



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:58 PM UTC

PDB ID : 6BM2 / pdb_00006bm2
Title : Pol II elongation complex with an abasic lesion at i-1 position
Authors : Wang, W.; Wang, D.
Deposited on : 2017-11-13
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
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

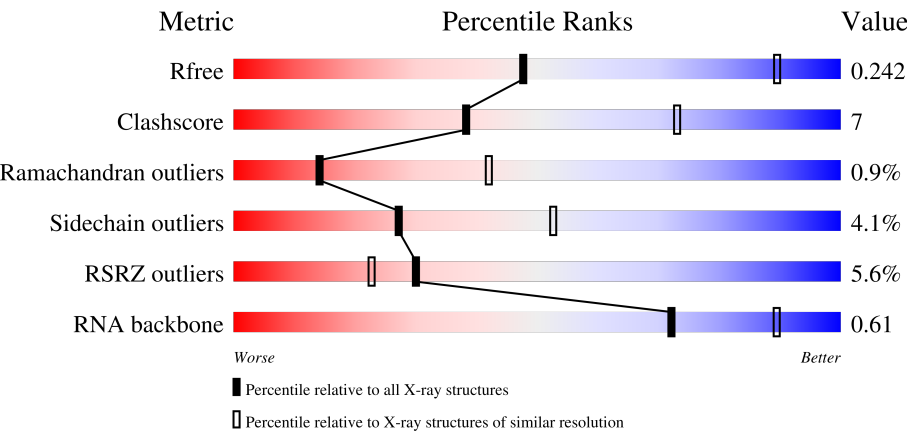
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)
RNA backbone	3983	1157 (3.80-3.00)

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	1733	5% 62%16%•21%
2	B	1224	4% 69%19%•10%
3	C	318	% 65%17%•16%
4	E	215	4% 87%12%•

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	155	2% 45% 8% 46%
6	H	146	8% 66% 22% 11%
7	I	122	3% 76% 17% 6%
8	J	70	3% 73% 17% 7%
9	K	120	72% 22% 5%
10	L	70	19% 43% 20% 37%
11	T	29	17% 21% 21% 59%
12	R	9	11% 56% 44%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 28244 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1372	Total	C	N	O	S	0	0	0
			10784	6802	1887	2034	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1097	Total	C	N	O	S	0	0	0
			8726	5526	1530	1615	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	213	Total	C	N	O	S	0	0	0
			1744	1107	308	318	11			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	130	Total	C	N	O	S	0	0	0
			1043	660	173	206	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	115	Total	C	N	O	S	0	0	0
			935	575	170	180	10			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	44	Total	C	N	O	S	0	0	0
			351	217	70	60	4			

- Molecule 11 is a DNA chain called DNA (5'-D(P*CP*AP*(3DR)P*CP*TP*CP*TP*TP*GP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	T	12	Total	C	N	O	P	0	0	0
			233	111	38	72	12			

- Molecule 12 is a RNA chain called RNA (5'-R(*AP*UP*CP*AP*AP*GP*AP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	R	9	Total	C	N	O	P	0	0	0
			194	88	40	58	8			

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	2	Total	Zn	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total 1	Zn 1	0	0
13	C	1	Total 1	Zn 1	0	0
13	I	2	Total 2	Zn 2	0	0
13	J	1	Total 1	Zn 1	0	0
13	L	1	Total 1	Zn 1	0	0

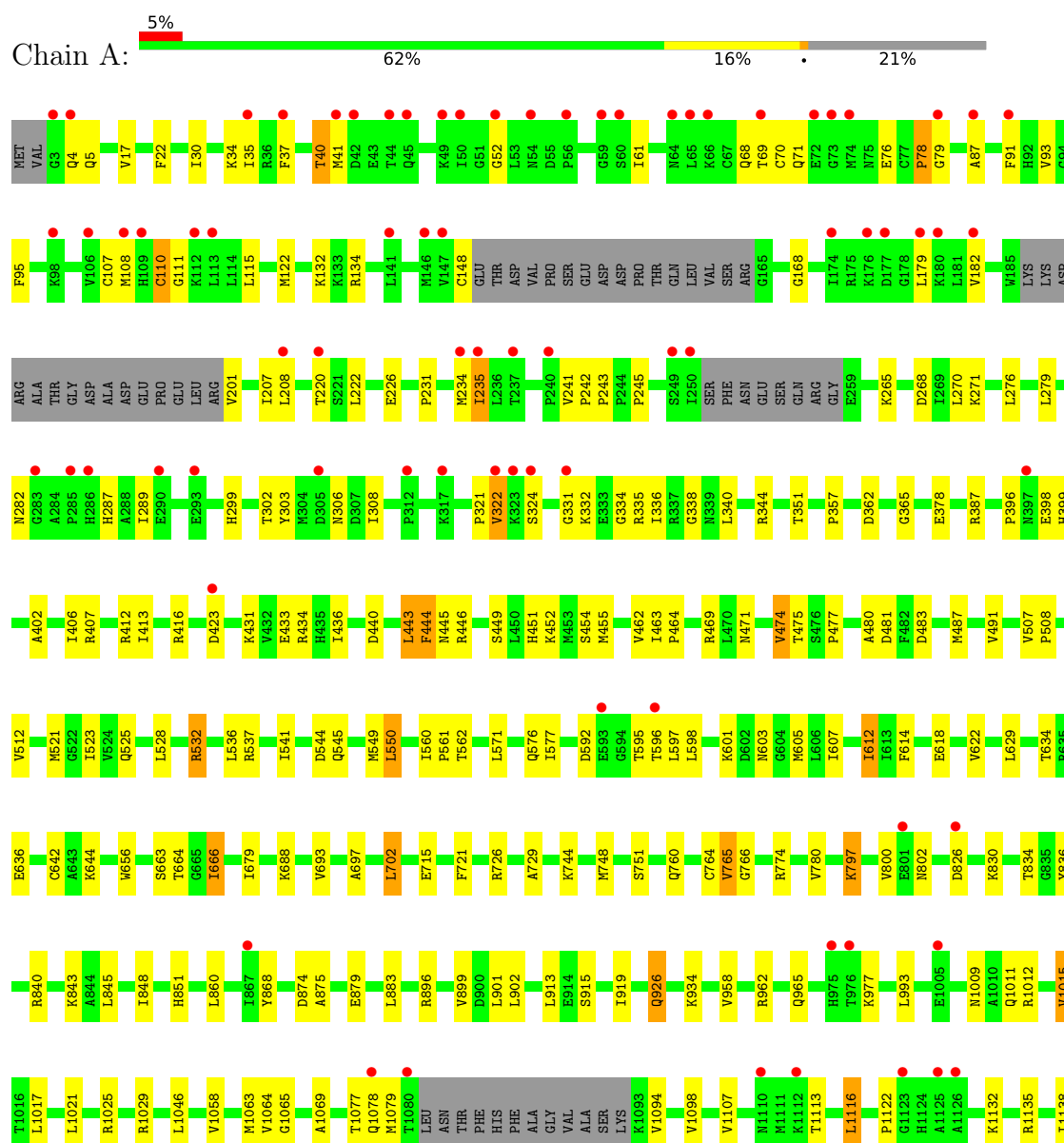
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

