



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:30 PM UTC

PDB ID : 4XYK / pdb_00004xyk
Title : Crystal structure of human phosphofructokinase-1 in complex with ADP, Northeast Structural Genomics Consortium Target HR9275
Authors : Forouhar, F.; Webb, B.A.; Szu, F.-E.; Seetharaman, J.; Barber, D.L.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2015-02-02
Resolution : 3.40 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

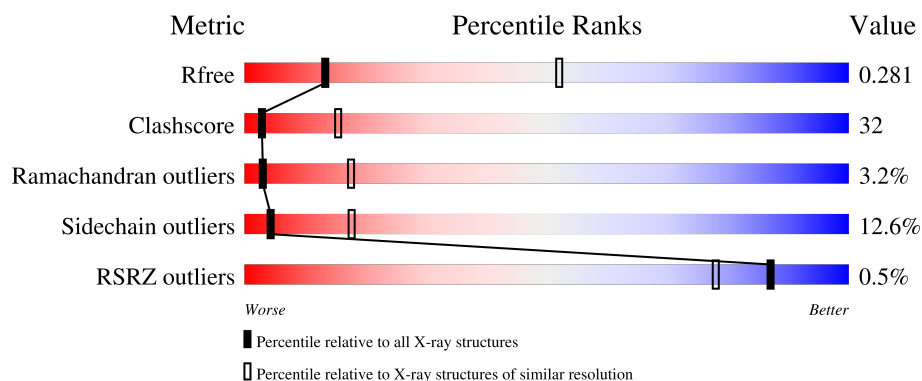
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	812	
1	B	812	
1	C	812	
1	D	812	

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	PO4	A	803	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22897 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 ATP-dependent 6-phosphofructokinase, platelet type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	737	Total	C	N	O	S	0	0	0
			5640	3542	1000	1059	39			
1	B	749	Total	C	N	O	S	0	0	0
			5727	3595	1019	1074	39			
1	C	743	Total	C	N	O	S	0	0	0
			5681	3566	1008	1068	39			
1	D	743	Total	C	N	O	S	0	0	0
			5681	3566	1008	1068	39			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP Q01813
A	-26	SER	-	expression tag	UNP Q01813
A	-25	TYR	-	expression tag	UNP Q01813
A	-24	TYR	-	expression tag	UNP Q01813
A	-23	HIS	-	expression tag	UNP Q01813
A	-22	HIS	-	expression tag	UNP Q01813
A	-21	HIS	-	expression tag	UNP Q01813
A	-20	HIS	-	expression tag	UNP Q01813
A	-19	HIS	-	expression tag	UNP Q01813
A	-18	HIS	-	expression tag	UNP Q01813
A	-17	ASP	-	expression tag	UNP Q01813
A	-16	TYR	-	expression tag	UNP Q01813
A	-15	ASP	-	expression tag	UNP Q01813
A	-14	ILE	-	expression tag	UNP Q01813
A	-13	PRO	-	expression tag	UNP Q01813
A	-12	THR	-	expression tag	UNP Q01813
A	-11	THR	-	expression tag	UNP Q01813
A	-10	GLU	-	expression tag	UNP Q01813
A	-9	ASN	-	expression tag	UNP Q01813
A	-8	LEU	-	expression tag	UNP Q01813
A	-7	TYR	-	expression tag	UNP Q01813

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	PHE	-	expression tag	UNP Q01813
A	-5	GLN	-	expression tag	UNP Q01813
A	-4	GLY	-	expression tag	UNP Q01813
A	-3	ALA	-	expression tag	UNP Q01813
A	-2	MET	-	expression tag	UNP Q01813
A	-1	ASP	-	expression tag	UNP Q01813
A	0	PRO	-	expression tag	UNP Q01813
B	-27	MET	-	initiating methionine	UNP Q01813
B	-26	SER	-	expression tag	UNP Q01813
B	-25	TYR	-	expression tag	UNP Q01813
B	-24	TYR	-	expression tag	UNP Q01813
B	-23	HIS	-	expression tag	UNP Q01813
B	-22	HIS	-	expression tag	UNP Q01813
B	-21	HIS	-	expression tag	UNP Q01813
B	-20	HIS	-	expression tag	UNP Q01813
B	-19	HIS	-	expression tag	UNP Q01813
B	-18	HIS	-	expression tag	UNP Q01813
B	-17	ASP	-	expression tag	UNP Q01813
B	-16	TYR	-	expression tag	UNP Q01813
B	-15	ASP	-	expression tag	UNP Q01813
B	-14	ILE	-	expression tag	UNP Q01813
B	-13	PRO	-	expression tag	UNP Q01813
B	-12	THR	-	expression tag	UNP Q01813
B	-11	THR	-	expression tag	UNP Q01813
B	-10	GLU	-	expression tag	UNP Q01813
B	-9	ASN	-	expression tag	UNP Q01813
B	-8	LEU	-	expression tag	UNP Q01813
B	-7	TYR	-	expression tag	UNP Q01813
B	-6	PHE	-	expression tag	UNP Q01813
B	-5	GLN	-	expression tag	UNP Q01813
B	-4	GLY	-	expression tag	UNP Q01813
B	-3	ALA	-	expression tag	UNP Q01813
B	-2	MET	-	expression tag	UNP Q01813
B	-1	ASP	-	expression tag	UNP Q01813
B	0	PRO	-	expression tag	UNP Q01813
C	-27	MET	-	initiating methionine	UNP Q01813
C	-26	SER	-	expression tag	UNP Q01813
C	-25	TYR	-	expression tag	UNP Q01813
C	-24	TYR	-	expression tag	UNP Q01813
C	-23	HIS	-	expression tag	UNP Q01813
C	-22	HIS	-	expression tag	UNP Q01813
C	-21	HIS	-	expression tag	UNP Q01813

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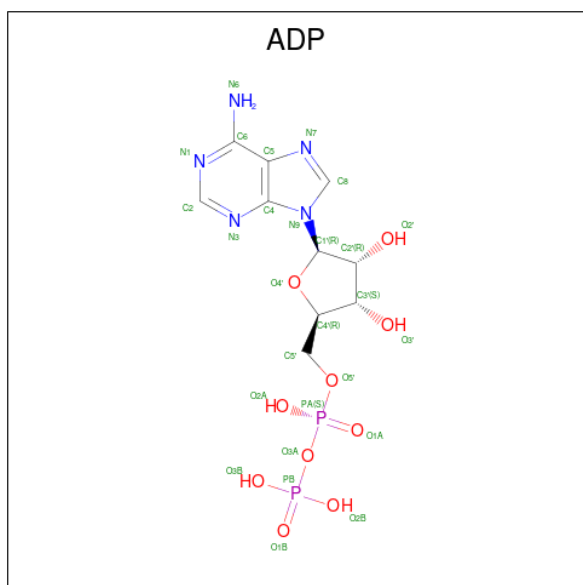
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C	-20	HIS	-	expression tag	UNP Q01813
C	-19	HIS	-	expression tag	UNP Q01813
C	-18	HIS	-	expression tag	UNP Q01813
C	-17	ASP	-	expression tag	UNP Q01813
C	-16	TYR	-	expression tag	UNP Q01813
C	-15	ASP	-	expression tag	UNP Q01813
C	-14	ILE	-	expression tag	UNP Q01813
C	-13	PRO	-	expression tag	UNP Q01813
C	-12	THR	-	expression tag	UNP Q01813
C	-11	THR	-	expression tag	UNP Q01813
C	-10	GLU	-	expression tag	UNP Q01813
C	-9	ASN	-	expression tag	UNP Q01813
C	-8	LEU	-	expression tag	UNP Q01813
C	-7	TYR	-	expression tag	UNP Q01813
C	-6	PHE	-	expression tag	UNP Q01813
C	-5	GLN	-	expression tag	UNP Q01813
C	-4	GLY	-	expression tag	UNP Q01813
C	-3	ALA	-	expression tag	UNP Q01813
C	-2	MET	-	expression tag	UNP Q01813
C	-1	ASP	-	expression tag	UNP Q01813
C	0	PRO	-	expression tag	UNP Q01813
D	-27	MET	-	initiating methionine	UNP Q01813
D	-26	SER	-	expression tag	UNP Q01813
D	-25	TYR	-	expression tag	UNP Q01813
D	-24	TYR	-	expression tag	UNP Q01813
D	-23	HIS	-	expression tag	UNP Q01813
D	-22	HIS	-	expression tag	UNP Q01813
D	-21	HIS	-	expression tag	UNP Q01813
D	-20	HIS	-	expression tag	UNP Q01813
D	-19	HIS	-	expression tag	UNP Q01813
D	-18	HIS	-	expression tag	UNP Q01813
D	-17	ASP	-	expression tag	UNP Q01813
D	-16	TYR	-	expression tag	UNP Q01813
D	-15	ASP	-	expression tag	UNP Q01813
D	-14	ILE	-	expression tag	UNP Q01813
D	-13	PRO	-	expression tag	UNP Q01813
D	-12	THR	-	expression tag	UNP Q01813
D	-11	THR	-	expression tag	UNP Q01813
D	-10	GLU	-	expression tag	UNP Q01813
D	-9	ASN	-	expression tag	UNP Q01813
D	-8	LEU	-	expression tag	UNP Q01813
D	-7	TYR	-	expression tag	UNP Q01813

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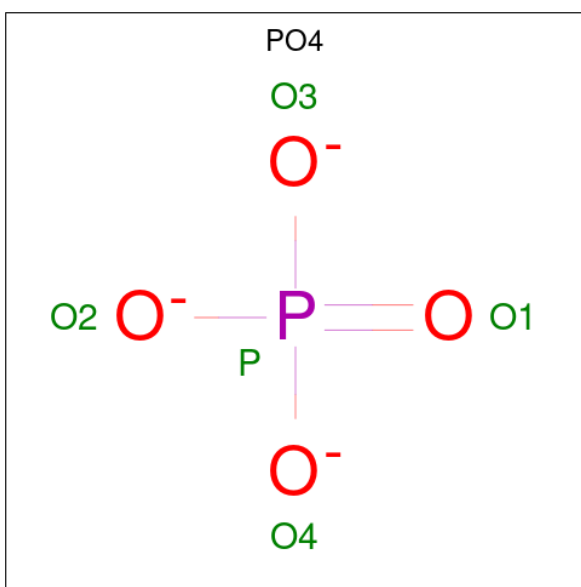
Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	PHE	-	expression tag	UNP Q01813
D	-5	GLN	-	expression tag	UNP Q01813
D	-4	GLY	-	expression tag	UNP Q01813
D	-3	ALA	-	expression tag	UNP Q01813
D	-2	MET	-	expression tag	UNP Q01813
D	-1	ASP	-	expression tag	UNP Q01813
D	0	PRO	-	expression tag	UNP Q01813

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

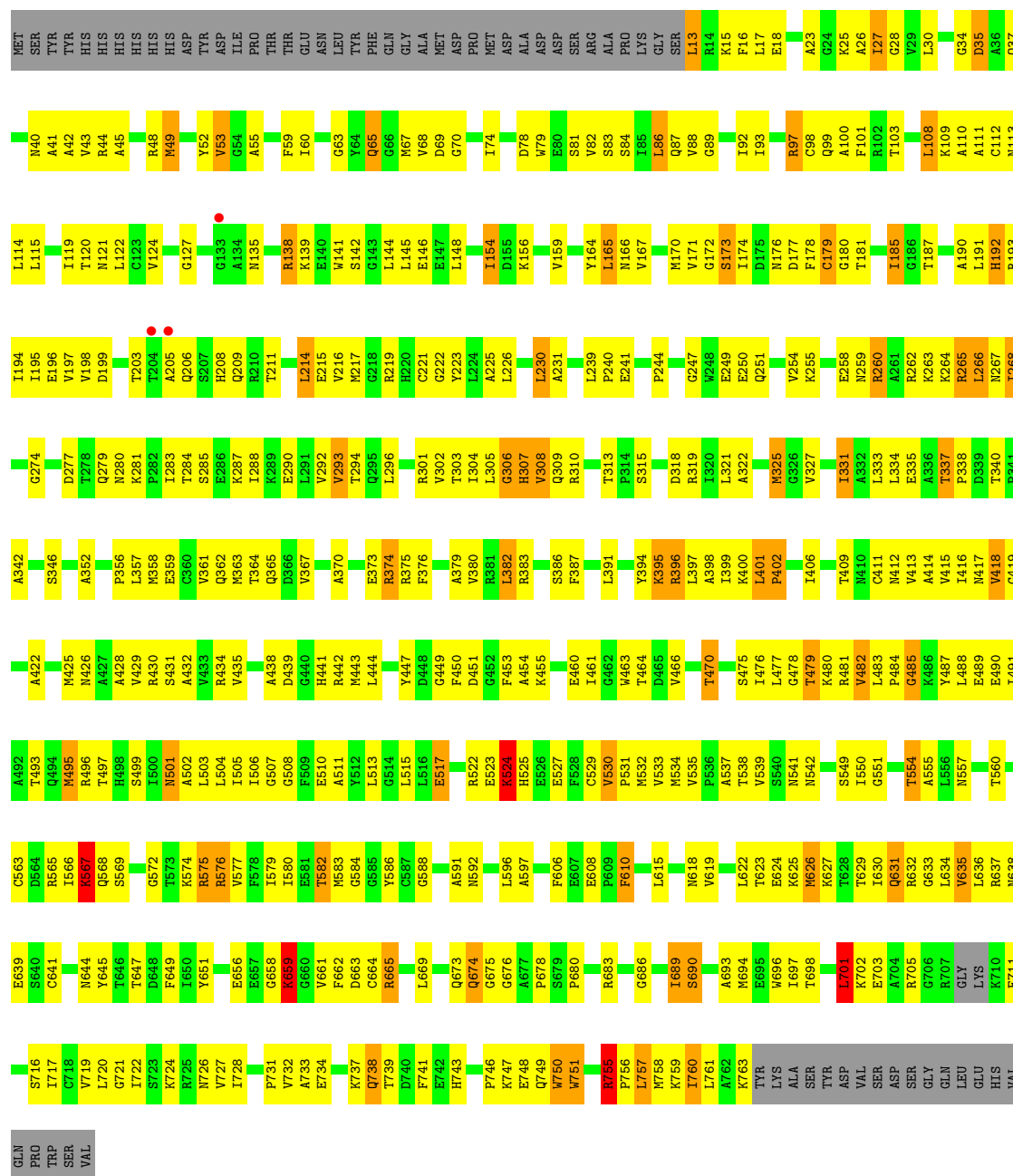


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

GLN
LEU
GLU
HIS
VAL
GLN
PRO
TRP
SER
VAL

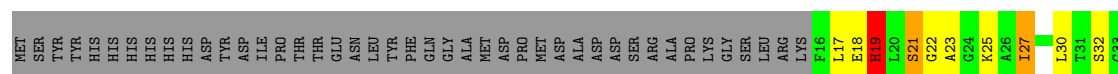
● Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

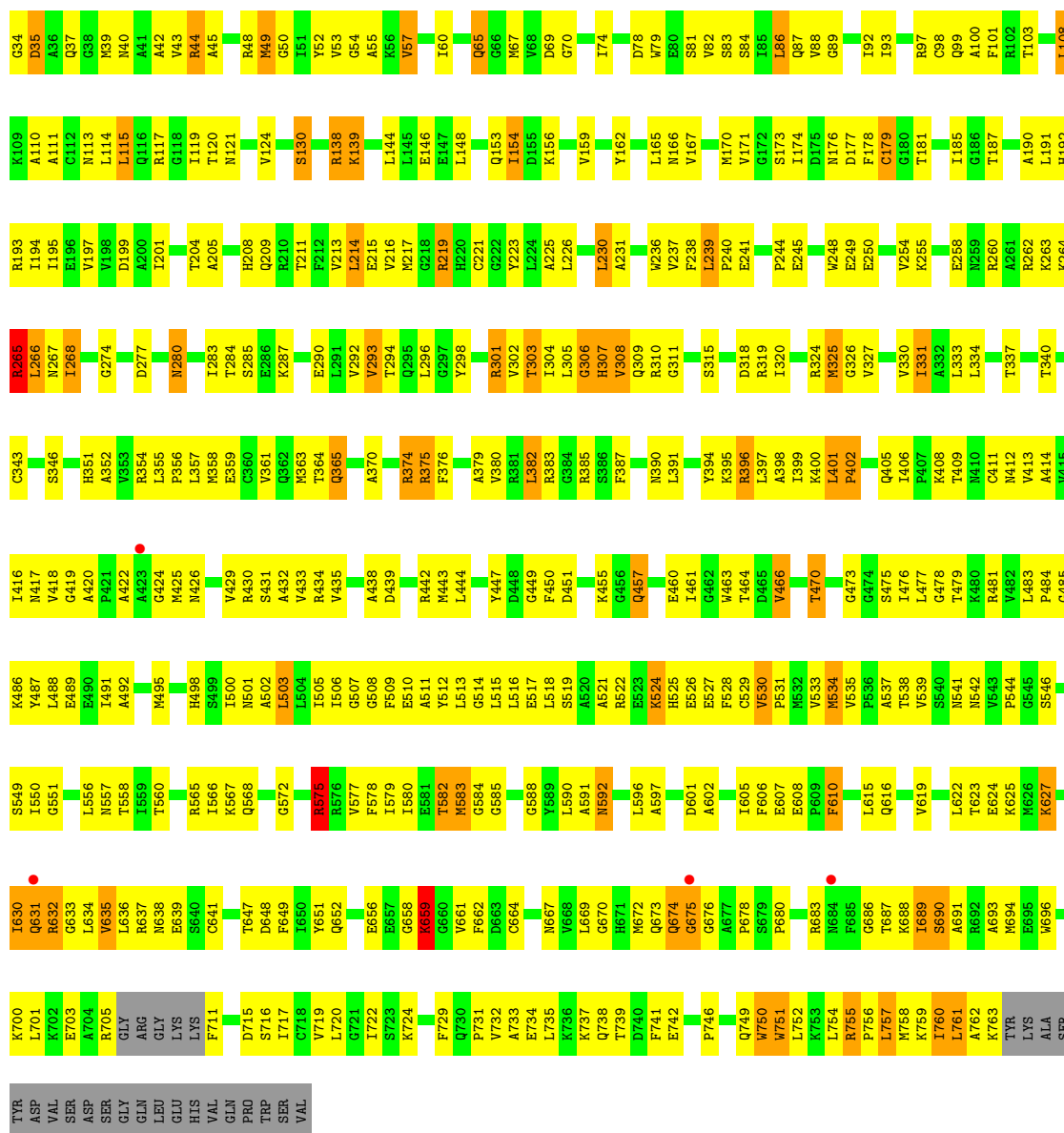
Chain B: 40% 45% 8% 8%



● Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

Chain C: 39% 44% 8% 8%





- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

TRP	V719	T647	L491	V418	R339	K264	L191
SER	L720	Q652	A492	G419	T340	R265	H192
VAL	G721	Q652	A420	P421	C343	L266	R193
	I722	S655	M495	A422	V344	N267	I194
	S723	E656	R496	A423	V345	I268	I195
	K724	E657	T497	A424	S346	E196	E196
	R725	G658	H498	G425		V197	
	N726	G658	S499	M425			
	V727	R575	T500	M426			
	L728	R576	N501				
	F729	V577	A502	V429			
	F730	F578	L503	R430			
	P731	I579	L504	S431			
	V732	D663	L505	A432			
	A733	C664	L506	V433			
	E734	L669	G507	R434			
	L735	T582	E510	V435			
	K736	M583	A511	D439			
	K737	H671	M512				
	K738	M672	Y512	R442			
	T739	Q673	Y512	M443			
	D740	Q674	C587	L444			
		G675	G588				
		G676	G588				
		A677	A591	Y447			
	H743	P678	N592	D448			
		S679	S519				
	P746	P680	A520	G449			
	K747	R683	A521	F450			
	E748	Q684	E523	A454			
	Q749	M684	E523				
	W750	F685	K524	T458			
	W751	G686	H525	R459			
	L752	T687	E526	E460			
		K688	E527	S386			
	R755	I689	F528	F387			
	P756	S690	C529				
	L757		V530	G463			
	M758	M694	P531	T464			
	K759	E695	H621	D465			
	I760	W696	L622	V466			
	L761	I697	T623				
	A762		E624				
	K763		M625	T470			
	TYR	K700	M626				
LYS	L701	R701	K627	G474			
ALA	K702	K702	T630	S475			
SER		R705	V539	L476			
TYR		GLY	S540	L477			
ASP		ARG	N541	G478			
VAL		GLY		T479			
SER		LYS	P544	K480			
ASP		LYS	G545	R481			
SER			S546	V482			
GLY			D547	L483			
GLN			F548	P484			
LEU			S549	G485			
GLU			I550	K486			
HIS			G541	Y487			
VAL			N557	L488			
GLN			N644	E489			
PRO			T560	E490			

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.34Å 168.37Å 133.27Å 90.00° 103.78° 90.00°	Depositor
Resolution (Å)	45.37 – 3.40 45.37 – 3.40	Depositor EDS
% Data completeness (in resolution range)	74.2 (45.37-3.40) 84.5 (45.37-3.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.40Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.256 , 0.290 0.269 , 0.281	Depositor DCC
R_{free} test set	3943 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	69.6	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	22897	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, PO4

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	0.70	0/5730	0.95	5/7735 (0.1%)
1	B	0.68	0/5819	0.97	20/7854 (0.3%)
1	C	0.69	1/5773 (0.0%)	0.96	12/7795 (0.2%)
1	D	0.68	1/5773 (0.0%)	1.00	21/7795 (0.3%)
All	All	0.68	2/23095 (0.0%)	0.97	58/31179 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
1	C	0	4
1	D	0	2
All	All	0	15

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	134	ALA	CA-CB	-5.33	1.44	1.53
1	C	55	ALA	CA-CB	-5.15	1.46	1.53

