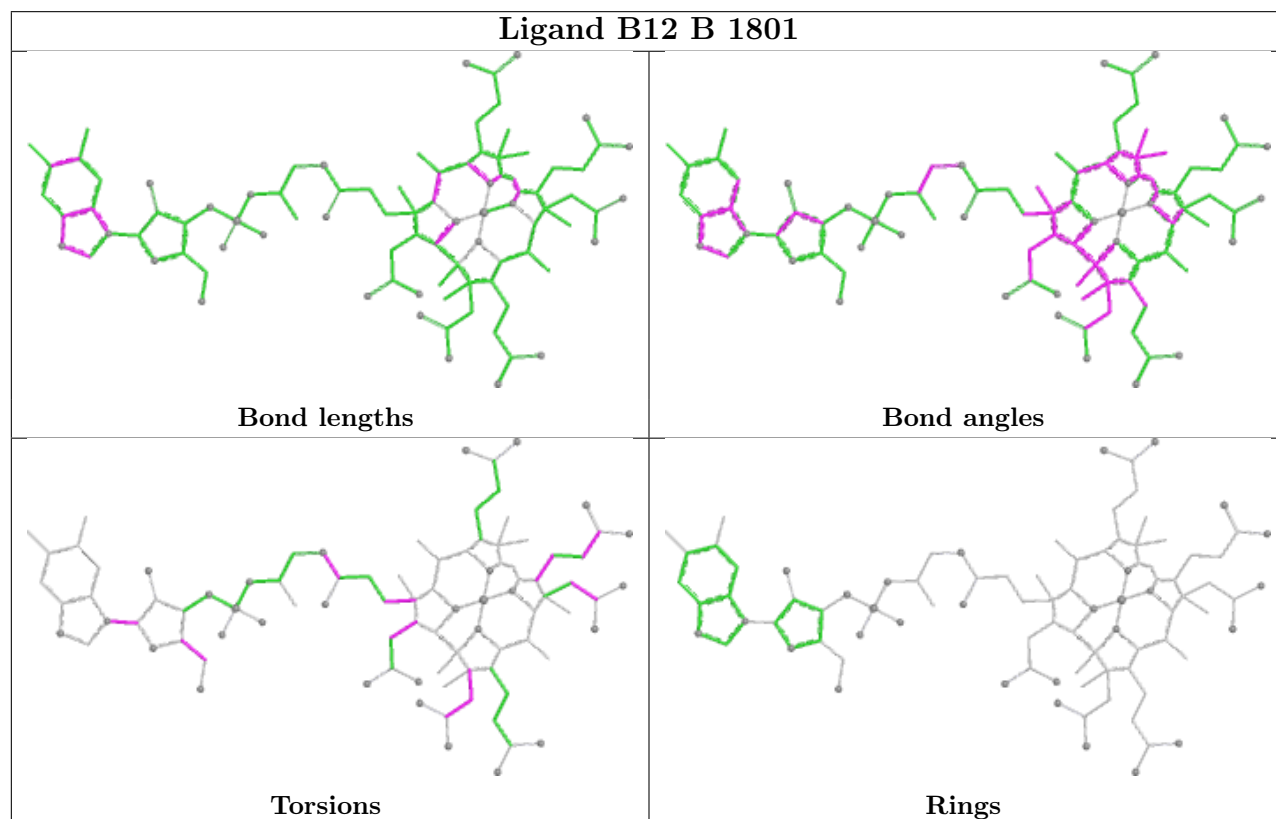
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1801	B12	25	0
3	C	1801	B12	26	0
4	C	767	Z97	2	0
3	A	1801	B12	22	0
5	B	1500	5AD	4	0
3	D	1801	B12	33	0
5	D	1500	5AD	4	0
4	B	767	Z97	4	0
4	D	767	Z97	2	0
5	A	1500	5AD	3	0

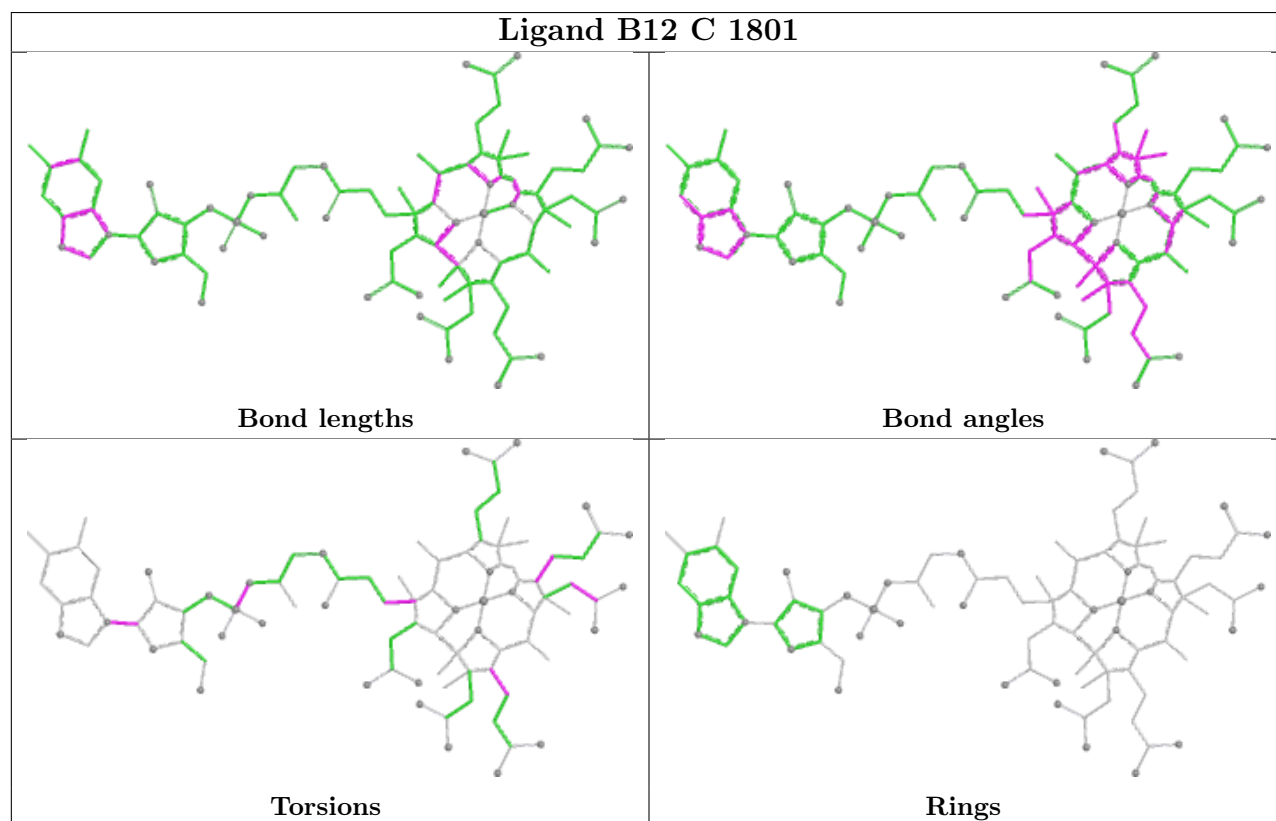
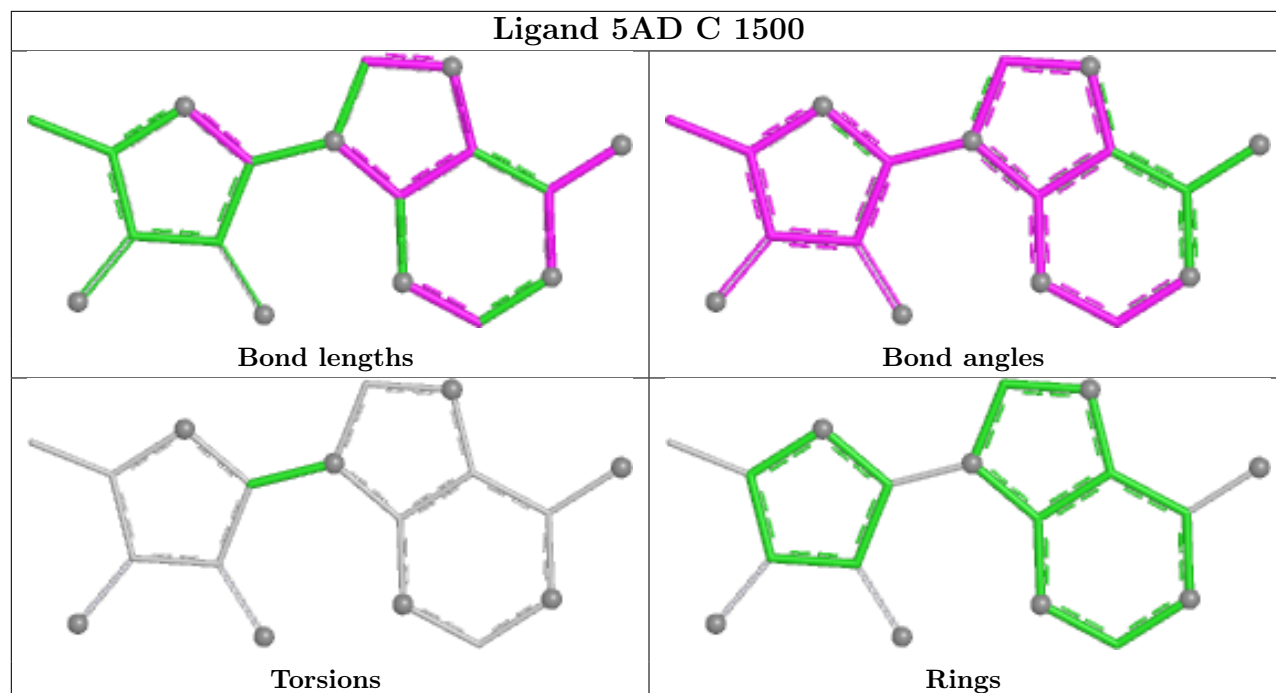
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 Z97 A 767

