



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:45 PM UTC

PDB ID : 6BQF / pdb_00006bqf
Title : Pol II elongation complex with 'dT-AP' at i+1, i-1 position
Authors : Wang, W.; Wang, D.
Deposited on : 2017-11-27
Resolution : 3.35 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

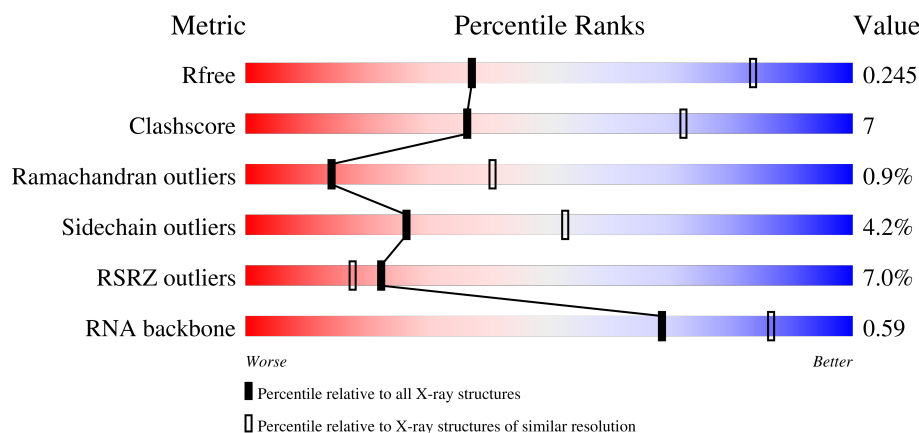
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)
RNA backbone	3983	1110 (3.72-3.00)

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	6% 61% 16% • 21%
2	B	1224	5% 68% 20% • 10%
3	C	318	2% 64% 18% • 16%
4	E	215	11% 88% 11% •

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Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	T	29	
12	R	9	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 28243 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*TP*(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
			232	111	35	74	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		

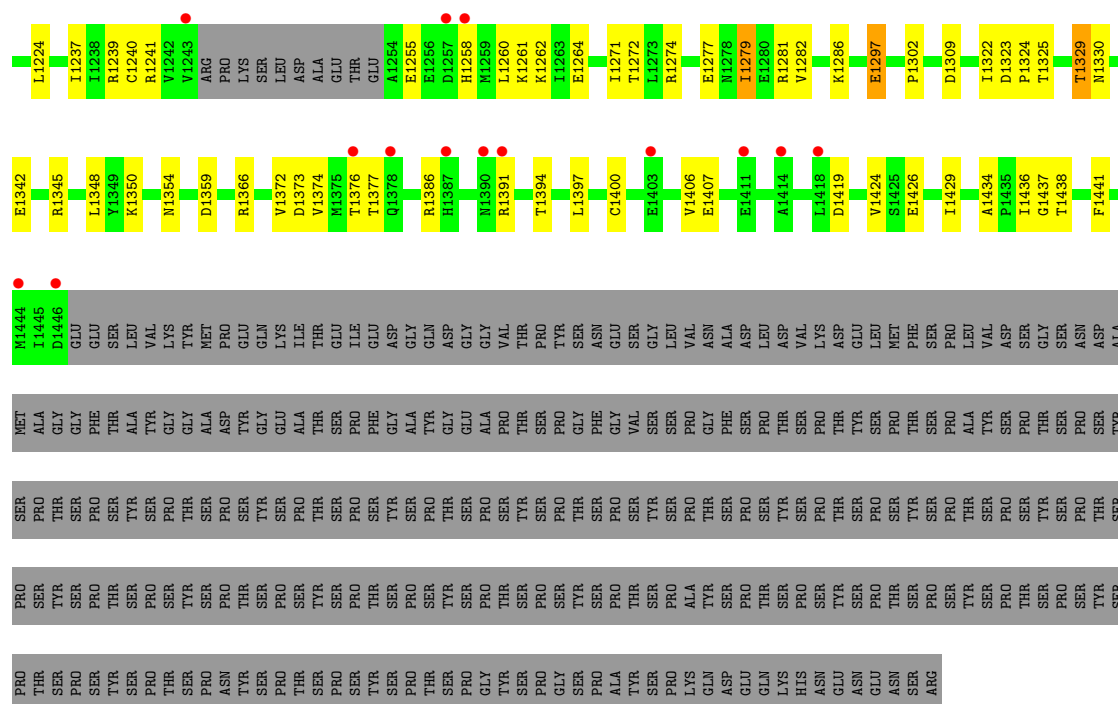
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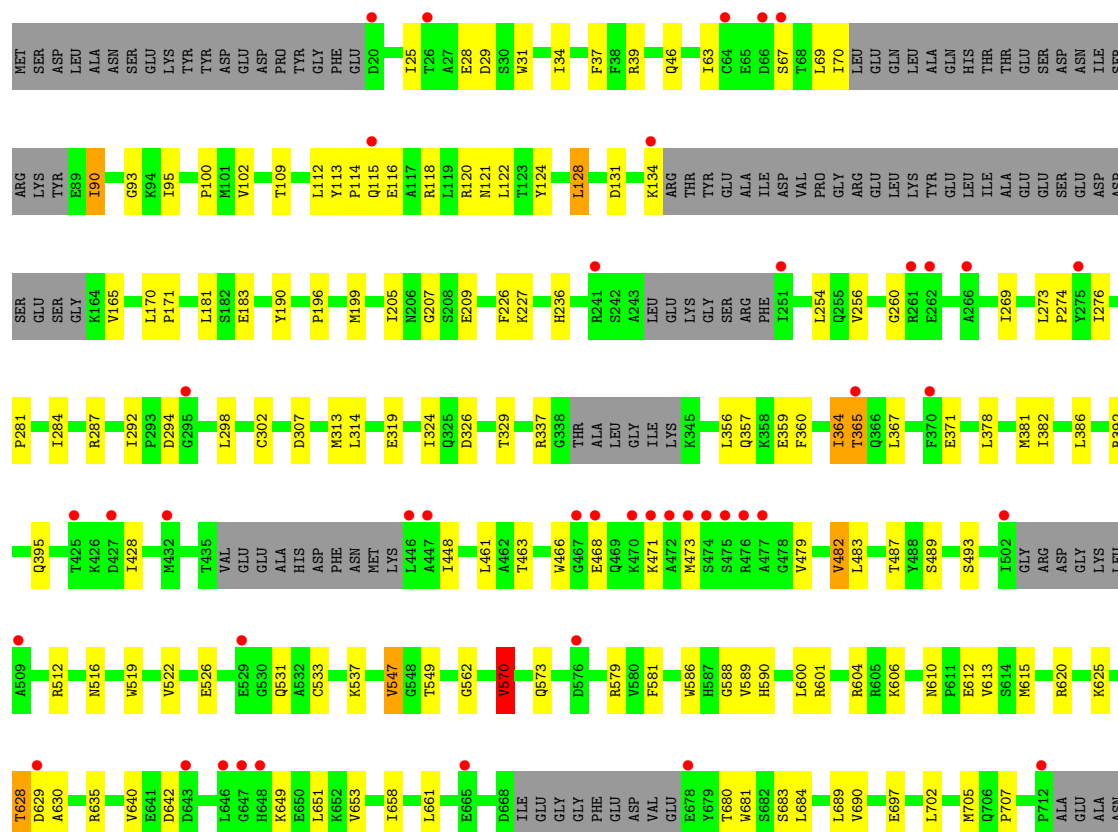
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total 1	Zn 1	0	0
13	C	1	Total 1	Zn 1	0	0
13	I	2	Total 2	Zn 2	0	0
13	J	1	Total 1	Zn 1	0	0
13	L	1	Total 1	Zn 1	0	0

