



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:27 AM UTC

PDB ID : 1YNN / pdb_00001ynn
Title : Taq RNA polymerase-rifampicin complex
Authors : Campbell, E.A.; Pavlova, O.; Zenkin, N.; Leon, F.; Irschik, H.; Jansen, R.;
Severinov, K.; Darst, S.A.
Deposited on : 2005-01-24
Resolution : 3.30 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:

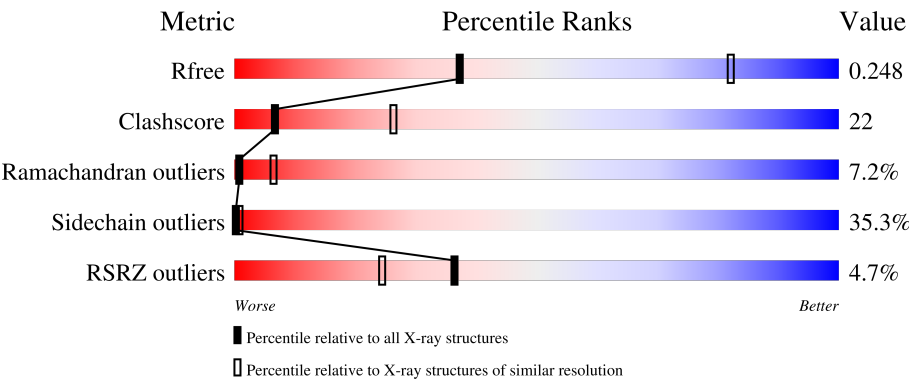
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

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

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	314	% 33% 28% 10% • 27%
1	B	314	% 31% 29% 11% • 28%
2	C	1119	3% 42% 40% 16% •
3	D	1524	6% 35% 32% 12% • 19%
3	J	1524	% 8% 6% • 84%

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Mol	Chain	Length	Quality of chain
4	K	99	6% 51% 33% 10%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24368 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 DNA-directed RNA polymerase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1763	1126	300	334	3			
1	B	225	Total	C	N	O	S	0	0	0
			1750	1118	300	329	3			

- Molecule 2 is a protein called DNA-directed RNA polymerase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1114	Total	C	N	O	S	0	0	0
			8576	5430	1513	1609	24			

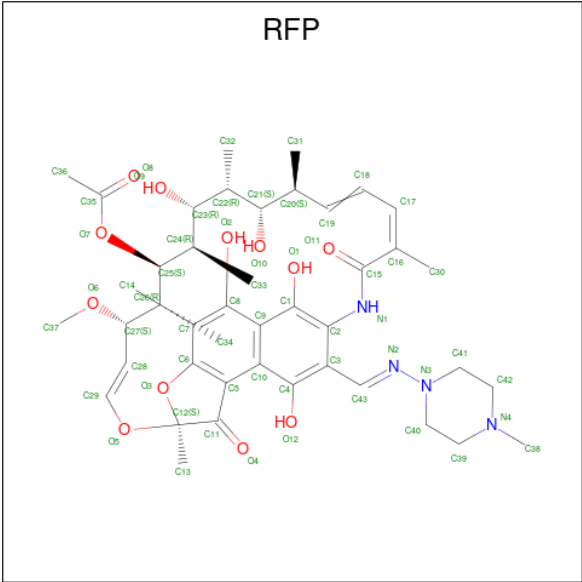
- Molecule 3 is a protein called DNA-directed RNA polymerase beta' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1238	Total	C	N	O	S	0	0	0
			9602	6065	1703	1798	36			
3	J	249	Total	C	N	O	S	0	0	0
			1869	1191	320	356	2			

- Molecule 4 is a protein called DNA-directed RNA polymerase omega chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	95	Total	C	N	O	S	0	0	0
			747	476	134	132	5			

- Molecule 5 is RIFAMPICIN (CCD ID: RFP) (formula: C₄₃H₅₈N₄O₁₂).



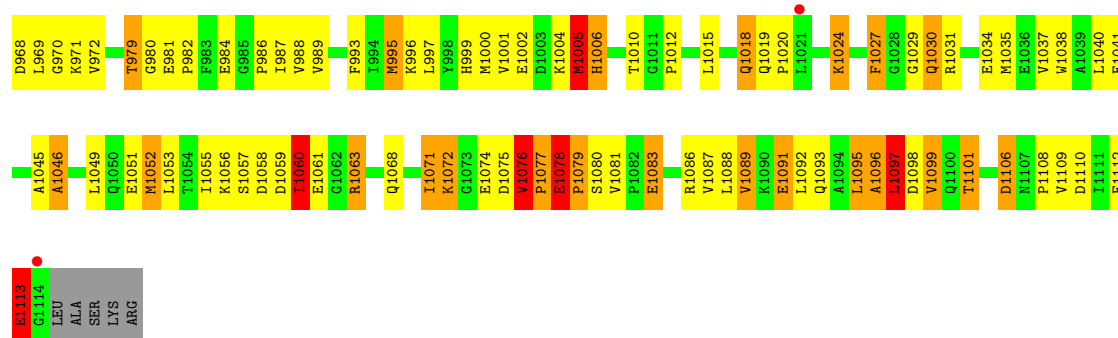
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			59	43	4	12		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

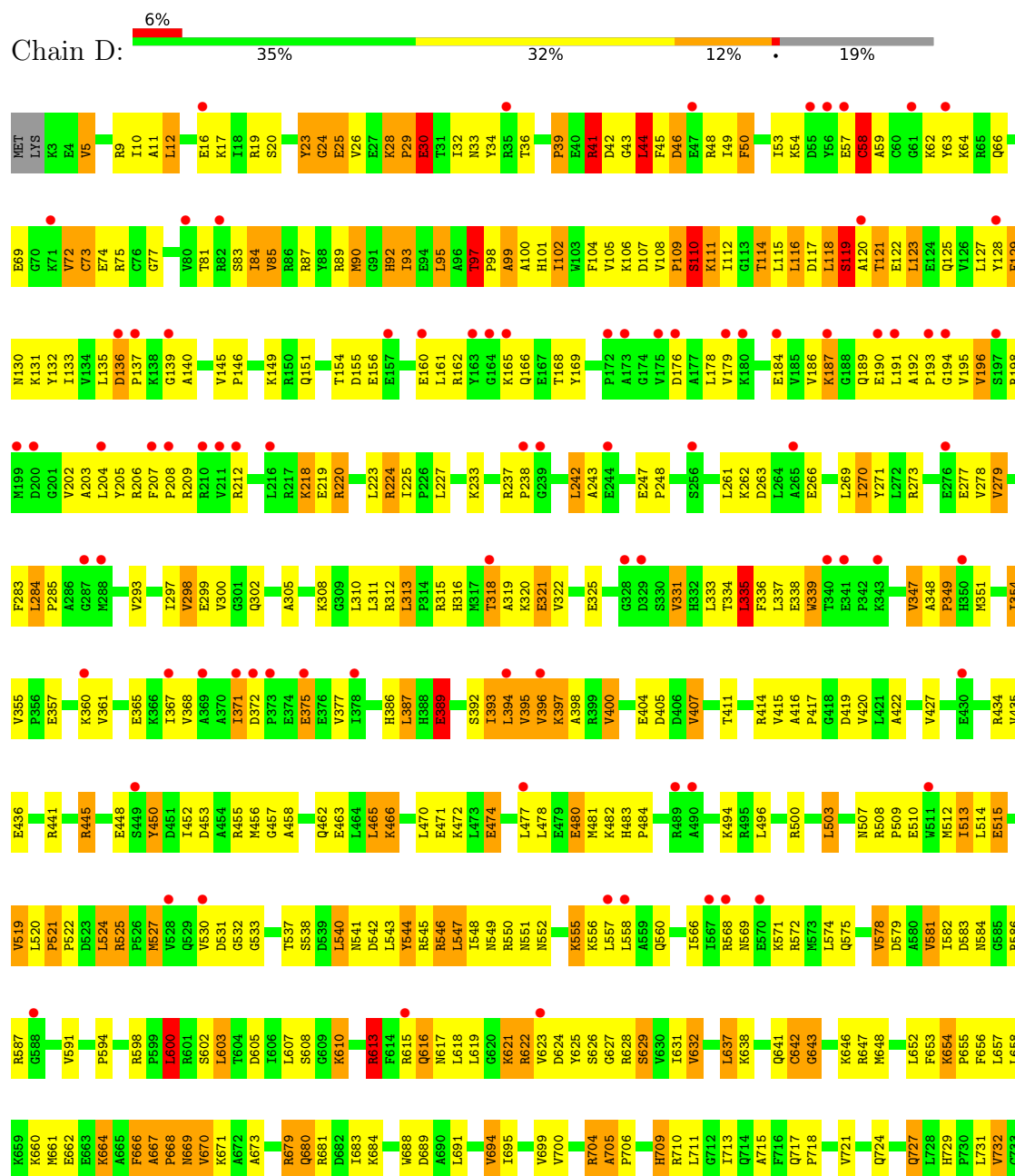
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	2	Total	Zn	0	0
			2	2		

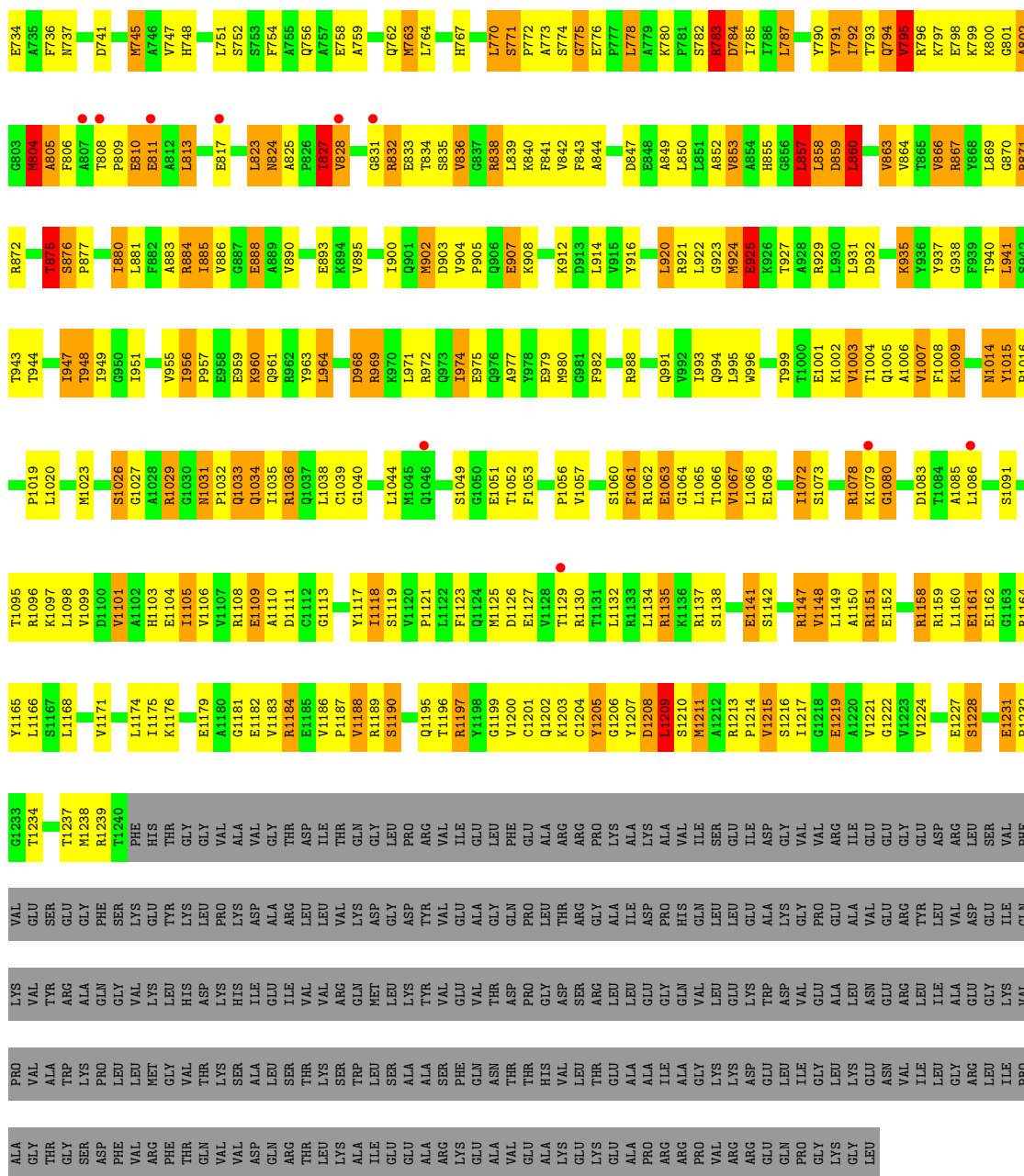
Chain C: 3% 42% 40% 16%

Category	Sub-Category	Node Label	Value (approx.)
Green (3%)	G800-G812	G808	0.1
		G809	0.1
		B810	0.1
		B811	0.1
		G812	0.1
	G813-G824	G813	0.1
		G814	0.1
		G815	0.1
		G816	0.1
		G817	0.1
Orange (42%)	O800-O812	O800	0.1
		O801	0.1
		O802	0.1
		O803	0.1
		O804	0.1
	O805-O817	O805	0.1
		O806	0.1
		O807	0.1
		O808	0.1
		O809	0.1
Red (40%)	R800-R812	R800	0.1
		R801	0.1
		R802	0.1
		R803	0.1
		R804	0.1
	R805-R817	R805	0.1
		R806	0.1
		R807	0.1
		R808	0.1
		R809	0.1
Grey (16%)	G800-G812	G800	0.1
		G801	0.1
		G802	0.1
		G803	0.1
		G804	0.1
	G805-G817	G805	0.1
		G806	0.1
		G807	0.1
		G808	0.1
		G809	0.1

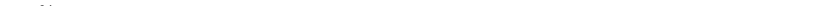


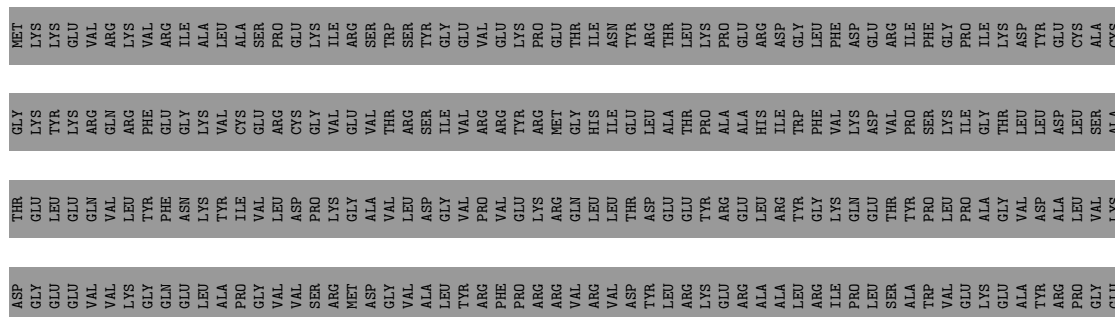
• Molecule 3: DNA-directed RNA polymerase beta' chain



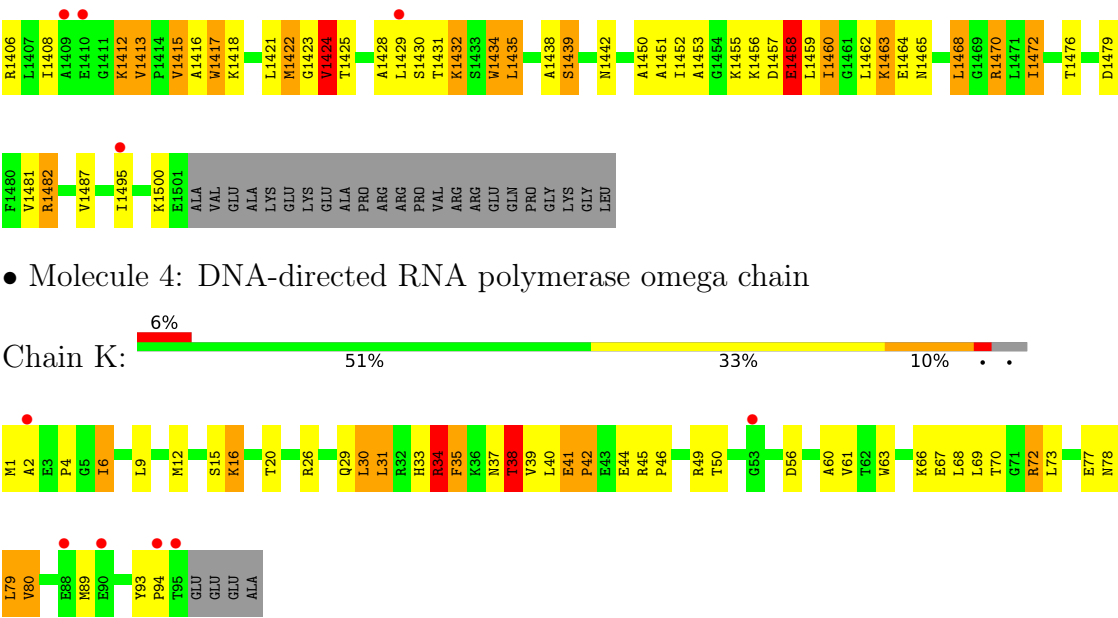


- Molecule 3: DNA-directed RNA polymerase beta' chain

Chain J:  %







• Molecule 4: DNA-directed RNA polymerase omega chain

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	200.76Å 200.76Å 292.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 30.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	84.9 (30.00-3.30) 84.8 (30.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.24Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.271 , 0.331 0.261 , 0.248	Depositor DCC
R_{free} test set	4075 reflections (4.12%)	wwPDB-VP
Wilson B-factor (Å ²)	87.9	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 130.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	24368	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.60	1/1798 (0.1%)	1.06	1/2453 (0.0%)
1	B	0.56	0/1784	0.99	1/2428 (0.0%)
2	C	0.56	0/8742	0.99	7/11848 (0.1%)
3	D	0.55	0/9772	0.99	14/13234 (0.1%)
3	J	0.56	0/1897	0.96	0/2570
4	K	0.56	0/762	1.00	0/1029
All	All	0.56	1/24755 (0.0%)	1.00	23/33562 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	C	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	ARG	CA-C	6.45	1.56	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	247	PRO	N-CA-C	8.09	120.57	110.70
2	C	831	ARG	N-CA-C	8.06	123.40	112.68
3	D	857	LEU	N-CA-C	8.00	119.69	110.97
3	D	1211	MET	N-CA-C	-7.76	102.89	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	52	PHE	N-CA-C	7.24	125.82	109.81
3	D	1064	GLY	N-CA-C	7.13	119.70	111.36
3	D	339	TRP	N-CA-C	6.67	116.67	107.73
3	D	524	LEU	N-CA-C	-6.07	104.30	113.89
3	D	1209	LEU	N-CA-C	-6.00	105.09	113.37
2	C	1029	GLY	N-CA-C	5.98	118.80	111.93
1	A	138	LEU	N-CA-C	5.93	122.09	114.56
3	D	642	CYS	N-CA-C	5.89	118.13	109.24
3	D	616	GLN	N-CA-C	5.76	118.05	111.02
3	D	875	THR	N-CA-C	5.59	122.70	110.80
3	D	279	VAL	N-CA-C	5.28	115.79	111.62
2	C	556	ASN	N-CA-C	5.25	116.69	111.07
2	C	547	ILE	N-CA-C	5.17	112.67	107.55
3	D	354	ILE	N-CA-C	5.11	117.02	112.17
1	B	148	VAL	N-CA-C	5.10	116.28	111.48
3	D	834	THR	N-CA-C	5.08	116.03	108.86
2	C	785	VAL	N-CA-C	5.08	115.97	108.45
3	D	335	LEU	N-CA-C	5.04	118.24	107.70
3	D	824	ASN	N-CA-C	5.03	121.52	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	PRO	Peptide
2	C	51	THR	Peptide