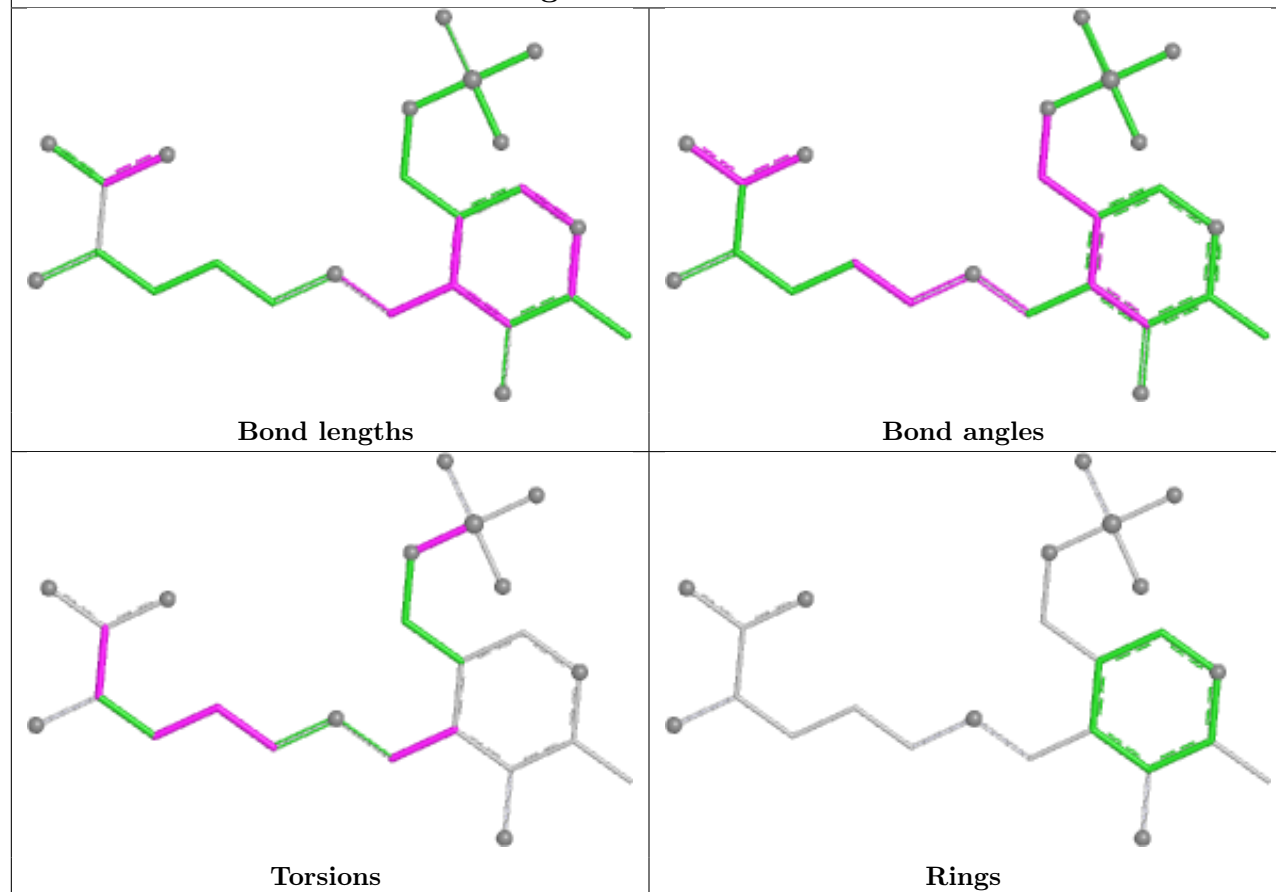


Ligand B12 B 1801

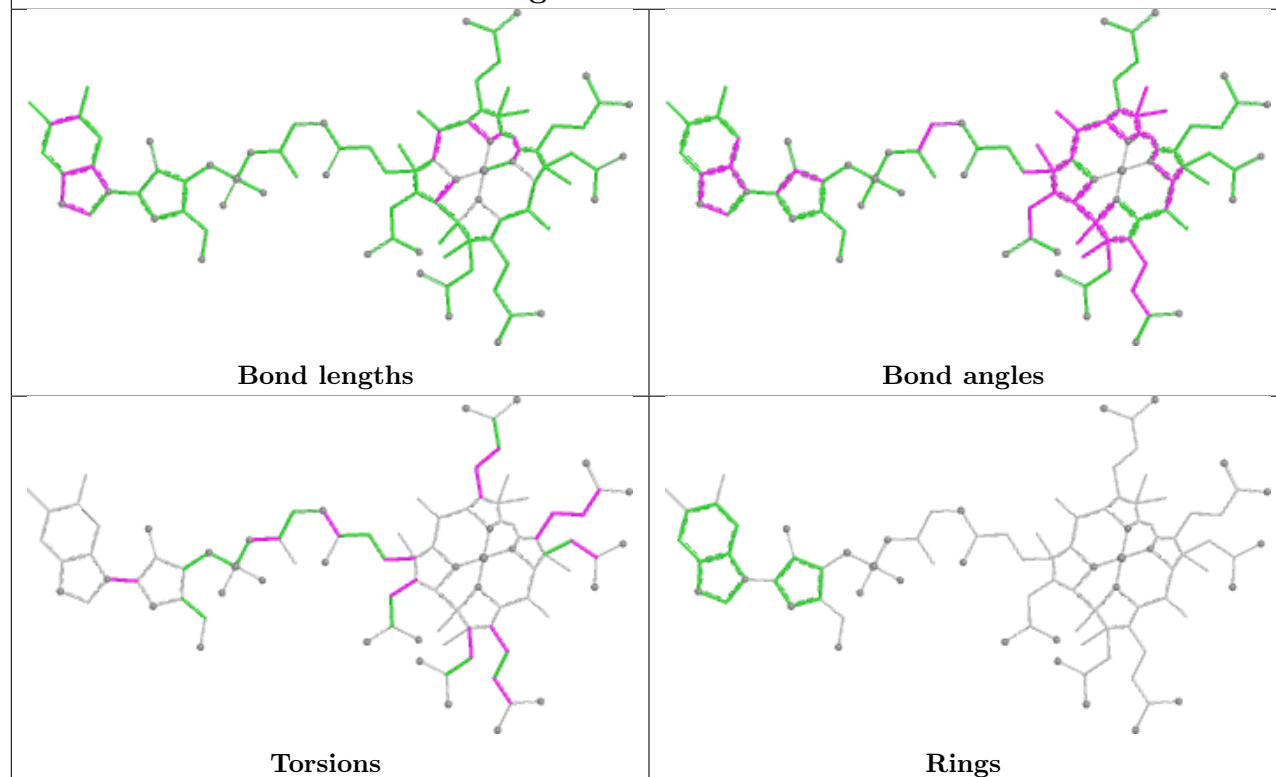