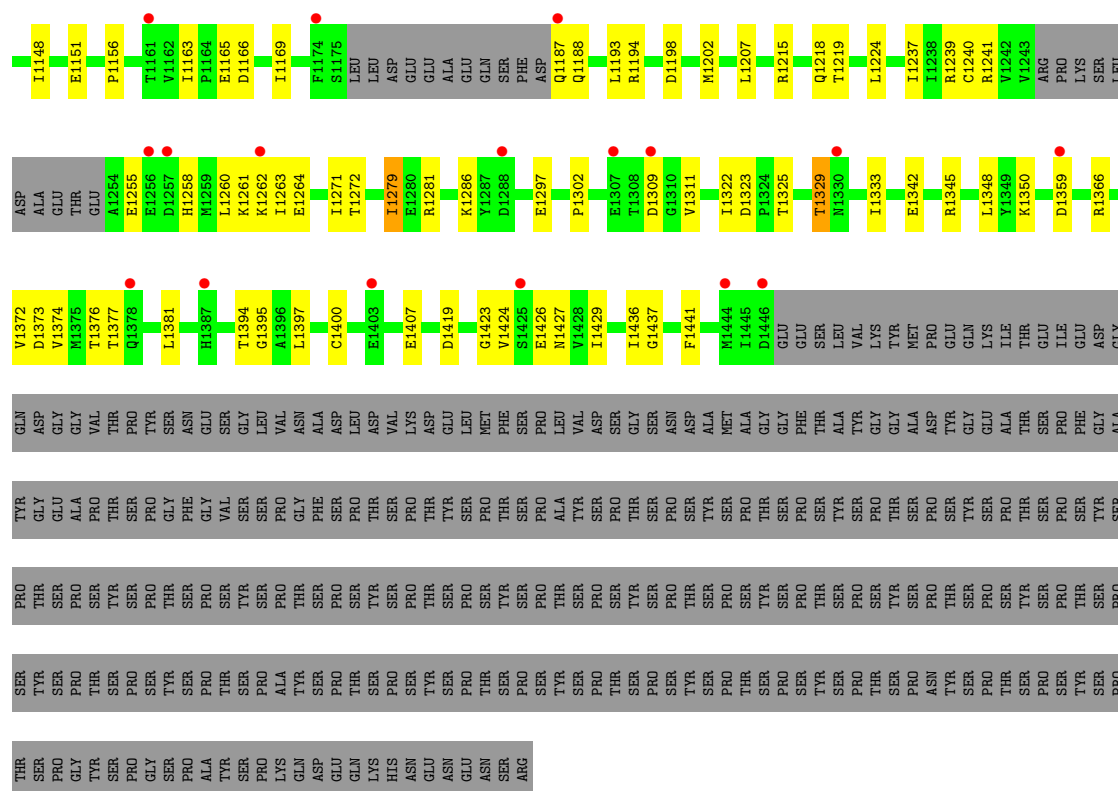
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total 1	Mg 1	0	0

3 Residue-property plots

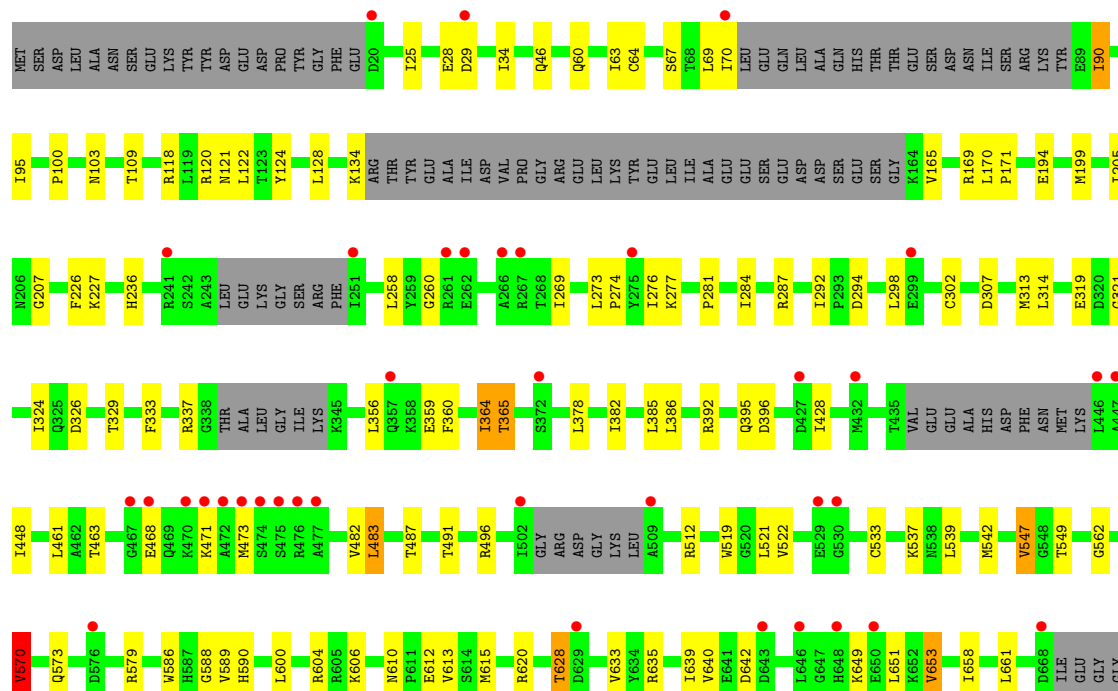
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



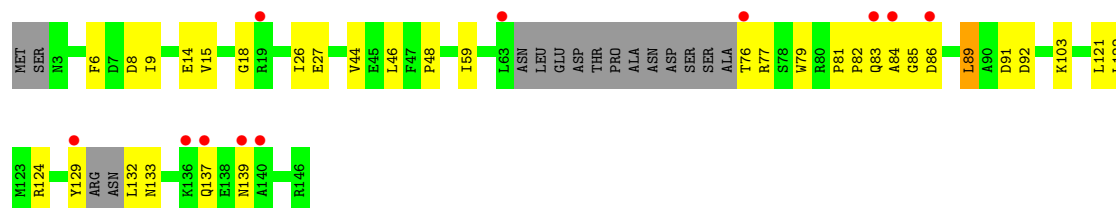


• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

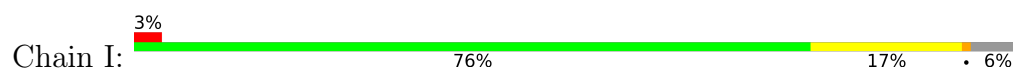




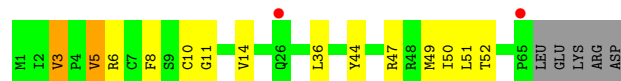
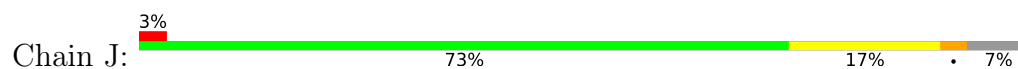
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



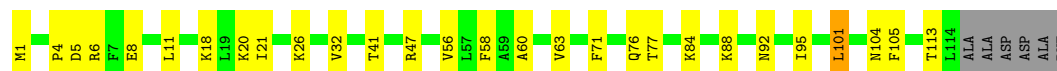
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



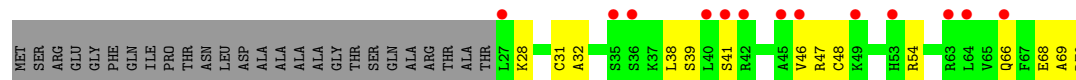
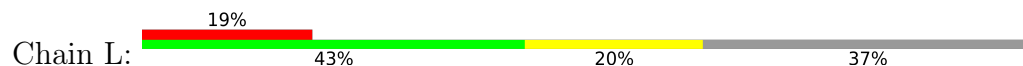
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 9: DNA-directed RNA polymerase II subunit RPB11

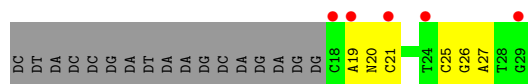


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

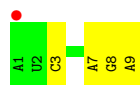


- Molecule 11: DNA (5'-D(P*CP*AP*(3DR)P*CP*TP*CP*TP*TP*GP*AP*TP*G)-3')





