



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 13, 2026 – 08:21 PM EDT

PDB ID : 8DH3 / pdb_00008dh3
Title : T7 RNA polymerase elongation complex with unnatural base dPa
Authors : Oh, J.; Wang, D.
Deposited on : 2022-06-24
Resolution : 3.00 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

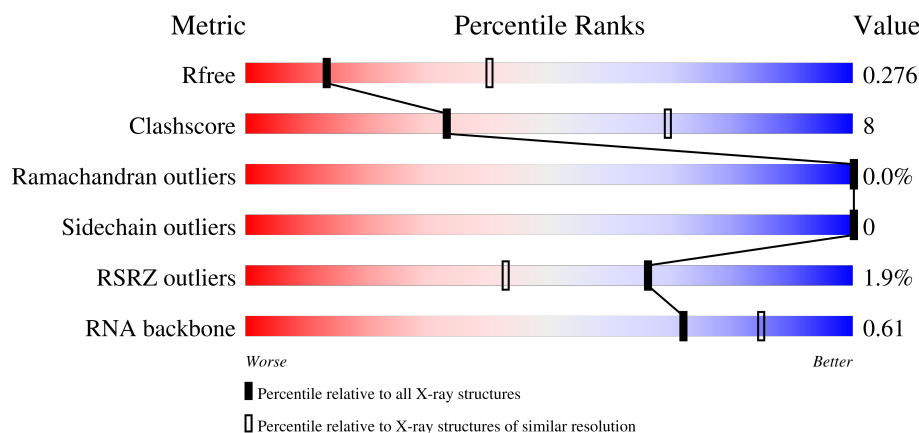
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



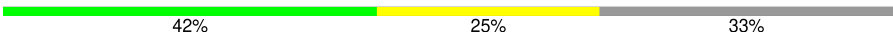
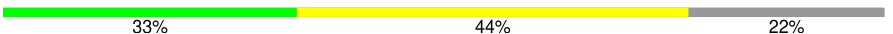
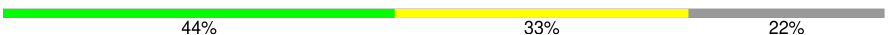
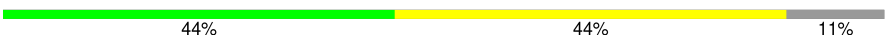
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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

Mol	Chain	Length	Quality of chain
1	B	883	79% 18% .
1	E	883	77% 17% 7%
1	I	883	3% 73% 21% 6%
1	M	883	2% 69% 18% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	A	18	
2	F	18	
2	J	18	
2	N	18	
3	C	12	
3	G	12	
3	K	12	
3	O	12	
4	D	9	
4	H	9	
4	L	9	
4	P	9	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28298 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 T7 RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	856	Total	C	N	O	S	0	0	0
			6728	4284	1169	1239	36			
1	E	825	Total	C	N	O	S	0	0	0
			6472	4130	1119	1189	34			
1	I	831	Total	C	N	O	S	0	0	0
			6530	4163	1142	1190	35			
1	M	775	Total	C	N	O	S	0	0	0
			5912	3755	1037	1088	32			

- Molecule 2 is a DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	16	Total	C	N	O	P	0	0	0
			325	155	60	94	16			
2	F	17	Total	C	N	O	P	0	0	0
			344	165	65	98	16			
2	J	16	Total	C	N	O	P	0	0	0
			325	155	60	94	16			
2	N	17	Total	C	N	O	P	0	0	0
			344	165	65	98	16			

- Molecule 3 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	P	0	0	0
			194	86	35	64	9			
3	G	8	Total	C	N	O	P	0	0	0
			174	77	33	56	8			
3	K	8	Total	C	N	O	P	0	0	0
			174	77	33	56	8			
3	O	8	Total	C	N	O	P	0	0	0
			174	77	33	56	8			

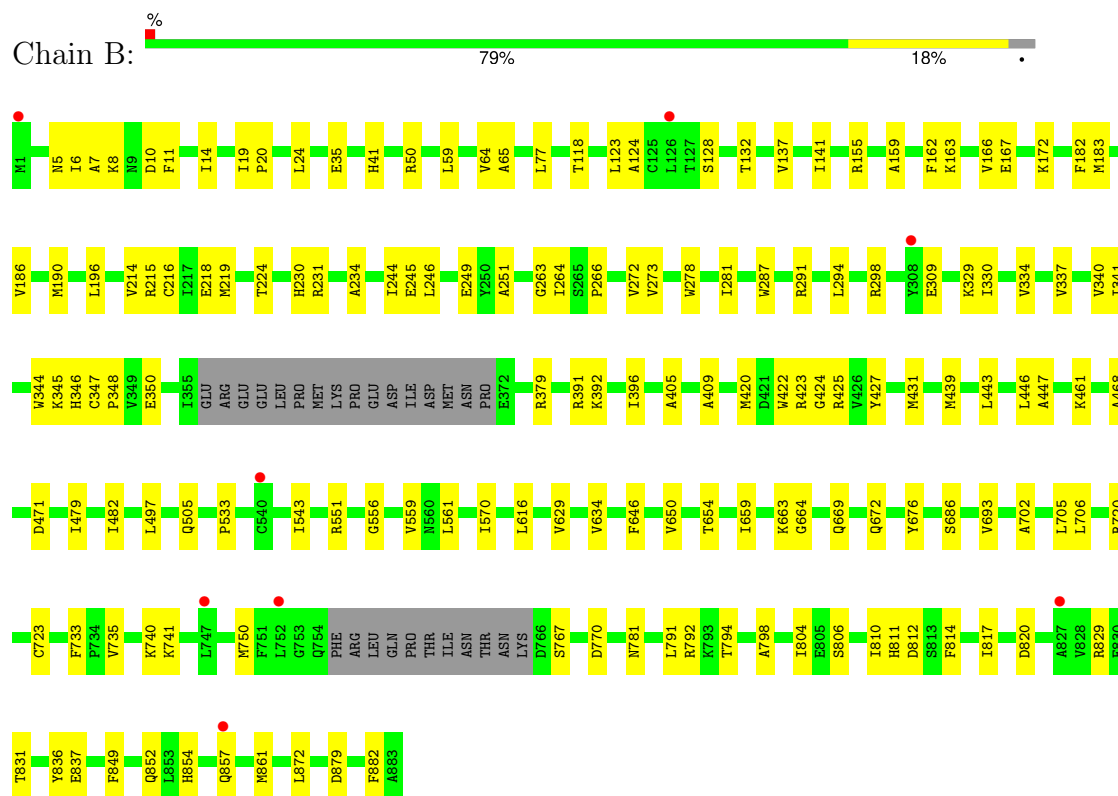
- Molecule 4 is a DNA chain called Non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	7	Total	C	N	O	P	0	0	0
			141	68	22	44	7			
4	H	8	Total	C	N	O	P	0	0	0
			160	77	25	50	8			
4	L	7	Total	C	N	O	P	0	0	0
			141	68	22	44	7			
4	P	8	Total	C	N	O	P	0	0	0
			160	77	25	50	8			

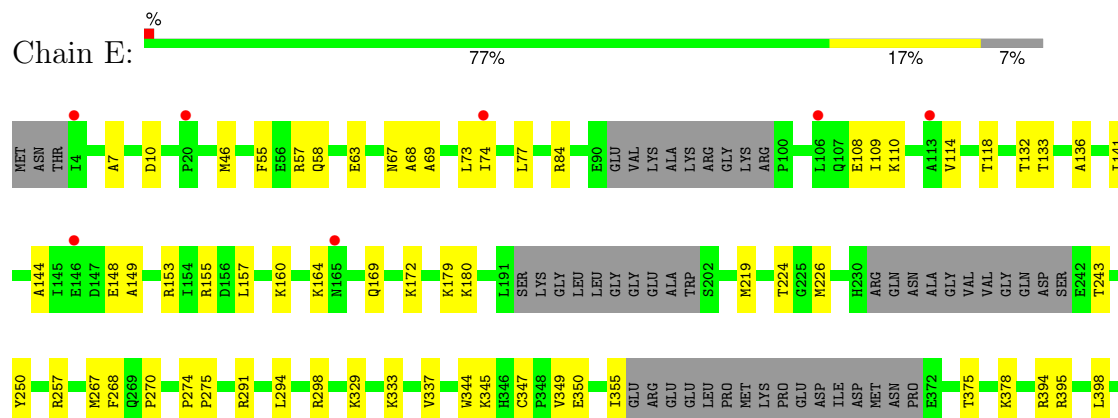
3 Residue-property plots [i](#)