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	374	ARG	NE-CZ-NH2	12.98	130.88	119.20
1	D	374	ARG	NE-CZ-NH1	-11.79	109.71	121.50
1	B	665	ARG	NE-CZ-NH1	-11.40	110.10	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	97	ARG	NE-CZ-NH2	-11.07	109.24	119.20
1	B	665	ARG	NE-CZ-NH2	10.87	128.98	119.20
1	D	150	ARG	NE-CZ-NH2	10.24	128.42	119.20
1	D	374	ARG	CD-NE-CZ	10.12	138.56	124.40
1	B	576	ARG	NE-CZ-NH2	9.86	128.07	119.20
1	B	576	ARG	NE-CZ-NH1	-9.34	112.16	121.50
1	C	97	ARG	CD-NE-CZ	8.88	136.83	124.40
1	C	97	ARG	NE-CZ-NH1	8.76	130.25	121.50
1	D	375	ARG	NE-CZ-NH2	-8.65	111.42	119.20
1	C	575	ARG	NE-CZ-NH2	8.57	126.91	119.20
1	B	665	ARG	CD-NE-CZ	8.05	135.67	124.40
1	B	701	LEU	N-CA-C	-8.04	103.60	113.41
1	B	575	ARG	NE-CZ-NH1	7.61	129.11	121.50
1	B	575	ARG	NE-CZ-NH2	-7.55	112.40	119.20
1	D	150	ARG	NE-CZ-NH1	-7.53	113.97	121.50
1	B	575	ARG	CD-NE-CZ	7.42	134.79	124.40
1	D	150	ARG	CD-NE-CZ	7.30	134.62	124.40
1	C	627	LYS	N-CA-C	-7.27	105.02	114.04
1	D	375	ARG	CD-NE-CZ	7.25	134.55	124.40
1	C	575	ARG	NE-CZ-NH1	-7.10	114.40	121.50
1	D	575	ARG	CD-NE-CZ	7.10	134.34	124.40
1	D	575	ARG	NE-CZ-NH1	7.05	128.55	121.50
1	D	375	ARG	NE-CZ-NH1	6.96	128.46	121.50
1	D	575	ARG	NE-CZ-NH2	-6.68	113.19	119.20
1	C	575	ARG	CD-NE-CZ	6.68	133.75	124.40
1	C	750	TRP	N-CA-C	6.63	118.17	111.07
1	A	575	ARG	CD-NE-CZ	6.61	133.66	124.40
1	B	576	ARG	CD-NE-CZ	6.36	133.31	124.40
1	D	701	LEU	N-CA-C	-6.21	105.87	113.50
1	A	575	ARG	NE-CZ-NH2	6.21	124.78	119.20
1	B	750	TRP	N-CA-C	6.18	117.68	111.07
1	D	523	GLU	N-CA-C	-6.13	105.73	112.72
1	D	750	TRP	N-CA-C	5.95	117.43	111.07
1	B	567	LYS	N-CA-C	-5.84	106.24	113.19
1	B	180	GLY	N-CA-C	-5.79	107.15	114.16
1	C	375	ARG	NE-CZ-NH2	5.76	124.38	119.20
1	B	386	SER	N-CA-C	-5.75	106.81	113.88
1	C	239	LEU	CA-C-N	5.74	125.28	119.19
1	C	239	LEU	C-N-CA	5.74	125.28	119.19
1	D	386	SER	N-CA-C	-5.57	107.03	113.88
1	D	696	TRP	N-CA-C	-5.54	105.62	112.38
1	D	476	ILE	N-CA-C	-5.49	107.51	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	THR	CA-C-N	5.48	125.83	119.47
1	B	337	THR	C-N-CA	5.48	125.83	119.47
1	C	716	SER	N-CA-C	-5.44	107.90	114.75
1	B	260	ARG	N-CA-C	-5.26	106.99	113.41
1	D	627	LYS	N-CA-C	-5.22	106.85	113.43
1	A	750	TRP	N-CA-C	5.22	116.65	111.07
1	A	567	LYS	N-CA-C	-5.16	107.01	113.15
1	A	375	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	B	375	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	D	401	LEU	CA-C-N	5.10	126.21	119.84
1	D	401	LEU	C-N-CA	5.10	126.21	119.84
1	B	696	TRP	N-CA-C	-5.03	105.93	111.71
1	B	97	ARG	NE-CZ-NH2	5.00	123.70	119.20

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	219	ARG	Sidechain
1	A	262	ARG	Sidechain
1	A	301	ARG	Sidechain
1	A	632	ARG	Sidechain
1	A	692	ARG	Sidechain
1	B	219	ARG	Sidechain
1	B	396	ARG	Sidechain
1	B	565	ARG	Sidechain
1	B	755	ARG	Sidechain
1	C	260	ARG	Sidechain
1	C	265	ARG	Sidechain
1	C	44	ARG	Sidechain
1	C	632	ARG	Sidechain
1	D	138	ARG	Sidechain
1	D	265	ARG	Sidechain

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	5640	0	5674	365	0
1	B	5727	0	5764	371	0
1	C	5681	0	5709	382	0
1	D	5681	0	5709	408	0
2	A	27	0	12	2	0
2	B	27	0	12	1	0
2	C	27	0	12	1	0
2	D	27	0	12	0	0
3	A	15	0	0	2	0
3	B	10	0	0	0	0
3	C	20	0	0	1	0
3	D	15	0	0	1	0
All	All	22897	0	22904	1487	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 32.

