



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 06:43 PM BST

PDB ID : 6UQ2
Title : RNA polymerase II elongation complex with dG in state 1
Authors : Oh, J.; Wang, D.
Deposited on : 2019-10-18
Resolution : 3.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

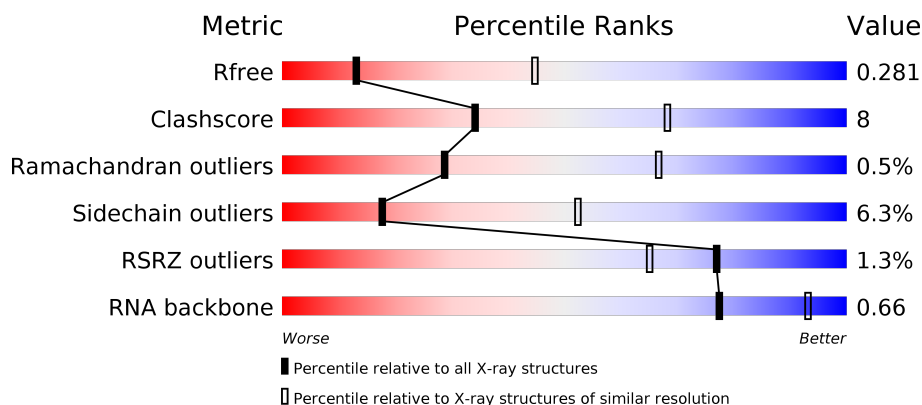
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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 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	R	9	<div> <div>78%</div> <div>22%</div> </div>
2	T	29	<div> <div>7%</div> <div>69%</div> <div>17%</div> <div>•</div> <div>10%</div> </div>
3	N	18	<div> <div>61%</div> <div>22%</div> <div>17%</div> </div>
4	A	1733	<div> <div>%</div> <div>59%</div> <div>19%</div> <div>•</div> <div>20%</div> </div>

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Mol	Chain	Length	Quality of chain
5	B	1224	
6	C	318	
7	E	215	
8	F	155	
9	H	146	
10	I	122	
11	J	70	
12	K	120	
13	L	70	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 29048 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 RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	9	Total	C	N	O	P	0	0	0
			195	88	40	59	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	26	Total	C	N	O	P	0	0	0
			520	250	80	164	26			

- Molecule 3 is a DNA chain called Non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	15	Total	C	N	O	P	0	0	0
			317	148	71	83	15			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1384	Total	C	N	O	S	0	0	0
			10828	6831	1896	2041	60			

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1123	Total	C	N	O	S	0	0	0
			8859	5607	1552	1647	53			

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	212	Total	C	N	O	S	0	0	0
			1731	1100	305	315	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	86	Total	C	N	O	S	0	0	0
			684	437	115	129	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	133	Total	C	N	O	S	0	0	0
			1064	670	179	211	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	118	Total	C	N	O	S	0	0	0
			952	585	173	184	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	43	Total	C	N	O	S	0	0	0
			337	208	66	59	4			

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

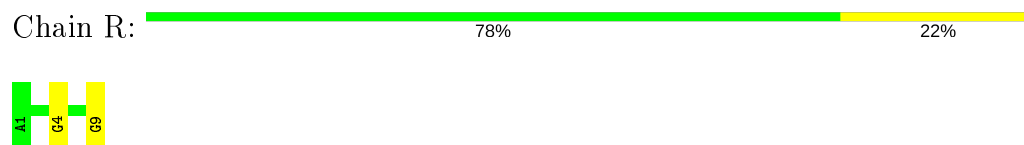
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

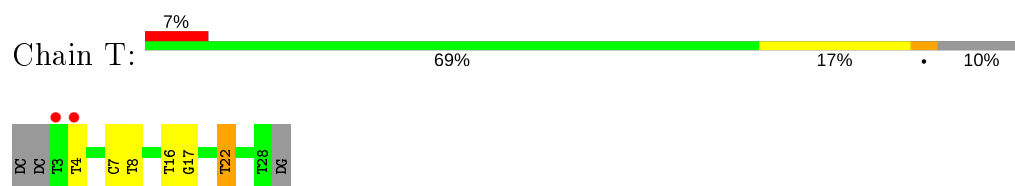
3 Residue-property plots [i](#)

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

- Molecule 1: RNA



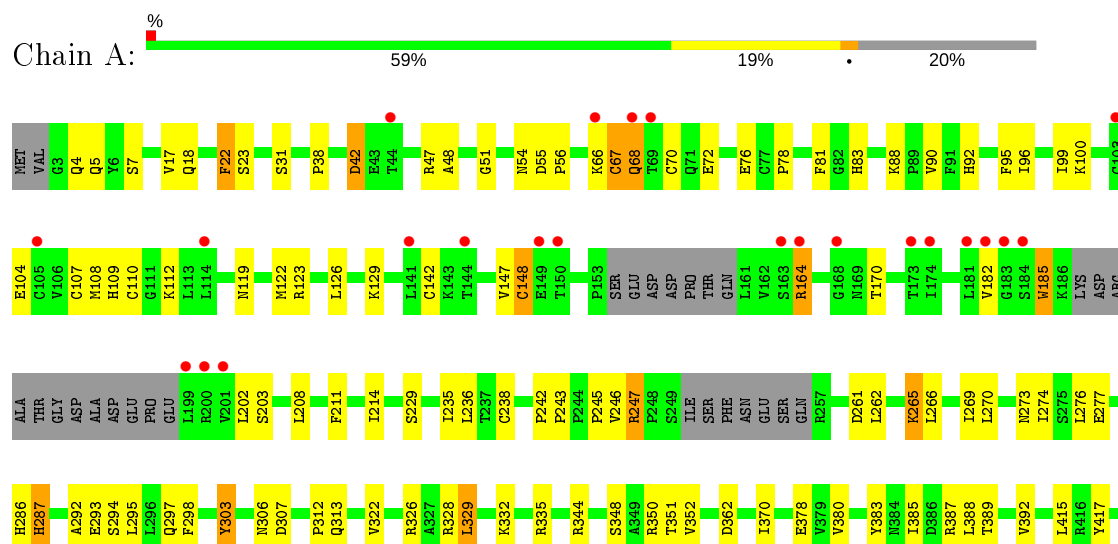
- Molecule 2: Template strand DNA



- Molecule 3: Non-template strand DNA



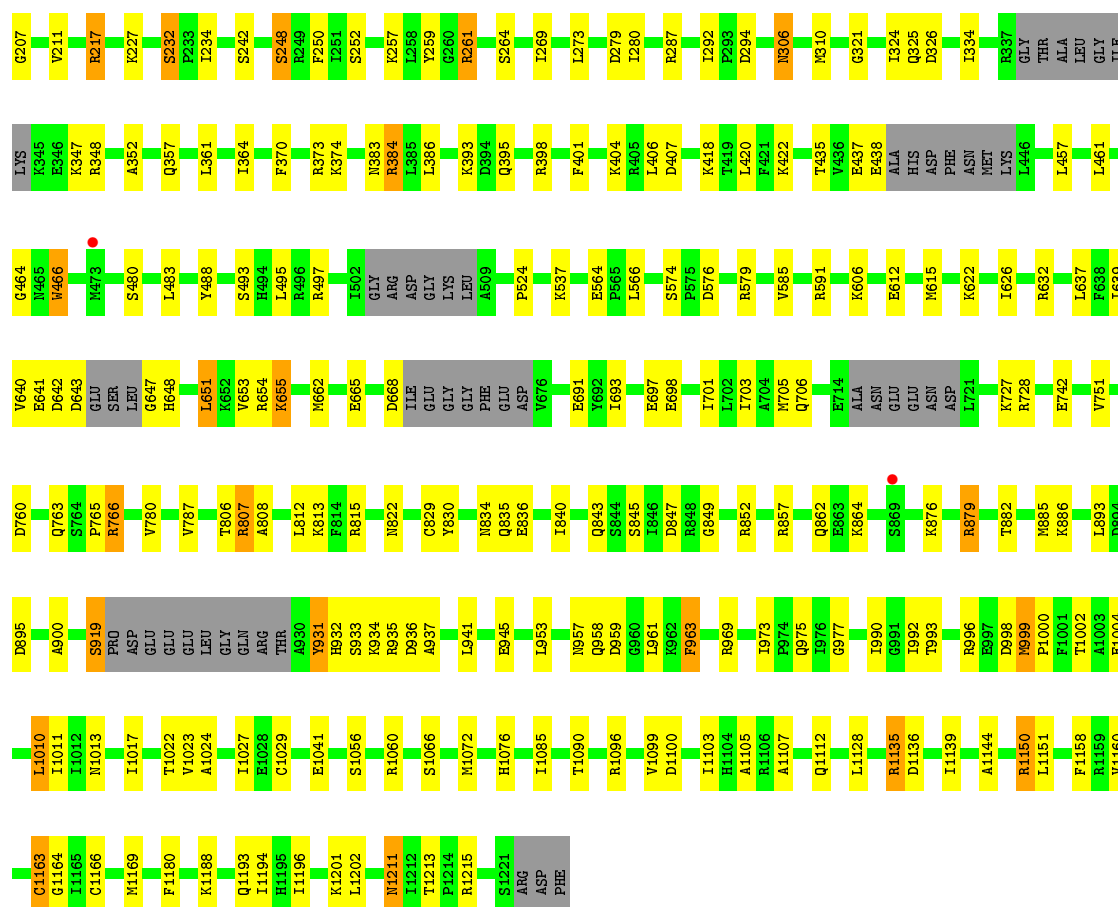
- Molecule 4: DNA-directed RNA polymerase II subunit RPB1