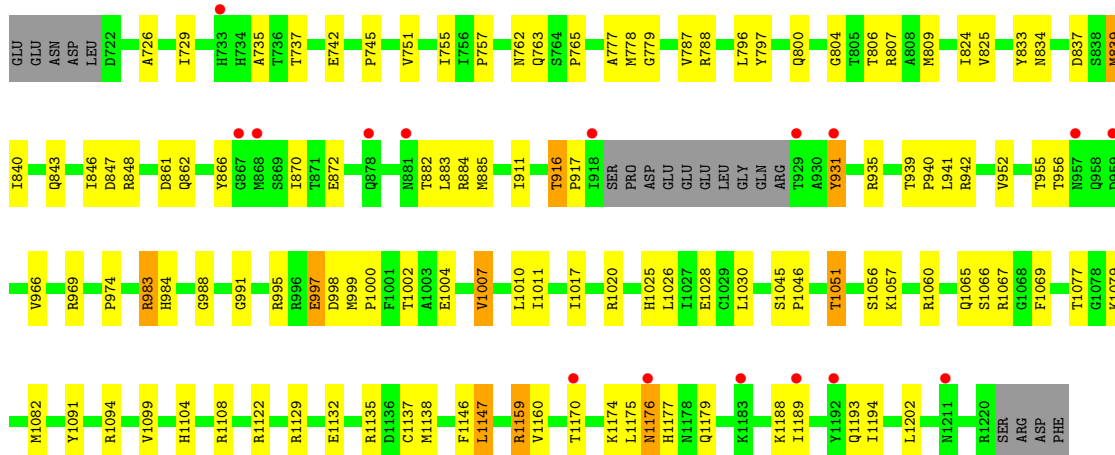
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

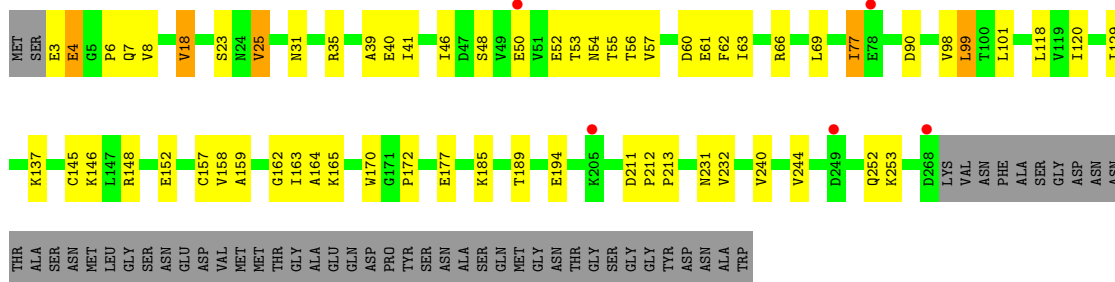


• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

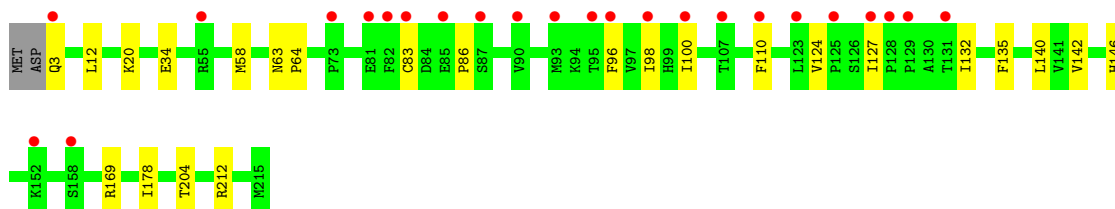
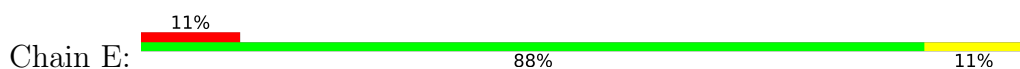




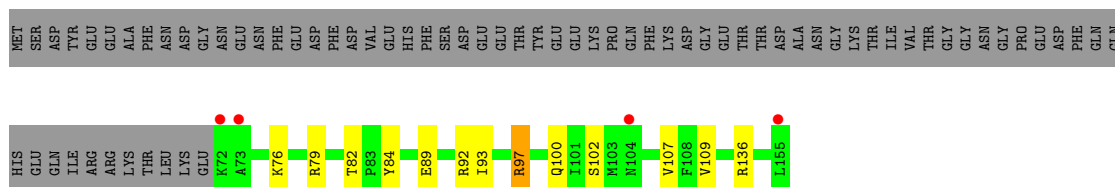
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



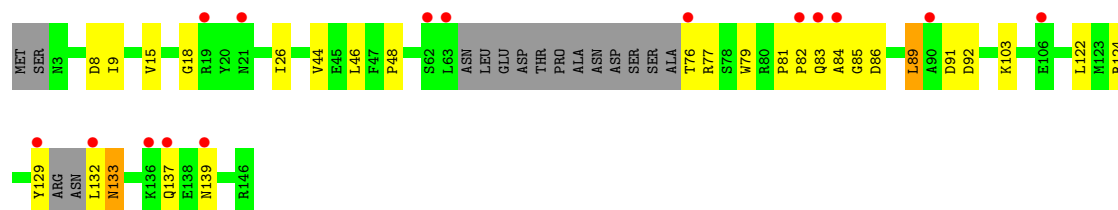
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



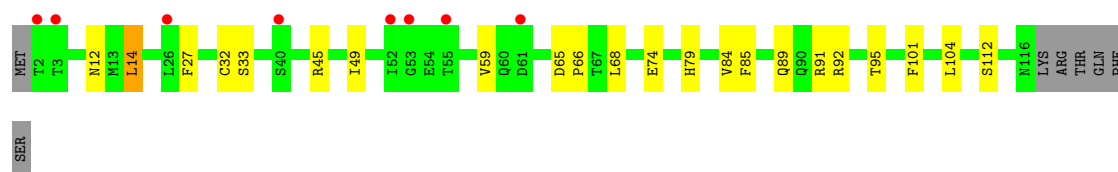
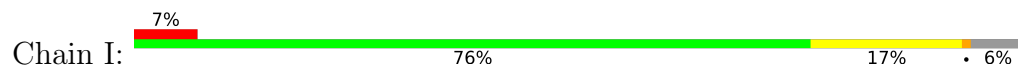
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



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



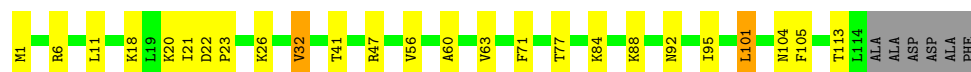
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



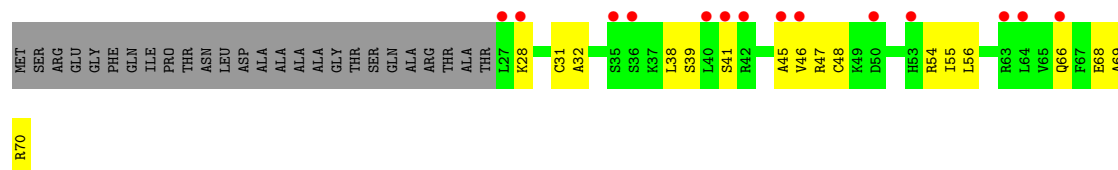
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



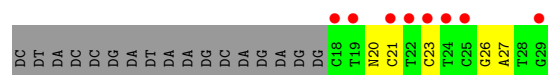
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



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

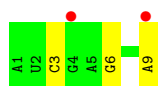


- Molecule 11: DNA (5'-D(P*CP*TP*(3DR)P*CP*TP*CP*TP*TP*GP*AP*TP*G)-3')