5.2 Too-close contacts [i](#)

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	1763	0	1760	70	0
1	B	1750	0	1775	69	0
2	C	8576	0	8510	431	0
3	D	9602	0	9558	444	0
3	J	1869	0	1876	81	0
4	K	747	0	735	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	59	0	55	10	0
6	D	2	0	0	0	0
All	All	24368	0	24269	1046	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (1046) 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)
3:D:136:ASP:HB3	3:D:137:PRO:HD3	1.14	1.10
2:C:432:ARG:O	2:C:433:THR:HB	1.49	1.09
2:C:263:ASP:HB3	2:C:264:PRO:HD3	1.12	1.09
1:B:26:GLU:HB3	1:B:27:PRO:HD3	1.29	1.09
2:C:650:LYS:HB3	2:C:653:ASP:HB2	1.35	1.07
3:D:28:LYS:HG3	3:D:42:ASP:HB3	1.10	1.07
3:D:705:ALA:HB1	3:D:706:PRO:CD	1.85	1.05
3:D:136:ASP:HB3	3:D:137:PRO:CD	1.87	1.04
2:C:442:GLU:O	2:C:442:GLU:HG3	1.55	1.02
3:D:1101:VAL:HG21	3:J:1424:VAL:HG22	1.41	1.02
3:J:1460:ILE:HD12	3:J:1460:ILE:H	1.23	1.02
3:D:705:ALA:CB	3:D:706:PRO:HD2	1.90	1.01
3:D:136:ASP:CB	3:D:137:PRO:HD3	1.90	1.01
3:D:30:GLU:HG3	3:D:545:ARG:HD2	1.41	1.00
3:D:805:ALA:HB3	3:D:832:ARG:H	1.20	1.00
2:C:474:VAL:HG21	2:C:529:VAL:CG1	1.92	1.00
2:C:1076:VAL:HB	2:C:1077:PRO:HD3	1.43	0.98
3:D:705:ALA:HB1	3:D:706:PRO:HD2	0.98	0.98
1:B:26:GLU:CB	1:B:27:PRO:HD3	1.94	0.97
3:D:98:PRO:HB2	3:D:458:ALA:HB3	1.46	0.97
2:C:650:LYS:CB	2:C:653:ASP:HB2	1.96	0.95
2:C:211:LEU:HD11	2:C:308:ARG:HA	1.49	0.94
2:C:263:ASP:CB	2:C:264:PRO:HD3	1.98	0.94
3:D:957:PRO:HD3	3:D:1007:VAL:HG23	1.45	0.94
3:D:655:PRO:HA	3:D:658:LEU:HD12	1.47	0.94
1:B:26:GLU:HB3	1:B:27:PRO:CD	1.98	0.93
3:D:28:LYS:HG3	3:D:42:ASP:CB	1.98	0.93
4:K:41:GLU:HG3	4:K:45:ARG:HH21	1.34	0.93
3:D:98:PRO:CB	3:D:458:ALA:HB3	2.01	0.91
3:D:1161:GLU:HG3	3:D:1164:ARG:HG3	1.50	0.91
3:D:783:ARG:HG3	3:D:783:ARG:HH11	1.37	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:806:PHE:HB2	3:D:808:THR:O	1.70	0.90
2:C:396:ASP:H	2:C:406:HIS:HD2	1.19	0.90
2:C:601:GLY:H	2:C:649:VAL:HG22	1.37	0.90
2:C:263:ASP:HB3	2:C:264:PRO:CD	2.01	0.89
3:D:699:VAL:H	3:D:756:GLN:NE2	1.72	0.88
3:D:841:PHE:HB2	3:D:864:VAL:HG13	1.54	0.88
3:D:28:LYS:CG	3:D:42:ASP:HB3	2.03	0.88
3:D:792:ILE:HD11	3:D:881:LEU:HD23	1.56	0.88
3:D:643:GLY:HA3	3:D:727:GLN:H	1.39	0.87
3:D:870:GLY:O	3:D:871:ARG:HB2	1.74	0.86
2:C:1076:VAL:CB	2:C:1077:PRO:HD3	2.05	0.85
3:J:1275:SER:OG	3:J:1294:VAL:HG21	1.77	0.85
2:C:474:VAL:HG21	2:C:529:VAL:HG13	1.58	0.85
3:D:1147:ARG:HB3	3:D:1188:VAL:HG21	1.57	0.84
2:C:577:PRO:HA	2:C:671:ASN:ND2	1.92	0.84
2:C:628:TYR:H	2:C:638:ASP:HB2	1.41	0.84
2:C:563:ASN:O	2:C:565:GLN:N	2.11	0.83
3:D:859:ASP:O	3:D:860:LEU:HB2	1.77	0.83
3:D:805:ALA:HB3	3:D:832:ARG:N	1.93	0.83
3:D:828:VAL:HG11	3:D:863:VAL:H	1.43	0.83
1:A:202:ASP:O	1:A:204:SER:N	2.12	0.82
1:A:126:ASP:O	1:A:127:LEU:HB3	1.79	0.82
2:C:874:LEU:O	3:D:1029:ARG:HD2	1.79	0.82
3:D:1148:VAL:HG21	3:D:1203:LYS:O	1.80	0.82
3:D:908:LYS:HB2	3:D:1027:GLY:HA3	1.62	0.82
3:D:1207:TYR:HA	3:D:1213:ARG:O	1.79	0.81
2:C:508:ILE:HD13	2:C:526:PRO:HB3	1.62	0.81
2:C:749:VAL:CG1	2:C:792:VAL:HG21	2.12	0.80
2:C:722:ILE:O	2:C:722:ILE:HG22	1.79	0.80
3:D:1068:LEU:O	3:D:1072:ILE:HG12	1.82	0.80
1:B:44:LEU:O	1:B:174:VAL:HG21	1.82	0.80
3:J:1264:GLU:OE2	3:J:1264:GLU:HA	1.81	0.80
2:C:637:PHE:HD1	2:C:659:PRO:HG3	1.48	0.79
2:C:575:GLN:HE21	2:C:670:GLN:HB3	1.48	0.79
3:D:843:PHE:HB2	3:D:866:VAL:HG22	1.63	0.79
3:D:1197:ARG:HD2	3:J:1396:GLU:HB3	1.64	0.79
1:B:33:GLY:O	1:B:195:LEU:HD13	1.83	0.78
3:D:100:ALA:N	3:D:575:GLN:OE1	2.17	0.78
3:D:1209:LEU:HG	3:D:1211:MET:HE2	1.65	0.78
2:C:841:ASN:C	2:C:841:ASN:HD22	1.91	0.78
2:C:946:ARG:HD2	2:C:984:GLU:HB2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1076:VAL:HB	2:C:1077:PRO:CD	2.12	0.78
3:D:1231:GLU:HG3	3:D:1232:PRO:HD3	1.66	0.78
1:A:198:ARG:O	1:A:199:ILE:HB	1.82	0.77
3:D:543:LEU:HD11	3:D:584:ASN:HD22	1.49	0.77
3:D:949:ILE:HD11	3:D:1023:MET:HE1	1.66	0.77
3:D:477:LEU:HA	3:D:480:GLU:HB2	1.66	0.77
2:C:693:GLU:HA	2:C:696:LYS:HD2	1.65	0.77
1:A:20:TYR:HD2	1:A:21:GLY:N	1.83	0.77
1:B:39:PRO:O	1:B:43:ILE:HD12	1.85	0.77
2:C:140:ILE:HG22	2:C:333:ILE:HD13	1.65	0.77
1:B:18:ASP:CG	1:B:19:HIS:H	1.93	0.77
3:D:1211:MET:HB2	3:D:1213:ARG:HD2	1.67	0.76
3:D:937:TYR:HB3	3:D:941:LEU:HD22	1.67	0.76
2:C:1112:PHE:O	2:C:1113:GLU:HB3	1.85	0.76
2:C:565:GLN:HA	2:C:995:MET:HE1	1.68	0.76
2:C:1087:VAL:O	2:C:1091:GLU:HG2	1.86	0.76
2:C:565:GLN:HA	2:C:995:MET:CE	2.16	0.75
3:D:805:ALA:C	3:D:832:ARG:HB2	2.11	0.75
3:D:704:ARG:HB2	3:D:745:MET:HG3	1.67	0.75
3:D:883:ALA:HB2	3:D:902:MET:HE1	1.69	0.75
3:D:1205:TYR:CE1	3:D:1221:VAL:HG11	2.22	0.75
2:C:632:ASN:HB3	2:C:633:GLN:NE2	2.01	0.74
3:D:1031:ASN:HD21	3:D:1033:GLN:HG2	1.51	0.74
3:J:1457:ASP:O	3:J:1458:GLU:HB2	1.86	0.74
1:A:59:GLU:HG2	1:A:139:TYR:HB3	1.68	0.74
3:D:795:VAL:HG12	3:D:863:VAL:HG22	1.69	0.73
1:A:225:PHE:HD2	1:B:11:PHE:CE1	2.06	0.73
3:D:841:PHE:HB2	3:D:864:VAL:CG1	2.18	0.73
1:A:124:ASN:ND2	1:A:127:LEU:HD22	2.03	0.73
2:C:261:LEU:HD21	2:C:263:ASP:HB2	1.70	0.73
3:D:552:ASN:HA	3:D:555:LYS:HB2	1.71	0.73
2:C:600:ASP:HB3	2:C:651:LYS:HG3	1.70	0.73
2:C:432:ARG:O	2:C:433:THR:CB	2.35	0.73
3:D:62:LYS:HG3	3:D:63:TYR:H	1.54	0.73
2:C:140:ILE:CG2	2:C:333:ILE:HD13	2.19	0.73
2:C:551:GLU:HA	2:C:906:PHE:HE2	1.54	0.72
2:C:719:PRO:HD2	2:C:761:PHE:CE1	2.23	0.72
2:C:632:ASN:C	2:C:633:GLN:HE21	1.96	0.72
2:C:936:VAL:HA	2:C:940:GLU:OE2	1.88	0.72
2:C:672:VAL:HG22	2:C:868:ASP:HB2	1.70	0.72
2:C:477:GLY:HA2	2:C:508:ILE:HD11	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:220:ARG:HH21	3:D:336:PHE:HB2	1.55	0.72
3:D:850:LEU:HA	3:D:853:VAL:HG23	1.70	0.72
2:C:1077:PRO:O	2:C:1078:GLU:HB2	1.90	0.72
2:C:3:ILE:HG23	2:C:902:ILE:HD13	1.72	0.71
2:C:1041:GLU:HG2	3:J:1472:ILE:HD11	1.72	0.71
3:D:270:ILE:HD12	3:D:284:LEU:HD21	1.70	0.71
2:C:441:VAL:HG12	2:C:442:GLU:H	1.54	0.71
2:C:258:PHE:N	2:C:258:PHE:CD1	2.58	0.71
2:C:437:ARG:NH2	2:C:491:GLU:OE1	2.24	0.71
3:D:176:ASP:HA	3:D:389:GLU:HB3	1.73	0.70
3:D:140:ALA:H	3:D:452:ILE:HG22	1.55	0.70
2:C:1051:GLU:HG2	2:C:1055:ILE:HD11	1.74	0.69
2:C:149:THR:HG22	2:C:150:PRO:HD2	1.72	0.69
2:C:1005:MET:HB2	3:D:629:SER:HB2	1.74	0.69
3:D:787:LEU:HG	3:D:947:ILE:HD11	1.73	0.69
4:K:26:ARG:NE	4:K:67:GLU:OE2	2.26	0.69
3:D:704:ARG:NH1	3:D:737:ASN:O	2.25	0.69
2:C:808:ARG:HB2	2:C:820:ARG:HB2	1.75	0.69
3:D:963:TYR:HE2	3:D:1002:LYS:CB	2.05	0.69
3:D:843:PHE:CE1	3:D:864:VAL:HG11	2.27	0.69
2:C:182:VAL:HG11	2:C:307:LEU:HD11	1.75	0.69
2:C:850:ALA:HA	3:D:632:VAL:HG21	1.73	0.69
2:C:988:VAL:HG12	3:D:948:THR:OG1	1.92	0.69
3:D:1095:THR:O	3:D:1099:VAL:HG23	1.92	0.69
2:C:474:VAL:HG21	2:C:529:VAL:HG12	1.73	0.69
2:C:606:VAL:HB	2:C:645:VAL:HG22	1.74	0.69
2:C:328:LEU:HB2	2:C:433:THR:HG23	1.74	0.68
5:C:1120:RFP:H18C	5:C:1120:RFP:HN1	1.57	0.68
3:D:643:GLY:HA3	3:D:727:GLN:N	2.08	0.68
1:A:158:ILE:H	1:A:166:PRO:HB3	1.56	0.68
3:D:283:PHE:CD2	3:D:335:LEU:HD13	2.29	0.68
2:C:1034:GLU:OE2	3:D:1096:ARG:NH1	2.23	0.68
3:D:1147:ARG:HB3	3:D:1188:VAL:CG2	2.22	0.68
2:C:134:ARG:HA	2:C:394:PHE:O	1.93	0.68
3:D:12:LEU:HB2	3:D:507:ASN:ND2	2.09	0.68
3:D:1208:ASP:C	3:D:1210:SER:H	2.01	0.68
2:C:1059:ASP:OD2	2:C:1083:GLU:HB2	1.94	0.68
3:D:699:VAL:H	3:D:756:GLN:HE22	1.42	0.68
2:C:682:TYR:CE1	2:C:851:LYS:HE3	2.28	0.67
2:C:751:PRO:HA	2:C:792:VAL:HG12	1.75	0.67
3:D:1197:ARG:CD	3:J:1396:GLU:HB3	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:289:THR:HG22	2:C:303:PHE:CE1	2.29	0.67
2:C:17:PRO:HD2	2:C:20:GLU:HG3	1.75	0.67
3:D:783:ARG:O	3:D:784:ASP:HB2	1.94	0.67
2:C:535:SER:O	2:C:538:GLN:HB2	1.94	0.67
2:C:580:MET:HB3	2:C:584:GLU:CD	2.19	0.67
2:C:722:ILE:O	2:C:722:ILE:CG2	2.43	0.67
3:D:1204:CYS:O	3:D:1206:GLY:N	2.28	0.67
2:C:757:GLY:HA2	2:C:789:SER:OG	1.94	0.67
3:D:1040:GLY:O	3:D:1060:SER:HB3	1.95	0.67
2:C:551:GLU:HA	2:C:906:PHE:CE2	2.29	0.67
2:C:650:LYS:C	2:C:652:GLY:H	2.01	0.66
2:C:374:ASN:HB3	2:C:377:PRO:HD2	1.77	0.66
2:C:710:ILE:HB	2:C:790:LEU:HD22	1.77	0.66
2:C:1101:THR:HB	2:C:1109:VAL:HG12	1.78	0.66
2:C:198:ARG:HD3	2:C:228:ALA:HA	1.77	0.66
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.36	0.66
2:C:1087:VAL:O	2:C:1091:GLU:CG	2.43	0.66
2:C:987:ILE:HA	3:D:948:THR:HG21	1.77	0.66
2:C:184:MET:HE2	2:C:303:PHE:CE2	2.30	0.66
2:C:701:THR:HG22	2:C:832:LYS:HA	1.78	0.66
2:C:1077:PRO:HG2	2:C:1079:PRO:HD3	1.79	0.65
1:A:73:GLU:O	1:A:74:ASP:HB3	1.95	0.65
1:B:17:GLY:O	1:B:18:ASP:HB3	1.95	0.65
2:C:577:PRO:HA	2:C:671:ASN:HD22	1.60	0.65
3:D:1105:ILE:HD11	3:J:1374:GLN:NE2	2.11	0.65
3:D:1031:ASN:HD21	3:D:1033:GLN:CG	2.08	0.65
2:C:271:GLU:HB3	2:C:464:LEU:HD22	1.79	0.65
3:D:224:ARG:HG3	3:D:331:VAL:O	1.97	0.65
1:A:9:PRO:HA	1:A:27:PRO:HD2	1.77	0.65
3:D:1211:MET:CB	3:D:1213:ARG:HD2	2.26	0.65
3:D:10:ILE:HG23	3:J:1451:ALA:HA	1.77	0.64
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.77	0.64
3:D:792:ILE:HG13	3:D:941:LEU:HG	1.79	0.64
3:D:859:ASP:O	3:D:860:LEU:CB	2.46	0.64
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.79	0.64
2:C:399:ASN:HD22	2:C:401:LEU:H	1.44	0.64
3:D:631:ILE:HG21	3:D:745:MET:SD	2.37	0.64
3:D:243:ALA:HB3	3:D:311:LEU:HD12	1.80	0.64
2:C:743:VAL:HG11	2:C:800:VAL:HG21	1.78	0.64
2:C:1056:LYS:O	3:D:624:ASP:HB2	1.98	0.64
3:D:145:VAL:CB	3:D:146:PRO:HD2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:SER:HA	1:B:14:THR:HA	1.79	0.64
2:C:881:ASN:H	2:C:881:ASN:HD22	1.43	0.64
2:C:393:GLN:HG3	2:C:406:HIS:HE1	1.62	0.64
2:C:45:GLN:HG2	2:C:71:TYR:HE2	1.63	0.64
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.79	0.64
2:C:261:LEU:HD21	2:C:263:ASP:CB	2.27	0.63
2:C:496:ILE:O	2:C:515:ALA:HB1	1.98	0.63
1:B:57:TYR:HB2	1:B:164:ALA:HB2	1.81	0.63
3:D:1237:THR:HG22	3:D:1239:ARG:H	1.63	0.63
2:C:1076:VAL:CG1	2:C:1077:PRO:HD3	2.28	0.63
3:D:643:GLY:CA	3:D:727:GLN:H	2.09	0.63
3:D:318:THR:HG22	3:D:338:GLU:HB2	1.81	0.63
3:J:1404:ASN:C	3:J:1406:ARG:H	2.06	0.63
3:D:623:VAL:HG12	3:D:625:TYR:H	1.64	0.63
2:C:469:THR:HG22	2:C:470:PRO:HD2	1.80	0.63
3:D:1078:ARG:C	3:D:1080:GLY:H	2.06	0.63
2:C:601:GLY:H	2:C:649:VAL:CG2	2.10	0.62
2:C:1098:ASP:HB3	3:D:11:ALA:HB3	1.80	0.62
3:D:116:LEU:HD11	3:D:465:LEU:HD23	1.81	0.62
3:J:1282:ARG:HB3	3:J:1293:PHE:HB2	1.81	0.62
2:C:672:VAL:HG22	2:C:868:ASP:CB	2.27	0.62
3:J:1396:GLU:HA	3:J:1399:ASP:HB2	1.82	0.62
2:C:575:GLN:HE21	2:C:670:GLN:CB	2.11	0.62
3:D:1031:ASN:HD21	3:D:1033:GLN:CD	2.08	0.62
1:B:183:ASP:N	1:B:183:ASP:OD1	2.32	0.62
2:C:343:GLN:HG2	2:C:385:PHE:HB2	1.82	0.62
3:D:1158:ARG:HH11	3:D:1160:LEU:HD21	1.65	0.62
2:C:879:ARG:H	2:C:879:ARG:HD3	1.65	0.62
1:B:18:ASP:CG	1:B:19:HIS:N	2.57	0.62
2:C:403:SER:O	2:C:407:LYS:HD2	2.00	0.62
2:C:707:ARG:HB2	2:C:826:PHE:CD2	2.35	0.61
2:C:1018:GLN:NE2	2:C:1063:ARG:HH22	1.98	0.61
3:J:1378:TYR:HE2	3:J:1394:VAL:HG22	1.64	0.61
2:C:676:ILE:O	3:D:948:THR:HB	2.00	0.61
2:C:850:ALA:HA	3:D:632:VAL:CG2	2.28	0.61
3:D:662:GLU:OE1	3:D:670:VAL:HG22	2.00	0.61
3:J:1258:ARG:HH11	3:J:1258:ARG:CG	2.13	0.61
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.82	0.61
2:C:1034:GLU:CD	3:D:1096:ARG:HH12	2.07	0.61
3:D:1103:HIS:HD2	3:J:1462:LEU:H	1.48	0.61
1:A:56:VAL:HG12	1:A:142:VAL:HG12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:708:TYR:OH	2:C:796:GLU:HG2	2.00	0.61
1:A:233:LEU:HB2	1:B:14:THR:HG22	1.82	0.61
2:C:72:ARG:NH1	2:C:112:GLU:OE1	2.34	0.61
4:K:46:PRO:HG2	4:K:63:TRP:NE1	2.14	0.61
2:C:944:LEU:HD11	2:C:963:LEU:HD23	1.82	0.61
3:J:1378:TYR:CD1	3:J:1422:MET:HE3	2.35	0.61
2:C:674:VAL:HB	2:C:869:VAL:HG13	1.83	0.61
2:C:876:VAL:O	2:C:879:ARG:O	2.18	0.61
3:D:806:PHE:CD1	3:D:809:PRO:HA	2.36	0.61
3:D:1205:TYR:HD2	3:D:1215:VAL:HG21	1.66	0.60
3:D:642:CYS:HB3	3:D:718:PRO:HA	1.83	0.60
3:D:774:SER:O	3:D:776:GLU:N	2.34	0.60
3:D:1035:ILE:HA	3:D:1038:LEU:HD12	1.83	0.60
2:C:717:LEU:HD12	3:D:533:GLY:HA2	1.82	0.60
2:C:944:LEU:HD22	2:C:962:GLN:HB3	1.84	0.60
3:D:617:ASN:OD1	3:D:621:LYS:HE3	2.01	0.60