All (1487) 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)
1:D:512:TYR:HA	1:D:534:MET:HE1	1.36	1.06
1:D:480:LYS:HB3	1:D:482:VAL:HG23	1.29	1.05
1:B:522:ARG:HH12	1:B:529:CYS:HA	1.25	1.00
1:D:532:MET:HB2	1:D:717:ILE:HG22	1.41	1.00
1:A:539:VAL:HG11	1:A:674:GLN:HB3	1.43	0.99
1:A:121:ASN:HB3	1:A:333:LEU:HD22	1.46	0.97
1:C:121:ASN:HB3	1:C:333:LEU:HD22	1.45	0.95
1:C:44:ARG:NH1	1:C:761:LEU:HD22	1.81	0.95
1:D:327:VAL:HG21	1:D:757:LEU:HD21	1.47	0.93
1:D:30:LEU:HD21	1:D:124:VAL:HG22	1.51	0.92
1:B:30:LEU:HD21	1:B:124:VAL:HG22	1.50	0.91
1:A:181:THR:HB	1:A:346:SER:HB2	1.53	0.91
1:B:588:GLY:HA2	1:B:638:ASN:HD22	1.36	0.90
1:A:284:THR:HG23	1:A:287:LYS:H	1.32	0.90
1:C:588:GLY:HA2	1:C:638:ASN:HD22	1.37	0.90
1:D:630:ILE:HD12	1:D:630:ILE:H	1.36	0.90
1:B:121:ASN:HB3	1:B:333:LEU:HD22	1.53	0.89
1:B:630:ILE:H	1:B:630:ILE:HD12	1.37	0.89
1:D:516:LEU:HD21	1:D:736:LYS:HE2	1.54	0.89
1:A:219:ARG:HG3	1:A:273:GLU:OE1	1.72	0.88
1:A:496:ARG:HB3	1:A:527:GLU:HG3	1.53	0.88
1:C:539:VAL:HG11	1:C:674:GLN:HB3	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ARG:HH11	1:D:44:ARG:HG3	1.38	0.87
1:A:678:PRO:HG2	1:A:683:ARG:HD3	1.57	0.87
1:C:630:ILE:HD12	1:C:630:ILE:H	1.39	0.86
1:B:284:THR:HG23	1:B:287:LYS:H	1.37	0.86
1:D:181:THR:HB	1:D:346:SER:HB2	1.54	0.86
1:D:678:PRO:HG2	1:D:683:ARG:HD3	1.55	0.86
1:D:488:LEU:HD23	1:D:488:LEU:H	1.40	0.85
1:C:534:MET:HG2	1:C:719:VAL:HG22	1.56	0.85
1:B:522:ARG:NH1	1:B:529:CYS:HA	1.91	0.84
1:C:30:LEU:HD21	1:C:124:VAL:HG22	1.59	0.84
1:A:30:LEU:HD21	1:A:124:VAL:HG22	1.59	0.84
1:C:284:THR:HG23	1:C:287:LYS:H	1.40	0.84
1:B:262:ARG:HH22	1:B:400:LYS:HD3	1.42	0.84
1:C:181:THR:HB	1:C:346:SER:HB2	1.58	0.84
1:A:480:LYS:HB3	1:A:482:VAL:HG23	1.57	0.83
1:B:539:VAL:HG11	1:B:674:GLN:HB3	1.60	0.82
1:B:669:LEU:HB3	1:B:673:GLN:HE21	1.44	0.82
1:A:630:ILE:HD12	1:A:630:ILE:H	1.44	0.82
1:D:121:ASN:HB3	1:D:333:LEU:HD22	1.58	0.82
1:A:515:LEU:CD2	1:A:732:VAL:HG11	2.10	0.82
1:D:575:ARG:HD3	1:D:661:VAL:O	1.79	0.82
1:B:678:PRO:HG2	1:B:683:ARG:HD3	1.60	0.82
1:A:527:GLU:CD	1:A:527:GLU:H	1.87	0.82
1:C:658:GLY:O	1:C:661:VAL:HG12	1.80	0.81
1:D:539:VAL:HG11	1:D:674:GLN:HB3	1.61	0.81
1:C:262:ARG:HH22	1:C:400:LYS:HD3	1.43	0.81
1:A:448:ASP:OD1	1:B:574:LYS:HG3	1.81	0.81
1:D:401:LEU:HD23	1:D:401:LEU:H	1.46	0.80
1:A:45:ALA:O	1:A:49:MET:HB2	1.82	0.80
1:B:26:ALA:HB3	1:B:119:ILE:HA	1.60	0.80
1:B:401:LEU:HD23	1:B:401:LEU:H	1.45	0.80
1:B:413:VAL:HG22	1:B:502:ALA:HB3	1.63	0.80
1:B:279:GLN:HG2	1:B:374:ARG:CZ	2.11	0.80
1:C:306:GLY:CA	1:D:303:THR:HG21	2.12	0.79
1:C:327:VAL:HG21	1:C:757:LEU:HD21	1.64	0.79
1:A:658:GLY:O	1:A:661:VAL:HG12	1.83	0.79
1:A:42:ALA:HB1	1:A:170:MET:HE1	1.63	0.79
1:C:522:ARG:NH1	1:C:529:CYS:HA	1.97	0.79
1:A:48:ARG:HH12	3:A:803:PO4:P	2.06	0.79
1:D:505:ILE:HG13	1:D:515:LEU:HD21	1.64	0.78
1:C:686:GLY:O	1:C:690:SER:HB2	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:THR:HG23	1:D:287:LYS:H	1.49	0.78
1:B:401:LEU:HD21	1:B:406:ILE:HD11	1.65	0.78
1:C:401:LEU:HD23	1:C:401:LEU:H	1.49	0.78
1:D:503:LEU:HB3	1:D:532:MET:HG2	1.65	0.77
1:D:515:LEU:HA	1:D:518:LEU:HD12	1.65	0.77
1:B:259:ASN:HD22	1:B:267:ASN:HD21	1.33	0.77
1:A:40:ASN:OD1	1:A:92:ILE:HG23	1.85	0.76
1:B:327:VAL:HG21	1:B:757:LEU:HD21	1.68	0.76
1:B:42:ALA:HB1	1:B:170:MET:HE1	1.67	0.76
1:B:181:THR:HB	1:B:346:SER:HB2	1.66	0.76
1:B:250:GLU:O	1:B:254:VAL:HG23	1.85	0.76
1:B:480:LYS:HB3	1:B:482:VAL:HG23	1.68	0.76
1:C:522:ARG:HE	1:C:717:ILE:HD11	1.51	0.76
1:D:630:ILE:HG22	1:D:632:ARG:HG2	1.68	0.76
1:B:70:GLY:HA3	1:B:113:ASN:ND2	2.00	0.75
1:D:266:LEU:HD22	1:D:267:ASN:N	2.02	0.75
1:D:658:GLY:O	1:D:661:VAL:HG12	1.85	0.75
1:C:412:ASN:OD1	1:C:442:ARG:HD3	1.86	0.75
1:D:262:ARG:HH22	1:D:400:LYS:HD3	1.52	0.75
1:A:515:LEU:HD22	1:A:732:VAL:HG11	1.69	0.75
1:C:413:VAL:HG22	1:C:502:ALA:HB3	1.67	0.74
1:B:606:PHE:HB2	1:B:641:CYS:HA	1.69	0.74
1:B:401:LEU:HD23	1:B:401:LEU:N	2.03	0.74
1:D:43:VAL:HG11	1:D:93:ILE:HD12	1.68	0.74
1:B:588:GLY:HA2	1:B:638:ASN:ND2	2.02	0.74
1:C:401:LEU:HD21	1:C:406:ILE:HD11	1.69	0.74
1:C:495:MET:SD	1:C:500:ILE:HD12	2.28	0.74
1:C:40:ASN:OD1	1:C:92:ILE:HG23	1.86	0.74
1:D:42:ALA:HB1	1:D:170:MET:HE1	1.70	0.74
1:A:530:VAL:HB	1:A:531:PRO:HD2	1.70	0.73
1:C:501:ASN:O	1:C:530:VAL:HB	1.88	0.73
1:D:577:VAL:HG21	1:D:622:LEU:HD21	1.70	0.73
1:C:44:ARG:NH1	1:C:761:LEU:CD2	2.52	0.73
1:C:431:SER:HB2	1:C:687:THR:HG23	1.70	0.73
1:D:401:LEU:H	1:D:401:LEU:CD2	2.01	0.73
1:B:534:MET:HB3	1:B:719:VAL:HG12	1.71	0.73
1:D:731:PRO:HG2	1:D:734:GLU:HG2	1.68	0.73
1:B:142:SER:O	1:B:146:GLU:HG2	1.88	0.73
1:D:541:ASN:HA	1:D:549:SER:OG	1.89	0.73
1:A:425:MET:HE2	1:A:475:SER:HB2	1.69	0.73
1:B:401:LEU:H	1:B:401:LEU:CD2	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:731:PRO:HG2	1:C:734:GLU:HG2	1.68	0.73
1:D:720:LEU:HD23	1:D:721:GLY:N	2.03	0.73
1:A:83:SER:HA	3:A:803:PO4:O3	1.89	0.72
1:A:108:LEU:HG	1:A:144:LEU:HD22	1.69	0.72
1:C:588:GLY:HA2	1:C:638:ASN:ND2	2.05	0.72
1:A:577:VAL:HG21	1:A:622:LEU:HD21	1.70	0.72
1:C:42:ALA:HB1	1:C:170:MET:HE1	1.69	0.72
1:C:171:VAL:HG11	1:C:181:THR:HG21	1.70	0.72
1:A:717:ILE:HG12	1:A:717:ILE:O	1.90	0.72
1:C:79:TRP:CZ2	1:C:763:LYS:HB2	2.25	0.72
1:C:515:LEU:HD11	1:C:534:MET:HB3	1.72	0.72
1:D:250:GLU:O	1:D:254:VAL:HG23	1.90	0.72
1:B:418:VAL:O	1:B:507:GLY:HA3	1.90	0.71
1:A:522:ARG:HH21	1:A:717:ILE:HG23	1.55	0.71
1:B:108:LEU:HG	1:B:144:LEU:HD22	1.71	0.71
1:C:250:GLU:O	1:C:254:VAL:HG23	1.90	0.71
1:D:320:ILE:HD11	1:D:597:ALA:HB2	1.70	0.71
1:D:412:ASN:OD1	1:D:442:ARG:HD3	1.90	0.71
1:D:84:SER:CB	1:D:632:ARG:HH22	2.03	0.71
1:C:301:ARG:HH21	1:C:301:ARG:CG	2.03	0.71
1:A:401:LEU:N	1:A:401:LEU:HD23	2.06	0.70
1:C:306:GLY:HA3	1:D:303:THR:HG21	1.72	0.70
1:B:503:LEU:HB3	1:B:532:MET:HG2	1.71	0.70
1:D:84:SER:HB2	1:D:632:ARG:HH22	1.55	0.70
1:B:43:VAL:HG11	1:B:93:ILE:HD12	1.71	0.70
1:C:401:LEU:HD23	1:C:401:LEU:N	2.05	0.70
1:A:191:LEU:HD22	1:A:680:PRO:HB3	1.73	0.70
1:C:401:LEU:H	1:C:401:LEU:CD2	2.04	0.70
1:B:583:MET:HG2	1:B:673:GLN:OE1	1.91	0.70
1:A:522:ARG:NH2	1:A:716:SER:HB2	2.06	0.70
1:B:731:PRO:HG2	1:B:734:GLU:HG2	1.72	0.70
1:D:40:ASN:OD1	1:D:92:ILE:HG23	1.91	0.70
1:A:700:LYS:O	1:A:711:PHE:HZ	1.75	0.70
1:B:86:LEU:HD21	1:B:597:ALA:O	1.92	0.70
1:C:505:ILE:HD12	1:C:515:LEU:HD21	1.74	0.70
1:A:401:LEU:H	1:A:401:LEU:CD2	2.06	0.69
1:B:84:SER:HB2	1:B:632:ARG:HH22	1.56	0.69
1:D:27:ILE:HG21	1:D:333:LEU:HD13	1.74	0.69
1:D:44:ARG:HG3	1:D:44:ARG:NH1	2.04	0.69
1:A:420:ALA:HB2	1:A:481:ARG:HD3	1.75	0.69
1:B:577:VAL:HG21	1:B:622:LEU:HD21	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:ILE:HD11	1:B:449:GLY:C	2.18	0.69
1:A:142:SER:O	1:A:146:GLU:HG2	1.93	0.69
1:D:45:ALA:O	1:D:49:MET:HB2	1.93	0.69
1:C:425:MET:HE2	1:C:475:SER:HB2	1.73	0.69
1:C:669:LEU:HB3	1:C:673:GLN:HE21	1.57	0.69
1:B:686:GLY:O	1:B:690:SER:HB2	1.91	0.69
1:C:108:LEU:HG	1:C:144:LEU:HD22	1.74	0.69
1:D:70:GLY:HA3	1:D:113:ASN:ND2	2.07	0.69
1:D:718:CYS:HB3	1:D:731:PRO:HA	1.75	0.69
1:C:306:GLY:HA2	1:D:303:THR:HG21	1.74	0.68
1:C:678:PRO:HG2	1:C:683:ARG:HD3	1.73	0.68
1:A:401:LEU:HD23	1:A:401:LEU:H	1.58	0.68
1:B:582:THR:HG21	1:B:591:ALA:HA	1.75	0.68
1:C:508:GLY:HA3	1:C:538:THR:HB	1.76	0.68
1:D:327:VAL:HG21	1:D:757:LEU:CD2	2.21	0.68
1:A:583:MET:HG2	1:A:673:GLN:OE1	1.93	0.68
1:B:515:LEU:HD12	1:B:732:VAL:HG11	1.75	0.68
1:B:532:MET:HB2	1:B:717:ILE:HG23	1.75	0.68
1:B:719:VAL:HG13	1:B:732:VAL:HG12	1.76	0.68
1:C:219:ARG:HH12	3:C:805:PO4:P	2.15	0.68
1:C:430:ARG:HD3	1:C:470:THR:HG23	1.73	0.68
1:C:623:THR:HG23	1:C:661:VAL:HG21	1.75	0.68
1:D:401:LEU:HD23	1:D:401:LEU:N	2.08	0.68
1:B:370:ALA:HB3	1:B:379:ALA:HB2	1.75	0.68
1:B:527:GLU:CD	1:B:527:GLU:H	2.01	0.68
1:C:301:ARG:HG2	1:C:301:ARG:NH2	2.07	0.68
1:D:515:LEU:HG	1:D:534:MET:HE2	1.74	0.68
1:C:43:VAL:HG11	1:C:93:ILE:HD12	1.76	0.68
1:D:430:ARG:HD3	1:D:470:THR:HG23	1.76	0.67
1:B:428:ALA:HB1	1:B:506:ILE:HD13	1.77	0.67
1:A:306:GLY:C	1:A:308:VAL:H	2.02	0.67
1:A:756:PRO:O	1:A:760:ILE:HG23	1.94	0.67
1:B:756:PRO:O	1:B:760:ILE:HG23	1.94	0.67
1:C:483:LEU:CD1	1:C:484:PRO:HD2	2.24	0.67
1:D:306:GLY:C	1:D:308:VAL:H	2.01	0.67
1:D:534:MET:HE3	1:D:719:VAL:HG12	1.77	0.67
1:A:731:PRO:HG2	1:A:734:GLU:HG2	1.75	0.67
1:B:532:MET:HB2	1:B:717:ILE:HG12	1.76	0.67
1:C:416:ILE:HD11	1:C:449:GLY:C	2.19	0.67
1:A:49:MET:O	1:A:53:VAL:HG22	1.95	0.67
1:D:370:ALA:HB3	1:D:379:ALA:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:GLU:O	1:A:254:VAL:HG23	1.96	0.66
1:A:430:ARG:HD3	1:A:470:THR:HG23	1.77	0.66
1:B:266:LEU:HD22	1:B:267:ASN:N	2.10	0.66
1:C:483:LEU:HD13	1:C:484:PRO:HD2	1.76	0.66
1:C:45:ALA:O	1:C:49:MET:HB2	1.95	0.66
1:A:294:THR:HG23	1:A:294:THR:O	1.96	0.66
1:A:669:LEU:HB3	1:A:673:GLN:HE21	1.60	0.66
1:D:376:PHE:O	1:D:380:VAL:HG23	1.96	0.66
1:D:398:ALA:O	1:D:399:ILE:HD13	1.95	0.66
1:A:416:ILE:HD11	1:A:449:GLY:C	2.21	0.65
1:A:717:ILE:HD13	1:A:717:ILE:H	1.61	0.65
1:C:575:ARG:H	1:C:631:GLN:HB2	1.60	0.65
1:C:478:GLY:HA2	1:D:572:GLY:O	1.96	0.65
1:C:226:LEU:HB2	1:C:239:LEU:HD11	1.77	0.65
1:D:483:LEU:HD13	1:D:484:PRO:HD2	1.78	0.65
1:B:588:GLY:CA	1:B:638:ASN:HD22	2.09	0.65
1:D:702:LYS:HA	1:D:705:ARG:HB2	1.77	0.65
1:A:418:VAL:O	1:A:507:GLY:HA3	1.96	0.65
1:C:280:ASN:H	1:C:374:ARG:HH21	1.43	0.65
1:D:515:LEU:HD11	1:D:534:MET:HB2	1.77	0.65
1:A:515:LEU:HD21	1:A:732:VAL:HG11	1.78	0.65
1:B:401:LEU:HG	1:B:406:ILE:HG12	1.78	0.65
1:D:583:MET:HG2	1:D:673:GLN:OE1	1.96	0.65
1:A:678:PRO:HG2	1:A:683:ARG:CD	2.27	0.65
1:A:358:MET:HG3	1:A:359:GLU:H	1.63	0.64
1:B:483:LEU:HD22	1:B:513:LEU:HD22	1.80	0.64
1:A:70:GLY:HA3	1:A:113:ASN:ND2	2.12	0.64
1:C:693:ALA:HB2	1:C:720:LEU:HD23	1.79	0.64
1:D:16:PHE:N	1:D:16:PHE:CD2	2.64	0.64
1:D:534:MET:HB3	1:D:719:VAL:HG12	1.80	0.64
1:D:108:LEU:HG	1:D:144:LEU:HD22	1.78	0.64
1:A:419:GLY:HA2	1:A:510:GLU:HG3	1.79	0.64
1:C:70:GLY:HA3	1:C:113:ASN:ND2	2.13	0.64
1:D:669:LEU:HB3	1:D:673:GLN:HE21	1.63	0.64
1:C:457:GLN:HA	1:C:457:GLN:NE2	2.12	0.64
1:D:412:ASN:ND2	1:D:499:SER:HB2	2.12	0.64
1:D:532:MET:O	1:D:717:ILE:HA	1.98	0.64
1:A:43:VAL:HG11	1:A:93:ILE:HD12	1.79	0.63
1:A:588:GLY:HA2	1:A:638:ASN:OD1	1.98	0.63
1:B:230:LEU:HG	1:B:394:TYR:HB2	1.79	0.63
1:B:630:ILE:HG22	1:B:632:ARG:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:MET:HG3	1:B:327:VAL:HG13	1.80	0.63
1:D:719:VAL:HG13	1:D:732:VAL:HG12	1.79	0.63
1:B:192:HIS:CE1	1:B:680:PRO:HD2	2.34	0.63
1:B:623:THR:HG23	1:B:661:VAL:HG21	1.80	0.63
1:C:746:PRO:HG2	1:C:749:GLN:HG2	1.81	0.63
1:D:419:GLY:HA2	1:D:510:GLU:HG3	1.81	0.63
1:C:266:LEU:HD22	1:C:267:ASN:N	2.13	0.63
1:D:262:ARG:O	1:D:263:LYS:HB2	1.98	0.63
1:D:697:ILE:O	1:D:701:LEU:HB2	1.99	0.63
1:D:280:ASN:H	1:D:374:ARG:NH2	1.97	0.63
1:A:171:VAL:HG11	1:A:181:THR:HG21	1.80	0.63
1:A:592:ASN:C	1:A:592:ASN:HD22	2.07	0.63
1:B:575:ARG:H	1:B:631:GLN:HB2	1.64	0.63
1:D:320:ILE:CD1	1:D:597:ALA:HB2	2.28	0.63
1:D:507:GLY:O	1:D:537:ALA:N	2.31	0.63
1:D:658:GLY:O	1:D:659:LYS:C	2.41	0.63
1:A:398:ALA:O	1:A:399:ILE:HD13	1.98	0.62
1:B:425:MET:HE2	1:B:475:SER:HB2	1.80	0.62
1:A:280:ASN:H	1:A:374:ARG:HH21	1.45	0.62
1:C:303:THR:HG21	1:D:306:GLY:CA	2.29	0.62
1:D:226:LEU:HB2	1:D:239:LEU:HD11	1.81	0.62
1:D:280:ASN:H	1:D:374:ARG:HH21	1.47	0.62
1:A:612:ILE:HG21	1:C:616:GLN:NE2	2.15	0.62
1:B:40:ASN:OD1	1:B:92:ILE:HG23	1.99	0.62
1:C:49:MET:HG3	1:C:327:VAL:HG13	1.79	0.62
1:D:203:THR:HA	1:D:206:GLN:HG2	1.82	0.62
1:D:722:ILE:HD13	1:D:727:VAL:HG12	1.80	0.62
1:D:678:PRO:HG2	1:D:683:ARG:CD	2.28	0.62
1:B:358:MET:HG3	1:B:359:GLU:H	1.62	0.62
1:B:541:ASN:HA	1:B:549:SER:OG	2.00	0.62
1:D:27:ILE:HD13	1:D:57:VAL:HG12	1.82	0.62
1:D:454:ALA:HB1	1:D:490:GLU:HB2	1.81	0.62
1:D:512:TYR:HE1	1:D:516:LEU:HD12	1.64	0.62
1:B:18:GLU:HB2	1:B:52:TYR:OH	1.98	0.62
1:B:480:LYS:HB3	1:B:482:VAL:CG2	2.30	0.62
1:B:505:ILE:HD12	1:B:515:LEU:HD21	1.81	0.62
1:D:171:VAL:HG11	1:D:181:THR:HG21	1.80	0.62
1:A:567:LYS:HG2	1:A:632:ARG:HD3	1.82	0.61
1:A:648:ASP:O	1:A:652:GLN:HG3	2.00	0.61
1:B:84:SER:CB	1:B:632:ARG:HH22	2.12	0.61
1:C:546:SER:HA	1:C:722:ILE:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:702:LYS:HD2	1:D:705:ARG:CB	2.31	0.61
1:D:148:LEU:HB3	1:D:154:ILE:HG23	1.81	0.61
1:D:592:ASN:C	1:D:592:ASN:HD22	2.08	0.61
1:A:422:ALA:O	1:A:425:MET:HB2	2.00	0.61
1:C:749:GLN:OE1	1:C:751:TRP:CZ2	2.54	0.61
1:D:49:MET:SD	1:D:760:ILE:HD11	2.41	0.61
1:D:337:THR:OG1	1:D:340:THR:HB	2.00	0.61
1:B:79:TRP:NE1	1:B:763:LYS:HB2	2.16	0.61
1:D:120:THR:HG23	1:D:121:ASN:ND2	2.15	0.61
1:B:409:THR:HB	1:B:705:ARG:HH22	1.65	0.61
1:B:658:GLY:O	1:B:661:VAL:HG12	2.00	0.61
1:D:49:MET:HG3	1:D:327:VAL:HG13	1.80	0.61
1:A:292:VAL:O	1:A:296:LEU:HB2	2.01	0.61
1:D:538:THR:HG23	1:D:541:ASN:H	1.66	0.61
1:D:458:ILE:HD12	1:D:498:HIS:CD2	2.36	0.61
1:B:259:ASN:HD22	1:B:267:ASN:ND2	1.99	0.60
1:C:176:ASN:C	1:C:178:PHE:H	2.08	0.60
1:B:171:VAL:HG11	1:B:181:THR:HG21	1.82	0.60
1:C:292:VAL:O	1:C:296:LEU:HB2	2.01	0.60
1:A:454:ALA:HB2	1:A:491:ILE:HD12	1.82	0.60
1:B:428:ALA:CB	1:B:506:ILE:HD13	2.32	0.60
1:C:65:GLN:HG2	1:C:98:CYS:HB2	1.84	0.60
1:C:301:ARG:CG	1:C:301:ARG:NH2	2.62	0.60
1:B:13:LEU:N	1:B:13:LEU:HD23	2.17	0.60
1:C:514:GLY:O	1:C:518:LEU:HD23	2.01	0.60
1:C:32:SER:HB3	1:C:130:SER:OG	2.02	0.60
1:C:148:LEU:HB3	1:C:154:ILE:HG23	1.83	0.60
1:A:575:ARG:H	1:A:631:GLN:HB2	1.67	0.60
1:A:714:ASP:OD2	1:A:733:ALA:HB2	2.02	0.60
1:D:567:LYS:HG2	1:D:632:ARG:HD3	1.84	0.60
1:B:70:GLY:HA3	1:B:113:ASN:HD22	1.67	0.60
1:C:358:MET:HA	1:C:358:MET:HE3	1.83	0.60
1:C:418:VAL:O	1:C:507:GLY:HA3	2.01	0.60
1:C:762:ALA:O	1:C:763:LYS:HB3	2.02	0.60
1:B:179:CYS:SG	1:B:363:MET:HB2	2.42	0.59
1:C:230:LEU:HG	1:C:394:TYR:HB2	1.84	0.59
1:D:532:MET:HE3	1:D:717:ILE:HG21	1.83	0.59
1:D:746:PRO:HG2	1:D:749:GLN:HG2	1.84	0.59
1:A:176:ASN:C	1:A:178:PHE:H	2.10	0.59
1:A:596:LEU:HB2	1:A:758:MET:HG3	1.83	0.59
1:B:415:VAL:HG12	1:B:504:LEU:HD23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:VAL:HG11	1:C:181:THR:CG2	2.31	0.59
1:D:48:ARG:HE	1:D:79:TRP:CD1	2.20	0.59
1:D:720:LEU:HD12	1:D:729:PHE:CE2	2.37	0.59
1:C:541:ASN:HA	1:C:549:SER:OG	2.02	0.59
1:D:221:CYS:HA	1:D:383:ARG:NH2	2.17	0.59
1:D:503:LEU:HD21	1:D:505:ILE:HD11	1.83	0.59
1:A:535:VAL:HG13	1:A:689:ILE:HD11	1.83	0.59
1:A:658:GLY:O	1:A:659:LYS:C	2.45	0.59
1:B:79:TRP:CZ2	1:B:763:LYS:HA	2.36	0.59
1:B:493:THR:O	1:B:497:THR:HG23	2.02	0.59
1:C:361:VAL:HG12	1:C:365:GLN:NE2	2.17	0.59
1:D:190:ALA:O	1:D:194:ILE:HG13	2.01	0.59
1:B:244:PRO:HD2	1:B:277:ASP:HA	1.84	0.59
1:B:398:ALA:O	1:B:399:ILE:HD13	2.02	0.59
1:C:25:LYS:CE	1:C:120:THR:HG21	2.33	0.59
1:C:398:ALA:O	1:C:399:ILE:HD13	2.02	0.59
1:D:418:VAL:O	1:D:507:GLY:HA3	2.02	0.59
1:A:226:LEU:HB2	1:A:239:LEU:HD11	1.85	0.59
1:A:582:THR:HG21	1:A:591:ALA:HA	1.84	0.59
1:B:45:ALA:O	1:B:49:MET:HB2	2.02	0.59
1:B:430:ARG:HD3	1:B:470:THR:HG23	1.84	0.59
1:C:606:PHE:HB2	1:C:641:CYS:HA	1.85	0.59
1:D:512:TYR:CE1	1:D:516:LEU:HD12	2.37	0.59
1:A:205:ALA:CB	1:A:266:LEU:HD23	2.33	0.59
1:B:37:GLN:NE2	1:B:310:ARG:C	2.61	0.59
1:B:266:LEU:HD11	1:B:268:ILE:HD11	1.84	0.59
1:D:290:GLU:O	1:D:294:THR:HG22	2.02	0.59
1:D:422:ALA:O	1:D:425:MET:HB2	2.01	0.59
1:A:205:ALA:HB3	1:A:266:LEU:HD23	1.85	0.59
1:C:473:GLY:CA	1:C:678:PRO:HD3	2.32	0.59
1:A:644:ASN:HD22	1:C:656:GLU:HB2	1.68	0.59
1:B:251:GLN:O	1:B:254:VAL:HB	2.03	0.58
1:B:758:MET:HE2	1:B:759:LYS:HG3	1.85	0.58
1:C:579:ILE:N	1:C:579:ILE:HD12	2.18	0.58
1:D:358:MET:HG3	1:D:359:GLU:H	1.67	0.58
1:D:534:MET:HE3	1:D:719:VAL:CG1	2.33	0.58
1:D:634:LEU:HD11	1:D:636:LEU:HD21	1.85	0.58
1:D:702:LYS:HD2	1:D:705:ARG:HB3	1.85	0.58
1:A:48:ARG:HE	1:A:79:TRP:CD1	2.21	0.58
1:C:756:PRO:O	1:C:760:ILE:HG23	2.03	0.58
1:D:216:VAL:HG21	1:D:225:ALA:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:487:TYR:N	1:D:487:TYR:HD2	2.01	0.58
1:C:658:GLY:O	1:C:659:LYS:C	2.45	0.58
1:D:579:ILE:HD12	1:D:579:ILE:N	2.18	0.58
1:A:203:THR:HA	1:A:206:GLN:HG2	1.84	0.58
1:C:221:CYS:HA	1:C:383:ARG:NH2	2.17	0.58
1:C:676:GLY:HA2	1:D:565:ARG:HG2	1.85	0.58
1:B:426:ASN:OD1	1:B:476:ILE:HG13	2.04	0.58
1:C:195:ILE:HD11	1:C:231:ALA:HB3	1.86	0.58
1:C:370:ALA:HB3	1:C:379:ALA:HB2	1.86	0.58
1:D:480:LYS:C	1:D:482:VAL:H	2.11	0.58
1:B:83:SER:O	1:B:84:SER:HB3	2.04	0.58
1:B:434:ARG:HG2	1:B:463:TRP:CD2	2.38	0.58
1:C:290:GLU:O	1:C:294:THR:HG22	2.04	0.58
1:A:426:ASN:OD1	1:A:476:ILE:HG13	2.04	0.58
1:B:148:LEU:HB3	1:B:154:ILE:HG23	1.84	0.58
1:D:217:MET:HG3	1:D:309:GLN:NE2	2.19	0.58
1:D:623:THR:HG23	1:D:661:VAL:HG21	1.85	0.58
1:C:542:ASN:O	1:C:746:PRO:HD3	2.04	0.58
1:A:477:LEU:HD12	1:A:477:LEU:H	1.67	0.57
1:B:625:LYS:C	1:B:627:LYS:H	2.11	0.57
1:B:634:LEU:HD11	1:B:636:LEU:HD21	1.86	0.57
1:C:37:GLN:NE2	1:C:310:ARG:C	2.62	0.57
1:A:401:LEU:N	1:A:401:LEU:CD2	2.66	0.57
1:B:190:ALA:O	1:B:194:ILE:HG13	2.04	0.57
1:B:195:ILE:HD11	1:B:231:ALA:HB3	1.86	0.57
1:B:658:GLY:O	1:B:659:LYS:C	2.47	0.57
1:A:649:PHE:CD1	1:C:649:PHE:CE1	2.93	0.57
1:D:176:ASN:C	1:D:178:PHE:H	2.13	0.57
1:D:762:ALA:O	1:D:763:LYS:HB2	2.04	0.57
1:A:515:LEU:HD23	1:A:515:LEU:C	2.29	0.57
1:A:630:ILE:HG22	1:A:632:ARG:HG2	1.87	0.57
1:B:630:ILE:H	1:B:630:ILE:CD1	2.14	0.57
1:D:401:LEU:HD21	1:D:406:ILE:HD11	1.86	0.57
1:B:30:LEU:H	1:B:30:LEU:HD23	1.70	0.57
1:B:337:THR:OG1	1:B:340:THR:HB	2.05	0.57
1:D:431:SER:HB2	1:D:687:THR:HG23	1.86	0.57
1:B:306:GLY:C	1:B:308:VAL:H	2.13	0.57
1:D:487:TYR:N	1:D:487:TYR:CD2	2.72	0.57
1:D:735:LEU:O	1:D:739:THR:HG22	2.05	0.57
1:B:327:VAL:HG21	1:B:757:LEU:CD2	2.35	0.57
1:C:25:LYS:HE2	1:C:120:THR:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:637:ARG:HE	1:C:647:THR:N	2.03	0.57
1:D:719:VAL:HG23	1:D:719:VAL:O	2.04	0.57
1:A:395:LYS:C	1:A:397:LEU:H	2.12	0.57
1:C:315:SER:O	1:C:319:ARG:HG3	2.05	0.57
1:C:583:MET:HG2	1:C:673:GLN:OE1	2.05	0.57
1:C:676:GLY:HA3	1:D:565:ARG:CD	2.34	0.57
1:D:715:ASP:C	1:D:717:ILE:H	2.13	0.57
1:C:483:LEU:HD12	1:C:517:GLU:OE1	2.05	0.56
1:B:358:MET:HG3	1:B:359:GLU:N	2.19	0.56
1:B:669:LEU:CB	1:B:673:GLN:HE21	2.15	0.56
1:D:756:PRO:O	1:D:760:ILE:HG23	2.04	0.56
1:A:402:PRO:HG2	1:A:405:GLN:HG3	1.88	0.56
1:A:539:VAL:HG11	1:A:674:GLN:CB	2.29	0.56
1:A:612:ILE:HG21	1:C:616:GLN:HE22	1.69	0.56
1:B:292:VAL:O	1:B:296:LEU:HB2	2.05	0.56
1:B:508:GLY:CA	1:B:538:THR:HB	2.35	0.56
1:C:592:ASN:C	1:C:592:ASN:HD22	2.13	0.56
1:C:608:GLU:OE1	1:C:755:ARG:HG2	2.05	0.56
1:C:757:LEU:C	1:C:757:LEU:HD22	2.30	0.56
1:D:625:LYS:C	1:D:627:LYS:H	2.14	0.56
1:B:176:ASN:C	1:B:178:PHE:H	2.13	0.56
1:B:484:PRO:HG2	1:B:517:GLU:HB3	1.87	0.56
1:B:525:HIS:HB3	1:B:527:GLU:OE1	2.06	0.56
1:B:678:PRO:HG2	1:B:683:ARG:CD	2.33	0.56
1:C:285:SER:HB3	1:C:302:VAL:HG21	1.87	0.56
1:D:92:ILE:HG13	1:D:93:ILE:N	2.19	0.56
1:A:181:THR:CB	1:A:346:SER:HB2	2.33	0.56
1:A:49:MET:HG3	1:A:327:VAL:HG13	1.86	0.56
1:C:419:GLY:HA2	1:C:510:GLU:HG3	1.86	0.56
1:A:606:PHE:HB2	1:A:641:CYS:HA	1.87	0.56
1:C:262:ARG:NH2	1:C:400:LYS:HD3	2.19	0.56
1:D:84:SER:HB2	1:D:632:ARG:NH2	2.21	0.56
1:A:575:ARG:HG2	1:A:661:VAL:O	2.05	0.56
1:C:156:LYS:O	1:C:159:VAL:HG12	2.06	0.56
1:D:416:ILE:HD11	1:D:449:GLY:C	2.30	0.56
1:D:577:VAL:HG21	1:D:622:LEU:CD2	2.36	0.56
1:A:401:LEU:HD21	1:A:406:ILE:HD11	1.88	0.56
1:A:479:THR:HG23	1:A:479:THR:O	2.05	0.56
1:A:527:GLU:CD	1:A:527:GLU:N	2.62	0.56
1:A:686:GLY:O	1:A:690:SER:HB2	2.06	0.56
1:B:531:PRO:HA	1:B:716:SER:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:701:LEU:O	1:B:705:ARG:HG3	2.06	0.56
1:A:454:ALA:HB2	1:A:491:ILE:CD1	2.36	0.56
1:B:477:LEU:HD12	1:B:477:LEU:H	1.70	0.56
1:B:592:ASN:C	1:B:592:ASN:HD22	2.14	0.56
1:C:35:ASP:OD2	1:D:204:THR:HA	2.06	0.56
1:D:390:ASN:OD1	1:D:688:LYS:HE2	2.05	0.56
1:A:99:GLN:C	1:A:101:PHE:H	2.14	0.55
1:A:236:TRP:HZ3	1:A:399:ILE:HD11	1.71	0.55
1:C:337:THR:OG1	1:C:340:THR:HB	2.05	0.55
1:C:487:TYR:O	1:C:491:ILE:HG13	2.06	0.55
1:C:720:LEU:HD22	1:C:729:PHE:CE2	2.41	0.55
1:C:303:THR:HG21	1:D:306:GLY:HA3	1.87	0.55
1:C:534:MET:CG	1:C:719:VAL:HG22	2.33	0.55
1:C:579:ILE:HG13	1:C:635:VAL:CG1	2.37	0.55
1:A:416:ILE:HG13	1:A:446:ILE:HB	1.87	0.55
1:B:577:VAL:HG21	1:B:622:LEU:CD2	2.36	0.55
1:A:370:ALA:HB3	1:A:379:ALA:HB2	1.88	0.55
1:A:397:LEU:HD21	1:A:430:ARG:NH2	2.22	0.55
1:C:397:LEU:HD11	1:C:431:SER:HA	1.88	0.55
1:A:450:PHE:CE1	1:A:484:PRO:HD3	2.42	0.55
1:C:306:GLY:C	1:C:308:VAL:H	2.14	0.55
1:B:78:ASP:OD2	1:B:78:ASP:N	2.34	0.55
1:D:292:VAL:O	1:D:296:LEU:HB2	2.06	0.55
1:D:567:LYS:HD3	1:D:632:ARG:NH1	2.21	0.55
1:D:606:PHE:HB2	1:D:641:CYS:HA	1.89	0.55
1:A:127:GLY:C	2:A:801:ADP:O3B	2.49	0.55
1:A:195:ILE:HD11	1:A:231:ALA:HB3	1.89	0.55
1:A:625:LYS:C	1:A:627:LYS:H	2.15	0.55
1:C:634:LEU:HD11	1:C:636:LEU:HD21	1.87	0.55
1:A:478:GLY:HA2	1:B:572:GLY:O	2.05	0.55
1:C:579:ILE:HG13	1:C:635:VAL:HG13	1.88	0.55
1:C:680:PRO:HA	1:C:683:ARG:HG3	1.89	0.55
1:D:305:LEU:HD12	1:D:305:LEU:H	1.72	0.55
1:D:722:ILE:HD13	1:D:727:VAL:CG1	2.36	0.55
1:B:192:HIS:O	1:B:196:GLU:HG3	2.06	0.55
1:B:221:CYS:HA	1:B:383:ARG:NH2	2.22	0.55
1:A:148:LEU:HB3	1:A:154:ILE:HD12	1.89	0.55
1:A:461:ILE:O	1:A:461:ILE:HD12	2.07	0.55
1:C:25:LYS:CD	1:C:120:THR:HG21	2.37	0.55
1:C:99:GLN:C	1:C:101:PHE:H	2.15	0.55
1:C:320:ILE:HD11	1:C:597:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:505:ILE:HG21	1:C:511:ALA:HB1	1.88	0.55
1:C:675:GLY:O	1:D:568:GLN:HG2	2.07	0.55
1:D:637:ARG:HE	1:D:647:THR:N	2.05	0.55
1:C:301:ARG:HH21	1:C:301:ARG:HG2	1.67	0.54
1:A:358:MET:HG3	1:A:359:GLU:N	2.22	0.54
1:A:506:ILE:HD13	1:A:535:VAL:HB	1.88	0.54
1:A:649:PHE:CE1	1:C:649:PHE:CE1	2.95	0.54
1:B:397:LEU:HD11	1:B:431:SER:HA	1.89	0.54
1:B:401:LEU:N	1:B:401:LEU:CD2	2.68	0.54
1:A:634:LEU:HD11	1:A:636:LEU:HD21	1.90	0.54
1:A:669:LEU:HB3	1:A:673:GLN:NE2	2.22	0.54
1:B:205:ALA:CB	1:B:266:LEU:HD23	2.37	0.54
1:B:461:ILE:HD12	1:B:461:ILE:O	2.08	0.54
1:C:240:PRO:HG3	1:C:274:GLY:O	2.08	0.54
1:B:177:ASP:O	1:B:364:THR:HG23	2.06	0.54
1:C:327:VAL:HG21	1:C:757:LEU:CD2	2.37	0.54
1:C:630:ILE:HG22	1:C:632:ARG:HG2	1.90	0.54
1:D:156:LYS:O	1:D:159:VAL:HG12	2.08	0.54