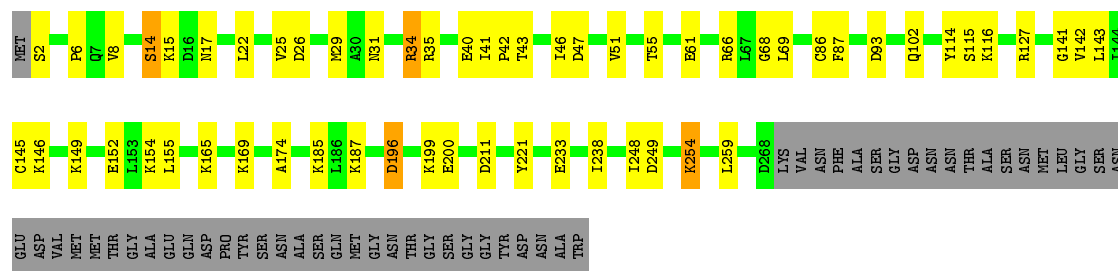
Device Type	Percentage
Smartphone	71%
Tablet	19%
Feature Phone	8%





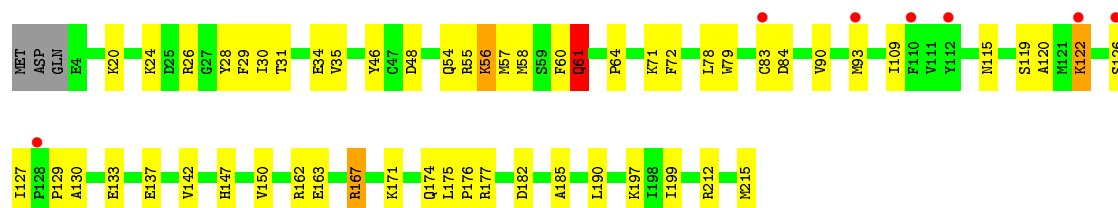
• Molecule 6: DNA-directed RNA polymerase II subunit RPB3

Chain C: 66% 17% 16%

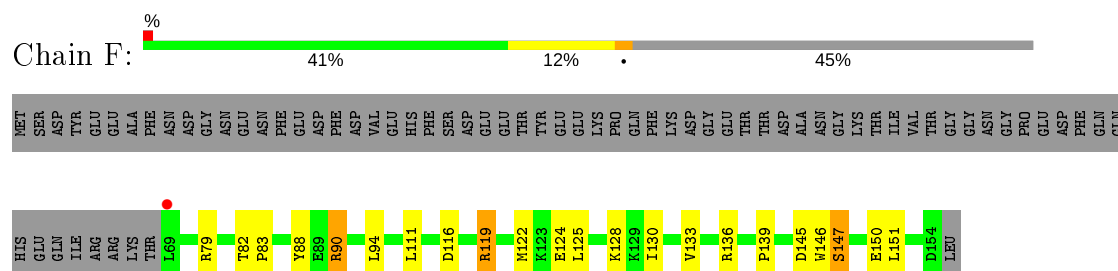


• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

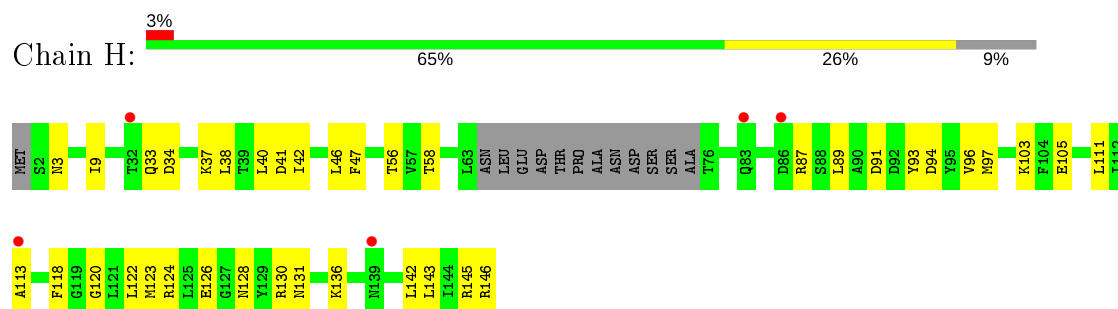
Chain E: 3% 73% 24%



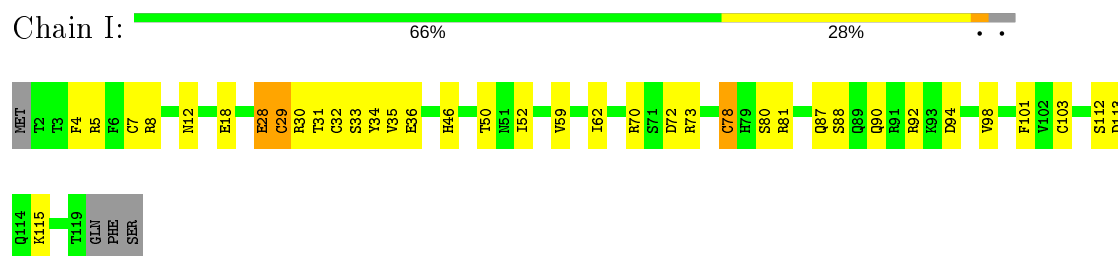
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2



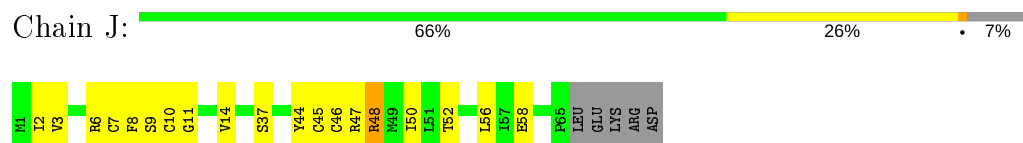
- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 10: DNA-directed RNA polymerase II subunit RPB9



- Molecule 11: 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	165.69Å 223.32Å 193.52Å 90.00° 99.37° 90.00°	Depositor
Resolution (Å)	49.75 – 3.20 49.76 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.75-3.20) 99.9 (49.76-3.20)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.13 _2998	Depositor
R, R_{free}	0.230 , 0.280 0.230 , 0.281	Depositor DCC
R_{free} test set	1801 reflections (1.58%)	wwPDB-VP
Wilson B-factor (Å ²)	80.5	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	29048	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	R	0.32	0/219	0.88	0/341
2	T	0.56	0/577	1.07	1/886 (0.1%)
3	N	0.57	0/359	0.94	1/553 (0.2%)
4	A	0.30	0/11020	0.59	6/14907 (0.0%)
5	B	0.31	0/9030	0.55	3/12186 (0.0%)
6	C	0.30	0/2139	0.56	0/2899
7	E	0.32	0/1767	0.60	1/2378 (0.0%)
8	F	0.28	0/696	0.55	0/943
9	H	0.33	0/1082	0.66	0/1466
10	I	0.32	0/970	0.58	0/1308
11	J	0.30	0/541	0.60	0/727
12	K	0.32	0/937	0.63	0/1265
13	L	0.32	0/339	0.57	0/450
All	All	0.32	0/29676	0.60	12/40309 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1150	ARG	NE-CZ-NH2	-6.48	117.06	120.30
4	A	472	LEU	CB-CG-CD2	-6.33	100.25	111.00
5	B	1150	ARG	CA-CB-CG	-6.27	99.60	113.40
4	A	550	LEU	CA-CB-CG	6.09	129.30	115.30
4	A	702	LEU	CB-CG-CD1	6.02	121.24	111.00
3	N	3	DA	O4'-C1'-N9	5.73	112.01	108.00
7	E	167	ARG	NE-CZ-NH1	5.58	123.09	120.30
4	A	691	LEU	CA-CB-CG	5.39	127.69	115.30
2	T	22	DT	O4'-C4'-C3'	-5.32	102.37	104.50
4	A	262	LEU	CA-CB-CG	5.27	127.43	115.30
4	A	702	LEU	CA-CB-CG	5.25	127.37	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	941	LEU	CA-CB-CG	5.20	127.26	115.30

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	R	195	0	99	0	0
2	T	520	0	297	6	0
3	N	317	0	166	3	0
4	A	10828	0	10876	203	0
5	B	8859	0	8816	153	0
6	C	2101	0	2056	38	0
7	E	1731	0	1758	37	0
8	F	684	0	692	16	0
9	H	1064	0	1029	22	0
10	I	952	0	897	29	0
11	J	532	0	542	13	0
12	K	919	0	929	12	0
13	L	337	0	352	7	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	29048	0	28509	477	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 8.