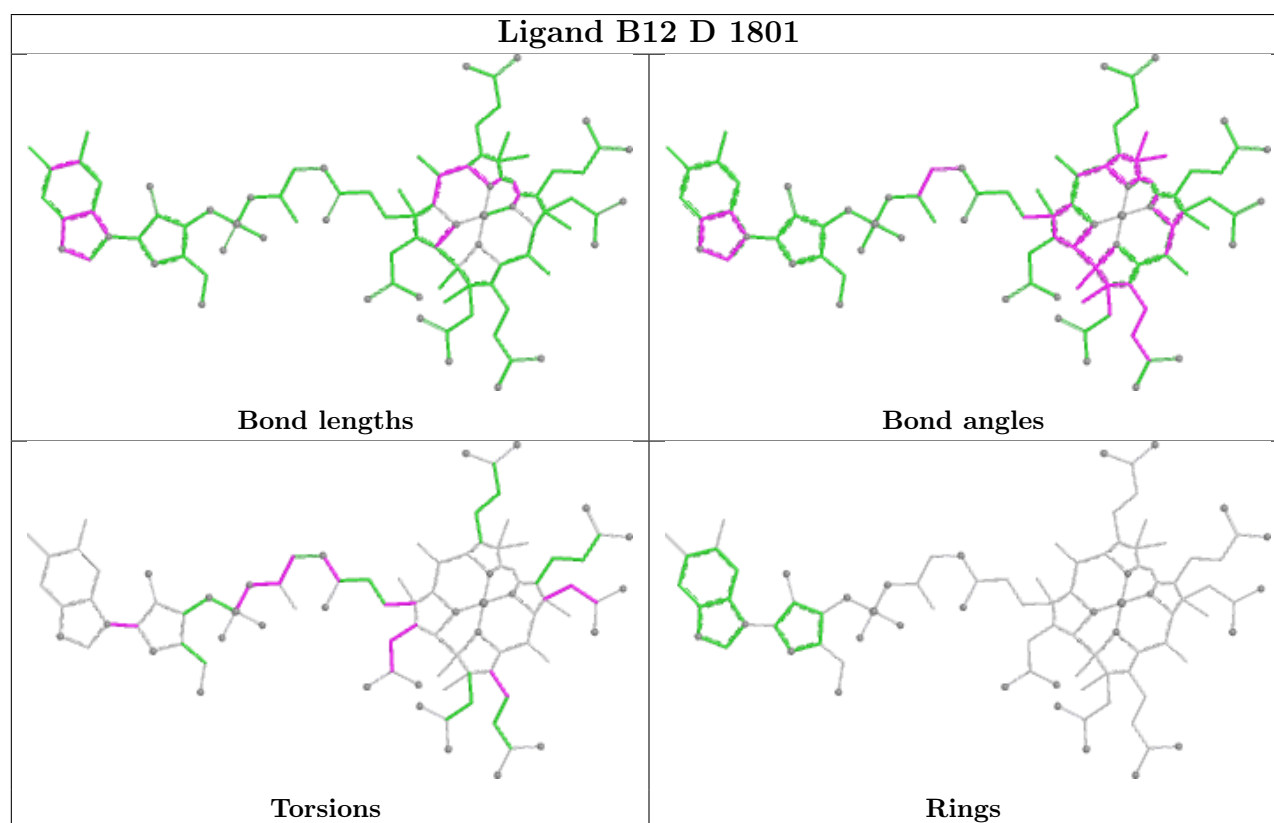
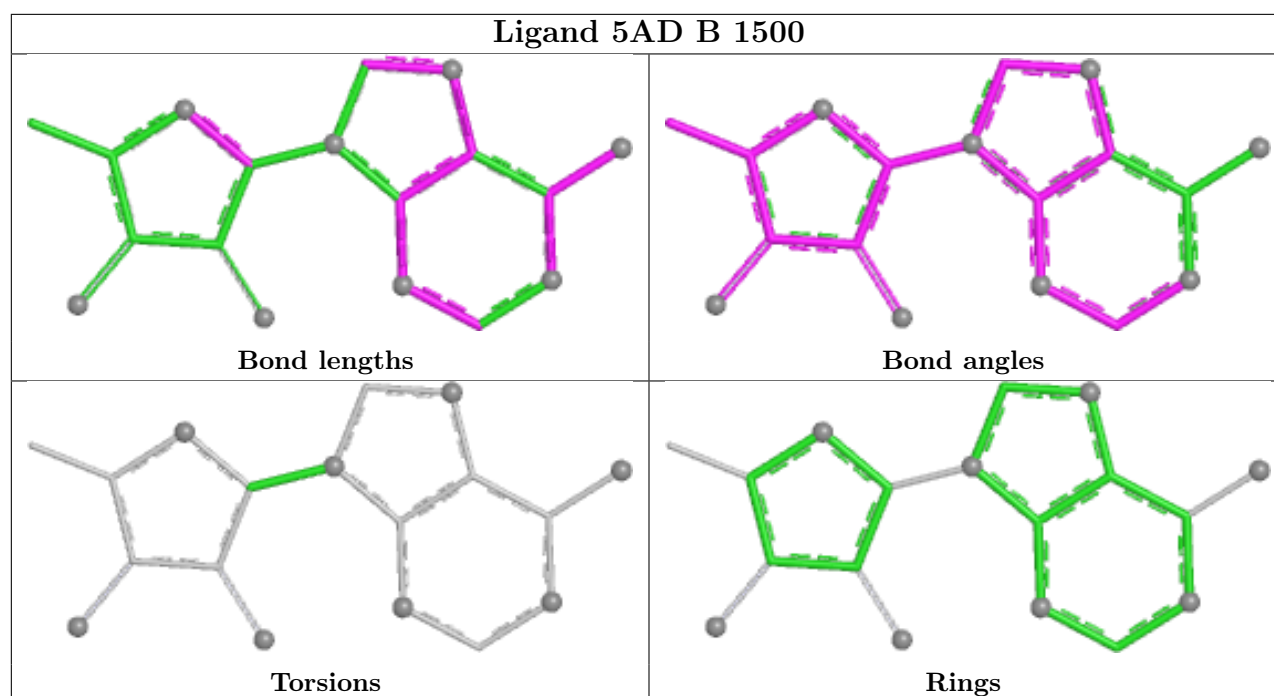