1:D:582:THR:HG21	1:D:591:ALA:HA	1.90	0.54
1:A:495:MET:HE3	1:A:500:ILE:CG2	2.38	0.54
1:D:83:SER:O	1:D:84:SER:HB3	2.07	0.54
1:D:588:GLY:HA2	1:D:638:ASN:HD22	1.71	0.54
1:A:541:ASN:HA	1:A:549:SER:OG	2.08	0.54
1:C:303:THR:HG21	1:D:306:GLY:HA2	1.89	0.54
1:D:395:LYS:C	1:D:397:LEU:H	2.15	0.54
1:D:434:ARG:HG2	1:D:463:TRP:CD2	2.43	0.54
1:D:661:VAL:HG13	1:D:662:PHE:CD2	2.43	0.54
1:A:315:SER:O	1:A:319:ARG:HG3	2.08	0.54
1:A:680:PRO:HA	1:A:683:ARG:HG3	1.88	0.54
1:B:417:ASN:HB3	1:B:425:MET:HE3	1.90	0.54
1:C:114:LEU:HD22	1:C:119:ILE:HB	1.90	0.54
1:C:376:PHE:O	1:C:380:VAL:HG23	2.07	0.54
1:D:236:TRP:CZ3	1:D:399:ILE:HD11	2.43	0.54
1:B:669:LEU:HB3	1:B:673:GLN:NE2	2.18	0.54
1:C:120:THR:HG23	1:C:121:ASN:ND2	2.23	0.54
1:B:395:LYS:C	1:B:397:LEU:H	2.15	0.54
1:D:370:ALA:CB	1:D:379:ALA:HB2	2.37	0.54
1:A:576:ARG:HA	1:A:663:ASP:O	2.08	0.53
1:A:746:PRO:HG2	1:A:749:GLN:HG2	1.90	0.53
1:B:266:LEU:CD1	1:B:268:ILE:HD11	2.38	0.53
1:C:560:THR:HG22	1:C:597:ALA:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:CYS:HA	1:A:383:ARG:NH2	2.24	0.53
1:A:758:MET:HE2	1:A:759:LYS:HG3	1.90	0.53
1:C:567:LYS:HG2	1:C:632:ARG:HD3	1.89	0.53
1:A:434:ARG:HG2	1:A:463:TRP:CD2	2.43	0.53
1:A:522:ARG:HG2	1:A:528:PHE:O	2.08	0.53
1:B:240:PRO:HG3	1:B:274:GLY:O	2.08	0.53
1:D:99:GLN:C	1:D:101:PHE:H	2.16	0.53
1:D:142:SER:O	1:D:146:GLU:HG2	2.08	0.53
1:D:503:LEU:CB	1:D:532:MET:HG2	2.36	0.53
1:D:535:VAL:HG13	1:D:689:ILE:HD11	1.91	0.53
1:A:65:GLN:HG2	1:A:98:CYS:HB2	1.90	0.53
1:A:483:LEU:HD12	1:A:483:LEU:H	1.74	0.53
1:B:262:ARG:O	1:B:263:LYS:HB2	2.07	0.53
1:C:138:ARG:HA	1:C:165:LEU:HD12	1.91	0.53
1:D:503:LEU:CD2	1:D:505:ILE:HD11	2.39	0.53
1:A:37:GLN:NE2	1:A:310:ARG:C	2.67	0.53
1:A:262:ARG:O	1:A:263:LYS:HB2	2.08	0.53
1:A:577:VAL:HG21	1:A:622:LEU:CD2	2.37	0.53
1:B:409:THR:HB	1:B:705:ARG:NH2	2.23	0.53
1:C:434:ARG:HG2	1:C:463:TRP:CD2	2.43	0.53
1:C:737:LYS:HG3	1:C:738:GLN:N	2.22	0.53
1:D:236:TRP:HZ3	1:D:399:ILE:HD11	1.73	0.53
1:D:397:LEU:HD21	1:D:430:ARG:NH2	2.24	0.53
1:D:488:LEU:H	1:D:488:LEU:CD2	2.16	0.53
1:A:529:CYS:O	1:A:711:PHE:HB2	2.08	0.53
1:C:638:ASN:HB3	1:C:641:CYS:HB3	1.90	0.53
1:C:757:LEU:HD22	1:C:757:LEU:O	2.09	0.53
1:D:193:ARG:O	1:D:197:VAL:HG23	2.09	0.53
1:B:120:THR:HG23	1:B:121:ASN:ND2	2.24	0.53
1:C:25:LYS:CG	1:C:120:THR:HG21	2.39	0.53
1:C:538:THR:HG23	1:C:541:ASN:H	1.74	0.53
1:C:669:LEU:HB3	1:C:673:GLN:NE2	2.23	0.53
1:A:431:SER:HB2	1:A:687:THR:HG23	1.89	0.53
1:B:739:THR:HG23	1:B:741:PHE:CE1	2.44	0.53
1:D:171:VAL:HG11	1:D:181:THR:CG2	2.38	0.53
1:D:240:PRO:HG3	1:D:274:GLY:O	2.08	0.53
1:A:83:SER:O	1:A:84:SER:HB3	2.09	0.53
1:A:138:ARG:HA	1:A:165:LEU:HD12	1.90	0.53
1:A:412:ASN:HB2	1:A:499:SER:O	2.08	0.53
1:B:84:SER:HB2	1:B:632:ARG:NH2	2.24	0.53
1:B:717:ILE:O	1:B:732:VAL:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:ILE:HG23	1:D:121:ASN:HB2	1.90	0.53
1:D:480:LYS:HB3	1:D:482:VAL:CG2	2.20	0.53
1:B:530:VAL:HB	1:B:531:PRO:HD2	1.90	0.52
1:C:49:MET:O	1:C:53:VAL:HG22	2.09	0.52
1:A:421:PRO:HG2	1:A:674:GLN:HE22	1.74	0.52
1:B:479:THR:HG23	1:B:479:THR:O	2.08	0.52
1:B:579:ILE:HD12	1:B:579:ILE:N	2.24	0.52
1:B:680:PRO:HA	1:B:683:ARG:HG3	1.91	0.52
1:C:174:ILE:HG21	1:C:190:ALA:HB2	1.90	0.52
1:C:280:ASN:H	1:C:374:ARG:NH2	2.06	0.52
1:C:488:LEU:HD22	1:C:528:PHE:CZ	2.44	0.52
1:C:746:PRO:HD2	1:C:749:GLN:NE2	2.24	0.52
1:C:758:MET:HE2	1:C:759:LYS:HG3	1.91	0.52
1:D:560:THR:HG22	1:D:597:ALA:HB3	1.91	0.52
1:B:315:SER:O	1:B:319:ARG:HG3	2.09	0.52
1:C:556:LEU:O	1:C:560:THR:HG23	2.09	0.52
1:C:700:LYS:HA	1:C:703:GLU:HG2	1.90	0.52
1:C:356:PRO:HG2	1:C:359:GLU:HB3	1.92	0.52
1:C:582:THR:HG21	1:C:591:ALA:HA	1.91	0.52
1:A:240:PRO:HG3	1:A:274:GLY:O	2.09	0.52
1:A:487:TYR:O	1:A:491:ILE:HD13	2.10	0.52
1:C:435:VAL:HG21	1:C:691:ALA:CB	2.40	0.52
1:D:27:ILE:N	1:D:27:ILE:HD12	2.24	0.52
1:D:397:LEU:HD11	1:D:431:SER:HA	1.91	0.52
1:D:758:MET:HE2	1:D:759:LYS:HG3	1.92	0.52
1:A:138:ARG:HD3	1:A:165:LEU:O	2.09	0.52
1:A:306:GLY:C	1:A:308:VAL:N	2.68	0.52
1:A:483:LEU:HD12	1:A:483:LEU:N	2.23	0.52
1:A:616:GLN:HA	1:A:616:GLN:HE21	1.74	0.52
1:A:236:TRP:CZ3	1:A:399:ILE:HD11	2.45	0.52
1:B:419:GLY:HA2	1:B:481:ARG:HG2	1.90	0.52
1:B:532:MET:CB	1:B:717:ILE:HG23	2.40	0.52
1:C:508:GLY:CA	1:C:538:THR:HB	2.39	0.52
1:C:516:LEU:HD22	1:C:732:VAL:HB	1.92	0.52
1:A:268:ILE:HD12	1:A:268:ILE:N	2.25	0.52
1:A:435:VAL:HG12	1:A:435:VAL:O	2.09	0.52
1:C:424:GLY:N	1:C:678:PRO:HB3	2.24	0.52
1:C:477:LEU:HD12	1:C:477:LEU:H	1.74	0.52
1:D:477:LEU:HD12	1:D:477:LEU:H	1.74	0.52
1:A:720:LEU:HD22	1:A:729:PHE:CE2	2.46	0.51
1:D:420:ALA:HB2	1:D:481:ARG:HH11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:680:PRO:HA	1:D:683:ARG:HG3	1.91	0.51
1:A:50:GLY:O	1:A:53:VAL:HG23	2.11	0.51
1:A:206:GLN:O	1:A:265:ARG:NH2	2.44	0.51
1:A:396:ARG:HB3	1:A:396:ARG:HH21	1.76	0.51
1:B:99:GLN:C	1:B:101:PHE:H	2.18	0.51
1:B:114:LEU:HD22	1:B:119:ILE:HB	1.93	0.51
1:B:376:PHE:O	1:B:380:VAL:HG23	2.10	0.51
1:B:483:LEU:HD21	1:B:513:LEU:HD13	1.92	0.51
1:C:187:THR:HG21	1:C:223:TYR:HE2	1.75	0.51
1:C:615:LEU:O	1:C:619:VAL:HG23	2.10	0.51
1:B:226:LEU:HB2	1:B:239:LEU:HD11	1.91	0.51
1:B:542:ASN:O	1:B:746:PRO:HD3	2.10	0.51
1:C:181:THR:CB	1:C:346:SER:HB2	2.35	0.51
1:C:199:ASP:CG	1:C:683:ARG:HH22	2.19	0.51
1:C:479:THR:HG23	1:C:479:THR:O	2.10	0.51
1:D:48:ARG:HG2	1:D:79:TRP:CE2	2.45	0.51
1:D:621:HIS:CE1	1:D:763:LYS:HB2	2.46	0.51
1:D:717:ILE:O	1:D:732:VAL:HG13	2.10	0.51
1:A:115:LEU:HD12	1:A:162:TYR:CD2	2.46	0.51
1:A:337:THR:OG1	1:A:340:THR:HB	2.10	0.51
1:B:560:THR:HG22	1:B:597:ALA:HB3	1.92	0.51
1:D:65:GLN:HG2	1:D:98:CYS:HB2	1.92	0.51
1:A:216:VAL:HG21	1:A:225:ALA:HA	1.93	0.51
1:A:623:THR:HG23	1:A:661:VAL:HG21	1.93	0.51
1:B:438:ALA:HB2	1:B:463:TRP:HZ3	1.74	0.51
1:D:101:PHE:C	1:D:103:THR:H	2.17	0.51
1:D:412:ASN:ND2	1:D:499:SER:CB	2.74	0.51
1:B:216:VAL:HG21	1:B:225:ALA:HA	1.91	0.51
1:B:262:ARG:NH2	1:B:400:LYS:HD3	2.18	0.51
1:D:32:SER:HB3	1:D:130:SER:OG	2.09	0.51
1:D:715:ASP:C	1:D:717:ILE:N	2.66	0.51
1:A:28:GLY:HA3	1:A:122:LEU:HD12	1.93	0.51
1:A:579:ILE:HG13	1:A:635:VAL:HG13	1.93	0.51
1:C:357:LEU:O	1:C:361:VAL:HG23	2.10	0.51
1:D:66:GLY:HA2	1:D:73:ASN:HD22	1.75	0.51
1:B:443:MET:O	1:B:460:GLU:HG3	2.11	0.51
1:B:615:LEU:O	1:B:619:VAL:HG23	2.11	0.51
1:B:630:ILE:HD12	1:B:630:ILE:N	2.17	0.51
1:C:572:GLY:O	1:D:478:GLY:HA2	2.10	0.51
1:B:48:ARG:HE	1:B:79:TRP:CD1	2.29	0.51
1:B:203:THR:HA	1:B:206:GLN:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:ARG:HB3	1:B:527:GLU:HG2	1.92	0.51
1:B:579:ILE:HG13	1:B:635:VAL:HG13	1.93	0.51
1:B:760:ILE:HG12	1:B:761:LEU:HD23	1.92	0.51
1:C:305:LEU:H	1:C:305:LEU:HD12	1.75	0.51
1:D:16:PHE:N	1:D:16:PHE:HD2	2.09	0.51
1:D:450:PHE:CD1	1:D:484:PRO:HD3	2.46	0.51
1:A:608:GLU:OE1	1:A:755:ARG:HG2	2.11	0.51
1:B:277:ASP:HB3	1:B:283:ILE:HD11	1.93	0.51
1:B:739:THR:N	1:B:747:LYS:HG3	2.26	0.51
1:C:190:ALA:O	1:C:194:ILE:HG13	2.11	0.51
1:C:262:ARG:HD3	1:C:464:THR:HG22	1.93	0.51
1:D:331:ILE:HG13	1:D:354:ARG:HH22	1.76	0.51
1:A:417:ASN:HB3	1:A:425:MET:HE3	1.93	0.50
1:A:538:THR:HG23	1:A:541:ASN:H	1.75	0.50
1:B:737:LYS:HG3	1:B:738:GLN:HG3	1.92	0.50
1:B:750:TRP:CG	1:B:751:TRP:N	2.78	0.50
1:C:516:LEU:CD2	1:C:732:VAL:HB	2.41	0.50
1:C:522:ARG:HH12	1:C:529:CYS:HA	1.72	0.50
1:D:358:MET:HG3	1:D:359:GLU:N	2.26	0.50
1:B:92:ILE:HG13	1:B:93:ILE:N	2.26	0.50
1:C:583:MET:HA	1:C:639:GLU:HB2	1.93	0.50
1:A:171:VAL:HG11	1:A:181:THR:CG2	2.41	0.50
1:A:522:ARG:C	1:A:524:LYS:H	2.18	0.50
1:B:206:GLN:O	1:B:265:ARG:NH2	2.44	0.50
1:A:174:ILE:HG21	1:A:190:ALA:HB2	1.93	0.50
1:A:483:LEU:HD23	1:A:513:LEU:HD12	1.94	0.50
1:B:26:ALA:CB	1:B:119:ILE:HA	2.35	0.50
1:B:192:HIS:HA	1:B:680:PRO:HG2	1.94	0.50
1:B:523:GLU:O	1:B:524:LYS:C	2.54	0.50
1:C:237:VAL:HG12	1:C:238:PHE:N	2.26	0.50
1:D:424:GLY:N	1:D:678:PRO:HB3	2.26	0.50
1:D:577:VAL:CG2	1:D:622:LEU:HD21	2.39	0.50
1:D:615:LEU:O	1:D:619:VAL:HG23	2.12	0.50
1:D:630:ILE:H	1:D:630:ILE:CD1	2.11	0.50
1:A:717:ILE:O	1:A:717:ILE:CG1	2.58	0.50
1:B:539:VAL:HG12	1:B:551:GLY:O	2.12	0.50
1:C:515:LEU:CD1	1:C:534:MET:HB3	2.42	0.50
1:D:211:THR:OG1	1:D:267:ASN:HB2	2.12	0.50
1:A:192:HIS:O	1:A:196:GLU:HG3	2.11	0.50
1:A:195:ILE:HG13	1:A:680:PRO:HG3	1.93	0.50
1:A:254:VAL:O	1:A:258:GLU:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:ALA:HB1	1:B:504:LEU:CD2	2.42	0.50
1:B:501:ASN:HA	1:B:530:VAL:HG11	1.92	0.50
1:B:746:PRO:HG2	1:B:749:GLN:HG2	1.94	0.50
1:C:255:LYS:HE3	1:C:399:ILE:HD13	1.93	0.50
1:C:395:LYS:C	1:C:397:LEU:H	2.19	0.50
1:C:396:ARG:HH21	1:C:396:ARG:HB3	1.75	0.50
1:C:565:ARG:HG2	1:D:676:GLY:HA2	1.92	0.50
1:A:305:LEU:HD12	1:A:305:LEU:H	1.77	0.50
1:C:522:ARG:NE	1:C:717:ILE:HD11	2.24	0.50
1:D:315:SER:O	1:D:319:ARG:HG3	2.11	0.50
1:A:611:ASP:OD1	1:A:613:ARG:HB2	2.11	0.50
1:C:84:SER:CB	1:C:632:ARG:HH22	2.25	0.50
1:D:580:ILE:N	1:D:580:ILE:HD12	2.26	0.50
1:B:290:GLU:O	1:B:294:THR:HG23	2.12	0.50
1:B:453:PHE:CG	1:B:491:ILE:HD12	2.46	0.50
1:B:538:THR:HG23	1:B:541:ASN:H	1.75	0.50
1:D:70:GLY:HA3	1:D:113:ASN:HD22	1.77	0.50
1:A:238:PHE:CD2	1:A:283:ILE:HG21	2.47	0.49
1:A:630:ILE:HD12	1:A:630:ILE:N	2.21	0.49
1:B:504:LEU:HD22	1:B:694:MET:HE2	1.93	0.49
1:C:44:ARG:HH11	1:C:761:LEU:CD2	2.21	0.49
1:A:114:LEU:HD22	1:A:119:ILE:HB	1.94	0.49
1:A:539:VAL:O	1:A:590:LEU:HD11	2.12	0.49
1:B:49:MET:O	1:B:53:VAL:HG22	2.12	0.49
1:C:201:ILE:HD11	1:D:308:VAL:HG12	1.95	0.49
1:C:429:VAL:HG11	1:C:477:LEU:HD11	1.93	0.49
1:A:49:MET:HE3	1:A:330:VAL:HG11	1.95	0.49
1:A:266:LEU:HD22	1:A:267:ASN:N	2.26	0.49
1:A:290:GLU:O	1:A:294:THR:HG22	2.12	0.49
1:A:560:THR:HG22	1:A:597:ALA:HB3	1.94	0.49
1:B:211:THR:OG1	1:B:267:ASN:HB2	2.12	0.49
1:B:255:LYS:HE3	1:B:399:ILE:HD13	1.93	0.49
1:C:262:ARG:O	1:C:263:LYS:HB2	2.11	0.49
1:C:670:GLY:C	1:C:672:MET:H	2.20	0.49
1:D:279:GLN:O	1:D:281:LYS:N	2.46	0.49
1:D:325:MET:HE3	1:D:325:MET:HA	1.94	0.49
1:A:230:LEU:HG	1:A:394:TYR:HB2	1.94	0.49
1:B:193:ARG:O	1:B:197:VAL:HG23	2.11	0.49
1:D:447:TYR:HD2	1:D:477:LEU:HA	1.77	0.49
1:D:461:ILE:HD12	1:D:461:ILE:O	2.11	0.49
1:D:512:TYR:CD1	1:D:512:TYR:C	2.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ASN:H	1:A:374:ARG:NH2	2.09	0.49
1:A:331:ILE:HG13	1:A:354:ARG:HH22	1.78	0.49
1:A:474:GLY:HA3	1:B:568:GLN:HE21	1.77	0.49
1:B:111:ALA:O	1:B:115:LEU:HD22	2.12	0.49
1:B:422:ALA:O	1:B:425:MET:HB2	2.12	0.49
1:C:447:TYR:HD2	1:C:477:LEU:HA	1.77	0.49
1:D:429:VAL:HG11	1:D:477:LEU:HD11	1.93	0.49
1:A:266:LEU:HD11	1:A:268:ILE:HD11	1.94	0.49
1:A:417:ASN:ND2	1:A:506:ILE:HB	2.28	0.49
1:A:542:ASN:O	1:A:746:PRO:HD3	2.13	0.49
1:A:693:ALA:HB2	1:A:720:LEU:HD23	1.93	0.49
1:B:48:ARG:HG2	1:B:79:TRP:CE2	2.48	0.49
1:B:181:THR:CB	1:B:346:SER:HB2	2.41	0.49
1:B:579:ILE:HG13	1:B:635:VAL:CG1	2.42	0.49
1:D:238:PHE:CD2	1:D:283:ILE:HG21	2.48	0.49
1:D:669:LEU:HB3	1:D:673:GLN:NE2	2.28	0.49
1:A:493:THR:O	1:A:497:THR:HB	2.13	0.49
1:B:539:VAL:HG11	1:B:674:GLN:CB	2.38	0.49
1:C:179:CYS:SG	1:C:363:MET:HB2	2.53	0.49
1:D:49:MET:O	1:D:53:VAL:HG22	2.12	0.49
1:A:44:ARG:HD3	1:A:86:LEU:HB2	1.95	0.49
1:D:195:ILE:HD11	1:D:231:ALA:HB3	1.95	0.49
1:D:696:TRP:CZ2	1:D:700:LYS:HD2	2.47	0.49
1:A:244:PRO:HD2	1:A:277:ASP:HA	1.94	0.49
1:A:470:THR:O	1:A:683:ARG:HD2	2.13	0.49
1:B:669:LEU:CB	1:B:673:GLN:NE2	2.75	0.49
1:C:65:GLN:HG2	1:C:98:CYS:CB	2.42	0.49
1:C:264:LYS:HG2	1:C:266:LEU:O	2.12	0.49
1:C:537:ALA:HA	1:C:550:ILE:HB	1.94	0.49
1:C:539:VAL:HG12	1:C:551:GLY:O	2.13	0.49
1:C:578:PHE:C	1:C:579:ILE:HD12	2.38	0.49
1:D:411:CYS:O	1:D:442:ARG:HG2	2.12	0.49
1:D:412:ASN:HB2	1:D:499:SER:O	2.12	0.49
1:D:495:MET:C	1:D:497:THR:H	2.21	0.49
1:B:42:ALA:HB1	1:B:170:MET:CE	2.39	0.49
1:B:737:LYS:HG3	1:B:738:GLN:N	2.27	0.49
1:C:208:HIS:O	1:C:209:GLN:C	2.56	0.49
1:C:397:LEU:HD21	1:C:430:ARG:NH2	2.28	0.49
1:C:605:ILE:HG12	1:C:755:ARG:HH21	1.76	0.49
1:C:610:PHE:N	1:C:610:PHE:CD1	2.80	0.49
1:D:27:ILE:HG21	1:D:333:LEU:CD1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:ASN:HB3	1:D:425:MET:HE3	1.95	0.49
1:A:268:ILE:HD12	1:A:268:ILE:H	1.77	0.48
1:C:223:TYR:C	1:C:225:ALA:N	2.69	0.48
1:D:192:HIS:O	1:D:196:GLU:HG3	2.13	0.48
1:D:501:ASN:HA	1:D:530:VAL:HG11	1.94	0.48
1:D:739:THR:N	1:D:747:LYS:HG3	2.28	0.48
1:A:266:LEU:CD1	1:A:268:ILE:HD11	2.42	0.48
1:A:532:MET:HB2	1:A:717:ILE:HG22	1.95	0.48
1:C:417:ASN:HB3	1:C:425:MET:HE3	1.95	0.48
1:D:205:ALA:CB	1:D:266:LEU:HD23	2.43	0.48
1:A:495:MET:HE3	1:A:500:ILE:HG22	1.95	0.48
1:B:174:ILE:HG21	1:B:190:ALA:HB2	1.94	0.48
1:B:223:TYR:C	1:B:225:ALA:N	2.70	0.48
1:B:645:TYR:CE1	1:D:656:GLU:HG2	2.48	0.48
1:C:501:ASN:O	1:C:531:PRO:HD2	2.13	0.48
1:D:746:PRO:HG2	1:D:749:GLN:CG	2.43	0.48
1:A:156:LYS:O	1:A:159:VAL:HG12	2.13	0.48
1:A:644:ASN:ND2	1:C:656:GLU:HB2	2.27	0.48
1:B:566:ILE:C	1:B:568:GLN:H	2.21	0.48
1:B:722:ILE:HD13	1:B:727:VAL:HG12	1.95	0.48
1:D:37:GLN:NE2	1:D:310:ARG:C	2.71	0.48
1:A:92:ILE:HG13	1:A:93:ILE:N	2.29	0.48
1:A:583:MET:HA	1:A:639:GLU:HB2	1.96	0.48
1:A:670:GLY:C	1:A:672:MET:H	2.21	0.48
1:A:480:LYS:C	1:A:482:VAL:H	2.20	0.48
1:B:495:MET:HE1	1:B:527:GLU:O	2.14	0.48
1:B:583:MET:HA	1:B:639:GLU:HB2	1.94	0.48
1:B:662:PHE:CD1	1:B:662:PHE:C	2.90	0.48
1:D:740:ASP:CG	1:D:743:HIS:HD1	2.21	0.48
1:A:522:ARG:NH1	1:A:529:CYS:HA	2.29	0.48
1:B:508:GLY:HA2	1:B:538:THR:HB	1.94	0.48
1:B:535:VAL:HG13	1:B:689:ILE:HD11	1.94	0.48
1:B:656:GLU:HB2	1:D:644:ASN:ND2	2.28	0.48
1:C:266:LEU:CD1	1:C:268:ILE:HD11	2.44	0.48
1:A:577:VAL:CG2	1:A:622:LEU:HD21	2.41	0.48
1:C:461:ILE:HD12	1:C:461:ILE:O	2.13	0.48
1:C:750:TRP:CG	1:C:751:TRP:N	2.81	0.48
1:D:181:THR:CB	1:D:346:SER:HB2	2.37	0.48
1:A:241:GLU:OE2	1:A:387:PHE:HE1	1.97	0.48
1:A:284:THR:HG22	1:A:287:LYS:HB2	1.96	0.48
1:A:443:MET:O	1:A:460:GLU:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:VAL:CG1	1:A:674:GLN:HB3	2.30	0.48
1:C:176:ASN:C	1:C:178:PHE:N	2.72	0.48
1:C:244:PRO:HD2	1:C:277:ASP:HA	1.93	0.48
1:C:533:VAL:HG22	1:C:696:TRP:CZ3	2.49	0.48
1:D:174:ILE:HG21	1:D:190:ALA:HB2	1.95	0.48
1:B:638:ASN:HB3	1:B:641:CYS:HB3	1.96	0.48
1:C:48:ARG:HE	1:C:79:TRP:CD1	2.31	0.48
1:C:238:PHE:CD2	1:C:283:ILE:HG21	2.48	0.48
1:D:49:MET:SD	1:D:760:ILE:CD1	3.01	0.48
1:D:52:TYR:CE2	1:D:760:ILE:HB	2.49	0.48
1:D:255:LYS:HE3	1:D:399:ILE:HD13	1.95	0.48
1:A:292:VAL:HG23	1:A:293:VAL:N	2.28	0.47
1:A:337:THR:O	1:A:340:THR:HG22	2.13	0.47
1:A:539:VAL:HG12	1:A:551:GLY:O	2.14	0.47
1:B:156:LYS:O	1:B:159:VAL:HG12	2.13	0.47
1:C:27:ILE:CG2	1:C:121:ASN:HB2	2.44	0.47
1:C:211:THR:OG1	1:C:267:ASN:HB2	2.14	0.47
1:D:87:GLN:HE22	1:D:567:LYS:HE3	1.79	0.47
1:D:560:THR:CG2	1:D:597:ALA:HB3	2.44	0.47
1:D:596:LEU:HB2	1:D:758:MET:HG3	1.96	0.47
1:A:191:LEU:HD22	1:A:680:PRO:CB	2.44	0.47
1:B:65:GLN:HG2	1:B:98:CYS:HB2	1.96	0.47
1:B:530:VAL:CB	1:B:531:PRO:HD2	2.45	0.47
1:B:750:TRP:CD2	1:B:751:TRP:N	2.82	0.47
1:C:48:ARG:HG2	1:C:79:TRP:CE2	2.49	0.47
1:C:205:ALA:CB	1:C:266:LEU:HD23	2.44	0.47
1:C:411:CYS:O	1:C:442:ARG:HG2	2.13	0.47
1:C:539:VAL:O	1:C:590:LEU:HD11	2.14	0.47
1:C:720:LEU:HD13	1:C:729:PHE:CD2	2.49	0.47
1:A:750:TRP:CG	1:A:751:TRP:N	2.82	0.47
1:D:27:ILE:CG2	1:D:333:LEU:HD13	2.41	0.47
1:B:84:SER:C	1:B:87:GLN:HE22	2.21	0.47
1:B:205:ALA:HB3	1:B:266:LEU:HD23	1.97	0.47
1:B:262:ARG:HD3	1:B:464:THR:HG22	1.96	0.47
1:C:27:ILE:HG13	1:C:57:VAL:HG12	1.96	0.47
1:C:192:HIS:CE1	1:C:680:PRO:HD2	2.48	0.47
1:D:450:PHE:CE1	1:D:484:PRO:HG3	2.49	0.47
1:B:199:ASP:CG	1:B:683:ARG:HH22	2.23	0.47
1:B:435:VAL:O	1:B:435:VAL:HG12	2.14	0.47
1:C:197:VAL:HG13	1:D:308:VAL:HG11	1.95	0.47
1:C:451:ASP:O	1:C:455:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:ARG:HA	1:D:165:LEU:HD12	1.95	0.47
1:D:164:TYR:CD2	1:D:338:PRO:HB3	2.50	0.47
1:D:262:ARG:HD3	1:D:464:THR:HG22	1.97	0.47
1:A:494:GLN:O	1:A:497:THR:HG22	2.14	0.47
1:A:547:ASP:HB3	1:A:750:TRP:NE1	2.30	0.47
1:A:651:TYR:HE2	1:A:664:CYS:O	1.98	0.47
1:B:44:ARG:HD3	1:B:86:LEU:HB2	1.96	0.47
1:B:478:GLY:O	1:B:479:THR:HB	2.15	0.47
1:C:148:LEU:HB3	1:C:154:ILE:CG2	2.45	0.47
1:C:414:ALA:HA	1:C:444:LEU:O	2.13	0.47
1:D:27:ILE:HD12	1:D:56:LYS:O	2.14	0.47
1:A:23:ALA:HB1	1:A:54:GLY:O	2.14	0.47
1:A:67:MET:HE2	1:A:67:MET:HB3	1.86	0.47
1:A:84:SER:C	1:A:87:GLN:HE22	2.23	0.47
1:A:476:ILE:C	1:A:478:GLY:H	2.23	0.47
1:A:579:ILE:HG13	1:A:635:VAL:CG1	2.44	0.47
1:A:661:VAL:HG13	1:A:662:PHE:CD2	2.49	0.47
1:A:731:PRO:C	1:A:733:ALA:N	2.72	0.47
1:C:193:ARG:O	1:C:197:VAL:HG23	2.14	0.47
1:C:223:TYR:C	1:C:225:ALA:H	2.23	0.47
1:C:241:GLU:OE2	1:C:387:PHE:HE1	1.97	0.47
1:C:661:VAL:HG13	1:C:662:PHE:CD2	2.50	0.47
1:C:662:PHE:CD1	1:C:662:PHE:C	2.93	0.47
1:D:87:GLN:CD	1:D:87:GLN:H	2.23	0.47
1:D:191:LEU:HD22	1:D:680:PRO:HB3	1.95	0.47
1:A:221:CYS:SG	1:A:223:TYR:HB2	2.55	0.47
1:A:380:VAL:C	1:A:382:LEU:H	2.22	0.47
1:A:487:TYR:N	1:A:487:TYR:CD2	2.81	0.47
1:A:565:ARG:O	1:A:568:GLN:HB3	2.15	0.47
1:B:171:VAL:HG11	1:B:181:THR:CG2	2.44	0.47
1:B:254:VAL:O	1:B:258:GLU:HG3	2.15	0.47
1:B:567:LYS:HG2	1:B:632:ARG:HD3	1.97	0.47
1:C:443:MET:O	1:C:460:GLU:HG3	2.15	0.47
1:D:337:THR:O	1:D:340:THR:HG22	2.14	0.47
1:D:610:PHE:CD1	1:D:610:PHE:N	2.82	0.47
1:A:260:ARG:NH2	1:A:267:ASN:HD22	2.13	0.47
1:A:739:THR:N	1:A:747:LYS:HG3	2.30	0.47
1:B:241:GLU:O	1:B:376:PHE:HB3	2.15	0.47
1:B:508:GLY:HA3	1:B:538:THR:HB	1.96	0.47
1:B:580:ILE:HG23	1:B:669:LEU:HG	1.96	0.47
1:B:630:ILE:CG2	1:B:632:ARG:HG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:GLN:HA	1:C:265:ARG:O	2.15	0.47
1:C:361:VAL:HG12	1:C:365:GLN:HE22	1.80	0.47
1:C:502:ALA:HB2	1:C:701:LEU:HD11	1.95	0.47
1:C:625:LYS:C	1:C:627:LYS:H	2.22	0.47
1:C:651:TYR:HE2	1:C:664:CYS:O	1.97	0.47
1:D:380:VAL:C	1:D:382:LEU:H	2.23	0.47
1:A:726:ASN:OD1	1:A:726:ASN:N	2.48	0.47
1:B:726:ASN:OD1	1:B:726:ASN:N	2.47	0.47
1:C:213:VAL:O	1:C:302:VAL:HG23	2.15	0.47
1:C:596:LEU:HB2	1:C:758:MET:HG3	1.96	0.47
1:D:332:ALA:HA	1:D:354:ARG:NH1	2.30	0.47
1:D:546:SER:HA	1:D:722:ILE:O	2.15	0.47
1:A:319:ARG:HD2	1:A:597:ALA:O	2.14	0.46
1:A:750:TRP:CD2	1:A:751:TRP:N	2.83	0.46
1:B:720:LEU:HD23	1:B:721:GLY:N	2.29	0.46
1:B:722:ILE:HD13	1:B:727:VAL:CG1	2.45	0.46
1:C:121:ASN:OD1	1:C:166:ASN:HB2	2.15	0.46
1:C:402:PRO:HG2	1:C:405:GLN:CD	2.40	0.46
1:C:676:GLY:HA3	1:D:565:ARG:HD2	1.96	0.46
1:D:713:THR:O	1:D:715:ASP:N	2.49	0.46
1:A:49:MET:HE3	1:A:330:VAL:CG1	2.46	0.46
1:A:198:VAL:HG12	1:A:199:ASP:N	2.29	0.46
1:A:413:VAL:HG22	1:A:502:ALA:HB3	1.97	0.46
1:B:198:VAL:HG22	1:B:214:LEU:HD21	1.96	0.46
1:B:414:ALA:HA	1:B:444:LEU:O	2.15	0.46
1:D:414:ALA:HA	1:D:444:LEU:O	2.14	0.46
1:D:670:GLY:C	1:D:672:MET:H	2.23	0.46
1:A:428:ALA:HB1	1:A:506:ILE:HD12	1.98	0.46
1:B:661:VAL:HG13	1:B:662:PHE:CD2	2.50	0.46
1:C:420:ALA:HB2	1:C:481:ARG:NH1	2.31	0.46
1:C:750:TRP:CD2	1:C:751:TRP:N	2.83	0.46
1:D:430:ARG:HA	1:D:466:VAL:HB	1.97	0.46
1:D:481:ARG:HH12	3:D:801:PO4:P	2.39	0.46
1:D:579:ILE:HG13	1:D:635:VAL:CG1	2.45	0.46
1:A:711:PHE:HD2	1:A:716:SER:HB3	1.81	0.46
1:B:223:TYR:C	1:B:225:ALA:H	2.24	0.46
1:C:509:PHE:HE2	1:C:513:LEU:HD21	1.80	0.46
1:D:65:GLN:HG2	1:D:98:CYS:CB	2.46	0.46
1:D:115:LEU:HD12	1:D:162:TYR:CD2	2.50	0.46
1:D:262:ARG:NH2	1:D:400:LYS:HD3	2.27	0.46
1:D:426:ASN:OD1	1:D:476:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:752:LEU:O	1:D:755:ARG:HB2	2.14	0.46
1:A:396:ARG:HD2	1:A:396:ARG:O	2.15	0.46
1:A:638:ASN:HB3	1:A:641:CYS:HB3	1.98	0.46
1:B:264:LYS:C	1:B:266:LEU:H	2.24	0.46
1:C:535:VAL:HG13	1:C:689:ILE:HD11	1.98	0.46
1:C:755:ARG:N	1:C:756:PRO:HD2	2.31	0.46
1:D:208:HIS:C	1:D:209:GLN:HG2	2.40	0.46
1:D:496:ARG:HB2	1:D:527:GLU:HG2	1.98	0.46
1:D:685:PHE:CE2	1:D:689:ILE:HG21	2.51	0.46
1:A:219:ARG:HG3	1:A:273:GLU:CD	2.38	0.46
1:A:526:GLU:C	1:A:528:PHE:H	2.24	0.46
1:B:185:ILE:HD11	1:B:322:ALA:HA	1.98	0.46
1:B:406:ILE:HG22	1:B:406:ILE:O	2.16	0.46
1:B:493:THR:HG22	1:B:496:ARG:NH2	2.30	0.46
1:D:718:CYS:HA	1:D:732:VAL:HG13	1.97	0.46
1:A:264:LYS:C	1:A:266:LEU:H	2.24	0.46
1:B:702:LYS:HA	1:B:705:ARG:HD2	1.97	0.46
1:C:92:ILE:HG13	1:C:93:ILE:N	2.30	0.46
1:D:512:TYR:C	1:D:512:TYR:HD1	2.24	0.46
1:A:492:ALA:HB1	1:A:527:GLU:OE1	2.15	0.46
1:A:494:GLN:C	1:A:497:THR:HG22	2.41	0.46
1:C:525:HIS:HB2	1:C:528:PHE:CE1	2.51	0.46
1:C:577:VAL:HG21	1:C:622:LEU:HD21	1.98	0.46
1:C:700:LYS:HA	1:C:703:GLU:CG	2.45	0.46
1:A:69:ASP:O	1:A:113:ASN:ND2	2.48	0.46
1:B:529:CYS:HB3	1:B:711:PHE:O	2.16	0.46
1:B:610:PHE:N	1:B:610:PHE:CD1	2.84	0.46
1:C:762:ALA:O	1:C:763:LYS:CB	2.64	0.46
1:A:546:SER:HB2	1:A:721:GLY:HA3	1.98	0.46
1:A:622:LEU:O	1:A:626:MET:HG2	2.16	0.46
1:A:717:ILE:HD13	1:A:717:ILE:N	2.30	0.46
1:A:735:LEU:O	1:A:739:THR:HG22	2.16	0.46
1:B:576:ARG:HD3	1:B:663:ASP:HB3	1.96	0.46
1:B:663:ASP:O	1:B:664:CYS:HB3	2.16	0.46
1:C:630:ILE:HD12	1:C:630:ILE:N	2.19	0.46
1:D:214:LEU:HB3	1:D:305:LEU:HD11	1.98	0.46
1:D:387:PHE:C	1:D:387:PHE:CD2	2.93	0.46
1:A:148:LEU:HB3	1:A:154:ILE:HG23	1.97	0.45
1:A:174:ILE:HD11	1:A:217:MET:SD	2.56	0.45
1:A:176:ASN:C	1:A:178:PHE:N	2.74	0.45
1:A:532:MET:O	1:A:717:ILE:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:TRP:CZ3	1:C:399:ILE:HD11	2.51	0.45
1:C:264:LYS:C	1:C:266:LEU:H	2.23	0.45
1:D:262:ARG:O	1:D:263:LYS:CB	2.64	0.45
1:D:387:PHE:C	1:D:387:PHE:HD2	2.24	0.45
1:D:486:LYS:C	1:D:487:TYR:HD2	2.24	0.45
1:D:712:THR:O	1:D:713:THR:C	2.58	0.45
1:A:27:ILE:HD13	1:A:57:VAL:CG1	2.46	0.45
1:A:138:ARG:CD	1:A:165:LEU:O	2.64	0.45
1:A:260:ARG:NH2	1:A:267:ASN:ND2	2.64	0.45
1:A:412:ASN:OD1	1:A:442:ARG:HD3	2.17	0.45
1:B:88:VAL:HG12	1:B:89:GLY:N	2.31	0.45
1:B:135:ASN:HB2	1:B:357:LEU:HD22	1.99	0.45
1:B:241:GLU:OE2	1:B:387:PHE:HE1	1.98	0.45
1:B:476:ILE:C	1:B:478:GLY:H	2.22	0.45
1:B:596:LEU:HB2	1:B:758:MET:HG3	1.98	0.45
1:B:719:VAL:HG23	1:B:719:VAL:O	2.15	0.45
1:D:401:LEU:HG	1:D:406:ILE:HG12	1.98	0.45
1:D:504:LEU:HD23	1:D:504:LEU:O	2.16	0.45
1:C:223:TYR:O	1:C:225:ALA:N	2.48	0.45
1:C:522:ARG:HE	1:C:717:ILE:CD1	2.23	0.45
1:D:507:GLY:N	1:D:537:ALA:HB3	2.32	0.45
1:A:81:SER:C	1:A:83:SER:H	2.24	0.45
1:C:115:LEU:HD12	1:C:162:TYR:CD2	2.52	0.45
1:C:426:ASN:OD1	1:C:476:ILE:HG13	2.16	0.45
1:C:489:GLU:OE2	1:C:525:HIS:CD2	2.69	0.45
