



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 11:59 PM EDT

PDB ID : 6BQF
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

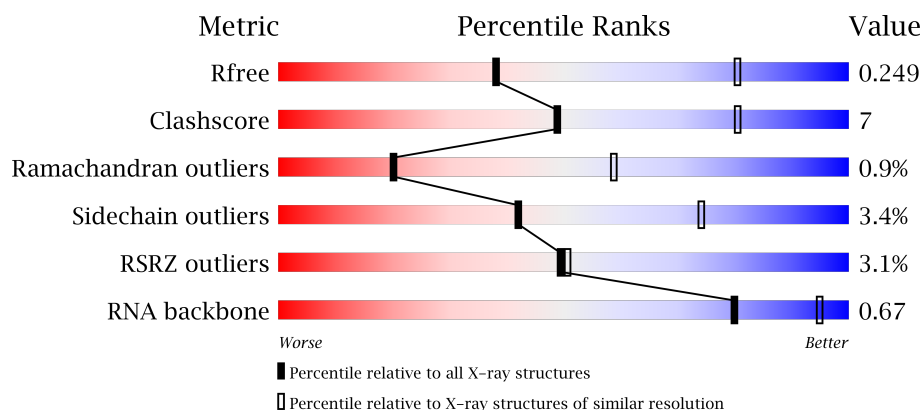
1 Overall quality at a glance

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}	100719	1156 (3.42-3.30)
Clashscore	112137	1231 (3.42-3.30)
Ramachandran outliers	110173	1212 (3.42-3.30)
Sidechain outliers	110143	1211 (3.42-3.30)
RSRZ outliers	101464	1165 (3.42-3.30)
RNA backbone	2435	1005 (3.90-2.82)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>3%</div> <div>63%</div> <div>15%</div> <div>•</div> <div>21%</div> </div>
2	B	1224	<div> <div>•</div> <div>70%</div> <div>19%</div> <div>•</div> <div>10%</div> </div>
3	C	318	<div> <div>64%</div> <div>18%</div> <div>•</div> <div>16%</div> </div>
4	E	215	<div> <div>14%</div> <div>88%</div> <div>10%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
5	F	155	<div><div></div><div>45%</div><div>8%</div><div></div><div>46%</div></div>
6	H	146	<div><div>2%</div><div></div><div>71%</div><div>17%</div><div>11%</div></div>
7	I	122	<div><div>%</div><div></div><div>77%</div><div>16%</div><div>6%</div></div>
8	J	70	<div><div>%</div><div></div><div>76%</div><div>14%</div><div>7%</div></div>
9	K	120	<div><div></div><div>78%</div><div>18%</div><div>5%</div></div>
10	L	70	<div><div>3%</div><div></div><div>40%</div><div>23%</div><div>37%</div></div>
11	T	29	<div><div>10%</div><div></div><div>28%</div><div>14%</div><div>59%</div></div>
12	R	9	<div><div>22%</div><div></div><div>67%</div><div>33%</div></div>

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 (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	J	1	Total	Zn	0	0
			1	1		