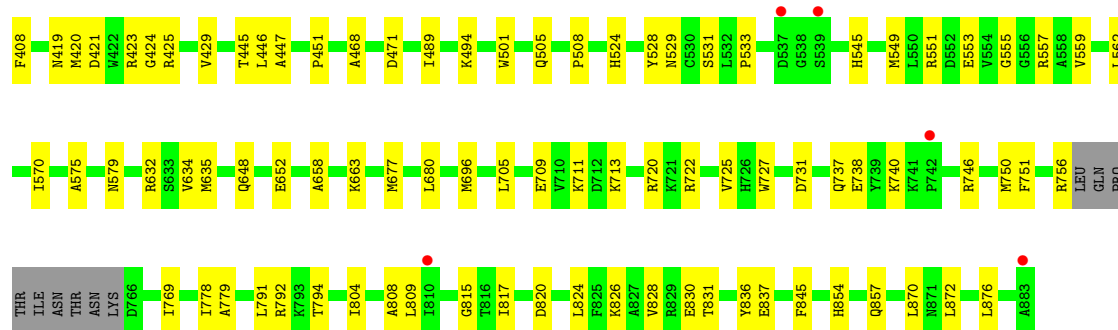
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: T7 RNA polymerase

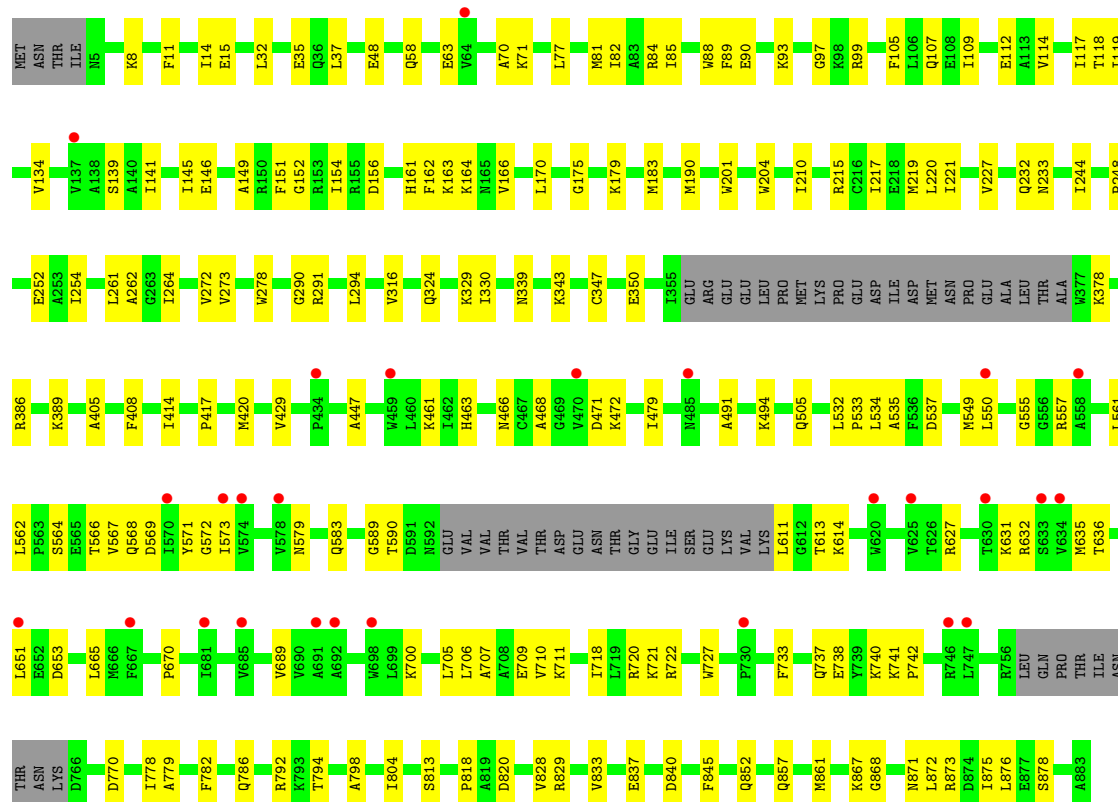


• Molecule 1: T7 RNA polymerase

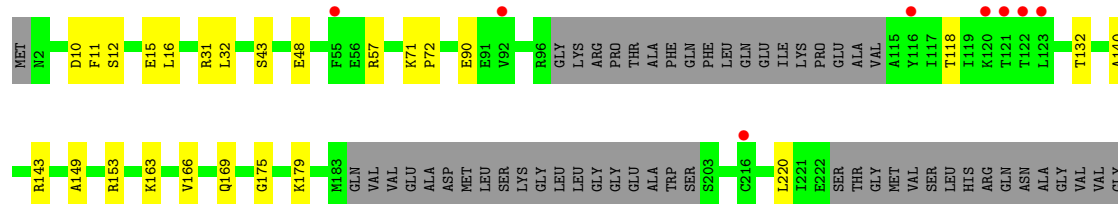


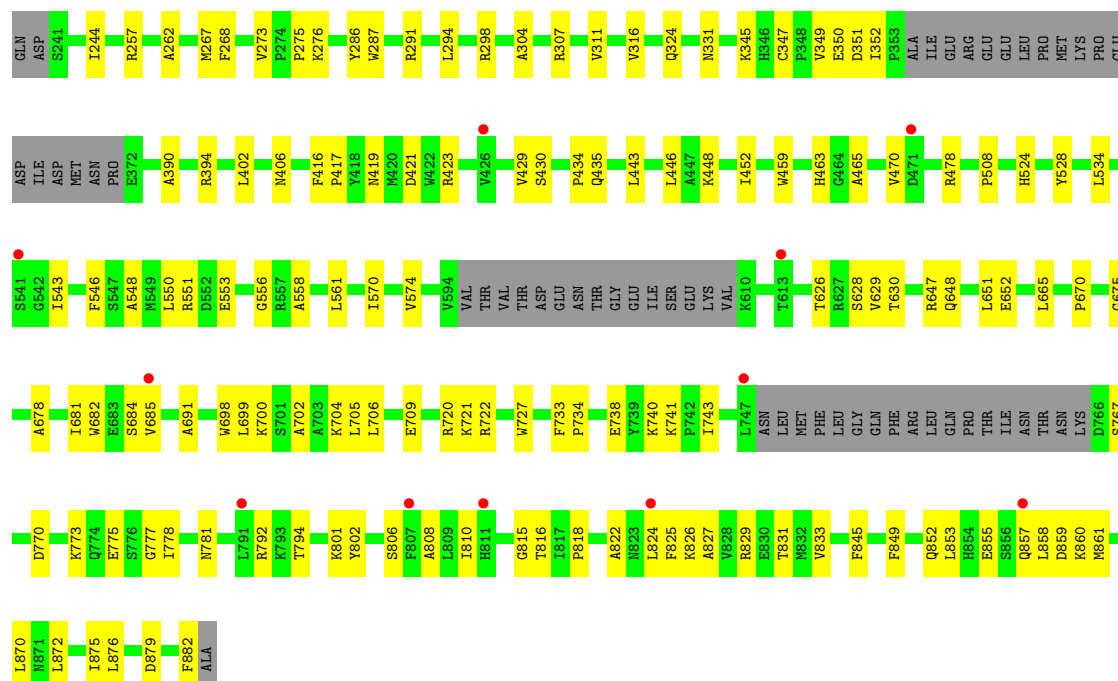


• Molecule 1: T7 RNA polymerase



• Molecule 1: T7 RNA polymerase





- Molecule 2: Template strand DNA

Chain A: 78% 11% 11%



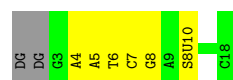
- Molecule 2: Template strand DNA

Chain F: 72% 22% 6%



- Molecule 2: Template strand DNA

Chain J: 56% 33% 11%



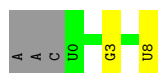
- Molecule 2: Template strand DNA

Chain N: 78% 17% 6%



- Molecule 3: RNA

Chain C:  58% 17% 25%

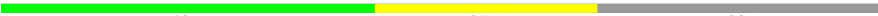


• Molecule 3: RNA

Chain G:  67% 33%



• Molecule 3: RNA

Chain K:  42% 25% 33%

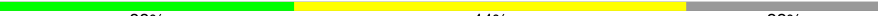


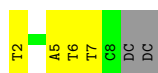
• Molecule 3: RNA

Chain O:  50% 17% 33%



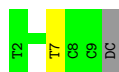
• Molecule 4: Non-template strand DNA

Chain D:  33% 44% 22%



• Molecule 4: Non-template strand DNA

Chain H:  78% 11% 11%



• Molecule 4: Non-template strand DNA

Chain L:  44% 33% 22%



• Molecule 4: Non-template strand DNA

Chain P:  44% 44% 11%

T2	A5	T6	T7	C8	C9	DC
----	----	----	----	----	----	----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.07Å 86.27Å 201.97Å 89.70° 86.01° 69.45°	Depositor
Resolution (Å)	47.98 – 3.00 47.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.98-3.00) 98.3 (47.98-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.19	Depositor
R, R_{free}	0.247 , 0.276 0.247 , 0.276	Depositor DCC
R_{free} test set	1994 reflections (1.86%)	wwPDB-VP
Wilson B-factor (Å ²)	90.7	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 103.7	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	0.93	EDS
Total number of atoms	28298	wwPDB-VP
Average B, all atoms (Å ²)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: S8U

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	B	0.14	0/6878	0.35	0/9304
1	E	0.14	0/6617	0.36	0/8952
1	I	0.15	0/6679	0.37	0/9030
1	M	0.15	0/6039	0.37	0/8181
2	A	0.20	0/343	0.39	0/524
2	F	0.16	0/365	0.34	0/559
2	J	0.16	0/343	0.34	0/524
2	N	0.17	0/365	0.38	0/559
3	C	0.09	0/216	0.22	0/335
3	G	0.09	0/194	0.21	0/301
3	K	0.09	0/194	0.21	0/301
3	O	0.10	0/194	0.24	0/301
4	D	0.20	0/156	0.46	0/238
4	H	0.17	0/177	0.42	0/270
4	L	0.19	0/156	0.43	0/238
4	P	0.19	0/177	0.44	0/270
All	All	0.15	0/29093	0.36	0/39887

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6728	0	6694	100	0
1	E	6472	0	6402	100	0
1	I	6530	0	6480	117	0
1	M	5912	0	5684	97	1
2	A	325	0	168	1	0
2	F	344	0	180	3	0
2	J	325	0	168	3	0
2	N	344	0	180	2	0
3	C	194	0	98	2	0
3	G	174	0	88	0	0
3	K	174	0	88	3	0
3	O	174	0	88	0	0
4	D	141	0	81	3	0
4	H	160	0	92	1	0
4	L	141	0	81	4	0
4	P	160	0	92	3	0
All	All	28298	0	26664	426	1

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 8.