3:D:704:ARG:HB2	3:D:745:MET:CG	2.32	0.60
3:D:783:ARG:HG3	3:D:783:ARG:NH1	2.15	0.60
1:B:213:GLN:O	1:B:217:ILE:HG12	2.00	0.60
2:C:682:TYR:CE1	2:C:851:LYS:CE	2.84	0.60
2:C:1081:VAL:HB	2:C:1086:ARG:NH2	2.17	0.60
3:D:133:ILE:HA	3:D:456:MET:HG3	1.83	0.60
3:D:618:LEU:HD22	3:J:1463:LYS:HG3	1.83	0.60
3:D:1105:ILE:HD11	3:J:1374:GLN:HE22	1.67	0.60
3:D:98:PRO:HB3	3:D:458:ALA:HB3	1.81	0.59
3:D:1224:VAL:O	3:D:1228:SER:HB2	2.02	0.59
2:C:64:LEU:HD23	2:C:100:LEU:HD21	1.83	0.59
2:C:196:LEU:O	2:C:200:LEU:HG	2.02	0.59
2:C:551:GLU:HG3	2:C:906:PHE:HD2	1.66	0.59
3:D:849:ALA:O	3:D:852:ALA:HB3	2.02	0.59
1:A:149:GLY:O	1:A:171:PHE:HB2	2.03	0.59
2:C:281:LEU:HD11	2:C:306:THR:HA	1.83	0.59
2:C:399:ASN:HB2	2:C:400:PRO:HD2	1.84	0.59
3:D:416:ALA:HB1	3:D:417:PRO:CD	2.32	0.59
2:C:1019:GLN:HB2	2:C:1020:PRO:HD2	1.83	0.59
4:K:79:LEU:O	4:K:80:VAL:HB	2.02	0.59
1:A:29:GLU:O	1:A:32:PHE:HB2	2.02	0.59
2:C:626:ARG:H	2:C:639:GLN:HE21	1.49	0.59
3:D:1029:ARG:HG2	3:D:1029:ARG:HH11	1.67	0.59
3:D:1121:PRO:O	3:D:1135:ARG:HD2	2.02	0.59
3:D:97:THR:CB	3:D:98:PRO:HD3	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1479:ASP:OD1	3:J:1482:ARG:NH1	2.36	0.59
1:B:185:ARG:HA	1:B:190:THR:HA	1.85	0.59
3:D:584:ASN:HB2	3:D:602:SER:HB3	1.85	0.59
3:D:796:ARG:HG3	3:D:796:ARG:HH11	1.68	0.59
5:C:1120:RFP:H363	5:C:1120:RFP:H372	1.85	0.59
3:J:1400:VAL:O	3:J:1404:ASN:HB3	2.03	0.59
1:A:94:MET:HE2	1:A:97:THR:HB	1.85	0.58
2:C:676:ILE:HB	2:C:988:VAL:HG13	1.85	0.58
1:A:133:GLU:HG2	1:A:134:GLU:N	2.17	0.58
2:C:1101:THR:HG22	3:D:5:VAL:HG13	1.85	0.58
3:D:578:VAL:O	3:D:582:ILE:HG12	2.02	0.58
5:C:1120:RFP:N1	5:C:1120:RFP:N2	2.51	0.58
3:D:218:LYS:HA	3:D:337:LEU:O	2.03	0.58
3:D:1150:ALA:HB3	3:D:1187:PRO:HB2	1.85	0.58
3:J:1330:ILE:O	3:J:1332:PRO:HD3	2.02	0.58
3:J:1425:THR:O	3:J:1428:ALA:HB3	2.04	0.58
1:A:225:PHE:HD2	1:B:11:PHE:HE1	1.49	0.58
3:D:843:PHE:HE1	3:D:864:VAL:HG11	1.66	0.58
2:C:545:ASN:HB3	2:C:583:LEU:HD12	1.84	0.58
1:B:80:LEU:HB3	3:D:867:ARG:HH11	1.69	0.58
2:C:1052:MET:HE3	2:C:1056:LYS:NZ	2.17	0.58
1:A:160:ASP:O	1:A:161:ARG:HB3	2.02	0.58
3:D:191:LEU:HD22	3:D:393:ILE:HG21	1.85	0.58
3:D:1006:ALA:HA	3:D:1009:LYS:HB2	1.86	0.58
3:D:1103:HIS:CD2	3:J:1462:LEU:H	2.21	0.58
3:D:1123:PHE:CD2	3:D:1184:ARG:HG3	2.39	0.58
3:D:1207:TYR:HA	3:D:1214:PRO:HA	1.85	0.58
2:C:261:LEU:CD2	2:C:263:ASP:HB2	2.34	0.58
2:C:1089:VAL:HG11	2:C:1112:PHE:HE1	1.69	0.58
3:D:44:LEU:HD22	3:D:544:TYR:HB3	1.86	0.58
3:D:804:MET:SD	3:D:831:GLY:HA3	2.44	0.58
1:B:179:PHE:HB2	1:B:197:LEU:HD12	1.86	0.57
2:C:545:ASN:HB3	2:C:583:LEU:CD1	2.34	0.57
2:C:650:LYS:O	2:C:652:GLY:N	2.37	0.57
3:D:783:ARG:O	3:D:784:ASP:CB	2.52	0.57
3:D:1207:TYR:O	3:D:1209:LEU:N	2.37	0.57
3:D:100:ALA:HA	3:D:513:ILE:HD13	1.85	0.57
3:D:154:THR:HG22	3:D:155:ASP:H	1.69	0.57
2:C:324:ASP:C	2:C:326:ASP:H	2.12	0.57
2:C:690:ILE:HG12	2:C:849:VAL:HG13	1.86	0.57
2:C:144:PRO:HA	2:C:163:ILE:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:719:PRO:HD2	2:C:761:PHE:HE1	1.66	0.57
3:D:102:ILE:HD11	3:D:579:ASP:HA	1.85	0.57
2:C:289:THR:HG23	2:C:302:VAL:HB	1.85	0.57
3:D:805:ALA:O	3:D:832:ARG:HB2	2.04	0.57
3:D:969:ARG:HD3	3:D:972:ARG:HD2	1.84	0.57
3:J:1423:GLY:O	3:J:1425:THR:N	2.37	0.57
1:B:176:ARG:HD3	1:B:200:TRP:CD1	2.40	0.57
2:C:39:ARG:HB3	2:C:45:GLN:HG3	1.86	0.57
2:C:568:ALA:HB2	2:C:995:MET:HE3	1.85	0.57
3:D:613:ARG:O	3:D:613:ARG:HG3	2.05	0.57
3:D:656:PHE:HB3	3:D:694:VAL:HG11	1.85	0.57
3:D:1057:VAL:HG22	3:D:1069:GLU:HG2	1.87	0.57
3:D:43:GLY:C	3:D:45:PHE:H	2.13	0.57
3:D:971:LEU:O	3:D:974:ILE:HG22	2.05	0.57
3:D:136:ASP:CB	3:D:137:PRO:CD	2.63	0.56
3:D:1031:ASN:OD1	3:D:1034:GLN:NE2	2.38	0.56
3:D:1197:ARG:HD2	3:J:1396:GLU:CB	2.33	0.56
3:D:1208:ASP:C	3:D:1210:SER:N	2.63	0.56
3:D:653:PHE:O	3:D:656:PHE:HB2	2.04	0.56
1:A:20:TYR:HD2	1:A:20:TYR:C	2.13	0.56
2:C:369:PRO:C	2:C:371:LYS:H	2.12	0.56
2:C:788:THR:O	2:C:788:THR:OG1	2.19	0.56
2:C:881:ASN:HD22	2:C:881:ASN:N	2.04	0.56
2:C:1005:MET:HE3	3:D:724:GLN:HG2	1.87	0.56
3:D:407:VAL:HG13	3:D:422:ALA:HB2	1.87	0.56
2:C:52:PHE:O	2:C:54:ILE:N	2.38	0.56
3:D:657:LEU:O	3:D:657:LEU:HG	2.06	0.56
3:D:771:SER:HB2	3:D:778:LEU:HD22	1.86	0.56
3:J:1396:GLU:O	3:J:1396:GLU:HG3	2.05	0.56
3:J:1258:ARG:HH21	3:J:1262:LEU:HD11	1.70	0.56
3:J:1310:ARG:HB3	3:J:1327:ARG:HD3	1.87	0.56
3:J:1412:LYS:HG3	3:J:1413:VAL:HG22	1.86	0.56
3:D:109:PRO:O	3:D:110:SER:HB2	2.05	0.56
3:D:631:ILE:HG23	3:D:745:MET:HB2	1.88	0.56
1:A:85:LEU:HA	1:A:124:ASN:HD21	1.70	0.56
2:C:57:GLY:O	2:C:58:ASP:HB2	2.05	0.56
3:D:1110:ALA:HA	3:D:1202:GLN:HB3	1.88	0.56
2:C:291:VAL:HG23	2:C:301:GLU:HG3	1.88	0.55
2:C:376:ARG:H	2:C:377:PRO:HD2	1.71	0.55
2:C:400:PRO:HG3	2:C:659:PRO:HD2	1.88	0.55
3:D:977:ALA:O	3:D:982:PHE:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:TYR:C	1:A:20:TYR:CD2	2.84	0.55
2:C:487:THR:HB	2:C:490:GLU:H	1.70	0.55
3:D:107:ASP:CG	3:D:108:VAL:H	2.15	0.55
2:C:569:VAL:O	2:C:571:LEU:HD12	2.07	0.55
2:C:289:THR:CG2	2:C:303:PHE:CE1	2.89	0.55
2:C:554:ASP:HB2	2:C:880:MET:HB2	1.89	0.55
2:C:724:ARG:HG2	2:C:724:ARG:O	2.05	0.55
2:C:903:SER:OG	2:C:908:GLY:HA3	2.06	0.55
2:C:1:MET:HG3	2:C:900:ARG:HE	1.71	0.55
2:C:394:PHE:HB2	5:C:1120:RFP:O8	2.06	0.55
2:C:631:SER:HB2	2:C:635:THR:HB	1.87	0.55
2:C:760:SER:H	2:C:788:THR:CG2	2.19	0.55
1:A:233:LEU:HD12	1:A:234:PRO:HD2	1.89	0.55
3:J:1277:ILE:HG13	3:J:1278:ASP:N	2.22	0.55
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.88	0.55
3:D:805:ALA:CB	3:D:832:ARG:H	2.07	0.55
2:C:399:ASN:HD21	2:C:401:LEU:HB3	1.72	0.54
1:A:53:VAL:HG21	1:A:82:LEU:O	2.06	0.54
1:A:199:ILE:HG21	1:A:207:PRO:HA	1.89	0.54
1:A:215:VAL:HG23	1:B:222:LEU:HD22	1.88	0.54
2:C:448:ASN:O	2:C:449:ILE:C	2.50	0.54
2:C:521:PRO:HB3	3:D:1068:LEU:CD2	2.38	0.54
2:C:1101:THR:CG2	3:D:5:VAL:HG13	2.37	0.54
1:A:73:GLU:HG3	1:A:130:ALA:HA	1.90	0.54
3:D:24:GLY:HA3	3:D:49:ILE:HB	1.89	0.54
4:K:41:GLU:HB3	4:K:42:PRO:CD	2.38	0.54
3:D:104:PHE:HD2	3:D:512:MET:SD	2.30	0.54
3:J:1465:ASN:HD21	3:J:1470:ARG:HH11	1.56	0.54
3:D:767:HIS:HA	3:D:924:MET:HE3	1.90	0.54
1:B:156:HIS:ND1	1:B:158:ILE:HG12	2.22	0.54
2:C:546:LEU:HB3	2:C:565:GLN:HE22	1.72	0.54
3:D:212:ARG:HB3	3:D:386:HIS:HB2	1.90	0.54
1:A:201:THR:HG21	1:A:205:VAL:O	2.07	0.54
2:C:50:GLU:OE2	2:C:345:ARG:NE	2.37	0.54
2:C:393:GLN:HG3	2:C:406:HIS:CE1	2.43	0.54
3:D:618:LEU:CD2	3:J:1463:LYS:HG3	2.37	0.54
3:D:860:LEU:HA	3:D:877:PRO:HB2	1.87	0.54
3:J:1258:ARG:HH11	3:J:1258:ARG:HG2	1.71	0.54
3:D:72:VAL:HG22	3:D:73:CYS:H	1.73	0.54
3:D:551:ASN:HA	3:D:574:LEU:HD12	1.89	0.54
3:J:1258:ARG:HG2	3:J:1258:ARG:NH1	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:650:LYS:C	2:C:652:GLY:N	2.66	0.54
2:C:807:ARG:HA	2:C:821:GLU:HA	1.90	0.54
3:J:1278:ASP:N	3:J:1278:ASP:OD1	2.36	0.54
1:B:128:HIS:O	1:B:130:ALA:N	2.40	0.53
1:B:179:PHE:CB	1:B:197:LEU:HD12	2.38	0.53
3:D:923:GLY:O	3:D:924:MET:C	2.51	0.53
3:J:1331:ASP:OD2	3:J:1334:GLN:HG3	2.08	0.53
1:A:38:ASN:H	1:A:39:PRO:HD2	1.74	0.53
2:C:1030:GLN:NE2	3:D:628:ARG:HG2	2.23	0.53
3:D:1109:GLU:HA	3:D:1217:ILE:HD13	1.90	0.53
1:A:44:LEU:HA	1:A:48:ILE:CD1	2.39	0.53
1:A:89:PHE:O	1:A:91:ASP:N	2.40	0.53
2:C:878:SER:HB2	3:D:1029:ARG:HD3	1.89	0.53
2:C:1059:ASP:CG	2:C:1083:GLU:HB2	2.33	0.53
3:D:1161:GLU:CG	3:D:1164:ARG:HG3	2.32	0.53
2:C:565:GLN:HA	2:C:995:MET:HE3	1.90	0.53
2:C:710:ILE:HG21	2:C:756:VAL:HG11	1.89	0.53
4:K:26:ARG:HD2	4:K:29:GLN:HE21	1.73	0.53
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.44	0.53
2:C:831:ARG:O	2:C:832:LYS:HB2	2.08	0.53
3:D:584:ASN:HD21	3:D:591:VAL:HB	1.74	0.53
2:C:577:PRO:HA	2:C:671:ASN:HD21	1.72	0.53
2:C:602:GLU:O	2:C:613:VAL:HG23	2.08	0.53
3:D:160:GLU:HG2	3:D:165:LYS:HB2	1.91	0.53
3:D:1105:ILE:HG23	3:D:1199:GLY:HA2	1.90	0.53
2:C:1095:LEU:O	2:C:1096:ALA:HB3	2.09	0.53
3:D:638:LYS:HA	3:D:932:ASP:OD2	2.09	0.53
3:J:1353:GLN:HG2	3:J:1368:ILE:HD12	1.90	0.53
2:C:1006:HIS:HB3	2:C:1027:PHE:CG	2.44	0.53
3:D:483:HIS:N	3:D:484:PRO:HD3	2.24	0.53
3:D:907:GLU:HB2	3:D:1026:SER:HA	1.91	0.53
2:C:1020:PRO:HG2	3:D:622:ARG:HB2	1.90	0.53
3:J:1417:TRP:CD1	3:J:1417:TRP:C	2.86	0.53
1:B:118:ALA:C	1:B:120:VAL:H	2.16	0.53
2:C:631:SER:CB	2:C:635:THR:HB	2.39	0.53
2:C:841:ASN:ND2	2:C:845:ASN:H	2.07	0.53
2:C:902:ILE:O	2:C:902:ILE:HG22	2.08	0.53
3:D:792:ILE:CD1	3:D:881:LEU:HD23	2.34	0.53
3:D:543:LEU:HG	3:D:600:LEU:HD11	1.90	0.52
3:J:1349:VAL:HG22	3:J:1368:ILE:HG22	1.91	0.52
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:203:ALA:HA	3:D:394:LEU:O	2.10	0.52
1:A:21:GLY:O	1:A:198:ARG:O	2.26	0.52
1:A:198:ARG:O	1:A:199:ILE:CB	2.55	0.52
1:A:211:LEU:O	1:A:215:VAL:HG12	2.10	0.52
2:C:393:GLN:HB3	5:C:1120:RFP:O9	2.09	0.52
2:C:793:PRO:HG2	2:C:796:GLU:HB2	1.91	0.52
3:D:396:VAL:C	3:D:398:ALA:H	2.16	0.52
3:J:1307:LYS:C	3:J:1309:ALA:H	2.16	0.52
2:C:327:HIS:HD2	2:C:329:GLY:H	1.57	0.52
3:D:90:MET:HA	3:D:521:PRO:HD3	1.91	0.52
3:D:319:ALA:HB2	3:D:337:LEU:HD23	1.92	0.52
2:C:84:ARG:HA	2:C:131:GLY:HA2	1.90	0.52
1:B:118:ALA:C	1:B:120:VAL:N	2.67	0.52
2:C:177:GLU:C	2:C:179:SER:H	2.18	0.52
2:C:650:LYS:HB2	2:C:653:ASP:HB2	1.89	0.52
3:D:97:THR:OG1	3:D:98:PRO:HD3	2.09	0.52
4:K:6:ILE:HD13	4:K:6:ILE:O	2.10	0.52
2:C:749:VAL:HG12	2:C:792:VAL:HG21	1.91	0.52
3:D:41:ARG:NH2	3:D:42:ASP:CG	2.68	0.52
3:D:372:ASP:HB3	3:D:375:GLU:HB2	1.92	0.52
3:D:957:PRO:CD	3:D:1007:VAL:HG23	2.31	0.52
3:D:1106:VAL:O	3:D:1108:ARG:HG2	2.10	0.52
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.92	0.52
1:B:129:ILE:HG22	1:B:130:ALA:N	2.25	0.52
2:C:441:VAL:HG12	2:C:442:GLU:N	2.24	0.52
3:D:1197:ARG:CG	3:J:1396:GLU:HB3	2.40	0.52
1:A:86:VAL:HG21	1:A:202:ASP:HB2	1.91	0.52
2:C:605:LYS:HB2	2:C:612:ALA:HB3	1.91	0.52
2:C:631:SER:HB3	2:C:633:GLN:H	1.75	0.52
3:D:129:PHE:O	3:D:131:LYS:N	2.42	0.52
3:D:190:GLU:HG2	3:D:196:VAL:HG13	1.91	0.52
2:C:271:GLU:HB3	2:C:464:LEU:CD2	2.40	0.51
2:C:967:PHE:HA	2:C:971:LYS:O	2.10	0.51
3:D:334:THR:C	3:D:335:LEU:HG	2.35	0.51
3:D:810:GLU:HG3	3:D:810:GLU:O	2.10	0.51
3:J:1277:ILE:HG13	3:J:1278:ASP:H	1.74	0.51
4:K:38:THR:HG22	4:K:40:LEU:H	1.75	0.51
2:C:628:TYR:N	2:C:638:ASP:HB2	2.18	0.51
3:D:30:GLU:HG3	3:D:545:ARG:CD	2.28	0.51
2:C:843:HIS:CD2	2:C:884:GLN:HA	2.44	0.51
3:D:783:ARG:HH11	3:D:783:ARG:CG	2.15	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:GLU:CB	1:B:27:PRO:CD	2.68	0.51
2:C:272:ALA:O	2:C:276:LYS:N	2.40	0.51
1:B:59:GLU:HB2	1:B:139:TYR:HB3	1.92	0.51
2:C:216:ASP:O	2:C:219:GLN:HB2	2.10	0.51
2:C:436:GLY:O	2:C:459:ALA:HB2	2.11	0.51
3:D:44:LEU:CD2	3:D:544:TYR:HB3	2.41	0.51
3:D:631:ILE:CG2	3:D:745:MET:HB2	2.40	0.51
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.91	0.51
2:C:617:ASP:O	2:C:619:ARG:N	2.44	0.51
3:D:732:VAL:HG13	3:D:736:PHE:CD1	2.46	0.51
2:C:285:LEU:HD11	2:C:302:VAL:HG22	1.93	0.51
3:D:519:VAL:HG22	3:D:544:TYR:CE1	2.46	0.51
2:C:261:LEU:HG	2:C:263:ASP:H	1.75	0.51
2:C:1101:THR:O	2:C:1108:PRO:HA	2.11	0.51
3:D:870:GLY:O	3:D:871:ARG:CB	2.52	0.51
3:D:1141:GLU:HA	3:D:1171:VAL:HG11	1.93	0.51
1:B:82:LEU:O	1:B:85:LEU:HB3	2.11	0.50
3:D:139:GLY:HA2	3:D:452:ILE:HG22	1.93	0.50
3:D:886:VAL:HG11	3:D:900:ILE:HD11	1.92	0.50
2:C:1113:GLU:O	2:C:1113:GLU:HG2	2.11	0.50
3:J:1311:LEU:HD12	3:J:1313:VAL:H	1.76	0.50
2:C:134:ARG:NH1	2:C:392:SER:O	2.44	0.50
2:C:496:ILE:HG12	2:C:531:PHE:HB2	1.94	0.50
1:B:33:GLY:HA3	1:B:181:VAL:HG21	1.93	0.50
2:C:477:GLY:HA2	2:C:508:ILE:CD1	2.40	0.50
2:C:856:GLU:CD	2:C:856:GLU:H	2.19	0.50
2:C:881:ASN:H	2:C:881:ASN:ND2	2.07	0.50
3:D:959:GLU:HB3	3:D:963:TYR:CD1	2.46	0.50
2:C:328:LEU:HB2	2:C:433:THR:CG2	2.41	0.50
2:C:874:LEU:HD21	3:D:787:LEU:HD22	1.92	0.50
3:D:100:ALA:HB1	3:D:105:VAL:HG21	1.93	0.50
3:D:1111:ASP:C	3:D:1113:GLY:N	2.70	0.50
1:B:32:PHE:HA	1:B:35:THR:HB	1.93	0.50
2:C:257:LEU:C	2:C:259:GLY:H	2.19	0.50
3:D:92:HIS:CD2	3:D:92:HIS:C	2.88	0.50
1:A:34:VAL:O	1:A:35:THR:C	2.54	0.50
2:C:847:GLY:HA2	3:D:741:ASP:HA	1.94	0.50