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

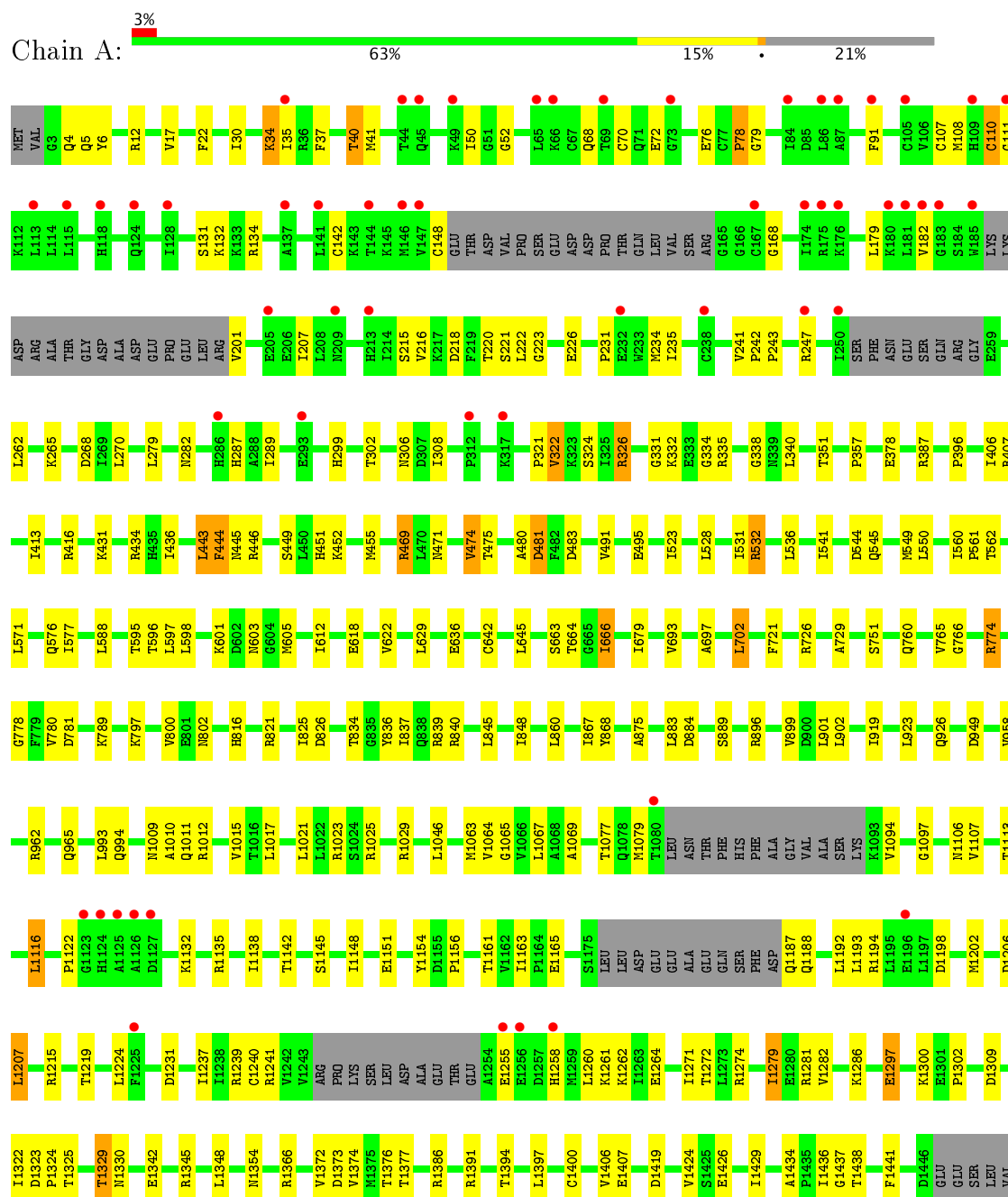
- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

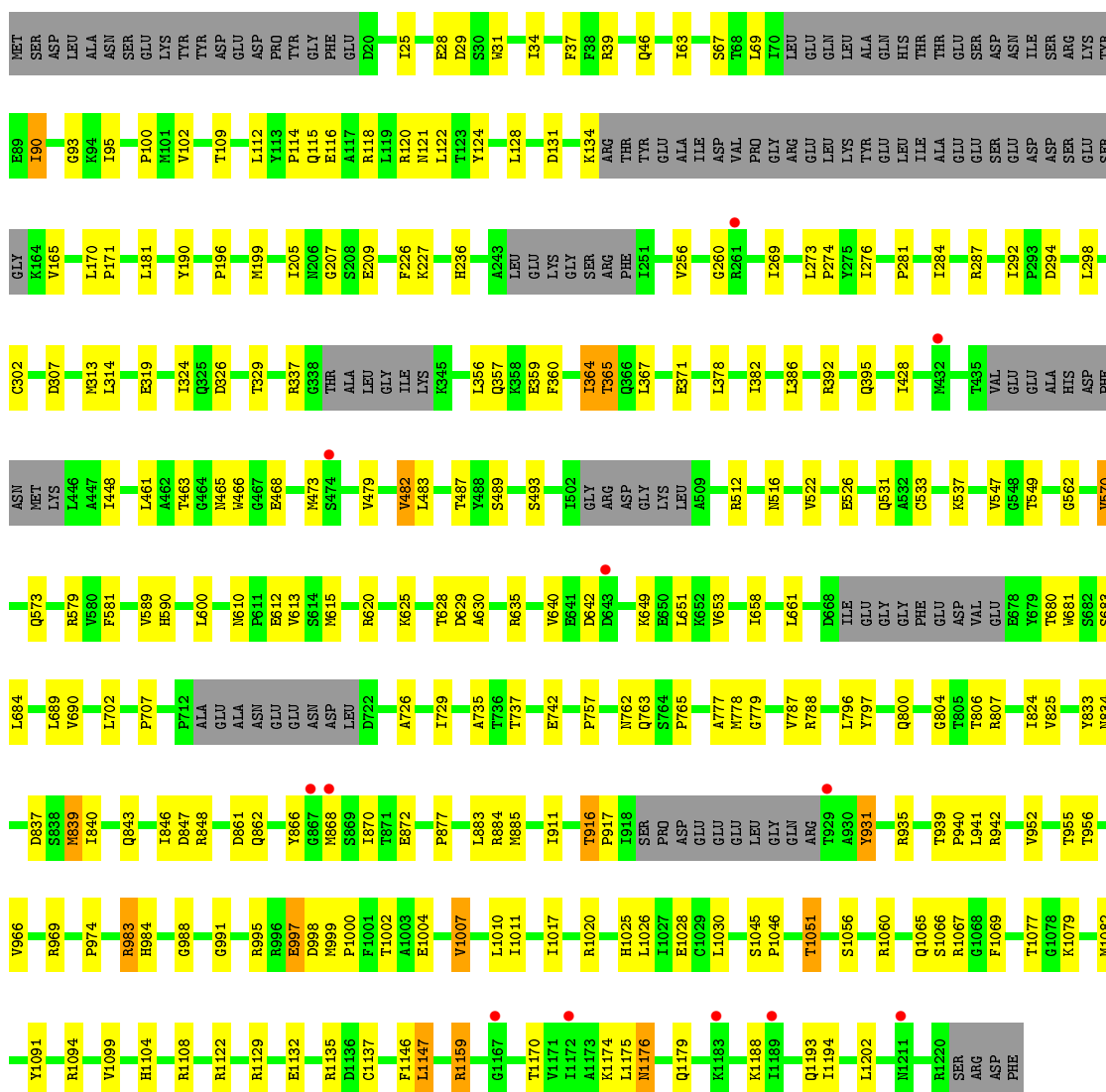
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