- Molecule 12: RNA (5'-R(*AP*UP*CP*AP*AP*GP*AP*GP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.11Å 222.27Å 193.71Å 90.00° 101.28° 90.00°	Depositor
Resolution (Å)	82.92 – 3.40 82.92 – 3.40	Depositor EDS
% Data completeness (in resolution range)	87.3 (82.92-3.40) 87.3 (82.92-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.219 , 0.244 0.221 , 0.242	Depositor DCC
R_{free} test set	4079 reflections (4.24%)	wwPDB-VP
Wilson B-factor (Å ²)	51.6	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	28244	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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: MG, ZN, 3DR

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	0.26	0/10975	0.69	3/14838 (0.0%)
2	B	0.25	0/8896	0.69	2/11996 (0.0%)
3	C	0.26	0/2133	0.70	2/2891 (0.1%)
4	E	0.25	0/1780	0.72	0/2395
5	F	0.25	0/691	0.72	0/933
6	H	0.27	0/1060	0.70	0/1434
7	I	0.24	0/953	0.66	0/1284
8	J	0.24	0/541	0.61	0/727
9	K	0.24	0/937	0.65	0/1265
10	L	0.23	0/353	0.56	0/468
11	T	0.13	0/246	0.28	0/374
12	R	0.05	0/218	0.11	0/339
All	All	0.25	0/28783	0.69	7/38944 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	525	GLN	CB-CA-C	-5.82	109.88	116.63
1	A	71	GLN	CB-CA-C	-5.42	109.86	117.23
3	C	211	ASP	CA-C-N	5.37	123.58	119.66
3	C	211	ASP	C-N-CA	5.37	123.58	119.66
2	B	570	VAL	CA-C-N	5.27	125.08	119.28
2	B	570	VAL	C-N-CA	5.27	125.08	119.28
1	A	1098	VAL	CB-CA-C	-5.03	109.02	114.35

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10784	0	10871	164	0
2	B	8726	0	8760	144	0
3	C	2095	0	2051	36	0
4	E	1744	0	1772	12	0
5	F	679	0	701	8	0
6	H	1043	0	1015	18	0
7	I	935	0	886	13	0
8	J	532	0	542	10	0
9	K	919	0	929	17	0
10	L	351	0	375	7	0
11	T	233	0	133	6	0
12	R	194	0	99	3	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
14	A	1	0	0	0	0
All	All	28244	0	28134	388	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 7.