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

Chain R: 22% 67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.40Å 221.35Å 193.70Å 90.00° 100.60° 90.00°	Depositor
Resolution (Å)	82.76 – 3.35 82.76 – 3.35	Depositor EDS
% Data completeness (in resolution range)	92.0 (82.76-3.35) 92.0 (82.76-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.217 , 0.245 0.219 , 0.245	Depositor DCC
R_{free} test set	4550 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	28243	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: ZN, 3DR, MG

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	0.70	4/14838 (0.0%)
2	B	0.25	0/8896	0.70	4/11996 (0.0%)
3	C	0.26	0/2133	0.70	0/2891
4	E	0.25	0/1780	0.72	0/2395
5	F	0.26	0/691	0.72	0/933
6	H	0.27	0/1060	0.70	0/1434
7	I	0.24	0/953	0.65	0/1284
8	J	0.25	0/541	0.62	0/727
9	K	0.23	0/937	0.67	0/1265
10	L	0.24	0/353	0.63	1/468 (0.2%)
11	T	0.13	0/244	0.30	0/371
12	R	0.07	0/218	0.12	0/339
All	All	0.25	0/28781	0.69	9/38941 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	525	GLN	CB-CA-C	-5.80	109.90	116.63
1	A	1098	VAL	CB-CA-C	-5.47	108.55	114.35
10	L	45	ALA	CB-CA-C	-5.47	110.29	116.63
1	A	71	GLN	CB-CA-C	-5.35	109.95	117.23
2	B	570	VAL	CA-C-N	5.24	124.86	119.05
2	B	570	VAL	C-N-CA	5.24	124.86	119.05
1	A	507	VAL	CB-CA-C	-5.16	108.88	114.35
2	B	113	TYR	CA-C-N	5.03	125.05	119.32
2	B	113	TYR	C-N-CA	5.03	125.05	119.32