All (477) 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)
5:B:29:ASP:OD2	5:B:655:LYS:NZ	1.65	1.27
10:I:59:VAL:O	10:I:62:ILE:HD13	1.54	1.06
10:I:59:VAL:H	10:I:62:ILE:CD1	1.68	1.05
7:E:55:ARG:NH2	7:E:137:GLU:OE1	2.01	0.93
10:I:59:VAL:H	10:I:62:ILE:HD11	1.35	0.90
10:I:59:VAL:H	10:I:62:ILE:HD13	1.40	0.86
10:I:59:VAL:N	10:I:62:ILE:HD13	1.95	0.81
10:I:59:VAL:N	10:I:62:ILE:CD1	2.44	0.80
4:A:445:ASN:ND2	4:A:455:MET:SD	2.63	0.72
4:A:326:ARG:HG3	4:A:1406:VAL:HG11	1.71	0.71
4:A:848:ILE:HG21	4:A:1370:LEU:HD21	1.73	0.70
4:A:666:ILE:HD12	4:A:667:GLY:N	2.07	0.70
5:B:998:ASP:OD1	6:C:35:ARG:NH2	2.26	0.69
10:I:59:VAL:C	10:I:62:ILE:HD13	2.13	0.68
5:B:806:THR:HG22	5:B:808:ALA:H	1.58	0.68
5:B:612:GLU:O	5:B:632:ARG:NH2	2.27	0.68
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.75	0.67
4:A:443:LEU:HB3	4:A:490:HIS:HB2	1.76	0.67
10:I:50:THR:HG22	10:I:52:ILE:H	1.59	0.67
4:A:535:THR:HG21	4:A:617:VAL:HG23	1.76	0.66
4:A:68:GLN:NE2	4:A:70:CYS:SG	2.69	0.66
7:E:46:TYR:HH	7:E:56:LYS:H	1.44	0.66
8:F:133:VAL:HG23	8:F:146:TRP:C	2.16	0.66
4:A:306:ASN:OD1	4:A:313:GLN:NE2	2.29	0.65
5:B:857:ARG:NH1	5:B:945:GLU:OE2	2.30	0.65
4:A:243:PRO:HB2	4:A:245:PRO:HD2	1.78	0.64
7:E:175:LEU:HD12	7:E:176:PRO:HD2	1.79	0.64
4:A:72:GLU:HB3	4:A:76:GLU:HB3	1.79	0.64
4:A:525:GLN:NE2	5:B:836:GLU:OE2	2.24	0.64
4:A:265:LYS:HG3	4:A:303:TYR:HB2	1.78	0.64
4:A:838:GLN:HG3	4:A:1073:GLY:HA3	1.79	0.64
6:C:31:ASN:OD1	6:C:34:ARG:NH1	2.31	0.63
4:A:170:THR:HG23	4:A:185:TRP:HE1	1.63	0.63
5:B:975:GLN:NE2	5:B:1100:ASP:OD2	2.30	0.63
5:B:1002:THR:HG23	5:B:1004:GLU:H	1.64	0.63
5:B:273:LEU:HD12	5:B:280:ILE:HD11	1.80	0.63
5:B:364:ILE:HD13	5:B:585:VAL:HG13	1.81	0.63
4:A:90:VAL:HG23	4:A:236:LEU:HB2	1.81	0.63
4:A:1064:VAL:O	4:A:1068:ALA:N	2.29	0.63
4:A:286:HIS:NE2	4:A:287:HIS:CE1	2.67	0.63
11:J:48:ARG:O	11:J:52:THR:OG1	2.16	0.63
5:B:1076:HIS:O	6:C:31:ASN:ND2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:526:ASP:OD1	5:B:835:GLN:NE2	2.32	0.62
4:A:38:PRO:HD3	4:A:270:LEU:HD22	1.81	0.62
5:B:40:GLU:OE1	5:B:41:LYS:HG2	2.00	0.62
4:A:864:ILE:HD12	4:A:1374:VAL:HG22	1.81	0.62
4:A:440:ASP:OD2	4:A:498:ARG:NH2	2.32	0.62
5:B:361:LEU:HD23	5:B:364:ILE:HG13	1.82	0.61
5:B:1029:CYS:SG	5:B:1090:THR:OG1	2.58	0.61
6:C:169:LYS:NZ	13:L:69:ALA:O	2.33	0.61
4:A:88:LYS:HD3	4:A:293:GLU:HG2	1.84	0.60
9:H:37:LYS:NZ	9:H:126:GLU:OE1	2.34	0.60
4:A:1312:ASN:ND2	4:A:1315:GLU:OE2	2.34	0.60
4:A:1436:ILE:HB	5:B:1144:ALA:HB2	1.82	0.60
7:E:127:ILE:HG22	7:E:129:PRO:HD2	1.83	0.60
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.34	0.60
6:C:40:GLU:OE1	6:C:254:LYS:NZ	2.27	0.60
4:A:446:ARG:NH1	4:A:447:GLN:O	2.34	0.60
5:B:193:LYS:HB3	5:B:787:VAL:HG11	1.84	0.60
4:A:211:PHE:HA	4:A:214:ILE:HG12	1.85	0.59
4:A:438:ASP:OD2	4:A:461:LYS:NZ	2.35	0.59
6:C:115:SER:HB3	6:C:142:VAL:HG12	1.82	0.59
10:I:59:VAL:O	10:I:62:ILE:CD1	2.39	0.59
4:A:1025:ARG:O	4:A:1035:TYR:OH	2.20	0.59
6:C:185:LYS:NZ	6:C:211:ASP:O	2.35	0.59
5:B:383:ASN:OD1	5:B:384:ARG:NH1	2.36	0.59
12:K:100:ALA:O	12:K:104:ASN:ND2	2.36	0.59
5:B:780:VAL:HG21	11:J:56:LEU:HD11	1.85	0.58
5:B:822:ASN:O	11:J:48:ARG:NH1	2.36	0.58
5:B:996:ARG:NH2	6:C:174:ALA:O	2.35	0.58
4:A:1350:LYS:O	4:A:1354:ASN:ND2	2.31	0.58
4:A:392:VAL:HG13	4:A:415:LEU:HD11	1.85	0.58
5:B:847:ASP:OD2	12:K:6:ARG:NH2	2.36	0.58
10:I:80:SER:OG	10:I:103:CYS:SG	2.60	0.58
8:F:79:ARG:NH2	8:F:150:GLU:OE1	2.36	0.58
5:B:102:VAL:HG22	5:B:112:LEU:HB2	1.85	0.58
10:I:59:VAL:N	10:I:62:ILE:HD11	2.13	0.58
4:A:1118:VAL:HG23	4:A:1327:ILE:HG13	1.84	0.58
4:A:445:ASN:HB3	4:A:488:ASN:HB2	1.86	0.58
7:E:55:ARG:N	7:E:84:ASP:OD2	2.36	0.57
4:A:503:GLN:OE1	8:F:90:ARG:NH2	2.36	0.57
6:C:86:CYS:SG	6:C:87:PHE:N	2.77	0.57
4:A:711:ARG:NH2	10:I:87:GLN:OE1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:165:LYS:O	12:K:6:ARG:NH1	2.37	0.57
4:A:1239:ARG:HH12	4:A:1241:ARG:HH12	1.51	0.57
4:A:808:LEU:O	5:B:728:ARG:NH1	2.37	0.57
4:A:107:CYS:SG	4:A:110:CYS:N	2.77	0.57
5:B:40:GLU:C	5:B:40:GLU:OE1	2.43	0.57
5:B:114:PRO:HG3	5:B:181:LEU:HD11	1.86	0.57
4:A:517:ASN:OD1	4:A:1364:ASN:ND2	2.37	0.56
7:E:177:ARG:HB3	7:E:215:MET:HG2	1.87	0.56
5:B:103:ASN:ND2	5:B:109:THR:OG1	2.38	0.56
4:A:457:ALA:HB3	4:A:506:ALA:HA	1.86	0.56
5:B:325:GLN:NE2	10:I:12:ASN:OD1	2.39	0.56
5:B:287:ARG:NH1	5:B:324:ILE:O	2.38	0.56
5:B:287:ARG:NH2	5:B:294:ASP:OD2	2.38	0.56
12:K:24:ASP:OD2	12:K:74:ARG:NH1	2.38	0.56
4:A:1166:ASP:HA	4:A:1169:ILE:HD13	1.88	0.56
4:A:871:ASP:OD1	4:A:1366:ARG:NH2	2.38	0.56
2:T:22:DT:OP1	4:A:344:ARG:NH1	2.38	0.56
4:A:1323:ASP:OD1	4:A:1325:THR:OG1	2.21	0.56
5:B:103:ASN:OD1	5:B:169:ARG:NH2	2.39	0.56
6:C:146:LYS:NZ	11:J:58:GLU:OE2	2.38	0.55
6:C:22:LEU:HD11	12:K:101:LEU:HD21	1.87	0.55
4:A:148:CYS:SG	4:A:164:ARG:NH1	2.80	0.55
4:A:352:VAL:HB	5:B:1099:VAL:HG12	1.88	0.55
4:A:903:ASN:O	4:A:907:THR:OG1	2.22	0.55
9:H:40:LEU:HD13	9:H:123:MET:HB2	1.86	0.55
9:H:94:ASP:OD1	9:H:94:ASP:N	2.39	0.55
5:B:66:ASP:OD2	5:B:422:LYS:NZ	2.39	0.55
5:B:118:ARG:HA	5:B:207:GLY:HA2	1.88	0.55
5:B:493:SER:OG	5:B:497:ARG:NH2	2.40	0.55
5:B:115:GLN:HG2	5:B:193:LYS:HB2	1.88	0.55
4:A:1339:LEU:HD13	7:E:147:HIS:HD2	1.72	0.55
4:A:824:LEU:HD21	5:B:765:PRO:HB3	1.89	0.54
5:B:287:ARG:HG2	5:B:292:ILE:HD13	1.89	0.54
7:E:171:LYS:HB2	7:E:174:GLN:HG3	1.90	0.54
4:A:1168:GLU:HA	4:A:1171:GLN:HB3	1.89	0.54
4:A:781:ASP:HB2	4:A:789:LYS:HG2	1.90	0.54
4:A:884:ASP:OD2	4:A:1030:ARG:NH2	2.39	0.54
5:B:334:ILE:HG21	5:B:352:ALA:HB2	1.88	0.54
6:C:66:ARG:NH1	6:C:143:LEU:O	2.41	0.54
10:I:28:GLU:HB3	10:I:35:VAL:HG13	1.88	0.54
5:B:1135:ARG:NH2	5:B:1136:ASP:OD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1063:MET:HG3	5:B:1139:ILE:HG22	1.90	0.54
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.90	0.54
7:E:56:LYS:HD3	7:E:84:ASP:OD1	2.08	0.54
12:K:18:LYS:NZ	12:K:36:GLU:O	2.33	0.54
4:A:4:GLN:NE2	4:A:76:GLU:OE1	2.41	0.54
6:C:69:LEU:HD12	11:J:6:ARG:HG3	1.89	0.54
4:A:1004:ASN:HB3	7:E:167:ARG:HH21	1.73	0.53
4:A:123:ARG:HA	4:A:126:LEU:HG	1.90	0.53
4:A:1118:VAL:HG12	4:A:1306:LEU:HB2	1.91	0.53
10:I:59:VAL:CA	10:I:62:ILE:HD13	2.39	0.53
5:B:882:THR:HG22	5:B:934:LYS:HD2	1.91	0.53
4:A:1193:LEU:HB2	4:A:1260:LEU:HD21	1.91	0.53
4:A:562:THR:O	4:A:576:GLN:NE2	2.42	0.53
4:A:1140:HIS:HA	4:A:1275:GLY:HA3	1.91	0.53
5:B:643:ASP:O	5:B:647:GLY:N	2.42	0.53
4:A:350:ARG:NE	4:A:486:GLU:OE2	2.35	0.53
4:A:51:GLY:HA2	4:A:56:PRO:HD3	1.90	0.53
10:I:101:PHE:HE1	10:I:112:SER:HB3	1.73	0.53
5:B:373:ARG:HA	5:B:566:LEU:HD23	1.91	0.52
5:B:900:ALA:HB3	13:L:61:THR:HG23	1.91	0.52
5:B:217:ARG:NH1	5:B:407:ASP:OD1	2.42	0.52
5:B:651:LEU:HD13	5:B:653:VAL:HG23	1.91	0.52
6:C:43:THR:HG22	6:C:238:ILE:HD13	1.92	0.52
4:A:147:VAL:HG12	4:A:170:THR:HA	1.91	0.52
6:C:14:SER:OG	6:C:15:LYS:N	2.42	0.52
8:F:133:VAL:HG23	8:F:147:SER:N	2.24	0.52
4:A:541:ILE:HD12	4:A:577:ILE:HG21	1.92	0.52
5:B:176:SER:OG	5:B:177:LYS:N	2.42	0.52
11:J:9:SER:OG	11:J:48:ARG:NH2	2.43	0.52
10:I:5:ARG:NH2	10:I:36:GLU:OE2	2.42	0.52
4:A:274:ILE:HD12	4:A:277:GLU:HB2	1.92	0.52
4:A:513:SER:OG	4:A:515:GLN:O	2.28	0.52
4:A:575:LYS:HE3	9:H:120:GLY:HA3	1.92	0.52
4:A:329:LEU:HA	4:A:335:ARG:H	1.74	0.51
6:C:145:CYS:SG	6:C:146:LYS:N	2.83	0.51
7:E:26:ARG:NH2	7:E:133:GLU:OE1	2.36	0.51
7:E:147:HIS:HB3	7:E:150:VAL:HG23	1.92	0.51
4:A:663:SER:OG	4:A:664:THR:N	2.42	0.51