All (426) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:347:CYS:CB	1:E:350:GLU:HG3	1.80	1.12
1:E:347:CYS:HB3	1:E:350:GLU:HG3	1.28	1.11
1:E:347:CYS:SG	1:E:350:GLU:HG3	2.03	0.96
1:E:179:LYS:NZ	1:E:750:MET:SD	2.50	0.85
1:B:35:GLU:HG2	1:B:272:VAL:HG21	1.66	0.77
1:M:705:LEU:HD13	1:M:857:GLN:HB3	1.66	0.77
1:I:589:GLY:HA3	1:I:614:LYS:HB3	1.66	0.77
1:E:347:CYS:HB3	1:E:350:GLU:CG	2.11	0.76
1:E:837:GLU:HG3	1:E:872:LEU:HD12	1.67	0.75
1:I:118:THR:HA	1:I:141:ILE:HD12	1.69	0.75
1:M:435:GLN:HB3	1:M:810:ILE:HD13	1.70	0.73
1:B:50:ARG:HH12	1:B:431:MET:HE1	1.54	0.72
1:I:347:CYS:HB2	1:I:350:GLU:HB2	1.71	0.70
1:E:148:GLU:HA	1:E:750:MET:HE3	1.74	0.70
1:M:72:PRO:HG3	1:M:257:ARG:HE	1.57	0.69
1:E:347:CYS:SG	1:E:350:GLU:CG	2.80	0.69
1:I:700:LYS:NZ	4:L:5:DA:OP1	2.28	0.66
1:M:32:LEU:HB3	1:M:273:VAL:HG12	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:571:TYR:HB2	1:I:627:ARG:HG3	1.77	0.66
1:B:172:LYS:HD2	3:C:3:G:H5''	1.77	0.66
1:M:316:VAL:HG21	1:M:733:PHE:HB2	1.77	0.66
1:E:84:ARG:HG3	1:E:219:MET:HE2	1.77	0.66
1:M:478:ARG:HH12	1:M:882:PHE:HZ	1.44	0.66
1:I:386:ARG:NH2	3:K:4:G:OP1	2.29	0.65
1:I:134:VAL:HG22	1:I:244:ILE:HG12	1.77	0.65
1:B:159:ALA:HB1	1:B:162:PHE:HB3	1.78	0.65
1:M:705:LEU:O	1:M:720:ARG:NH2	2.31	0.65
1:I:316:VAL:HG11	1:I:733:PHE:HB2	1.79	0.64
1:I:738:GLU:HG2	1:I:740:LYS:HD3	1.77	0.64
1:B:837:GLU:HG3	1:B:872:LEU:HD12	1.79	0.64
1:I:420:MET:HE1	1:I:792:ARG:HD3	1.80	0.63
1:M:647:ARG:HD2	1:M:675:GLY:HA2	1.80	0.63
1:B:10:ASP:HB3	1:B:291:ARG:HE	1.63	0.63
1:M:57:ARG:HH12	2:N:17:DG:H5''	1.62	0.63
1:E:468:ALA:HA	1:E:505:GLN:HB3	1.79	0.63
1:I:857:GLN:N	1:I:857:GLN:OE1	2.31	0.63
1:B:345:LYS:NZ	1:E:344:TRP:O	2.28	0.63
1:E:421:ASP:OD2	1:E:423:ARG:NH1	2.31	0.63
1:E:830:GLU:HG3	1:E:876:LEU:HD21	1.81	0.62
1:M:720:ARG:NH1	1:M:852:GLN:O	2.32	0.62
1:E:791:LEU:HD11	1:E:809:LEU:HB3	1.81	0.62
1:I:118:THR:HG22	1:I:141:ILE:HD11	1.82	0.61
1:E:746:ARG:HH22	1:E:756:ARG:HB2	1.66	0.61
1:E:46:MET:HB3	1:E:267:MET:HE2	1.82	0.61
1:M:833:VAL:HG23	1:M:872:LEU:HB3	1.82	0.61
1:B:19:ILE:HG23	1:B:20:PRO:HD3	1.82	0.61
1:B:854:HIS:HB3	1:B:857:GLN:HG3	1.82	0.61
1:I:15:GLU:HB2	1:I:37:LEU:HD23	1.82	0.61
1:B:155:ARG:HB2	1:B:163:LYS:HE3	1.83	0.61
1:E:722:ARG:HD3	1:E:769:ILE:HG12	1.83	0.61
1:M:347:CYS:HB3	1:M:350:GLU:HB2	1.83	0.60
1:M:574:VAL:HG23	1:M:684:SER:HB3	1.83	0.60
1:I:590:THR:HG22	1:I:613:THR:H	1.66	0.60
1:M:720:ARG:HH12	1:M:853:LEU:HA	1.67	0.60
1:B:425:ARG:NH2	3:C:8:U:O2'	2.35	0.59
1:B:159:ALA:O	1:B:163:LYS:N	2.33	0.59
1:B:24:LEU:HD11	1:B:273:VAL:HG21	1.84	0.59
1:B:669:GLN:OE1	1:B:672:GLN:NE2	2.36	0.59
1:B:379:ARG:HH12	1:B:659:ILE:HD11	1.68	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:THR:HG22	1:E:141:ILE:HD11	1.84	0.59
1:E:575:ALA:O	1:E:579:ASN:ND2	2.34	0.59
1:I:829:ARG:NH2	1:I:878:SER:O	2.36	0.58
1:M:704:LYS:NZ	1:M:775:GLU:OE1	2.35	0.58
1:M:738:GLU:HG2	1:M:740:LYS:HD3	1.84	0.58
1:B:215:ARG:NH1	1:B:218:GLU:OE1	2.37	0.58
1:B:706:LEU:HD21	1:B:849:PHE:HB2	1.86	0.58
1:E:10:ASP:HB2	1:E:291:ARG:HE	1.69	0.57
1:M:12:SER:HA	1:M:15:GLU:HG2	1.86	0.57
1:M:11:PHE:HD2	1:M:291:ARG:HH21	1.53	0.57
1:B:298:ARG:HH21	1:B:427:TYR:HB2	1.70	0.57
1:B:163:LYS:HA	1:B:166:VAL:HG22	1.86	0.57
1:B:817:ILE:HG13	1:B:820:ASP:HB2	1.87	0.57
1:I:798:ALA:HB1	1:I:804:ILE:HD12	1.86	0.57
1:I:706:LEU:O	1:I:720:ARG:NH2	2.38	0.56
1:B:810:ILE:O	1:B:812:ASP:N	2.38	0.56
1:E:108:GLU:HG3	1:E:109:ILE:HD12	1.86	0.56
1:E:298:ARG:HH21	1:E:419:ASN:HB3	1.70	0.56
1:I:220:LEU:HB3	1:I:227:VAL:HG21	1.86	0.56
1:I:278:TRP:HD1	1:I:324:GLN:HE22	1.52	0.56
1:B:329:LYS:HG2	1:B:447:ALA:HA	1.87	0.56
1:M:276:LYS:HE3	1:M:287:TRP:HA	1.86	0.56
1:B:77:LEU:HG	1:B:224:THR:HG21	1.88	0.56
1:I:294:LEU:HD21	1:I:429:VAL:HG11	1.87	0.56
1:M:118:THR:HB	1:M:220:LEU:HD11	1.87	0.56
1:E:791:LEU:HD21	1:E:809:LEU:HD13	1.88	0.56
1:E:375:THR:HA	1:E:378:LYS:HE3	1.87	0.56
1:E:524:HIS:HB2	1:E:528:TYR:HB2	1.87	0.56
1:I:389:LYS:HD2	3:K:4:G:H4'	1.88	0.55
1:I:35:GLU:HG2	1:I:272:VAL:HG21	1.87	0.55
1:I:837:GLU:HG3	1:I:872:LEU:HD12	1.88	0.55
1:M:550:LEU:HD22	1:M:691:ALA:HA	1.88	0.55
1:M:741:LYS:HB3	1:M:770:ASP:HB2	1.88	0.55
1:B:705:LEU:HD13	1:B:857:GLN:HB3	1.87	0.55
1:M:345:LYS:NZ	1:M:351:ASP:O	2.40	0.55
1:B:345:LYS:HD3	1:B:348:PRO:HA	1.89	0.55
1:I:564:SER:OG	1:I:566:THR:O	2.24	0.55
1:I:631:LYS:HG2	1:I:635:MET:HE2	1.89	0.55
1:I:561:LEU:HD22	1:I:875:ILE:HG12	1.86	0.55
1:M:802:TYR:HE2	1:M:827:ALA:HB2	1.72	0.55
1:B:334:VAL:HG23	1:B:443:LEU:HD23	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:224:THR:HG22	1:E:226:MET:H	1.73	0.54
1:I:77:LEU:HD21	1:I:119:ILE:HG12	1.87	0.54
1:I:162:PHE:HD1	1:I:190:MET:HE2	1.73	0.54
4:L:5:DA:H2''	4:L:6:DT:H5'	1.89	0.54
