



Full wwPDB X-ray Structure Validation Report

Mar 31, 2014 – 03:43 PM BST

PDB ID : 4A3I
Title : RNA Polymerase II binary complex with DNA
Authors : Cheung, A.C.M.; Sainsbury, S.; Cramer, P.
Deposited on : 2011-09-30
Resolution : 3.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

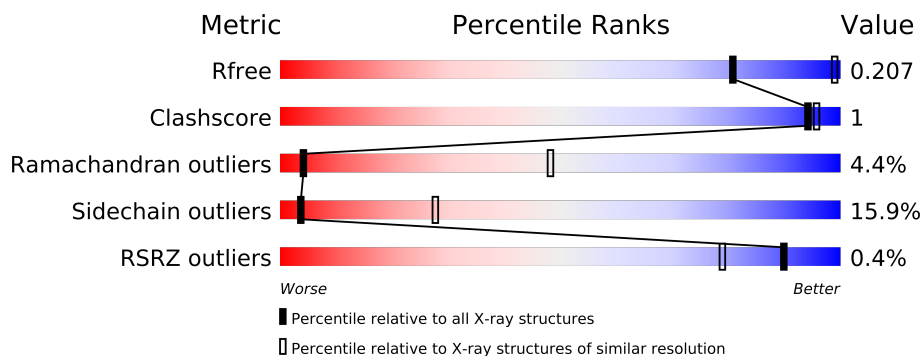
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable23004
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23004

1 Overall quality at a glance

The reported resolution of this entry is 3.80 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}	66092	1162 (4.20-3.40)
Clashscore	79885	1100 (4.10-3.50)
Ramachandran outliers	78287	1050 (4.10-3.50)
Sidechain outliers	78261	1042 (4.10-3.50)
RSRZ outliers	66119	1163 (4.20-3.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1732	
2	B	1224	
3	C	318	
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	15	
14	T	27	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
16	MG	A	2458	-	X

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 31768 atoms, of which 0 are hydrogen and 0 are deuterium.

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	1422	Total	C	N	O	S	0	0	0
			11174	7037	1954	2121	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1115	Total	C	N	O	S	0	0	0
			8859	5609	1554	1641	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 POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

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

- Molecule 7 is a protein called RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

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

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	1
			920	590	157	171	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is a DNA chain called 5'-D(*GP*GP*CP*AP*CP*AP*AP*CP*TP*GP*CP*GP*GP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	11	Total	C	N	O	P	0	0	0
			222	106	44	62	10			

- Molecule 14 is a DNA chain called TEMPLATE DNA 27-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	17	Total	Br	C	N	O	P	0	0
			350	1	166	61	105	17		