5:B:248:SER:OG	5:B:248:SER:O	2.29	0.51
5:B:919:SER:OG	5:B:919:SER:O	2.29	0.51
11:J:37:SER:OG	11:J:47:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1127:ASP:HB3	4:A:1130:GLN:HB3	1.92	0.51
4:A:1012:ARG:O	4:A:1016:THR:OG1	2.27	0.51
5:B:287:ARG:NH1	5:B:321:GLY:O	2.44	0.51
7:E:185:ALA:HA	7:E:190:LEU:HD23	1.92	0.51
7:E:31:THR:HB	7:E:34:GLU:HB3	1.93	0.51
5:B:564:GLU:OE2	5:B:591:ARG:NH2	2.41	0.51
4:A:868:TYR:CE1	4:A:1064:VAL:HG11	2.46	0.51
7:E:127:ILE:HB	7:E:130:ALA:HB3	1.92	0.51
5:B:876:LYS:HD2	5:B:893:LEU:HB2	1.93	0.50
4:A:861:GLY:O	7:E:174:GLN:NE2	2.44	0.50
6:C:249:ASP:OD1	12:K:102:LYS:NZ	2.44	0.50
4:A:451:HIS:HB3	4:A:453:MET:H	1.76	0.50
4:A:739:ASP:OD1	4:A:739:ASP:N	2.44	0.50
5:B:574:SER:HB3	5:B:591:ARG:HH12	1.77	0.50
9:H:89:LEU:HD13	9:H:91:ASP:O	2.11	0.50
10:I:59:VAL:CA	10:I:62:ILE:CD1	2.90	0.50
11:J:44:TYR:HA	11:J:47:ARG:HB2	1.94	0.50
13:L:47:ARG:HG3	13:L:54:ARG:HG2	1.93	0.50
4:A:1356:ILE:HG23	4:A:1361:SER:HB2	1.93	0.50
4:A:666:ILE:C	4:A:666:ILE:HD12	2.32	0.50
5:B:27:ALA:O	5:B:30:SER:OG	2.30	0.50
11:J:10:CYS:SG	11:J:11:GLY:N	2.84	0.50
4:A:508:PRO:HA	4:A:511:ILE:HG13	1.94	0.50
5:B:173:MET:HB2	5:B:203:PHE:HE2	1.77	0.50
5:B:834:ASN:HD22	5:B:1011:ILE:HG22	1.77	0.50
10:I:78:CYS:SG	10:I:80:SER:OG	2.65	0.50
4:A:999:VAL:HG12	4:A:1000:LEU:HD12	1.93	0.50
5:B:464:GLY:HA2	5:B:480:SER:HB3	1.94	0.50
7:E:48:ASP:OD1	7:E:54:GLN:NE2	2.45	0.50
4:A:1111:MET:HG3	4:A:1114:PRO:HG3	1.94	0.49
4:A:549:MET:HG2	4:A:652:VAL:HG13	1.92	0.49
4:A:208:LEU:HD23	4:A:235:ILE:HD11	1.94	0.49
9:H:41:ASP:HB2	9:H:122:LEU:H	1.76	0.49
4:A:42:ASP:OD1	4:A:42:ASP:N	2.36	0.49
4:A:7:SER:HB3	5:B:1193:GLN:HE22	1.76	0.49
5:B:1213:THR:OG1	5:B:1215:ARG:NH2	2.44	0.49
4:A:96:ILE:HA	4:A:99:ILE:HB	1.93	0.49
4:A:1235:LYS:HB3	4:A:1237:ILE:HD11	1.95	0.49
4:A:982:THR:HG22	4:A:984:LYS:H	1.75	0.49
5:B:40:GLU:O	5:B:40:GLU:OE1	2.29	0.49
4:A:662:PHE:HB3	5:B:829:CYS:SG	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:835:GLN:HE21	5:B:1013:ASN:HD21	1.59	0.49
5:B:852:ARG:HD3	5:B:973:ILE:HG23	1.94	0.49
5:B:44:VAL:HG11	5:B:495:LEU:HD13	1.95	0.49
4:A:975:HIS:O	4:A:1036:ARG:NH2	2.38	0.49
5:B:849:GLY:HA2	5:B:852:ARG:HG3	1.95	0.49
13:L:41:SER:N	13:L:44:ASP:OD2	2.46	0.49
4:A:443:LEU:HD21	4:A:455:MET:HB3	1.94	0.49
4:A:335:ARG:HD2	5:B:1202:LEU:HD12	1.93	0.49
5:B:205:ILE:HG13	5:B:461:LEU:HB3	1.95	0.49
4:A:785:PRO:HG2	5:B:703:ILE:HD12	1.94	0.49
4:A:54:ASN:ND2	4:A:54:ASN:O	2.46	0.49
4:A:899:VAL:HG21	4:A:908:LEU:HG	1.95	0.49
8:F:94:LEU:HD13	8:F:122:MET:HG2	1.94	0.48
13:L:28:LYS:N	13:L:38:LEU:O	2.46	0.48
4:A:1138:ILE:HD11	4:A:1316:VAL:HG13	1.96	0.48
4:A:266:LEU:HA	4:A:269:ILE:HD12	1.95	0.48
4:A:888:GLY:O	4:A:940:ARG:NH2	2.46	0.48
9:H:89:LEU:HD12	9:H:91:ASP:H	1.79	0.48
4:A:821:ARG:NH1	5:B:524:PRO:O	2.46	0.48
5:B:1060:ARG:NH1	6:C:200:GLU:O	2.46	0.48
5:B:1194:ILE:HD13	5:B:1196:ILE:HG23	1.94	0.48
7:E:28:TYR:HA	7:E:64:PRO:HA	1.96	0.48
4:A:457:ALA:HB2	4:A:501:LEU:HD12	1.96	0.48
9:H:58:THR:HB	9:H:143:LEU:HB2	1.95	0.48
4:A:295:LEU:HA	4:A:298:PHE:HB3	1.96	0.48
4:A:839:ARG:NH2	4:A:1402:PHE:HA	2.29	0.48
5:B:29:ASP:CG	5:B:655:LYS:NZ	2.57	0.48
4:A:1339:LEU:HD13	7:E:147:HIS:CD2	2.49	0.48
9:H:9:ILE:HG12	9:H:56:THR:HG23	1.96	0.48
5:B:815:ARG:NH2	5:B:1041:GLU:OE1	2.46	0.48
5:B:693:ILE:HG23	5:B:697:GLU:HG2	1.95	0.48
4:A:246:VAL:O	4:A:328:ARG:NH1	2.47	0.47
5:B:882:THR:OG1	5:B:885:MET:SD	2.72	0.47
4:A:351:THR:OG1	4:A:352:VAL:N	2.47	0.47
5:B:1024:ALA:HA	5:B:1027:ILE:HD12	1.96	0.47
5:B:843:GLN:HB2	5:B:993:THR:HB	1.95	0.47
9:H:89:LEU:CD1	9:H:91:ASP:H	2.27	0.47
4:A:608:ILE:HB	4:A:613:ILE:HD11	1.96	0.47
5:B:234:ILE:HD12	5:B:257:LYS:HB3	1.96	0.47
4:A:66:LYS:HD3	4:A:66:LYS:HA	1.72	0.47
5:B:615:MET:HG3	5:B:626:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1025:ARG:HA	4:A:1030:ARG:HH11	1.78	0.47
10:I:90:GLN:HG2	10:I:92:ARG:HG3	1.96	0.47
11:J:14:VAL:HB	11:J:50:ILE:HD11	1.96	0.47
4:A:702:LEU:HD12	4:A:710:LEU:HD12	1.97	0.47
4:A:1002:GLY:O	4:A:1008:GLN:NE2	2.43	0.47
4:A:95:PHE:O	4:A:99:ILE:N	2.42	0.47
7:E:56:LYS:HE2	7:E:84:ASP:OD1	2.15	0.47
4:A:306:ASN:HD22	4:A:322:VAL:HG22	1.80	0.47
4:A:31:SER:HB2	4:A:83:HIS:HB3	1.96	0.47
5:B:766:ARG:HG3	5:B:1022:THR:HG22	1.96	0.47
5:B:1023:VAL:HG12	5:B:1027:ILE:HD11	1.96	0.47
5:B:698:GLU:HA	5:B:701:ILE:HG12	1.95	0.47
5:B:862:GLN:HG2	5:B:963:PHE:HB2	1.96	0.47
4:A:848:ILE:HB	4:A:1065:GLY:HA3	1.96	0.47
4:A:901:LEU:HA	4:A:907:THR:HG23	1.96	0.47
5:B:1211:ASN:O	5:B:1211:ASN:ND2	2.39	0.47
5:B:310:MET:HG3	5:B:386:LEU:HD12	1.97	0.47
4:A:38:PRO:HB3	4:A:270:LEU:HB3	1.96	0.46
4:A:919:ILE:HD11	4:A:925:LEU:HD12	1.96	0.46
9:H:93:TYR:HA	9:H:145:ARG:HG3	1.97	0.46
4:A:998:LEU:HD12	4:A:1001:ARG:HG3	1.97	0.46
4:A:466:SER:OG	5:B:975:GLN:OE1	2.31	0.46
5:B:227:LYS:N	5:B:395:GLN:OE1	2.45	0.46
6:C:55:THR:HG1	6:C:152:GLU:H	1.58	0.46
2:T:7:DC:N4	3:N:11:DA:N1	2.63	0.46
5:B:576:ASP:OD1	5:B:576:ASP:N	2.41	0.46
6:C:8:VAL:HG22	6:C:22:LEU:HD12	1.98	0.46
4:A:537:ARG:NH1	4:A:602:ASP:OD1	2.49	0.46
5:B:118:ARG:NH2	5:B:194:GLU:OE2	2.48	0.46
4:A:567:LYS:HB2	9:H:96:VAL:HB	1.98	0.46
4:A:1436:ILE:HG22	4:A:1437:GLY:H	1.81	0.46
4:A:380:VAL:HG12	4:A:388:LEU:HD12	1.97	0.46
4:A:852:TYR:CZ	8:F:136:ARG:HG2	2.51	0.46
4:A:898:ARG:NH1	4:A:930:ASP:OD1	2.37	0.46
5:B:117:ALA:HA	5:B:122:LEU:HB2	1.97	0.46
5:B:864:LYS:HB3	5:B:864:LYS:HE2	1.69	0.46
4:A:90:VAL:HG12	4:A:297:GLN:HB2	1.98	0.46
6:C:93:ASP:O	6:C:127:ARG:NH2	2.48	0.46
10:I:32:CYS:SG	10:I:33:SER:N	2.89	0.46
4:A:913:LEU:HG	4:A:1032:LEU:HD13	1.98	0.46
4:A:92:HIS:HB3	4:A:95:PHE:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:17:ASN:HB3	6:C:233:GLU:HG3	1.98	0.46
5:B:969:ARG:NH1	6:C:61:GLU:OE1	2.40	0.46
9:H:128:ASN:OD1	9:H:131:ASN:ND2	2.36	0.46
4:A:1385:THR:HG22	4:A:1386:ARG:H	1.81	0.46
8:F:116:ASP:HB3	8:F:119:ARG:HB2	1.97	0.46
9:H:118:PHE:HE1	9:H:123:MET:HB3	1.81	0.46
10:I:34:TYR:CE2	10:I:36:GLU:HB3	2.51	0.45
4:A:370:ILE:HD13	5:B:1105:ALA:HB2	1.97	0.45
5:B:46:GLN:HG3	5:B:46:GLN:H	1.60	0.45
6:C:51:VAL:HG23	6:C:155:LEU:HB3	1.98	0.45
6:C:6:PRO:HB3	6:C:25:VAL:HG22	1.97	0.45
4:A:514:PRO:HB3	4:A:875:ALA:HB3	1.99	0.45
5:B:420:LEU:HD12	5:B:457:LEU:HD23	1.98	0.45
5:B:760:ASP:OD1	5:B:760:ASP:N	2.49	0.45
4:A:590:ARG:NH1	4:A:592:ASP:OD2	2.33	0.45
5:B:931:TYR:HD2	5:B:932:HIS:H	1.63	0.45
4:A:1154:TYR:OH	10:I:18:GLU:OE2	2.21	0.45
12:K:114:LEU:HA	12:K:114:LEU:HD23	1.84	0.45
4:A:119:ASN:HB3	4:A:122:MET:HB3	1.98	0.45
4:A:839:ARG:HH21	4:A:1402:PHE:HA	1.81	0.45
4:A:806:ARG:NH2	5:B:727:LYS:O	2.49	0.45
7:E:90:VAL:HB	7:E:119:SER:HB2	1.98	0.45
5:B:242:SER:OG	5:B:252:SER:OG	2.27	0.45
7:E:24:LYS:HB3	7:E:30:ILE:HB	1.99	0.45
9:H:122:LEU:HA	9:H:122:LEU:HD23	1.82	0.45
2:T:8:DT:H3	3:N:11:DA:H2	1.64	0.45
4:A:1006:ILE:HD11	7:E:163:GLU:HG3	1.98	0.45
4:A:1202:MET:HE3	4:A:1207:LEU:HB3	1.99	0.45
4:A:773:LYS:HB3	4:A:773:LYS:HE2	1.73	0.45
5:B:115:GLN:NE2	5:B:193:LYS:O	2.46	0.45
5:B:199:MET:N	5:B:199:MET:SD	2.76	0.45
5:B:840:ILE:HG12	5:B:992:ILE:HG22	1.99	0.45
7:E:20:LYS:HD2	7:E:35:VAL:HA	1.98	0.45
7:E:46:TYR:OH	7:E:56:LYS:N	2.41	0.45
12:K:57:LEU:HB2	12:K:76:GLN:HB3	1.98	0.45
4:A:18:GLN:NE2	4:A:1417:GLU:O	2.50	0.45
4:A:378:GLU:OE2	4:A:387:ARG:NH2	2.49	0.45
5:B:957:ASN:HD21	5:B:961:LEU:HD12	1.82	0.45
8:F:79:ARG:NH1	8:F:145:ASP:O	2.50	0.45
9:H:111:LEU:HA	9:H:111:LEU:HD23	1.87	0.45