All (388) 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:B:653:VAL:HG22	2:B:689:LEU:HB3	1.69	0.74
8:J:5:VAL:HG22	8:J:6:ARG:HG3	1.70	0.72
1:A:899:VAL:HG22	1:A:1029:ARG:HG2	1.73	0.70
2:B:911:ILE:HD11	2:B:941:LEU:HD23	1.73	0.70
7:I:92:ARG:HB3	7:I:95:THR:HG23	1.74	0.69
2:B:1174:LYS:HB2	2:B:1179:GLN:HB2	1.74	0.69
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.73	0.69
3:C:66:ARG:NH2	8:J:3:VAL:O	2.26	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.74	0.68
2:B:1065:GLN:HG2	2:B:1069:PHE:HB2	1.75	0.68
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.74	0.68
3:C:6:PRO:HB2	9:K:101:LEU:HD23	1.76	0.67
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.77	0.67
2:B:287:ARG:NH1	2:B:324:ILE:O	2.28	0.66
2:B:642:ASP:HB3	2:B:649:LYS:HG2	1.76	0.66
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.78	0.65
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.28	0.65
2:B:1175:LEU:O	2:B:1176:ASN:ND2	2.29	0.65
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.77	0.65
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.77	0.65
1:A:40:THR:HG22	1:A:41:MET:HG3	1.78	0.64
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.80	0.64
1:A:446:ARG:NH2	12:R:9:A:O2'	2.30	0.64
2:B:839:MET:HE2	2:B:1010:LEU:HD21	1.79	0.64
1:A:134:ARG:NH1	1:A:220:THR:O	2.31	0.64
4:E:178:ILE:HB	4:E:212:ARG:HD3	1.80	0.63
3:C:48:SER:HB3	3:C:158:VAL:HB	1.80	0.63
1:A:4:GLN:OE1	2:B:1159:ARG:NH1	2.32	0.62
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.82	0.62
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.82	0.62
1:A:1009:ASN:OD1	1:A:1012:ARG:NH2	2.32	0.62
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.65	0.62
2:B:165:VAL:HG21	2:B:448:ILE:HD12	1.82	0.61
4:E:12:LEU:HD11	4:E:58:MET:HE1	1.82	0.61
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.33	0.61
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.83	0.61
5:F:82:THR:HG22	5:F:84:TYR:H	1.64	0.61
2:B:463:THR:HG22	11:T:27:DA:H2''	1.82	0.61
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.82	0.61
1:A:601:LYS:HB2	1:A:603:ASN:HD22	1.65	0.61
1:A:634:THR:HG1	1:A:642:CYS:HG	1.49	0.61
2:B:882:THR:HB	2:B:885:MET:HE2	1.83	0.61
3:C:3:GLU:HG3	3:C:4:GLU:HG3	1.80	0.61
3:C:46:ILE:HD13	3:C:159:ALA:HB2	1.83	0.61
3:C:145:CYS:SG	3:C:146:LYS:N	2.73	0.60
2:B:778:MET:HE1	2:B:1094:ARG:HH11	1.66	0.60
6:H:129:TYR:O	6:H:132:LEU:N	2.35	0.60
1:A:1187:GLN:HG3	1:A:1188:GLN:HG3	1.84	0.60
1:A:477:PRO:HG3	1:A:521:MET:HE2	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ARG:NH2	2:B:991:GLY:O	2.35	0.59
1:A:693:VAL:HG21	1:A:721:PHE:HE2	1.66	0.59
2:B:916:THR:HG23	2:B:935:ARG:HB2	1.84	0.59
1:A:774:ARG:HG3	1:A:797:LYS:HZ2	1.68	0.59
3:C:77:ILE:HG12	3:C:129:ILE:HD11	1.84	0.59
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.35	0.59
1:A:1079:MET:HE3	1:A:1359:ASP:HB2	1.84	0.59
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.83	0.59
1:A:68:GLN:O	1:A:70:CYS:N	2.34	0.58
1:A:338:GLY:HA2	2:B:1129:ARG:HH21	1.68	0.58
7:I:32:CYS:SG	7:I:33:SER:N	2.76	0.58
5:F:76:LYS:O	5:F:79:ARG:NH1	2.32	0.58
2:B:28:GLU:OE1	2:B:807:ARG:NH1	2.33	0.58
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.37	0.58
1:A:1116:LEU:HD22	1:A:1329:THR:HB	1.85	0.58
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.85	0.57
1:A:1122:PRO:HD3	1:A:1323:ASP:HB2	1.86	0.57
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.84	0.57
3:C:69:LEU:HD12	8:J:6:ARG:HD3	1.85	0.57
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.86	0.57
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.85	0.57
2:B:613:VAL:HG22	2:B:628:THR:HG23	1.87	0.57
1:A:993:LEU:HD22	1:A:1046:LEU:HG	1.87	0.57
1:A:306:ASN:ND2	1:A:321:PRO:O	2.38	0.57
1:A:365:GLY:HA3	1:A:469:ARG:HB2	1.87	0.57
2:B:103:ASN:OD1	2:B:169:ARG:NH2	2.38	0.57
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.87	0.56
1:A:1423:GLY:O	1:A:1427:ASN:ND2	2.36	0.56
6:H:89:LEU:H	6:H:89:LEU:HD13	1.70	0.56
1:A:30:ILE:HG23	2:B:1170:THR:HG23	1.88	0.56
1:A:76:GLU:OE2	2:B:1159:ARG:NH1	2.39	0.56
2:B:60:GLN:NE2	2:B:64:CYS:SG	2.79	0.56
3:C:46:ILE:HD12	3:C:157:CYS:HB3	1.86	0.56
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.87	0.56
3:C:185:LYS:HG2	3:C:213:PRO:HG3	1.87	0.56
6:H:91:ASP:OD1	6:H:92:ASP:N	2.38	0.56
1:A:1148:ILE:HD13	7:I:49:ILE:HD12	1.89	0.55
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.88	0.55
1:A:34:LYS:H	1:A:34:LYS:HD3	1.72	0.55
2:B:857:ARG:NH2	11:T:25:DC:OP1	2.40	0.55
1:A:110:CYS:SG	1:A:111:GLY:N	2.73	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1239:ARG:HH22	1:A:1241:ARG:HH21	1.54	0.55
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.88	0.55
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.89	0.54
1:A:802:ASN:OD1	2:B:729:ILE:N	2.36	0.54
1:A:1151:GLU:OE2	7:I:45:ARG:NH1	2.40	0.54
8:J:36:LEU:HD11	8:J:51:LEU:HB2	1.89	0.54
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.89	0.54
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.89	0.54
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.40	0.54
1:A:562:THR:O	1:A:576:GLN:NE2	2.40	0.54
5:F:97:ARG:NH1	5:F:100:GLN:OE1	2.41	0.54
7:I:74:GLU:OE1	7:I:79:HIS:ND1	2.38	0.54
2:B:471:LYS:HA	2:B:473:MET:HE2	1.90	0.53
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.90	0.53
1:A:697:ALA:HA	1:A:702:LEU:HB2	1.89	0.53
1:A:744:LYS:HE2	1:A:748:MET:HE3	1.90	0.53
9:K:56:VAL:HG22	9:K:77:THR:HG22	1.90	0.53
2:B:806:THR:HG22	2:B:808:ALA:H	1.74	0.53
3:C:6:PRO:HB3	3:C:25:VAL:HG13	1.91	0.53
8:J:8:PHE:H	8:J:49:MET:HE3	1.74	0.53
1:A:532:ARG:HE	1:A:536:LEU:HD21	1.73	0.53
1:A:1193:LEU:HB3	1:A:1240:CYS:HB2	1.90	0.53
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.73	0.53
1:A:332:LYS:HE2	11:T:19:DA:H3'	1.91	0.53
6:H:137:GLN:HG3	6:H:139:ASN:H	1.73	0.53
1:A:868:TYR:CE1	1:A:1064:VAL:HG21	2.43	0.53
2:B:855:PHE:HZ	2:B:857:ARG:HH11	1.57	0.52
4:E:20:LYS:NZ	4:E:34:GLU:O	2.37	0.52
6:H:85:GLY:HA2	6:H:86:ASP:HB3	1.91	0.52
2:B:547:VAL:N	2:B:612:GLU:OE2	2.40	0.52
2:B:995:ARG:NH1	2:B:997:GLU:OE1	2.43	0.52
1:A:378:GLU:OE2	1:A:387:ARG:NH2	2.41	0.52
1:A:550:LEU:HD21	1:A:561:PRO:HD2	1.90	0.52
1:A:1281:ARG:HG2	1:A:1309:ASP:HB2	1.91	0.52
1:A:528:LEU:HD23	1:A:751:SER:HA	1.92	0.52
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.91	0.52
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.90	0.52
6:H:8:ASP:OD1	6:H:9:ILE:N	2.43	0.52
3:C:50:GLU:HG2	10:L:66:GLN:HG2	1.92	0.51
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.92	0.51
1:A:1138:ILE:HG22	1:A:1279:ILE:HG21	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.93	0.51
1:A:1286:LYS:HE2	1:A:1302:PRO:HB2	1.92	0.51
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.91	0.51
3:C:99:LEU:HB3	3:C:120:ILE:HD13	1.93	0.51
2:B:586:TRP:CD1	2:B:588:GLY:H	2.29	0.51
10:L:38:LEU:HD21	10:L:48:CYS:HA	1.92	0.51
12:R:7:A:H2'	12:R:8:G:C8	2.45	0.51
2:B:284:ILE:HG21	2:B:333:PHE:HD2	1.75	0.51
10:L:47:ARG:HG2	10:L:54:ARG:HG2	1.93	0.51
2:B:963:PHE:HE2	2:B:965:LYS:HE3	1.76	0.51
2:B:95:ILE:HD11	2:B:128:LEU:HB3	1.93	0.51
4:E:83:CYS:HB2	4:E:110:PHE:HE1	1.75	0.51
1:A:1325:THR:OG1	4:E:146:HIS:O	2.28	0.50
1:A:560:ILE:HB	6:H:79:TRP:H	1.75	0.50
8:J:10:CYS:SG	8:J:11:GLY:N	2.84	0.50
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.94	0.50
1:A:834:THR:HG21	1:A:1077:THR:HA	1.93	0.50
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.44	0.50
3:C:165:LYS:O	9:K:6:ARG:NH1	2.44	0.50
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.93	0.50
5:F:107:VAL:HG12	5:F:109:VAL:H	1.76	0.50
1:A:545:GLN:HG2	1:A:549:MET:HE3	1.94	0.50
2:B:298:LEU:O	2:B:302:CYS:N	2.40	0.50
2:B:579:ARG:HA	2:B:589:VAL:HA	1.92	0.50
2:B:378:LEU:O	2:B:382:ILE:HG12	2.12	0.50
3:C:98:VAL:HG22	3:C:158:VAL:HG22	1.93	0.50
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.94	0.50
2:B:680:THR:O	2:B:683:SER:OG	2.29	0.50
1:A:182:VAL:HA	1:A:201:VAL:HA	1.94	0.49
3:C:252:GLN:HG3	9:K:95:ILE:HG23	1.92	0.49
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.93	0.49
2:B:810:GLU:OE1	2:B:815:ARG:NH2	2.45	0.49
6:H:84:ALA:HB3	6:H:86:ASP:HB3	1.94	0.49
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.94	0.49
2:B:839:MET:HG3	2:B:1010:LEU:HD11	1.95	0.49
1:A:412:ARG:NH1	1:A:433:GLU:OE2	2.43	0.48
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.52	0.48
2:B:428:ILE:HD11	2:B:448:ILE:HG23	1.95	0.48
2:B:482:VAL:HG11	11:T:26:DG:H5''	1.94	0.48
2:B:956:THR:HG22	10:L:46:VAL:HG11	1.95	0.48
1:A:544:ASP:OD1	1:A:545:GLN:N	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:LEU:HD23	1:A:1311:VAL:HA	1.95	0.48
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.95	0.48
2:B:522:VAL:HG11	2:B:537:LYS:HD2	1.96	0.48
1:A:95:PHE:HB3	1:A:234:MET:HE2	1.95	0.48
2:B:620:ARG:NH2	7:I:89:GLN:OE1	2.46	0.48
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.47	0.48
1:A:596:THR:C	1:A:598:LEU:H	2.21	0.48
1:A:1163:ILE:HG22	1:A:1165:GLU:H	1.79	0.48
2:B:298:LEU:HD22	2:B:314:LEU:HD13	1.95	0.48
9:K:21:ILE:HD13	9:K:84:LYS:HE2	1.96	0.48
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.96	0.48
1:A:868:TYR:OH	1:A:1366:ARG:HD3	2.14	0.47
3:C:163:ILE:HG22	3:C:165:LYS:H	1.79	0.47
1:A:115:LEU:HB2	1:A:122:MET:HE3	1.96	0.47
1:A:306:ASN:HB2	1:A:324:SER:HB3	1.96	0.47
1:A:860:LEU:HD21	1:A:1394:THR:HA	1.96	0.47
2:B:843:GLN:HB2	2:B:993:THR:HB	1.96	0.47
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.96	0.47
2:B:562:GLY:O	2:B:590:HIS:ND1	2.40	0.47
2:B:1017:ILE:H	2:B:1018:PRO:HD2	1.79	0.47
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.96	0.47
1:A:663:SER:OG	1:A:664:THR:N	2.47	0.47
1:A:868:TYR:CZ	1:A:1064:VAL:HG21	2.49	0.47
1:A:1166:ASP:HA	1:A:1169:ILE:HD13	1.97	0.47