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

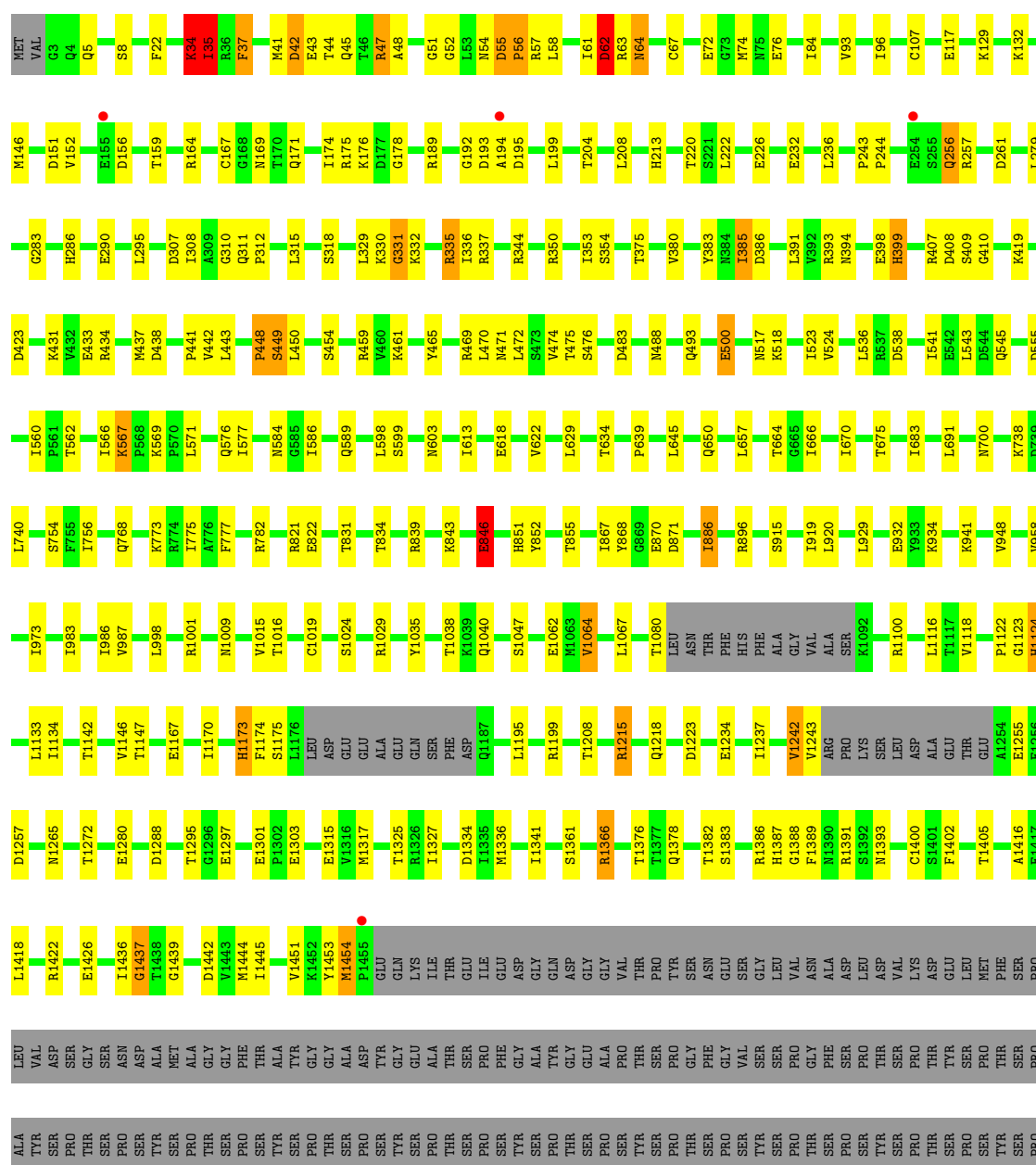
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		

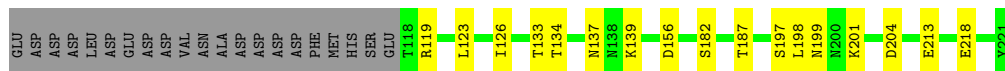
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

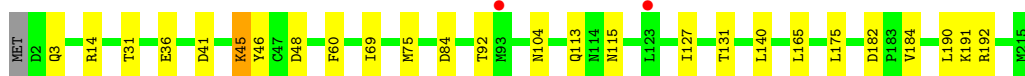
Chain A:





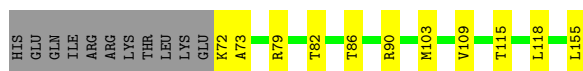
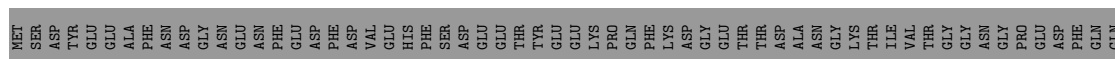
- Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

Chain E:



- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain F:



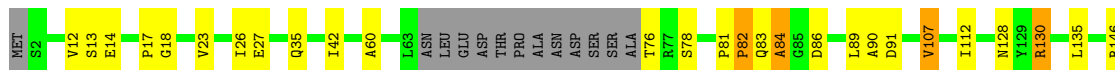
- Molecule 7: RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G:



- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H:



- Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

Chain I:



- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J:



- Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K:



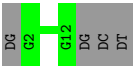
• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L:



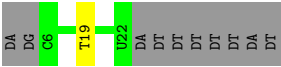
• Molecule 13: 5'-D(*GP*GP*CP*AP*CP*AP*AP*CP*TP*GP*CP*GP*GP*CP*T)-3'

Chain N:



• Molecule 14: TEMPLATE DNA 27-MER

Chain T:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	221.14Å 393.18Å 282.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.80 – 3.80 49.80 – 3.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.80-3.80) 100.0 (49.80-3.80)	Depositor EDS
R_{merge}	0.89	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 3.77Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.159 , 0.191 0.179 , 0.207	Depositor DCC
R_{free} test set	2400 reflections (1.99%)	DCC
Wilson B-factor (Å ²)	111.3	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 107.8	EDS
Estimated twinning fraction	0.026 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.034 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 120651 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31768	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, BRU

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	0.54	0/11374	0.86	10/15383 (0.1%)
2	B	0.52	0/9029	0.81	4/12171 (0.0%)
3	C	0.49	0/2133	0.80	0/2891
4	D	0.53	0/1444	0.83	0/1935
5	E	0.48	0/1788	0.76	0/2406
6	F	0.60	0/691	0.82	0/933
7	G	0.52	0/1368	0.82	0/1844
8	H	0.51	0/1086	0.83	0/1470
9	I	0.45	0/989	0.77	0/1331
10	J	0.57	0/541	0.90	0/727
11	K	0.49	0/938	0.77	0/1267
12	L	0.57	0/365	1.00	0/485
13	N	1.12	0/248	0.95	0/380
14	T	1.20	1/369 (0.3%)	0.96	0/568
All	All	0.54	1/32363 (0.0%)	0.83	14/43791 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	19	DT	C1'-N1	5.82	1.56	1.49

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	HIS	N-CA-CB	7.68	124.42	110.60
1	A	56	PRO	C-N-CA	7.07	139.38	121.70
2	B	339	THR	C-N-CA	6.22	137.25	121.70
1	A	34	LYS	C-N-CA	6.11	136.96	121.70
1	A	194	ALA	C-N-CA	5.80	136.19	121.70
1	A	35	ILE	N-CA-CB	5.72	123.97	110.80
1	A	55	ASP	N-CA-CB	5.60	120.68	110.60
2	B	1121	GLY	N-CA-C	5.50	126.85	113.10
1	A	331	GLY	N-CA-C	5.41	126.61	113.10
1	A	34	LYS	N-CA-C	-5.28	96.73	111.00
2	B	340	ALA	C-N-CA	5.25	134.83	121.70
1	A	47	ARG	C-N-CA	5.17	134.62	121.70
1	A	35	ILE	CB-CA-C	5.14	121.89	111.60
2	B	340	ALA	N-CA-C	-5.03	97.41	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	LYS	Mainchain,Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11174	0	0	23	0
2	B	8859	0	0	12	0
3	C	2095	0	0	3	0
4	D	1434	0	0	2	0
5	E	1752	0	0	0	0
6	F	679	0	0	0	0
7	G	1340	0	0	4	0
8	H	1068	0	0	3	0
9	I	971	0	0	0	0
10	J	532	0	0	5	0
11	K	920	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	363	0	0	0	0
13	N	222	0	0	0	0
14	T	350	0	0	0	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	A	1	0	0	0	0
All	All	31768	0	0	46	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