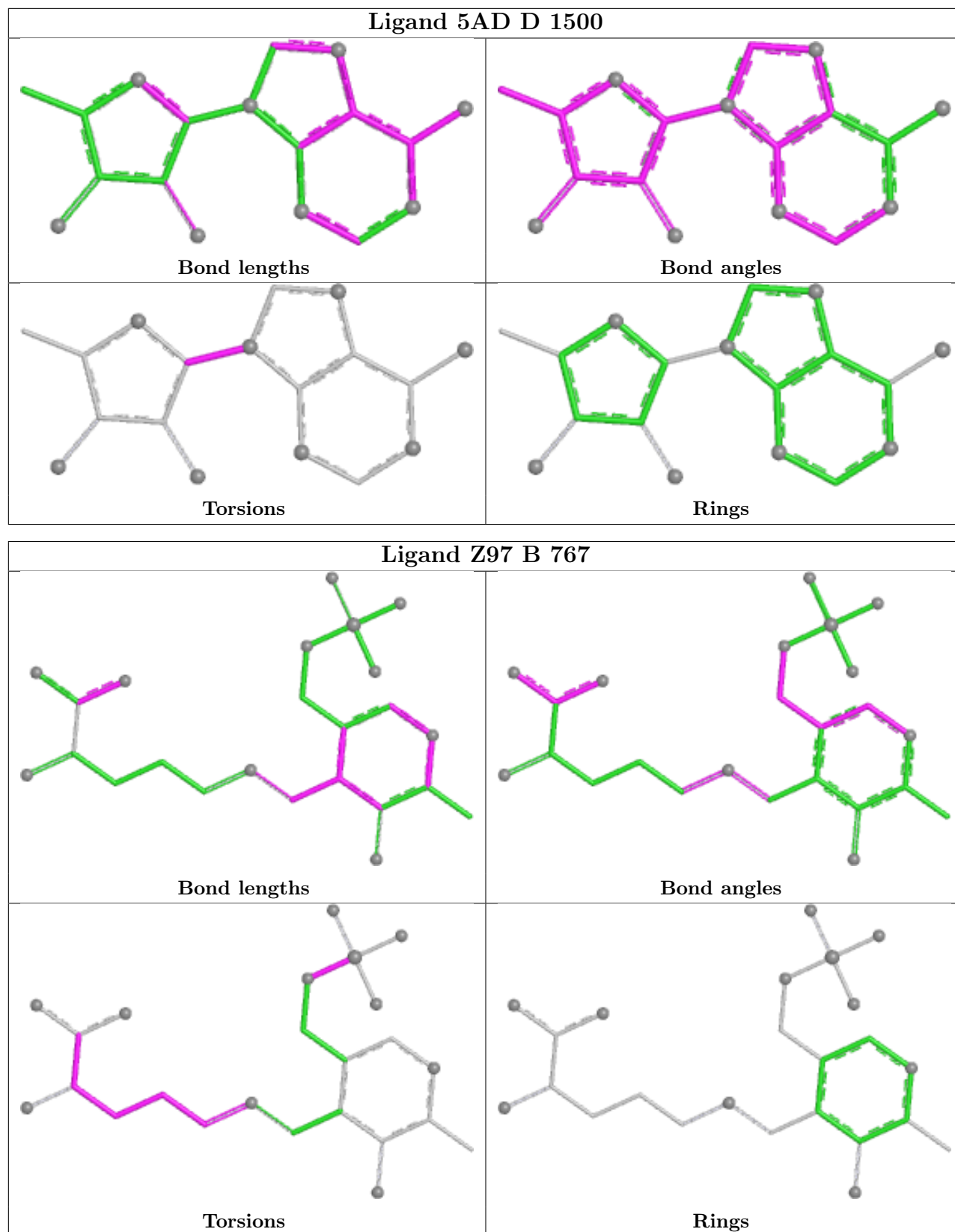
Ligand Z97 C 767



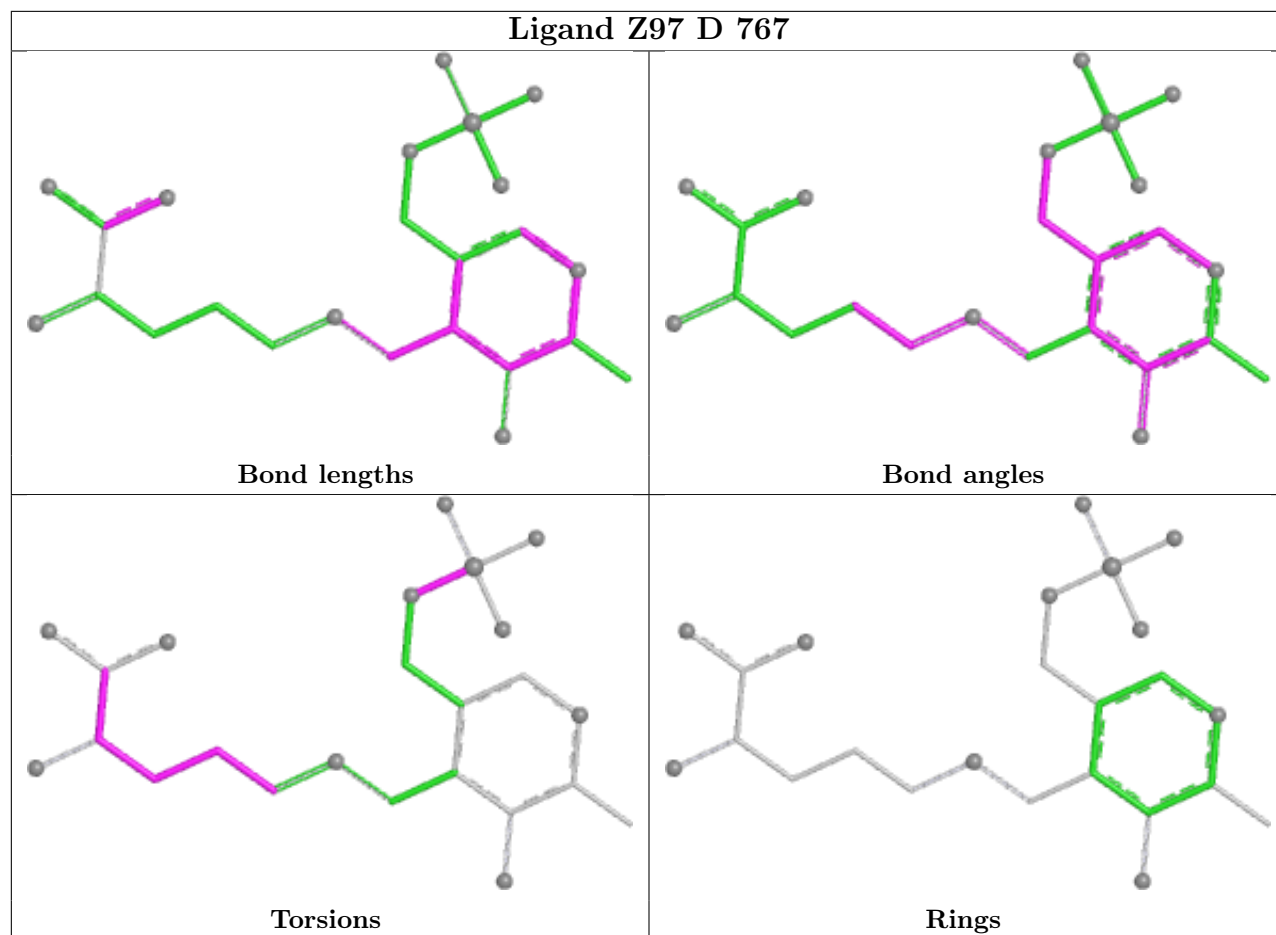
Ligand B12 A 1801



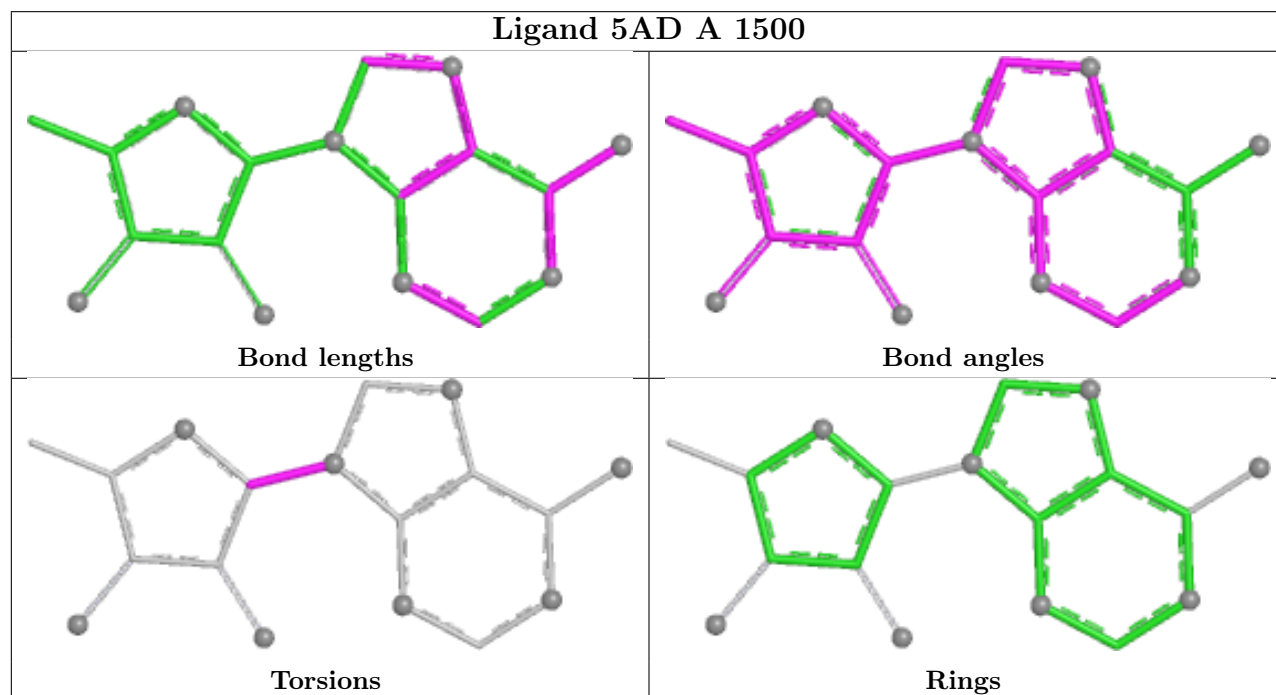




Ligand Z97 D 767



Ligand 5AD A 1500



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	A	728/763 (95%)	-0.28	12 (1%) 70 61	16, 34, 103, 118	0
1	B	728/763 (95%)	-0.45	2 (0%) 90 86	15, 33, 66, 95	0
1	C	728/763 (95%)	-0.46	2 (0%) 90 86	19, 38, 61, 83	0
1	D	728/763 (95%)	-0.38	12 (1%) 70 61	17, 32, 89, 104	0
2	E	110/121 (90%)	-0.44	1 (0%) 81 74	25, 40, 62, 73	0
2	F	110/121 (90%)	-0.42	1 (0%) 81 74	26, 38, 53, 72	0
2	G	110/121 (90%)	-0.28	2 (1%) 67 58	32, 45, 69, 80	0
2	H	110/121 (90%)	-0.40	0 100 100	25, 38, 57, 86	0
All	All	3352/3536 (94%)	-0.39	32 (0%) 79 72	15, 36, 83, 118	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	5	ASP	3.6
1	A	591	ILE	3.3
1	A	5	LEU	3.2
1	C	5	LEU	3.1
1	D	5	LEU	2.8
1	C	587	PRO	2.8