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	10873	172	0
2	B	8726	0	8760	157	0
3	C	2095	0	2051	43	0
4	E	1744	0	1772	11	0
5	F	679	0	701	8	0
6	H	1043	0	1015	14	0
7	I	935	0	886	16	0
8	J	532	0	542	11	0
9	K	919	0	929	16	0
10	L	351	0	375	9	0
11	T	232	0	134	5	0
12	R	194	0	99	2	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	28243	0	28137	404	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 (404) 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	1.67	0.76
1:A:899:VAL:HG22	1:A:1029:ARG:HG2	1.70	0.73
8:J:5:VAL:HG22	8:J:6:ARG:HG3	1.69	0.73
3:C:66:ARG:NH2	8:J:3:VAL:O	2.23	0.72
3:C:6:PRO:HB2	9:K:101:LEU:HD23	1.70	0.72
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.72	0.71
2:B:911:ILE:HD11	2:B:941:LEU:HD23	1.73	0.71
2:B:1174:LYS:HB2	2:B:1179:GLN:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.73	0.69
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.75	0.69
2:B:287:ARG:NH1	2:B:324:ILE:O	2.27	0.68
7:I:92:ARG:HB3	7:I:95:THR:HG23	1.76	0.68
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.75	0.68
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.75	0.67
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.77	0.67
3:C:46:ILE:HD13	3:C:159:ALA:HB2	1.76	0.66
1:A:338:GLY:HA2	2:B:1129:ARG:HH21	1.58	0.66
2:B:1175:LEU:O	2:B:1176:ASN:ND2	2.29	0.66
1:A:134:ARG:NH1	1:A:220:THR:O	2.29	0.66
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.30	0.65
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.79	0.65
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.77	0.64
2:B:165:VAL:HG21	2:B:448:ILE:HD12	1.79	0.64
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.80	0.64
2:B:1065:GLN:HG2	2:B:1069:PHE:HB2	1.79	0.64
1:A:4:GLN:OE1	2:B:1159:ARG:NH1	2.31	0.64
4:E:12:LEU:HD11	4:E:58:MET:HE1	1.80	0.64
1:A:40:THR:HG22	1:A:41:MET:HG3	1.79	0.63
3:C:50:GLU:HG2	10:L:66:GLN:HG2	1.80	0.63
3:C:99:LEU:HB3	3:C:120:ILE:HD13	1.80	0.63
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.81	0.63
3:C:3:GLU:HG3	3:C:4:GLU:HG3	1.80	0.63
2:B:839:MET:HE2	2:B:1010:LEU:HD21	1.81	0.62
1:A:1079:MET:HE3	1:A:1359:ASP:HB2	1.82	0.62
2:B:1129:ARG:NH1	11:T:21:DC:OP1	2.33	0.62
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.82	0.61
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.82	0.61
1:A:744:LYS:HE2	1:A:748:MET:HE3	1.82	0.61
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.82	0.61
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.33	0.61
2:B:28:GLU:OE1	2:B:807:ARG:NH1	2.33	0.61
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.83	0.61
1:A:1187:GLN:HG3	1:A:1188:GLN:HG3	1.83	0.61
1:A:601:LYS:HB2	1:A:603:ASN:HD22	1.66	0.60
1:A:693:VAL:HG21	1:A:721:PHE:HE2	1.64	0.60
6:H:91:ASP:OD1	6:H:92:ASP:N	2.33	0.60
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.82	0.60
1:A:1281:ARG:HG2	1:A:1309:ASP:HB2	1.83	0.60
1:A:1009:ASN:OD1	1:A:1012:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.28	0.60
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.84	0.60
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.83	0.60
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.84	0.60
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.67	0.60
5:F:82:THR:HG22	5:F:84:TYR:H	1.66	0.60
1:A:1239:ARG:HH22	1:A:1241:ARG:HH21	1.49	0.59
2:B:916:THR:HG23	2:B:935:ARG:HB2	1.84	0.59
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.85	0.59
6:H:129:TYR:O	6:H:132:LEU:N	2.37	0.58
1:A:1148:ILE:HD13	7:I:49:ILE:HD12	1.86	0.58
1:A:1207:LEU:HD23	1:A:1274:ARG:HD2	1.85	0.58
2:B:778:MET:HE1	2:B:1094:ARG:HH11	1.69	0.58
1:A:1116:LEU:HD22	1:A:1329:THR:HB	1.86	0.58
1:A:68:GLN:O	1:A:70:CYS:N	2.35	0.57
1:A:110:CYS:SG	1:A:111:GLY:N	2.71	0.57
1:A:993:LEU:HD22	1:A:1046:LEU:HG	1.85	0.57
4:E:178:ILE:HB	4:E:212:ARG:HD3	1.85	0.57
2:B:620:ARG:NH2	7:I:89:GLN:OE1	2.38	0.57
7:I:32:CYS:SG	7:I:33:SER:N	2.76	0.57
1:A:1122:PRO:HD3	1:A:1323:ASP:HB2	1.87	0.57
3:C:145:CYS:SG	3:C:146:LYS:N	2.77	0.57
3:C:6:PRO:HB3	3:C:25:VAL:HG13	1.85	0.57
5:F:76:LYS:O	5:F:79:ARG:NH1	2.35	0.57
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.38	0.56
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.86	0.56
2:B:95:ILE:HD11	2:B:128:LEU:HB3	1.85	0.56
2:B:642:ASP:HB3	2:B:649:LYS:HG2	1.87	0.56
2:B:983:ARG:NH1	2:B:1028:GLU:OE1	2.35	0.56
1:A:697:ALA:HA	1:A:702:LEU:HB2	1.87	0.56
1:A:802:ASN:OD1	2:B:729:ILE:N	2.39	0.56
1:A:1151:GLU:OE2	7:I:45:ARG:NH1	2.38	0.56
1:A:30:ILE:HG23	2:B:1170:THR:HG23	1.88	0.56
1:A:1325:THR:OG1	4:E:146:HIS:O	2.21	0.56
1:A:1342:GLU:OE2	4:E:212:ARG:NH1	2.39	0.56
3:C:46:ILE:HD12	3:C:157:CYS:HB3	1.87	0.55
1:A:34:LYS:H	1:A:34:LYS:HD3	1.72	0.55
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.40	0.55
1:A:306:ASN:ND2	1:A:321:PRO:O	2.39	0.55
2:B:463:THR:HG22	11:T:27:DA:H2"	1.89	0.54
2:B:613:VAL:HG22	2:B:628:THR:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.88	0.54
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.88	0.54
3:C:7:GLN:HB2	3:C:23:SER:HB2	1.89	0.54
2:B:882:THR:HB	2:B:885:MET:HE2	1.89	0.54
1:A:378:GLU:OE2	1:A:387:ARG:NH2	2.40	0.54
1:A:528:LEU:HD23	1:A:751:SER:HA	1.89	0.54
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.90	0.54
1:A:636:GLU:OE2	1:A:962:ARG:NH1	2.40	0.54
3:C:163:ILE:HG22	3:C:165:LYS:H	1.73	0.54
2:B:620:ARG:HD2	7:I:68:LEU:HD11	1.90	0.53
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.72	0.53
9:K:88:LYS:O	9:K:92:ASN:ND2	2.39	0.53
2:B:702:LEU:HD21	2:B:735:ALA:HB1	1.89	0.53
1:A:868:TYR:CE1	1:A:1064:VAL:HG21	2.43	0.53
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.91	0.53
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.91	0.53
1:A:406:ILE:HB	1:A:431:LYS:HB2	1.90	0.53
3:C:185:LYS:HG2	3:C:213:PRO:HG3	1.91	0.53
6:H:85:GLY:HA2	6:H:86:ASP:HB3	1.90	0.53
1:A:562:THR:O	1:A:576:GLN:NE2	2.42	0.53
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.91	0.52
1:A:634:THR:HG1	1:A:642:CYS:HG	1.57	0.52
1:A:469:ARG:NH2	2:B:991:GLY:O	2.43	0.52
2:B:487:THR:OG1	2:B:777:ALA:O	2.26	0.52
2:B:779:GLY:HA2	2:B:796:LEU:HB2	1.92	0.52
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.42	0.52
6:H:8:ASP:OD1	6:H:9:ILE:N	2.41	0.52
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.42	0.52
6:H:137:GLN:HG3	6:H:139:ASN:H	1.73	0.52
10:L:38:LEU:HD21	10:L:48:CYS:HA	1.92	0.52
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.92	0.52
2:B:586:TRP:CD1	2:B:588:GLY:H	2.28	0.52
3:C:77:ILE:HG12	3:C:129:ILE:HD11	1.92	0.52
7:I:84:VAL:HG23	7:I:104:LEU:HD11	1.92	0.52
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.50	0.51
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.90	0.51
3:C:69:LEU:HD12	8:J:6:ARG:HD3	1.91	0.51
1:A:477:PRO:HG3	1:A:521:MET:HE2	1.91	0.51