3:D:101:HIS:C	3:D:101:HIS:CD2	2.90	0.50
3:J:1353:GLN:O	3:J:1357:ARG:HB2	2.12	0.50
2:C:175:GLU:O	2:C:175:GLU:HG3	2.12	0.50
2:C:202:TYR:HE1	2:C:300:ASP:OD1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:886:LEU:HD23	3:D:951:ILE:HD12	1.93	0.50
2:C:1030:GLN:HB2	3:D:626:SER:HB2	1.94	0.50
4:K:35:PHE:C	4:K:37:ASN:H	2.19	0.50
2:C:396:ASP:H	2:C:406:HIS:CD2	2.11	0.49
2:C:1093:GLN:C	2:C:1095:LEU:H	2.20	0.49
1:B:80:LEU:HD13	3:D:844:ALA:HA	1.95	0.49
1:B:215:VAL:O	1:B:219:LYS:HB2	2.12	0.49
2:C:673:LEU:HD23	2:C:867:VAL:HG12	1.95	0.49
2:C:707:ARG:HB2	2:C:826:PHE:HD2	1.74	0.49
2:C:1076:VAL:CB	2:C:1077:PRO:CD	2.79	0.49
3:D:12:LEU:HD21	3:D:104:PHE:HE2	1.77	0.49
3:D:116:LEU:HD21	3:D:465:LEU:HD23	1.94	0.49
3:D:666:PHE:O	3:D:667:ALA:HB3	2.11	0.49
2:C:435:TYR:OH	2:C:533:ASP:OD2	2.26	0.49
2:C:1041:GLU:HG2	3:J:1472:ILE:CD1	2.40	0.49
3:D:219:GLU:HG2	3:D:271:TYR:OH	2.12	0.49
2:C:256:TYR:HD2	2:C:261:LEU:HD22	1.78	0.49
3:D:136:ASP:CG	3:D:137:PRO:HD3	2.36	0.49
3:D:208:PRO:HG2	3:D:347:VAL:HG21	1.95	0.49
1:B:20:TYR:HA	1:B:199:ILE:O	2.12	0.49
2:C:110:GLU:HB2	2:C:369:PRO:HG2	1.94	0.49
2:C:760:SER:H	2:C:788:THR:HG21	1.76	0.49
2:C:1034:GLU:CD	3:D:1096:ARG:NH1	2.68	0.49
3:D:660:LYS:O	3:D:664:LYS:HB2	2.13	0.49
1:A:58:ILE:HG23	1:A:140:MET:HG3	1.95	0.49
2:C:26:TYR:HB2	2:C:121:MET:HE1	1.95	0.49
2:C:714:ASP:HA	2:C:719:PRO:HA	1.95	0.49
3:D:543:LEU:HD11	3:D:584:ASN:ND2	2.23	0.49
2:C:637:PHE:CD1	2:C:659:PRO:HG3	2.38	0.49
5:C:1120:RFP:H18C	5:C:1120:RFP:N1	2.27	0.49
3:D:191:LEU:HD13	3:D:393:ILE:HG21	1.95	0.49
3:D:450:TYR:N	3:D:450:TYR:CD1	2.80	0.49
1:B:186:LEU:N	1:B:189:ARG:O	2.31	0.49
2:C:260:LEU:O	2:C:261:LEU:HD23	2.12	0.49
2:C:436:GLY:HA3	2:C:469:THR:HG21	1.94	0.49
2:C:846:LYS:HG3	3:D:741:ASP:HB2	1.94	0.49
3:D:46:ASP:OD2	3:D:49:ILE:HG12	2.13	0.49
3:D:666:PHE:CD1	3:D:666:PHE:C	2.91	0.49
3:J:1347:TYR:CZ	3:J:1351:GLU:HG3	2.48	0.49
2:C:263:ASP:CB	2:C:264:PRO:CD	2.74	0.49
3:D:112:ILE:C	3:D:114:THR:H	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1336:LEU:HG	3:J:1337:GLU:N	2.27	0.49
2:C:809:GLY:O	2:C:810:ASP:C	2.57	0.48
3:D:416:ALA:HB1	3:D:417:PRO:HD2	1.94	0.48
3:D:540:LEU:HD11	3:D:603:LEU:HD13	1.95	0.48
3:J:1396:GLU:O	3:J:1396:GLU:CG	2.60	0.48
2:C:1006:HIS:O	3:D:627:GLY:HA3	2.13	0.48
3:D:84:ILE:H	3:D:84:ILE:HG13	1.45	0.48
3:D:759:ALA:HA	3:D:763:MET:HG3	1.95	0.48
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.48	0.48
2:C:442:GLU:O	2:C:442:GLU:CG	2.41	0.48
2:C:540:PHE:CZ	2:C:906:PHE:HE1	2.32	0.48
2:C:546:LEU:HD11	2:C:666:LEU:HD23	1.94	0.48
2:C:564:MET:O	2:C:567:GLN:N	2.46	0.48
3:D:963:TYR:CE2	3:D:1002:LYS:CB	2.92	0.48
2:C:632:ASN:HB3	2:C:633:GLN:HE21	1.76	0.48
2:C:953:VAL:HG22	2:C:966:LEU:HD13	1.96	0.48
3:D:19:ARG:NH2	3:D:515:GLU:HB3	2.29	0.48
3:D:937:TYR:O	3:D:938:GLY:C	2.57	0.48
3:D:1008:PHE:CZ	3:D:1032:PRO:HA	2.48	0.48
3:D:1014:ASN:O	3:D:1015:TYR:CB	2.62	0.48
3:D:1111:ASP:C	3:D:1113:GLY:H	2.21	0.48
2:C:139:GLN:NE2	2:C:334:ARG:HH21	2.11	0.48
3:D:1007:VAL:HG21	3:D:1039:CYS:HB2	1.95	0.48
3:D:1029:ARG:HG2	3:D:1029:ARG:NH1	2.27	0.48
3:D:1031:ASN:ND2	3:D:1033:GLN:HG2	2.22	0.48
3:J:1342:GLU:H	3:J:1342:GLU:CD	2.21	0.48
1:A:62:LEU:HD12	1:A:62:LEU:H	1.79	0.48
2:C:351:LEU:HD11	2:C:373:VAL:HG22	1.95	0.48
3:J:1462:LEU:O	3:J:1463:LYS:C	2.56	0.48
2:C:25:SER:HA	2:C:28:LYS:HE2	1.96	0.48
2:C:147:TYR:O	2:C:148:PHE:HB2	2.13	0.48
2:C:230:ARG:HB3	2:C:233:GLU:HB2	1.96	0.48
3:J:1335:LEU:HD23	3:J:1344:VAL:CG2	2.43	0.48
2:C:544:THR:HG22	2:C:550:LEU:HD21	1.95	0.48
2:C:712:ALA:HB2	2:C:722:ILE:HD12	1.95	0.48
3:D:85:VAL:HG11	3:D:89:ARG:HE	1.77	0.48
3:D:465:LEU:HD13	3:D:509:PRO:O	2.14	0.48
3:D:1060:SER:O	3:D:1062:ARG:N	2.47	0.48
3:J:1382:THR:O	3:J:1416:ALA:HB3	2.13	0.48
2:C:109:LYS:HZ2	2:C:109:LYS:HB3	1.78	0.48
3:D:852:ALA:O	3:D:857:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:256:TYR:CD2	2:C:261:LEU:HD22	2.49	0.47
2:C:475:LYS:O	2:C:476:ASN:C	2.56	0.47
2:C:968:ASP:C	2:C:970:GLY:H	2.22	0.47
3:D:24:GLY:O	3:D:25:GLU:CB	2.62	0.47
2:C:333:ILE:HD11	2:C:467:ILE:HD11	1.96	0.47
2:C:486:MET:HE3	2:C:491:GLU:HA	1.96	0.47
2:C:508:ILE:HD13	2:C:526:PRO:CB	2.40	0.47
3:D:262:LYS:N	3:D:269:LEU:O	2.47	0.47
3:D:368:VAL:H	3:D:377:VAL:HB	1.79	0.47
3:D:762:GLN:HE21	4:K:20:THR:HG21	1.79	0.47
3:D:810:GLU:O	3:D:811:GLU:C	2.58	0.47
2:C:684:PHE:CE2	2:C:685:GLU:HG2	2.49	0.47
2:C:815:LEU:HD13	2:C:822:VAL:HG23	1.95	0.47
2:C:856:GLU:CD	2:C:856:GLU:N	2.72	0.47
3:D:1060:SER:O	3:D:1061:PHE:C	2.57	0.47
2:C:580:MET:HB3	2:C:584:GLU:OE2	2.14	0.47
2:C:599:GLU:O	2:C:600:ASP:C	2.57	0.47
2:C:732:ALA:HA	2:C:735:ARG:HD2	1.96	0.47
3:D:242:LEU:HD13	3:D:313:LEU:HD21	1.97	0.47
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.96	0.47
2:C:327:HIS:CD2	2:C:329:GLY:H	2.31	0.47
3:D:841:PHE:CB	3:D:864:VAL:CG1	2.92	0.47
1:A:143:ARG:NE	1:A:145:ASP:OD1	2.47	0.47
1:A:206:THR:O	1:A:207:PRO:C	2.57	0.47
1:B:19:HIS:HA	1:B:201:THR:OG1	2.14	0.47
3:D:804:MET:CG	3:D:805:ALA:H	2.26	0.47
3:J:1258:ARG:CG	3:J:1258:ARG:NH1	2.76	0.47
1:A:26:GLU:HB3	1:A:27:PRO:HD3	1.96	0.47
1:A:68:ILE:HB	1:A:71:VAL:CG2	2.45	0.47
1:A:90:LEU:HG	1:A:119:ASP:C	2.39	0.47
1:B:86:VAL:HB	1:B:123:MET:HB2	1.96	0.47
1:B:176:ARG:HB3	1:B:200:TRP:CD1	2.49	0.47
2:C:193:LEU:HD22	2:C:197:LEU:HG	1.97	0.47
2:C:948:GLU:HB3	2:C:953:VAL:HB	1.96	0.47
3:D:458:ALA:O	3:D:462:GLN:HB2	2.15	0.47
3:D:1066:THR:O	3:D:1069:GLU:N	2.48	0.47
3:D:1211:MET:SD	4:K:16:LYS:HE3	2.54	0.47
2:C:549:PHE:HB3	2:C:552:HIS:HD2	1.80	0.47
2:C:1088:LEU:O	2:C:1089:VAL:C	2.57	0.47
3:D:73:CYS:HB2	3:D:77:GLY:HA2	1.97	0.47
3:D:1125:MET:HE3	3:D:1132:LEU:HG	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:396:ASP:HA	2:C:633:GLN:OE1	2.15	0.47
3:D:95:LEU:HD12	3:D:574:LEU:HD21	1.96	0.47
1:B:53:VAL:HG11	1:B:82:LEU:HD12	1.96	0.47
2:C:89:THR:HG22	2:C:91:GLN:HG3	1.96	0.47
2:C:147:TYR:O	2:C:323:ASP:HB2	2.15	0.47
2:C:379:GLU:O	2:C:383:ARG:HB2	2.15	0.47
3:D:762:GLN:NE2	4:K:20:THR:HG21	2.30	0.47
3:D:813:LEU:HD11	3:D:839:LEU:HD22	1.97	0.47
4:K:33:HIS:O	4:K:34:ARG:C	2.58	0.47
1:B:44:LEU:HD13	1:B:214:ALA:HB2	1.95	0.46
2:C:160:ALA:HB2	2:C:310:LEU:HD13	1.96	0.46
2:C:857:ASP:O	2:C:858:MET:HB2	2.15	0.46
2:C:967:PHE:O	2:C:970:GLY:N	2.45	0.46
2:C:1071:ILE:HG13	3:D:670:VAL:HG11	1.97	0.46
3:D:202:VAL:O	3:D:395:VAL:HA	2.15	0.46
3:D:796:ARG:HG3	3:D:796:ARG:NH1	2.27	0.46
3:D:956:ILE:HG23	3:D:1039:CYS:O	2.15	0.46
1:A:151:VAL:HA	1:A:152:PRO:HD3	1.77	0.46
2:C:1046:ALA:HA	3:J:1472:ILE:HG22	1.98	0.46
3:D:25:GLU:HA	3:D:92:HIS:O	2.16	0.46
3:D:371:ILE:H	3:D:371:ILE:HG13	1.55	0.46
2:C:256:TYR:HE2	2:C:261:LEU:HB3	1.79	0.46
2:C:462:ASP:O	2:C:463:ALA:C	2.57	0.46
2:C:565:GLN:CA	2:C:995:MET:HE1	2.43	0.46
3:D:804:MET:HE2	3:D:804:MET:HB2	1.83	0.46
3:D:1014:ASN:O	3:D:1015:TYR:CG	2.68	0.46
3:D:1031:ASN:HD21	3:D:1033:GLN:H	1.63	0.46
3:J:1372:VAL:HG22	3:J:1375:MET:HE2	1.96	0.46
1:B:24:VAL:HG22	1:B:196:THR:HG23	1.97	0.46
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.98	0.46
2:C:1038:TRP:CD1	3:D:1099:VAL:HG11	2.49	0.46
3:D:179:VAL:HG21	3:D:191:LEU:HD23	1.96	0.46
3:D:705:ALA:CB	3:D:706:PRO:CD	2.64	0.46
3:D:709:HIS:O	3:D:710:ARG:C	2.57	0.46
3:D:1015:TYR:N	3:D:1016:PRO:CD	2.78	0.46
1:A:34:VAL:HG12	1:A:179:PHE:HZ	1.80	0.46
1:B:132:LEU:HD22	1:B:132:LEU:H	1.80	0.46
3:D:121:THR:O	3:D:123:LEU:N	2.48	0.46
3:D:932:ASP:O	3:D:935:LYS:HB3	2.16	0.46
2:C:979:THR:O	2:C:981:GLU:N	2.49	0.46
3:D:102:ILE:HD11	3:D:579:ASP:CA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:456:MET:HG2	3:D:457:GLY:H	1.81	0.46
3:D:668:PRO:HD2	3:D:669:ASN:H	1.81	0.46
2:C:26:TYR:HB2	2:C:121:MET:CE	2.46	0.46
3:D:530:VAL:O	3:D:532:GLY:N	2.49	0.46
3:D:583:ASP:O	3:D:586:ARG:HG2	2.16	0.46
3:D:646:LYS:HB2	3:D:688:TRP:CZ3	2.51	0.46
2:C:850:ALA:CB	3:D:632:VAL:HG22	2.46	0.46
3:D:284:LEU:HD13	3:D:305:ALA:HB2	1.98	0.46
2:C:603:VAL:HG21	2:C:643:VAL:CG1	2.45	0.46
2:C:1095:LEU:O	2:C:1096:ALA:CB	2.63	0.46
3:D:12:LEU:HD21	3:D:104:PHE:CE2	2.51	0.46
4:K:15:SER:O	4:K:16:LYS:C	2.59	0.46
1:B:65:PHE:CD1	3:D:813:LEU:HG	2.51	0.46
1:B:120:VAL:HG12	1:B:120:VAL:O	2.15	0.46
2:C:1076:VAL:HG12	2:C:1077:PRO:HD3	1.97	0.46
3:D:186:VAL:CG1	3:D:187:LYS:N	2.79	0.46
4:K:26:ARG:O	4:K:30:LEU:HB2	2.16	0.46
2:C:313:LEU:O	2:C:313:LEU:HG	2.16	0.45
2:C:324:ASP:C	2:C:326:ASP:N	2.73	0.45
3:D:367:ILE:HB	3:D:377:VAL:HG12	1.98	0.45
3:D:400:VAL:HG23	3:D:445:ARG:HB3	1.98	0.45
3:D:959:GLU:HB3	3:D:963:TYR:CE1	2.51	0.45
2:C:447:ALA:H	3:D:1085:ALA:HB1	1.80	0.45
2:C:494:TYR:HB3	2:C:530:GLU:HB2	1.98	0.45
2:C:524:VAL:HG13	2:C:528:GLU:HB2	1.97	0.45
3:D:29:PRO:HB2	3:D:30:GLU:H	1.55	0.45
3:D:960:LYS:O	3:D:964:LEU:HB2	2.16	0.45
3:D:1066:THR:O	3:D:1068:LEU:N	2.48	0.45
2:C:901:TYR:HE2	2:C:917:LEU:CD1	2.30	0.45
3:D:860:LEU:HD12	3:D:877:PRO:HB2	1.98	0.45
1:B:216:ALA:O	1:B:220:GLU:HB2	2.17	0.45
2:C:575:GLN:NE2	2:C:670:GLN:HB3	2.25	0.45
2:C:582:GLY:O	2:C:584:GLU:N	2.50	0.45
2:C:941:LYS:O	2:C:942:GLU:C	2.59	0.45
2:C:971:LYS:HA	2:C:988:VAL:HA	1.99	0.45
3:D:396:VAL:C	3:D:398:ALA:N	2.75	0.45
3:D:827:ILE:O	3:D:836:VAL:HG13	2.16	0.45
1:B:188:GLN:HG2	3:D:688:TRP:NE1	2.31	0.45
2:C:399:ASN:ND2	2:C:401:LEU:HB3	2.31	0.45
3:D:112:ILE:HD11	3:D:512:MET:HB3	1.98	0.45
3:D:508:ARG:C	3:D:510:GLU:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:SER:O	1:B:142:VAL:HA	2.17	0.45
1:B:208:LEU:HG	1:B:212:ASN:ND2	2.32	0.45
2:C:21:ILE:H	2:C:21:ILE:HG13	1.46	0.45
2:C:210:GLU:O	2:C:308:ARG:HD2	2.16	0.45
2:C:363:SER:HA	2:C:364:PRO:HD3	1.80	0.45
2:C:966:LEU:HD11	2:C:986:PRO:HG3	1.99	0.45
3:D:39:PRO:HB3	3:D:45:PHE:HB3	1.98	0.45
3:D:835:SER:H	3:D:838:ARG:HG3	1.82	0.45
3:D:929:ARG:NH1	4:K:1:MET:HA	2.31	0.45
3:D:937:TYR:HA	3:D:940:THR:HG22	1.98	0.45
2:C:431:HIS:HB3	2:C:434:HIS:CE1	2.52	0.45
2:C:856:GLU:N	2:C:856:GLU:OE2	2.50	0.45
3:D:118:LEU:O	3:D:119:SER:C	2.60	0.45
3:D:137:PRO:HD2	3:D:453:ASP:HB3	1.99	0.45
3:D:338:GLU:O	3:D:339:TRP:HB3	2.17	0.45
3:D:792:ILE:HG23	3:D:793:THR:HG23	1.98	0.45
2:C:261:LEU:CD2	2:C:263:ASP:CB	2.93	0.45
2:C:726:ILE:HB	2:C:729:LEU:HD22	1.99	0.45
3:D:602:SER:H	3:D:605:ASP:HB2	1.81	0.45
4:K:41:GLU:O	4:K:42:PRO:C	2.60	0.45
2:C:198:ARG:HD2	2:C:198:ARG:HA	1.74	0.45
2:C:443:THR:OG1	2:C:444:PRO:HD2	2.17	0.45
2:C:809:GLY:O	2:C:810:ASP:O	2.35	0.45
3:D:178:LEU:HG	3:D:193:PRO:HD3	1.99	0.45
3:J:1457:ASP:O	3:J:1458:GLU:CB	2.61	0.45
4:K:70:THR:C	4:K:72:ARG:H	2.25	0.45
2:C:901:TYR:HE2	2:C:917:LEU:HD11	1.82	0.45
3:D:186:VAL:HG12	3:D:187:LYS:N	2.32	0.45
3:D:875:THR:OG1	3:D:876:SER:N	2.48	0.45
3:J:1438:ALA:O	3:J:1439:SER:C	2.60	0.45
3:D:828:VAL:HG11	3:D:863:VAL:HG23	1.99	0.44
3:D:1031:ASN:ND2	3:D:1033:GLN:H	2.15	0.44
3:D:1149:LEU:HD23	3:D:1187:PRO:O	2.16	0.44
3:J:1258:ARG:NH2	3:J:1262:LEU:HD11	2.32	0.44
1:A:57:TYR:CD2	1:A:57:TYR:C	2.95	0.44
1:B:184:THR:N	1:B:192:LEU:O	2.45	0.44
2:C:110:GLU:HB2	2:C:369:PRO:CG	2.48	0.44
3:D:729:HIS:CE1	3:D:731:LEU:HB2	2.51	0.44
3:D:1117:TYR:HE2	3:D:1151:ARG:HE	1.66	0.44
2:C:194:VAL:HA	2:C:197:LEU:HD12	1.99	0.44
2:C:439:CYS:CB	2:C:541:SER:HB3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:29:PRO:HB2	3:D:30:GLU:OE1	2.18	0.44
3:D:581:VAL:O	3:D:581:VAL:CG1	2.66	0.44
3:J:1272:ALA:HA	3:J:1326:THR:HG22	1.99	0.44
1:B:17:GLY:O	1:B:18:ASP:CB	2.62	0.44
2:C:501:THR:HA	2:C:502:PRO:HD3	1.81	0.44
2:C:550:LEU:HB3	2:C:905:VAL:HG13	1.99	0.44
3:D:104:PHE:N	3:D:104:PHE:CD1	2.85	0.44
3:D:1174:LEU:HD13	3:D:1186:VAL:HG21	1.98	0.44
3:J:1307:LYS:C	3:J:1309:ALA:N	2.76	0.44
3:J:1363:LEU:C	3:J:1363:LEU:HD12	2.42	0.44
2:C:20:GLU:OE1	2:C:460:ARG:HD3	2.17	0.44
2:C:54:ILE:HD11	2:C:356:ARG:HG3	1.99	0.44
2:C:981:GLU:HB3	2:C:982:PRO:HD2	1.99	0.44
2:C:1018:GLN:HE21	2:C:1063:ARG:HH22	1.63	0.44
3:D:704:ARG:HG3	3:D:705:ALA:CB	2.48	0.44
3:J:1256:LEU:N	3:J:1257:PRO:CD	2.81	0.44
3:J:1314:LYS:H	3:J:1314:LYS:HG2	1.60	0.44