1:B:741:LYS:HB3	1:B:770:ASP:HB2	1.88	0.54
1:I:491:ALA:HA	1:I:494:LYS:HD2	1.90	0.54
1:B:64:VAL:HB	1:B:123:LEU:HD13	1.89	0.54
1:E:74:ILE:HA	1:E:77:LEU:HB2	1.89	0.54
1:B:468:ALA:HA	1:B:505:GLN:HG3	1.89	0.54
1:B:798:ALA:HB1	1:B:804:ILE:HD12	1.90	0.54
1:I:632:ARG:HH21	1:I:653:ASP:HB3	1.73	0.54
1:I:468:ALA:HA	1:I:505:GLN:HB3	1.88	0.53
1:M:698:TRP:HE3	1:M:699:LEU:HD12	1.73	0.53
1:I:710:VAL:HG21	1:I:857:GLN:HE21	1.73	0.53
1:B:733:PHE:HB2	1:B:792:ARG:HH12	1.72	0.53
1:I:232:GLN:HG3	1:I:233:ASN:HD22	1.73	0.53
1:I:161:HIS:HA	1:I:164:LYS:HD2	1.90	0.53
1:E:132:THR:HB	1:E:243:THR:HB	1.91	0.53
1:I:93:LYS:HA	1:I:99:ARG:HE	1.73	0.53
1:I:58:GLN:NE2	1:I:63:GLU:O	2.41	0.52
1:I:741:LYS:HB3	1:I:770:ASP:HB2	1.92	0.52
1:B:59:LEU:HD12	1:B:64:VAL:HG22	1.91	0.52
1:M:794:THR:HA	1:M:831:THR:HG21	1.90	0.52
1:M:702:ALA:HA	1:M:861:MET:HE1	1.91	0.52
1:B:461:LYS:HG2	1:B:482:ILE:HG21	1.91	0.52
1:B:720:ARG:HD3	1:B:854:HIS:HB2	1.90	0.52
1:I:557:ARG:HG2	1:I:562:LEU:HD13	1.91	0.52
1:I:114:VAL:O	1:I:118:THR:HG23	2.09	0.52
1:E:705:LEU:HD13	1:E:857:GLN:HB3	1.91	0.52
1:E:713:LYS:NZ	2:F:2:DG:N7	2.57	0.52
2:J:5:DA:H1'	2:J:6:DT:H5'	1.92	0.51
1:I:532:LEU:HD12	1:I:533:PRO:HD2	1.92	0.51
1:M:855:GLU:HA	1:M:858:LEU:HD23	1.92	0.51
1:E:709:GLU:OE1	1:E:711:LYS:NZ	2.41	0.51
1:M:524:HIS:HB2	1:M:528:TYR:HB2	1.92	0.51
1:I:11:PHE:HA	1:I:14:ILE:HG12	1.91	0.51
1:I:324:GLN:HG2	1:I:417:PRO:HA	1.91	0.51
1:I:718:ILE:HD13	1:I:721:LYS:HD3	1.93	0.51
1:E:738:GLU:HG2	1:E:740:LYS:HD3	1.92	0.51
1:M:421:ASP:OD1	1:M:423:ARG:NH1	2.32	0.51
1:M:709:GLU:HB3	1:M:722:ARG:HG2	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:ALA:O	1:E:257:ARG:NH2	2.43	0.51
1:I:97:GLY:O	1:I:99:ARG:NH1	2.44	0.51
1:M:720:ARG:HD2	1:M:721:LYS:O	2.11	0.51
1:B:246:LEU:HD22	1:B:251:ALA:HB2	1.92	0.51
1:B:420:MET:HE3	1:B:424:GLY:HA2	1.93	0.51
1:E:109:ILE:HD11	1:E:149:ALA:HB2	1.92	0.51
1:B:471:ASP:N	1:B:471:ASP:OD2	2.44	0.50
1:B:5:ASN:HB3	1:B:8:LYS:HE3	1.92	0.50
1:E:148:GLU:OE2	1:E:155:ARG:NH1	2.42	0.50
1:E:794:THR:HG21	1:E:828:VAL:HG22	1.93	0.50
1:M:682:TRP:HA	1:M:685:VAL:HG22	1.93	0.50
1:M:402:LEU:O	1:M:406:ASN:ND2	2.44	0.50
1:M:459:TRP:HE1	1:M:822:ALA:HB2	1.76	0.50
1:E:57:ARG:HH22	2:F:17:DG:H5"	1.76	0.50
1:I:408:PHE:HB3	1:I:414:ILE:HG21	1.92	0.50
1:M:294:LEU:HD21	1:M:429:VAL:HG21	1.93	0.50
1:M:311:VAL:HG11	1:M:734:PRO:HG3	1.93	0.50
1:B:347:CYS:HB3	1:B:350:GLU:HB3	1.94	0.50
1:E:329:LYS:HG2	1:E:447:ALA:HA	1.93	0.50
1:E:808:ALA:HB3	1:E:815:GLY:HA3	1.93	0.50
1:I:32:LEU:HB3	1:I:273:VAL:HG12	1.94	0.50
1:I:217:ILE:HA	1:I:220:LEU:HB2	1.94	0.50
1:I:651:LEU:HD11	1:I:670:PRO:HB3	1.94	0.50
1:E:7:ALA:O	1:E:291:ARG:NH2	2.44	0.50
1:M:169:GLN:OE1	1:M:169:GLN:N	2.43	0.50
1:B:446:LEU:HG	1:B:533:PRO:HG3	1.93	0.50
1:I:707:ALA:O	1:I:722:ARG:NE	2.37	0.50
1:M:140:ALA:HA	1:M:143:ARG:HH11	1.77	0.50
1:M:465:ALA:HB1	1:M:470:VAL:HB	1.93	0.50
1:B:132:THR:OG1	1:B:244:ILE:O	2.30	0.49
1:E:160:LYS:O	1:E:164:LYS:N	2.39	0.49
1:M:561:LEU:HB3	1:M:875:ILE:HG13	1.94	0.49
1:B:741:LYS:O	1:B:767:SER:OG	2.28	0.49
1:I:466:ASN:HA	1:I:471:ASP:HB3	1.93	0.49
1:E:55:PHE:HA	1:E:58:GLN:NE2	2.28	0.49
1:M:665:LEU:H	1:M:665:LEU:HD23	1.77	0.49
1:B:163:LYS:O	1:B:167:GLU:N	2.45	0.49
1:B:124:ALA:O	1:B:128:SER:OG	2.30	0.49
1:I:555:GLY:HA2	1:I:689:VAL:HG22	1.95	0.49
1:B:10:ASP:O	1:B:291:ARG:NH2	2.39	0.49
1:M:268:PHE:HB3	1:M:430:SER:HA	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:LEU:HD21	1:E:250:TYR:HD1	1.78	0.48
1:E:144:ALA:HB1	1:E:751:PHE:HZ	1.76	0.48
1:I:88:TRP:CD1	1:I:215:ARG:HH21	2.31	0.48
1:B:791:LEU:HA	1:B:814:PHE:HE2	1.79	0.48
1:I:14:ILE:HD12	1:I:290:GLY:HA2	1.95	0.48
1:I:70:ALA:HA	1:I:254:ILE:HG22	1.95	0.48
1:I:109:ILE:HD11	1:I:149:ALA:HA	1.94	0.48
1:E:826:LYS:NZ	1:E:876:LEU:O	2.46	0.48
1:E:570:ILE:HG12	1:E:634:VAL:HG11	1.96	0.48
1:M:12:SER:O	1:M:16:LEU:HD13	2.13	0.48
1:B:543:ILE:HB	1:B:559:VAL:HG11	1.96	0.48
1:I:170:LEU:HD13	1:I:183:MET:HE3	1.96	0.48
1:E:632:ARG:HA	1:E:635:MET:HE2	1.94	0.48
1:E:804:ILE:HG12	1:E:820:ASP:HB3	1.94	0.48
1:M:826:LYS:NZ	1:M:876:LEU:O	2.46	0.48
1:B:570:ILE:HG12	1:B:634:VAL:HG11	1.96	0.48
1:I:278:TRP:CD1	1:I:324:GLN:HE22	2.30	0.48
1:M:777:GLY:O	1:M:781:ASN:ND2	2.46	0.47
1:B:231:ARG:HG2	1:B:234:ALA:HB2	1.96	0.47
1:E:69:ALA:HA	1:E:257:ARG:HE	1.79	0.47
1:I:778:ILE:HD12	1:I:779:ALA:N	2.29	0.47
1:B:423:ARG:NH1	1:B:781:ASN:OD1	2.43	0.47
1:I:537:ASP:OD2	1:I:537:ASP:N	2.45	0.47
1:M:626:THR:HB	1:M:629:VAL:HG13	1.97	0.47
1:E:329:LYS:HG3	1:E:445:THR:HG23	1.96	0.47
1:B:6:ILE:HD13	1:B:263:GLY:HA3	1.95	0.47
1:E:349:VAL:HG11	1:E:508:PRO:HG3	1.96	0.47
1:I:8:LYS:HA	1:I:8:LYS:HD3	1.62	0.47
1:M:829:ARG:HH22	1:M:882:PHE:H	1.61	0.47
1:I:632:ARG:O	1:I:636:THR:OG1	2.23	0.47
