



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:51 PM UTC

PDB ID : 8DH0 / pdb_00008dh0
Title : T7 RNA polymerase elongation complex with unnatural base dDs
Authors : Oh, J.; Wang, D.
Deposited on : 2022-06-24
Resolution : 2.90 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
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

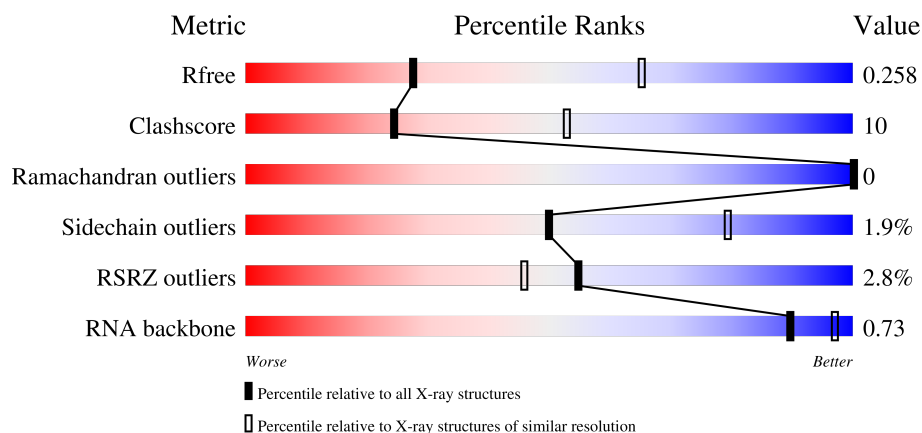
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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	18	44% 28% 28%
1	E	18	61% 22% 17%
1	I	18	56% 11% 33%
1	M	18	61% 17% 22%

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Mol	Chain	Length	Quality of chain
2	B	883	% 76% 18% 5%
2	F	883	2% 74% 16% 10%
2	J	883	4% 64% 26% 9%
2	N	883	3% 67% 19% 12%
3	C	12	67% 33%
3	G	12	67% 33%
3	K	12	67% 33%
3	O	12	50% 17% 33%
4	H	9	11% 56% 33%
4	P	9	11% 44% 44%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26201 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 DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	13	Total	C	N	O	P	S	0	0	0
			268	130	47	77	13	1			
1	E	15	Total	C	N	O	P	S	0	0	0
			310	150	57	87	15	1			
1	I	12	Total	C	N	O	P	S	0	0	0
			248	120	45	70	12	1			
1	M	14	Total	C	N	O	P	S	0	0	0
			289	140	52	82	14	1			

- Molecule 2 is a protein called T7 RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	840	Total	C	N	O	S	0	0	0
			6503	4142	1129	1196	36			
2	F	796	Total	C	N	O	S	0	0	0
			5875	3734	1028	1082	31			
2	J	805	Total	C	N	O	S	0	0	0
			6058	3859	1051	1114	34			
2	N	773	Total	C	N	O	S	0	0	0
			5706	3622	1006	1050	28			

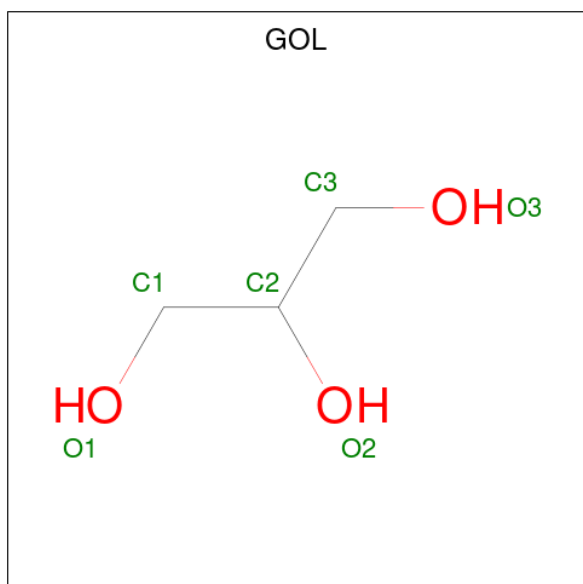
- Molecule 3 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	8	Total 174	C 77	N 33	O 56	P 8	0	0	0
3	G	8	Total 174	C 77	N 33	O 56	P 8	0	0	0
3	K	8	Total 174	C 77	N 33	O 56	P 8	0	0	0
3	O	8	Total 174	C 77	N 33	O 56	P 8	0	0	0

- Molecule 4 is a DNA chain called Non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	6	Total	C	N	O	P	0	0	0
			122	59	19	38	6			
4	P	5	Total	C	N	O	P	0	0	0
			102	49	17	31	5			

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

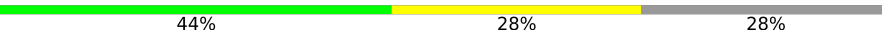


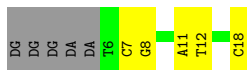
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	J	1	Total	C	O	0	0
			6	3	3		
5	N	1	Total	C	O	0	0
			6	3	3		

3 Residue-property plots [i](#)

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

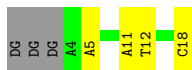
- Molecule 1: Template strand DNA

Chain A: 



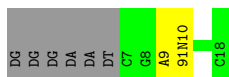
- Molecule 1: Template strand DNA

Chain E: 



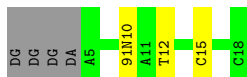
- Molecule 1: Template strand DNA

Chain I: 



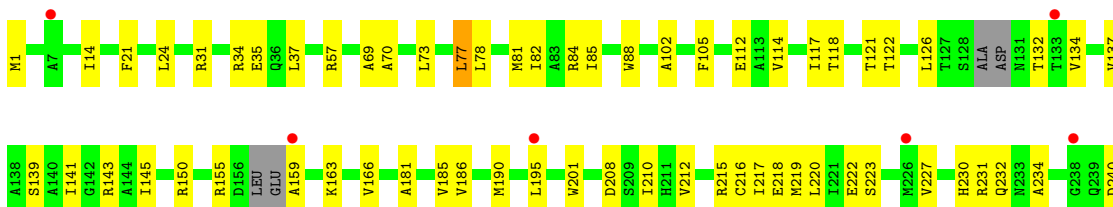
- Molecule 1: Template strand DNA

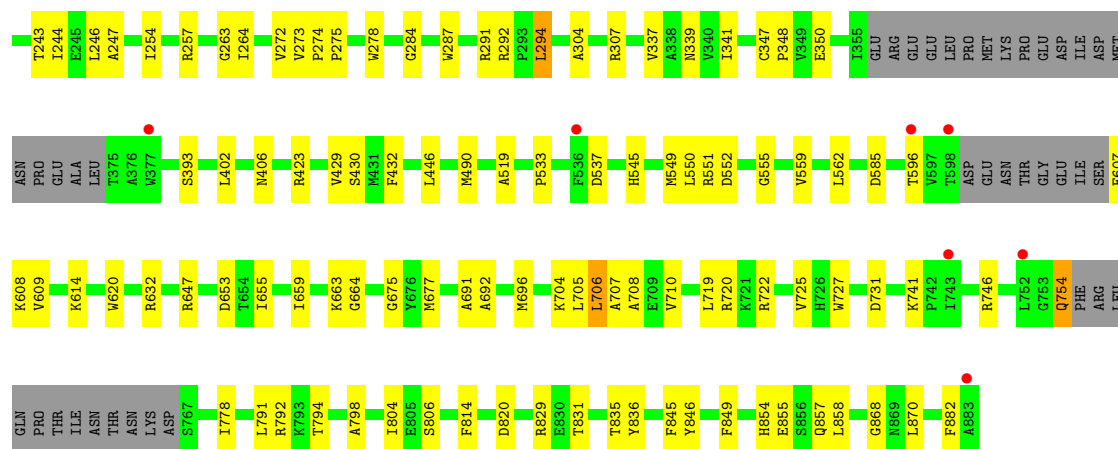
Chain M: 