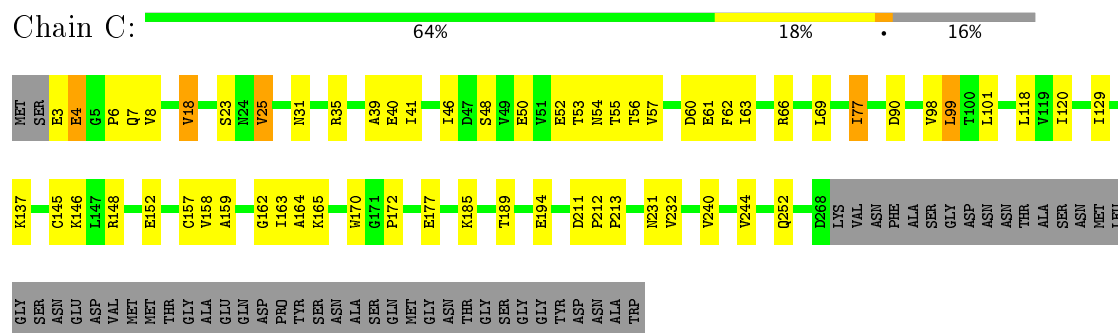
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



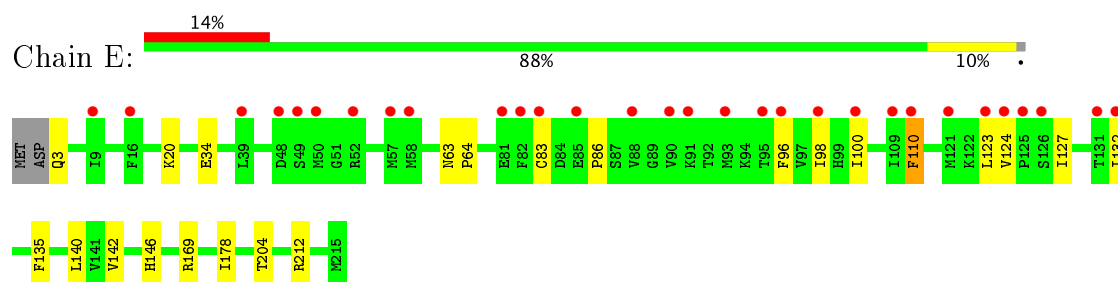
- Molecule 2: DNA-directed RNA polymerase II subunit RPB2