1:A:1215:ARG:NH2	1:A:1218:GLN:OE1	2.47	0.47
1:A:362:ASP:HB3	1:A:508:PRO:HD3	1.97	0.47
1:A:336:ILE:HA	1:A:340:LEU:HD12	1.95	0.47
3:C:7:GLN:HB2	3:C:23:SER:HB2	1.96	0.47
10:L:68:GLU:O	10:L:70:ARG:N	2.48	0.47
1:A:1194:ARG:HH21	1:A:1237:ILE:HD13	1.80	0.47
4:E:4:GLU:OE1	4:E:7:ARG:NH2	2.34	0.46
1:A:962:ARG:HA	1:A:965:GLN:HG2	1.96	0.46
2:B:1082:MET:HA	3:C:189:THR:HA	1.97	0.46
3:C:3:GLU:N	9:K:104:ASN:HD21	2.12	0.46
9:K:5:ASP:HB2	9:K:8:GLU:HG3	1.96	0.46
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.97	0.46
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.96	0.46
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.98	0.46
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.98	0.46
1:A:544:ASP:HB2	9:K:47:ARG:HH21	1.81	0.46
2:B:702:LEU:HD21	2:B:735:ALA:HB1	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.97	0.46
1:A:483:ASP:HA	2:B:988:GLY:HA2	1.98	0.46
6:H:81:PRO:O	6:H:83:GLN:N	2.49	0.46
10:L:31:CYS:SG	10:L:32:ALA:N	2.88	0.46
1:A:108:MET:O	1:A:110:CYS:N	2.48	0.46
1:A:443:LEU:HD13	1:A:455:MET:HE2	1.98	0.46
1:A:449:SER:HB3	2:B:1137:CYS:SG	2.56	0.46
1:A:760:GLN:HG2	1:A:765:VAL:HA	1.97	0.46
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.98	0.46
2:B:883:LEU:O	2:B:885:MET:N	2.49	0.46
1:A:148:CYS:HB2	1:A:168:GLY:HA2	1.98	0.46
1:A:614:PHE:HB3	6:H:122:LEU:HD21	1.98	0.45
1:A:883:LEU:HD23	1:A:1021:LEU:HD13	1.98	0.45
2:B:1175:LEU:C	2:B:1177:HIS:H	2.23	0.45
3:C:52:GLU:HG2	3:C:53:THR:HG23	1.97	0.45
7:I:84:VAL:HG23	7:I:104:LEU:HD11	1.98	0.45
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.81	0.45
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.82	0.45
1:A:279:LEU:HB3	1:A:289:ILE:HG22	1.98	0.45
4:E:124:VAL:HG13	4:E:132:ILE:HB	1.99	0.45
3:C:77:ILE:O	3:C:161:LYS:NZ	2.36	0.45
1:A:406:ILE:HB	1:A:431:LYS:HB2	1.98	0.45
1:A:634:THR:OG1	1:A:642:CYS:SG	2.64	0.45
2:B:34:ILE:HG23	2:B:542:MET:HE3	1.98	0.45
7:I:65:ASP:HA	7:I:66:PRO:HD3	1.83	0.45
1:A:446:ARG:HB2	1:A:487:MET:HG2	1.98	0.45
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.99	0.45
2:B:326:ASP:OD1	2:B:329:THR:OG1	2.24	0.45
1:A:595:THR:OG1	1:A:603:ASN:OD1	2.31	0.44
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.98	0.44
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.99	0.44
3:C:33:LEU:HG	3:C:37:MET:HE2	1.99	0.44
4:E:24:LYS:HB3	4:E:30:ILE:HB	1.99	0.44
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.99	0.44
2:B:281:PRO:HB2	2:B:284:ILE:HG12	1.99	0.44
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.98	0.44
2:B:941:LEU:HD22	2:B:942:ARG:H	1.82	0.44
2:B:1060:ARG:HA	2:B:1060:ARG:HD2	1.84	0.44
1:A:396:PRO:C	1:A:398:GLU:H	2.26	0.44
2:B:610:ASN:HB3	2:B:613:VAL:HG23	2.00	0.44
1:A:235:ILE:H	1:A:235:ILE:HG13	1.55	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:PRO:HA	1:A:243:PRO:HD3	1.80	0.44
1:A:1397:LEU:HB2	1:A:1426:GLU:HG2	2.00	0.44
3:C:108:GLU:HA	3:C:149:LYS:HD3	2.00	0.44
7:I:101:PHE:HE1	7:I:112:SER:HB3	1.82	0.44
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.98	0.44
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.98	0.44
1:A:1132:LYS:HG3	1:A:1135:ARG:HH12	1.83	0.43
2:B:939:THR:HA	2:B:940:PRO:HD3	1.82	0.43
2:B:999:MET:HG3	2:B:1000:PRO:HD2	2.00	0.43
1:A:396:PRO:HG3	1:A:416:ARG:HB3	1.99	0.43
1:A:507:VAL:HG13	1:A:521:MET:HE1	2.00	0.43
3:C:62:PHE:O	3:C:66:ARG:HG3	2.18	0.43
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	2.00	0.43
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.33	0.43
5:F:82:THR:O	5:F:136:ARG:NH1	2.31	0.43
2:B:199:MET:SD	2:B:199:MET:N	2.82	0.43
2:B:483:LEU:HD21	2:B:491:THR:HG23	2.00	0.43
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	2.00	0.43
2:B:916:THR:HA	2:B:917:PRO:HD3	1.80	0.43
1:A:541:ILE:HD12	1:A:577:ILE:HG12	2.01	0.43
1:A:1333:ILE:HD13	1:A:1381:LEU:HD12	2.01	0.43
2:B:512:ARG:NH1	2:B:533:CYS:O	2.51	0.43
2:B:984:HIS:CE1	2:B:1025:HIS:HA	2.54	0.43
1:A:765:VAL:HG22	1:A:800:VAL:HB	1.99	0.43
2:B:307:ASP:OD1	2:B:392:ARG:NH1	2.45	0.43
2:B:600:LEU:HB3	2:B:615:MET:SD	2.59	0.43
2:B:857:ARG:HH21	2:B:942:ARG:NH2	2.17	0.43
10:L:28:LYS:HA	10:L:39:SER:HA	2.00	0.43
1:A:444:PHE:HD1	1:A:444:PHE:HA	1.71	0.43
1:A:1261:LYS:HE3	1:A:1261:LYS:HB2	1.84	0.43
2:B:861:ASP:OD1	2:B:862:GLN:N	2.50	0.43
6:H:76:THR:OG1	6:H:77:ARG:N	2.52	0.43
2:B:827:ILE:HG12	2:B:1012:ILE:HD11	2.01	0.42
1:A:87:ALA:HB3	1:A:276:LEU:HD23	2.01	0.42
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.54	0.42
1:A:402:ALA:HA	1:A:434:ARG:HA	2.01	0.42
1:A:1261:LYS:O	1:A:1264:GLU:HG3	2.19	0.42
2:B:287:ARG:NH1	2:B:321:GLY:O	2.52	0.42
2:B:227:LYS:HG2	2:B:236:HIS:CD2	2.54	0.42
1:A:331:GLY:HA2	1:A:334:GLY:H	1.85	0.42
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:LEU:HB2	2:B:90:ILE:HG12	2.01	0.42
2:B:771:SER:O	2:B:775:LYS:HE3	2.20	0.42
2:B:1013:ASN:OD1	2:B:1015:HIS:ND1	2.49	0.42
2:B:1129:ARG:NH1	11:T:21:DC:OP1	2.52	0.42
2:B:1138:MET:HE2	2:B:1146:PHE:CD1	2.54	0.42
5:F:128:LYS:HD2	5:F:149:GLU:HA	2.02	0.42
7:I:85:PHE:HB3	7:I:101:PHE:CD2	2.54	0.42
1:A:78:PRO:HB2	1:A:79:GLY:H	1.62	0.42
1:A:302:THR:OG1	1:A:306:ASN:OD1	2.37	0.42
1:A:644:LYS:HD2	1:A:644:LYS:HA	1.91	0.42
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	2.02	0.42
1:A:1255:GLU:HB3	1:A:1258:HIS:CE1	2.55	0.42
4:E:63:ASN:HA	4:E:64:PRO:HD3	1.88	0.42
8:J:44:TYR:HA	8:J:47:ARG:HB3	2.01	0.42
1:A:265:LYS:HZ1	1:A:303:TYR:HA	1.85	0.42
1:A:445:ASN:HA	1:A:454:SER:O	2.20	0.42
1:A:571:LEU:HD12	6:H:46:LEU:HD11	2.01	0.42
7:I:65:ASP:HB3	7:I:68:LEU:HD12	2.00	0.42
1:A:471:ASN:O	1:A:474:VAL:HG12	2.20	0.42
1:A:537:ARG:HD2	6:H:121:LEU:HD23	2.02	0.42
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.20	0.42
2:B:604:ARG:HH22	2:B:697:GLU:CD	2.27	0.42
2:B:1106:ARG:HH11	2:B:1126:GLY:HA2	1.85	0.42
2:B:1135:ARG:NH2	2:B:1136:ASP:OD1	2.53	0.42
9:K:88:LYS:O	9:K:92:ASN:ND2	2.43	0.42
1:A:423:ASP:OD1	1:A:423:ASP:N	2.49	0.42
1:A:879:GLU:OE1	1:A:962:ARG:NH2	2.53	0.42
1:A:913:LEU:HG	1:A:915:SER:H	1.84	0.42
1:A:1342:GLU:OE2	4:E:212:ARG:NH1	2.53	0.42
2:B:100:PRO:HG2	2:B:124:TYR:CZ	2.55	0.42
2:B:570:VAL:HB	2:B:573:GLN:HG2	2.02	0.42
6:H:6:PHE:HB3	6:H:59:ILE:HB	2.02	0.42
1:A:231:PRO:HA	1:A:234:MET:HG3	2.02	0.41
1:A:1260:LEU:HD12	1:A:1263:ILE:HD12	2.02	0.41
2:B:63:ILE:O	2:B:67:SER:OG	2.30	0.41
2:B:898:LEU:HD11	2:B:964:VAL:HG21	2.02	0.41
11:T:26:DG:H1	12:R:3:C:H42	1.67	0.41
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.20	0.41
3:C:41:ILE:HB	3:C:172:PRO:HG3	2.02	0.41
3:C:212:PRO:HA	3:C:213:PRO:HD3	1.86	0.41
6:H:14:GLU:HB3	6:H:27:GLU:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:CYS:SG	1:A:108:MET:N	2.93	0.41
1:A:868:TYR:HD2	1:A:1058:VAL:HG11	1.84	0.41
1:A:1395:GLY:HA3	1:A:1426:GLU:OE2	2.19	0.41
3:C:8:VAL:HG11	9:K:105:PHE:HD1	1.86	0.41
2:B:843:GLN:NE2	2:B:847:ASP:OD1	2.53	0.41
2:B:872:GLU:HG2	2:B:916:THR:HB	2.03	0.41
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.85	0.41
3:C:56:THR:HG21	3:C:63:ILE:HD11	2.02	0.41
4:E:135:PHE:HB3	4:E:140:LEU:HD11	2.03	0.41
6:H:133:ASN:OD1	6:H:133:ASN:N	2.54	0.41
1:A:91:PHE:HZ	1:A:207:ILE:HD12	1.85	0.41
1:A:523:ILE:HD13	1:A:622:VAL:HG22	2.03	0.41
1:A:598:LEU:O	6:H:122:LEU:HD12	2.21	0.41
2:B:170:LEU:HD12	2:B:171:PRO:HD2	2.02	0.41
2:B:792:MET:HE3	2:B:855:PHE:HE1	1.85	0.41
1:A:399:HIS:CE1	1:A:462:VAL:HG21	2.56	0.41
1:A:1215:ARG:HD3	1:A:1272:THR:O	2.21	0.41
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.49	0.41
2:B:128:LEU:HD21	2:B:170:LEU:HB2	2.03	0.41
2:B:487:THR:OG1	2:B:777:ALA:O	2.39	0.41
2:B:1156:ASP:OD1	2:B:1156:ASP:N	2.52	0.41
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.03	0.41
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.56	0.41
1:A:843:LYS:HD3	1:A:843:LYS:HA	1.94	0.41
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.56	0.41
2:B:364:ILE:HG13	2:B:365:THR:OG1	2.21	0.41
2:B:496:ARG:NH1	2:B:539:LEU:O	2.54	0.41
7:I:14:LEU:HD13	7:I:27:PHE:HB3	2.03	0.41
1:A:445:ASN:HD22	1:A:455:MET:HG2	1.86	0.40
1:A:607:ILE:HG12	1:A:612:ILE:HA	2.03	0.40
1:A:851:HIS:CG	5:F:139:PRO:HG3	2.56	0.40
2:B:122:LEU:HD22	2:B:958:GLN:HB2	2.03	0.40
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.21	0.40
8:J:36:LEU:HD13	8:J:47:ARG:HG3	2.04	0.40
9:K:47:ARG:HH11	9:K:47:ARG:HB3	1.85	0.40
9:K:63:VAL:HG22	9:K:71:PHE:HB3	2.03	0.40
1:A:577:ILE:H	1:A:577:ILE:HG13	1.71	0.40
1:A:636:GLU:OE2	1:A:962:ARG:NH1	2.54	0.40
1:A:874:ASP:HB2	1:A:1058:VAL:HA	2.04	0.40
1:A:1021:LEU:HD11	1:A:1025:ARG:NH1	2.36	0.40
1:A:1373:ASP:HA	1:A:1376:THR:HG22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:651:LEU:HD11	2:B:707:PRO:HB3	2.02	0.40
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.20	0.40
2:B:118:ARG:NH2	2:B:194:GLU:OE2	2.52	0.40
4:E:201:LYS:HA	4:E:201:LYS:HD3	1.95	0.40
1:A:464:PRO:HB2	9:K:4:PRO:HD3	2.04	0.40
2:B:63:ILE:HD12	2:B:95:ILE:HB	2.03	0.40
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.56	0.40
1:A:848:ILE:HB	1:A:1065:GLY:HA3	2.02	0.40
2:B:762:ASN:OD1	2:B:984:HIS:HD2	2.05	0.40
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	2.04	0.40
9:K:47:ARG:HD2	9:K:60:ALA:HA	2.03	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	1358/1733 (78%)	1238 (91%)	106 (8%)	14 (1%)	12	40
2	B	1077/1224 (88%)	1001 (93%)	67 (6%)	9 (1%)	16	44
3	C	264/318 (83%)	243 (92%)	19 (7%)	2 (1%)	16	44
4	E	211/215 (98%)	201 (95%)	9 (4%)	1 (0%)	24	54
5	F	82/155 (53%)	79 (96%)	3 (4%)	0	100	100
6	H	124/146 (85%)	107 (86%)	15 (12%)	2 (2%)	7	29
7	I	113/122 (93%)	100 (88%)	13 (12%)	0	100	100
8	J	63/70 (90%)	58 (92%)	5 (8%)	0	100	100
9	K	112/120 (93%)	108 (96%)	3 (3%)	1 (1%)	14	42
10	L	42/70 (60%)	34 (81%)	6 (14%)	2 (5%)	2	11
All	All	3446/4173 (83%)	3169 (92%)	246 (7%)	31 (1%)	14	42