1	D	667	SER	2.6
1	A	649	VAL	2.6
1	D	668	THR	2.6
1	B	5	LEU	2.5
1	D	591	ILE	2.5
1	A	668	THR	2.4
1	D	672	HIS	2.4
1	D	691	GLY	2.4
1	D	717	ALA	2.4
1	A	509	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	6	GLN	2.4
1	A	594	GLU	2.2
1	A	657	ILE	2.2
1	A	683	ILE	2.2
1	A	692	ILE	2.2
1	D	594	GLU	2.2
1	D	738	GLU	2.2
2	E	5	ASP	2.2
1	A	661	ALA	2.2
2	G	5	ASP	2.1
1	D	711	VAL	2.1
1	D	699	GLY	2.1
1	A	672	HIS	2.1
1	D	710	ALA	2.1
1	A	429	ASN	2.0
2	G	20	GLU	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.

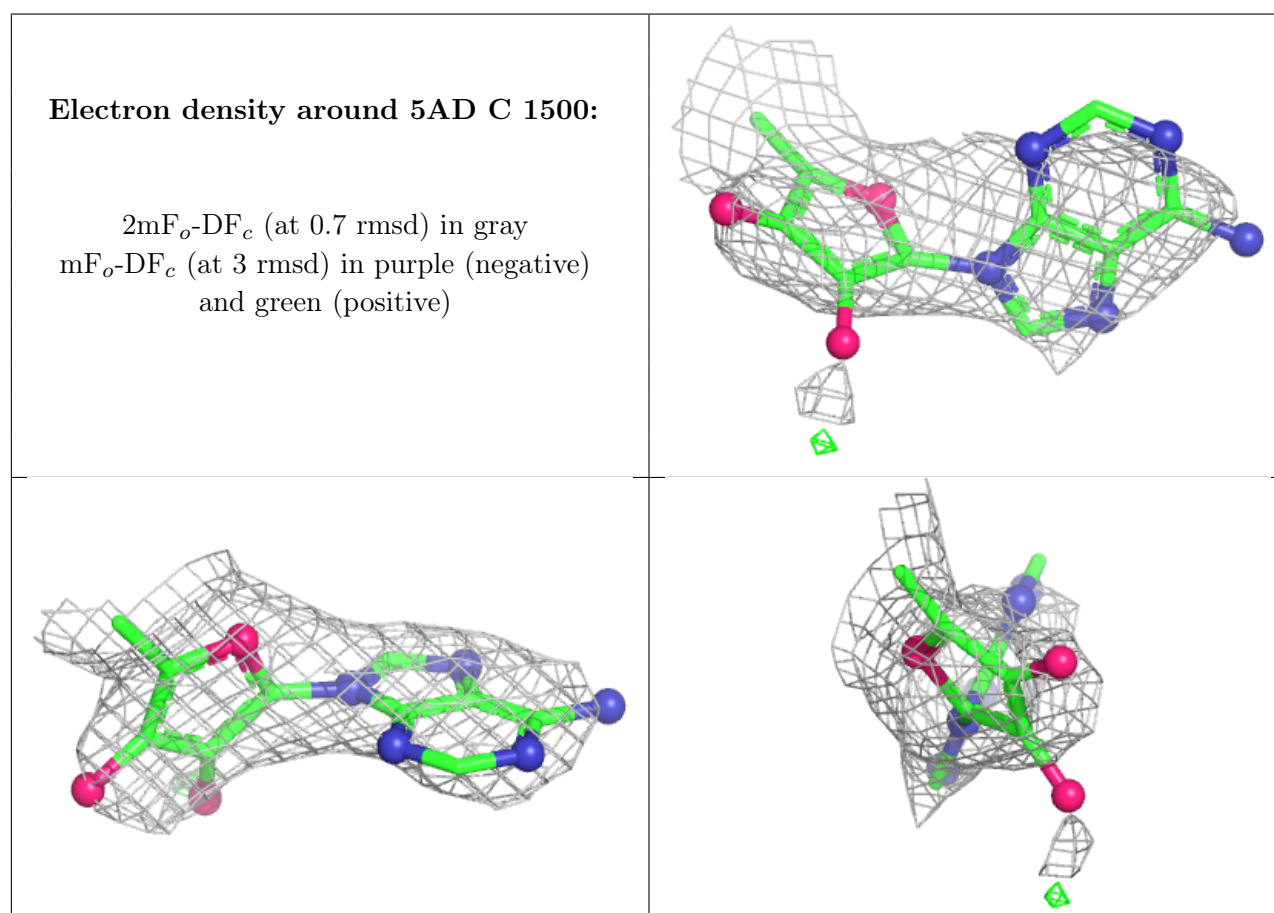
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	5AD	C	1500	18/18	0.81	0.13	78,87,94,97	0
5	5AD	B	1500	18/18	0.83	0.13	64,76,83,84	0
5	5AD	D	1500	18/18	0.87	0.11	48,60,65,66	0
3	B12	A	1801	91/91	0.89	0.12	57,87,98,99	0
5	5AD	A	1500	18/18	0.91	0.10	37,46,54,55	0
3	B12	D	1801	91/91	0.91	0.11	40,73,84,86	0
3	B12	B	1801	91/91	0.94	0.10	35,55,67,70	0