All (46) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:867:ILE:CD1	1:A:867:ILE:CG1	1.81	1.53
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.28	0.66
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.32	0.62
1:A:37:PHE:CD1	1:A:52:GLY:CA	2.82	0.62
2:B:933:SER:O	2:B:935:ARG:N	2.34	0.61
1:A:42:ASP:O	1:A:44:THR:N	2.36	0.58
3:C:183:TRP:O	3:C:185:LYS:N	2.39	0.55
3:C:66:ARG:NH2	10:J:3:VAL:O	2.39	0.55
7:G:1:MET:CE	7:G:80:LYS:O	2.54	0.55
7:G:1:MET:CG	7:G:2:PHE:N	2.70	0.54
7:G:1:MET:SD	7:G:2:PHE:N	2.81	0.54
10:J:48:ARG:O	10:J:52:THR:CG2	2.56	0.53
2:B:996:ARG:NH2	3:C:174:ALA:O	2.43	0.52
8:H:82:PRO:O	8:H:84:ALA:N	2.42	0.52
2:B:744:HIS:ND1	2:B:746:SER:OG	2.43	0.51
1:A:1389:PHE:CZ	1:A:1402:PHE:CE2	2.99	0.51
1:A:843:LYS:NZ	1:A:846:GLU:OE2	2.45	0.49
1:A:55:ASP:N	1:A:56:PRO:CD	2.77	0.47
8:H:82:PRO:C	8:H:84:ALA:N	2.68	0.47
1:A:469:ARG:NH2	2:B:991:GLY:O	2.48	0.46
1:A:1035:TYR:N	1:A:1035:TYR:CD1	2.82	0.46
10:J:9:SER:OG	10:J:48:ARG:NH2	2.48	0.46
1:A:62:ASP:O	1:A:64:ASN:N	2.50	0.45
10:J:37:SER:OG	10:J:47:ARG:NH2	2.50	0.45
4:D:14:ARG:O	4:D:16:LYS:N	2.50	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:21:ARG:NH1	7:G:24:GLN:OE1	2.50	0.44
2:B:847:ASP:OD2	11:K:6:ARG:NH2	2.51	0.44
2:B:881:ASN:OD1	2:B:933:SER:N	2.51	0.44
1:A:1436:ILE:O	1:A:1437:GLY:C	2.57	0.43
1:A:433:GLU:OE1	2:B:1108:ARG:NH2	2.52	0.43
1:A:562:THR:O	1:A:576:GLN:NE2	2.51	0.43
4:D:39:ASN:O	4:D:42:GLY:N	2.52	0.43
1:A:350:ARG:NH1	1:A:488:ASN:OD1	2.51	0.42
1:A:471:ASN:ND2	1:A:650:GLN:OE1	2.52	0.42
1:A:1436:ILE:O	1:A:1439:GLY:N	2.53	0.42
2:B:221:ASN:N	2:B:241:ARG:O	2.53	0.42
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	3.02	0.42
1:A:146:MET:O	1:A:171:GLN:N	2.52	0.41
8:H:13:SER:N	8:H:27:GLU:O	2.53	0.41
1:A:35:ILE:CG2	1:A:84:ILE:CG2	2.98	0.41
2:B:842:ASN:OD1	2:B:845:SER:OG	2.38	0.41
1:A:448:PRO:O	1:A:449:SER:CB	2.68	0.41
1:A:500:GLU:OE2	2:B:1145:SER:N	2.54	0.41
10:J:10:CYS:SG	10:J:43:ARG:NH2	2.94	0.41
2:B:350:GLN:O	2:B:351:TYR:C	2.58	0.41
1:A:1215:ARG:NE	1:A:1272:THR:O	2.54	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	1414/1732 (82%)	1207 (85%)	137 (10%)	70 (5%)	3	44
2	B	1095/1224 (90%)	929 (85%)	122 (11%)	44 (4%)	5	51
3	C	264/318 (83%)	231 (88%)	25 (10%)	8 (3%)	7	59
4	D	174/221 (79%)	152 (87%)	13 (8%)	9 (5%)	3	43
5	E	212/215 (99%)	186 (88%)	19 (9%)	7 (3%)	6	57
6	F	82/155 (53%)	75 (92%)	6 (7%)	1 (1%)	19	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	169/171 (99%)	149 (88%)	17 (10%)	3 (2%)	13	70
8	H	129/146 (88%)	102 (79%)	16 (12%)	11 (8%)	1	27
9	I	117/122 (96%)	91 (78%)	23 (20%)	3 (3%)	8	62
10	J	63/70 (90%)	52 (82%)	6 (10%)	5 (8%)	1	29
11	K	113/120 (94%)	107 (95%)	6 (5%)	0	100	100
12	L	44/70 (63%)	26 (59%)	10 (23%)	8 (18%)	0	5
All	All	3876/4564 (85%)	3307 (85%)	400 (10%)	169 (4%)	4	48