1:D:306:GLY:O	1:D:308:VAL:N	2.50	0.45
1:D:487:TYR:O	1:D:491:ILE:HD12	2.17	0.45
1:D:750:TRP:CG	1:D:751:TRP:N	2.83	0.45
1:B:447:TYR:HD2	1:B:477:LEU:HA	1.82	0.45
1:C:30:LEU:HB3	1:C:60:ILE:HB	1.99	0.45
1:C:277:ASP:HB3	1:C:283:ILE:HD11	1.99	0.45
1:C:577:VAL:HG22	1:C:633:GLY:HA3	1.99	0.45
1:C:746:PRO:HG2	1:C:749:GLN:CG	2.45	0.45
1:D:223:TYR:C	1:D:225:ALA:N	2.74	0.45
1:B:363:MET:O	1:B:367:VAL:HG23	2.17	0.45
1:B:483:LEU:CD2	1:B:513:LEU:HD22	2.45	0.45
1:D:536:PRO:HD3	1:D:720:LEU:O	2.16	0.45
1:D:580:ILE:HG23	1:D:669:LEU:HG	1.99	0.45
1:A:332:ALA:HA	1:A:354:ARG:NH1	2.31	0.45
1:B:537:ALA:HA	1:B:550:ILE:HB	1.98	0.45
1:C:327:VAL:O	1:C:331:ILE:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:PHE:CE1	1:C:484:PRO:HD3	2.52	0.45
1:C:558:THR:CG2	1:C:672:MET:HE2	2.46	0.45
1:D:81:SER:C	1:D:83:SER:H	2.25	0.45
1:D:470:THR:O	1:D:683:ARG:HD2	2.17	0.45
1:D:701:LEU:HD23	1:D:701:LEU:HA	1.83	0.45
1:D:729:PHE:CD1	1:D:729:PHE:N	2.85	0.45
1:D:755:ARG:N	1:D:756:PRO:HD2	2.31	0.45
1:A:120:THR:HG23	1:A:121:ASN:ND2	2.31	0.45
1:A:168:VAL:O	1:A:168:VAL:HG13	2.16	0.45
1:B:356:PRO:HG2	1:B:359:GLU:HB3	1.99	0.45
1:C:409:THR:HB	1:C:705:ARG:NH2	2.32	0.45
1:C:473:GLY:HA2	1:C:678:PRO:HD3	1.98	0.45
1:D:419:GLY:CA	1:D:510:GLU:HG3	2.47	0.45
1:D:481:ARG:HG3	1:D:510:GLU:CG	2.47	0.45
1:D:485:GLY:O	1:D:488:LEU:HD22	2.17	0.45
1:D:685:PHE:HE2	1:D:689:ILE:HG21	1.81	0.45
1:A:293:VAL:HG23	1:A:298:TYR:O	2.16	0.45
1:A:354:ARG:O	1:A:355:LEU:HD23	2.16	0.45
1:A:556:LEU:O	1:A:560:THR:HG23	2.16	0.45
1:B:30:LEU:HB3	1:B:60:ILE:HB	1.98	0.45
1:B:67:MET:HE2	1:B:67:MET:HB3	1.83	0.45
1:B:285:SER:HB3	1:B:302:VAL:HG21	1.98	0.45
1:B:325:MET:HE1	1:B:352:ALA:HB1	1.98	0.45
1:C:307:HIS:C	1:C:309:GLN:H	2.24	0.45
1:C:476:ILE:C	1:C:478:GLY:H	2.23	0.45
1:D:435:VAL:HG12	1:D:435:VAL:O	2.16	0.45
1:D:757:LEU:C	1:D:757:LEU:HD22	2.42	0.45
1:A:39:MET:O	1:A:42:ALA:HB3	2.16	0.45
1:A:70:GLY:HA3	1:A:113:ASN:HD22	1.79	0.45
1:A:187:THR:HG21	1:A:223:TYR:HE2	1.82	0.45
1:A:258:GLU:O	1:A:262:ARG:HG3	2.17	0.45
1:A:417:ASN:HD22	1:A:506:ILE:HB	1.82	0.45
1:B:450:PHE:HD1	1:B:482:VAL:O	2.00	0.45
1:B:515:LEU:HD11	1:B:534:MET:HB2	1.98	0.45
1:B:586:TYR:CG	1:B:743:HIS:HB3	2.51	0.45
1:C:101:PHE:C	1:C:103:THR:H	2.23	0.45
1:C:519:SER:O	1:C:522:ARG:HD2	2.16	0.45
1:D:30:LEU:HB3	1:D:60:ILE:HB	1.99	0.45
1:D:59:PHE:O	1:D:74:ILE:HA	2.17	0.45
1:D:285:SER:HB3	1:D:302:VAL:HG21	1.99	0.45
1:D:726:ASN:OD1	1:D:726:ASN:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:GLY:O	1:A:251:GLN:HG2	2.17	0.44
1:A:397:LEU:HD11	1:A:431:SER:HA	1.99	0.44
1:A:685:PHE:CE2	1:A:689:ILE:HG21	2.53	0.44
1:B:25:LYS:O	1:B:55:ALA:HB1	2.17	0.44
1:B:79:TRP:CZ2	1:B:763:LYS:CA	3.00	0.44
1:B:566:ILE:C	1:B:568:GLN:N	2.74	0.44
1:B:577:VAL:CG2	1:B:622:LEU:HD21	2.44	0.44
1:C:488:LEU:HD22	1:C:528:PHE:CE1	2.52	0.44
1:C:735:LEU:O	1:C:739:THR:HG22	2.17	0.44
1:D:306:GLY:C	1:D:308:VAL:N	2.65	0.44
1:D:578:PHE:C	1:D:579:ILE:HD12	2.42	0.44
1:A:26:ALA:HA	1:A:56:LYS:O	2.16	0.44
1:A:174:ILE:CG2	1:A:190:ALA:HB2	2.48	0.44
1:A:284:THR:CG2	1:A:287:LYS:HB2	2.46	0.44
1:B:306:GLY:C	1:B:308:VAL:N	2.76	0.44
1:B:533:VAL:HG21	1:B:693:ALA:HB1	1.99	0.44
1:C:50:GLY:O	1:C:53:VAL:HG23	2.18	0.44
1:C:83:SER:O	1:C:84:SER:HB3	2.18	0.44
1:C:432:ALA:O	1:C:694:MET:HE3	2.17	0.44
1:C:731:PRO:C	1:C:733:ALA:N	2.74	0.44
1:D:286:GLU:C	1:D:288:ILE:N	2.75	0.44
1:D:480:LYS:C	1:D:482:VAL:N	2.76	0.44
1:D:495:MET:HE1	1:D:527:GLU:O	2.17	0.44
1:D:583:MET:HA	1:D:639:GLU:HB2	1.98	0.44
1:A:696:TRP:CZ2	1:A:700:LYS:HD2	2.52	0.44
1:B:79:TRP:CE2	1:B:763:LYS:HB2	2.51	0.44
1:C:320:ILE:CD1	1:C:597:ALA:HB2	2.47	0.44
1:C:461:ILE:HD12	1:C:461:ILE:C	2.43	0.44
1:C:566:ILE:C	1:C:568:GLN:H	2.24	0.44
1:D:52:TYR:CD2	1:D:760:ILE:HB	2.52	0.44
1:D:221:CYS:HA	1:D:383:ARG:HH21	1.80	0.44
1:D:521:ALA:O	1:D:525:HIS:HB2	2.17	0.44
1:D:530:VAL:HG12	1:D:531:PRO:HD2	1.99	0.44
1:D:579:ILE:HA	1:D:635:VAL:HG13	1.98	0.44
1:B:215:GLU:OE1	1:B:304:ILE:HG12	2.18	0.44
1:C:165:LEU:HD13	1:C:167:VAL:HG13	2.00	0.44
1:D:387:PHE:HD2	1:D:387:PHE:O	2.01	0.44
1:D:532:MET:HE3	1:D:717:ILE:CG2	2.46	0.44
1:A:395:LYS:C	1:A:397:LEU:N	2.76	0.44
1:A:496:ARG:HH21	1:A:496:ARG:HG3	1.83	0.44
1:A:496:ARG:C	1:A:498:HIS:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ARG:HA	1:B:165:LEU:HD12	1.98	0.44
1:B:221:CYS:HA	1:B:383:ARG:HH21	1.82	0.44
1:B:483:LEU:CD2	1:B:513:LEU:HB3	2.48	0.44
1:D:266:LEU:HD11	1:D:268:ILE:HD11	1.99	0.44
1:D:293:VAL:HG23	1:D:298:TYR:O	2.18	0.44
1:D:416:ILE:HG22	1:D:505:ILE:HD13	1.99	0.44
1:A:285:SER:HB3	1:A:302:VAL:HG21	2.00	0.44
1:B:101:PHE:C	1:B:103:THR:H	2.25	0.44
1:B:205:ALA:HB1	1:B:266:LEU:HD23	1.99	0.44
1:B:451:ASP:O	1:B:455:LYS:HG3	2.17	0.44
1:B:524:LYS:HD3	1:B:524:LYS:H	1.82	0.44
1:B:608:GLU:OE1	1:B:755:ARG:HG2	2.18	0.44
1:B:644:ASN:HD21	1:D:655:SER:HB3	1.83	0.44
1:C:23:ALA:HA	1:C:54:GLY:O	2.17	0.44
1:C:326:GLY:O	1:C:330:VAL:HG23	2.18	0.44
1:D:27:ILE:HD12	1:D:27:ILE:H	1.83	0.44
1:D:413:VAL:HA	1:D:502:ALA:HB3	1.98	0.44
1:D:479:THR:HG23	1:D:479:THR:O	2.16	0.44
1:D:537:ALA:HA	1:D:550:ILE:HB	1.99	0.44
1:D:638:ASN:O	1:D:639:GLU:C	2.61	0.44
1:A:78:ASP:OD2	1:A:78:ASP:N	2.43	0.44
1:A:306:GLY:O	1:A:308:VAL:N	2.51	0.44
1:A:720:LEU:HD13	1:A:729:PHE:CD2	2.53	0.44
1:B:30:LEU:HD23	1:B:30:LEU:N	2.32	0.44
1:B:209:GLN:HA	1:B:265:ARG:O	2.18	0.44
1:B:327:VAL:O	1:B:331:ILE:HG23	2.18	0.44
1:B:380:VAL:C	1:B:382:LEU:H	2.25	0.44
1:C:81:SER:C	1:C:83:SER:H	2.26	0.44
1:C:221:CYS:HA	1:C:383:ARG:HH21	1.80	0.44
1:D:74:ILE:HG21	1:D:117:ARG:HG3	1.99	0.44
1:D:512:TYR:CE2	1:D:544:PRO:HG2	2.53	0.44
1:A:260:ARG:HH22	1:A:267:ASN:HD22	1.66	0.44
1:B:27:ILE:HG12	1:B:333:LEU:HD13	1.99	0.44
1:B:554:THR:HG22	1:B:555:ALA:N	2.33	0.44
1:C:266:LEU:HD11	1:C:268:ILE:HD11	1.99	0.44
1:C:387:PHE:HD2	1:C:387:PHE:C	2.26	0.44
1:C:541:ASN:C	1:C:541:ASN:HD22	2.23	0.44
1:D:26:ALA:HA	1:D:56:LYS:O	2.17	0.44
1:D:244:PRO:HB2	1:D:248:TRP:CG	2.53	0.44
1:A:42:ALA:HB1	1:A:170:MET:CE	2.40	0.44
1:A:279:GLN:O	1:A:281:LYS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:VAL:O	1:A:331:ILE:HG23	2.18	0.44
1:A:411:CYS:O	1:A:442:ARG:HG2	2.17	0.44
1:A:718:CYS:SG	1:A:731:PRO:HA	2.58	0.44
1:C:525:HIS:C	1:C:527:GLU:H	2.26	0.44
1:C:701:LEU:HD23	1:C:701:LEU:HA	1.89	0.44
1:A:101:PHE:C	1:A:103:THR:H	2.26	0.43
1:A:370:ALA:HB2	1:A:375:ARG:NH1	2.33	0.43
1:A:414:ALA:HA	1:A:444:LEU:O	2.18	0.43
1:A:496:ARG:C	1:A:498:HIS:H	2.25	0.43
1:B:411:CYS:O	1:B:442:ARG:HG2	2.17	0.43
1:B:454:ALA:N	1:B:491:ILE:HD11	2.33	0.43
1:B:504:LEU:HD12	1:B:533:VAL:HG13	1.99	0.43
1:B:541:ASN:O	1:B:541:ASN:ND2	2.48	0.43
1:C:580:ILE:N	1:C:580:ILE:HD12	2.33	0.43
1:D:717:ILE:O	1:D:717:ILE:HG13	2.18	0.43
1:A:193:ARG:O	1:A:197:VAL:HG23	2.18	0.43
1:A:211:THR:OG1	1:A:267:ASN:HB2	2.17	0.43
1:A:327:VAL:HG21	1:A:757:LEU:HD21	2.01	0.43
1:A:731:PRO:C	1:A:733:ALA:H	2.27	0.43
1:B:370:ALA:CB	1:B:379:ALA:HB2	2.45	0.43
1:B:412:ASN:OD1	1:B:442:ARG:HD3	2.19	0.43
1:B:429:VAL:HG11	1:B:477:LEU:HD11	1.99	0.43
1:B:577:VAL:O	1:B:664:CYS:HA	2.18	0.43
1:C:70:GLY:HA3	1:C:113:ASN:HD22	1.83	0.43
1:C:414:ALA:O	1:C:503:LEU:HA	2.18	0.43
1:D:230:LEU:HG	1:D:394:TYR:HB2	2.00	0.43
1:D:244:PRO:HD2	1:D:277:ASP:HA	1.99	0.43
1:D:327:VAL:O	1:D:331:ILE:HG23	2.17	0.43
1:D:496:ARG:HD3	1:D:527:GLU:OE1	2.17	0.43
1:A:465:ASP:C	1:A:467:GLY:H	2.25	0.43
1:B:419:GLY:HA2	1:B:510:GLU:HG3	2.00	0.43
1:C:311:GLY:HA3	1:D:200:ALA:O	2.18	0.43
1:C:433:VAL:HG21	1:C:466:VAL:HG11	1.99	0.43
1:D:187:THR:HG21	1:D:223:TYR:HE2	1.83	0.43
1:A:99:GLN:C	1:A:101:PHE:N	2.77	0.43
1:A:209:GLN:HA	1:A:265:ARG:O	2.19	0.43
1:A:535:VAL:HG13	1:A:689:ILE:CD1	2.48	0.43
1:A:649:PHE:CD1	1:C:649:PHE:CD1	3.06	0.43
1:A:739:THR:HG23	1:A:741:PHE:CE1	2.53	0.43
1:C:325:MET:HE1	1:C:352:ALA:HB1	2.01	0.43
1:D:27:ILE:HD13	1:D:57:VAL:CG1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:738:GLN:O	1:D:738:GLN:HG2	2.18	0.43
1:A:244:PRO:HB2	1:A:248:TRP:CG	2.54	0.43
1:A:255:LYS:HE3	1:A:399:ILE:HD13	2.01	0.43
1:B:187:THR:HG21	1:B:223:TYR:HE2	1.82	0.43
1:B:208:HIS:C	1:B:209:GLN:HG2	2.43	0.43
1:B:217:MET:HG3	1:B:309:GLN:NE2	2.33	0.43
1:B:637:ARG:HE	1:B:647:THR:N	2.17	0.43
1:B:755:ARG:HD2	1:B:755:ARG:HA	1.70	0.43
1:C:262:ARG:HD3	1:C:464:THR:CG2	2.48	0.43
1:D:25:LYS:H	1:D:25:LYS:HG3	1.50	0.43
1:A:170:MET:HG3	1:A:345:VAL:HG23	2.01	0.43
1:A:668:VAL:O	1:A:669:LEU:C	2.61	0.43
1:B:649:PHE:HD1	1:D:652:GLN:OE1	2.01	0.43
1:B:717:ILE:O	1:B:717:ILE:HG22	2.18	0.43
1:C:370:ALA:HB2	1:C:375:ARG:NH1	2.34	0.43
1:C:565:ARG:HG2	1:D:676:GLY:CA	2.49	0.43
1:C:579:ILE:HA	1:C:635:VAL:HG13	2.00	0.43
1:D:87:GLN:NE2	1:D:567:LYS:HE3	2.33	0.43
1:B:35:ASP:O	1:B:310:ARG:HD2	2.19	0.43
1:B:731:PRO:C	1:B:733:ALA:H	2.27	0.43
1:B:748:GLU:CD	1:B:748:GLU:O	2.61	0.43
1:C:402:PRO:HB2	1:C:405:GLN:HG3	2.01	0.43
1:C:568:GLN:HG3	1:D:474:GLY:HA3	2.01	0.43
1:C:608:GLU:OE1	1:C:755:ARG:CG	2.66	0.43
1:A:59:PHE:O	1:A:74:ILE:HA	2.18	0.43
1:A:448:ASP:CG	1:B:574:LYS:HG3	2.42	0.43
1:A:477:LEU:HD12	1:A:477:LEU:N	2.33	0.43
1:A:722:ILE:HD13	1:A:727:VAL:HG12	2.01	0.43
1:B:23:ALA:C	1:B:25:LYS:H	2.27	0.43
1:B:67:MET:HE2	1:B:110:ALA:HB1	1.99	0.43
1:B:284:THR:O	1:B:288:ILE:HG13	2.18	0.43
1:B:493:THR:O	1:B:496:ARG:N	2.49	0.43
1:C:88:VAL:HG12	1:C:89:GLY:N	2.34	0.43
1:C:402:PRO:HG2	1:C:405:GLN:HG3	2.01	0.43
1:D:277:ASP:HB3	1:D:283:ILE:HD11	2.01	0.43
1:D:526:GLU:HA	1:D:529:CYS:SG	2.59	0.43
1:D:584:GLY:O	1:D:585:GLY:C	2.61	0.43
1:A:30:LEU:N	1:A:30:LEU:HD23	2.34	0.43
1:A:223:TYR:C	1:A:225:ALA:N	2.76	0.43
1:B:41:ALA:CB	1:B:86:LEU:HD12	2.48	0.43
1:C:42:ALA:HB1	1:C:170:MET:CE	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:601:ASP:O	1:C:602:ALA:HB2	2.19	0.43
1:D:37:GLN:CD	1:D:37:GLN:H	2.27	0.43
1:D:154:ILE:O	1:D:155:ASP:C	2.62	0.43
1:A:438:ALA:HB2	1:A:463:TRP:HZ3	1.84	0.43
1:B:292:VAL:HG23	1:B:293:VAL:N	2.34	0.43
1:B:331:ILE:O	1:B:335:GLU:HB2	2.19	0.43
1:C:30:LEU:N	1:C:30:LEU:HD23	2.33	0.43
1:C:49:MET:HG2	1:C:760:ILE:HD11	2.01	0.43
1:C:308:VAL:HG12	1:D:201:ILE:HD11	2.00	0.43
1:C:324:ARG:NE	1:C:754:LEU:HD21	2.34	0.43
1:D:148:LEU:HB3	1:D:154:ILE:CG2	2.47	0.43
1:D:481:ARG:HG3	1:D:510:GLU:HB3	2.00	0.43
1:D:486:LYS:C	1:D:488:LEU:HD23	2.43	0.43
1:D:519:SER:OG	1:D:717:ILE:HD11	2.18	0.43
1:A:610:PHE:N	1:A:610:PHE:CD1	2.87	0.42
1:A:685:PHE:HE2	1:A:689:ILE:HG21	1.84	0.42
1:B:68:VAL:O	1:B:109:LYS:HG3	2.19	0.42
1:B:121:ASN:OD1	1:B:166:ASN:HB2	2.18	0.42
1:B:247:GLY:O	1:B:251:GLN:HG2	2.19	0.42
1:B:321:LEU:HD23	1:B:321:LEU:O	2.19	0.42
1:B:567:LYS:HD3	1:B:632:ARG:NH1	2.33	0.42
1:B:702:LYS:HD2	1:B:705:ARG:HD2	2.01	0.42
1:C:25:LYS:HG2	1:C:120:THR:HG21	1.99	0.42
1:C:483:LEU:HD13	1:C:484:PRO:CD	2.47	0.42
1:C:731:PRO:C	1:C:733:ALA:H	2.27	0.42
1:C:739:THR:HG23	1:C:741:PHE:CE1	2.54	0.42
1:D:638:ASN:HB3	1:D:641:CYS:HB3	1.99	0.42
1:B:16:PHE:C	1:B:18:GLU:H	2.27	0.42
1:B:279:GLN:O	1:B:281:LYS:N	2.52	0.42
1:B:625:LYS:C	1:B:627:LYS:N	2.77	0.42
1:B:629:THR:O	1:B:631:GLN:HG3	2.18	0.42
1:C:67:MET:HB3	1:C:67:MET:HE2	1.79	0.42
1:C:177:ASP:O	1:C:364:THR:HG23	2.19	0.42
1:D:179:CYS:SG	1:D:363:MET:CB	3.07	0.42
1:D:443:MET:O	1:D:460:GLU:HG3	2.18	0.42
1:A:222:GLY:HA3	1:A:240:PRO:HD2	2.01	0.42
1:A:629:THR:O	1:A:631:GLN:HG3	2.19	0.42
1:B:222:GLY:HA3	1:B:240:PRO:HD2	2.01	0.42
1:B:337:THR:O	1:B:340:THR:HG22	2.19	0.42
1:C:86:LEU:HD21	1:C:597:ALA:O	2.19	0.42
1:C:541:ASN:O	1:C:541:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:TYR:O	1:D:225:ALA:N	2.52	0.42
1:D:402:PRO:HB2	1:D:405:GLN:HG3	2.00	0.42
1:D:637:ARG:HH11	1:D:637:ARG:CG	2.32	0.42
1:A:357:LEU:O	1:A:361:VAL:HG23	2.19	0.42
1:A:489:GLU:O	1:A:490:GLU:C	2.61	0.42
1:B:164:TYR:CD2	1:B:338:PRO:HB3	2.54	0.42
1:C:217:MET:HG3	1:C:309:GLN:NE2	2.35	0.42
1:C:755:ARG:HD2	1:C:755:ARG:HA	1.83	0.42
1:D:540:SER:O	1:D:541:ASN:HB3	2.19	0.42
1:D:694:MET:O	1:D:697:ILE:HB	2.20	0.42
1:A:190:ALA:O	1:A:194:ILE:HG13	2.18	0.42
1:A:376:PHE:O	1:A:380:VAL:HG23	2.19	0.42
1:A:731:PRO:O	1:A:733:ALA:N	2.52	0.42
1:B:28:GLY:HA3	1:B:122:LEU:HD12	2.01	0.42
1:B:217:MET:HE1	1:B:310:ARG:NH1	2.34	0.42
1:B:441:HIS:NE2	1:B:698:THR:HG23	2.34	0.42
1:C:27:ILE:HG23	1:C:121:ASN:HB2	2.01	0.42
1:C:408:LYS:H	1:C:408:LYS:HG2	1.68	0.42
1:C:438:ALA:HB2	1:C:463:TRP:HZ3	1.84	0.42
1:D:78:ASP:OD2	1:D:78:ASP:N	2.42	0.42
1:D:266:LEU:HD22	1:D:266:LEU:C	2.43	0.42
1:D:492:ALA:HB2	1:D:528:PHE:CZ	2.55	0.42
1:A:74:ILE:HG21	1:A:117:ARG:HG3	2.01	0.42
1:A:171:VAL:HG23	1:A:171:VAL:O	2.19	0.42
1:A:411:CYS:SG	1:A:701:LEU:HD21	2.60	0.42
1:A:422:ALA:HB2	1:A:538:THR:HA	2.01	0.42
1:A:448:ASP:O	1:A:449:GLY:C	2.61	0.42
1:A:566:ILE:C	1:A:568:GLN:H	2.26	0.42
1:B:477:LEU:HD12	1:B:477:LEU:N	2.33	0.42
1:C:505:ILE:HD12	1:C:515:LEU:CD2	2.48	0.42
1:C:750:TRP:C	1:C:752:LEU:H	2.27	0.42
1:D:577:VAL:O	1:D:664:CYS:HA	2.20	0.42
1:D:750:TRP:C	1:D:752:LEU:H	2.27	0.42
1:A:277:ASP:HB3	1:A:283:ILE:HD11	2.00	0.42
1:A:580:ILE:N	1:A:580:ILE:HD12	2.34	0.42
1:B:112:CYS:HB2	1:B:148:LEU:CD2	2.49	0.42
1:C:21:SER:HB2	1:C:22:GLY:H	1.60	0.42
1:C:236:TRP:HZ3	1:C:399:ILE:HD11	1.85	0.42
1:C:492:ALA:O	1:C:495:MET:HB2	2.19	0.42
1:D:179:CYS:SG	1:D:363:MET:HB2	2.59	0.42
1:D:395:LYS:C	1:D:397:LEU:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:HIS:C	1:A:209:GLN:HG2	2.45	0.42
1:A:537:ALA:HA	1:A:550:ILE:HB	2.01	0.42
1:A:630:ILE:H	1:A:630:ILE:CD1	2.18	0.42
1:B:127:GLY:HA3	2:B:801:ADP:O2B	2.19	0.42
1:B:541:ASN:HD22	1:B:541:ASN:C	2.28	0.42
1:C:84:SER:HB2	1:C:632:ARG:HH22	1.83	0.42
1:C:241:GLU:O	1:C:376:PHE:HB3	2.20	0.42
1:C:307:HIS:NE2	1:D:301:ARG:HG2	2.34	0.42
1:C:355:LEU:HB3	1:C:356:PRO:HD2	2.01	0.42
1:C:435:VAL:O	1:C:435:VAL:HG12	2.20	0.42
1:C:667:ASN:HD22	1:C:667:ASN:HA	1.64	0.42
1:D:478:GLY:O	1:D:479:THR:HB	2.19	0.42
1:D:547:ASP:HB3	1:D:750:TRP:NE1	2.35	0.42
1:A:156:LYS:HA	1:A:156:LYS:HD2	1.84	0.42
1:A:447:TYR:HD2	1:A:477:LEU:HA	1.83	0.42
1:C:293:VAL:HG23	1:C:298:TYR:O	2.20	0.42
1:C:483:LEU:HD12	1:C:517:GLU:CD	2.45	0.42
1:C:521:ALA:O	1:C:528:PHE:HD1	2.02	0.42
1:D:275:ALA:C	1:D:276:ILE:HG23	2.45	0.42
1:D:413:VAL:HG22	1:D:502:ALA:HB3	2.01	0.42
1:D:416:ILE:CG2	1:D:505:ILE:HD13	2.50	0.42
1:A:729:PHE:N	1:A:729:PHE:CD1	2.87	0.42
1:B:30:LEU:HD12	1:B:63:GLY:C	2.44	0.42
1:B:148:LEU:HB3	1:B:154:ILE:CG2	2.49	0.42
1:C:48:ARG:HD3	1:C:761:LEU:O	2.20	0.42
1:C:179:CYS:SG	1:C:363:MET:CB	3.08	0.42
1:C:244:PRO:HB2	1:C:248:TRP:CG	2.55	0.42
1:C:422:ALA:O	1:C:425:MET:HB2	2.20	0.42
1:C:717:ILE:O	1:C:732:VAL:HG22	2.20	0.42
1:C:729:PHE:CD1	1:C:729:PHE:N	2.88	0.42
1:D:61:TYR:HA	1:D:93:ILE:O	2.20	0.42
1:D:567:LYS:HD3	1:D:632:ARG:CD	2.50	0.42
1:A:637:ARG:HE	1:A:647:THR:N	2.18	0.41
1:B:156:LYS:HA	1:B:156:LYS:HD2	1.85	0.41
1:B:504:LEU:HD22	1:B:694:MET:CE	2.50	0.41
1:B:504:LEU:CD1	1:B:533:VAL:HG13	2.50	0.41
1:C:412:ASN:OD1	1:C:442:ARG:CD	2.63	0.41
1:C:412:ASN:ND2	1:C:498:HIS:O	2.53	0.41
1:C:495:MET:HE1	1:C:500:ILE:HB	2.02	0.41
1:D:205:ALA:HB3	1:D:266:LEU:HD23	2.02	0.41
1:D:717:ILE:O	1:D:732:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:748:GLU:CD	1:D:748:GLU:O	2.63	0.41
1:A:208:HIS:O	1:A:209:GLN:C	2.63	0.41
1:B:59:PHE:O	1:B:74:ILE:HA	2.19	0.41
1:B:656:GLU:HB2	1:D:644:ASN:HD22	1.84	0.41
1:C:67:MET:HE2	1:C:110:ALA:HB1	2.02	0.41
1:C:648:ASP:O	1:C:652:GLN:HG3	2.20	0.41
1:D:174:ILE:CG2	1:D:190:ALA:HB2	2.50	0.41
1:D:217:MET:HE1	1:D:310:ARG:NH1	2.35	0.41
1:D:279:GLN:C	1:D:281:LYS:N	2.77	0.41
1:A:406:ILE:O	1:A:406:ILE:HG22	2.20	0.41
1:A:501:ASN:O	1:A:531:PRO:HD2	2.19	0.41
1:A:546:SER:HA	1:A:722:ILE:O	2.20	0.41
1:B:214:LEU:HB3	1:B:305:LEU:HD11	2.02	0.41
1:B:279:GLN:C	1:B:281:LYS:N	2.79	0.41
1:B:401:LEU:O	1:B:402:PRO:C	2.63	0.41
1:B:530:VAL:HA	1:B:711:PHE:CD2	2.55	0.41
1:C:74:ILE:HG21	1:C:117:ARG:HG3	2.02	0.41
1:C:370:ALA:CB	1:C:379:ALA:HB2	2.49	0.41
1:D:48:ARG:NE	1:D:79:TRP:NE1	2.68	0.41
1:D:67:MET:HE3	1:D:114:LEU:HG	2.01	0.41
1:D:264:LYS:C	1:D:266:LEU:H	2.29	0.41
1:D:279:GLN:C	1:D:281:LYS:H	2.28	0.41
1:D:294:THR:O	1:D:294:THR:HG23	2.19	0.41
1:D:731:PRO:C	1:D:733:ALA:N	2.74	0.41
1:A:432:ALA:HB1	1:A:504:LEU:HD23	2.02	0.41
1:A:717:ILE:O	1:A:732:VAL:HG13	2.20	0.41
1:B:357:LEU:O	1:B:361:VAL:HG23	2.20	0.41
1:B:430:ARG:HH21	1:B:470:THR:CG2	2.33	0.41
1:D:101:PHE:C	1:D:103:THR:N	2.78	0.41
1:D:354:ARG:O	1:D:355:LEU:HD23	2.20	0.41
1:D:432:ALA:O	1:D:694:MET:HE3	2.20	0.41
1:D:476:ILE:C	1:D:478:GLY:H	2.27	0.41
1:D:735:LEU:O	1:D:739:THR:CG2	2.67	0.41
1:A:88:VAL:HG12	1:A:89:GLY:N	2.35	0.41
1:B:65:GLN:HG2	1:B:98:CYS:CB	2.50	0.41
1:B:395:LYS:C	1:B:397:LEU:N	2.78	0.41
1:B:622:LEU:O	1:B:626:MET:HG2	2.20	0.41
1:D:515:LEU:CG	1:D:534:MET:HE2	2.46	0.41
1:A:86:LEU:HD21	1:A:597:ALA:O	2.20	0.41
1:A:129:GLY:N	2:A:801:ADP:O3B	2.53	0.41
1:B:412:ASN:ND2	1:B:442:ARG:HH11	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:VAL:C	1:C:382:LEU:H	2.28	0.41
1:C:566:ILE:C	1:C:568:GLN:N	2.77	0.41
1:D:67:MET:HE2	1:D:67:MET:HB3	1.88	0.41
1:D:184:THR:O	1:D:185:ILE:C	2.62	0.41
1:D:424:GLY:CA	1:D:678:PRO:HB3	2.50	0.41
1:D:481:ARG:HD3	1:D:510:GLU:OE1	2.20	0.41
1:D:720:LEU:HD23	1:D:720:LEU:C	2.46	0.41
1:A:157:GLU:CD	1:A:157:GLU:C	2.89	0.41
1:B:138:ARG:HH11	1:B:342:ALA:HA	1.86	0.41
1:B:268:ILE:H	1:B:268:ILE:HD12	1.85	0.41
1:B:284:THR:CG2	1:B:287:LYS:HB2	2.51	0.41
1:B:397:LEU:HD21	1:B:430:ARG:NH2	2.36	0.41
1:B:511:ALA:HB3	1:B:534:MET:HE3	2.03	0.41
1:C:52:TYR:CE2	1:C:760:ILE:HB	2.56	0.41
1:D:325:MET:HE1	1:D:352:ALA:HB1	2.01	0.41
1:D:461:ILE:HD12	1:D:461:ILE:C	2.45	0.41
1:D:586:TYR:HB2	1:D:743:HIS:O	2.21	0.41
1:A:30:LEU:HB3	1:A:60:ILE:HB	2.02	0.41
1:A:122:LEU:O	1:A:167:VAL:HA	2.21	0.41
1:B:122:LEU:O	1:B:167:VAL:HA	2.20	0.41
1:B:172:GLY:O	1:B:173:SER:HB2	2.19	0.41
1:B:524:LYS:H	1:B:524:LYS:CD	2.34	0.41
1:C:130:SER:HB2	2:C:801:ADP:O2A	2.20	0.41
1:C:201:ILE:HD11	1:D:308:VAL:CG1	2.50	0.41
1:C:354:ARG:O	1:C:355:LEU:HD23	2.21	0.41
1:C:512:TYR:O	1:C:516:LEU:HD23	2.21	0.41
1:D:79:TRP:CZ2	1:D:763:LYS:HA	2.55	0.41
1:A:164:TYR:CD2	1:A:338:PRO:HB3	2.56	0.41
1:A:331:ILE:O	1:A:335:GLU:HB2	2.21	0.41
1:A:334:LEU:H	1:A:334:LEU:HG	1.68	0.41
1:A:447:TYR:CD2	1:A:477:LEU:HA	2.56	0.41
1:A:697:ILE:O	1:A:701:LEU:N	2.51	0.41
1:A:755:ARG:N	1:A:756:PRO:HD2	2.35	0.41
1:B:176:ASN:C	1:B:178:PHE:N	2.79	0.41
1:B:412:ASN:HB2	1:B:499:SER:O	2.21	0.41
1:B:461:ILE:HD12	1:B:461:ILE:C	2.45	0.41
1:B:485:GLY:O	1:B:488:LEU:HB2	2.21	0.41
1:B:755:ARG:N	1:B:756:PRO:HD2	2.36	0.41
1:C:37:GLN:HE21	1:C:310:ARG:C	2.29	0.41
1:C:214:LEU:N	1:C:214:LEU:CD1	2.84	0.41
1:C:216:VAL:HG21	1:C:225:ALA:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:PHE:C	1:C:387:PHE:CD2	2.97	0.41
1:D:150:ARG:C	1:D:152:GLY:H	2.28	0.41
1:D:209:GLN:HA	1:D:265:ARG:O	2.20	0.41
1:D:254:VAL:O	1:D:258:GLU:HG3	2.20	0.41
1:D:284:THR:CG2	1:D:287:LYS:HB2	2.51	0.41
1:A:279:GLN:C	1:A:281:LYS:N	2.79	0.41
1:A:325:MET:HA	1:A:325:MET:HE3	2.02	0.41
1:A:478:GLY:O	1:A:479:THR:HB	2.20	0.41
1:B:223:TYR:O	1:B:225:ALA:N	2.54	0.41
1:B:731:PRO:C	1:B:733:ALA:N	2.74	0.41
1:B:757:LEU:C	1:B:757:LEU:HD22	2.46	0.41
1:C:515:LEU:HB3	1:C:717:ILE:CG2	2.51	0.41
1:C:539:VAL:HG11	1:C:674:GLN:CB	2.36	0.41
1:C:580:ILE:HG23	1:C:669:LEU:HG	2.03	0.41
1:C:584:GLY:O	1:C:585:GLY:C	2.64	0.41
1:D:222:GLY:HA3	1:D:240:PRO:HD2	2.01	0.41
1:D:266:LEU:CD1	1:D:268:ILE:HD11	2.51	0.41
1:D:579:ILE:HG13	1:D:635:VAL:HG13	2.02	0.41
1:A:251:GLN:O	1:A:254:VAL:HB	2.21	0.40
1:B:511:ALA:HB1	1:B:534:MET:HG3	2.03	0.40
1:C:78:ASP:OD2	1:C:81:SER:HB2	2.21	0.40
1:C:111:ALA:O	1:C:115:LEU:HD22	2.21	0.40
1:C:215:GLU:OE1	1:C:304:ILE:HG12	2.21	0.40
1:C:530:VAL:HB	1:C:531:PRO:HD2	2.02	0.40
1:D:176:ASN:C	1:D:178:PHE:N	2.73	0.40
1:D:239:LEU:HA	1:D:240:PRO:HD3	1.86	0.40
1:D:416:ILE:HG12	1:D:417:ASN:N	2.36	0.40
1:D:750:TRP:CD2	1:D:751:TRP:N	2.89	0.40
1:A:255:LYS:HB2	1:A:255:LYS:HE2	1.91	0.40
1:A:615:LEU:O	1:A:619:VAL:HG23	2.22	0.40
1:A:722:ILE:HD13	1:A:727:VAL:CG1	2.51	0.40
1:B:141:TRP:CG	1:B:165:LEU:HB2	2.56	0.40
1:B:577:VAL:HG22	1:B:633:GLY:HA3	2.03	0.40
1:C:139:LYS:HD3	1:C:139:LYS:HA	1.80	0.40
1:C:174:ILE:CG2	1:C:190:ALA:HB2	2.50	0.40
1:C:205:ALA:HB1	1:C:266:LEU:HD23	2.03	0.40
1:C:268:ILE:HD12	1:C:268:ILE:H	1.86	0.40
1:C:473:GLY:HA3	1:C:678:PRO:HD3	2.03	0.40
1:D:223:TYR:C	1:D:225:ALA:H	2.29	0.40
1:A:430:ARG:HA	1:A:466:VAL:HB	2.02	0.40
1:B:81:SER:C	1:B:83:SER:H	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:GLN:C	1:B:281:LYS:H	2.29	0.40
1:B:307:HIS:C	1:B:309:GLN:H	2.29	0.40
1:B:502:ALA:HB1	1:B:697:ILE:CG2	2.51	0.40
1:C:506:ILE:HG22	1:C:537:ALA:CB	2.52	0.40
1:D:83:SER:O	1:D:84:SER:CB	2.69	0.40
1:A:111:ALA:O	1:A:115:LEU:HD22	2.21	0.40
1:A:224:LEU:HA	1:A:227:VAL:CG2	2.51	0.40
1:A:579:ILE:HD12	1:A:579:ILE:N	2.36	0.40
1:B:728:ILE:HD12	1:B:728:ILE:HA	1.97	0.40
1:B:756:PRO:HG2	1:B:757:LEU:H	1.86	0.40
1:C:17:LEU:C	1:C:19:HIS:H	2.29	0.40
1:C:25:LYS:HB3	1:C:120:THR:CG2	2.50	0.40
1:C:307:HIS:C	1:C:309:GLN:N	2.80	0.40
1:C:544:PRO:HB3	1:C:746:PRO:HB3	2.04	0.40
1:D:531:PRO:HD3	1:D:711:PHE:CD1	2.57	0.40
1:A:179:CYS:SG	1:A:363:MET:HB2	2.62	0.40
1:A:491:ILE:HG22	1:A:492:ALA:N	2.36	0.40
1:A:530:VAL:HB	1:A:531:PRO:CD	2.47	0.40
1:A:577:VAL:O	1:A:664:CYS:HA	2.21	0.40
1:A:750:TRP:C	1:A:752:LEU:H	2.29	0.40
1:B:239:LEU:HA	1:B:240:PRO:HD3	1.83	0.40
1:B:373:GLU:O	1:B:374:ARG:C	2.64	0.40
1:B:586:TYR:CE1	1:B:743:HIS:HD2	2.40	0.40
1:B:651:TYR:HE2	1:B:664:CYS:O	2.03	0.40
1:C:390:ASN:OD1	1:C:688:LYS:HE2	2.21	0.40
1:C:667:ASN:OD1	1:D:670:GLY:HA3	2.22	0.40
1:D:23:ALA:O	1:D:25:LYS:HG3	2.21	0.40
1:D:156:LYS:HA	1:D:156:LYS:HD2	1.82	0.40
1:D:506:ILE:HG23	1:D:537:ALA:HB2	2.03	0.40
1:D:592:ASN:C	1:D:592:ASN:ND2	2.78	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	731/812 (90%)	610 (83%)	95 (13%)	26 (4%)	2	16
1	B	745/812 (92%)	631 (85%)	87 (12%)	27 (4%)	2	16
1	C	739/812 (91%)	620 (84%)	97 (13%)	22 (3%)	3	18
1	D	739/812 (91%)	618 (84%)	101 (14%)	20 (3%)	4	20
All	All	2954/3248 (91%)	2479 (84%)	380 (13%)	95 (3%)	3	17