3:J:1376:LEU:O	3:J:1378:TYR:N	2.51	0.44
1:A:43:ILE:HG12	1:B:32:PHE:CE1	2.52	0.44
2:C:304:LEU:N	2:C:305:PRO:HD2	2.33	0.44
2:C:999:HIS:HB3	2:C:1004:LYS:NZ	2.32	0.44
3:D:98:PRO:O	3:D:99:ALA:HB2	2.18	0.44
3:D:764:LEU:HD23	3:D:767:HIS:CE1	2.52	0.44
3:D:923:GLY:O	3:D:925:GLU:N	2.51	0.44
3:D:955:VAL:O	3:D:1039:CYS:HB3	2.17	0.44
3:J:1435:LEU:HD21	3:J:1468:LEU:HD21	1.99	0.44
1:A:218:LEU:O	1:A:222:LEU:HB2	2.17	0.44
1:B:52:ALA:CB	1:B:170:ILE:HD12	2.47	0.44
2:C:193:LEU:HD13	2:C:197:LEU:HD11	1.98	0.44
2:C:311:PHE:C	2:C:313:LEU:H	2.24	0.44
2:C:699:PHE:C	2:C:701:THR:H	2.25	0.44
2:C:1072:LYS:HD3	2:C:1074:GLU:CD	2.42	0.44
3:D:43:GLY:C	3:D:45:PHE:N	2.75	0.44
3:D:996:TRP:CE2	3:D:1056:PRO:HG3	2.52	0.44
2:C:8:ARG:HD2	2:C:8:ARG:HA	1.64	0.44
2:C:232:GLU:HA	2:C:235:MET:HE3	2.00	0.44
2:C:397:GLU:O	2:C:398:THR:C	2.61	0.44
2:C:462:ASP:O	2:C:465:GLY:N	2.35	0.44
2:C:768:SER:O	2:C:771:GLU:HG3	2.17	0.44
3:J:1413:VAL:HB	3:J:1415:VAL:H	1.82	0.44
3:J:1450:ALA:O	3:J:1453:ALA:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:52:PHE:CG	2:C:68:PHE:HB2	2.53	0.44
2:C:393:GLN:OE1	5:C:1120:RFP:H343	2.18	0.44
2:C:1034:GLU:OE1	3:D:1096:ARG:NH1	2.51	0.44
3:D:1165:TYR:CZ	3:D:1214:PRO:HB3	2.53	0.44
1:A:115:THR:HA	1:A:116:PRO:HD3	1.83	0.43
1:A:231:SER:HB3	1:B:15:THR:HG22	2.00	0.43
2:C:168:ARG:NH2	2:C:262:ALA:HB1	2.33	0.43
2:C:498:GLN:OE1	3:D:1068:LEU:HB2	2.18	0.43
2:C:1052:MET:HE1	3:D:748:HIS:HB3	1.99	0.43
2:C:1097:LEU:N	2:C:1097:LEU:HD23	2.33	0.43
3:D:771:SER:HA	3:D:772:PRO:HD3	1.87	0.43
2:C:274:ARG:O	2:C:278:GLU:N	2.44	0.43
2:C:601:GLY:N	2:C:649:VAL:HG22	2.19	0.43
3:D:111:LYS:HG2	3:J:1452:ILE:CD1	2.48	0.43
3:D:320:LYS:O	3:D:321:GLU:C	2.61	0.43
3:D:547:LEU:HD11	3:D:578:VAL:HG22	2.00	0.43
3:D:661:MET:HG2	3:D:666:PHE:CZ	2.52	0.43
1:B:80:LEU:HB3	3:D:867:ARG:NH1	2.31	0.43
2:C:576:ALA:HB1	2:C:580:MET:HE2	2.00	0.43
2:C:699:PHE:O	2:C:701:THR:N	2.50	0.43
2:C:751:PRO:HA	2:C:792:VAL:CG1	2.46	0.43
3:D:666:PHE:O	3:D:666:PHE:CD1	2.71	0.43
3:D:699:VAL:H	3:D:756:GLN:HE21	1.55	0.43
3:D:884:ARG:O	3:D:885:ILE:C	2.61	0.43
3:J:1269:LYS:O	3:J:1270:ALA:HB3	2.17	0.43
2:C:1074:GLU:O	2:C:1076:VAL:N	2.45	0.43
3:D:770:LEU:HB3	3:D:775:GLY:O	2.17	0.43
3:D:806:PHE:HD2	3:D:810:GLU:HG2	1.84	0.43
3:D:1209:LEU:HD12	3:D:1209:LEU:O	2.18	0.43
4:K:33:HIS:O	4:K:35:PHE:N	2.51	0.43
2:C:131:GLY:O	2:C:132:ALA:O	2.36	0.43
2:C:272:ALA:O	2:C:273:GLY:C	2.59	0.43
2:C:436:GLY:HA2	2:C:538:GLN:O	2.19	0.43
2:C:508:ILE:H	2:C:508:ILE:HG13	1.41	0.43
2:C:928:LYS:O	2:C:929:ARG:C	2.61	0.43
3:D:397:LYS:O	3:D:448:GLU:HB2	2.18	0.43
3:D:951:ILE:HG12	3:D:1062:ARG:HD3	2.01	0.43
3:J:1460:ILE:H	3:J:1460:ILE:CD1	1.99	0.43
5:C:1120:RFP:H363	5:C:1120:RFP:C37	2.48	0.43
3:D:858:LEU:HD22	3:D:864:VAL:HG21	2.00	0.43
3:D:880:ILE:HD13	3:D:880:ILE:HA	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:974:ILE:HD11	3:D:991:GLN:HB3	1.99	0.43
3:D:999:THR:O	3:D:1003:VAL:HG23	2.19	0.43
3:D:1060:SER:O	3:D:1063:GLU:N	2.51	0.43
3:J:1432:LYS:HD2	3:J:1432:LYS:N	2.34	0.43
2:C:25:SER:O	2:C:26:TYR:C	2.61	0.43
2:C:139:GLN:HB3	2:C:391:LEU:HD21	2.00	0.43
2:C:289:THR:HG22	2:C:303:PHE:CD1	2.54	0.43
2:C:489:SER:C	2:C:491:GLU:H	2.27	0.43
2:C:604:VAL:HG21	2:C:614:ARG:HB2	1.99	0.43
2:C:734:LEU:O	2:C:736:ASP:N	2.51	0.43
3:D:145:VAL:CB	3:D:146:PRO:CD	2.96	0.43
3:D:823:LEU:O	3:D:825:ALA:N	2.49	0.43
1:B:78:ILE:HG13	1:B:130:ALA:HB2	2.00	0.43
2:C:99:GLN:HB3	2:C:109:LYS:HG3	2.01	0.43
2:C:140:ILE:CD1	2:C:331:ARG:HH21	2.31	0.43
3:D:195:VAL:HG12	3:D:196:VAL:N	2.34	0.43
3:D:351:MET:HE2	3:D:368:VAL:HG11	2.00	0.43
3:D:773:ALA:HA	3:J:1367:HIS:NE2	2.34	0.43
3:D:1221:VAL:O	3:D:1222:GLY:C	2.62	0.43
3:D:41:ARG:HH22	3:D:48:ARG:NE	2.17	0.43
3:D:732:VAL:CG1	3:D:736:PHE:HD1	2.32	0.43
1:A:44:LEU:HD23	1:A:48:ILE:HD13	2.01	0.43
3:D:774:SER:C	3:D:776:GLU:H	2.27	0.43
4:K:31:LEU:HD13	4:K:60:ALA:HB2	2.01	0.43
1:B:101:LEU:HD21	1:B:109:VAL:HG11	2.00	0.42
2:C:42:VAL:N	2:C:46:ALA:HB2	2.34	0.42
2:C:143:SER:HA	2:C:144:PRO:HD2	1.87	0.42
2:C:317:VAL:HB	2:C:320:HIS:CD2	2.54	0.42
2:C:841:ASN:HD21	2:C:845:ASN:H	1.65	0.42
3:D:638:LYS:H	3:D:641:GLN:HE21	1.66	0.42
3:D:1099:VAL:O	3:D:1103:HIS:HB3	2.19	0.42
2:C:194:VAL:O	2:C:195:LEU:C	2.61	0.42
2:C:683:ASN:CG	2:C:872:ASN:HB2	2.44	0.42
2:C:886:LEU:HD23	3:D:951:ILE:CD1	2.48	0.42
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	2.01	0.42
3:D:298:VAL:HG23	3:D:302:GLN:CD	2.44	0.42
3:D:790:TYR:CE2	3:D:794:GLN:HG3	2.54	0.42
1:A:23:PHE:O	1:A:196:THR:HA	2.18	0.42
1:A:48:ILE:HA	1:A:49:PRO:HD3	1.79	0.42
2:C:124:ASP:HA	2:C:592:LEU:HD12	2.01	0.42
2:C:272:ALA:HA	2:C:275:TYR:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:810:ASP:O	2:C:811:PRO:C	2.62	0.42
3:D:804:MET:O	3:D:805:ALA:O	2.37	0.42
1:A:186:LEU:O	1:A:188:GLN:N	2.52	0.42
1:B:93:LYS:HD2	1:B:93:LYS:HA	1.76	0.42
2:C:20:GLU:O	2:C:21:ILE:C	2.62	0.42
2:C:790:LEU:O	2:C:791:ARG:HB2	2.19	0.42
2:C:876:VAL:H	2:C:877:PRO:CD	2.32	0.42
3:D:12:LEU:HD23	3:D:507:ASN:HD22	1.84	0.42
3:D:45:PHE:CZ	3:D:527:MET:HB2	2.55	0.42
2:C:879:ARG:H	2:C:879:ARG:CD	2.24	0.42
3:D:704:ARG:HG3	3:D:705:ALA:HB3	2.02	0.42
3:D:1205:TYR:CE1	3:D:1221:VAL:CG1	2.98	0.42
1:A:96:SER:HB3	1:A:145:ASP:HA	2.02	0.42
1:B:115:THR:HA	1:B:116:PRO:HD3	1.86	0.42
2:C:20:GLU:OE1	2:C:460:ARG:CD	2.67	0.42
2:C:144:PRO:HG3	2:C:165:LEU:HG	2.00	0.42
2:C:513:VAL:HG12	2:C:524:VAL:HG12	2.00	0.42
2:C:958:SER:HB3	2:C:961:GLU:OE2	2.20	0.42
3:D:1211:MET:O	3:D:1213:ARG:HG3	2.19	0.42
2:C:141:HIS:CE1	2:C:334:ARG:HG3	2.55	0.42
2:C:717:LEU:HD13	2:C:762:LYS:HA	2.01	0.42
2:C:1012:PRO:HG2	2:C:1024:LYS:H	1.85	0.42
3:D:710:ARG:N	3:D:1227:GLU:OE1	2.51	0.42
2:C:11:GLU:H	2:C:11:GLU:HG2	1.63	0.42
2:C:390:GLN:HE21	2:C:414:GLY:HA2	1.85	0.42
2:C:439:CYS:HB2	2:C:541:SER:HB3	2.01	0.42
2:C:1030:GLN:HB2	3:D:626:SER:CB	2.49	0.42
3:D:205:TYR:CD2	3:D:387:LEU:HD12	2.55	0.42
3:D:237:ARG:HB3	3:D:238:PRO:HD2	2.01	0.42
1:A:179:PHE:HB3	1:A:197:LEU:HD23	2.00	0.42
2:C:38:LYS:O	2:C:39:ARG:C	2.63	0.42
2:C:711:GLU:HG2	2:C:822:VAL:HG22	2.01	0.42
3:D:49:ILE:HG13	3:D:50:PHE:N	2.34	0.42
3:D:137:PRO:HD2	3:D:453:ASP:O	2.19	0.42
3:D:545:ARG:C	3:D:547:LEU:N	2.77	0.42
3:D:1123:PHE:HA	3:D:1134:LEU:HA	2.01	0.42
3:J:1335:LEU:HD23	3:J:1344:VAL:HG23	2.02	0.42
1:A:184:THR:HB	1:A:194:LYS:HB2	2.01	0.42
2:C:30:LEU:HA	2:C:44:ILE:HD12	2.02	0.42
2:C:42:VAL:HA	2:C:46:ALA:HB2	2.01	0.42
2:C:78:PHE:CZ	2:C:812:GLY:HA3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:538:SER:HB3	3:D:541:ASN:ND2	2.35	0.42
3:D:1205:TYR:CD2	3:D:1215:VAL:HG21	2.51	0.42
1:A:225:PHE:CD2	1:B:11:PHE:CE1	2.97	0.41
2:C:193:LEU:HD12	2:C:307:LEU:HD13	2.02	0.41
2:C:343:GLN:HA	2:C:346:VAL:HG23	2.02	0.41
2:C:369:PRO:C	2:C:371:LYS:N	2.77	0.41
2:C:550:LEU:O	2:C:551:GLU:C	2.62	0.41
2:C:753:ASP:O	2:C:791:ARG:HA	2.20	0.41
2:C:1045:ALA:O	2:C:1046:ALA:C	2.62	0.41
3:D:169:TYR:HB2	3:D:393:ILE:HG22	2.02	0.41
3:D:548:ILE:H	3:D:548:ILE:HG13	1.69	0.41
3:J:1434:TRP:CE2	3:J:1435:LEU:HD13	2.55	0.41
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.91	0.41
1:B:202:ASP:OD2	1:B:204:SER:N	2.53	0.41
2:C:30:LEU:O	2:C:31:GLN:C	2.62	0.41
2:C:42:VAL:CA	2:C:46:ALA:HB2	2.49	0.41
2:C:762:LYS:HB3	2:C:764:GLU:OE1	2.20	0.41
2:C:971:LYS:HB3	2:C:986:PRO:HB2	2.02	0.41
3:D:26:VAL:HG13	3:D:93:ILE:HG12	2.02	0.41
3:D:964:LEU:O	3:D:968:ASP:HB2	2.20	0.41
3:D:1053:PHE:CE1	3:D:1072:ILE:HG22	2.56	0.41
3:D:1202:GLN:O	3:D:1204:CYS:O	2.38	0.41
3:D:732:VAL:CG1	3:D:736:PHE:CD1	3.04	0.41
1:B:5:LYS:HB3	1:B:6:LEU:H	1.74	0.41
1:B:36:LEU:O	1:B:39:PRO:HD2	2.20	0.41
1:B:85:LEU:HA	1:B:124:ASN:HD21	1.85	0.41
2:C:10:ARG:HA	2:C:10:ARG:HD2	1.85	0.41
2:C:853:LEU:HA	2:C:854:PRO:HD2	1.90	0.41
3:D:237:ARG:HB3	3:D:238:PRO:CD	2.50	0.41
3:D:247:GLU:HA	3:D:248:PRO:HD3	1.95	0.41
4:K:68:LEU:HA	4:K:73:LEU:HD12	2.03	0.41
1:A:222:LEU:C	1:A:224:TYR:H	2.29	0.41
2:C:261:LEU:C	2:C:263:ASP:H	2.28	0.41
2:C:551:GLU:HB2	2:C:552:HIS:CD2	2.56	0.41
2:C:605:LYS:HB3	2:C:610:ARG:NH1	2.35	0.41
2:C:755:LEU:HD22	2:C:825:VAL:HG11	2.02	0.41
2:C:807:ARG:H	2:C:807:ARG:HG2	1.75	0.41
2:C:922:PHE:CD2	2:C:922:PHE:C	2.98	0.41
3:D:161:LEU:HD23	3:D:452:ILE:HD13	2.01	0.41
1:B:25:LEU:HD23	1:B:28:LEU:HD11	2.03	0.41
2:C:87:ASP:OD2	2:C:824:ARG:NH2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:375:SER:O	2:C:375:SER:OG	2.30	0.41
2:C:474:VAL:HG12	2:C:479:VAL:HA	2.02	0.41
2:C:755:LEU:HG	2:C:792:VAL:HG23	2.02	0.41
2:C:1005:MET:HB2	3:D:629:SER:CB	2.47	0.41
3:D:416:ALA:O	3:D:419:ASP:HB2	2.21	0.41
2:C:809:GLY:C	2:C:810:ASP:O	2.63	0.41
2:C:841:ASN:C	2:C:841:ASN:ND2	2.63	0.41
3:D:23:TYR:CE2	3:D:89:ARG:HD3	2.55	0.41
3:D:466:LYS:HA	3:D:510:GLU:HG2	2.02	0.41
3:J:1372:VAL:HA	3:J:1375:MET:HE2	2.03	0.41
4:K:6:ILE:HA	4:K:9:LEU:HD12	2.03	0.41
1:A:34:VAL:HG12	1:A:179:PHE:CZ	2.55	0.41
1:A:43:ILE:HD12	1:A:218:LEU:HB2	2.03	0.41
1:A:90:LEU:HD23	1:A:90:LEU:N	2.35	0.41
2:C:94:LEU:HD21	2:C:344:PHE:HZ	1.86	0.41
3:D:335:LEU:O	3:D:337:LEU:HG	2.21	0.41
3:D:348:ALA:O	3:D:349:PRO:C	2.64	0.41
3:D:474:GLU:HG3	3:D:503:LEU:HD13	2.02	0.41
3:D:731:LEU:HD23	3:D:731:LEU:HA	1.92	0.41
3:D:794:GLN:HG2	3:D:905:PRO:HB3	2.03	0.41
3:D:920:LEU:HA	3:D:920:LEU:HD13	1.89	0.41
3:D:1004:THR:OG1	3:D:1036:ARG:HD3	2.21	0.41
1:A:77:GLU:HG3	2:C:640:ARG:NH2	2.35	0.41
2:C:154:ARG:NH1	2:C:176:VAL:O	2.54	0.41
2:C:549:PHE:CE2	2:C:909:ALA:HB3	2.55	0.41
2:C:721:ARG:O	2:C:758:ARG:HA	2.21	0.41
2:C:889:HIS:HE1	3:D:951:ILE:H	1.67	0.41
2:C:1006:HIS:HB3	2:C:1027:PHE:CD1	2.56	0.41
5:C:1120:RFP:O12	5:C:1120:RFP:O4	2.39	0.41
3:D:520:LEU:HD23	3:D:525:ARG:HG2	2.02	0.41
3:D:801:GLY:O	3:D:802:ALA:HB2	2.21	0.41
3:D:804:MET:SD	3:D:805:ALA:N	2.86	0.41
3:D:884:ARG:O	3:D:888:GLU:N	2.38	0.41
3:D:968:ASP:O	3:D:971:LEU:HB3	2.21	0.41
3:D:1147:ARG:CB	3:D:1188:VAL:HG21	2.40	0.41
3:D:1206:GLY:O	3:J:1366:LYS:NZ	2.50	0.41
1:A:135:GLY:O	1:A:136:GLY:C	2.64	0.41
2:C:710:ILE:HG21	2:C:756:VAL:CG1	2.51	0.41
5:C:1120:RFP:H342	5:C:1120:RFP:H24C	1.91	0.41
3:D:192:ALA:C	3:D:194:GLY:H	2.29	0.41
3:D:223:LEU:HG	3:D:224:ARG:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:285:PRO:HG2	3:D:311:LEU:HD22	2.02	0.41
3:D:804:MET:SD	3:D:805:ALA:HB2	2.61	0.41
3:D:1118:ILE:CG1	3:D:1190:SER:HB3	2.51	0.41
3:D:1174:LEU:O	3:D:1175:ILE:C	2.63	0.41
1:A:86:VAL:O	1:A:86:VAL:CG2	2.68	0.40
1:A:138:LEU:O	1:A:139:TYR:C	2.63	0.40
1:A:192:LEU:O	2:C:938:LYS:NZ	2.54	0.40
1:B:176:ARG:HB3	1:B:200:TRP:HB2	2.03	0.40
2:C:17:PRO:HD2	2:C:20:GLU:CG	2.47	0.40
3:D:135:LEU:O	3:D:136:ASP:C	2.63	0.40
3:D:661:MET:HE3	3:D:673:ALA:HB1	2.02	0.40
3:D:1219:GLU:HG2	3:D:1221:VAL:HG22	2.04	0.40
3:J:1363:LEU:HD12	3:J:1363:LEU:O	2.21	0.40
2:C:177:GLU:H	2:C:177:GLU:HG2	1.66	0.40
2:C:261:LEU:CG	2:C:263:ASP:HB2	2.51	0.40
3:D:618:LEU:HD22	3:J:1463:LYS:HE3	2.03	0.40
3:D:916:TYR:CD2	3:D:916:TYR:C	2.99	0.40
3:J:1306:PRO:O	3:J:1307:LYS:CB	2.69	0.40
4:K:44:GLU:OE2	4:K:72:ARG:NH2	2.54	0.40
2:C:911:GLU:HA	2:C:914:ILE:HD12	2.02	0.40
3:D:191:LEU:HD13	3:D:393:ILE:CG2	2.51	0.40
3:J:1262:LEU:HD12	3:J:1262:LEU:HA	1.78	0.40
2:C:1059:ASP:O	2:C:1060:ILE:C	2.65	0.40
3:D:855:HIS:HB2	3:D:857:LEU:HD22	2.02	0.40
3:D:1174:LEU:HD23	3:D:1174:LEU:HA	1.83	0.40
2:C:368:THR:HB	2:C:369:PRO:CD	2.52	0.40
2:C:431:HIS:HB3	2:C:434:HIS:ND1	2.37	0.40
3:D:58:CYS:HB3	3:D:59:ALA:H	1.61	0.40
3:D:637:LEU:HB2	3:D:641:GLN:HB2	2.04	0.40
3:D:1063:GLU:H	3:D:1063:GLU:HG3	1.67	0.40
3:D:1072:ILE:HG12	3:D:1072:ILE:H	1.66	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	228/314 (73%)	173 (76%)	38 (17%)	17 (8%)	1	6
1	B	223/314 (71%)	177 (79%)	31 (14%)	15 (7%)	1	7
2	C	1112/1119 (99%)	871 (78%)	153 (14%)	88 (8%)	1	5
3	D	1236/1524 (81%)	968 (78%)	187 (15%)	81 (7%)	1	7
3	J	247/1524 (16%)	194 (78%)	40 (16%)	13 (5%)	1	10
4	K	93/99 (94%)	74 (80%)	8 (9%)	11 (12%)	0	1
All	All	3139/4894 (64%)	2457 (78%)	457 (15%)	225 (7%)	1	6