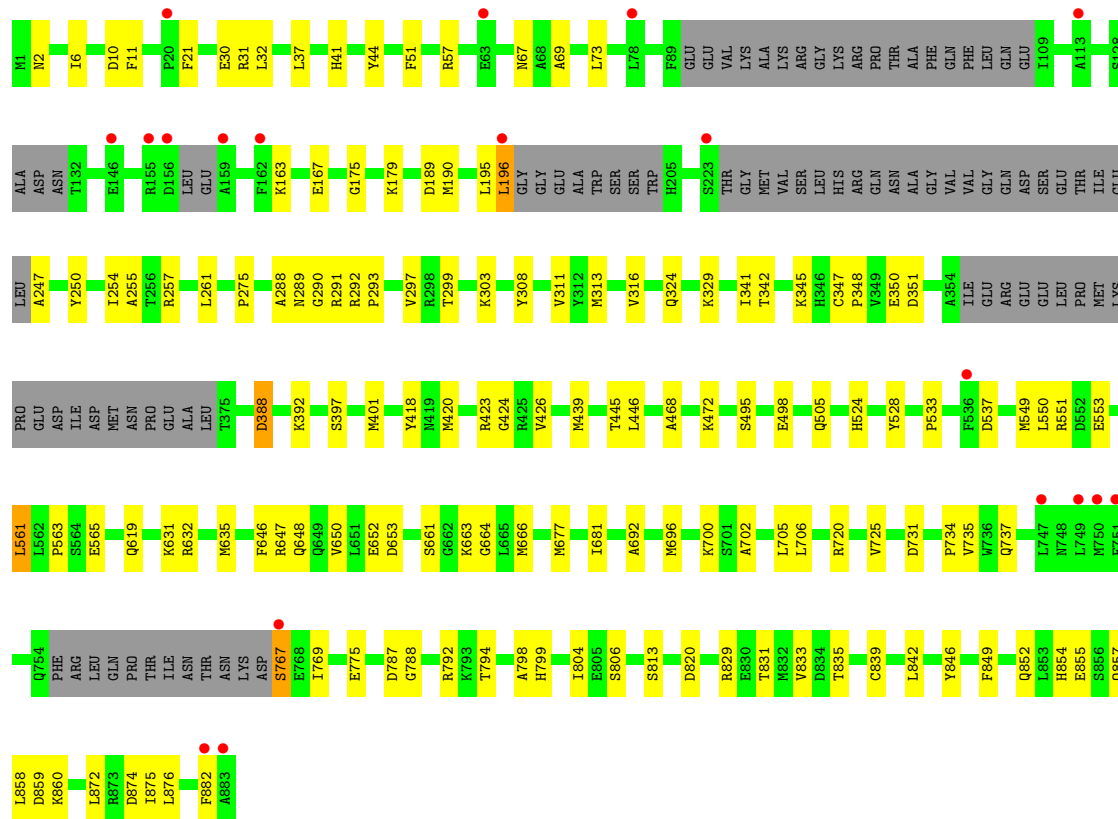
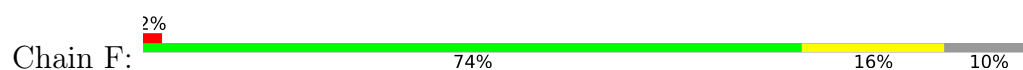
- Molecule 2: T7 RNA polymerase

Chain B: 

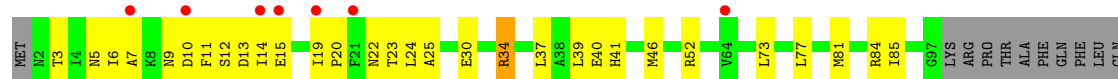




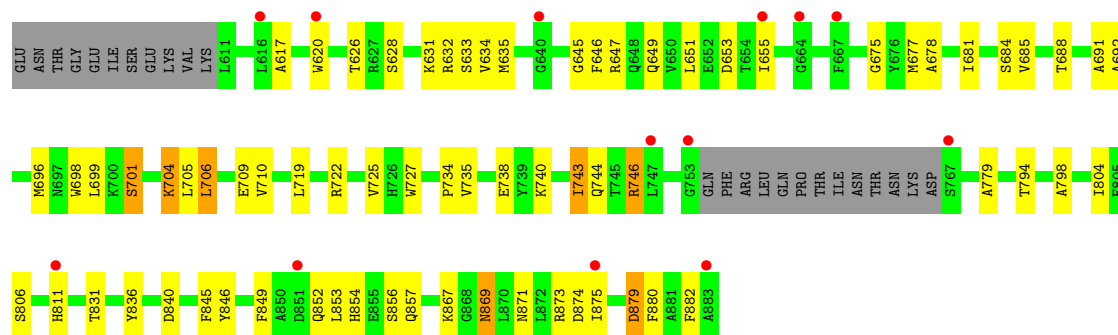
• Molecule 2: T7 RNA polymerase



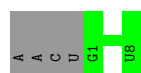
• Molecule 2: T7 RNA polymerase







- Molecule 3: RNA



- Molecule 3: RNA



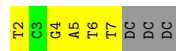
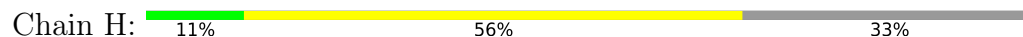
- Molecule 3: RNA



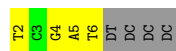
- Molecule 3: RNA



- Molecule 4: Non-template strand DNA



- Molecule 4: Non-template strand DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.71Å 86.23Å 201.22Å 89.91° 85.23° 69.50°	Depositor
Resolution (Å)	42.03 – 2.90 42.03 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.9 (42.03-2.90) 96.9 (42.03-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.19	Depositor
R, R_{free}	0.221 , 0.261 0.217 , 0.258	Depositor DCC
R_{free} test set	2000 reflections (1.65%)	wwPDB-VP
Wilson B-factor (Å ²)	82.5	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 85.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26201	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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: GOL, 91N

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	0.19	0/270	0.37	0/411
1	E	0.21	0/318	0.43	0/485
1	I	0.19	0/248	0.35	0/377
1	M	0.25	0/294	0.41	0/448
2	B	0.16	0/6646	0.40	1/9000 (0.0%)
2	F	0.18	0/5999	0.39	0/8142
2	J	0.22	0/6192	0.47	2/8399 (0.0%)
2	N	0.21	0/5824	0.45	1/7906 (0.0%)
3	C	0.12	0/194	0.32	0/301
3	G	0.10	0/194	0.24	0/301
3	K	0.10	0/194	0.25	0/301
3	O	0.10	0/194	0.24	0/301
4	H	0.23	0/135	0.47	0/206
4	P	0.20	0/113	0.41	0/172
All	All	0.19	0/26815	0.42	4/36750 (0.0%)

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
2	J	0	3
2	N	0	1
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	215	ARG	CG-CD-NE	5.54	124.18	112.00
2	B	31	ARG	CA-CB-CG	-5.42	103.26	114.10
2	N	306	MET	CB-CG-SD	5.18	128.23	112.70
2	J	215	ARG	CB-CG-CD	-5.07	99.64	111.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	J	215	ARG	Sidechain
2	J	34	ARG	Sidechain
2	J	394	ARG	Sidechain
2	N	291	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	268	0	135	4	0
1	E	310	0	157	5	0
1	I	248	0	123	3	0
1	M	289	0	146	3	0
2	B	6503	0	6377	107	0
2	F	5875	0	5480	89	0
2	J	6058	0	5747	157	0
2	N	5706	0	5328	131	0
3	C	174	0	88	0	0
3	G	174	0	88	0	0
3	K	174	0	88	0	0
3	O	174	0	88	2	0
4	H	122	0	70	4	0
4	P	102	0	58	3	0
5	B	6	0	8	0	0
5	F	6	0	8	0	0
5	J	6	0	8	0	0
5	N	6	0	8	0	0
All	All	26201	0	24005	495	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 10.