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.91	0.51
9:K:56:VAL:HG22	9:K:77:THR:HG22	1.93	0.51
2:B:680:THR:O	2:B:683:SER:OG	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:ARG:HE	1:A:536:LEU:HD21	1.75	0.51
2:B:522:VAL:HG11	2:B:537:LYS:HD2	1.93	0.51
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.43	0.51
3:C:252:GLN:HG3	9:K:95:ILE:HG23	1.91	0.51
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.75	0.51
2:B:487:THR:HG22	2:B:489:SER:H	1.76	0.51
3:C:165:LYS:O	9:K:6:ARG:NH1	2.44	0.51
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.92	0.51
1:A:834:THR:HG21	1:A:1077:THR:HA	1.93	0.51
1:A:1286:LYS:HE2	1:A:1302:PRO:HB2	1.93	0.51
1:A:95:PHE:HB3	1:A:234:MET:HE2	1.93	0.50
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.93	0.50
10:L:68:GLU:O	10:L:70:ARG:N	2.44	0.50
1:A:544:ASP:OD1	1:A:545:GLN:N	2.42	0.50
2:B:839:MET:HG3	2:B:1010:LEU:HD11	1.94	0.50
4:E:83:CYS:HB2	4:E:110:PHE:HE1	1.76	0.50
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.47	0.50
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.94	0.50
2:B:116:GLU:HG3	10:L:55:ILE:HD11	1.93	0.50
1:A:306:ASN:HB2	1:A:324:SER:HB3	1.93	0.50
7:I:14:LEU:HD13	7:I:27:PHE:HB3	1.94	0.50
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.94	0.50
5:F:107:VAL:HG12	5:F:109:VAL:H	1.76	0.50
1:A:148:CYS:HB2	1:A:168:GLY:HA2	1.94	0.49
5:F:82:THR:O	5:F:136:ARG:NH1	2.32	0.49
1:A:76:GLU:OE2	2:B:1159:ARG:NH1	2.45	0.49
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.94	0.49
1:A:760:GLN:HG2	1:A:765:VAL:HA	1.95	0.49
1:A:1142:THR:O	1:A:1145:SER:OG	2.29	0.49
2:B:287:ARG:NH2	2:B:294:ASP:OD1	2.45	0.49
2:B:471:LYS:HA	2:B:473:MET:HE2	1.93	0.49
1:A:443:LEU:HD13	1:A:455:MET:HE2	1.93	0.49
1:A:634:THR:OG1	1:A:642:CYS:SG	2.69	0.49
2:B:512:ARG:NH1	2:B:533:CYS:O	2.44	0.49
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.93	0.49
2:B:281:PRO:HB2	2:B:284:ILE:HG12	1.94	0.49
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.78	0.49
1:A:825:ILE:HD12	2:B:512:ARG:HD3	1.94	0.49
1:A:868:TYR:OH	1:A:1366:ARG:HD3	2.13	0.49
2:B:872:GLU:HG2	2:B:916:THR:HB	1.95	0.49
1:A:868:TYR:CZ	1:A:1064:VAL:HG21	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:21:ILE:HD13	9:K:84:LYS:HE2	1.96	0.48
2:B:298:LEU:HD22	2:B:314:LEU:HD13	1.95	0.48
6:H:84:ALA:HB3	6:H:86:ASP:HB3	1.95	0.48
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.96	0.48
1:A:560:ILE:HB	6:H:79:TRP:H	1.78	0.48
1:A:1064:VAL:HG23	1:A:1067:LEU:HD23	1.95	0.48
2:B:995:ARG:NH1	2:B:997:GLU:OE1	2.46	0.48
1:A:596:THR:C	1:A:598:LEU:H	2.21	0.48
1:A:962:ARG:HA	1:A:965:GLN:HG2	1.96	0.48
6:H:81:PRO:O	6:H:83:GLN:N	2.47	0.48
8:J:8:PHE:H	8:J:49:MET:HE3	1.78	0.48
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.95	0.48
3:C:3:GLU:N	9:K:104:ASN:HD21	2.12	0.48
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.96	0.48
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.95	0.48
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.29	0.47
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.96	0.47
3:C:54:ASN:ND2	3:C:60:ASP:OD1	2.41	0.47
1:A:550:LEU:HD21	1:A:561:PRO:HD2	1.95	0.47
1:A:1138:ILE:HG22	1:A:1279:ILE:HG21	1.96	0.47
11:T:26:DG:H1	12:R:3:C:H42	1.62	0.47
1:A:1373:ASP:HA	1:A:1376:THR:HG22	1.95	0.47
1:A:471:ASN:O	1:A:474:VAL:HG12	2.14	0.47
2:B:357:GLN:NE2	2:B:371:GLU:OE1	2.41	0.47
3:C:56:THR:HG21	3:C:63:ILE:HD11	1.95	0.47
1:A:541:ILE:HD12	1:A:577:ILE:HG12	1.97	0.47
3:C:48:SER:HB3	3:C:158:VAL:HB	1.96	0.47
2:B:493:SER:OG	2:B:526:GLU:OE2	2.29	0.47
2:B:651:LEU:HD11	2:B:707:PRO:HB3	1.97	0.47
2:B:952:VAL:HG13	2:B:966:VAL:HG22	1.95	0.47
6:H:89:LEU:H	6:H:89:LEU:HD13	1.79	0.47
1:A:93:VAL:HG12	1:A:304:MET:HE3	1.97	0.47
1:A:115:LEU:HB2	1:A:122:MET:HE3	1.96	0.47
1:A:396:PRO:HG3	1:A:416:ARG:HB3	1.96	0.47
2:B:307:ASP:OD1	2:B:392:ARG:NH1	2.37	0.47
2:B:482:VAL:HG11	11:T:26:DG:H5"	1.97	0.47
2:B:1082:MET:HA	3:C:189:THR:HA	1.97	0.47
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.97	0.46
1:A:182:VAL:HA	1:A:201:VAL:HA	1.96	0.46
1:A:781:ASP:OD1	7:I:91:ARG:NH2	2.48	0.46
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:570:VAL:HB	2:B:573:GLN:HG2	1.97	0.46
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.97	0.46
2:B:579:ARG:HA	2:B:589:VAL:HA	1.95	0.46
2:B:956:THR:HG22	10:L:46:VAL:HG11	1.97	0.46
1:A:108:MET:O	1:A:110:CYS:N	2.47	0.46
1:A:1386:ARG:O	1:A:1391:ARG:NH1	2.48	0.46
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.96	0.46
4:E:124:VAL:HG13	4:E:132:ILE:HB	1.98	0.46
3:C:55:THR:HG1	3:C:152:GLU:H	1.63	0.46
2:B:428:ILE:HD11	2:B:448:ILE:HG23	1.97	0.46
3:C:98:VAL:HG22	3:C:158:VAL:HG22	1.97	0.46
7:I:65:ASP:HB3	7:I:68:LEU:HD12	1.96	0.46
1:A:1206:ASP:O	1:A:1274:ARG:NH1	2.49	0.46
2:B:209:GLU:OE1	2:B:788:ARG:NH2	2.49	0.46
3:C:101:LEU:HB2	3:C:118:LEU:HD23	1.98	0.46
5:F:97:ARG:NH1	5:F:100:GLN:OE1	2.49	0.46
1:A:780:VAL:HG23	1:A:789:LYS:HE2	1.98	0.46
2:B:378:LEU:O	2:B:382:ILE:HG12	2.16	0.46
3:C:8:VAL:HG11	9:K:105:PHE:HD1	1.81	0.46
1:A:774:ARG:HG3	1:A:797:LYS:HZ2	1.81	0.45
1:A:1324:PRO:HB2	4:E:142:VAL:HG11	1.97	0.45
2:B:69:LEU:HB2	2:B:90:ILE:HG12	1.98	0.45
1:A:279:LEU:HB3	1:A:289:ILE:HG22	1.96	0.45
2:B:512:ARG:NH2	2:B:531:GLN:O	2.38	0.45
1:A:131:SER:HB3	1:A:223:GLY:HA2	1.98	0.45
1:A:235:ILE:H	1:A:235:ILE:HG13	1.55	0.45
1:A:588:LEU:HD22	1:A:629:LEU:HD23	1.98	0.45
1:A:1194:ARG:HH21	1:A:1237:ILE:HD13	1.80	0.45
1:A:1438:THR:HG23	5:F:92:ARG:HB2	1.97	0.45
1:A:242:PRO:HA	1:A:243:PRO:HD3	1.82	0.45
2:B:562:GLY:O	2:B:590:HIS:ND1	2.41	0.45
2:B:939:THR:HA	2:B:940:PRO:HD3	1.82	0.45
3:C:52:GLU:HG2	3:C:53:THR:HG23	1.98	0.45
10:L:47:ARG:HG2	10:L:54:ARG:HG2	1.99	0.45
1:A:481:ASP:OD1	1:A:481:ASP:N	2.47	0.45
1:A:449:SER:HB3	2:B:1137:CYS:SG	2.57	0.45
2:B:298:LEU:O	2:B:302:CYS:N	2.41	0.45
2:B:843:GLN:HE21	9:K:6:ARG:HH21	1.65	0.45
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.52	0.45
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.52	0.45
1:A:663:SER:OG	1:A:664:THR:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:949:ASP:OD1	1:A:949:ASP:N	2.50	0.45
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.98	0.45
1:A:1064:VAL:HA	1:A:1067:LEU:HB3	1.99	0.45
2:B:941:LEU:HD22	2:B:942:ARG:H	1.82	0.45
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.98	0.44
2:B:848:ARG:NH1	8:J:8:PHE:O	2.49	0.44
2:B:999:MET:HG3	2:B:1000:PRO:HD2	2.00	0.44
7:I:101:PHE:HE1	7:I:112:SER:HB3	1.81	0.44
2:B:1175:LEU:C	2:B:1177:HIS:H	2.24	0.44
2:B:916:THR:HA	2:B:917:PRO:HD3	1.80	0.44
1:A:867:ILE:HD11	1:A:1010:ALA:HB1	1.99	0.44
2:B:199:MET:SD	2:B:199:MET:N	2.84	0.44
2:B:610:ASN:HB3	2:B:613:VAL:HG23	1.99	0.44
2:B:1135:ARG:HG3	2:B:1147:LEU:HD21	2.00	0.44
2:B:726:ALA:HB1	2:B:1051:THR:HG21	2.00	0.44
1:A:544:ASP:HB2	9:K:47:ARG:HH21	1.82	0.44