4:A:827:THR:O	4:A:831:THR:OG1	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:269:ILE:HD11	5:B:386:LEU:HD21	1.98	0.45
7:E:93:MET:HE3	7:E:120:ALA:HB1	1.99	0.45
10:I:29:CYS:SG	10:I:30:ARG:N	2.90	0.45
5:B:259:TYR:OH	5:B:279:ASP:OD2	2.33	0.45
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.98	0.45
8:F:94:LEU:HD21	8:F:125:LEU:HD22	1.99	0.45
5:B:393:LYS:HD3	5:B:393:LYS:HA	1.62	0.44
6:C:47:ASP:OD1	13:L:70:ARG:NH1	2.49	0.44
5:B:101:MET:HG2	5:B:111:ALA:HA	1.98	0.44
4:A:472:LEU:HD11	5:B:835:GLN:HB3	1.98	0.44
4:A:362:ASP:N	4:A:362:ASP:OD2	2.37	0.44
4:A:868:TYR:CZ	4:A:1064:VAL:HG11	2.52	0.44
5:B:418:LYS:HE2	5:B:418:LYS:HB3	1.88	0.44
10:I:98:VAL:HG11	10:I:113:ASP:HB2	1.99	0.44
3:N:6:DG:H2"	3:N:7:DA:H5"	2.00	0.44
4:A:1281:ARG:NH2	4:A:1309:ASP:OD1	2.46	0.44
5:B:1160:VAL:HG11	5:B:1169:MET:HB3	1.97	0.44
4:A:490:HIS:CG	5:B:1150:ARG:HH12	2.36	0.44
5:B:406:LEU:HA	5:B:406:LEU:HD23	1.86	0.44
6:C:196:ASP:HB3	6:C:199:LYS:HB2	1.99	0.44
4:A:1324:PRO:HB2	7:E:142:VAL:HG11	2.00	0.44
7:E:20:LYS:HB3	7:E:35:VAL:HG22	2.00	0.44
4:A:876:ALA:O	4:A:877:HIS:ND1	2.50	0.44
4:A:882:SER:O	4:A:1025:ARG:NH1	2.51	0.44
5:B:119:LEU:HD22	5:B:953:LEU:HD13	1.98	0.44
4:A:1138:ILE:HG23	4:A:1282:VAL:HG21	1.98	0.44
5:B:637:LEU:HD23	5:B:742:GLU:HA	2.00	0.44
4:A:1376:THR:HG22	7:E:212:ARG:HH12	1.81	0.44
4:A:512:VAL:HA	4:A:519:PRO:HA	1.99	0.44
4:A:913:LEU:HD23	4:A:913:LEU:HA	1.84	0.44
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.52	0.44
7:E:197:LYS:HE2	7:E:199:ILE:HD11	2.00	0.44
4:A:1062:GLU:OE2	8:F:88:TYR:OH	2.35	0.44
4:A:276:LEU:HD21	4:A:292:ALA:HB1	1.99	0.44
4:A:78:PRO:O	5:B:1201:LYS:NZ	2.42	0.44
10:I:29:CYS:SG	10:I:31:THR:N	2.87	0.44
4:A:100:LYS:O	4:A:104:GLU:N	2.51	0.43
4:A:901:LEU:N	4:A:926:GLN:OE1	2.38	0.43
9:H:103:LYS:HA	9:H:103:LYS:HD3	1.80	0.43
4:A:535:THR:HG23	4:A:575:LYS:HG2	2.00	0.43
4:A:880:LYS:HA	4:A:955:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:640:VAL:HA	5:B:651:LEU:HA	1.99	0.43
9:H:40:LEU:HG	9:H:42:ILE:HG12	2.00	0.43
4:A:466:SER:HB3	5:B:1103:ILE:HD11	2.00	0.43
4:A:592:ASP:O	4:A:595:THR:OG1	2.35	0.43
4:A:785:PRO:HD2	4:A:786:HIS:CD2	2.53	0.43
4:A:851:HIS:ND1	8:F:139:PRO:HG3	2.34	0.43
5:B:232:SER:O	5:B:261:ARG:NH2	2.45	0.43
4:A:571:LEU:HD23	9:H:46:LEU:HD11	1.99	0.43
4:A:67:CYS:HB3	4:A:68:GLN:H	1.47	0.43
5:B:879:ARG:HA	5:B:885:MET:SD	2.59	0.43
7:E:24:LYS:HE3	7:E:24:LYS:HB2	1.74	0.43
10:I:72:ASP:OD1	10:I:72:ASP:N	2.37	0.43
5:B:705:MET:HB3	5:B:706:GLN:H	1.70	0.43
5:B:845:SER:HB2	11:J:8:PHE:HB3	2.01	0.43
6:C:41:ILE:HA	6:C:42:PRO:HD3	1.88	0.43
8:F:82:THR:O	8:F:136:ARG:NH1	2.42	0.43
13:L:38:LEU:HD21	13:L:48:CYS:HA	1.99	0.43
4:A:387:ARG:HE	4:A:387:ARG:HB3	1.59	0.43
4:A:592:ASP:N	4:A:595:THR:OG1	2.51	0.43
4:A:864:ILE:HD13	4:A:1377:THR:HG21	2.00	0.43
4:A:944:ARG:NH2	4:A:1296:GLY:O	2.38	0.43
4:A:608:ILE:HA	4:A:608:ILE:HD13	1.91	0.43
5:B:211:VAL:HG13	5:B:495:LEU:HD23	2.00	0.43
7:E:56:LYS:CE	7:E:84:ASP:OD1	2.66	0.43
4:A:182:VAL:HA	4:A:202:LEU:HD13	2.00	0.43
4:A:348:SER:HB2	5:B:1128:LEU:HB2	2.00	0.43
5:B:116:GLU:OE2	5:B:120:ARG:NH1	2.52	0.43
7:E:177:ARG:O	7:E:212:ARG:NH2	2.50	0.43
11:J:2:ILE:HG12	11:J:3:VAL:H	1.84	0.43
6:C:26:ASP:OD1	6:C:26:ASP:N	2.49	0.42
2:T:16:DT:H2"	2:T:17:DG:C8	2.54	0.42
4:A:688:LYS:HB2	4:A:688:LYS:HE2	1.70	0.42
4:A:666:ILE:O	4:A:669:THR:OG1	2.28	0.42
8:F:128:LYS:NZ	8:F:151:LEU:O	2.52	0.42
10:I:94:ASP:OD1	10:I:94:ASP:N	2.52	0.42
4:A:1329:THR:HG22	4:A:1331:SER:H	1.84	0.42
4:A:471:ASN:OD1	4:A:472:LEU:N	2.53	0.42
4:A:584:ASN:HA	4:A:610:GLY:HA3	2.02	0.42
4:A:332:LYS:HB3	4:A:332:LYS:HE2	1.75	0.42
5:B:435:THR:HG23	5:B:438:GLU:HB2	2.02	0.42
5:B:763:GLN:HG3	5:B:765:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:488:TYR:HE2	5:B:813:LYS:HB2	1.83	0.42
4:A:742:ASN:N	4:A:742:ASN:OD1	2.53	0.42
4:A:800:VAL:HG13	4:A:812:GLU:HB3	2.01	0.42
5:B:751:VAL:HG23	5:B:812:LEU:HD22	2.02	0.42
5:B:840:ILE:HB	5:B:1011:ILE:HB	2.02	0.42
6:C:248:ILE:HD11	12:K:101:LEU:HD22	2.02	0.42
4:A:385:ILE:O	4:A:389:THR:OG1	2.34	0.42
7:E:78:LEU:HD21	7:E:109:ILE:HD13	2.01	0.42
9:H:142:LEU:HD23	9:H:142:LEU:HA	1.80	0.42
11:J:45:CYS:SG	11:J:46:CYS:N	2.93	0.42
4:A:1128:GLN:H	4:A:1128:GLN:HG3	1.52	0.41
4:A:760:GLN:HA	4:A:765:VAL:HA	2.02	0.41
5:B:1158:PHE:HE2	5:B:1201:LYS:HE3	1.84	0.41
4:A:1428:VAL:HG13	5:B:1151:LEU:HD21	2.00	0.41
4:A:444:PHE:CE2	4:A:470:LEU:HD23	2.55	0.41
4:A:579:SER:HA	4:A:582:ILE:HG13	2.01	0.41
4:A:910:PRO:HA	4:A:916:GLY:HA3	2.01	0.41
5:B:977:GLY:H	5:B:990:ILE:HB	1.86	0.41
7:E:122:LYS:HA	7:E:122:LYS:HD2	1.85	0.41
4:A:211:PHE:HD1	4:A:211:PHE:HA	1.77	0.41
4:A:899:VAL:HG13	4:A:929:LEU:HD13	2.02	0.41
5:B:227:LYS:HG3	5:B:395:GLN:HG3	2.00	0.41
5:B:1010:LEU:HD23	5:B:1010:LEU:HA	1.85	0.41
5:B:1163:CYS:SG	5:B:1164:GLY:N	2.94	0.41
6:C:29:MET:HE2	12:K:45:LEU:HD21	2.02	0.41
6:C:46:ILE:HB	6:C:68:GLY:HA2	2.02	0.41
6:C:55:THR:HG1	6:C:55:THR:H	1.65	0.41
4:A:523:ILE:HG23	4:A:527:THR:HB	2.01	0.41
5:B:579:ARG:NH2	5:B:622:LYS:O	2.53	0.41
8:F:124:GLU:HB3	8:F:130:ILE:HD11	2.03	0.41
2:T:7:DC:H6	2:T:7:DC:H2'	1.67	0.41
4:A:993:LEU:HD22	4:A:1046:LEU:HG	2.03	0.41
8:F:128:LYS:HB3	8:F:128:LYS:HE3	1.82	0.41
5:B:326:ASP:N	5:B:326:ASP:OD1	2.54	0.41
5:B:62:ILE:HG23	5:B:418:LYS:HG2	2.01	0.41
5:B:936:ASP:OD1	5:B:937:ALA:N	2.53	0.41
7:E:46:TYR:CE1	7:E:57:MET:HB3	2.55	0.41
6:C:114:TYR:HB3	6:C:141:GLY:H	1.86	0.41
9:H:46:LEU:HD23	9:H:46:LEU:HA	1.93	0.41
4:A:229:SER:HB3	4:A:1416:ALA:HB2	2.03	0.41
4:A:17:VAL:HG23	4:A:1421:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:4:DT:H2'	2:T:4:DT:H6	1.74	0.41
5:B:1158:PHE:CE2	5:B:1201:LYS:HE3	2.56	0.41
7:E:61:GLN:HB2	7:E:79:TRP:HE3	1.86	0.41
10:I:115:LYS:HD3	10:I:115:LYS:HA	1.85	0.41
4:A:1116:LEU:O	4:A:1308:THR:HG23	2.21	0.40
4:A:286:HIS:CE1	4:A:287:HIS:ND1	2.89	0.40
4:A:669:THR:O	4:A:762:SER:OG	2.32	0.40
5:B:1072:MET:HG3	5:B:1085:ILE:HB	2.03	0.40
6:C:102:GLN:HB3	6:C:154:LYS:HG3	2.02	0.40
9:H:105:GLU:HB3	9:H:113:ALA:HB3	2.03	0.40
4:A:1345:ARG:NH1	4:A:1373:ASP:OD2	2.45	0.40
4:A:618:GLU:HB2	4:A:619:LYS:H	1.78	0.40
5:B:1160:VAL:HB	5:B:1194:ILE:HD11	2.02	0.40
5:B:28:GLU:OE2	5:B:807:ARG:NH2	2.48	0.40
5:B:306:ASN:OD1	5:B:306:ASN:N	2.54	0.40
5:B:537:LYS:HB2	5:B:537:LYS:HE2	1.90	0.40
8:F:83:PRO:HA	8:F:146:TRP:CZ3	2.56	0.40
4:A:1373:ASP:O	4:A:1377:THR:N	2.53	0.40
4:A:1392:SER:HB2	4:A:1394:THR:HG23	2.03	0.40
6:C:259:LEU:HD12	6:C:259:LEU:HA	1.93	0.40
4:A:269:ILE:O	4:A:273:ASN:N	2.52	0.40
4:A:242:PRO:O	4:A:247:ARG:NH2	2.51	0.40
5:B:100:PRO:HG3	5:B:172:ILE:HG13	2.02	0.40
4:A:22:PHE:HB2	5:B:1211:ASN:ND2	2.36	0.40
5:B:357:GLN:HA	5:B:374:LYS:NZ	2.36	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
4	A	1370/1733 (79%)	1276 (93%)	85 (6%)	9 (1%)	22 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	B	1103/1224 (90%)	1040 (94%)	60 (5%)	3 (0%)	41	74
6	C	265/318 (83%)	246 (93%)	19 (7%)	0	100	100
7	E	210/215 (98%)	192 (91%)	16 (8%)	2 (1%)	15	54
8	F	84/155 (54%)	75 (89%)	9 (11%)	0	100	100
9	H	129/146 (88%)	116 (90%)	12 (9%)	1 (1%)	19	58
10	I	116/122 (95%)	107 (92%)	9 (8%)	0	100	100
11	J	63/70 (90%)	60 (95%)	3 (5%)	0	100	100
12	K	112/120 (93%)	106 (95%)	5 (4%)	1 (1%)	17	56
13	L	41/70 (59%)	36 (88%)	5 (12%)	0	100	100
All	All	3493/4173 (84%)	3254 (93%)	223 (6%)	16 (0%)	29	67