All (495) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:30:GLU:OE1	2:J:34:ARG:NH2	2.14	0.80
2:N:317:TYR:O	2:N:321:ASN:ND2	2.17	0.77
2:N:19:ILE:HG13	2:N:20:PRO:HD3	1.67	0.76
2:J:30:GLU:HB2	2:J:34:ARG:HH21	1.51	0.76
2:J:561:LEU:HG	2:J:875:ILE:HG12	1.68	0.76
2:J:696:MET:HG2	2:J:779:ALA:HB1	1.67	0.75
2:N:798:ALA:HB1	2:N:804:ILE:HD12	1.67	0.74
2:N:81:MET:HG3	2:N:115:ALA:HB1	1.69	0.74
2:B:339:ASN:HD21	2:B:406:ASN:HD21	1.35	0.73
2:B:102:ALA:HB3	2:B:215:ARG:HD2	1.69	0.73
2:B:232:GLN:HE22	2:B:243:THR:HB	1.55	0.72
2:B:35:GLU:HG2	2:B:272:VAL:HG21	1.72	0.72
2:J:320:ILE:HD11	2:J:420:MET:HE3	1.71	0.71
2:J:46:MET:HB3	2:J:267:MET:HE2	1.71	0.71
2:J:461:LYS:NZ	2:J:483:GLU:OE1	2.22	0.71
2:F:347:CYS:HB3	2:F:350:GLU:HB2	1.73	0.70
2:B:746:ARG:HH21	2:B:754:GLN:HB3	1.56	0.70
2:B:132:THR:OG1	2:B:243:THR:OG1	2.09	0.70
2:B:155:ARG:HA	2:B:163:LYS:HG3	1.72	0.70
2:J:450:LYS:HD3	2:J:817:ILE:HD11	1.73	0.70
2:N:871:ASN:HD21	2:N:873:ARG:HB2	1.56	0.70
2:F:190:MET:HG2	2:F:195:LEU:HB2	1.75	0.69
2:F:700:LYS:HE3	2:F:775:GLU:HB3	1.74	0.69
2:J:611:LEU:HD23	2:J:619:GLN:HE22	1.55	0.68
2:J:854:HIS:HB3	2:J:857:GLN:HG3	1.75	0.68
2:J:457:TYR:CE2	2:J:461:LYS:HE2	2.29	0.67
2:J:22:ASN:HA	2:J:25:ALA:HB3	1.75	0.66
2:B:347:CYS:HB3	2:B:350:GLU:HB2	1.77	0.65
2:N:854:HIS:HD1	2:N:856:SER:H	1.45	0.65
2:B:490:MET:HE1	2:B:519:ALA:HA	1.79	0.64
2:B:69:ALA:HA	2:B:257:ARG:HG2	1.78	0.64
2:J:6:ILE:HD11	2:J:259:GLY:HA2	1.78	0.64
2:N:561:LEU:HG	2:N:875:ILE:HG12	1.80	0.64
2:J:220:LEU:HD11	2:J:226:MET:HE3	1.79	0.64
2:J:347:CYS:HB3	2:J:350:GLU:HB2	1.81	0.63
2:N:540:CYS:HB3	2:N:543:ILE:HD13	1.80	0.63
2:J:594:VAL:HA	2:J:609:VAL:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:LEU:O	2:B:77:LEU:HD22	1.99	0.63
1:E:18:DC:OP2	2:F:57:ARG:NH2	2.29	0.63
2:J:590:THR:HG22	2:J:613:THR:H	1.62	0.63
2:N:347:CYS:HB2	2:N:350:GLU:HB2	1.81	0.63
2:N:275:PRO:HG2	2:N:324:GLN:HB3	1.81	0.63
2:J:6:ILE:HG22	2:J:10:ASP:HB3	1.80	0.62
2:J:677:MET:HG3	2:J:681:ILE:HD11	1.81	0.62
2:J:19:ILE:HD12	2:J:20:PRO:HD2	1.81	0.62
2:J:524:HIS:HB2	2:J:528:TYR:HB2	1.80	0.62
2:F:561:LEU:HG	2:F:875:ILE:HG12	1.81	0.62
2:B:114:VAL:O	2:B:118:THR:HG23	2.00	0.62
2:F:619:GLN:NE2	2:F:666:MET:O	2.33	0.62
2:J:205:HIS:HB3	2:J:208:ASP:HB2	1.80	0.62
2:N:743:ILE:HD12	2:N:744:GLN:HG3	1.81	0.62
2:F:446:LEU:HG	2:F:533:PRO:HG3	1.81	0.62
2:N:631:LYS:HD2	2:N:632:ARG:H	1.64	0.61
2:J:420:MET:HE1	2:J:792:ARG:HD3	1.82	0.61
2:N:471:ASP:OD1	2:N:471:ASP:N	2.33	0.61
2:J:281:ILE:HG22	2:J:282:THR:HG23	1.83	0.61
2:B:663:LYS:HG3	2:B:664:GLY:H	1.66	0.60
2:F:69:ALA:HA	2:F:257:ARG:HG2	1.82	0.60
2:J:215:ARG:HE	2:J:219:MET:HE2	1.66	0.60
2:N:704:LYS:NZ	4:P:6:DT:OP1	2.35	0.60
2:J:311:VAL:HG11	2:J:734:PRO:HG3	1.82	0.60
2:B:746:ARG:HE	2:B:754:GLN:H	1.50	0.59
2:B:692:ALA:O	2:B:696:MET:HG3	2.02	0.59
2:N:699:LEU:HD12	2:N:779:ALA:HA	1.85	0.59
2:N:709:GLU:HG3	2:N:722:ARG:HG3	1.83	0.59
2:F:190:MET:HE1	2:F:196:LEU:HD23	1.84	0.59
2:J:345:LYS:NZ	2:J:347:CYS:O	2.34	0.59
2:J:446:LEU:HG	2:J:533:PRO:HG3	1.84	0.59
2:N:692:ALA:O	2:N:696:MET:HG3	2.02	0.59
2:J:175:GLY:O	2:J:178:TYR:N	2.35	0.59
2:N:840:ASP:OD2	2:N:867:LYS:NZ	2.35	0.59
2:J:545:HIS:HD1	2:J:836:TYR:HH	1.51	0.58
2:J:837:GLU:HG2	2:J:872:LEU:HD22	1.85	0.58
2:N:854:HIS:HB3	2:N:857:GLN:HG3	1.84	0.58
2:J:6:ILE:HG22	2:J:10:ASP:CB	2.33	0.58
2:F:794:THR:HA	2:F:831:THR:HG21	1.86	0.58
2:B:186:VAL:O	2:B:190:MET:HG3	2.04	0.58
2:F:297:VAL:HG12	2:F:299:THR:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:584:ALA:HA	2:J:587:ILE:HD12	1.86	0.58
2:B:21:PHE:HE2	2:B:34:ARG:HD2	1.70	0.57
2:B:537:ASP:OD1	2:B:537:ASP:N	2.35	0.57
2:F:11:PHE:CE1	2:F:44:TYR:HB3	2.39	0.57
2:F:705:LEU:O	2:F:720:ARG:NH2	2.37	0.57
2:F:692:ALA:O	2:F:696:MET:HG3	2.04	0.57
2:B:632:ARG:NH1	2:B:653:ASP:OD2	2.38	0.57
2:J:208:ASP:O	2:J:212:VAL:HG23	2.04	0.57
2:J:537:ASP:OD1	2:J:537:ASP:N	2.36	0.57
2:F:833:VAL:HG21	2:F:876:LEU:HG	1.87	0.57
2:J:20:PRO:HB2	2:J:23:THR:HG23	1.87	0.57
2:N:681:ILE:O	2:N:685:VAL:HG23	2.05	0.57
2:J:632:ARG:HA	2:J:635:MET:HE3	1.86	0.57
2:N:6:ILE:HD12	2:N:6:ILE:H	1.70	0.56
2:B:218:GLU:O	2:B:222:GLU:HG3	2.06	0.56
2:J:84:ARG:HH21	2:J:222:GLU:C	2.13	0.56
2:F:163:LYS:O	2:F:167:GLU:N	2.38	0.56
2:J:457:TYR:HE2	2:J:461:LYS:HE2	1.69	0.56
2:N:10:ASP:O	2:N:291:ARG:NH2	2.39	0.56
2:J:849:PHE:HA	2:J:852:GLN:HG3	1.88	0.56
2:B:710:VAL:O	2:B:719:LEU:N	2.37	0.56
2:N:552:ASP:HB2	2:N:691:ALA:HB2	1.88	0.56
2:N:879:ASP:OD2	2:N:879:ASP:N	2.38	0.55
2:J:11:PHE:HA	2:J:14:ILE:HG22	1.88	0.55
2:J:77:LEU:HD12	2:J:226:MET:HE2	1.88	0.55
2:J:804:ILE:HG12	2:J:820:ASP:HB3	1.88	0.55
2:N:10:ASP:HB3	2:N:291:ARG:CZ	2.37	0.55
2:B:446:LEU:HG	2:B:533:PRO:HG3	1.89	0.55
2:N:626:THR:HG23	2:N:628:SER:H	1.70	0.55
2:B:139:SER:O	2:B:143:ARG:HG3	2.06	0.55
2:N:678:ALA:HA	2:N:681:ILE:HD12	1.89	0.55
2:N:137:VAL:O	2:N:141:ILE:HG13	2.07	0.55
2:B:446:LEU:HD13	2:B:806:SER:HB3	1.88	0.55
2:J:213:GLY:O	2:J:217:ILE:HG13	2.07	0.54
2:F:854:HIS:HB3	2:F:857:GLN:HG3	1.89	0.54
2:J:303:LYS:H	2:J:303:LYS:HD2	1.71	0.54
2:N:549:MET:HG2	2:N:836:TYR:HE1	1.72	0.54
2:B:608:LYS:HD2	2:B:609:VAL:H	1.72	0.54
2:B:230:HIS:HB2	2:B:243:THR:HG22	1.89	0.54
2:B:21:PHE:CE2	2:B:34:ARG:HD2	2.43	0.54
2:F:341:ILE:HD12	2:F:348:PRO:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:646:PHE:O	2:J:650:VAL:HG23	2.08	0.54
2:N:82:ILE:HD12	2:N:112:GLU:HA	1.89	0.54
2:B:430:SER:OG	2:B:432:PHE:O	2.25	0.54
2:F:6:ILE:HD12	2:F:291:ARG:HH12	1.72	0.54
2:B:159:ALA:N	2:B:195:LEU:HD11	2.23	0.53
2:B:798:ALA:HB1	2:B:804:ILE:HD12	1.90	0.53