1:I:665:LEU:HD23	1:I:665:LEU:H	1.79	0.47
1:I:741:LYS:NZ	1:I:742:PRO:O	2.47	0.47
1:I:794:THR:HG22	1:I:828:VAL:HA	1.96	0.47
1:I:840:ASP:OD2	1:I:867:LYS:NZ	2.47	0.47
1:I:90:GLU:HA	1:I:93:LYS:HG2	1.96	0.47
1:M:463:HIS:HB2	1:M:534:LEU:HG	1.97	0.47
1:M:558:ALA:HB1	1:M:570:ILE:HD13	1.97	0.47
1:M:574:VAL:HG13	1:M:630:THR:HG21	1.97	0.47
4:P:5:DA:H2''	4:P:6:DT:H2'	1.97	0.47
1:B:720:ARG:HH12	1:B:723:CYS:HB2	1.80	0.46
1:I:215:ARG:HG3	1:I:219:MET:HE2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:550:LEU:O	1:I:868:GLY:N	2.48	0.46
1:M:570:ILE:O	1:M:574:VAL:HG12	2.15	0.46
1:B:337:VAL:O	1:B:341:ILE:HG12	2.16	0.46
1:E:419:ASN:HB2	1:E:429:VAL:HG22	1.96	0.46
1:E:424:GLY:O	1:E:792:ARG:NH1	2.48	0.46
1:I:84:ARG:HG3	1:I:219:MET:HG2	1.97	0.46
1:M:543:ILE:HA	1:M:546:PHE:HB2	1.98	0.46
1:B:190:MET:HE2	1:B:196:LEU:HG	1.97	0.46
1:I:261:LEU:HA	1:I:264:ILE:HG12	1.97	0.46
1:E:494:LYS:HB2	1:E:494:LYS:HE3	1.77	0.46
1:E:531:SER:HA	1:E:817:ILE:HD12	1.98	0.46
1:M:648:GLN:NE2	1:M:652:GLU:OE2	2.41	0.46
1:M:548:ALA:O	1:M:551:ARG:NH1	2.49	0.46
1:M:700:LYS:HB2	1:M:700:LYS:HE3	1.69	0.46
1:E:658:ALA:HB1	1:E:663:LYS:HB3	1.97	0.46
1:M:43:SER:HB3	1:M:267:MET:O	2.15	0.46
1:I:217:ILE:O	1:I:221:ILE:HG13	2.16	0.46
1:B:330:ILE:HD12	1:B:405:ALA:HA	1.98	0.46
1:B:11:PHE:HZ	1:B:263:GLY:HA2	1.81	0.45
1:I:81:MET:HE1	1:I:219:MET:HB3	1.98	0.45
1:M:743:ILE:HD12	1:M:743:ILE:H	1.81	0.45
1:B:14:ILE:HD11	1:B:41:HIS:HA	1.98	0.45
1:B:159:ALA:HB2	1:B:190:MET:HE1	1.98	0.45
1:B:249:GLU:H	1:B:249:GLU:CD	2.24	0.45
4:P:8:DC:H1'	4:P:9:DC:H5'	1.98	0.45
1:E:419:ASN:OD1	1:E:420:MET:N	2.48	0.45
1:E:854:HIS:HB3	1:E:857:GLN:HG3	1.97	0.45
1:B:686:SER:HA	1:B:693:VAL:HG21	1.99	0.45
1:E:731:ASP:OD1	1:E:792:ARG:NE	2.43	0.45
1:E:268:PHE:CZ	1:E:294:LEU:HD21	2.52	0.45
1:I:89:PHE:HE1	1:I:107:GLN:HE22	1.65	0.45
1:I:329:LYS:HG2	1:I:447:ALA:HA	1.98	0.45
1:I:534:LEU:HD13	1:I:818:PRO:HG3	1.99	0.45
1:I:549:MET:HE2	1:I:786:GLN:HG3	1.98	0.45
1:I:569:ASP:OD1	1:I:572:GLY:N	2.47	0.45
1:E:725:VAL:HG23	1:E:737:GLN:HB3	1.98	0.45
1:I:833:VAL:HG11	1:I:876:LEU:HD11	1.99	0.45
1:M:286:TYR:CZ	1:M:417:PRO:HG2	2.51	0.45
1:I:710:VAL:HG21	1:I:857:GLN:NE2	2.30	0.45
1:M:626:THR:HG22	1:M:628:SER:H	1.80	0.45
2:A:6:DT:H3	4:D:5:DA:H61	1.65	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:GLN:HA	1:E:172:LYS:HB2	1.99	0.44
1:E:446:LEU:HG	1:E:533:PRO:HG3	1.99	0.44
1:I:579:ASN:O	1:I:583:GLN:NE2	2.50	0.44
4:D:2:DT:H6	4:D:2:DT:H2'	1.64	0.44
1:B:556:GLY:O	1:B:561:LEU:N	2.47	0.44
1:I:88:TRP:NE1	1:I:215:ARG:HE	2.15	0.44
1:I:139:SER:HB3	1:I:210:ILE:HG12	1.99	0.44
1:E:355:ILE:HD12	1:E:355:ILE:H	1.83	0.44
1:M:149:ALA:O	1:M:153:ARG:HG2	2.17	0.44
1:E:270:PRO:HD2	1:E:408:PHE:HE1	1.81	0.44
1:I:461:LYS:HZ2	1:I:479:ILE:HG23	1.82	0.44
1:M:808:ALA:O	1:M:815:GLY:N	2.50	0.44
1:B:214:VAL:O	1:B:218:GLU:HG3	2.17	0.44
1:I:871:ASN:OD1	1:I:873:ARG:HB2	2.17	0.44
2:N:5:DA:H61	4:P:6:DT:H3	1.66	0.44
1:B:740:LYS:HZ1	1:B:767:SER:H	1.65	0.44
1:E:133:THR:HG22	1:E:136:ALA:H	1.83	0.44
1:M:316:VAL:HG22	1:M:792:ARG:HE	1.83	0.44
1:M:741:LYS:O	1:M:767:SER:HB3	2.18	0.44
1:B:278:TRP:HH2	1:B:294:LEU:HB3	1.83	0.43
1:E:114:VAL:O	1:E:118:THR:HG23	2.17	0.43
1:E:350:GLU:OE1	1:E:394:ARG:NH2	2.51	0.43
1:E:551:ARG:NH2	1:E:836:TYR:O	2.51	0.43
1:B:663:LYS:HG3	1:B:664:GLY:H	1.83	0.43
1:E:545:HIS:O	1:E:549:MET:HG3	2.17	0.43
1:E:557:ARG:CZ	1:E:562:LEU:HD23	2.48	0.43
1:I:804:ILE:HG12	1:I:820:ASP:HB3	2.00	0.43
1:M:720:ARG:NH2	1:M:857:GLN:OE1	2.51	0.43
1:B:59:LEU:O	1:B:128:SER:HB3	2.18	0.43
1:B:166:VAL:HB	1:B:182:PHE:HZ	1.83	0.43
1:B:346:HIS:HB2	1:B:391:ARG:HH21	1.83	0.43
1:B:616:LEU:HD13	1:B:676:TYR:HB2	1.99	0.43
1:E:451:PRO:HA	1:E:529:ASN:HA	2.00	0.43
1:I:48:GLU:HA	1:I:262:ALA:HB1	2.00	0.43
1:I:463:HIS:HB2	1:I:534:LEU:HG	2.01	0.43
1:I:535:ALA:HB1	1:I:813:SER:OG	2.18	0.43
1:B:794:THR:HA	1:B:831:THR:HG21	1.99	0.43
1:M:816:THR:HB	1:M:824:LEU:HD13	2.00	0.43
1:B:551:ARG:NH2	1:B:836:TYR:O	2.51	0.43
1:E:421:ASP:OD1	1:E:424:GLY:N	2.50	0.43
4:L:4:DG:H2''	4:L:5:DA:H8	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:390:ALA:O	1:M:394:ARG:HG3	2.18	0.43
1:B:702:ALA:HB2	1:B:861:MET:HE1	2.00	0.43
1:B:750:MET:HB3	1:B:750:MET:HE3	1.71	0.43
1:E:7:ALA:HB1	1:E:291:ARG:HH22	1.83	0.43
1:I:175:GLY:O	1:I:179:LYS:HG3	2.17	0.43
1:M:678:ALA:HA	1:M:681:ILE:HG12	2.01	0.43
1:B:392:LYS:HE2	1:B:396:ILE:HD13	1.99	0.43
1:E:224:THR:HG21	1:E:226:MET:HE3	2.01	0.43
1:M:773:LYS:HD2	1:M:773:LYS:HA	1.75	0.43
1:B:461:LYS:HE3	1:B:479:ILE:HD12	2.01	0.43
1:I:117:ILE:HG21	1:I:145:ILE:HG13	2.01	0.43
1:I:711:LYS:HB3	1:I:718:ILE:HA	2.00	0.43
1:M:71:LYS:HB2	1:M:71:LYS:HE2	1.77	0.43
1:E:395:ARG:HD2	1:E:398:LEU:HD23	2.01	0.43
1:E:489:ILE:HG13	1:E:501:TRP:HZ3	1.84	0.43