2:B:118:ARG:HA	2:B:207:GLY:HA2	2.00	0.44
2:B:883:LEU:O	2:B:885:MET:N	2.51	0.44
2:B:114:PRO:HG2	2:B:181:LEU:HD11	2.00	0.44
2:B:600:LEU:HB3	2:B:615:MET:SD	2.58	0.44
2:B:601:ARG:HA	2:B:615:MET:HE1	1.98	0.44
2:B:681:TRP:CH2	2:B:690:VAL:HG11	2.53	0.44
6:H:76:THR:OG1	6:H:77:ARG:N	2.51	0.44
6:H:133:ASN:OD1	6:H:133:ASN:N	2.42	0.44
1:A:331:GLY:HA2	1:A:334:GLY:H	1.83	0.44
2:B:466:TRP:HB2	2:B:479:VAL:HG21	1.99	0.44
2:B:806:THR:HG23	2:B:1045:SER:HA	2.00	0.44
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.99	0.44
1:A:571:LEU:HD12	6:H:46:LEU:HD11	1.99	0.43
3:C:57:VAL:HG11	8:J:60:PHE:HB3	2.00	0.43
3:C:62:PHE:O	3:C:66:ARG:HG3	2.18	0.43
1:A:483:ASP:HA	2:B:988:GLY:HA2	2.01	0.43
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.54	0.43
3:C:41:ILE:HB	3:C:172:PRO:HG3	2.00	0.43
1:A:396:PRO:C	1:A:398:GLU:H	2.27	0.43
2:B:115:GLN:NE2	2:B:787:VAL:O	2.51	0.43
2:B:547:VAL:N	2:B:612:GLU:OE2	2.45	0.43
1:A:78:PRO:HB2	1:A:79:GLY:H	1.65	0.43
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.53	0.43
1:A:595:THR:OG1	1:A:603:ASN:OD1	2.32	0.43
1:A:839:ARG:NH2	2:B:1132:GLU:OE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:18:VAL:HG23	3:C:232:VAL:HB	2.01	0.43
10:L:28:LYS:HA	10:L:39:SER:HA	2.01	0.43
1:A:523:ILE:HD13	1:A:622:VAL:HG22	2.01	0.43
2:B:25:ILE:HG23	2:B:29:ASP:HB2	2.01	0.43
2:B:256:VAL:HG11	2:B:382:ILE:HD13	2.00	0.43
11:T:23:DC:H42	12:R:6:G:H1	1.66	0.43
1:A:445:ASN:ND2	1:A:455:MET:HG2	2.34	0.43
2:B:931:TYR:HD1	2:B:931:TYR:HA	1.74	0.43
2:B:999:MET:HG2	2:B:1007:VAL:HG13	2.01	0.43
4:E:63:ASN:HA	4:E:64:PRO:HD3	1.88	0.43
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	2.00	0.43
2:B:861:ASP:OD1	2:B:862:GLN:N	2.51	0.43
7:I:85:PHE:HB3	7:I:101:PHE:CD2	2.54	0.43
1:A:326:ARG:HG2	1:A:1406:VAL:HG11	2.01	0.42
2:B:93:GLY:N	2:B:131:ASP:O	2.48	0.42
2:B:326:ASP:OD1	2:B:329:THR:OG1	2.24	0.42
2:B:1138:MET:HE2	2:B:1146:PHE:CD1	2.54	0.42
8:J:44:TYR:HA	8:J:47:ARG:HB3	2.01	0.42
1:A:50:ILE:HG23	1:A:52:GLY:H	1.85	0.42
1:A:765:VAL:HG22	1:A:800:VAL:HB	2.01	0.42
1:A:889:SER:HB3	1:A:1297:GLU:HG3	2.01	0.42
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	2.00	0.42
2:B:804:GLY:O	2:B:983:ARG:NH2	2.53	0.42
10:L:31:CYS:SG	10:L:32:ALA:N	2.93	0.42
1:A:247:ARG:HB3	1:A:262:LEU:HB2	2.01	0.42
2:B:63:ILE:O	2:B:67:SER:OG	2.33	0.42
8:J:36:LEU:HD11	8:J:51:LEU:HB2	2.01	0.42
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.99	0.42
1:A:231:PRO:HA	1:A:234:MET:HG3	2.02	0.42
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	2.01	0.42
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.19	0.42
1:A:1215:ARG:HD3	1:A:1272:THR:O	2.20	0.42
2:B:63:ILE:HD12	2:B:95:ILE:HB	2.01	0.42
1:A:91:PHE:HZ	1:A:207:ILE:HD12	1.85	0.42
1:A:107:CYS:SG	1:A:108:MET:N	2.93	0.42
1:A:837:ILE:HA	1:A:840:ARG:HD3	2.02	0.42
2:B:604:ARG:HH22	2:B:697:GLU:CD	2.27	0.42
3:C:211:ASP:HA	3:C:212:PRO:HD3	1.93	0.42
1:A:1255:GLU:HB3	1:A:1258:HIS:CE1	2.55	0.42
1:A:1261:LYS:O	1:A:1264:GLU:HG3	2.20	0.42
10:L:31:CYS:HA	10:L:56:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1104:HIS:CG	2:B:1122:ARG:HG3	2.54	0.42
7:I:74:GLU:OE1	7:I:79:HIS:ND1	2.49	0.42
1:A:528:LEU:O	1:A:531:ILE:HG22	2.19	0.41
1:A:598:LEU:O	6:H:122:LEU:HD12	2.20	0.41
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	2.02	0.41
2:B:866:TYR:HB2	2:B:870:ILE:HB	2.00	0.41
1:A:452:LYS:NZ	1:A:1067:LEU:HD13	2.35	0.41
1:A:778:GLY:HA3	2:B:516:ASN:HB2	2.00	0.41
1:A:1163:ILE:HG22	1:A:1165:GLU:H	1.84	0.41
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.56	0.41
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.85	0.41
4:E:20:LYS:NZ	4:E:34:GLU:O	2.44	0.41
9:K:22:ASP:HA	9:K:23:PRO:HD3	1.90	0.41
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.55	0.41
1:A:883:LEU:HD23	1:A:1021:LEU:HD13	2.03	0.41
1:A:1132:LYS:HG3	1:A:1135:ARG:HH22	1.85	0.41
2:B:120:ARG:HB2	2:B:122:LEU:HG	2.03	0.41
2:B:364:ILE:HG13	2:B:365:THR:OG1	2.20	0.41
2:B:755:ILE:HG23	2:B:809:MET:HE2	2.02	0.41
2:B:1060:ARG:HA	2:B:1060:ARG:HD2	1.92	0.41
3:C:39:ALA:O	3:C:41:ILE:N	2.53	0.41
1:A:218:ASP:O	1:A:221:SER:OG	2.33	0.41
1:A:1397:LEU:HB2	1:A:1426:GLU:HG2	2.02	0.41
2:B:102:VAL:HG23	2:B:112:LEU:HB2	2.03	0.41
3:C:31:ASN:O	3:C:35:ARG:HG3	2.21	0.41
6:H:44:VAL:HG13	6:H:48:PRO:HA	2.02	0.41
1:A:215:SER:OG	1:A:216:VAL:N	2.52	0.41
1:A:816:HIS:HE2	2:B:763:GLN:HA	1.86	0.41
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.21	0.41
1:A:1154:TYR:CE1	1:A:1156:PRO:HG3	2.56	0.41
2:B:629:ASP:OD1	2:B:630:ALA:N	2.54	0.41
1:A:902:LEU:HD21	1:A:923:LEU:HD23	2.03	0.41
2:B:100:PRO:HG2	2:B:124:TYR:CZ	2.55	0.41
3:C:212:PRO:HA	3:C:213:PRO:HD3	1.84	0.41
9:K:22:ASP:HB2	9:K:32:VAL:HG13	2.03	0.41
1:A:444:PHE:HD1	1:A:444:PHE:HA	1.72	0.41
1:A:642:CYS:O	1:A:645:LEU:HB3	2.20	0.41
1:A:666:ILE:H	1:A:666:ILE:HG13	1.56	0.41
1:A:860:LEU:HD21	1:A:1394:THR:HA	2.01	0.41
1:A:1094:VAL:HA	1:A:1113:THR:HG21	2.02	0.41
1:A:1436:ILE:O	1:A:1438:THR:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:LEU:HD12	2:B:171:PRO:HD2	2.03	0.41
2:B:581:PHE:HB2	2:B:625:LYS:HG2	2.03	0.41
2:B:620:ARG:HH21	7:I:89:GLN:CD	2.29	0.41
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.55	0.41
1:A:70:CYS:O	1:A:72:GLU:HG2	2.21	0.41
1:A:774:ARG:H	1:A:774:ARG:HG2	1.69	0.41
1:A:848:ILE:HB	1:A:1065:GLY:HA3	2.02	0.41
1:A:994:GLN:HE22	1:A:1023:ARG:HH21	1.69	0.41
2:B:227:LYS:HG2	2:B:236:HIS:CD2	2.56	0.41
2:B:984:HIS:CE1	2:B:1025:HIS:HA	2.56	0.41
1:A:1135:ARG:HG3	1:A:1282:VAL:HB	2.02	0.40
2:B:37:PHE:O	2:B:39:ARG:N	2.47	0.40
4:E:135:PHE:HB3	4:E:140:LEU:HD11	2.03	0.40
7:I:65:ASP:HA	7:I:66:PRO:HD3	1.87	0.40
9:K:63:VAL:HG22	9:K:71:PHE:HB3	2.04	0.40
1:A:265:LYS:NZ	1:A:302:THR:HG23	2.35	0.40
2:B:762:ASN:OD1	2:B:984:HIS:HD2	2.04	0.40
3:C:69:LEU:O	8:J:6:ARG:HD2	2.22	0.40
1:A:495:GLU:HG3	5:F:102:SER:HB3	2.02	0.40
2:B:254:LEU:HD23	2:B:381:MET:HE1	2.04	0.40
2:B:1067:ARG:NE	3:C:194:GLU:OE1	2.42	0.40
1:A:1261:LYS:HE3	1:A:1261:LYS:HB2	1.84	0.40
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.56	0.40
1:A:1113:THR:O	1:A:1330:ASN:ND2	2.43	0.40
1:A:1277:GLU:C	1:A:1279:ILE:H	2.30	0.40
1:A:1434:ALA:O	1:A:1436:ILE:N	2.51	0.40
2:B:190:TYR:CZ	2:B:196:PRO:HG3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1358/1733 (78%)	1234 (91%)	112 (8%)	12 (1%)	14	41
2	B	1077/1224 (88%)	994 (92%)	74 (7%)	9 (1%)	16	44
3	C	264/318 (83%)	246 (93%)	14 (5%)	4 (2%)	8	29
4	E	211/215 (98%)	200 (95%)	10 (5%)	1 (0%)	24	52
5	F	82/155 (53%)	77 (94%)	5 (6%)	0	100	100
6	H	124/146 (85%)	107 (86%)	15 (12%)	2 (2%)	7	28
7	I	113/122 (93%)	102 (90%)	11 (10%)	0	100	100
8	J	63/70 (90%)	60 (95%)	3 (5%)	0	100	100
9	K	112/120 (93%)	108 (96%)	3 (3%)	1 (1%)	14	41
10	L	42/70 (60%)	33 (79%)	7 (17%)	2 (5%)	2	11
All	All	3446/4173 (83%)	3161 (92%)	254 (7%)	31 (1%)	14	41