2:J:183:MET:HA	2:J:186:VAL:HG22	1.90	0.53
2:J:565:GLU:HG2	2:J:566:THR:HG23	1.88	0.53
2:J:155:ARG:HA	2:J:163:LYS:HG2	1.91	0.53
2:J:190:MET:O	2:J:195:LEU:N	2.32	0.53
2:B:263:GLY:HA3	2:B:291:ARG:HH11	1.73	0.53
2:F:495:SER:HB3	2:F:498:GLU:HB2	1.91	0.53
2:J:6:ILE:HD12	2:J:6:ILE:H	1.73	0.53
2:J:190:MET:O	2:J:194:GLY:N	2.32	0.53
2:N:25:ALA:HB1	2:N:30:GLU:HG2	1.89	0.53
1:E:18:DC:P	2:F:57:ARG:HH21	2.31	0.53
4:H:4:DG:H2'	4:H:5:DA:C8	2.44	0.53
2:N:350:GLU:OE1	2:N:391:ARG:NH1	2.42	0.53
2:J:730:PRO:HB2	2:J:793:LYS:HE3	1.91	0.52
2:B:731:ASP:OD1	2:B:792:ARG:NE	2.28	0.52
2:J:275:PRO:HG2	2:J:324:GLN:HB3	1.91	0.52
2:J:646:PHE:O	2:J:649:GLN:HG2	2.09	0.52
2:J:138:ALA:HB2	2:J:217:ILE:HD11	1.91	0.52
2:N:30:GLU:O	2:N:34:ARG:HD2	2.10	0.52
2:F:524:HIS:HB2	2:F:528:TYR:HB2	1.89	0.52
2:B:829:ARG:NH2	2:B:882:PHE:H	2.08	0.52
2:F:731:ASP:HB3	2:F:792:ARG:HH21	1.75	0.52
2:N:727:TRP:HB3	2:N:845:PHE:CD2	2.45	0.52
4:H:6:DT:H2''	4:H:7:DT:H5'	1.91	0.52
2:F:663:LYS:HD3	2:F:664:GLY:H	1.75	0.52
2:N:557:ARG:HG2	2:N:568:GLN:OE1	2.10	0.51
2:N:698:TRP:HE3	2:N:699:LEU:HD23	1.75	0.51
2:N:794:THR:HA	2:N:831:THR:HG21	1.92	0.51
2:J:657:PRO:O	2:J:661:SER:OG	2.22	0.51
2:J:307:ARG:NH1	2:J:738:GLU:OE1	2.44	0.51
1:M:12:DT:H4'	2:N:423:ARG:HD2	1.93	0.51
2:N:306:MET:HE3	2:N:306:MET:HA	1.93	0.51
3:O:2:C:H2'	3:O:3:G:C8	2.46	0.51
2:B:552:ASP:HB2	2:B:691:ALA:HB2	1.92	0.51
2:N:6:ILE:HG22	2:N:10:ASP:HB2	1.91	0.51
2:N:267:MET:HG2	2:N:431:MET:SD	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:226:MET:HG3	2:J:227:VAL:HG23	1.92	0.51
2:B:562:LEU:HD11	2:B:870:LEU:HD12	1.93	0.51
2:J:24:LEU:HD21	2:J:287:TRP:CE2	2.45	0.51
2:N:632:ARG:NH2	2:N:653:ASP:HB3	2.26	0.51
2:F:345:LYS:HZ3	2:F:351:ASP:H	1.59	0.51
2:F:446:LEU:HD13	2:F:806:SER:HB3	1.93	0.51
2:F:720:ARG:HD2	2:F:852:GLN:O	2.11	0.51
2:J:329:LYS:HG3	2:J:445:THR:HG23	1.93	0.51
2:N:11:PHE:HB3	2:N:41:HIS:CD2	2.46	0.50
2:N:78:LEU:O	2:N:82:ILE:HG12	2.10	0.50
2:J:318:LYS:O	2:J:322:ILE:HG13	2.11	0.50
2:N:294:LEU:HD11	2:N:429:VAL:HG21	1.93	0.50
2:N:306:MET:O	2:N:309:GLU:HG2	2.11	0.50
2:N:710:VAL:O	2:N:719:LEU:N	2.44	0.50
2:B:118:THR:HG21	2:B:216:CYS:HB3	1.92	0.50
2:B:217:ILE:HG21	2:B:244:ILE:HD11	1.92	0.50
2:N:446:LEU:HG	2:N:533:PRO:HG3	1.92	0.50
2:N:10:ASP:HB3	2:N:291:ARG:HE	1.76	0.50
2:B:707:ALA:O	2:B:722:ARG:NH1	2.35	0.50
2:B:659:ILE:HD13	2:B:664:GLY:HA3	1.94	0.50
2:N:423:ARG:HH21	2:N:425:ARG:HE	1.60	0.50
2:N:631:LYS:O	2:N:635:MET:HG3	2.11	0.50
2:N:565:GLU:H	2:N:565:GLU:CD	2.20	0.49
2:B:831:THR:O	2:B:835:THR:HG23	2.13	0.49
2:F:831:THR:O	2:F:835:THR:HG23	2.12	0.49
2:B:81:MET:O	2:B:85:ILE:HG12	2.13	0.49
2:J:204:TRP:CZ3	2:J:212:VAL:HG21	2.47	0.49
2:J:801:LYS:HG2	2:J:802:TYR:CZ	2.47	0.49
2:J:13:ASP:OD1	2:J:14:ILE:N	2.46	0.49
2:N:651:LEU:HA	2:N:655:ILE:HB	1.95	0.49
2:B:705:LEU:HD13	2:B:857:GLN:HB3	1.95	0.49
2:J:215:ARG:C	2:J:215:ARG:HD2	2.34	0.49
2:B:596:THR:HA	2:B:607:GLU:HA	1.93	0.49
2:J:430:SER:O	2:J:433:ASN:ND2	2.43	0.49
2:J:551:ARG:NE	2:J:872:LEU:HD11	2.28	0.49
2:B:337:VAL:O	2:B:341:ILE:HG12	2.13	0.49
2:J:462:ILE:O	2:J:466:ASN:ND2	2.45	0.49
2:B:855:GLU:HA	2:B:858:LEU:HD23	1.95	0.48
2:J:251:ALA:O	2:J:254:ILE:HG13	2.13	0.48
2:N:746:ARG:H	2:N:746:ARG:HD2	1.76	0.48
2:B:804:ILE:HG12	2:B:820:ASP:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:476:PRO:O	2:J:480:LYS:HG2	2.13	0.48
2:B:708:ALA:O	2:B:720:ARG:NH2	2.46	0.48
2:B:854:HIS:HB3	2:B:857:GLN:HG3	1.95	0.48
2:J:708:ALA:HA	2:J:722:ARG:HH21	1.78	0.48
2:B:181:ALA:O	2:B:185:VAL:HG23	2.14	0.48
2:J:215:ARG:HD2	2:J:215:ARG:HA	1.67	0.48
2:N:727:TRP:HB3	2:N:845:PHE:HD2	1.78	0.48
2:B:24:LEU:HD11	2:B:273:VAL:HG21	1.95	0.48
2:N:30:GLU:HB3	2:N:34:ARG:HE	1.78	0.48
2:N:311:VAL:HG11	2:N:734:PRO:HG3	1.95	0.48
1:A:18:DC:OP2	2:B:57:ARG:NH2	2.41	0.48
2:F:67:ASN:ND2	2:F:69:ALA:H	2.12	0.48
2:J:205:HIS:CE1	2:J:207:GLU:HG2	2.49	0.48
2:N:684:SER:O	2:N:688:THR:OG1	2.28	0.48
2:B:791:LEU:HA	2:B:814:PHE:HE2	1.79	0.48
2:J:207:GLU:HA	2:J:210:ILE:HG22	1.96	0.48
2:J:337:VAL:O	2:J:341:ILE:HG12	2.13	0.48
2:B:304:ALA:HA	2:B:307:ARG:HE	1.79	0.48
2:B:731:ASP:HB3	2:B:792:ARG:HH21	1.79	0.48
2:J:485:ASN:O	2:J:489:ILE:HG13	2.13	0.48
2:B:82:ILE:HD13	2:B:112:GLU:HG3	1.95	0.48
2:F:829:ARG:HH22	2:F:882:PHE:H	1.61	0.48
2:J:556:GLY:O	2:J:561:LEU:N	2.46	0.48
2:F:313:MET:HB2	2:F:316:VAL:HB	1.95	0.47
2:B:725:VAL:HG11	2:B:778:ILE:HD13	1.95	0.47
2:F:725:VAL:HG13	2:F:737:GLN:HB3	1.96	0.47
2:J:578:VAL:HA	2:J:581:ILE:HD12	1.95	0.47
2:J:822:ALA:O	2:J:826:LYS:HG3	2.14	0.47
2:N:47:GLY:HA3	2:N:265:SER:O	2.14	0.47
2:B:231:ARG:HD3	2:B:234:ALA:HB2	1.95	0.47
2:F:551:ARG:NE	2:F:872:LEU:HD11	2.28	0.47
2:J:163:LYS:HA	2:J:166:VAL:HG22	1.97	0.47
2:J:249:GLU:H	2:J:249:GLU:CD	2.21	0.47
3:O:2:C:H2'	3:O:3:G:H8	1.80	0.47
2:J:589:GLY:HA3	2:J:614:LYS:HB3	1.95	0.47
2:B:585:ASP:O	2:B:614:LYS:HA	2.14	0.47
2:F:11:PHE:HB3	2:F:41:HIS:CE1	2.49	0.47
2:F:31:ARG:H	2:F:31:ARG:HD3	1.79	0.47
2:F:846:TYR:HA	2:F:849:PHE:CE2	2.49	0.47
1:M:10:91N:C10	2:N:649:GLN:HG2	2.44	0.47
2:N:846:TYR:HA	2:N:849:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:DT:H4'	2:B:423:ARG:HD2	1.96	0.47
2:B:105:PHE:CE1	2:B:208:ASP:HB3	2.49	0.47
2:J:417:PRO:HG2	2:J:429:VAL:HB	1.97	0.47
2:J:705:LEU:O	2:J:720:ARG:NH2	2.46	0.47
2:N:84:ARG:HD2	2:N:84:ARG:HA	1.70	0.47
2:N:701:SER:O	2:N:705:LEU:HG	2.15	0.47
2:B:85:ILE:HD13	2:B:219:MET:SD	2.55	0.47
2:J:22:ASN:OD1	2:J:23:THR:N	2.48	0.47
2:J:475:PHE:CE2	2:J:879:ASP:HB2	2.49	0.47
2:J:573:ILE:O	2:J:577:LYS:HG3	2.15	0.47
2:N:545:HIS:O	2:N:549:MET:HG3	2.15	0.47