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	K	28	PRO
4	A	55	ASP
4	A	704	ALA
4	A	1036	ARG
4	A	1242	VAL
5	B	466	TRP
4	A	48	ALA
4	A	67	CYS
5	B	1107	ALA
7	E	61	GLN
7	E	115	ASN
4	A	312	PRO
5	B	1017	ILE
9	H	33	GLN
4	A	464	PRO
4	A	1436	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	
4	A	1194/1520 (79%)	1116 (94%)	78 (6%)	17	51
5	B	955/1061 (90%)	900 (94%)	55 (6%)	20	55
6	C	235/274 (86%)	226 (96%)	9 (4%)	33	67
7	E	193/197 (98%)	181 (94%)	12 (6%)	18	53
8	F	73/137 (53%)	69 (94%)	4 (6%)	21	57
9	H	116/128 (91%)	106 (91%)	10 (9%)	10	38
10	I	110/116 (95%)	99 (90%)	11 (10%)	7	30
11	J	60/65 (92%)	58 (97%)	2 (3%)	38	71
12	K	99/102 (97%)	91 (92%)	8 (8%)	11	42
13	L	37/57 (65%)	33 (89%)	4 (11%)	6	27
All	All	3072/3657 (84%)	2879 (94%)	193 (6%)	18	52