All (225) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	LEU
1	A	161	ARG
1	A	203	GLY
1	B	18	ASP
1	B	26	GLU
1	B	129	ILE
2	C	9	ILE
2	C	42	VAL
2	C	132	ALA
2	C	148	PHE
2	C	183	THR
2	C	213	ALA
2	C	264	PRO
2	C	283	VAL
2	C	315	ALA
2	C	394	PHE
2	C	422	ARG
2	C	449	ILE
2	C	564	MET
2	C	735	ARG
2	C	762	LYS
2	C	764	GLU
2	C	780	GLU
2	C	907	ASP
2	C	936	VAL
2	C	1046	ALA
2	C	1077	PRO

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Mol	Chain	Res	Type
2	C	1096	ALA
2	C	1097	LEU
2	C	1106	ASP
3	D	41	ARG
3	D	99	ALA
3	D	110	SER
3	D	130	ASN
3	D	136	ASP
3	D	531	ASP
3	D	666	PHE
3	D	679	ARG
3	D	795	VAL
3	D	802	ALA
3	D	805	ALA
3	D	827	ILE
3	D	860	LEU
3	D	871	ARG
3	D	875	THR
3	D	924	MET
3	D	1061	PHE
3	D	1067	VAL
3	D	1197	ARG
3	D	1208	ASP
3	J	1377	LYS
3	J	1424	VAL
3	J	1455	LYS
4	K	2	ALA
4	K	34	ARG
4	K	41	GLU
4	K	42	PRO
1	A	59	GLU
1	A	126	ASP
1	A	139	TYR
1	A	157	GLY
1	A	187	GLY
1	A	199	ILE
1	B	30	ARG
1	B	61	VAL
1	B	119	ASP
2	C	64	LEU
2	C	111	ASP
2	C	242	LEU

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Mol	Chain	Res	Type
2	C	257	LEU
2	C	284	GLY
2	C	316	GLY
2	C	433	THR
2	C	476	ASN
2	C	563	ASN
2	C	583	LEU
2	C	618	GLY
2	C	699	PHE
2	C	716	LYS
2	C	740	GLU
2	C	811	PRO
2	C	1060	ILE
2	C	1076	VAL
2	C	1078	GLU
3	D	25	GLU
3	D	30	GLU
3	D	32	ILE
3	D	97	THR
3	D	119	SER
3	D	132	TYR
3	D	321	GLU
3	D	427	VAL
3	D	643	GLY
3	D	705	ALA
3	D	775	GLY
3	D	783	ARG
3	D	784	ASP
3	D	791	TYR
3	D	824	ASN
3	D	925	GLU
3	D	1181	GLY
3	D	1205	TYR
4	K	16	LYS
4	K	35	PHE
1	A	20	TYR
1	A	27	PRO
1	A	74	ASP
1	A	165	ILE
1	B	5	LYS
1	B	6	LEU
1	B	20	TYR

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Mol	Chain	Res	Type
2	C	112	GLU
2	C	247	PRO
2	C	290	LEU
2	C	292	ARG
2	C	293	PHE
2	C	325	ILE
2	C	463	ALA
2	C	538	GLN
2	C	651	LYS
2	C	659	PRO
2	C	700	TYR
2	C	739	GLU
2	C	788	THR
3	D	24	GLY
3	D	29	PRO
3	D	44	LEU
3	D	50	PHE
3	D	69	GLU
3	D	349	PRO
3	D	397	LYS
3	D	546	ARG
3	D	600	LEU
3	D	610	LYS
3	D	629	SER
3	D	758	GLU
3	D	804	MET
3	D	823	LEU
3	D	1015	TYR
3	D	1091	SER
3	J	1270	ALA
3	J	1307	LYS
4	K	80	VAL
1	A	118	ALA
1	A	136	GLY
1	A	234	PRO
1	B	17	GLY
1	B	75	VAL
1	B	104	GLU
1	B	118	ALA
2	C	8	ARG
2	C	41	ASN
2	C	66	LEU

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Mol	Chain	Res	Type
2	C	178	ALA
2	C	252	LYS
2	C	258	PHE
2	C	619	ARG
2	C	652	GLY
2	C	858	MET
2	C	980	GLY
2	C	1075	ASP
2	C	1110	ASP
3	D	39	PRO
3	D	57	GLU
3	D	58	CYS
3	D	117	ASP
3	D	122	GLU
3	D	207	PHE
3	D	594	PRO
3	D	613	ARG
3	D	667	ALA
3	D	680	GLN
3	D	800	LYS
3	J	1315	ASP
3	J	1458	GLU
4	K	38	THR
1	A	38	ASN
1	B	133	GLU
2	C	53	PRO
2	C	261	LEU
2	C	262	ALA
2	C	336	VAL
2	C	376	ARG
2	C	629	ALA
2	C	685	GLU
2	C	810	ASP
2	C	821	GLU
2	C	1005	MET
2	C	1099	VAL
3	D	72	VAL
3	D	109	PRO
3	D	120	ALA
3	D	127	LEU
3	D	389	GLU
3	D	521	PRO

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Mol	Chain	Res	Type
3	D	587	ARG
3	D	621	LYS
3	D	668	PRO
3	D	1026	SER
3	J	1285	GLU
3	J	1383	ASP
3	J	1405	GLU
3	J	1415	VAL
4	K	4	PRO
4	K	93	TYR
2	C	876	VAL
2	C	959	PRO
2	C	1113	GLU
3	D	522	PRO
3	D	1079	LYS
3	J	1327	ARG
3	J	1408	ILE
2	C	645	VAL
2	C	1079	PRO
3	D	828	VAL
1	B	120	VAL
2	C	248	PRO
3	D	885	ILE
3	D	1080	GLY
4	K	94	PRO
2	C	186	VAL
2	C	263	ASP
3	D	1019	PRO
2	C	548	PRO
2	C	194	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	189/270 (70%)	127 (67%)	62 (33%)	0 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	191/270 (71%)	121 (63%)	70 (37%)	0	1
2	C	889/936 (95%)	585 (66%)	304 (34%)	0	1
3	D	992/1281 (77%)	631 (64%)	361 (36%)	0	1
3	J	191/1281 (15%)	115 (60%)	76 (40%)	0	0
4	K	75/88 (85%)	57 (76%)	18 (24%)	1	3
All	All	2527/4126 (61%)	1636 (65%)	891 (35%)	0	1