2:B:24:LEU:HD13	2:B:287:TRP:CD2	2.49	0.47
2:B:704:LYS:HB3	2:B:704:LYS:HE2	1.80	0.47
2:J:9:ASN:O	2:J:12:SER:OG	2.28	0.47
2:B:78:LEU:O	2:B:82:ILE:HG13	2.14	0.46
2:B:231:ARG:NH2	2:B:240:ASP:OD2	2.46	0.46
1:E:5:DA:H61	4:H:5:DA:H61	1.62	0.46
2:F:829:ARG:HB3	2:F:876:LEU:HD23	1.97	0.46
2:B:1:MET:N	2:B:254:ILE:HD11	2.29	0.46
2:B:139:SER:HB2	2:B:210:ILE:HD13	1.97	0.46
1:I:9:DA:H2'	2:J:644:PHE:CD1	2.50	0.46
1:E:12:DT:H4'	2:F:423:ARG:HD2	1.97	0.46
2:F:702:ALA:O	2:F:706:LEU:HG	2.14	0.46
2:J:787:ASP:OD2	2:J:788:GLY:N	2.48	0.46
2:F:21:PHE:CZ	2:F:30:GLU:HG2	2.50	0.46
2:F:663:LYS:HE2	2:F:663:LYS:HA	1.97	0.46
2:N:565:GLU:HG2	2:N:566:THR:HG23	1.97	0.46
2:B:727:TRP:HB3	2:B:845:PHE:HD1	1.79	0.46
1:I:9:DA:H2'	2:J:644:PHE:HD1	1.80	0.46
2:J:560:ASN:HB3	2:J:880:PHE:HB2	1.96	0.46
2:J:725:VAL:HG21	2:J:778:ILE:HD13	1.98	0.46
1:A:7:DC:H2''	1:A:8:DG:C8	2.50	0.46
2:F:51:PHE:CE1	2:F:261:LEU:HB2	2.51	0.46
2:J:710:VAL:O	2:J:719:LEU:N	2.45	0.46
2:J:829:ARG:O	2:J:833:VAL:HG23	2.16	0.46
2:N:337:VAL:O	2:N:341:ILE:HG12	2.16	0.46
4:H:2:DT:H6	4:H:2:DT:H2'	1.63	0.46
2:J:304:ALA:HA	2:J:307:ARG:HD2	1.96	0.46
2:J:315:GLU:HA	2:J:318:LYS:HD3	1.98	0.46
2:J:616:LEU:HD13	2:J:676:TYR:HB2	1.97	0.46
2:B:655:ILE:O	2:B:659:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:DA:H2'	1:E:12:DT:C6	2.51	0.45
2:J:77:LEU:HB3	2:J:224:THR:HG21	1.98	0.45
2:J:559:VAL:HG23	2:J:561:LEU:HB2	1.98	0.45
2:N:555:GLY:O	2:N:559:VAL:HG22	2.16	0.45
2:B:551:ARG:NH2	2:B:836:TYR:O	2.50	0.45
2:J:333:LYS:H	2:J:333:LYS:HD2	1.81	0.45
2:B:220:LEU:HD11	2:B:227:VAL:HB	1.98	0.45
2:F:289:ASN:HD22	2:F:290:GLY:N	2.14	0.45
2:J:555:GLY:O	2:J:559:VAL:HG22	2.15	0.45
2:N:645:GLY:O	2:N:649:GLN:HG3	2.16	0.45
2:B:720:ARG:HE	2:B:720:ARG:HB3	1.65	0.45
2:N:78:LEU:HD11	2:N:116:TYR:HA	1.97	0.45
2:N:86:ASN:HA	2:N:89:PHE:CD2	2.51	0.45
2:N:489:ILE:HG23	2:N:515:CYS:SG	2.56	0.45
2:N:578:VAL:HG11	2:N:677:MET:HE1	1.98	0.45
2:N:871:ASN:ND2	2:N:874:ASP:OD1	2.49	0.45
2:F:37:LEU:HD12	2:F:288:ALA:HB2	1.99	0.45
2:F:799:HIS:O	2:F:799:HIS:ND1	2.48	0.45
2:J:822:ALA:O	2:J:825:PHE:HB3	2.16	0.45
2:N:849:PHE:HA	2:N:852:GLN:OE1	2.16	0.45
2:B:402:LEU:HD23	2:B:402:LEU:HA	1.81	0.45
2:B:141:ILE:O	2:B:145:ILE:HG12	2.17	0.45
2:F:631:LYS:O	2:F:635:MET:HG3	2.16	0.45
2:F:292:ARG:NH1	2:F:293:PRO:O	2.49	0.45
2:F:798:ALA:HB1	2:F:804:ILE:HD12	1.98	0.45
1:I:10:91N:OP2	2:J:645:GLY:HA3	2.17	0.45
2:J:5:ASN:HA	2:J:52:ARG:NH2	2.31	0.45
2:J:40:GLU:CD	2:J:286:TYR:HB3	2.41	0.45
2:N:10:ASP:HB3	2:N:291:ARG:NE	2.31	0.45
2:N:307:ARG:NH1	2:N:738:GLU:OE1	2.50	0.45
2:B:278:TRP:CD2	2:B:284:GLY:HA3	2.52	0.44
2:N:50:ARG:HH21	2:N:267:MET:HG3	1.80	0.44
2:F:313:MET:HE2	2:F:313:MET:HB3	1.60	0.44
2:N:536:PHE:HB3	2:N:882:PHE:HB3	1.99	0.44
2:B:70:ALA:O	2:B:73:LEU:HD23	2.18	0.44
2:F:418:TYR:HD1	2:F:426:VAL:HG12	1.82	0.44
2:J:6:ILE:HD13	2:J:262:ALA:HB3	2.00	0.44
2:J:73:LEU:O	2:J:77:LEU:HG	2.17	0.44
2:J:6:ILE:O	2:J:10:ASP:HB3	2.18	0.44
2:J:197:GLY:C	2:J:199:GLU:H	2.26	0.44
2:J:655:ILE:O	2:J:659:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:338:ALA:O	2:N:342:THR:OG1	2.19	0.44
2:B:134:VAL:HG22	2:B:244:ILE:HG13	1.99	0.44
2:F:787:ASP:OD1	2:F:788:GLY:N	2.50	0.44
2:J:545:HIS:O	2:J:549:MET:HG2	2.18	0.44
2:N:17:ALA:O	2:N:20:PRO:HD2	2.17	0.44
2:F:21:PHE:HZ	2:F:30:GLU:HG2	1.83	0.44
2:F:632:ARG:HD2	2:F:653:ASP:OD1	2.18	0.44
2:F:646:PHE:O	2:F:650:VAL:HG23	2.18	0.44
2:J:457:TYR:CD1	2:J:521:VAL:HG11	2.52	0.44
2:J:631:LYS:HG2	2:J:635:MET:HE2	2.00	0.44
2:J:707:ALA:O	2:J:722:ARG:NE	2.49	0.44
2:B:117:ILE:O	2:B:121:THR:OG1	2.22	0.44
2:F:11:PHE:CZ	2:F:44:TYR:HB3	2.53	0.44
2:F:308:TYR:O	2:F:311:VAL:HG12	2.18	0.44
2:F:397:SER:O	2:F:401:MET:HG2	2.18	0.44
2:F:550:LEU:HD11	2:F:842:LEU:HD12	1.99	0.44
2:F:720:ARG:HD3	2:F:854:HIS:HB2	1.98	0.44
2:J:181:ALA:O	2:J:185:VAL:HG23	2.18	0.44
2:B:846:TYR:HA	2:B:849:PHE:CE1	2.53	0.44
2:J:571:TYR:HB2	2:J:627:ARG:HB2	2.00	0.44
2:J:701:SER:O	2:J:705:LEU:HG	2.18	0.44
1:M:15:DC:H5"	2:N:431:MET:HE3	1.99	0.44
2:B:647:ARG:HE	2:B:675:GLY:HA2	1.83	0.43
2:J:307:ARG:HH12	2:J:738:GLU:CD	2.26	0.43
2:J:727:TRP:HB3	2:J:845:PHE:HD1	1.83	0.43
2:N:738:GLU:O	2:N:740:LYS:HE3	2.18	0.43
2:F:663:LYS:HD2	2:F:666:MET:HE1	2.00	0.43
2:J:39:LEU:HD21	2:J:408:PHE:HE2	1.83	0.43
2:N:550:LEU:HD12	2:N:691:ALA:HA	1.98	0.43
2:N:550:LEU:HB2	2:N:691:ALA:HB1	1.99	0.43
2:N:647:ARG:HD2	2:N:675:GLY:HA2	2.00	0.43
2:N:474:PRO:HA	2:N:880:PHE:CZ	2.53	0.43
2:N:578:VAL:CG1	2:N:677:MET:HE1	2.48	0.43
2:B:232:GLN:NE2	2:B:243:THR:HB	2.28	0.43
2:N:873:ARG:HA	2:N:873:ARG:HD2	1.88	0.43
2:B:112:GLU:N	2:B:112:GLU:OE1	2.51	0.43
2:F:420:MET:HE2	2:F:424:GLY:HA2	2.00	0.43
2:B:126:LEU:HD21	2:B:244:ILE:HG22	1.99	0.43
2:F:190:MET:HE2	2:F:190:MET:HB3	1.90	0.43
2:F:804:ILE:HG12	2:F:820:ASP:HB3	2.01	0.43
2:J:462:ILE:HG22	2:J:466:ASN:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:709:GLU:HG2	2:J:722:ARG:HG2	2.01	0.43
2:N:14:ILE:HD12	2:N:289:ASN:O	2.18	0.43
2:F:2:ASN:O	2:F:255:ALA:HB1	2.18	0.43
2:F:73:LEU:HD23	2:F:73:LEU:H	1.83	0.43
2:J:81:MET:HG3	2:J:85:ILE:HD11	2.01	0.43
2:N:448:LYS:HA	2:N:448:LYS:HD3	1.60	0.43
2:N:633:SER:HB3	2:N:646:PHE:CE1	2.54	0.43
2:B:294:LEU:HD21	2:B:429:VAL:HG11	1.99	0.43
2:B:545:HIS:O	2:B:549:MET:HG3	2.19	0.43
2:N:36:GLN:O	2:N:40:GLU:HG3	2.19	0.43
2:F:439:MET:HE2	2:F:439:MET:HB3	1.92	0.43
2:N:628:SER:HA	2:N:631:LYS:HG3	2.00	0.43
2:J:812:ASP:N	2:J:812:ASP:OD2	2.50	0.43
2:N:342:THR:HG23	2:N:398:LEU:HD21	2.00	0.43
2:N:402:LEU:HD23	2:N:402:LEU:HA	1.92	0.43
2:N:710:VAL:HG12	2:N:719:LEU:HB2	2.00	0.43