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	ASP
1	A	724	LYS
1	B	724	LYS
1	C	19	HIS
1	C	724	LYS
1	D	714	ASP
1	A	402	PRO
1	A	523	GLU
1	A	659	LYS
1	A	675	GLY
1	B	69	ASP
1	B	374	ARG
1	B	402	PRO
1	B	485	GLY
1	B	659	LYS
1	B	675	GLY
1	B	676	GLY
1	C	69	ASP
1	C	486	LYS
1	C	659	LYS
1	C	675	GLY
1	D	69	ASP
1	D	280	ASN
1	D	307	HIS
1	D	402	PRO
1	D	659	LYS
1	D	675	GLY
1	D	724	LYS
1	D	751	TRP
1	A	19	HIS

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Mol	Chain	Res	Type
1	A	34	GLY
1	A	158	ALA
1	A	280	ASN
1	A	307	HIS
1	A	751	TRP
1	A	762	ALA
1	B	82	VAL
1	B	280	ASN
1	B	490	GLU
1	B	524	LYS
1	B	703	GLU
1	B	751	TRP
1	C	35	ASP
1	C	82	VAL
1	C	173	SER
1	C	185	ILE
1	C	307	HIS
1	C	402	PRO
1	C	524	LYS
1	D	82	VAL
1	D	100	ALA
1	D	466	VAL
1	D	676	GLY
1	D	713	THR
1	D	715	ASP
1	A	18	GLU
1	A	35	ASP
1	A	265	ARG
1	A	396	ARG
1	A	466	VAL
1	A	676	GLY
1	B	35	ASP
1	B	100	ALA
1	B	173	SER
1	B	185	ILE
1	B	265	ARG
1	B	307	HIS
1	B	466	VAL
1	B	479	THR
1	C	34	GLY
1	C	100	ALA
1	C	280	ASN