All (891) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	A	19	HIS
1	A	24	VAL
1	A	29	GLU
1	A	34	VAL
1	A	40	LEU
1	A	44	LEU
1	A	53	VAL
1	A	54	THR
1	A	55	SER
1	A	58	ILE
1	A	59	GLU
1	A	62	LEU
1	A	64	GLU
1	A	67	THR
1	A	68	ILE
1	A	72	LYS
1	A	74	ASP
1	A	77	GLU
1	A	79	ILE
1	A	83	LYS
1	A	86	VAL
1	A	87	VAL
1	A	90	LEU
1	A	94	MET
1	A	101	LEU
1	A	107	LYS
1	A	108	GLU
1	A	109	VAL
1	A	114	PHE

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Mol	Chain	Res	Type
1	A	115	THR
1	A	119	ASP
1	A	120	VAL
1	A	126	ASP
1	A	127	LEU
1	A	131	THR
1	A	133	GLU
1	A	134	GLU
1	A	137	LYS
1	A	144	VAL
1	A	145	ASP
1	A	148	VAL
1	A	151	VAL
1	A	159	LYS
1	A	160	ASP
1	A	161	ARG
1	A	167	VAL
1	A	172	SER
1	A	176	ARG
1	A	183	ASP
1	A	186	LEU
1	A	190	THR
1	A	195	LEU
1	A	196	THR
1	A	198	ARG
1	A	201	THR
1	A	215	VAL
1	A	219	LYS
1	A	222	LEU
1	A	223	ASN
1	A	229	GLU
1	A	231	SER
1	B	4	SER
1	B	5	LYS
1	B	6	LEU
1	B	7	LYS
1	B	10	VAL
1	B	30	ARG
1	B	34	VAL
1	B	41	ARG
1	B	43	ILE
1	B	44	LEU

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Mol	Chain	Res	Type
1	B	51	THR
1	B	55	SER
1	B	56	VAL
1	B	59	GLU
1	B	60	ASP
1	B	61	VAL
1	B	64	GLU
1	B	66	SER
1	B	67	THR
1	B	78	ILE
1	B	79	ILE
1	B	81	ASN
1	B	82	LEU
1	B	85	LEU
1	B	86	VAL
1	B	88	ARG
1	B	93	LYS
1	B	96	SER
1	B	97	THR
1	B	101	LEU
1	B	104	GLU
1	B	108	GLU
1	B	110	ARG
1	B	119	ASP
1	B	120	VAL
1	B	122	ILE
1	B	126	ASP
1	B	132	LEU
1	B	134	GLU
1	B	138	LEU
1	B	140	MET
1	B	142	VAL
1	B	145	ASP
1	B	146	ARG
1	B	148	VAL
1	B	151	VAL
1	B	159	LYS
1	B	160	ASP
1	B	161	ARG
1	B	162	ILE
1	B	165	ILE
1	B	167	VAL

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Mol	Chain	Res	Type
1	B	170	ILE
1	B	171	PHE
1	B	174	VAL
1	B	175	ARG
1	B	176	ARG
1	B	177	VAL
1	B	180	GLN
1	B	182	GLU
1	B	183	ASP
1	B	184	THR
1	B	186	LEU
1	B	188	GLN
1	B	197	LEU
1	B	198	ARG
1	B	213	GLN
1	B	217	ILE
1	B	219	LYS
1	B	220	GLU
2	C	1	MET
2	C	3	ILE
2	C	4	LYS
2	C	8	ARG
2	C	9	ILE
2	C	10	ARG
2	C	11	GLU
2	C	12	VAL
2	C	20	GLU
2	C	21	ILE
2	C	27	LYS
2	C	28	LYS
2	C	30	LEU
2	C	33	ASP
2	C	34	VAL
2	C	37	GLU
2	C	42	VAL
2	C	50	GLU
2	C	51	THR
2	C	52	PHE
2	C	55	GLU
2	C	56	GLU
2	C	58	ASP
2	C	61	LYS

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Mol	Chain	Res	Type
2	C	65	VAL
2	C	73	ILE
2	C	79	SER
2	C	80	GLN
2	C	88	LEU
2	C	94	LEU
2	C	95	TYR
2	C	97	ARG
2	C	98	LEU
2	C	101	ILE
2	C	103	LYS
2	C	104	ASP
2	C	105	THR
2	C	109	LYS
2	C	111	ASP
2	C	113	VAL
2	C	115	LEU
2	C	118	LEU
2	C	124	ASP
2	C	137	VAL
2	C	138	SER
2	C	139	GLN
2	C	142	ARG
2	C	149	THR
2	C	159	ILE
2	C	161	SER
2	C	163	ILE
2	C	165	LEU
2	C	167	LYS
2	C	175	GLU
2	C	177	GLU
2	C	179	SER
2	C	181	VAL
2	C	184	MET
2	C	193	LEU
2	C	194	VAL
2	C	195	LEU
2	C	196	LEU
2	C	198	ARG
2	C	200	LEU
2	C	204	GLN
2	C	207	LEU

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Mol	Chain	Res	Type
2	C	210	GLU
2	C	211	LEU
2	C	214	TYR
2	C	218	VAL
2	C	219	GLN
2	C	222	LEU
2	C	227	LEU
2	C	232	GLU
2	C	233	GLU
2	C	237	ARG
2	C	241	LEU
2	C	242	LEU
2	C	246	ASP
2	C	250	LYS
2	C	258	PHE
2	C	261	LEU
2	C	271	GLU
2	C	283	VAL
2	C	285	LEU
2	C	290	LEU
2	C	295	ASP
2	C	299	LYS
2	C	304	LEU
2	C	308	ARG
2	C	310	LEU
2	C	314	THR
2	C	321	GLU
2	C	322	VAL
2	C	323	ASP
2	C	328	LEU
2	C	333	ILE
2	C	335	THR
2	C	345	ARG
2	C	348	LEU
2	C	351	LEU
2	C	371	LYS
2	C	373	VAL
2	C	375	SER
2	C	376	ARG
2	C	378	LEU
2	C	382	LEU
2	C	389	SER

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Mol	Chain	Res	Type
2	C	391	LEU
2	C	393	GLN
2	C	395	LYS
2	C	397	GLU
2	C	402	SER
2	C	403	SER
2	C	404	LEU
2	C	407	LYS
2	C	408	ARG
2	C	413	LEU
2	C	429	ASP
2	C	432	ARG
2	C	433	THR
2	C	442	GLU
2	C	443	THR
2	C	445	GLU
2	C	449	ILE
2	C	453	THR
2	C	454	SER
2	C	460	ARG
2	C	462	ASP
2	C	469	THR
2	C	472	ARG
2	C	473	ARG
2	C	474	VAL
2	C	476	ASN
2	C	478	VAL
2	C	480	THR
2	C	481	GLU
2	C	486	MET
2	C	487	THR
2	C	493	ARG
2	C	495	THR
2	C	498	GLN
2	C	500	ASN
2	C	501	THR
2	C	508	ILE
2	C	513	VAL
2	C	514	VAL
2	C	516	ARG
2	C	517	ARG
2	C	518	ARG

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Mol	Chain	Res	Type
2	C	520	GLU
2	C	522	VAL
2	C	523	ILE
2	C	524	VAL
2	C	529	VAL
2	C	535	SER
2	C	539	VAL
2	C	541	SER
2	C	542	LEU
2	C	544	THR
2	C	545	ASN
2	C	546	LEU
2	C	550	LEU
2	C	556	ASN
2	C	557	ARG
2	C	559	LEU
2	C	569	VAL
2	C	579	VAL
2	C	584	GLU
2	C	589	ARG
2	C	595	LEU
2	C	598	GLU
2	C	599	GLU
2	C	603	VAL
2	C	607	ASP
2	C	609	THR
2	C	610	ARG
2	C	613	VAL
2	C	620	LEU
2	C	621	VAL
2	C	625	LEU
2	C	626	ARG
2	C	630	ARG
2	C	631	SER
2	C	632	ASN
2	C	633	GLN
2	C	635	THR
2	C	637	PHE
2	C	638	ASP
2	C	645	VAL
2	C	650	LYS
2	C	655	LEU

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Mol	Chain	Res	Type
2	C	657	ASP
2	C	671	ASN
2	C	674	VAL
2	C	688	ILE
2	C	692	GLU
2	C	694	LEU
2	C	698	ASP
2	C	699	PHE
2	C	704	HIS
2	C	707	ARG
2	C	713	ARG
2	C	714	ASP
2	C	715	THR
2	C	720	GLU
2	C	722	ILE
2	C	728	HIS
2	C	731	GLU
2	C	735	ARG
2	C	737	LEU
2	C	743	VAL
2	C	749	VAL
2	C	754	ILE
2	C	758	ARG
2	C	765	GLN
2	C	770	GLU
2	C	771	GLU
2	C	772	ARG
2	C	774	LEU
2	C	784	ASP
2	C	785	VAL
2	C	788	THR
2	C	790	LEU
2	C	796	GLU
2	C	799	ILE
2	C	801	VAL
2	C	804	LEU
2	C	805	ARG
2	C	806	LEU
2	C	807	ARG
2	C	815	LEU
2	C	820	ARG
2	C	823	VAL

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Mol	Chain	Res	Type
2	C	830	LYS
2	C	835	VAL
2	C	841	ASN
2	C	846	LYS
2	C	848	VAL
2	C	853	LEU
2	C	855	VAL
2	C	857	ASP
2	C	861	LEU
2	C	871	LEU
2	C	878	SER
2	C	879	ARG
2	C	881	ASN
2	C	882	LEU
2	C	886	LEU
2	C	902	ILE
2	C	911	GLU
2	C	917	LEU
2	C	918	LEU
2	C	939	ARG
2	C	941	LYS
2	C	942	GLU
2	C	949	LYS
2	C	952	LEU
2	C	958	SER
2	C	961	GLU
2	C	963	LEU
2	C	964	LYS
2	C	969	LEU
2	C	972	VAL
2	C	979	THR
2	C	989	VAL
2	C	995	MET
2	C	996	LYS
2	C	997	LEU
2	C	1000	MET
2	C	1001	VAL
2	C	1002	GLU
2	C	1005	MET
2	C	1006	HIS
2	C	1010	THR
2	C	1015	LEU

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Mol	Chain	Res	Type
2	C	1018	GLN
2	C	1024	LYS
2	C	1027	PHE
2	C	1030	GLN
2	C	1031	ARG
2	C	1035	MET
2	C	1040	LEU
2	C	1052	MET
2	C	1053	LEU
2	C	1057	SER
2	C	1058	ASP
2	C	1060	ILE
2	C	1061	GLU
2	C	1063	ARG
2	C	1068	GLN
2	C	1071	ILE
2	C	1072	LYS
2	C	1076	VAL
2	C	1078	GLU
2	C	1080	SER
2	C	1083	GLU
2	C	1089	VAL
2	C	1091	GLU
2	C	1095	LEU
2	C	1097	LEU
2	C	1101	THR
2	C	1106	ASP
2	C	1113	GLU
3	D	5	VAL
3	D	9	ARG
3	D	12	LEU
3	D	16	GLU
3	D	17	LYS
3	D	20	SER
3	D	23	TYR
3	D	28	LYS
3	D	30	GLU
3	D	33	ASN
3	D	34	TYR
3	D	36	THR
3	D	41	ARG
3	D	44	LEU

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Mol	Chain	Res	Type
3	D	46	ASP
3	D	53	ILE
3	D	54	LYS
3	D	58	CYS
3	D	64	LYS
3	D	66	GLN
3	D	73	CYS
3	D	74	GLU
3	D	75	ARG
3	D	81	THR
3	D	83	SER
3	D	84	ILE
3	D	85	VAL
3	D	87	ARG
3	D	90	MET
3	D	92	HIS
3	D	93	ILE
3	D	95	LEU
3	D	97	THR
3	D	102	ILE
3	D	106	LYS
3	D	110	SER
3	D	111	LYS
3	D	114	THR
3	D	115	LEU
3	D	116	LEU
3	D	118	LEU
3	D	119	SER
3	D	121	THR
3	D	123	LEU
3	D	125	GLN
3	D	128	TYR
3	D	129	PHE
3	D	149	LYS
3	D	151	GLN
3	D	156	GLU
3	D	162	ARG
3	D	166	GLN
3	D	168	THR
3	D	184	GLU
3	D	187	LYS
3	D	189	GLN

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Mol	Chain	Res	Type
3	D	196	VAL
3	D	198	ARG
3	D	204	LEU
3	D	206	ARG
3	D	209	ARG
3	D	218	LYS
3	D	220	ARG
3	D	224	ARG
3	D	225	ILE
3	D	227	LEU
3	D	233	LYS
3	D	242	LEU
3	D	261	LEU
3	D	263	ASP
3	D	266	GLU
3	D	270	ILE
3	D	273	ARG
3	D	277	GLU
3	D	278	VAL
3	D	279	VAL
3	D	284	LEU
3	D	293	VAL
3	D	297	ILE
3	D	298	VAL
3	D	299	GLU
3	D	300	VAL
3	D	308	LYS
3	D	310	LEU
3	D	312	ARG
3	D	313	LEU
3	D	315	ARG
3	D	316	HIS
3	D	318	THR
3	D	322	VAL
3	D	325	GLU
3	D	331	VAL
3	D	333	LEU
3	D	335	LEU
3	D	347	VAL
3	D	354	ILE
3	D	355	VAL
3	D	357	GLU

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Mol	Chain	Res	Type
3	D	360	LYS
3	D	361	VAL
3	D	365	GLU
3	D	371	ILE
3	D	375	GLU
3	D	387	LEU
3	D	389	GLU
3	D	392	SER
3	D	393	ILE
3	D	394	LEU
3	D	395	VAL
3	D	396	VAL
3	D	400	VAL
3	D	404	GLU
3	D	405	ASP
3	D	407	VAL
3	D	411	THR
3	D	414	ARG
3	D	415	VAL
3	D	420	VAL
3	D	434	ARG
3	D	435	VAL
3	D	436	GLU
3	D	441	ARG
3	D	445	ARG
3	D	450	TYR
3	D	455	ARG
3	D	463	GLU
3	D	465	LEU
3	D	466	LYS
3	D	470	LEU
3	D	471	GLU
3	D	472	LYS
3	D	474	GLU
3	D	478	LEU
3	D	480	GLU
3	D	481	MET
3	D	482	LYS
3	D	494	LYS
3	D	496	LEU
3	D	500	ARG
3	D	503	LEU

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Mol	Chain	Res	Type
3	D	513	ILE
3	D	514	LEU
3	D	515	GLU
3	D	519	VAL
3	D	524	LEU
3	D	525	ARG
3	D	527	MET
3	D	537	THR
3	D	540	LEU
3	D	542	ASP
3	D	544	TYR
3	D	546	ARG
3	D	547	LEU
3	D	549	ASN
3	D	550	ARG
3	D	555	LYS
3	D	556	LYS
3	D	557	LEU
3	D	558	LEU
3	D	560	GLN
3	D	566	ILE
3	D	568	ARG
3	D	569	ASN
3	D	571	LYS
3	D	572	ARG
3	D	578	VAL
3	D	581	VAL
3	D	598	ARG
3	D	600	LEU
3	D	603	LEU
3	D	607	LEU
3	D	608	SER
3	D	610	LYS
3	D	613	ARG
3	D	615	ARG
3	D	616	GLN
3	D	619	LEU
3	D	622	ARG
3	D	632	VAL
3	D	637	LEU
3	D	647	ARG
3	D	648	MET

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Mol	Chain	Res	Type
3	D	652	LEU
3	D	654	LYS
3	D	664	LYS
3	D	669	ASN
3	D	670	VAL
3	D	671	LYS
3	D	679	ARG
3	D	680	GLN
3	D	681	ARG
3	D	683	ILE
3	D	684	LYS
3	D	689	ASP
3	D	691	LEU
3	D	694	VAL
3	D	695	ILE
3	D	700	VAL
3	D	704	ARG
3	D	709	HIS
3	D	711	LEU
3	D	713	ILE
3	D	717	GLN
3	D	721	VAL
3	D	727	GLN
3	D	732	VAL
3	D	734	GLU
3	D	745	MET
3	D	747	VAL
3	D	751	LEU
3	D	752	SER
3	D	754	PHE
3	D	763	MET
3	D	770	LEU
3	D	771	SER
3	D	778	LEU
3	D	780	LYS
3	D	782	SER
3	D	783	ARG
3	D	785	ILE
3	D	787	LEU
3	D	791	TYR
3	D	792	ILE
3	D	794	GLN

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Mol	Chain	Res	Type
3	D	795	VAL
3	D	797	LYS
3	D	798	GLU
3	D	799	LYS
3	D	804	MET
3	D	810	GLU
3	D	811	GLU
3	D	813	LEU
3	D	817	GLU
3	D	827	ILE
3	D	832	ARG
3	D	833	GLU
3	D	836	VAL
3	D	838	ARG
3	D	840	LYS
3	D	842	VAL
3	D	847	ASP
3	D	853	VAL
3	D	857	LEU
3	D	858	LEU
3	D	859	ASP
3	D	860	LEU
3	D	863	VAL
3	D	866	VAL
3	D	867	ARG
3	D	869	LEU
3	D	872	ARG
3	D	876	SER
3	D	880	ILE
3	D	884	ARG
3	D	888	GLU
3	D	890	VAL
3	D	893	GLU
3	D	895	VAL
3	D	902	MET
3	D	903	ASP
3	D	904	VAL
3	D	907	GLU
3	D	912	LYS
3	D	914	LEU
3	D	920	LEU
3	D	921	ARG

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Mol	Chain	Res	Type
3	D	922	LEU
3	D	925	GLU
3	D	927	THR
3	D	931	LEU
3	D	935	LYS
3	D	941	LEU
3	D	943	THR
3	D	944	THR
3	D	947	ILE
3	D	948	THR
3	D	956	ILE
3	D	960	LYS
3	D	961	GLN
3	D	964	LEU
3	D	968	ASP
3	D	969	ARG
3	D	974	ILE
3	D	975	GLU
3	D	979	GLU
3	D	980	MET
3	D	988	ARG
3	D	993	ILE
3	D	994	GLN
3	D	995	LEU
3	D	1001	GLU
3	D	1003	VAL
3	D	1005	GLN
3	D	1007	VAL
3	D	1009	LYS
3	D	1014	ASN
3	D	1020	LEU
3	D	1029	ARG
3	D	1031	ASN
3	D	1033	GLN
3	D	1034	GLN
3	D	1036	ARG
3	D	1044	LEU
3	D	1049	SER
3	D	1051	GLU
3	D	1052	THR
3	D	1063	GLU
3	D	1065	LEU

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Mol	Chain	Res	Type
3	D	1067	VAL
3	D	1072	ILE
3	D	1073	SER
3	D	1078	ARG
3	D	1083	ASP
3	D	1086	LEU
3	D	1097	LYS
3	D	1098	LEU
3	D	1101	VAL
3	D	1104	GLU
3	D	1105	ILE
3	D	1109	GLU
3	D	1118	ILE
3	D	1119	SER
3	D	1126	ASP
3	D	1127	GLU
3	D	1129	THR
3	D	1130	ARG
3	D	1135	ARG
3	D	1137	ARG
3	D	1138	SER
3	D	1141	GLU
3	D	1142	SER
3	D	1147	ARG
3	D	1148	VAL
3	D	1151	ARG
3	D	1152	GLU
3	D	1158	ARG
3	D	1159	ARG
3	D	1161	GLU
3	D	1162	GLU
3	D	1166	LEU
3	D	1168	LEU
3	D	1176	LYS
3	D	1179	GLU
3	D	1182	GLU
3	D	1183	VAL
3	D	1184	ARG
3	D	1188	VAL
3	D	1189	ARG
3	D	1190	SER
3	D	1195	GLN