2:B:163:LYS:HA	2:B:166:VAL:HG22	2.00	0.42
2:J:385:TYR:O	2:J:389:LYS:HG3	2.19	0.42
2:N:446:LEU:HD13	2:N:806:SER:HB2	2.01	0.42
2:F:275:PRO:HG2	2:F:324:GLN:HB3	2.01	0.42
2:F:537:ASP:OD2	2:F:813:SER:HB2	2.19	0.42
2:J:345:LYS:HE3	2:J:352:ILE:HD13	2.01	0.42
2:J:560:ASN:O	2:J:878:SER:OG	2.36	0.42
2:J:608:LYS:HD3	2:J:608:LYS:HA	1.63	0.42
2:J:825:PHE:O	2:J:829:ARG:NH1	2.51	0.42
2:N:571:TYR:CD2	2:N:631:LYS:HA	2.54	0.42
2:B:794:THR:HA	2:B:831:THR:HG21	2.01	0.42
2:F:835:THR:O	2:F:839:CYS:N	2.52	0.42
2:F:257:ARG:O	2:F:261:LEU:HG	2.19	0.42
2:J:329:LYS:HG2	2:J:447:ALA:HA	2.00	0.42
2:J:563:PRO:CD	2:J:874:ASP:HB3	2.49	0.42
2:J:644:PHE:O	2:J:647:ARG:HG2	2.19	0.42
2:N:706:LEU:HD22	2:N:725:VAL:HG22	2.01	0.42
2:B:274:PRO:HA	2:B:275:PRO:HD3	1.92	0.42
2:F:289:ASN:HD22	2:F:289:ASN:C	2.28	0.42
2:J:801:LYS:HG2	2:J:802:TYR:CE1	2.55	0.42
2:N:853:LEU:HD23	2:N:853:LEU:HA	1.80	0.42
2:F:855:GLU:HA	2:F:858:LEU:CD2	2.49	0.42
2:J:278:TRP:CD2	2:J:284:GLY:HA3	2.54	0.42
2:N:375:THR:OG1	2:N:376:ALA:N	2.53	0.42
2:N:465:ALA:HB1	2:N:470:VAL:HG23	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:DA:H2'	1:A:12:DT:C6	2.55	0.42
2:F:859:ASP:OD1	2:F:860:LYS:N	2.52	0.42
2:J:180:LYS:HG3	2:J:750:MET:HE2	2.01	0.42
2:N:53:LYS:HA	2:N:53:LYS:HD3	1.65	0.42
2:N:60:LYS:HD2	2:N:60:LYS:HA	1.73	0.42
2:N:294:LEU:HD11	2:N:429:VAL:HG11	2.01	0.42
2:B:550:LEU:O	2:B:868:GLY:N	2.50	0.42
2:B:706:LEU:HD21	2:B:849:PHE:HB2	2.02	0.42
2:B:741:LYS:HB2	2:B:741:LYS:HE3	1.86	0.42
2:B:122:THR:HG23	2:B:141:ILE:HD11	2.02	0.42
2:B:227:VAL:HG13	2:B:244:ILE:HG23	2.02	0.42
2:J:536:PHE:HB3	2:J:882:PHE:CD2	2.55	0.42
2:B:208:ASP:O	2:B:212:VAL:HG23	2.20	0.42
2:F:565:GLU:CD	2:F:565:GLU:H	2.27	0.42
2:B:829:ARG:HH22	2:B:882:PHE:H	1.65	0.41
2:B:150:ARG:HD2	2:B:201:TRP:CD1	2.56	0.41
2:B:246:LEU:HD12	2:B:247:ALA:N	2.35	0.41
2:B:727:TRP:HB3	2:B:845:PHE:CD1	2.54	0.41
2:J:552:ASP:CG	2:J:555:GLY:H	2.28	0.41
2:N:59:LEU:HD12	2:N:59:LEU:HA	1.88	0.41
2:N:88:TRP:HE3	2:N:89:PHE:HD1	1.69	0.41
2:F:468:ALA:HA	2:F:505:GLN:HB3	2.02	0.41
2:N:313:MET:HB2	2:N:316:VAL:HB	2.02	0.41
2:F:329:LYS:HG3	2:F:445:THR:HG23	2.01	0.41
2:N:278:TRP:CD2	2:N:284:GLY:HA3	2.55	0.41
2:N:540:CYS:HB2	2:N:559:VAL:HG12	2.02	0.41
2:B:555:GLY:O	2:B:559:VAL:HG22	2.20	0.41
2:J:392:LYS:O	2:J:396:ILE:HD12	2.21	0.41
4:P:2:DT:H6	4:P:2:DT:H2'	1.62	0.41
2:F:31:ARG:HG2	2:F:32:LEU:N	2.34	0.41
2:J:7:ALA:O	2:J:11:PHE:HB2	2.20	0.41
2:J:677:MET:O	2:J:681:ILE:HD12	2.20	0.41
2:J:697:ASN:O	2:J:701:SER:OG	2.29	0.41
2:N:74:ILE:O	2:N:77:LEU:N	2.53	0.41
2:N:141:ILE:HG13	2:N:141:ILE:H	1.64	0.41
2:N:317:TYR:C	2:N:321:ASN:HD22	2.21	0.41
2:N:544:GLN:HG2	2:N:561:LEU:HD13	2.02	0.41
4:P:4:DG:H2'	4:P:5:DA:C8	2.56	0.41
2:J:135:GLN:HA	2:J:210:ILE:HD11	2.03	0.41
2:J:854:HIS:CG	2:J:855:GLU:N	2.89	0.41
2:F:6:ILE:HG23	2:F:10:ASP:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:388:ASP:O	2:F:392:LYS:HG2	2.21	0.41
2:J:782:PHE:O	2:J:786:GLN:HG2	2.20	0.41
2:N:278:TRP:HZ2	2:N:294:LEU:HD22	1.85	0.41
2:N:425:ARG:HH11	2:N:811:HIS:HB3	1.86	0.41
2:B:84:ARG:HB2	2:B:223:SER:HB3	2.03	0.41
2:B:620:TRP:CD2	2:B:677:MET:HE3	2.55	0.41
2:F:175:GLY:O	2:F:179:LYS:HG2	2.21	0.41
2:F:648:GLN:NE2	2:F:652:GLU:OE2	2.54	0.41
2:J:552:ASP:HB2	2:J:691:ALA:HB2	2.02	0.41
2:N:24:LEU:HD12	2:N:24:LEU:HA	1.90	0.41
2:N:392:LYS:HD3	2:N:392:LYS:O	2.21	0.41
2:N:402:LEU:HG	2:N:439:MET:HE1	2.03	0.41
2:N:461:LYS:HG2	2:N:482:ILE:HG21	2.03	0.41
2:N:569:ASP:OD1	2:N:572:GLY:N	2.45	0.41
2:N:577:LYS:HD3	2:N:577:LYS:HA	1.79	0.41
2:N:617:ALA:O	2:N:620:TRP:N	2.54	0.41
2:B:14:ILE:O	2:B:37:LEU:HD12	2.21	0.41
2:F:767:SER:O	2:F:767:SER:OG	2.38	0.41
2:J:500:THR:O	2:J:504:GLU:HG3	2.21	0.41
2:J:829:ARG:HG2	2:J:876:LEU:HA	2.04	0.41
2:N:461:LYS:HD2	2:N:479:ILE:HD12	2.02	0.41
2:N:482:ILE:HD13	2:N:482:ILE:HA	1.93	0.41
2:B:264:ILE:HG13	2:B:292:ARG:HB2	2.03	0.40
2:F:563:PRO:HD3	2:F:874:ASP:HB3	2.03	0.40
2:F:677:MET:HG3	2:F:681:ILE:HD11	2.03	0.40
2:J:876:LEU:HD12	2:J:876:LEU:H	1.84	0.40
2:N:552:ASP:OD2	2:N:554:VAL:HG22	2.21	0.40
2:N:743:ILE:H	2:N:743:ILE:HG13	1.65	0.40
2:B:347:CYS:HA	2:B:348:PRO:HD3	1.93	0.40
2:F:247:ALA:HB3	2:F:250:TYR:HD1	1.86	0.40
2:F:313:MET:HE1	2:F:734:PRO:HD3	2.03	0.40
2:F:549:MET:HE3	2:F:842:LEU:HG	2.03	0.40
2:J:574:VAL:HG13	2:J:684:SER:HB2	2.02	0.40
2:N:553:GLU:OE2	2:N:869:ASN:N	2.52	0.40
2:B:190:MET:HE2	2:B:195:LEU:HD12	2.02	0.40
2:J:11:PHE:HB3	2:J:41:HIS:CE1	2.55	0.40
2:J:15:GLU:O	2:J:37:LEU:HD12	2.20	0.40
2:J:557:ARG:HG2	2:J:562:LEU:CD1	2.52	0.40
2:N:71:LYS:HA	2:N:74:ILE:HG12	2.04	0.40
2:B:88:TRP:HZ2	2:B:215:ARG:HE	1.70	0.40
2:B:137:VAL:HG23	2:B:217:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:472:LYS:HD3	2:F:472:LYS:HA	1.73	0.40
2:J:578:VAL:HG13	2:J:680:LEU:HD23	2.02	0.40
2:J:727:TRP:HB3	2:J:845:PHE:CD1	2.57	0.40
2:N:6:ILE:HD11	2:N:259:GLY:C	2.47	0.40
2:F:303:LYS:HE2	2:F:303:LYS:HB2	1.81	0.40
2:J:24:LEU:HD23	2:J:24:LEU:HA	1.79	0.40
2:N:647:ARG:HG2	2:N:678:ALA:HB3	2.04	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	
2	B	828/883 (94%)	811 (98%)	17 (2%)	0	100	100
2	F	780/883 (88%)	770 (99%)	10 (1%)	0	100	100
2	J	789/883 (89%)	774 (98%)	15 (2%)	0	100	100
2	N	755/883 (86%)	745 (99%)	10 (1%)	0	100	100
All	All	3152/3532 (89%)	3100 (98%)	52 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	
2	B	662/729 (91%)	657 (99%)	5 (1%)	73	90
2	F	542/729 (74%)	530 (98%)	12 (2%)	45	77
2	J	583/729 (80%)	572 (98%)	11 (2%)	50	79
2	N	526/729 (72%)	509 (97%)	17 (3%)	34	68
All	All	2313/2916 (79%)	2268 (98%)	45 (2%)	50	79