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Mol	Chain	Res	Type
1	D	34	GLY
1	D	35	ASP
1	D	498	HIS
1	A	82	VAL
1	A	295	GLN
1	A	479	THR
1	A	485	GLY
1	A	527	GLU
1	B	626	MET
1	C	265	ARG
1	C	466	VAL
1	C	607	GLU
1	D	265	ARG
1	A	100	ALA
1	B	489	GLU
1	C	751	TRP
1	C	306	GLY
1	C	485	GLY
1	D	306	GLY
1	B	34	GLY
1	B	306	GLY
1	A	185	ILE
1	B	584	GLY

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	594/658 (90%)	517 (87%)	77 (13%)	4	16
1	B	602/658 (92%)	531 (88%)	71 (12%)	5	20
1	C	598/658 (91%)	523 (88%)	75 (12%)	4	18
1	D	598/658 (91%)	520 (87%)	78 (13%)	4	16
All	All	2392/2632 (91%)	2091 (87%)	301 (13%)	4	18

All (301) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	25	LYS
1	A	39	MET
1	A	49	MET
1	A	53	VAL
1	A	57	VAL
1	A	65	GLN
1	A	86	LEU
1	A	97	ARG
1	A	105	GLU
1	A	108	LEU
1	A	138	ARG
1	A	139	LYS
1	A	147	GLU
1	A	154	ILE
1	A	179	CYS
1	A	191	LEU
1	A	192	HIS
1	A	198	VAL
1	A	204	THR
1	A	206	GLN
1	A	214	LEU
1	A	230	LEU
1	A	249	GLU
1	A	260	ARG
1	A	266	LEU
1	A	268	ILE
1	A	293	VAL
1	A	294	THR
1	A	301	ARG
1	A	303	THR
1	A	308	VAL
1	A	313	THR
1	A	318	ASP
1	A	325	MET
1	A	331	ILE
1	A	334	LEU
1	A	365	GLN
1	A	374	ARG
1	A	382	LEU
1	A	391	LEU
1	A	396	ARG
1	A	401	LEU

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Mol	Chain	Res	Type
1	A	418	VAL
1	A	439	ASP
1	A	470	THR
1	A	483	LEU
1	A	489	GLU
1	A	491	ILE
1	A	510	GLU
1	A	516	LEU
1	A	525	HIS
1	A	541	ASN
1	A	557	ASN
1	A	566	ILE
1	A	575	ARG
1	A	582	THR
1	A	611	ASP
1	A	616	GLN
1	A	617	SER
1	A	624	GLU
1	A	630	ILE
1	A	631	GLN
1	A	635	VAL
1	A	659	LYS
1	A	674	GLN
1	A	689	ILE
1	A	690	SER
1	A	714	ASP
1	A	715	ASP
1	A	717	ILE
1	A	748	GLU
1	A	755	ARG
1	A	757	LEU
1	A	760	ILE
1	A	761	LEU
1	A	763	LYS
1	B	13	LEU
1	B	15	LYS
1	B	17	LEU
1	B	27	ILE
1	B	49	MET
1	B	53	VAL
1	B	65	GLN
1	B	86	LEU

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Mol	Chain	Res	Type
1	B	97	ARG
1	B	108	LEU
1	B	138	ARG
1	B	139	LYS
1	B	145	LEU
1	B	154	ILE
1	B	165	LEU
1	B	179	CYS
1	B	191	LEU
1	B	192	HIS
1	B	214	LEU
1	B	230	LEU
1	B	249	GLU
1	B	260	ARG
1	B	266	LEU
1	B	268	ILE
1	B	293	VAL
1	B	301	ARG
1	B	303	THR
1	B	308	VAL
1	B	313	THR
1	B	318	ASP
1	B	325	MET
1	B	331	ILE
1	B	334	LEU
1	B	362	GLN
1	B	365	GLN
1	B	382	LEU
1	B	391	LEU
1	B	395	LYS
1	B	396	ARG
1	B	401	LEU
1	B	418	VAL
1	B	439	ASP
1	B	470	THR
1	B	482	VAL
1	B	487	TYR
1	B	495	MET
1	B	501	ASN
1	B	517	GLU
1	B	524	LYS
1	B	530	VAL

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Mol	Chain	Res	Type
1	B	554	THR
1	B	557	ASN
1	B	563	CYS
1	B	567	LYS
1	B	569	SER
1	B	582	THR
1	B	610	PHE
1	B	618	ASN
1	B	624	GLU
1	B	631	GLN
1	B	635	VAL
1	B	659	LYS
1	B	665	ARG
1	B	674	GLN
1	B	689	ILE
1	B	690	SER
1	B	701	LEU
1	B	738	GLN
1	B	755	ARG
1	B	757	LEU
1	B	760	ILE
1	C	18	GLU
1	C	19	HIS
1	C	21	SER
1	C	27	ILE
1	C	39	MET
1	C	49	MET
1	C	57	VAL
1	C	65	GLN
1	C	86	LEU
1	C	87	GLN
1	C	108	LEU
1	C	115	LEU
1	C	130	SER
1	C	138	ARG
1	C	139	LYS
1	C	146	GLU
1	C	153	GLN
1	C	154	ILE
1	C	179	CYS
1	C	191	LEU
1	C	204	THR

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Mol	Chain	Res	Type
1	C	214	LEU
1	C	219	ARG
1	C	230	LEU
1	C	245	GLU
1	C	249	GLU
1	C	258	GLU
1	C	266	LEU
1	C	268	ILE
1	C	293	VAL
1	C	301	ARG
1	C	303	THR
1	C	308	VAL
1	C	318	ASP
1	C	325	MET
1	C	331	ILE
1	C	334	LEU
1	C	343	CYS
1	C	351	HIS
1	C	365	GLN
1	C	374	ARG
1	C	382	LEU
1	C	385	ARG
1	C	391	LEU
1	C	396	ARG
1	C	401	LEU
1	C	439	ASP
1	C	457	GLN
1	C	470	THR
1	C	503	LEU
1	C	524	LYS
1	C	526	GLU
1	C	530	VAL
1	C	534	MET
1	C	557	ASN
1	C	575	ARG
1	C	582	THR
1	C	583	MET
1	C	592	ASN
1	C	610	PHE
1	C	624	GLU
1	C	630	ILE
1	C	631	GLN

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Mol	Chain	Res	Type
1	C	635	VAL
1	C	659	LYS
1	C	674	GLN
1	C	689	ILE
1	C	690	SER
1	C	711	PHE
1	C	715	ASP
1	C	742	GLU
1	C	755	ARG
1	C	757	LEU
1	C	760	ILE
1	C	761	LEU
1	D	16	PHE
1	D	20	LEU
1	D	27	ILE
1	D	29	VAL
1	D	39	MET
1	D	44	ARG
1	D	49	MET
1	D	53	VAL
1	D	65	GLN
1	D	86	LEU
1	D	87	GLN
1	D	97	ARG
1	D	99	GLN
1	D	105	GLU
1	D	108	LEU
1	D	115	LEU
1	D	130	SER
1	D	138	ARG
1	D	139	LYS
1	D	142	SER
1	D	154	ILE
1	D	179	CYS
1	D	191	LEU
1	D	192	HIS
1	D	206	GLN
1	D	214	LEU
1	D	219	ARG
1	D	230	LEU
1	D	249	GLU
1	D	251	GLN

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Mol	Chain	Res	Type
1	D	260	ARG
1	D	266	LEU
1	D	268	ILE
1	D	293	VAL
1	D	301	ARG
1	D	303	THR
1	D	318	ASP
1	D	325	MET
1	D	331	ILE
1	D	334	LEU
1	D	365	GLN
1	D	382	LEU
1	D	385	ARG
1	D	391	LEU
1	D	396	ARG
1	D	401	LEU
1	D	403	ASP
1	D	439	ASP
1	D	470	THR
1	D	487	TYR
1	D	488	LEU
1	D	510	GLU
1	D	512	TYR
1	D	516	LEU
1	D	519	SER
1	D	530	VAL
1	D	533	VAL
1	D	540	SER
1	D	557	ASN
1	D	567	LYS
1	D	582	THR
1	D	592	ASN
1	D	610	PHE
1	D	624	GLU
1	D	630	ILE
1	D	635	VAL
1	D	659	LYS
1	D	674	GLN
1	D	689	ILE
1	D	690	SER
1	D	701	LEU
1	D	714	ASP

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Mol	Chain	Res	Type
1	D	715	ASP
1	D	718	CYS
1	D	755	ARG
1	D	757	LEU
1	D	760	ILE
1	D	763	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	73	ASN
1	A	87	GLN
1	A	116	GLN
1	A	135	ASN
1	A	153	GLN
1	A	206	GLN
1	A	259	ASN
1	A	267	ASN
1	A	348	ASN
1	A	362	GLN
1	A	365	GLN
1	A	417	ASN
1	A	457	GLN
1	A	557	ASN
1	A	616	GLN
1	A	618	ASN
1	A	652	GLN
1	A	667	ASN
1	A	674	GLN
1	B	19	HIS
1	B	65	GLN
1	B	113	ASN
1	B	116	GLN
1	B	135	ASN
1	B	192	HIS
1	B	208	HIS
1	B	259	ASN
1	B	279	GLN
1	B	348	ASN
1	B	417	ASN
1	B	498	HIS