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	5	GLN
4	A	22	PHE
4	A	23	SER
4	A	42	ASP
4	A	47	ARG
4	A	68	GLN
4	A	81	PHE
4	A	108	MET
4	A	109	HIS
4	A	112	LYS
4	A	129	LYS
4	A	142	CYS
4	A	148	CYS
4	A	164	ARG
4	A	185	TRP
4	A	203	SER
4	A	238	CYS
4	A	247	ARG
4	A	261	ASP
4	A	265	LYS
4	A	287	HIS
4	A	294	SER
4	A	303	TYR
4	A	307	ASP

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Mol	Chain	Res	Type
4	A	329	LEU
4	A	383	TYR
4	A	417	TYR
4	A	425	GLN
4	A	444	PHE
4	A	453	MET
4	A	455	MET
4	A	468	PHE
4	A	470	LEU
4	A	518	LYS
4	A	526	ASP
4	A	532	ARG
4	A	537	ARG
4	A	573	SER
4	A	583	PRO
4	A	584	ASN
4	A	603	ASN
4	A	618	GLU
4	A	672	ASP
4	A	677	ARG
4	A	688	LYS
4	A	739	ASP
4	A	742	ASN
4	A	764	CYS
4	A	813	PHE
4	A	816	HIS
4	A	821	ARG
4	A	873	MET
4	A	877	HIS
4	A	884	ASP
4	A	890	ASP
4	A	896	ARG
4	A	913	LEU
4	A	934	LYS
4	A	941	LYS
4	A	1001	ARG
4	A	1029	ARG
4	A	1030	ARG
4	A	1093	LYS
4	A	1100	ARG
4	A	1112	LYS
4	A	1150	SER