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	77	LEU
2	B	294	LEU
2	B	393	SER
2	B	706	LEU
2	B	754	GLN
2	F	189	ASP
2	F	196	LEU
2	F	254	ILE
2	F	342	THR
2	F	388	ASP
2	F	553	GLU
2	F	561	LEU
2	F	647	ARG
2	F	661	SER
2	F	735	VAL
2	F	767	SER
2	F	769	ILE
2	J	3	THR
2	J	333	LYS
2	J	495	SER
2	J	634	VAL
2	J	641	SER
2	J	752	LEU
2	J	795	VAL
2	J	813	SER
2	J	870	LEU
2	J	872	LEU
2	J	879	ASP
2	N	35	GLU
2	N	264	ILE
2	N	289	ASN
2	N	425	ARG
2	N	448	LYS

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Mol	Chain	Res	Type
2	N	471	ASP
2	N	526	LEU
2	N	564	SER
2	N	634	VAL
2	N	701	SER
2	N	704	LYS
2	N	706	LEU
2	N	735	VAL
2	N	743	ILE
2	N	746	ARG
2	N	869	ASN
2	N	879	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	184	GLN
2	B	232	GLN
2	B	289	ASN
2	B	300	HIS
2	B	406	ASN
2	B	499	ASN
2	B	648	GLN
2	F	5	ASN
2	F	176	HIS
2	F	289	ASN
2	F	485	ASN
2	F	488	ASN
2	F	499	ASN
2	F	522	GLN
2	F	619	GLN
2	F	726	HIS
2	F	772	HIS
2	J	404	GLN
2	J	466	ASN
2	J	485	ASN
2	J	488	ASN
2	J	499	ASN
2	J	619	GLN
2	N	27	HIS
2	N	339	ASN
2	N	404	GLN