1:I:152:GLY:O	1:I:156:ASP:N	2.47	0.43
1:B:446:LEU:HD22	1:B:806:SER:HB3	2.00	0.42
1:M:48:GLU:HG2	1:M:262:ALA:HB1	2.01	0.42
1:B:350:GLU:OE1	1:B:391:ARG:NH2	2.53	0.42
1:I:857:GLN:O	1:I:861:MET:N	2.52	0.42
1:M:10:ASP:OD2	1:M:11:PHE:N	2.52	0.42
1:M:452:ILE:HG13	1:M:818:PRO:HB2	2.00	0.42
1:B:264:ILE:O	1:B:266:PRO:HD3	2.19	0.42
1:E:153:ARG:O	1:E:157:LEU:N	2.46	0.42
1:I:568:GLN:HB3	1:I:573:ILE:HD11	2.00	0.42
1:I:705:LEU:O	1:I:720:ARG:NH1	2.48	0.42
1:M:446:LEU:HD22	1:M:806:SER:HB3	2.01	0.42
1:B:281:ILE:HD12	1:B:309:GLU:HB3	2.01	0.42
1:B:829:ARG:HH22	1:B:882:PHE:H	1.66	0.42
1:I:81:MET:O	1:I:85:ILE:HG12	2.19	0.42
1:M:132:THR:OG1	1:M:244:ILE:O	2.38	0.42
1:M:163:LYS:HA	1:M:166:VAL:HG22	2.01	0.42
1:E:58:GLN:HB2	1:E:63:GLU:HB2	2.01	0.42
1:E:696:MET:HG2	1:E:779:ALA:HB1	2.01	0.42
1:E:727:TRP:HB3	1:E:845:PHE:CD2	2.55	0.42
4:L:5:DA:H2'	4:L:6:DT:C6	2.55	0.42
1:E:824:LEU:O	1:E:828:VAL:HG23	2.19	0.42
1:I:8:LYS:NZ	1:I:291:ARG:HH22	2.17	0.42
2:J:4:DA:H2''	2:J:5:DA:H5'	2.01	0.42
1:M:416:PHE:CE1	1:M:434:PRO:HD3	2.55	0.42
1:B:215:ARG:HH21	1:B:219:MET:HG3	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:794:THR:HA	1:E:831:THR:HG21	2.02	0.42
1:I:706:LEU:HD11	1:I:852:GLN:HB2	2.01	0.42
1:M:556:GLY:O	1:M:561:LEU:N	2.48	0.42
1:M:879:ASP:OD2	1:M:879:ASP:N	2.52	0.42
1:B:629:VAL:HG13	1:B:654:THR:HG21	2.02	0.42
1:B:740:LYS:HB3	1:B:740:LYS:HE3	1.72	0.42
1:B:740:LYS:NZ	1:B:767:SER:H	2.18	0.42
1:E:705:LEU:O	1:E:720:ARG:NH2	2.53	0.42
2:F:4:DA:H61	4:H:7:DT:H3	1.68	0.42
1:M:651:LEU:HD12	1:M:670:PRO:HB2	2.02	0.42
1:M:801:LYS:HA	1:M:801:LYS:HD2	1.84	0.42
1:E:172:LYS:HD3	1:E:172:LYS:HA	1.70	0.42
1:E:423:ARG:NH2	1:E:425:ARG:HD2	2.35	0.42
1:I:248:PRO:O	1:I:252:GLU:HG2	2.20	0.42
1:B:646:PHE:O	1:B:650:VAL:HG22	2.20	0.41
1:E:709:GLU:HG3	1:E:722:ARG:HE	1.85	0.41
1:I:151:PHE:HA	1:I:154:ILE:HD12	2.02	0.41
1:I:163:LYS:HA	1:I:166:VAL:HG22	2.01	0.41
1:I:782:PHE:O	1:I:786:GLN:HG2	2.20	0.41
1:M:825:PHE:HZ	1:M:879:ASP:HA	1.84	0.41
1:M:859:ASP:OD1	1:M:860:LYS:N	2.53	0.41
1:B:24:LEU:HD13	1:B:287:TRP:CE2	2.55	0.41
1:B:422:TRP:O	1:B:735:VAL:HG23	2.19	0.41
1:E:274:PRO:HA	1:E:275:PRO:HD3	1.85	0.41
1:E:677:MET:HE3	1:E:680:LEU:HB2	2.02	0.41
1:I:472:LYS:HD2	1:I:567:VAL:HG21	2.02	0.41
1:I:709:GLU:HG2	1:I:718:ILE:HG21	2.01	0.41
1:M:298:ARG:HE	1:M:419:ASN:ND2	2.18	0.41
1:M:706:LEU:HD11	1:M:849:PHE:HB2	2.01	0.41
1:E:555:GLY:O	1:E:559:VAL:HG22	2.20	0.41
1:E:722:ARG:NH1	1:E:769:ILE:O	2.53	0.41
1:B:7:ALA:HA	1:B:11:PHE:HB2	2.01	0.41
1:B:230:HIS:NE2	1:B:245:GLU:HB2	2.36	0.41
1:I:378:LYS:H	1:I:378:LYS:HD2	1.85	0.41
1:B:137:VAL:O	1:B:141:ILE:HG13	2.21	0.41
1:E:471:ASP:OD2	1:E:471:ASP:N	2.51	0.41
1:E:553:GLU:HA	1:E:870:LEU:HD12	2.03	0.41
1:E:737:GLN:HE22	1:E:778:ILE:HA	1.84	0.41
1:M:626:THR:O	1:M:629:VAL:HG22	2.20	0.41
1:M:699:LEU:HD23	1:M:778:ILE:HG13	2.02	0.41
1:M:727:TRP:HB3	1:M:845:PHE:CD2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:648:GLN:O	1:E:652:GLU:HG3	2.20	0.41
1:I:105:PHE:HB3	1:I:204:TRP:CH2	2.56	0.41
1:M:553:GLU:HA	1:M:870:LEU:HB2	2.01	0.41
1:B:879:ASP:OD2	1:B:879:ASP:N	2.52	0.41
4:D:6:DT:H2''	4:D:7:DT:H5'	2.03	0.41
1:I:118:THR:HG22	1:I:141:ILE:CD1	2.48	0.41
1:I:162:PHE:CD1	1:I:190:MET:HE2	2.55	0.41
1:M:304:ALA:HA	1:M:307:ARG:HG3	2.02	0.41
1:B:65:ALA:HB2	1:B:123:LEU:HD21	2.03	0.41
1:B:344:TRP:O	1:E:345:LYS:NZ	2.54	0.41
1:I:737:GLN:NE2	1:I:778:ILE:HG23	2.36	0.41
1:E:180:LYS:HD2	1:E:180:LYS:HA	1.88	0.41
1:I:330:ILE:HD13	1:I:405:ALA:HA	2.03	0.41
1:I:339:ASN:O	1:I:343:LYS:HG3	2.21	0.41
1:I:727:TRP:HB3	1:I:845:PHE:CD1	2.55	0.41
1:M:345:LYS:HZ1	1:M:352:ILE:HD13	1.86	0.41
1:M:349:VAL:HG21	1:M:508:PRO:HG3	2.02	0.41
1:B:439:MET:HE2	1:B:439:MET:HB3	1.83	0.41
1:E:58:GLN:HE22	1:E:67:ASN:ND2	2.18	0.41
1:I:82:ILE:HD13	1:I:112:GLU:HG3	2.03	0.41
1:I:71:LYS:HD2	1:I:71:LYS:HA	1.88	0.40
1:I:611:LEU:HD23	1:I:611:LEU:HA	1.98	0.40
1:M:331:ASN:N	1:M:443:LEU:O	2.49	0.40
1:M:740:LYS:HA	1:M:740:LYS:HD2	1.91	0.40
1:B:849:PHE:HA	1:B:852:GLN:HG3	2.02	0.40
1:B:330:ILE:HB	1:B:409:ALA:HA	2.03	0.40
3:K:2:C:H2'	3:K:3:G:C8	2.56	0.40
1:M:275:PRO:HG2	1:M:324:GLN:HB3	2.02	0.40
1:B:340:VAL:HG21	1:B:497:LEU:HD11	2.02	0.40
1:M:175:GLY:O	1:M:179:LYS:HG2	2.22	0.40
1:M:448:LYS:HD2	1:M:448:LYS:HA	1.67	0.40
1:B:118:THR:HG21	1:B:216:CYS:HB3	2.03	0.40
1:B:183:MET:HA	1:B:186:VAL:HG12	2.04	0.40
1:B:829:ARG:NH2	1:B:882:PHE:H	2.20	0.40
1:E:110:LYS:H	1:E:110:LYS:HG3	1.71	0.40
1:E:333:LYS:O	1:E:337:VAL:HG23	2.22	0.40
1:I:146:GLU:HG3	1:I:201:TRP:HE1	1.85	0.40
1:I:561:LEU:HD23	1:I:561:LEU:HA	1.89	0.40
2:J:7:DC:H2''	2:J:8:DG:C8	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:31:ARG:NH2	1:M:90:GLU:O[1_655]	2.16	0.04