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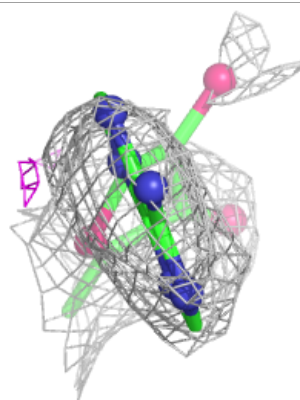
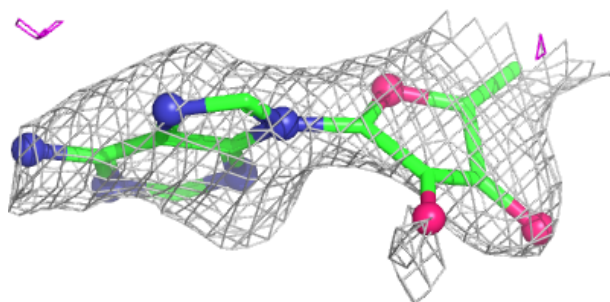
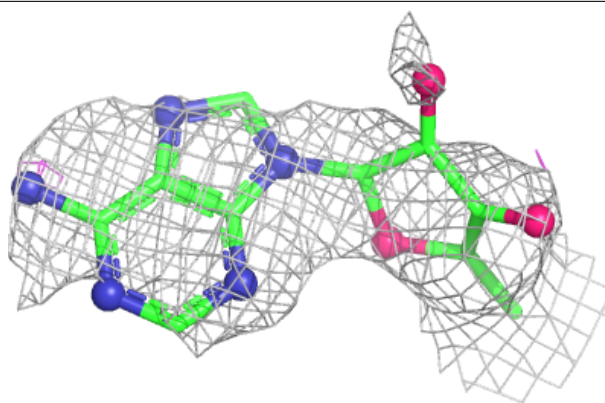
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	Z97	B	767	24/24	0.95	0.08	22,32,46,50	0
4	Z97	C	767	24/24	0.96	0.07	35,40,50,56	0
4	Z97	D	767	24/24	0.96	0.07	25,36,41,44	0
4	Z97	A	767	24/24	0.96	0.08	22,29,36,38	0
3	B12	C	1801	91/91	0.97	0.08	20,34,46,51	0

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.

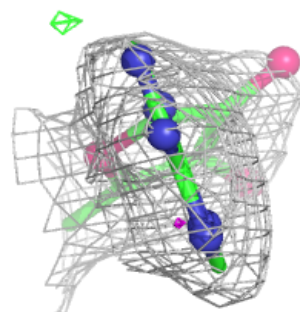
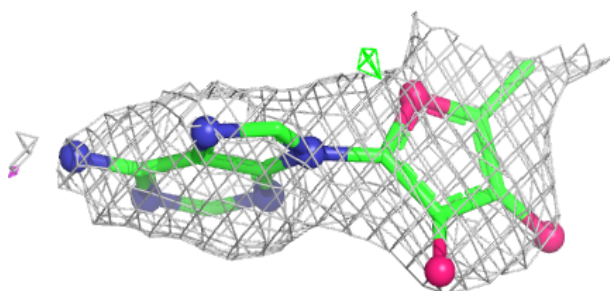
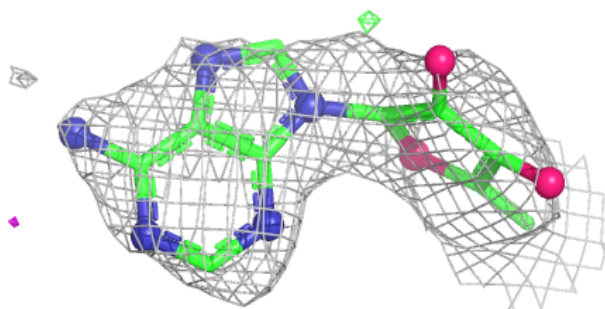


Electron density around 5AD B 1500:

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

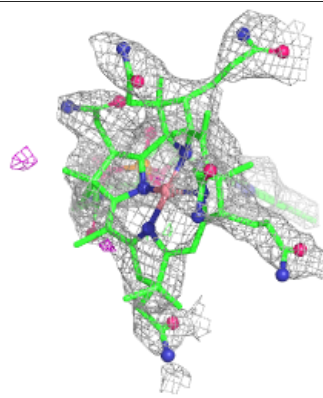
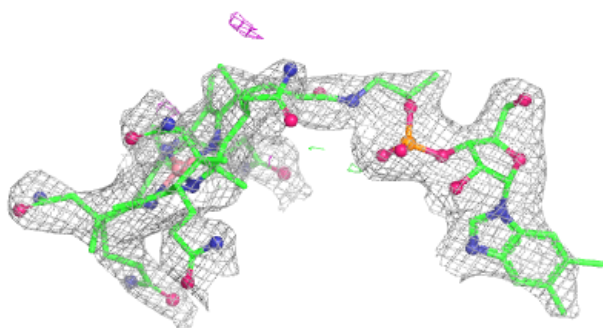
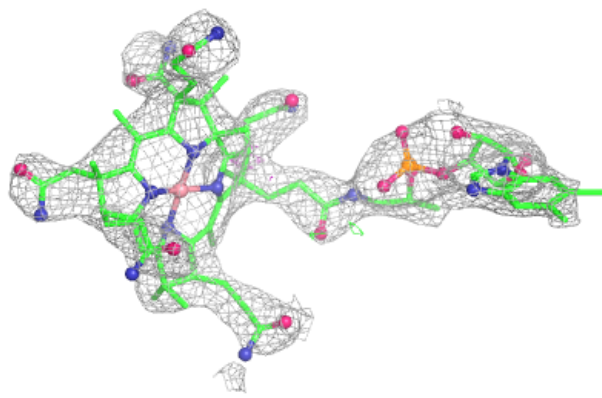
**Electron density around 5AD D 1500:**