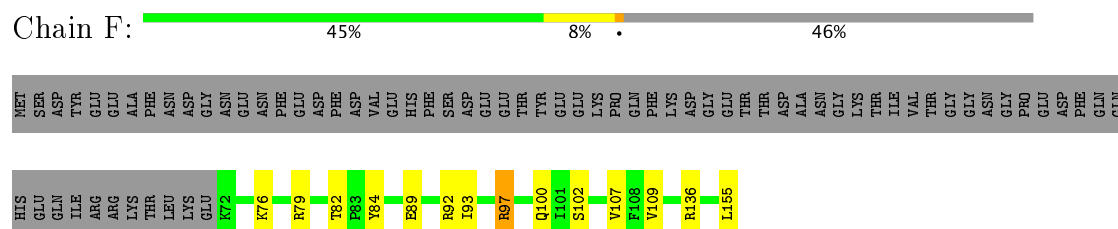
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



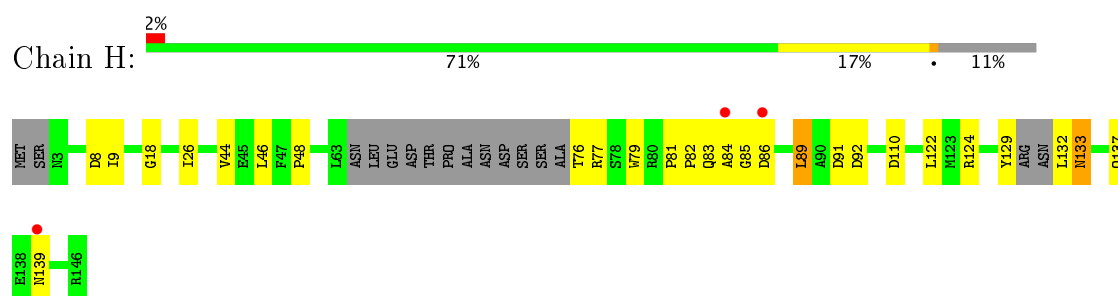
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



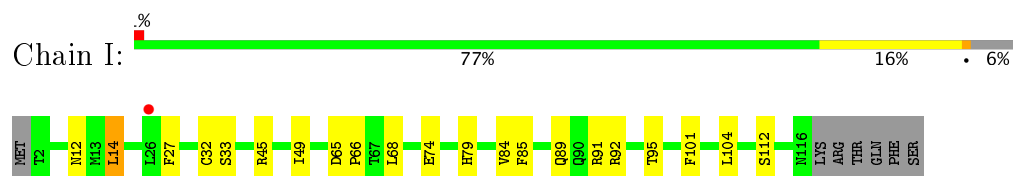
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



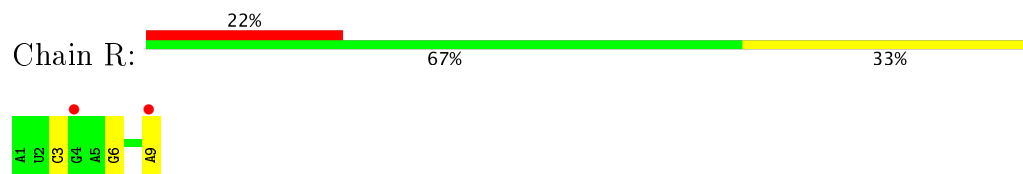
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



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



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



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 0.229 , 0.249	Depositor DCC
R_{free} test set	4550 reflections (5.20%)	DCC
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 46.2	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, MG, 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	0.21	0/10975	0.37	0/14838
2	B	0.21	0/8896	0.38	0/11996
3	C	0.20	0/2133	0.38	0/2891
4	E	0.21	0/1780	0.36	0/2395
5	F	0.20	0/691	0.38	0/933
6	H	0.21	0/1060	0.40	0/1434
7	I	0.21	0/953	0.36	0/1284
8	J	0.21	0/541	0.34	0/727
9	K	0.21	0/937	0.35	0/1265
10	L	0.20	0/353	0.36	0/468
11	T	0.46	0/244	0.92	0/371
12	R	0.17	0/218	0.62	0/339
All	All	0.21	0/28781	0.38	0/38941