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	B	850/883 (96%)	834 (98%)	15 (2%)	1 (0%)	48	80
1	E	813/883 (92%)	798 (98%)	15 (2%)	0	100	100
1	I	823/883 (93%)	815 (99%)	8 (1%)	0	100	100
1	M	761/883 (86%)	750 (99%)	11 (1%)	0	100	100
All	All	3247/3532 (92%)	3197 (98%)	49 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	811	HIS

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	
1	B	701/729 (96%)	701 (100%)	0	100	100
1	E	670/729 (92%)	670 (100%)	0	100	100
1	I	674/729 (92%)	674 (100%)	0	100	100
1	M	582/729 (80%)	582 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2627/2916 (90%)	2627 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	B	22	ASN
1	B	86	ASN
1	B	463	HIS
1	B	499	ASN
1	B	505	GLN
1	E	22	ASN
1	E	58	GLN
1	E	406	ASN
1	E	499	ASN
1	E	522	GLN
1	E	857	GLN
1	I	5	ASN
1	I	324	GLN
1	I	433	ASN
1	I	648	GLN
1	I	786	GLN
1	M	176	HIS
1	M	325	ASN
1	M	499	ASN
1	M	656	GLN
1	M	744	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	8/12 (66%)	0	0
3	G	7/12 (58%)	0	0
3	K	7/12 (58%)	0	0
3	O	7/12 (58%)	2 (28%)	0
All	All	29/48 (60%)	2 (6%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	O	2	C
3	O	3	G