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	337	ARG
2	B	468	GLU
2	B	1046	PRO
4	E	86	PRO
10	L	69	ALA
1	A	40	THR
1	A	282	ASN
2	B	884	ARG
3	C	90	ASP
9	K	26	LYS
10	L	41	SER
1	A	226	GLU
2	B	1108	ARG
3	C	40	GLU
3	C	148	ARG
1	A	597	LEU
1	A	958	VAL
1	A	1279	ILE
2	B	367	LEU
2	B	1017	ILE

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Mol	Chain	Res	Type
1	A	142	CYS
2	B	260	GLY
3	C	4	GLU
6	H	18	GLY
6	H	82	PRO
1	A	1107	VAL
2	B	824	ILE

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	49
2	B	952/1061 (90%)	914 (96%)	38 (4%)	28	53
3	C	234/274 (85%)	226 (97%)	8 (3%)	32	58
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%)	108 (95%)	6 (5%)	20	48
7	I	109/116 (94%)	107 (98%)	2 (2%)	51	66
8	J	60/65 (92%)	56 (93%)	4 (7%)	15	41
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%)	2942 (96%)	130 (4%)	26	52

All (130) 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

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Mol	Chain	Res	Type
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	463	ILE
1	A	469	ARG
1	A	474	VAL
1	A	475	THR
1	A	481	ASP
1	A	512	VAL
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	740	LEU
1	A	765	VAL
1	A	797	LYS
1	A	821	ARG
1	A	826	ASP
1	A	884	ASP
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

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Mol	Chain	Res	Type
1	A	1262	LYS
1	A	1297	GLU
1	A	1322	ILE
1	A	1329	THR
1	A	1350	LYS
1	A	1354	ASN
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	128	LEU
2	B	134	LYS
2	B	183	GLU
2	B	319	GLU
2	B	364	ILE
2	B	365	THR
2	B	482	VAL
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	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	997	GLU
2	B	1007	VAL
2	B	1051	THR
2	B	1057	LYS
2	B	1099	VAL
2	B	1147	LEU
2	B	1159	ARG

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Mol	Chain	Res	Type
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
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
6	H	133	ASN
7	I	14	LEU
7	I	59	VAL
8	J	3	VAL
8	J	5	VAL
8	J	46	CYS
8	J	52	THR
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 (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	316	GLN
1	A	394	ASN
1	A	445	ASN
1	A	659	HIS
1	A	935	GLN
1	A	1188	GLN
1	A	1258	HIS
1	A	1390	ASN
2	B	366	GLN
2	B	449	ASN
2	B	762	ASN
2	B	767	ASN
2	B	770	GLN
2	B	843	GLN
2	B	862	GLN
2	B	881	ASN
2	B	984	HIS
2	B	1093	GLN
2	B	1195	HIS
3	C	131	HIS
3	C	242	GLN
4	E	63	ASN
4	E	153	HIS
5	F	104	ASN
6	H	128	ASN
7	I	60	GLN
9	K	112	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	R	8/9 (88%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	R	9	A

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	1.43	1 (12%)	7,14,17	1.13	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	-	2/3/15/16	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'	-2.67	1.39	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'	2.15	106.89	103.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	T	20	3DR	O4'-C4'-C5'-O5'
11	T	20	3DR	C3'-C4'-C5'-O5'

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%)	0.52	104 (7%) 20 16	9, 62, 158, 299	0
2	B	1097/1224 (89%)	0.35	59 (5%) 31 23	8, 47, 120, 257	0
3	C	266/318 (83%)	0.19	5 (1%) 66 49	8, 47, 95, 170	0
4	E	213/215 (99%)	0.77	24 (11%) 10 10	29, 93, 176, 288	0
5	F	84/155 (54%)	0.24	4 (4%) 35 25	25, 62, 109, 161	0
6	H	130/146 (89%)	0.97	15 (11%) 9 10	40, 84, 139, 188	0
7	I	115/122 (94%)	0.52	8 (6%) 22 17	20, 62, 106, 127	0
8	J	65/70 (92%)	0.05	2 (3%) 51 38	18, 37, 82, 177	0
9	K	114/120 (95%)	0.10	0 100 100	18, 54, 95, 122	0
10	L	44/70 (62%)	1.38	14 (31%) 1 1	23, 86, 186, 240	0
11	T	11/29 (37%)	2.46	8 (72%) 0 0	107, 132, 166, 203	0
12	R	9/9 (100%)	1.70	2 (22%) 2 3	95, 110, 141, 173	0
All	All	3520/4211 (83%)	0.46	245 (6%) 22 17	8, 57, 147, 299	0