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Mol	Chain	Res	Type
3	D	1196	THR
3	D	1200	VAL
3	D	1201	CYS
3	D	1209	LEU
3	D	1215	VAL
3	D	1216	SER
3	D	1219	GLU
3	D	1228	SER
3	D	1231	GLU
3	D	1234	THR
3	D	1238	MET
3	J	1253	THR
3	J	1254	GLN
3	J	1258	ARG
3	J	1262	LEU
3	J	1264	GLU
3	J	1266	ARG
3	J	1269	LYS
3	J	1274	ILE
3	J	1275	SER
3	J	1278	ASP
3	J	1290	LEU
3	J	1292	VAL
3	J	1294	VAL
3	J	1304	LYS
3	J	1307	LYS
3	J	1310	ARG
3	J	1311	LEU
3	J	1312	LEU
3	J	1314	LYS
3	J	1315	ASP
3	J	1317	ASP
3	J	1319	VAL
3	J	1325	LEU
3	J	1326	THR
3	J	1327	ARG
3	J	1336	LEU
3	J	1339	LYS
3	J	1342	GLU
3	J	1344	VAL
3	J	1346	ARG
3	J	1348	LEU

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Mol	Chain	Res	Type
3	J	1354	LYS
3	J	1355	VAL
3	J	1357	ARG
3	J	1359	GLN
3	J	1361	VAL
3	J	1366	LYS
3	J	1376	LEU
3	J	1379	VAL
3	J	1381	VAL
3	J	1386	ASP
3	J	1387	SER
3	J	1389	LEU
3	J	1397	LYS
3	J	1400	VAL
3	J	1403	LEU
3	J	1412	LYS
3	J	1413	VAL
3	J	1417	TRP
3	J	1418	LYS
3	J	1421	LEU
3	J	1422	MET
3	J	1424	VAL
3	J	1429	LEU
3	J	1430	SER
3	J	1431	THR
3	J	1432	LYS
3	J	1434	TRP
3	J	1435	LEU
3	J	1439	SER
3	J	1442	ASN
3	J	1456	LYS
3	J	1458	GLU
3	J	1459	LEU
3	J	1460	ILE
3	J	1463	LYS
3	J	1464	GLU
3	J	1468	LEU
3	J	1470	ARG
3	J	1472	ILE
3	J	1476	THR
3	J	1481	VAL
3	J	1482	ARG

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Mol	Chain	Res	Type
3	J	1487	VAL
3	J	1495	ILE
3	J	1500	LYS
4	K	6	ILE
4	K	12	MET
4	K	30	LEU
4	K	31	LEU
4	K	34	ARG
4	K	38	THR
4	K	39	VAL
4	K	49	ARG
4	K	50	THR
4	K	56	ASP
4	K	61	VAL
4	K	66	LYS
4	K	69	LEU
4	K	72	ARG
4	K	77	GLU
4	K	78	ASN
4	K	79	LEU
4	K	89	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	221	HIS
1	B	19	HIS
1	B	212	ASN
1	B	213	GLN
1	B	223	ASN
2	C	102	HIS
2	C	139	GLN
2	C	141	HIS
2	C	219	GLN
2	C	320	HIS
2	C	327	HIS
2	C	390	GLN
2	C	399	ASN
2	C	406	HIS
2	C	431	HIS
2	C	500	ASN

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Mol	Chain	Res	Type
2	C	565	GLN
2	C	567	GLN
2	C	575	GLN
2	C	623	HIS
2	C	632	ASN
2	C	633	GLN
2	C	639	GLN
2	C	647	GLN
2	C	671	ASN
2	C	765	GLN
2	C	841	ASN
2	C	845	ASN
2	C	881	ASN
2	C	884	GLN
2	C	923	ASN
2	C	1018	GLN
3	D	166	GLN
3	D	350	HIS
3	D	507	ASN
3	D	552	ASN
3	D	584	ASN
3	D	616	GLN
3	D	636	GLN
3	D	640	HIS
3	D	641	GLN
3	D	717	GLN
3	D	724	GLN
3	D	744	GLN
3	D	756	GLN
3	D	1031	ASN
3	D	1034	GLN
3	D	1103	HIS
3	D	1124	GLN
3	D	1172	HIS
3	J	1353	GLN
3	J	1374	GLN
3	J	1465	ASN
4	K	28	GLN
4	K	29	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 ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	RFP	C	1120	-	63,63,63	1.52	10 (15%)	94,94,94	2.15	21 (22%)

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
5	RFP	C	1120	-	-	12/60/85/85	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1120	RFP	C43-N2	6.02	1.44	1.27
5	C	1120	RFP	O7-C35	4.53	1.45	1.35
5	C	1120	RFP	O2-C8	-3.27	1.24	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1120	RFP	O5-C29	3.14	1.47	1.39
5	C	1120	RFP	C8-C9	2.85	1.51	1.43
5	C	1120	RFP	N3-N2	-2.84	1.31	1.38
5	C	1120	RFP	C10-C9	2.83	1.49	1.42
5	C	1120	RFP	C5-C10	2.74	1.48	1.42
5	C	1120	RFP	C3-C43	2.46	1.51	1.46
5	C	1120	RFP	C8-C7	2.23	1.49	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1120	RFP	C42-N4-C39	11.84	128.40	109.54
5	C	1120	RFP	C3-C43-N2	-7.08	110.01	121.58
5	C	1120	RFP	C41-N3-C40	5.31	128.93	113.44
5	C	1120	RFP	O7-C35-C36	4.25	118.67	111.09
5	C	1120	RFP	C12-O5-C29	3.82	127.24	117.84
5	C	1120	RFP	C30-C16-C17	-3.50	115.17	123.67
5	C	1120	RFP	C42-C41-N3	3.39	116.01	110.51
5	C	1120	RFP	C40-C39-N4	3.34	116.23	110.86
5	C	1120	RFP	C38-N4-C39	3.33	116.98	110.63
5	C	1120	RFP	C25-O7-C35	-2.99	113.08	117.72
5	C	1120	RFP	O3-C6-C7	2.81	125.92	121.16
5	C	1120	RFP	C39-C40-N3	2.80	115.07	110.51
5	C	1120	RFP	C41-C42-N4	2.80	115.35	110.86
5	C	1120	RFP	C17-C18-C19	-2.63	118.33	124.43
5	C	1120	RFP	C43-N2-N3	2.36	123.93	120.55
5	C	1120	RFP	O7-C35-O8	-2.36	118.44	122.99
5	C	1120	RFP	C2-C3-C4	2.12	120.54	119.19
5	C	1120	RFP	C38-N4-C42	2.09	114.62	110.63
5	C	1120	RFP	O4-C11-C12	2.08	124.76	120.56
5	C	1120	RFP	C4-C3-C43	-2.03	114.02	116.63
5	C	1120	RFP	C12-O3-C6	2.01	111.05	107.69

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1120	RFP	C16-C15-N1-C2
5	C	1120	RFP	O11-C15-N1-C2
5	C	1120	RFP	C43-N2-N3-C40
5	C	1120	RFP	C43-N2-N3-C41
5	C	1120	RFP	C36-C35-O7-C25

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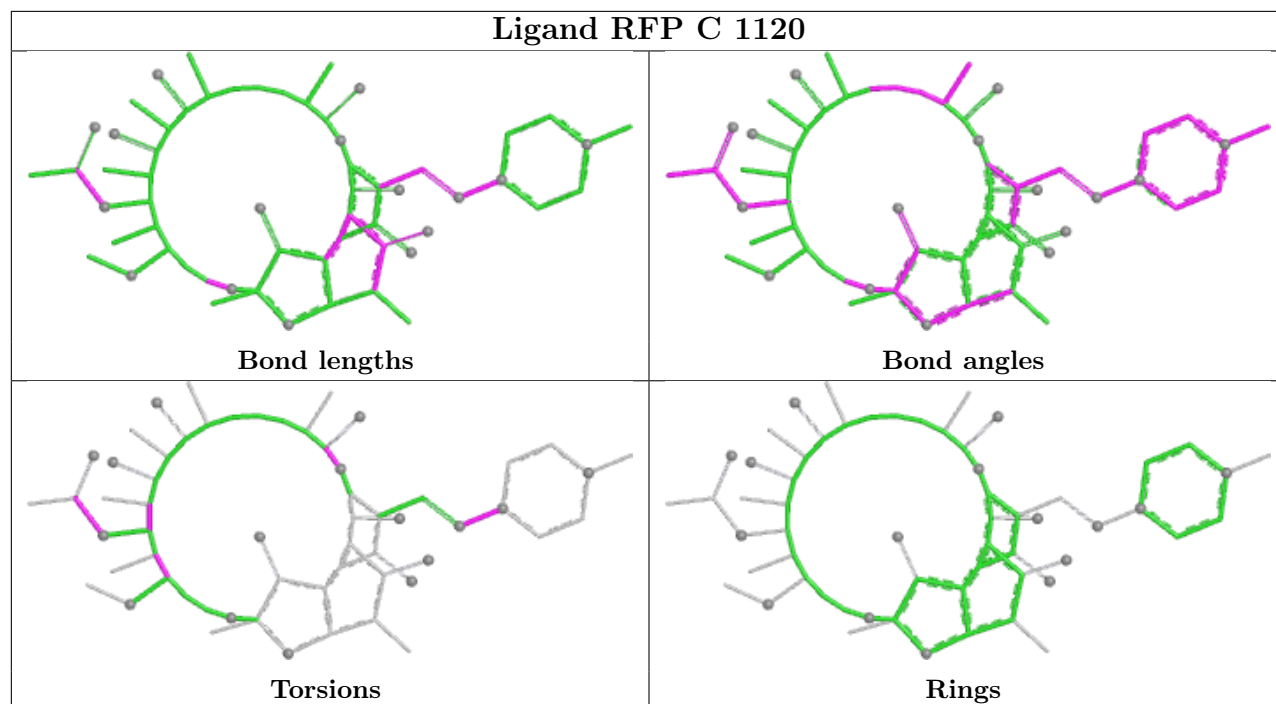
Mol	Chain	Res	Type	Atoms
5	C	1120	RFP	O8-C35-O7-C25
5	C	1120	RFP	C33-C24-C25-O7
5	C	1120	RFP	C33-C24-C25-C26
5	C	1120	RFP	C23-C24-C25-O7
5	C	1120	RFP	C23-C24-C25-C26
5	C	1120	RFP	C34-C26-C27-O6
5	C	1120	RFP	C34-C26-C27-C28

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1120	RFP	10	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	230/314 (73%)	-0.19	2 (0%) 81 65	17, 38, 68, 98	0
1	B	225/314 (71%)	-0.09	2 (0%) 81 65	24, 48, 73, 76	0
2	C	1114/1119 (99%)	-0.04	29 (2%) 57 38	17, 44, 76, 93	0
3	D	1238/1524 (81%)	0.29	94 (7%) 20 14	15, 49, 87, 130	0
3	J	249/1524 (16%)	0.24	16 (6%) 25 17	17, 45, 114, 122	0
4	K	95/99 (95%)	0.26	6 (6%) 26 17	20, 59, 140, 154	0
All	All	3151/4894 (64%)	0.11	149 (4%) 36 24	15, 46, 85, 154	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	1403	LEU	9.1
3	D	191	LEU	6.8
3	D	328	GLY	5.4
3	D	173	ALA	5.1
3	D	341	GLU	5.0
3	D	57	GLU	4.8
3	D	216	LEU	4.7
3	D	360	LYS	4.6
3	D	164	GLY	4.4
2	C	270	GLY	4.2
4	K	95	THR	4.2
3	D	489	ARG	4.2
3	D	157	GLU	4.1
3	D	207	PHE	3.9
3	D	256	SER	3.9
3	D	318	THR	3.8
2	C	111	ASP	3.7
3	D	208	PRO	3.6
3	D	490	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
2	C	418	LEU	3.5
3	J	1495	ILE	3.5
3	D	197	SER	3.5
3	D	558	LEU	3.4
3	D	807	ALA	3.4
3	D	375	GLU	3.4
3	J	1393	GLN	3.4
3	D	180	LYS	3.4
3	D	175	VAL	3.3
3	J	1308	ASP	3.3
3	D	200	ASP	3.3
3	D	160	GLU	3.2
3	D	244	GLU	3.2
3	D	372	ASP	3.2
3	D	588	GLY	3.2
3	D	16	GLU	3.2
3	D	204	LEU	3.2
2	C	739	GLU	3.1
3	D	139	GLY	3.1
3	D	528	VAL	3.1
3	D	120	ALA	3.0
3	D	373	PRO	2.9
3	J	1398	TRP	2.9
2	C	269	LEU	2.9
4	K	90	GLU	2.9
3	D	163	TYR	2.9
3	D	568	ARG	2.9
3	D	350	HIS	2.9
3	D	82	ARG	2.9
3	J	1402	ALA	2.8
3	D	811	GLU	2.8
3	D	165	LYS	2.8
2	C	935	GLY	2.7
3	D	367	ILE	2.7
3	D	623	VAL	2.7
2	C	267	TYR	2.7
2	C	227	LEU	2.6
3	D	136	ASP	2.6
3	D	371	ILE	2.6
3	D	56	TYR	2.6
3	D	193	PRO	2.6
4	K	53	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	615	ARG	2.6
3	D	176	ASP	2.6
2	C	220	GLY	2.5
2	C	932	GLU	2.5
3	D	1086	LEU	2.5
2	C	288	ARG	2.5
2	C	271	GLU	2.5
3	D	47	GLU	2.5
3	D	172	PRO	2.5
3	D	194	GLY	2.5
1	B	62	LEU	2.5
1	A	203	GLY	2.5
2	C	712	ALA	2.5
2	C	4	LYS	2.5
3	D	477	LEU	2.4
2	C	1114	GLY	2.4
3	D	430	GLU	2.4
4	K	94	PRO	2.4
3	D	831	GLY	2.4
2	C	294	GLU	2.4
3	D	343	LYS	2.4
3	D	35	ARG	2.4
3	D	449	SER	2.4
3	D	238	PRO	2.4
3	D	396	VAL	2.4
3	D	61	GLY	2.3
3	J	1409	ALA	2.3
3	D	276	GLU	2.3
4	K	88	GLU	2.3
3	D	179	VAL	2.3
3	D	63	TYR	2.3
3	J	1285	GLU	2.3
3	J	1410	GLU	2.3
2	C	427	VAL	2.3
3	D	211	VAL	2.3
3	D	287	GLY	2.3
2	C	171	TRP	2.3
3	D	265	ALA	2.3
3	D	199	MET	2.3
2	C	290	LEU	2.3
3	D	329	ASP	2.3
3	D	1079	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	184	GLU	2.3
4	K	2	ALA	2.3
3	J	1287	GLU	2.2
3	J	1429	LEU	2.2
3	D	511	TRP	2.2
3	D	340	THR	2.2
2	C	268	ASP	2.2
3	D	567	ILE	2.2
2	C	958	SER	2.2
2	C	704	HIS	2.2
3	D	828	VAL	2.2
3	D	1129	THR	2.2
3	J	1395	LEU	2.2
3	D	570	GLU	2.2
3	D	239	GLY	2.2
3	D	808	THR	2.1
3	D	817	GLU	2.1
3	D	80	VAL	2.1
3	D	378	ILE	2.1
3	D	557	LEU	2.1
3	D	190	GLU	2.1
2	C	621	VAL	2.1
3	D	530	VAL	2.1
3	J	1394	VAL	2.1
2	C	265	LYS	2.1
3	D	55	ASP	2.1
3	D	187	LYS	2.1
3	J	1288	ASP	2.1
3	D	128	TYR	2.1
1	B	8	ALA	2.1
2	C	442	GLU	2.1
2	C	107	LEU	2.1
3	D	212	ARG	2.1
2	C	596	TYR	2.1
3	D	369	ALA	2.1
3	D	394	LEU	2.0
3	D	1046	GLN	2.0
2	C	624	PRO	2.0
3	J	1405	GLU	2.0
1	A	109	VAL	2.0
2	C	1021	LEU	2.0
3	D	210	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
3	D	288	MET	2.0
3	J	1392	GLY	2.0
3	D	71	LYS	2.0
3	D	137	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

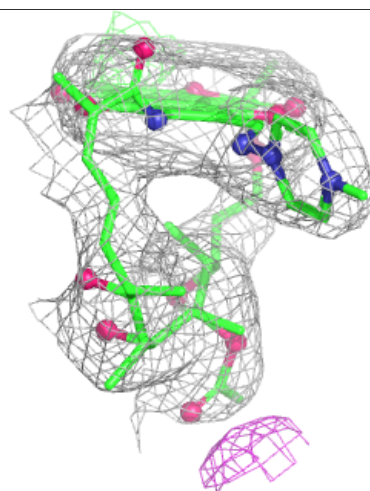
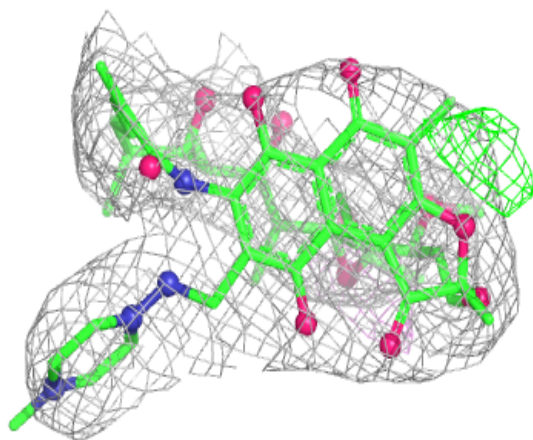
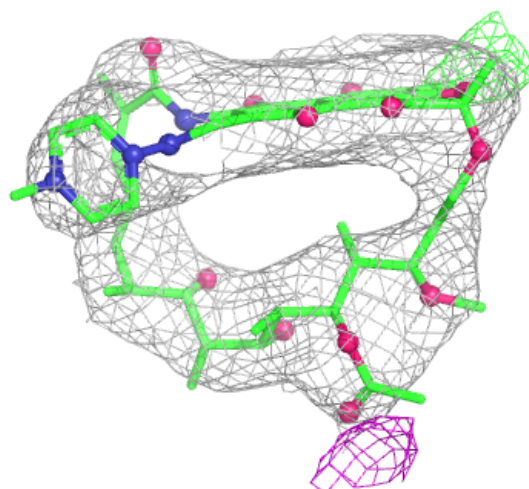
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	RFP	C	1120	59/59	0.90	0.12	44,47,60,63	0
6	ZN	D	1525	1/1	0.95	0.04	90,90,90,90	0
6	ZN	D	1526	1/1	0.97	0.17	52,52,52,52	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 RFP C 1120:

$2mF_o-DF_c$ (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.