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

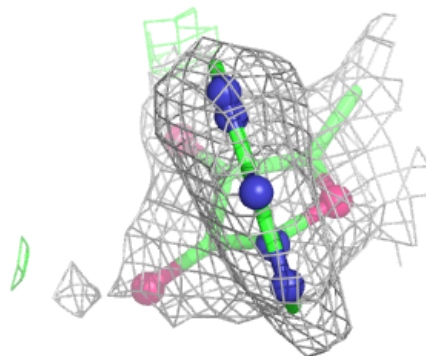
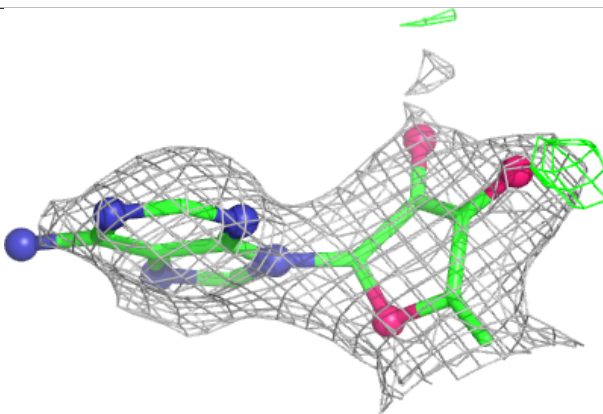
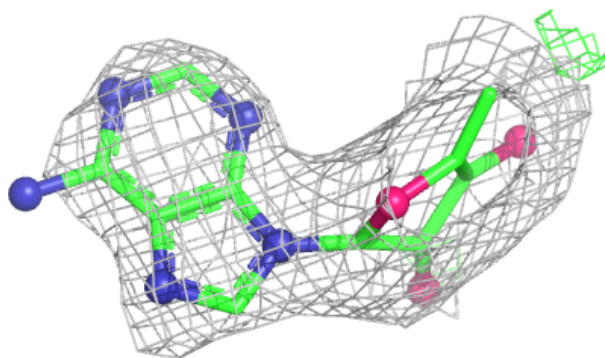


Electron density around B12 A 1801:

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

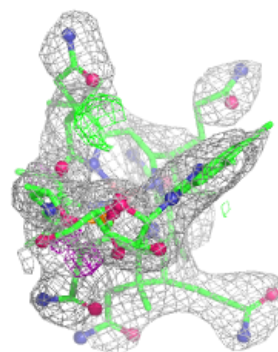
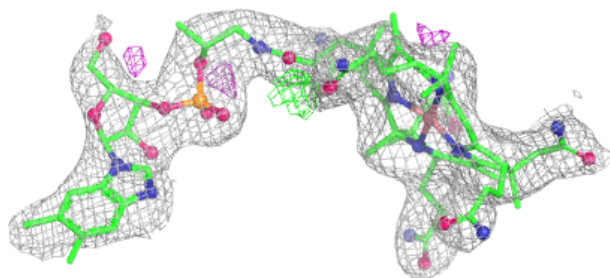
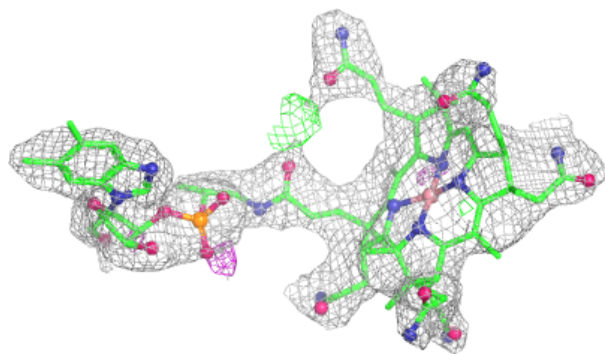
**Electron density around 5AD A 1500:**

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

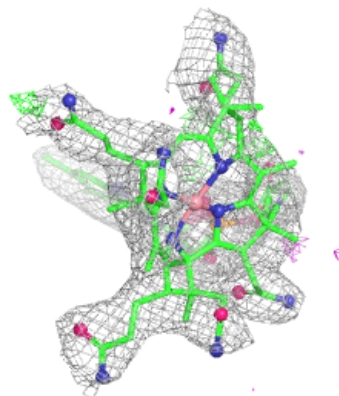
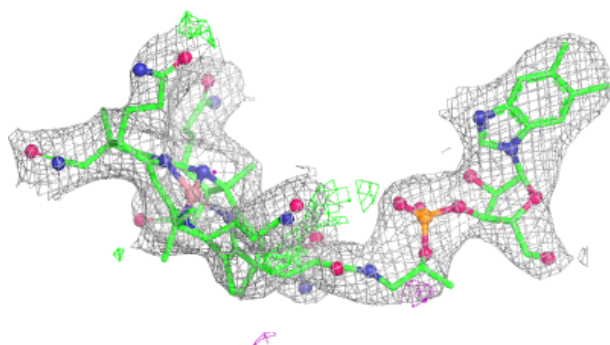
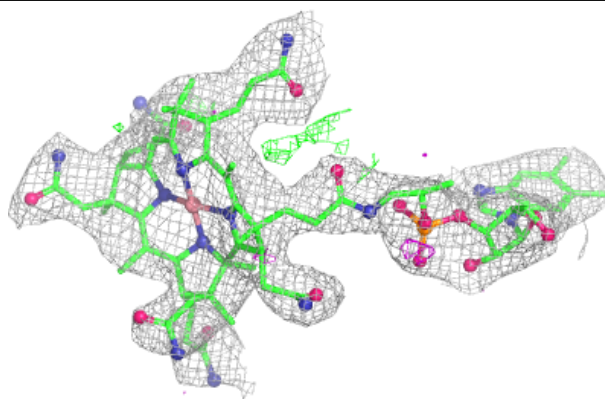


Electron density around B12 D 1801:

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

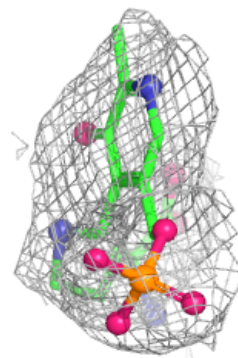
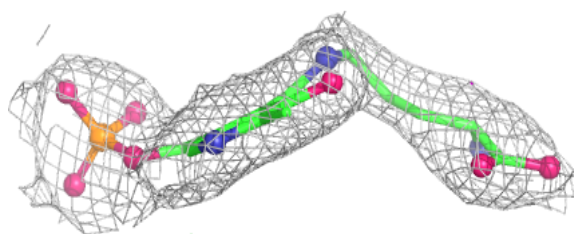
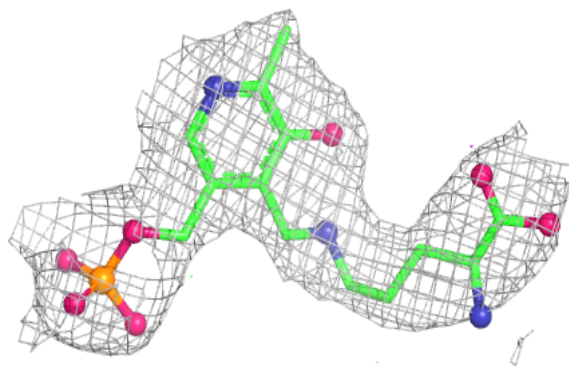
**Electron density around B12 B 1801:**