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Mol	Chain	Res	Type
4	A	1215	ARG
4	A	1218	GLN
4	A	1261	LYS
4	A	1289	ARG
4	A	1300	LYS
4	A	1313	LEU
4	A	1350	LYS
4	A	1366	ARG
4	A	1368	MET
4	A	1400	CYS
4	A	1410	PHE
4	A	1444	MET
5	B	39	ARG
5	B	40	GLU
5	B	46	GLN
5	B	106	ASP
5	B	126	SER
5	B	199	MET
5	B	217	ARG
5	B	232	SER
5	B	248	SER
5	B	250	PHE
5	B	261	ARG
5	B	264	SER
5	B	306	ASN
5	B	347	LYS
5	B	348	ARG
5	B	370	PHE
5	B	384	ARG
5	B	398	ARG
5	B	401	PHE
5	B	404	LYS
5	B	437	GLU
5	B	466	TRP
5	B	483	LEU
5	B	606	LYS
5	B	641	GLU
5	B	642	ASP
5	B	648	HIS
5	B	651	LEU
5	B	654	ARG
5	B	655	LYS

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Mol	Chain	Res	Type
5	B	662	MET
5	B	665	GLU
5	B	668	ASP
5	B	766	ARG
5	B	807	ARG
5	B	879	ARG
5	B	886	LYS
5	B	895	ASP
5	B	919	SER
5	B	931	TYR
5	B	933	SER
5	B	935	ARG
5	B	958	GLN
5	B	959	ASP
5	B	963	PHE
5	B	999	MET
5	B	1010	LEU
5	B	1096	ARG
5	B	1112	GLN
5	B	1135	ARG
5	B	1163	CYS
5	B	1166	CYS
5	B	1180	PHE
5	B	1188	LYS
5	B	1211	ASN
6	C	2	SER
6	C	14	SER
6	C	34	ARG
6	C	116	LYS
6	C	149	LYS
6	C	187	LYS
6	C	196	ASP
6	C	221	TYR
6	C	254	LYS
7	E	29	PHE
7	E	56	LYS
7	E	58	MET
7	E	60	PHE
7	E	61	GLN
7	E	71	LYS
7	E	72	PHE
7	E	83	CYS

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Mol	Chain	Res	Type
7	E	122	LYS
7	E	126	SER
7	E	162	ARG
7	E	182	ASP
8	F	90	ARG
8	F	111	LEU
8	F	119	ARG
8	F	147	SER
9	H	3	ASN
9	H	34	ASP
9	H	38	LEU
9	H	47	PHE
9	H	87	ARG
9	H	97	MET
9	H	124	ARG
9	H	130	ARG
9	H	136	LYS
9	H	146	ARG
10	I	4	PHE
10	I	7	CYS
10	I	8	ARG
10	I	28	GLU
10	I	29	CYS
10	I	46	HIS
10	I	70	ARG
10	I	73	ARG
10	I	78	CYS
10	I	81	ARG
10	I	88	SER
11	J	7	CYS
11	J	48	ARG
12	K	2	ASN
12	K	14	GLU
12	K	20	LYS
12	K	22	ASP
12	K	29	ASN
12	K	54	ARG
12	K	81	TYR
12	K	114	LEU
13	L	31	CYS
13	L	34	CYS
13	L	49	LYS

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Mol	Chain	Res	Type
13	L	58	LYS

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

Mol	Chain	Res	Type
5	B	103	ASN
5	B	835	GLN
5	B	1193	GLN
5	B	1211	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	8/9 (88%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	4	G
1	R	9	G

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides 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

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	R	9/9 (100%)	-0.51	0 100 100	85, 102, 180, 188	0
2	T	26/29 (89%)	-0.22	2 (7%) 13 7	85, 159, 230, 258	0
3	N	15/18 (83%)	0.17	0 100 100	181, 217, 240, 254	0
4	A	1384/1733 (79%)	-0.14	24 (1%) 70 57	46, 92, 174, 257	0
5	B	1123/1224 (91%)	-0.23	3 (0%) 94 92	37, 74, 140, 220	0
6	C	267/318 (83%)	-0.35	0 100 100	46, 78, 123, 146	0
7	E	212/215 (98%)	-0.06	7 (3%) 46 30	74, 117, 180, 247	0
8	F	86/155 (55%)	-0.42	1 (1%) 79 67	62, 91, 136, 185	0
9	H	133/146 (91%)	0.07	5 (3%) 40 26	80, 123, 169, 233	0
10	I	118/122 (96%)	-0.31	0 100 100	65, 99, 138, 176	0
11	J	65/70 (92%)	-0.40	0 100 100	49, 69, 104, 129	0
12	K	114/120 (95%)	-0.30	0 100 100	50, 84, 121, 133	0
13	L	43/70 (61%)	0.36	3 (6%) 16 9	64, 141, 209, 232	0
All	All	3595/4229 (85%)	-0.19	45 (1%) 77 65	37, 88, 168, 258	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	69	THR	8.0
4	A	144	THR	6.1
4	A	183	GLY	5.6
4	A	141	LEU	5.5
4	A	182	VAL	5.0
4	A	173	THR	4.1
9	H	83	GLN	3.9
4	A	114	LEU	3.7
5	B	869	SER	3.5

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Mol	Chain	Res	Type	RSRZ
4	A	181	LEU	3.4
4	A	200	ARG	3.4
7	E	93	MET	3.3
4	A	1126	ALA	3.2
4	A	184	SER	3.1
4	A	149	GLU	3.1
4	A	66	LYS	3.1
7	E	83	CYS	3.1
4	A	103	CYS	3.1
13	L	41	SER	3.0
9	H	86	ASP	3.0
4	A	150	THR	2.9
8	F	69	LEU	2.9
7	E	128	PRO	2.9
7	E	122	LYS	2.8
13	L	46	VAL	2.7
4	A	68	GLN	2.6
13	L	45	ALA	2.6
4	A	163	SER	2.6
4	A	44	THR	2.5
9	H	113	ALA	2.5
4	A	201	VAL	2.5
4	A	164	ARG	2.5
9	H	139	ASN	2.4
7	E	112	TYR	2.3
4	A	199	LEU	2.3
4	A	168	GLY	2.2
4	A	174	ILE	2.2
2	T	4	DT	2.2
9	H	32	THR	2.2
4	A	105	CYS	2.2
7	E	126	SER	2.1
5	B	106	ASP	2.1
7	E	110	PHE	2.1
2	T	3	DT	2.1
5	B	473	MET	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
14	ZN	I	201	1/1	0.86	0.10	100,100,100,100	0
14	ZN	L	101	1/1	0.88	0.07	208,208,208,208	0
14	ZN	A	1801	1/1	0.88	0.08	204,204,204,204	0
15	MG	A	1803	1/1	0.92	0.06	81,81,81,81	0
14	ZN	J	101	1/1	0.95	0.25	74,74,74,74	0
14	ZN	B	1301	1/1	0.96	0.09	152,152,152,152	0
14	ZN	C	401	1/1	0.96	0.06	69,69,69,69	0
14	ZN	A	1802	1/1	0.97	0.11	128,128,128,128	0
14	ZN	I	202	1/1	0.99	0.14	101,101,101,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.