All (245) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	474	SER	7.9
8	J	65	PRO	7.6
2	B	477	ALA	7.2
2	B	472	ALA	5.4
1	A	312	PRO	5.3
6	H	139	ASN	5.2
10	L	45	ALA	5.2
1	A	65	LEU	4.9
1	A	1080	THR	4.8
1	A	250	ILE	4.8
1	A	179	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
2	B	1183	LYS	4.7
1	A	49	LYS	4.5
2	B	471	LYS	4.3
4	E	93	MET	4.3
1	A	237	THR	4.3
2	B	646	LEU	4.3
6	H	136	LYS	4.2
1	A	98	LYS	4.2
1	A	79	GLY	4.1
1	A	147	VAL	4.1
2	B	918	ILE	4.1
1	A	1126	ALA	4.1
10	L	27	LEU	4.0
1	A	64	ASN	3.9
2	B	467	GLY	3.8
2	B	502	ILE	3.7
4	E	95	THR	3.7
1	A	826	ASP	3.7
1	A	182	VAL	3.6
6	H	84	ALA	3.6
10	L	66	GLN	3.6
1	A	60	SER	3.6
6	H	76	THR	3.6
1	A	73	GLY	3.6
11	T	18	DC	3.6
6	H	137	GLN	3.5
5	F	73	ALA	3.5
2	B	447	ALA	3.5
1	A	1156	PRO	3.5
2	B	468	GLU	3.5
1	A	1446	ASP	3.5
2	B	576	ASP	3.5
1	A	111	GLY	3.4
12	R	9	A	3.4
2	B	446	LEU	3.4
1	A	177	ASP	3.4
1	A	1403	GLU	3.4
1	A	44	THR	3.4
5	F	72	LYS	3.4
2	B	733	HIS	3.4
2	B	1189	ILE	3.3
12	R	4	G	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	221	SER	3.3
1	A	323	LYS	3.3
1	A	59	GLY	3.3
2	B	643	ASP	3.3
7	I	52	ILE	3.3
4	E	127	ILE	3.2
4	E	100	ILE	3.2
1	A	223	GLY	3.2
2	B	295	GLY	3.2
6	H	129	TYR	3.2
1	A	180	LYS	3.1
1	A	1196	GLU	3.1
1	A	69	THR	3.1
1	A	318	SER	3.1
2	B	1170	THR	3.1
11	T	19	DT	3.1
10	L	63	ARG	3.1
7	I	55	THR	3.1
2	B	476	ARG	3.1
2	B	251	ILE	3.1
2	B	648	HIS	3.1
2	B	647	GLY	3.1
1	A	115	LEU	3.0
2	B	509	ALA	3.0
11	T	25	DC	3.0
1	A	324	SER	3.0
2	B	275	TYR	3.0
1	A	91	PHE	3.0
2	B	432	MET	3.0
6	H	132	LEU	3.0
1	A	980	ASP	3.0
4	E	83	CYS	3.0
2	B	473	MET	3.0
10	L	35	SER	2.9
10	L	46	VAL	2.9
1	A	107	CYS	2.9
2	B	475	SER	2.9
1	A	975	HIS	2.9
1	A	235	ILE	2.9
1	A	45	GLN	2.9
2	B	529	GLU	2.9
4	E	96	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	315	LEU	2.9
4	E	98	ILE	2.9
1	A	331	GLY	2.8
1	A	1174	PHE	2.8
2	B	261	ARG	2.8
3	C	78	GLU	2.8
10	L	41	SER	2.8
4	E	131	THR	2.8
7	I	3	THR	2.8
2	B	868	MET	2.8
2	B	1176	ASN	2.8
11	T	29	DG	2.8
2	B	115	GLN	2.8
1	A	310	GLY	2.7
1	A	593	GLU	2.7
1	A	183	GLY	2.7
4	E	123	LEU	2.7
8	J	26	GLN	2.7
1	A	973	ILE	2.7
5	F	104	ASN	2.7
1	A	801	GLU	2.7
4	E	107	THR	2.7
2	B	629	ASP	2.7
2	B	1211	ASN	2.7
4	E	82	PHE	2.6
6	H	83	GLN	2.6
1	A	247	ARG	2.6
10	L	36	SER	2.6
1	A	1378	GLN	2.6
2	B	266	ALA	2.6
11	T	21	DC	2.6
2	B	67	SER	2.6
4	E	73	PRO	2.6
1	A	108	MET	2.6
1	A	142	CYS	2.6
1	A	181	LEU	2.6
2	B	262	GLU	2.6
1	A	66	LYS	2.6
4	E	110	PHE	2.5
1	A	271	LYS	2.5
1	A	1257	ASP	2.5
1	A	1390	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	20	ASP	2.5
6	H	21	ASN	2.5
1	A	105	CYS	2.5
1	A	1243	VAL	2.5
1	A	397	ASN	2.5
2	B	959	ASP	2.5
1	A	1444	MET	2.5
2	B	929	THR	2.5
4	E	129	PRO	2.5
6	H	82	PRO	2.5
1	A	287	HIS	2.5
1	A	1258	HIS	2.5
10	L	53	HIS	2.5
1	A	219	PHE	2.4
3	C	249	ASP	2.4
6	H	19	ARG	2.4
10	L	40	LEU	2.4
4	E	125	PRO	2.4
1	A	109	HIS	2.4
1	A	234	MET	2.4
1	A	1411	GLU	2.4
1	A	317	LYS	2.4
4	E	90	VAL	2.4
1	A	74	MET	2.4
11	T	24	DT	2.4
2	B	370	PHE	2.4
1	A	54	ASN	2.4
2	B	881	ASN	2.4
2	B	241	ARG	2.4
4	E	81	GLU	2.4
1	A	1161	THR	2.3
1	A	573	SER	2.3
1	A	292	ALA	2.3
2	B	470	LYS	2.3
1	A	272	ALA	2.3
1	A	1108	ALA	2.3
4	E	55	ARG	2.3
10	L	42	ARG	2.3
1	A	84	ILE	2.3
1	A	266	LEU	2.3
1	A	174	ILE	2.3
1	A	114	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
5	F	155	LEU	2.3
2	B	931	TYR	2.3
2	B	665	GLU	2.2
3	C	50	GLU	2.2
1	A	615	GLY	2.2
2	B	712	PRO	2.2
2	B	425	THR	2.2
4	E	158	SER	2.2
4	E	85	GLU	2.2
6	H	63	LEU	2.2
1	A	140	THR	2.2
4	E	152	LYS	2.2
7	I	2	THR	2.2
4	E	128	PRO	2.2
1	A	977	LYS	2.2
1	A	175	ARG	2.2
2	B	26	THR	2.2
2	B	878	GLN	2.2
1	A	141	LEU	2.2
11	T	22	DT	2.2
1	A	185	TRP	2.2
1	A	106	VAL	2.2
4	E	3	GLN	2.2
1	A	1110	ASN	2.2
2	B	867	GLY	2.2
1	A	1391	ARG	2.2
7	I	61	ASP	2.2
1	A	1376	THR	2.1
1	A	1418	LEU	2.1
1	A	52	GLY	2.1
1	A	167	CYS	2.1
2	B	427	ASP	2.1
6	H	90	ALA	2.1
1	A	76	GLU	2.1
4	E	87	SER	2.1
6	H	62	SER	2.1
7	I	40	SER	2.1
3	C	268	ASP	2.1
10	L	50	ASP	2.1
1	A	1387	HIS	2.1
1	A	596	THR	2.1
1	A	705	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
10	L	64	LEU	2.1
1	A	1414	ALA	2.1
2	B	957	ASN	2.1
2	B	1192	TYR	2.1
1	A	137	ALA	2.1
3	C	205	LYS	2.1
1	A	139	TRP	2.1
1	A	542	GLU	2.1
2	B	678	GLU	2.1
6	H	106	GLU	2.1
1	A	513	SER	2.0
1	A	128	ILE	2.0
1	A	233	TRP	2.0
2	B	365	THR	2.0
2	B	64	CYS	2.0
7	I	53	GLY	2.0
1	A	10	PRO	2.0
1	A	285	PRO	2.0
10	L	28	LYS	2.0
7	I	26	LEU	2.0
2	B	66	ASP	2.0
2	B	134	LYS	2.0
1	A	280	GLU	2.0
11	T	23	DC	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	0.64	0.24	134,145,157,187	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
14	MG	A	1803	1/1	0.93	0.12	36,36,36,36	0
13	ZN	A	1801	1/1	0.94	0.07	149,149,149,149	0
13	ZN	A	1802	1/1	0.96	0.07	83,83,83,83	0
13	ZN	B	1301	1/1	0.99	0.04	95,95,95,95	0
13	ZN	I	201	1/1	1.00	0.05	52,52,52,52	0
13	ZN	I	202	1/1	1.00	0.03	33,33,33,33	0
13	ZN	J	101	1/1	1.00	0.03	34,34,34,34	0
13	ZN	L	101	1/1	1.00	0.02	73,73,73,73	0
13	ZN	C	401	1/1	1.00	0.02	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.