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	A	10784	0	10873	163	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8726	0	8760	146	0
3	C	2095	0	2051	43	0
4	E	1744	0	1772	10	0
5	F	679	0	701	8	0
6	H	1043	0	1015	14	0
7	I	935	0	886	15	0
8	J	532	0	542	10	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	382	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 (382) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:165:VAL:HG21	2:B:448:ILE:HD12	1.79	0.64
1:A:4:GLN:OE1	2:B:1159:ARG:NH1	2.31	0.64
1:A:40:THR:HG22	1:A:41:MET:HG3	1.79	0.63
2:B:778:MET:HE1	2:B:1094:ARG:HH11	1.63	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: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: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:273:LEU:HB2	2:B:276:ILE:HD12	1.83	0.61
2:B:28:GLU:OE1	2:B:807:ARG:NH1	2.33	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
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:1077:THR:HG23	2:B:1079:LYS:H	1.67	0.60
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.84	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:1207:LEU:HD23	1:A:1274:ARG:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1148:ILE:HD13	7:I:49:ILE:HD12	1.86	0.58
1:A:1116:LEU:HD22	1:A:1329:THR:HB	1.86	0.58
1:A:993:LEU:HD22	1:A:1046:LEU:HG	1.85	0.57
1:A:110:CYS:SG	1:A:111:GLY:N	2.71	0.57
1:A:68:GLN:O	1:A:70:CYS:N	2.35	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:613:VAL:HG22	2:B:628:THR:HG23	1.90	0.54
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.88	0.54
2:B:463:THR:HG22	11:T:27:DA:H2"	1.89	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
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:1065:GLN:HG3	2:B:1067:ARG:H	1.72	0.53
2:B:620:ARG:HD2	7:I:68:LEU:HD11	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:A:469:ARG:NH2	2:B:991:GLY:O	2.43	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
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: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
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
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:834:THR:HG21	1:A:1077:THR:HA	1.93	0.51
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.92	0.51
1:A:1286:LYS:HE2	1:A:1302:PRO:HB2	1.93	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1345:ARG:HG3	1:A:1376:THR:HG21	1.94	0.49
1:A:76:GLU:OE2	2:B:1159:ARG:NH1	2.45	0.49
1:A:760:GLN:HG2	1:A:765:VAL:HA	1.95	0.49
2:B:287:ARG:NH2	2:B:294:ASP:OD1	2.45	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
1:A:868:TYR:OH	1:A:1366:ARG:HD3	2.13	0.49
1:A:825:ILE:HD12	2:B:512:ARG:HD3	1.94	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
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:1064:VAL:HG23	1:A:1067:LEU:HD23	1.95	0.48
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.96	0.48
2:B:995:ARG:NH1	2:B:997:GLU:OE1	2.46	0.48
1:A:560:ILE:HB	6:H:79:TRP:H	1.78	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
1:A:774:ARG:HG3	1:A:797:LYS:HZ2	1.77	0.48
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.96	0.48
3:C:3:GLU:N	9:K:104:ASN:HD21	2.12	0.48
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.95	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:1138:ILE:HG22	1:A:1279:ILE:HG21	1.96	0.47
1:A:550:LEU:HD21	1:A:561:PRO:HD2	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD13	6:H:89:LEU:H	1.79	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:1082:MET:HA	3:C:189:THR:HA	1.97	0.47
2:B:482:VAL:HG11	11:T:26:DG:H5"	1.97	0.47
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.80	0.46
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
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
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: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:1194:ARG:HH21	1:A:1237:ILE:HD13	1.80	0.45
1:A:131:SER:HB3	1:A:223:GLY:HA2	1.98	0.45
1:A:235:ILE:HG13	1:A:235:ILE:H	1.55	0.45
1:A:588:LEU:HD22	1:A:629:LEU:HD23	1.98	0.45
1:A:1438:THR:HG23	5:F:92:ARG:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1219:THR:HG21	1:A:1271:ILE:HD11	1.98	0.45
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.52	0.45
1:A:663:SER:OG	1:A:664:THR:N	2.50	0.45