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PRO
1	A	322	VAL
1	A	110	CYS
1	A	1437	GLY
2	B	468	GLU
2	B	1046	PRO
4	E	86	PRO
2	B	337	ARG
2	B	884	ARG
2	B	1017	ILE
3	C	90	ASP
3	C	148	ARG
10	L	69	ALA
1	A	40	THR
1	A	282	ASN
2	B	277	LYS
2	B	1108	ARG
9	K	26	LYS
10	L	41	SER
1	A	226	GLU
1	A	958	VAL
1	A	1156	PRO
1	A	1279	ILE
6	H	82	PRO
1	A	69	THR
1	A	592	ASP
1	A	597	LEU
2	B	260	GLY
6	H	18	GLY
2	B	824	ILE
1	A	1107	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	1196/1520 (79%)	1138 (95%)	58 (5%)	23	50
2	B	952/1061 (90%)	915 (96%)	37 (4%)	28	53
3	C	234/274 (85%)	226 (97%)	8 (3%)	32	57
4	E	195/197 (99%)	190 (97%)	5 (3%)	40	61
5	F	74/137 (54%)	72 (97%)	2 (3%)	39	60
6	H	114/128 (89%)	109 (96%)	5 (4%)	25	51
7	I	109/116 (94%)	106 (97%)	3 (3%)	38	60
8	J	60/65 (92%)	58 (97%)	2 (3%)	33	57
9	K	99/102 (97%)	92 (93%)	7 (7%)	13	39
10	L	39/57 (68%)	39 (100%)	0	100	100
All	All	3072/3657 (84%)	2945 (96%)	127 (4%)	27	52