All (169) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	48	ALA
1	A	54	ASN
1	A	57	ARG
1	A	58	LEU
1	A	72	GLU
1	A	76	GLU
1	A	195	ASP
1	A	286	HIS
1	A	311	GLN
1	A	312	PRO
1	A	318	SER
1	A	335	ARG
1	A	385	ILE
1	A	449	SER
1	A	775	ILE
1	A	1016	THR
1	A	1124	HIS
2	B	67	SER
2	B	229	ALA
2	B	344	LYS
2	B	364	ILE
2	B	476	ARG
2	B	629	ASP
2	B	707	PRO
2	B	1155	SER
2	B	1175	LEU
3	C	161	LYS
3	C	184	ASN

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Mol	Chain	Res	Type
4	D	18	VAL
5	E	36	GLU
5	E	104	ASN
7	G	2	PHE
9	I	95	THR
12	L	50	ASP
12	L	53	HIS
1	A	178	GLY
1	A	257	ARG
1	A	331	GLY
1	A	410	GLY
1	A	586	ILE
1	A	777	PHE
1	A	886	ILE
1	A	986	ILE
1	A	987	VAL
1	A	1123	GLY
1	A	1167	GLU
1	A	1175	SER
1	A	1437	GLY
2	B	108	VAL
2	B	184	ALA
2	B	322	PHE
2	B	338	GLY
2	B	341	LEU
2	B	343	ILE
2	B	368	GLU
2	B	369	GLY
2	B	531	GLN
2	B	533	CYS
2	B	655	LYS
2	B	711	GLU
2	B	731	VAL
2	B	751	VAL
2	B	792	MET
2	B	879	ARG
2	B	881	ASN
2	B	1046	PRO
2	B	1223	ASP
4	D	16	LYS
4	D	20	GLU
4	D	53	SER

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Mol	Chain	Res	Type
5	E	45	LYS
6	F	73	ALA
8	H	81	PRO
8	H	82	PRO
8	H	83	GLN
10	J	2	ILE
10	J	6	ARG
12	L	59	ALA
1	A	74	MET
1	A	167	CYS
1	A	189	ARG
1	A	310	GLY
1	A	332	LYS
1	A	569	LYS
1	A	846	GLU
1	A	852	TYR
1	A	870	GLU
1	A	1122	PRO
1	A	1173	HIS
1	A	1361	SER
1	A	1388	GLY
2	B	58	THR
2	B	68	THR
2	B	275	TYR
2	B	880	THR
2	B	883	LEU
2	B	1066	SER
4	D	199	ASN
4	D	218	GLU
5	E	3	GLN
5	E	48	ASP
5	E	75	MET
7	G	154	VAL
8	H	17	PRO
8	H	84	ALA
9	I	3	THR
10	J	17	LYS
12	L	26	THR
12	L	56	LEU
1	A	62	ASP
1	A	256	GLN
1	A	419	LYS

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Mol	Chain	Res	Type
1	A	448	PRO
1	A	465	TYR
1	A	567	LYS
1	A	599	SER
1	A	639	PRO
1	A	700	ASN
1	A	1280	GLU
1	A	1416	ALA
2	B	340	ALA
2	B	526	GLU
2	B	643	ASP
2	B	667	GLN
2	B	1157	ALA
2	B	1176	ASN
4	D	119	ARG
4	D	198	LEU
5	E	113	GLN
8	H	60	ALA
9	I	113	ASP
10	J	64	ASN
1	A	169	ASN
1	A	399	HIS
1	A	409	SER
1	A	958	VAL
1	A	1378	GLN
2	B	510	LYS
2	B	1169	MET
3	C	90	ASP
4	D	40	HIS
7	G	63	PRO
8	H	107	VAL
8	H	128	ASN
8	H	130	ARG
10	J	13	VAL
12	L	39	SER
12	L	45	ALA
12	L	46	VAL
1	A	51	GLY
1	A	1454	MET
2	B	644	GLU
3	C	214	ASN
8	H	18	GLY