1:A:949:ASP:N	1:A:949:ASP:OD1	2.50	0.45
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.52	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:877:PRO:HB2	2:B:885:MET:HE1	1.99	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:848:ARG:NH1	8:J:8:PHE:O	2.49	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:1135:ARG:HG3	2:B:1147:LEU:HD21	2.00	0.44
2:B:199:MET:N	2:B:199:MET:SD	2.84	0.44
2:B:610:ASN:HB3	2:B:613:VAL:HG23	1.99	0.44
3:C:55:THR:HG1	3:C:152:GLU:H	1.64	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:681:TRP:CH2	2:B:690:VAL:HG11	2.53	0.44
6:H:133:ASN:N	6:H:133:ASN:OD1	2.42	0.44
6:H:76:THR:OG1	6:H:77:ARG:N	2.51	0.44
1:A:331:GLY:HA2	1:A:334:GLY:H	1.83	0.44
2:B:806:THR:HG23	2:B:1045:SER:HA	2.00	0.44
2:B:466:TRP:HB2	2:B:479:VAL:HG21	1.99	0.44
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.99	0.44
1:A:596:THR:C	1:A:598:LEU:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:LEU:HD12	6:H:46:LEU:HD11	1.99	0.43
3:C:62:PHE:O	3:C:66:ARG:HG3	2.18	0.43
3:C:57:VAL:HG11	8:J:60:PHE:HB3	2.00	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
2:B:547:VAL:N	2:B:612:GLU:OE2	2.45	0.43
2:B:115:GLN:NE2	2:B:787:VAL:O	2.51	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:78:PRO:HB2	1:A:79:GLY:H	1.65	0.43
1:A:839:ARG:NH2	2:B:1132:GLU:OE2	2.52	0.43
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:HA	2:B:931:TYR:HD1	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:1079:MET:HE1	1:A:1097:GLY:HA2	2.00	0.42
1:A:326:ARG:HG2	1:A:1406:VAL:HG11	2.01	0.42
1:A:541:ILE:HD13	1:A:549:MET:HE1	2.00	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
8:J:44:TYR:HA	8:J:47:ARG:HB3	2.01	0.42
1:A:1142:THR:O	1:A:1145:SER:OG	2.29	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:465:ASN:HB3	2:B:473:MET:HE1	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:231:PRO:HA	1:A:234:MET:HG3	2.02	0.42
2:B:63:ILE:HD12	2:B:95:ILE:HB	2.01	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
1:A:91:PHE:HZ	1:A:207:ILE:HD12	1.85	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
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:1163:ILE:HG22	1:A:1165:GLU:H	1.84	0.41
1:A:452:LYS:NZ	1:A:1067:LEU:HD13	2.35	0.41
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.85	0.41
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.56	0.41
1:A:778:GLY:HA3	2:B:516:ASN:HB2	2.00	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
2:B:778:MET:HE1	2:B:1094:ARG:NH1	2.31	0.41
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.55	0.41
1:A:1132:LYS:HG3	1:A:1135:ARG:HH22	1.85	0.41
1:A:883:LEU:HD23	1:A:1021:LEU:HD13	2.03	0.41
2:B:1060:ARG:HA	2:B:1060:ARG:HD2	1.92	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
3:C:39:ALA:O	3:C:41:ILE:N	2.53	0.41
1:A:1397:LEU:HB2	1:A:1426:GLU:HG2	2.02	0.41
1:A:218:ASP:O	1:A:221:SER:OG	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:545:GLN:HG2	1:A:549:MET:HE3	2.02	0.41
1:A:816:HIS:HE2	2:B:763:GLN:HA	1.86	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:HA	1:A:444:PHE:HD1	1.72	0.41
1:A:860:LEU:HD21	1:A:1394:THR:HA	2.01	0.41
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
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
1:A:642:CYS:O	1:A:645:LEU:HB3	2.20	0.41
1:A:666:ILE:HG13	1:A:666:ILE:H	1.56	0.41
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.55	0.41
1:A:848:ILE:HB	1:A:1065:GLY:HA3	2.02	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:994:GLN:HE22	1:A:1023:ARG:HH21	1.69	0.41
2:B:984:HIS:CE1	2:B:1025:HIS:HA	2.56	0.41
2:B:227:LYS:HG2	2:B:236:HIS:CD2	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:1067:ARG:NE	3:C:194:GLU:OE1	2.42	0.40
1:A:1261:LYS:HB2	1:A:1261:LYS:HE3	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: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%)	20	59
2	B	1077/1224 (88%)	994 (92%)	74 (7%)	9 (1%)	22	61
3	C	264/318 (83%)	246 (93%)	14 (5%)	4 (2%)	12	46
4	E	211/215 (98%)	200 (95%)	10 (5%)	1 (0%)	32	70
5	F	82/155 (53%)	77 (94%)	5 (6%)	0	100	100
6	H	124/146 (85%)	107 (86%)	15 (12%)	2 (2%)	11	45
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%)	20	59
10	L	42/70 (60%)	33 (79%)	7 (17%)	2 (5%)	2	20
All	All	3446/4173 (83%)	3161 (92%)	254 (7%)	31 (1%)	20	59