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
1	A	61	ILE
1	A	93	VAL
1	A	132	LYS
1	A	179	LEU
1	A	208	LEU
1	A	222	LEU
1	A	235	ILE
1	A	270	LEU
1	A	271	LYS
1	A	287	HIS
1	A	308	ILE
1	A	322	VAL
1	A	335	ARG
1	A	351	THR
1	A	443	LEU
1	A	444	PHE
1	A	451	HIS
1	A	452	LYS
1	A	463	ILE
1	A	474	VAL
1	A	475	THR
1	A	481	ASP
1	A	512	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	532	ARG
1	A	550	LEU
1	A	605	MET
1	A	612	ILE
1	A	618	GLU
1	A	629	LEU
1	A	666	ILE
1	A	688	LYS
1	A	702	LEU
1	A	764	CYS
1	A	765	VAL
1	A	780	VAL
1	A	797	LYS
1	A	826	ASP
1	A	830	LYS
1	A	896	ARG
1	A	919	ILE
1	A	926	GLN
1	A	934	LYS
1	A	977	LYS
1	A	1015	VAL
1	A	1017	LEU
1	A	1078	GLN
1	A	1116	LEU
1	A	1207	LEU
1	A	1262	LYS
1	A	1297	GLU
1	A	1322	ILE
1	A	1329	THR
1	A	1350	LYS
1	A	1374	VAL
1	A	1377	THR
1	A	1400	CYS
1	A	1407	GLU
2	B	46	GLN
2	B	70	ILE
2	B	90	ILE
2	B	109	THR
2	B	134	LYS
2	B	319	GLU
2	B	364	ILE
2	B	365	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	396	ASP
2	B	483	LEU
2	B	547	VAL
2	B	549	THR
2	B	570	VAL
2	B	606	LYS
2	B	628	THR
2	B	653	VAL
2	B	737	THR
2	B	751	VAL
2	B	797	TYR
2	B	825	VAL
2	B	839	MET
2	B	916	THR
2	B	931	TYR
2	B	983	ARG
2	B	1007	VAL
2	B	1028	GLU
2	B	1051	THR
2	B	1057	LYS
2	B	1099	VAL
2	B	1147	LEU
2	B	1159	ARG
2	B	1160	VAL
2	B	1176	ASN
2	B	1188	LYS
2	B	1189	ILE
2	B	1194	ILE
2	B	1202	LEU
3	C	18	VAL
3	C	25	VAL
3	C	77	ILE
3	C	99	LEU
3	C	137	LYS
3	C	240	VAL
3	C	244	VAL
3	C	253	LYS
4	E	3	GLN
4	E	98	ILE
4	E	127	ILE
4	E	169	ARG
4	E	204	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	F	93	ILE
5	F	97	ARG
6	H	15	VAL
6	H	26	ILE
6	H	89	LEU
6	H	103	LYS
6	H	124	ARG
7	I	14	LEU
7	I	59	VAL
7	I	111	THR
8	J	3	VAL
8	J	5	VAL
9	K	1	MET
9	K	11	LEU
9	K	18	LYS
9	K	20	LYS
9	K	32	VAL
9	K	101	LEU
9	K	113	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	GLN
1	A	390	GLN
1	A	394	ASN
1	A	425	GLN
1	A	445	ASN
1	A	659	HIS
1	A	742	ASN
1	A	966	ASN
1	A	1048	ASN
1	A	1052	GLN
1	A	1258	HIS
2	B	115	GLN
2	B	255	GLN
2	B	350	GLN
2	B	449	ASN
2	B	538	ASN
2	B	587	HIS
2	B	686	ASN
2	B	762	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	770	GLN
2	B	843	GLN
2	B	951	GLN
2	B	984	HIS
2	B	986	GLN
2	B	1093	GLN
2	B	1195	HIS
3	C	131	HIS
3	C	242	GLN
4	E	63	ASN
5	F	104	ASN
6	H	128	ASN
7	I	22	ASN
7	I	60	GLN
7	I	90	GLN
9	K	112	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	R	8/9 (88%)	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 ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
11	3DR	T	20	11	8,11,12	1.37	1 (12%)	7,14,17	1.22	1 (14%)