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Mol	Chain	Res	Type
1	B	568	GLN
1	B	652	GLN
1	B	667	ASN
1	B	673	GLN
1	C	73	ASN
1	C	113	ASN
1	C	116	GLN
1	C	153	GLN
1	C	192	HIS
1	C	295	GLN
1	C	365	GLN
1	C	457	GLN
1	C	498	HIS
1	C	568	GLN
1	C	616	GLN
1	C	621	HIS
1	C	684	ASN
1	D	65	GLN
1	D	73	ASN
1	D	87	GLN
1	D	113	ASN
1	D	116	GLN
1	D	135	ASN
1	D	166	ASN
1	D	192	HIS
1	D	206	GLN
1	D	208	HIS
1	D	280	ASN
1	D	350	ASN
1	D	365	GLN
1	D	417	ASN
1	D	494	GLN
1	D	498	HIS
1	D	541	ASN
1	D	592	ASN
1	D	631	GLN
1	D	644	ASN
1	D	667	ASN
1	D	674	GLN
1	D	730	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 ⓘ

16 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	$\# Z > 2$
3	PO4	C	803	-	4,4,4	1.62	0	6,6,6	0.54	0
3	PO4	A	803	-	4,4,4	1.44	0	6,6,6	0.43	0
3	PO4	B	802	-	4,4,4	1.57	1 (25%)	6,6,6	0.44	0
3	PO4	D	804	-	4,4,4	1.61	0	6,6,6	0.49	0
3	PO4	B	803	-	4,4,4	1.57	0	6,6,6	0.47	0
3	PO4	A	802	-	4,4,4	1.69	0	6,6,6	0.48	0
3	PO4	D	803	-	4,4,4	1.66	1 (25%)	6,6,6	0.45	0
2	ADP	C	801	-	28,29,29	1.87	4 (14%)	43,45,45	0.95	2 (4%)
2	ADP	B	801	-	28,29,29	2.21	4 (14%)	43,45,45	1.11	5 (11%)
3	PO4	C	805	-	4,4,4	1.61	1 (25%)	6,6,6	0.44	0
2	ADP	D	802	-	28,29,29	2.42	6 (21%)	43,45,45	1.24	5 (11%)
3	PO4	A	804	-	4,4,4	1.69	1 (25%)	6,6,6	0.49	0
3	PO4	C	804	-	4,4,4	1.52	0	6,6,6	0.46	0
3	PO4	C	802	-	4,4,4	1.70	1 (25%)	6,6,6	0.43	0
3	PO4	D	801	-	4,4,4	1.59	1 (25%)	6,6,6	0.50	0
2	ADP	A	801	-	28,29,29	1.73	3 (10%)	43,45,45	1.11	3 (6%)

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
2	ADP	C	801	-	-	3/16/32/32	0/3/3/3
2	ADP	A	801	-	-	3/16/32/32	0/3/3/3
2	ADP	B	801	-	-	0/16/32/32	0/3/3/3
2	ADP	D	802	-	-	0/16/32/32	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	802	ADP	PA-O3A	-8.98	1.49	1.59
2	B	801	ADP	PA-O3A	-7.67	1.51	1.59
2	A	801	ADP	PA-O3A	-6.87	1.52	1.59
2	D	802	ADP	PB-O1B	6.66	1.71	1.50
2	C	801	ADP	PA-O3A	-6.62	1.52	1.59
2	B	801	ADP	PB-O1B	6.19	1.69	1.50
2	C	801	ADP	PB-O3B	4.00	1.69	1.54
2	A	801	ADP	PB-O3B	3.69	1.68	1.54
2	C	801	ADP	C4-N3	2.86	1.39	1.34
2	B	801	ADP	C4-N3	2.63	1.39	1.34
2	B	801	ADP	C1'-N9	2.44	1.53	1.46
2	D	802	ADP	C4-N3	2.33	1.38	1.34
3	D	803	PO4	P-O2	-2.29	1.48	1.54
2	A	801	ADP	C1'-N9	2.26	1.52	1.46
2	D	802	ADP	C1'-N9	2.21	1.52	1.46
3	A	804	PO4	P-O4	-2.12	1.48	1.54
3	C	802	PO4	P-O4	-2.11	1.48	1.54
2	D	802	ADP	PB-O2B	-2.09	1.47	1.54
2	C	801	ADP	C5-C6	2.09	1.46	1.41
3	D	801	PO4	P-O2	-2.06	1.48	1.54
3	C	805	PO4	P-O4	-2.05	1.48	1.54
3	B	802	PO4	P-O3	-2.02	1.48	1.54
2	D	802	ADP	C5-C6	2.02	1.46	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	802	ADP	O4'-C1'-N9	3.46	114.73	108.09
2	A	801	ADP	O2B-PB-O3A	3.38	115.98	104.64
2	D	802	ADP	O5'-C5'-C4'	3.21	119.92	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	ADP	O4'-C1'-N9	2.93	113.72	108.09
2	C	801	ADP	O2B-PB-O3A	2.80	114.03	104.64
2	A	801	ADP	O5'-C5'-C4'	2.77	118.42	108.99
2	B	801	ADP	O2B-PB-O3A	2.76	113.88	104.64
2	D	802	ADP	O2B-PB-O3A	2.74	113.83	104.64
2	C	801	ADP	O5'-C5'-C4'	2.50	117.50	108.99
2	B	801	ADP	O5'-C5'-C4'	2.40	117.17	108.99
2	D	802	ADP	C1'-N9-C8	2.25	132.09	127.09
2	B	801	ADP	O3B-PB-O3A	2.23	112.10	104.64
2	B	801	ADP	C1'-N9-C8	2.16	131.88	127.09
2	D	802	ADP	O2B-PB-O1B	-2.14	102.49	110.83
2	B	801	ADP	O4'-C1'-N9	2.07	112.07	108.09

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ADP	PA-O3A-PB-O2B
2	A	801	ADP	C5'-O5'-PA-O1A
2	C	801	ADP	C3'-C4'-C5'-O5'
2	C	801	ADP	O4'-C4'-C5'-O5'
2	C	801	ADP	C4'-C5'-O5'-PA
2	A	801	ADP	PA-O3A-PB-O3B

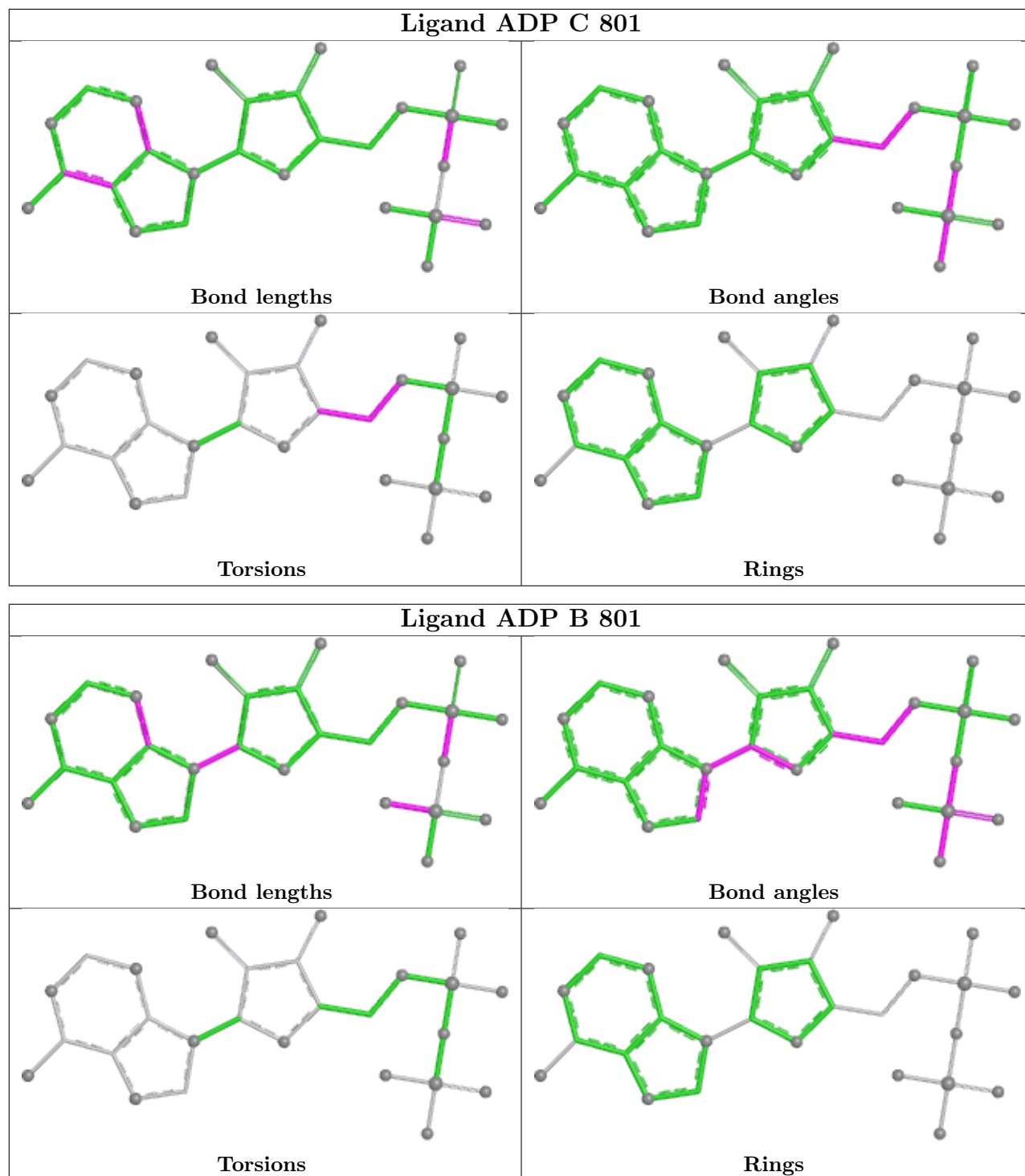
There are no ring outliers.

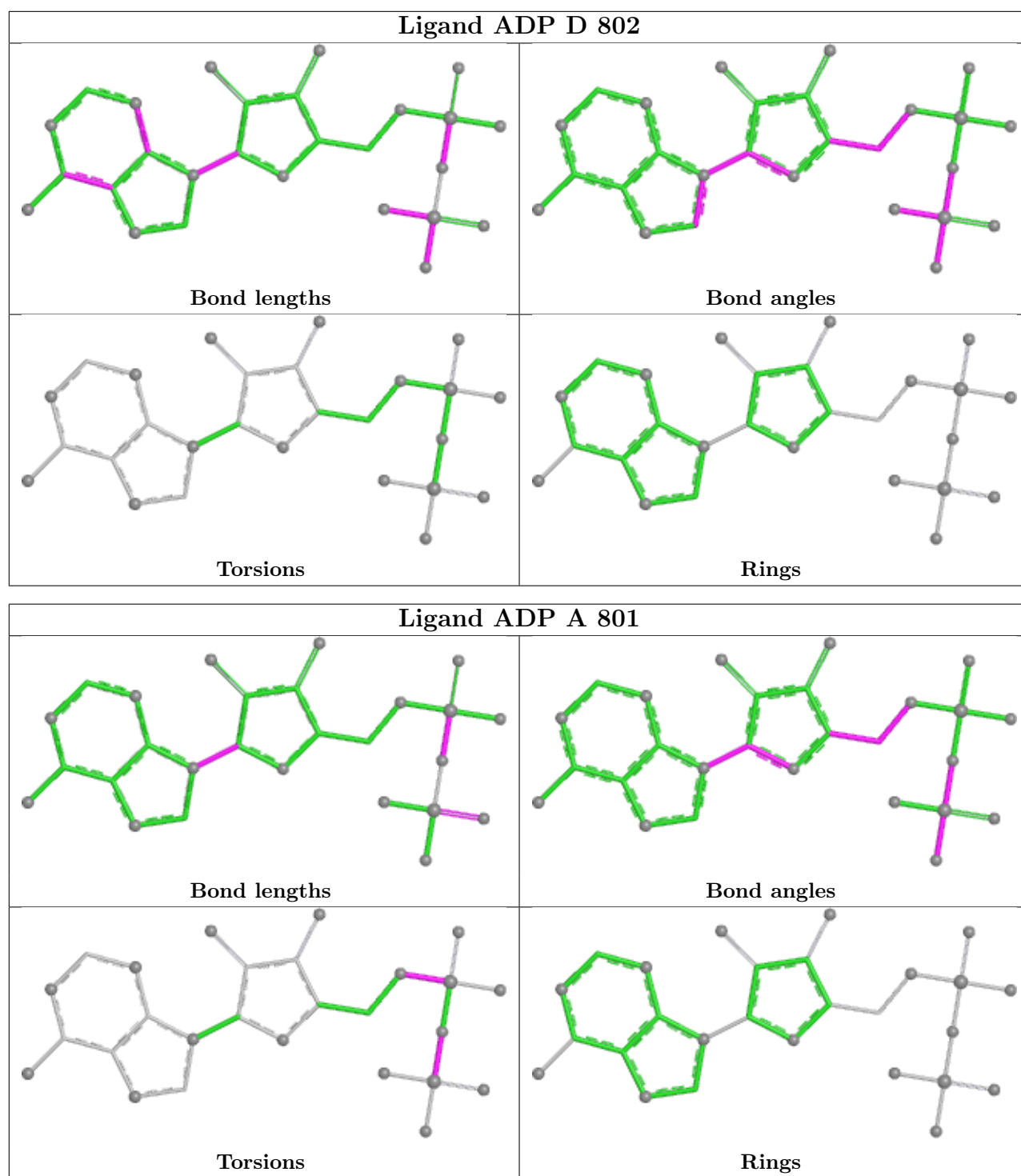
6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	PO4	2	0
2	C	801	ADP	1	0
2	B	801	ADP	1	0
3	C	805	PO4	1	0
3	D	801	PO4	1	0
2	A	801	ADP	2	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.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	737/812 (90%)	-0.06	3 (0%) 88 81	27, 73, 113, 162	0
1	B	749/812 (92%)	-0.06	3 (0%) 88 81	25, 75, 114, 162	0
1	C	743/812 (91%)	-0.13	4 (0%) 87 78	26, 73, 112, 161	0
1	D	743/812 (91%)	-0.12	6 (0%) 82 71	28, 74, 113, 162	0
All	All	2972/3248 (91%)	-0.09	16 (0%) 87 78	25, 74, 113, 162	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	205	ALA	3.3
1	D	435	VAL	3.0
1	B	204	THR	3.0
1	D	122	LEU	2.7
1	D	344	VAL	2.7
1	A	566	ILE	2.7
1	B	133	GLY	2.6
1	D	674	GLN	2.6
1	C	675	GLY	2.5
1	D	675	GLY	2.4
1	D	343	CYS	2.3
1	C	631	GLN	2.3
1	A	675	GLY	2.2
1	C	684	ASN	2.1
1	C	423	ALA	2.1
1	A	231	ALA	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](#)

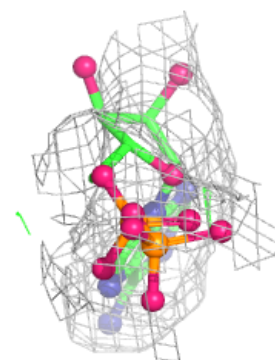
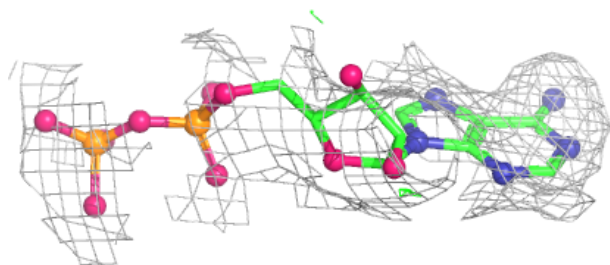
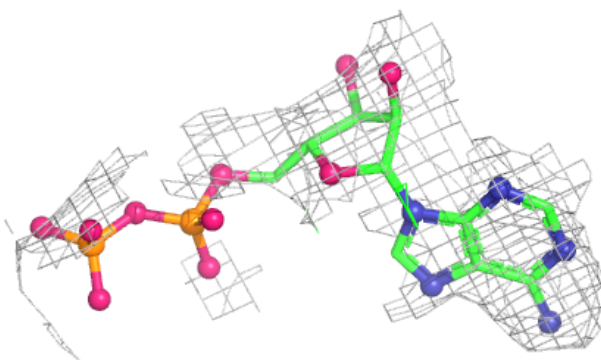
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PO4	C	804	5/5	0.79	0.11	6,89,105,127	0
2	ADP	C	801	27/27	0.87	0.09	35,98,135,151	0
2	ADP	B	801	27/27	0.87	0.09	21,98,154,163	0
3	PO4	B	802	5/5	0.88	0.09	16,71,134,135	0
2	ADP	A	801	27/27	0.88	0.09	1,73,118,137	0
3	PO4	D	803	5/5	0.88	0.09	31,32,74,82	0
3	PO4	D	801	5/5	0.89	0.07	14,27,57,97	0
3	PO4	C	805	5/5	0.91	0.06	65,81,155,163	0
3	PO4	A	802	5/5	0.92	0.08	1,67,103,108	0
3	PO4	A	803	5/5	0.93	0.10	17,29,126,144	0
3	PO4	C	803	5/5	0.93	0.07	1,20,85,87	0
3	PO4	C	802	5/5	0.94	0.05	1,66,70,97	0
2	ADP	D	802	27/27	0.94	0.08	1,91,129,134	0
3	PO4	B	803	5/5	0.94	0.07	7,34,89,107	0
3	PO4	D	804	5/5	0.96	0.06	18,41,68,78	0
3	PO4	A	804	5/5	0.97	0.04	4,10,57,70	0

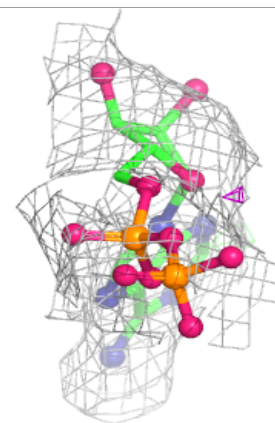
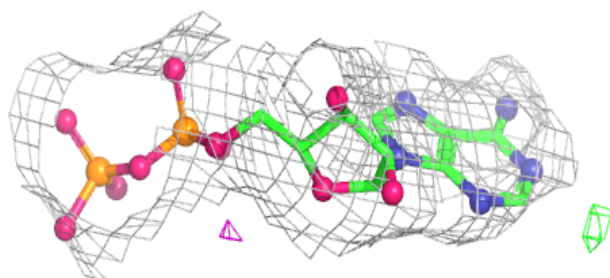
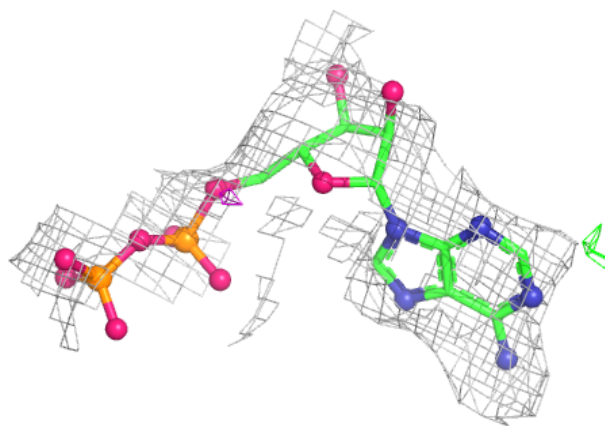
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP C 801:

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

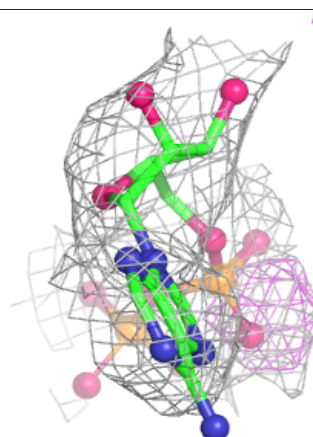
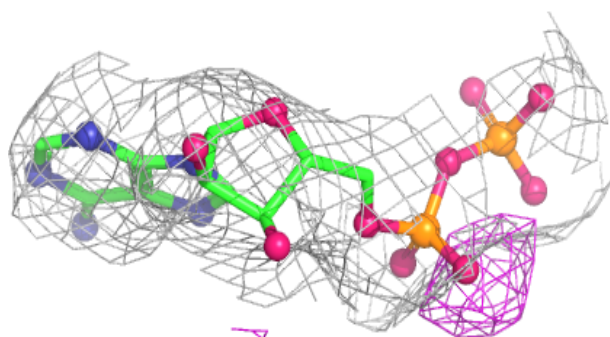
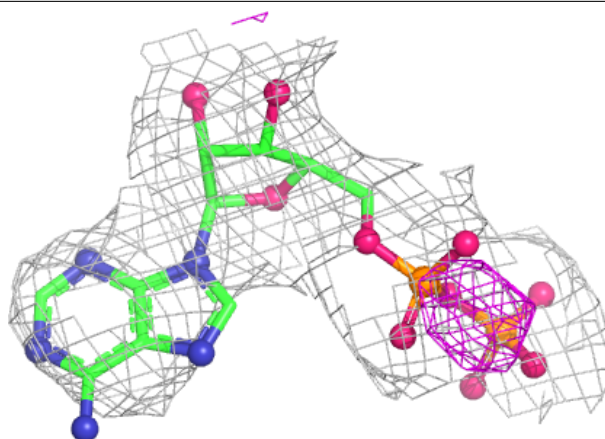
**Electron density around ADP B 801:**

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

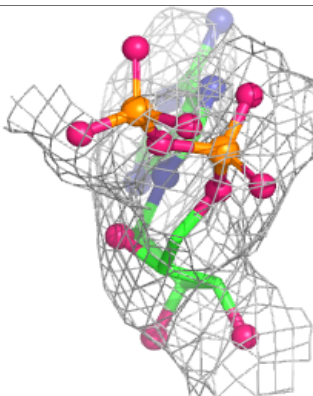
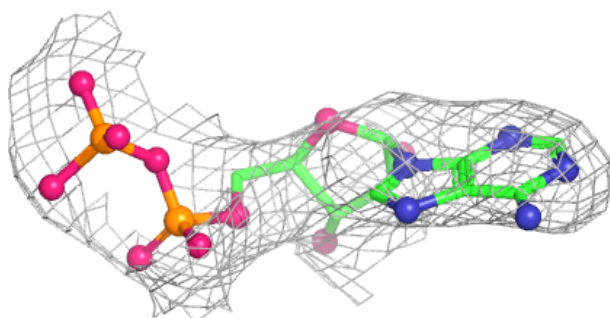
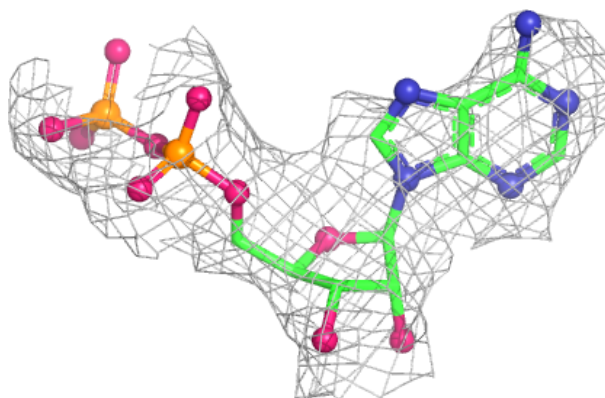


Electron density around ADP A 801:

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

**Electron density around ADP D 802:**

$2mF_o-DF_c$ (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.