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

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Mol	Chain	Res	Type
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
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%)	1147 (96%)	49 (4%)	35	70
2	B	952/1061 (90%)	922 (97%)	30 (3%)	44	76
3	C	234/274 (85%)	227 (97%)	7 (3%)	46	77
4	E	195/197 (99%)	188 (96%)	7 (4%)	40	73
5	F	74/137 (54%)	71 (96%)	3 (4%)	35	70
6	H	114/128 (89%)	109 (96%)	5 (4%)	33	68
7	I	109/116 (94%)	108 (99%)	1 (1%)	82	92
8	J	60/65 (92%)	58 (97%)	2 (3%)	43	75
9	K	99/102 (97%)	98 (99%)	1 (1%)	80	90
10	L	39/57 (68%)	39 (100%)	0	100	100
All	All	3072/3657 (84%)	2967 (97%)	105 (3%)	42	74

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	TYR
1	A	12	ARG
1	A	22	PHE
1	A	34	LYS
1	A	132	LYS
1	A	179	LEU
1	A	222	LEU
1	A	270	LEU
1	A	287	HIS
1	A	308	ILE
1	A	322	VAL
1	A	326	ARG
1	A	332	LYS
1	A	335	ARG
1	A	351	THR
1	A	434	ARG
1	A	443	LEU
1	A	444	PHE
1	A	451	HIS
1	A	469	ARG
1	A	474	VAL
1	A	475	THR
1	A	481	ASP
1	A	532	ARG
1	A	605	MET
1	A	612	ILE
1	A	618	GLU
1	A	666	ILE
1	A	702	LEU
1	A	774	ARG
1	A	821	ARG
1	A	826	ASP
1	A	884	ASP
1	A	896	ARG
1	A	1017	LEU
1	A	1025	ARG
1	A	1116	LEU
1	A	1207	LEU
1	A	1231	ASP
1	A	1262	LYS
1	A	1297	GLU
1	A	1300	LYS

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Mol	Chain	Res	Type
1	A	1322	ILE
1	A	1329	THR
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	90	ILE
2	B	109	THR
2	B	134	LYS
2	B	313	MET
2	B	319	GLU
2	B	364	ILE
2	B	365	THR
2	B	482	VAL
2	B	483	LEU
2	B	549	THR
2	B	570	VAL
2	B	737	THR
2	B	797	TYR
2	B	825	VAL
2	B	839	MET
2	B	868	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	1099	VAL
2	B	1147	LEU
2	B	1159	ARG
2	B	1176	ASN
2	B	1188	LYS
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

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Mol	Chain	Res	Type
3	C	240	VAL
3	C	244	VAL
4	E	3	GLN
4	E	98	ILE
4	E	110	PHE
4	E	123	LEU
4	E	127	ILE
4	E	169	ARG
4	E	204	THR
5	F	93	ILE
5	F	97	ARG
5	F	155	LEU
6	H	26	ILE
6	H	89	LEU
6	H	110	ASP
6	H	124	ARG
6	H	133	ASN
7	I	14	LEU
8	J	5	VAL
8	J	52	THR
9	K	1	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	325	GLN
2	B	366	GLN
2	B	762	ASN
2	B	984	HIS

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	1.81	2 (25%)	8,14,17	1.00	1 (12%)

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	-	0/3/15/16	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	20	3DR	O5'-C5'	-3.49	1.39	1.44
11	T	20	3DR	O4'-C4'	-2.68	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.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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	A	1372/1733 (79%)	0.17	56 (4%) 38 38	9, 62, 158, 299	0
2	B	1097/1224 (89%)	-0.04	12 (1%) 80 82	8, 47, 120, 257	0
3	C	266/318 (83%)	-0.21	0 100 100	8, 47, 95, 170	0
4	E	213/215 (99%)	0.57	30 (14%) 3 3	29, 93, 176, 288	0
5	F	84/155 (54%)	-0.21	0 100 100	25, 62, 109, 161	0
6	H	130/146 (89%)	0.17	3 (2%) 61 61	40, 84, 139, 188	0
7	I	115/122 (94%)	0.02	1 (0%) 84 86	20, 62, 106, 127	0
8	J	65/70 (92%)	-0.34	1 (1%) 74 74	18, 37, 82, 177	0
9	K	114/120 (95%)	-0.19	0 100 100	18, 54, 95, 122	0
10	L	44/70 (62%)	0.26	2 (4%) 34 34	23, 86, 186, 240	0
11	T	11/29 (37%)	1.15	3 (27%) 1 1	107, 132, 166, 203	0
12	R	9/9 (100%)	1.17	2 (22%) 1 1	95, 110, 141, 173	0
All	All	3520/4211 (83%)	0.07	110 (3%) 49 51	8, 57, 147, 299	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	93	MET	7.8
1	A	183	GLY	7.1
1	A	1126	ALA	6.3
1	A	44	THR	5.3
10	L	45	ALA	5.1
1	A	49	LYS	4.7
4	E	100	ILE	4.5
2	B	868	MET	4.0
1	A	174	ILE	4.0
6	H	139	ASN	4.0
1	A	69	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	286	HIS	3.9
4	E	98	ILE	3.8
4	E	123	LEU	3.8
4	E	110	PHE	3.7
1	A	45	GLN	3.7
4	E	85	GLU	3.6
1	A	1080	THR	3.5
2	B	474	SER	3.5
1	A	1125	ALA	3.5
1	A	1124	HIS	3.5
1	A	147	VAL	3.4
2	B	1183	LYS	3.4
1	A	213	HIS	3.3
1	A	128	ILE	3.3
4	E	125	PRO	3.3
1	A	175	ARG	3.3
4	E	96	PHE	3.3
1	A	111	GLY	3.2
12	R	9	A	3.2
2	B	643	ASP	3.1
4	E	83	CYS	3.1
1	A	141	LEU	3.1
1	A	73	GLY	3.0
1	A	91	PHE	3.0
1	A	180	LYS	2.9
1	A	86	LEU	2.9
4	E	57	MET	2.9
11	T	18	DC	2.9
1	A	105	CYS	2.9
1	A	87	ALA	2.8
1	A	113	LEU	2.8
4	E	95	THR	2.8
6	H	84	ALA	2.8
1	A	182	VAL	2.8
2	B	1172	ILE	2.7
1	A	205	GLU	2.7
1	A	109	HIS	2.7
1	A	115	LEU	2.7
1	A	181	LEU	2.7
1	A	209	ASN	2.6
1	A	1225	PHE	2.6
4	E	50	MET	2.6