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
11	3DR	T	20	11	-	1/3/15/16	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	20	3DR	O4'-C4'	-2.60	1.40	1.44

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	T	20	3DR	O4'-C4'-C3'	2.27	107.06	103.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	T	20	3DR	C4'-C5'-O5'-P

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](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	1372/1733 (79%)	0.47	94 (6%)	23	18	13, 57, 149, 257	0
2	B	1097/1224 (89%)	0.31	53 (4%)	35	26	11, 45, 111, 194	0
3	C	266/318 (83%)	0.18	4 (1%)	72	57	18, 46, 89, 158	0
4	E	213/215 (99%)	0.51	8 (3%)	44	31	31, 82, 157, 206	0
5	F	84/155 (54%)	0.16	3 (3%)	46	33	27, 60, 104, 162	0
6	H	130/146 (89%)	0.72	11 (8%)	16	15	35, 80, 141, 196	0
7	I	115/122 (94%)	0.41	4 (3%)	47	34	24, 59, 99, 112	0
8	J	65/70 (92%)	0.00	2 (3%)	51	38	19, 35, 72, 146	0
9	K	114/120 (95%)	0.01	0	100	100	22, 51, 86, 115	0
10	L	44/70 (62%)	1.30	13 (29%)	1	2	24, 89, 158, 208	0
11	T	11/29 (37%)	2.29	5 (45%)	0	1	107, 128, 181, 183	0
12	R	9/9 (100%)	1.52	1 (11%)	10	11	82, 102, 140, 147	0
All	All	3520/4211 (83%)	0.40	198 (5%)	30	23	11, 54, 138, 257	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	ILE	7.6
2	B	477	ALA	7.5
2	B	474	SER	6.2
1	A	65	LEU	5.8
1	A	1080	THR	5.6
10	L	45	ALA	5.4
8	J	65	PRO	5.3
1	A	397	ASN	5.0
6	H	139	ASN	5.0
10	L	27	LEU	4.9
1	A	60	SER	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	147	VAL	4.7
1	A	49	LYS	4.5
2	B	472	ALA	4.5
6	H	136	LYS	4.4
1	A	312	PRO	4.4
1	A	323	LYS	4.3
1	A	44	THR	4.3
6	H	84	ALA	4.2
1	A	98	LYS	4.2
1	A	73	GLY	4.2
2	B	509	ALA	4.1
2	B	1189	ILE	4.1
1	A	331	GLY	4.1
10	L	46	VAL	4.0
2	B	529	GLU	4.0
1	A	179	LEU	4.0
11	T	19	DA	4.0
1	A	1446	ASP	3.9
1	A	826	ASP	3.9
1	A	182	VAL	3.8
2	B	476	ARG	3.7
2	B	733	HIS	3.7
5	F	72	LYS	3.7
3	C	78	GLU	3.7
2	B	646	LEU	3.7
10	L	66	GLN	3.6
2	B	868	MET	3.6
2	B	918	ILE	3.6
2	B	266	ALA	3.5
1	A	79	GLY	3.5
2	B	275	TYR	3.5
1	A	1174	PHE	3.5
1	A	45	GLN	3.4
2	B	446	LEU	3.4
2	B	643	ASP	3.4
2	B	929	THR	3.4
1	A	1110	ASN	3.4
6	H	76	THR	3.4
2	B	470	LYS	3.3
2	B	468	GLU	3.3
1	A	317	LYS	3.3
2	B	1183	LYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	R	1	A	3.3
1	A	1126	ALA	3.3
1	A	91	PHE	3.2
1	A	1403	GLU	3.2
5	F	73	ALA	3.2
6	H	137	GLN	3.1
2	B	447	ALA	3.1
2	B	475	SER	3.1
11	T	24	DT	3.1
11	T	29	DG	3.1
1	A	74	MET	3.0
2	B	251	ILE	3.0
2	B	372	SER	3.0
1	A	975	HIS	3.0
1	A	64	ASN	3.0
4	E	9	ILE	2.9
1	A	1387	HIS	2.9
6	H	83	GLN	2.9
1	A	69	THR	2.9
6	H	129	TYR	2.9
1	A	177	ASP	2.9
2	B	576	ASP	2.9
1	A	180	LYS	2.9
7	I	116	ASN	2.9
10	L	35	SER	2.8
10	L	41	SER	2.8
1	A	42	ASP	2.8
1	A	3	GLY	2.8
1	A	286	HIS	2.8
10	L	53	HIS	2.8
2	B	712	PRO	2.8
1	A	240	PRO	2.8
1	A	174	ILE	2.8
1	A	235	ILE	2.8
1	A	1378	GLN	2.8
1	A	801	GLU	2.8
7	I	3	THR	2.7
1	A	423	ASP	2.7
6	H	19	ARG	2.7
10	L	63	ARG	2.7
8	J	26	GLN	2.7
1	A	37	PHE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1005	GLU	2.7
1	A	283	GLY	2.7
1	A	54	ASN	2.7
1	A	285	PRO	2.6
2	B	502	ILE	2.6
1	A	1262	LYS	2.6
1	A	322	VAL	2.6
10	L	36	SER	2.6
1	A	146	MET	2.6
2	B	884	ARG	2.6
1	A	87	ALA	2.6
2	B	887	HIS	2.6
1	A	596	THR	2.6
2	B	895	ASP	2.6
1	A	208	LEU	2.6
1	A	1288	ASP	2.5
1	A	56	PRO	2.5
2	B	530	GLY	2.5
3	C	268	ASP	2.5
4	E	93	MET	2.5
1	A	1161	THR	2.5
6	H	63	LEU	2.5
1	A	59	GLY	2.5
1	A	108	MET	2.4
2	B	241	ARG	2.4
2	B	427	ASP	2.4
2	B	648	HIS	2.4
6	H	140	ALA	2.4
2	B	261	ARG	2.4
1	A	220	THR	2.4
1	A	1425	SER	2.4
2	B	629	ASP	2.4
1	A	593	GLU	2.4
10	L	40	LEU	2.4
1	A	1330	ASN	2.4
1	A	234	MET	2.4
1	A	237	THR	2.3
1	A	66	LYS	2.3
1	A	112	LYS	2.3
2	B	29	ASP	2.3
2	B	267	ARG	2.3
1	A	72	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	249	SER	2.3
1	A	35	ILE	2.3
1	A	41	MET	2.3
1	A	290	GLU	2.3
4	E	152	LYS	2.3
2	B	869	SER	2.3
2	B	931	TYR	2.3
1	A	141	LEU	2.3
5	F	155	LEU	2.3
1	A	1257	ASP	2.3
2	B	650	GLU	2.3
1	A	1123	GLY	2.2
7	I	13	MET	2.2
1	A	109	HIS	2.2
1	A	1307	GLU	2.2
1	A	50	ILE	2.2
1	A	1125	ALA	2.2
2	B	473	MET	2.2
10	L	64	LEU	2.2
2	B	932	HIS	2.2
2	B	432	MET	2.2
6	H	86	ASP	2.2
1	A	4	GLN	2.2
2	B	262	GLU	2.2
2	B	467	GLY	2.2
2	B	20	ASP	2.2
2	B	471	LYS	2.2
1	A	976	THR	2.2
7	I	55	THR	2.2
1	A	1187	GLN	2.2
1	A	1309	ASP	2.2
11	T	18	DC	2.1
1	A	1256	GLU	2.1
1	A	305	ASP	2.1
2	B	668	ASP	2.1
1	A	106	VAL	2.1
1	A	867	ILE	2.1
2	B	70	ILE	2.1
3	C	163	ILE	2.1
1	A	176	LYS	2.1
1	A	1112	LYS	2.1
1	A	324	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	113	LEU	2.1
4	E	98	ILE	2.1
1	A	1444	MET	2.1
3	C	39	ALA	2.1
2	B	917	PRO	2.1
4	E	125	PRO	2.1
4	E	110	PHE	2.1
2	B	357	GLN	2.1
1	A	52	GLY	2.1
10	L	49	LYS	2.1
4	E	127	ILE	2.1
11	T	21	DC	2.1
1	A	293	GLU	2.1
2	B	299	GLU	2.1
4	E	102	GLU	2.1
1	A	1078	GLN	2.0
2	B	878	GLN	2.0
1	A	1359	ASP	2.0
10	L	42	ARG	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
11	3DR	T	20	11/12	0.82	0.20	136,143,151,154	0

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
13	ZN	A	1801	1/1	0.95	0.06	132,132,132,132	0
13	ZN	A	1802	1/1	0.97	0.05	82,82,82,82	0
13	ZN	B	1301	1/1	0.99	0.02	79,79,79,79	0
13	ZN	I	202	1/1	0.99	0.03	28,28,28,28	0
14	MG	A	1803	1/1	0.99	0.07	10,10,10,10	0
13	ZN	C	401	1/1	1.00	0.01	36,36,36,36	0
13	ZN	J	101	1/1	1.00	0.02	27,27,27,27	0
13	ZN	L	101	1/1	1.00	0.02	83,83,83,83	0
13	ZN	I	201	1/1	1.00	0.04	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.