There are no RNA pucker outliers to report.

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

4 non-standard protein/DNA/RNA residues 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
2	S8U	A	10	2	15,19,20	4.69	8 (53%)	19,26,29	1.25	2 (10%)
2	S8U	N	10	2	15,19,20	4.67	8 (53%)	19,26,29	1.39	3 (15%)
2	S8U	J	10	2	15,19,20	4.65	8 (53%)	19,26,29	1.44	4 (21%)
2	S8U	F	10	2	15,19,20	4.67	8 (53%)	19,26,29	1.34	2 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	S8U	A	10	2	-	5/9/23/24	0/2/2/2
2	S8U	N	10	2	-	3/9/23/24	0/2/2/2
2	S8U	J	10	2	-	5/9/23/24	0/2/2/2
2	S8U	F	10	2	-	2/9/23/24	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	10	S8U	C2'-C3'	-12.00	1.22	1.52
2	N	10	S8U	C2'-C3'	-11.84	1.22	1.52
2	J	10	S8U	C2'-C3'	-11.83	1.22	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	10	S8U	C2'-C3'	-11.80	1.22	1.52
2	F	10	S8U	O4'-C4'	-8.15	1.26	1.45
2	N	10	S8U	O4'-C4'	-8.13	1.26	1.45
2	J	10	S8U	O4'-C4'	-8.00	1.27	1.45
2	A	10	S8U	O4'-C4'	-7.96	1.27	1.45
2	A	10	S8U	C1'-N1	-5.64	1.33	1.48
2	F	10	S8U	C1'-N1	-5.62	1.33	1.48
2	N	10	S8U	C1'-N1	-5.61	1.34	1.48
2	A	10	S8U	C3'-C4'	5.39	1.67	1.53
2	J	10	S8U	C1'-N1	-5.27	1.34	1.48
2	J	10	S8U	C3'-C4'	5.25	1.66	1.53
2	N	10	S8U	C3'-C4'	5.22	1.66	1.53
2	F	10	S8U	C3'-C4'	5.16	1.66	1.53
2	F	10	S8U	C13-C12	4.65	1.53	1.44
2	N	10	S8U	C13-C12	4.59	1.53	1.44
2	A	10	S8U	C13-C12	4.53	1.52	1.44
2	J	10	S8U	C13-C12	4.35	1.52	1.44
2	J	10	S8U	O4'-C1'	4.33	1.52	1.42
2	A	10	S8U	O4'-C1'	4.18	1.51	1.42
2	N	10	S8U	O4'-C1'	4.13	1.51	1.42
2	F	10	S8U	O4'-C1'	4.12	1.51	1.42
2	J	10	S8U	O3'-C3'	3.30	1.50	1.43
2	A	10	S8U	O3'-C3'	3.09	1.49	1.43
2	F	10	S8U	O3'-C3'	3.05	1.49	1.43
2	N	10	S8U	O3'-C3'	3.00	1.49	1.43
2	N	10	S8U	O14-C13	-2.35	1.16	1.22
2	J	10	S8U	O14-C13	-2.31	1.17	1.22
2	F	10	S8U	O14-C13	-2.30	1.17	1.22
2	A	10	S8U	O14-C13	-2.30	1.17	1.22

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	10	S8U	C17-N1-C12	-3.12	107.21	109.18
2	N	10	S8U	C2'-C3'-C4'	3.02	108.93	102.80
2	F	10	S8U	C2'-C3'-C4'	2.97	108.82	102.80
2	J	10	S8U	O14-C13-C12	-2.85	120.04	126.63
2	F	10	S8U	O14-C13-C12	-2.54	120.77	126.63
2	A	10	S8U	O14-C13-C12	-2.54	120.77	126.63
2	N	10	S8U	O14-C13-C12	-2.52	120.81	126.63
2	J	10	S8U	C2'-C3'-C4'	2.46	107.78	102.80
2	J	10	S8U	O4'-C1'-N1	2.13	111.65	107.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	10	S8U	O4'-C1'-N1	2.11	111.60	107.86
2	N	10	S8U	C2'-C1'-N1	-2.01	108.80	113.81

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	10	S8U	C15-C12-C13-O14
2	A	10	S8U	N1-C12-C13-O14
2	A	10	S8U	O4'-C4'-C5'-O5'
2	F	10	S8U	C15-C12-C13-O14
2	F	10	S8U	N1-C12-C13-O14
2	J	10	S8U	C3'-C4'-C5'-O5'
2	J	10	S8U	O4'-C4'-C5'-O5'
2	N	10	S8U	C15-C12-C13-O14
2	N	10	S8U	N1-C12-C13-O14
2	A	10	S8U	C3'-C4'-C5'-O5'
2	J	10	S8U	N1-C12-C13-O14
2	J	10	S8U	C4'-C5'-O5'-P
2	J	10	S8U	C15-C12-C13-O14
2	A	10	S8U	C4'-C5'-O5'-P
2	N	10	S8U	C2'-C1'-N1-C17

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	B	856/883 (96%)	-0.05	8 (0%) 81 61	46, 89, 172, 247	0
1	E	825/883 (93%)	-0.00	12 (1%) 72 49	54, 100, 243, 301	0
1	I	831/883 (94%)	0.18	27 (3%) 50 29	70, 137, 216, 307	0
1	M	775/883 (87%)	0.08	19 (2%) 58 35	97, 155, 236, 309	0
2	A	15/18 (83%)	-0.31	0 100 100	65, 97, 305, 307	0
2	F	16/18 (88%)	-0.06	0 100 100	97, 148, 228, 231	0
2	J	15/18 (83%)	-0.25	0 100 100	99, 128, 332, 358	0
2	N	16/18 (88%)	-0.16	0 100 100	110, 198, 390, 393	0
3	C	9/12 (75%)	-0.60	0 100 100	67, 77, 127, 185	0
3	G	8/12 (66%)	-0.73	0 100 100	87, 106, 157, 158	0
3	K	8/12 (66%)	-0.65	0 100 100	96, 115, 163, 181	0
3	O	8/12 (66%)	-0.33	0 100 100	117, 142, 206, 219	0
4	D	7/9 (77%)	0.13	0 100 100	208, 254, 295, 309	0
4	H	8/9 (88%)	0.12	0 100 100	221, 228, 281, 295	0
4	L	7/9 (77%)	-0.14	0 100 100	271, 281, 301, 303	0
4	P	8/9 (88%)	-0.17	0 100 100	291, 298, 333, 336	0
All	All	3412/3688 (92%)	0.04	66 (1%) 66 43	46, 127, 233, 393	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	116	TYR	5.1
1	I	570	ILE	4.8
1	M	216	CYS	4.3
1	M	120	LYS	4.1
1	M	122	THR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	64	VAL	3.5
1	E	539	SER	3.4
1	B	752	LEU	3.3
1	E	106	LEU	3.1
1	E	113	ALA	3.0
1	I	558	ALA	2.9
1	M	811	HIS	2.9
1	E	74	ILE	2.8
1	M	857	GLN	2.8
1	E	4	ILE	2.8
1	I	681	ILE	2.8
1	M	613	THR	2.8
1	B	857	GLN	2.7
1	B	1	MET	2.7
1	I	574	VAL	2.6
1	M	824	LEU	2.6
1	M	685	VAL	2.6
1	I	620	TRP	2.5
1	E	883	ALA	2.5
1	M	121	THR	2.5
1	I	625	VAL	2.5
1	I	692	ALA	2.5
1	I	746	ARG	2.5
1	B	126	LEU	2.4
1	E	20	PRO	2.4
1	I	634	VAL	2.4
1	E	537	ASP	2.4
1	I	137	VAL	2.4
1	E	146	GLU	2.4
1	I	633	SER	2.4
1	I	434	PRO	2.4
1	I	459	TRP	2.4
1	I	730	PRO	2.3
1	B	540	CYS	2.3
1	B	747	LEU	2.3
1	I	578	VAL	2.3
1	M	426	VAL	2.3
1	I	550	LEU	2.3
1	I	667	PHE	2.3
1	E	810	ILE	2.2
1	B	827	ALA	2.2
1	I	651	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	471	ASP	2.2
1	E	742	PRO	2.2
1	I	485	ASN	2.2
1	I	630	THR	2.2
1	M	747	LEU	2.1
1	M	791	LEU	2.1
1	M	541	SER	2.1
1	B	308	TYR	2.1
1	I	573	ILE	2.1
1	I	691	ALA	2.1
1	M	123	LEU	2.1
1	E	165	ASN	2.1
1	I	698	TRP	2.1
1	I	470	VAL	2.0
1	I	747	LEU	2.0
1	I	685	VAL	2.0
1	M	92	VAL	2.0
1	M	55	PHE	2.0
1	M	807	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	S8U	J	10	18/19	0.83	0.13	126,150,175,183	0
2	S8U	F	10	18/19	0.86	0.12	105,116,135,147	0
2	S8U	N	10	18/19	0.86	0.14	119,144,161,170	0
2	S8U	A	10	18/19	0.94	0.13	71,90,110,124	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.