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Mol	Chain	Res	Type	RSRZ
4	E	124	VAL	2.6
1	A	250	ILE	2.6
1	A	84	ILE	2.6
8	J	65	PRO	2.6
1	A	65	LEU	2.6
1	A	238	CYS	2.6
2	B	1189	ILE	2.6
4	E	39	LEU	2.6
4	E	90	VAL	2.6
1	A	35	ILE	2.5
4	E	126	SER	2.5
4	E	81	GLU	2.5
4	E	109	ILE	2.5
11	T	19	DT	2.5
4	E	9	ILE	2.4
1	A	146	MET	2.4
4	E	82	PHE	2.4
2	B	867	GLY	2.4
1	A	167	CYS	2.4
6	H	86	ASP	2.3
1	A	118	HIS	2.3
1	A	176	LYS	2.3
4	E	88	VAL	2.3
2	B	432	MET	2.3
2	B	1167	GLY	2.3
1	A	317	LYS	2.2
12	R	4	G	2.2
4	E	52	ARG	2.2
1	A	137	ALA	2.2
4	E	49	SER	2.2
4	E	58	MET	2.2
4	E	132	ILE	2.2
4	E	121	MET	2.2
1	A	1255	GLU	2.2
1	A	1123	GLY	2.2
1	A	293	GLU	2.2
10	L	35	SER	2.2
1	A	1196	GLU	2.2
4	E	16	PHE	2.1
4	E	91	LYS	2.1
1	A	1256	GLU	2.1
2	B	929	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1258	HIS	2.1
1	A	1127	ASP	2.1
1	A	124	GLN	2.1
1	A	312	PRO	2.1
1	A	144	THR	2.1
2	B	1211	ASN	2.1
7	I	26	LEU	2.0
4	E	48	ASP	2.0
1	A	66	LYS	2.0
1	A	185	TRP	2.0
1	A	247	ARG	2.0
11	T	21	DC	2.0
4	E	131	THR	2.0
1	A	232	GLU	2.0
2	B	261	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
11	3DR	T	20	11/12	0.71	0.38	-	134,145,157,187	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
13	ZN	I	202	1/1	0.99	0.15	0.08	33,33,33,33	0
13	ZN	C	401	1/1	0.98	0.14	-0.87	37,37,37,37	0
13	ZN	I	201	1/1	0.99	0.13	-1.15	52,52,52,52	0
13	ZN	B	1301	1/1	0.97	0.10	-1.54	95,95,95,95	0
13	ZN	L	101	1/1	0.98	0.08	-1.74	73,73,73,73	0
13	ZN	J	101	1/1	0.99	0.16	-1.91	34,34,34,34	0
13	ZN	A	1802	1/1	0.94	0.12	-2.04	83,83,83,83	0
13	ZN	A	1801	1/1	0.89	0.08	-3.65	149,149,149,149	0
14	MG	A	1803	1/1	0.87	0.32	-	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.