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

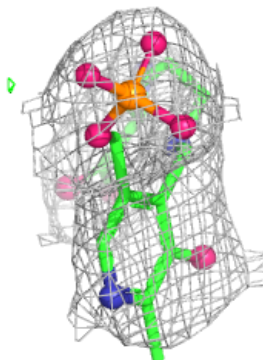
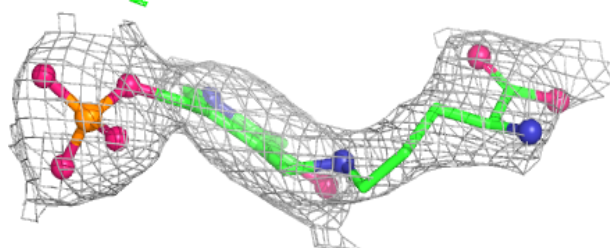


Electron density around Z97 B 767:

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

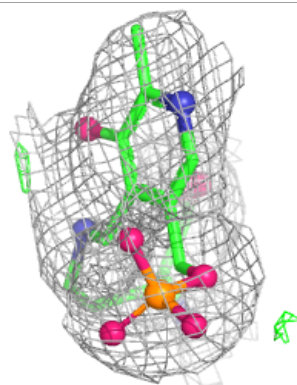
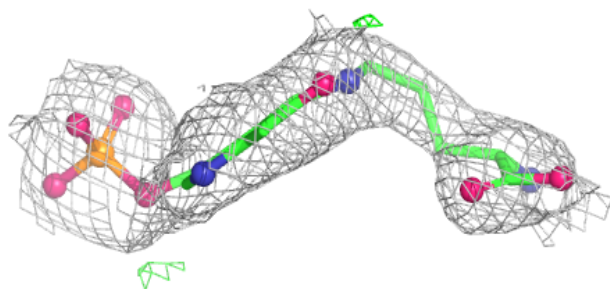
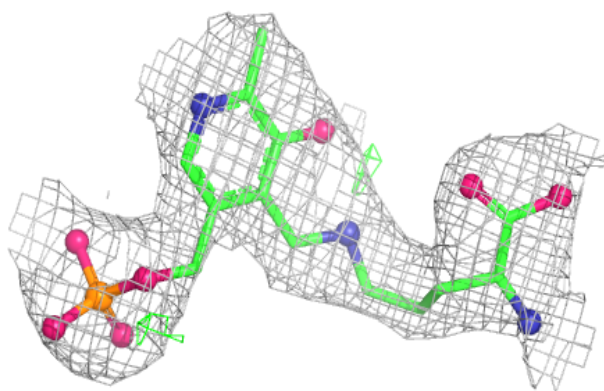
**Electron density around Z97 C 767:**

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

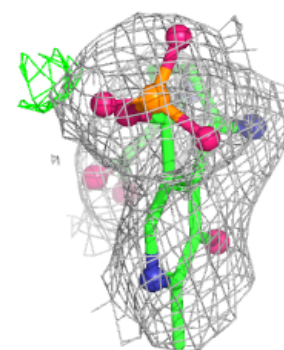
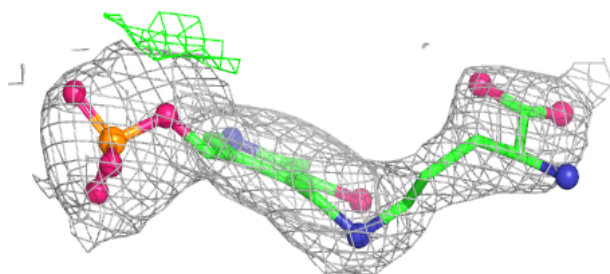
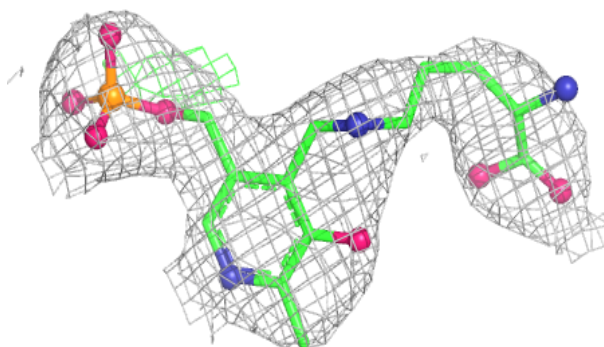


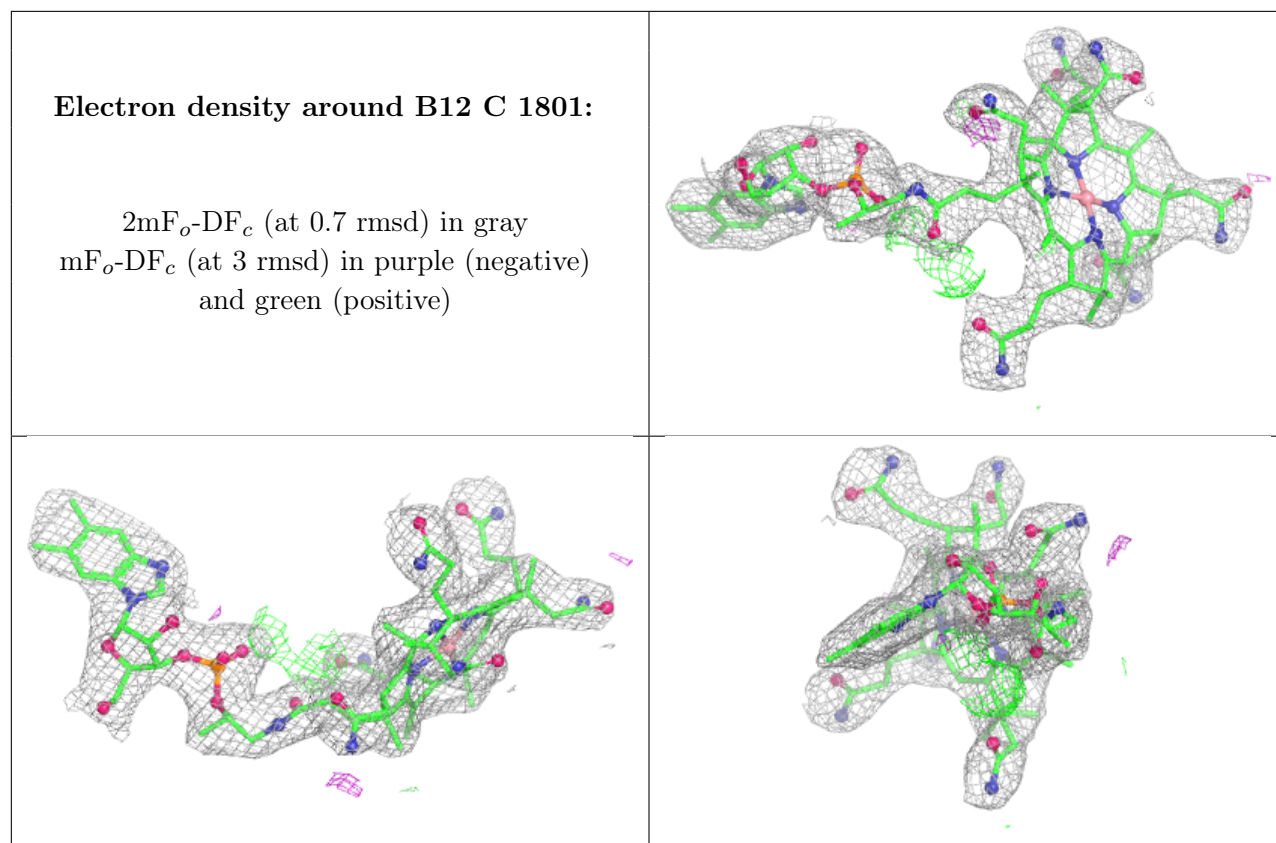
Electron density around Z97 D 767:

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

**Electron density around Z97 A 767:**

$2mF_o-DF_c$ (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.