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Mol	Chain	Res	Type
2	N	406	ASN
2	N	437	ASN
2	N	499	ASN
2	N	737	GLN
2	N	744	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	7/12 (58%)	0	0
3	G	7/12 (58%)	0	0
3	K	7/12 (58%)	0	0
3	O	7/12 (58%)	0	0
All	All	28/48 (58%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 ⓘ

4 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
5	GOL	J	901	-	5,5,5	0.91	0	5,5,5	1.12	1 (20%)
5	GOL	N	901	-	5,5,5	0.91	0	5,5,5	1.11	0
5	GOL	F	901	-	5,5,5	0.86	0	5,5,5	1.11	0
5	GOL	B	901	-	5,5,5	0.95	0	5,5,5	1.06	0

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	GOL	J	901	-	-	2/4/4/4	-
5	GOL	N	901	-	-	0/4/4/4	-
5	GOL	F	901	-	-	0/4/4/4	-
5	GOL	B	901	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	901	GOL	C3-C2-C1	-2.04	104.31	111.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	901	GOL	C1-C2-C3-O3
5	J	901	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	12/18 (66%)	-0.73	0 100 100	49, 60, 153, 172	0
1	E	14/18 (77%)	-0.52	0 100 100	65, 99, 229, 260	0
1	I	11/18 (61%)	-0.45	0 100 100	68, 80, 208, 218	0
1	M	13/18 (72%)	-0.02	0 100 100	85, 108, 198, 228	0
2	B	840/883 (95%)	-0.14	13 (1%) 72 64	40, 69, 134, 191	0
2	F	796/883 (90%)	0.02	19 (2%) 59 50	44, 79, 169, 209	0
2	J	805/883 (91%)	0.20	35 (4%) 40 31	58, 106, 169, 246	0
2	N	773/883 (87%)	0.25	26 (3%) 48 39	72, 118, 192, 258	0
3	C	8/12 (66%)	-0.81	0 100 100	52, 60, 85, 100	0
3	G	8/12 (66%)	-0.89	0 100 100	56, 80, 124, 138	0
3	K	8/12 (66%)	-0.66	0 100 100	77, 96, 122, 152	0
3	O	8/12 (66%)	-0.24	0 100 100	90, 113, 177, 193	0
4	H	6/9 (66%)	0.06	0 100 100	199, 205, 233, 253	0
4	P	5/9 (55%)	0.26	0 100 100	203, 206, 221, 252	0
All	All	3307/3670 (90%)	0.07	93 (2%) 55 46	40, 96, 175, 260	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	883	ALA	6.2
2	J	752	LEU	4.6
2	F	113	ALA	4.3
2	N	667	PHE	4.0
2	N	753	GLY	4.0
2	J	748	ASN	3.8
2	J	625	VAL	3.8
2	N	620	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
2	J	687	VAL	3.6
2	F	20	PRO	3.2
2	F	883	ALA	3.2
2	B	752	LEU	3.2
2	J	536	PHE	3.2
2	F	536	PHE	3.1
2	N	135	GLN	3.1
2	N	172	LYS	3.1
2	J	10	ASP	3.0
2	N	616	LEU	2.9
2	B	238	GLY	2.9
2	F	162	PHE	2.9
2	F	146	GLU	2.8
2	J	731	ASP	2.8
2	J	15	GLU	2.8
2	N	173	ARG	2.8
2	J	883	ALA	2.8
2	F	747	LEU	2.8
2	J	671	ASN	2.8
2	J	21	PHE	2.7
2	N	664	GLY	2.7
2	F	159	ALA	2.7
2	F	196	LEU	2.7
2	N	14	ILE	2.7
2	N	875	ILE	2.7
2	J	140	ALA	2.7
2	J	825	PHE	2.7
2	J	767	SER	2.7
2	J	570	ILE	2.7
2	B	596	THR	2.7
2	J	64	VAL	2.6
2	J	606	SER	2.6
2	N	216	CYS	2.6
2	F	156	ASP	2.6
2	N	95	LYS	2.6
2	J	159	ALA	2.6
2	N	536	PHE	2.6
2	N	851	ASP	2.5
2	B	159	ALA	2.5
2	B	883	ALA	2.5
2	N	125	CYS	2.5
2	N	747	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	155	ARG	2.4
2	J	541	SER	2.4
2	J	857	GLN	2.4
2	J	227	VAL	2.4
2	J	642	LYS	2.4
2	B	7	ALA	2.4
2	N	163	LYS	2.3
2	B	536	PHE	2.3
2	N	811	HIS	2.3
2	J	747	LEU	2.3
2	B	195	LEU	2.3
2	B	743	ILE	2.3
2	J	19	ILE	2.3
2	J	629	VAL	2.3
2	J	14	ILE	2.2
2	N	164	LYS	2.2
2	B	598	THR	2.2
2	N	767	SER	2.2
2	J	7	ALA	2.2
2	N	246	LEU	2.2
2	N	655	ILE	2.2
2	N	227	VAL	2.2
2	F	78	LEU	2.1
2	F	882	PHE	2.1
2	F	767	SER	2.1
2	B	226	MET	2.1
2	F	750	MET	2.1
2	F	63	GLU	2.1
2	N	640	GLY	2.1
2	B	133	THR	2.1
2	J	754	GLN	2.1
2	J	697	ASN	2.1
2	B	377	TRP	2.1
2	J	811	HIS	2.0
2	F	751	PHE	2.0
2	J	538	GLY	2.0
2	N	377	TRP	2.0
2	F	223	SER	2.0
2	J	128	SER	2.0
2	J	686	SER	2.0
2	F	749	LEU	2.0
2	J	665	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	J	577	LYS	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
5	GOL	J	901	6/6	0.85	0.10	86,93,105,109	0
5	GOL	N	901	6/6	0.90	0.11	86,98,101,102	0
5	GOL	B	901	6/6	0.92	0.14	52,61,68,87	0
5	GOL	F	901	6/6	0.93	0.09	66,75,81,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.