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Mol	Chain	Res	Type
8	H	90	ALA
1	A	35	ILE
2	B	251	ILE
3	C	38	ILE
1	A	244	PRO
3	C	150	GLY
3	C	212	PRO
1	A	192	GLY
1	A	283	GLY
1	A	380	VAL
1	A	1242	VAL
1	A	61	ILE
1	A	336	ILE
3	C	240	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1240/1519 (82%)	1029 (83%)	211 (17%)	3	24
2	B	966/1061 (91%)	813 (84%)	153 (16%)	4	28
3	C	234/274 (85%)	200 (86%)	34 (14%)	5	32
4	D	160/200 (80%)	132 (82%)	28 (18%)	3	21
5	E	196/197 (100%)	176 (90%)	20 (10%)	11	52
6	F	74/137 (54%)	64 (86%)	10 (14%)	6	36
7	G	152/152 (100%)	131 (86%)	21 (14%)	5	35
8	H	117/128 (91%)	101 (86%)	16 (14%)	5	36
9	I	113/116 (97%)	101 (89%)	12 (11%)	10	49
10	J	60/65 (92%)	45 (75%)	15 (25%)	1	8
11	K	99/102 (97%)	82 (83%)	17 (17%)	3	22
12	L	40/57 (70%)	28 (70%)	12 (30%)	0	5
All	All	3451/4008 (86%)	2902 (84%)	549 (16%)	4	28

All (549) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	22	PHE
1	A	34	LYS
1	A	37	PHE
1	A	41	MET
1	A	42	ASP
1	A	45	GLN
1	A	47	ARG
1	A	62	ASP
1	A	63	ARG
1	A	64	ASN
1	A	67	CYS
1	A	93	VAL
1	A	96	ILE
1	A	107	CYS
1	A	117	GLU
1	A	129	LYS
1	A	132	LYS
1	A	151	ASP
1	A	152	VAL
1	A	156	ASP
1	A	159	THR
1	A	164	ARG
1	A	174	ILE
1	A	175	ARG
1	A	176	LYS
1	A	193	ASP
1	A	199	LEU
1	A	204	THR
1	A	208	LEU
1	A	213	HIS
1	A	220	THR
1	A	222	LEU
1	A	226	GLU
1	A	232	GLU
1	A	236	LEU
1	A	243	PRO
1	A	256	GLN
1	A	261	ASP
1	A	279	LEU
1	A	290	GLU
1	A	295	LEU
1	A	307	ASP

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Mol	Chain	Res	Type
1	A	308	ILE
1	A	315	LEU
1	A	329	LEU
1	A	330	LYS
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	353	ILE
1	A	354	SER
1	A	375	THR
1	A	383	TYR
1	A	385	ILE
1	A	386	ASP
1	A	391	LEU
1	A	393	ARG
1	A	394	ASN
1	A	398	GLU
1	A	407	ARG
1	A	408	ASP
1	A	423	ASP
1	A	431	LYS
1	A	434	ARG
1	A	437	MET
1	A	438	ASP
1	A	441	PRO
1	A	442	VAL
1	A	443	LEU
1	A	450	LEU
1	A	454	SER
1	A	459	ARG
1	A	461	LYS
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	483	ASP
1	A	493	GLN
1	A	500	GLU
1	A	517	ASN
1	A	518	LYS
1	A	523	ILE

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Mol	Chain	Res	Type
1	A	524	VAL
1	A	536	LEU
1	A	538	ASP
1	A	541	ILE
1	A	543	LEU
1	A	545	GLN
1	A	555	ASP
1	A	560	ILE
1	A	566	ILE
1	A	567	LYS
1	A	571	LEU
1	A	577	ILE
1	A	584	ASN
1	A	589	GLN
1	A	598	LEU
1	A	603	ASN
1	A	613	ILE
1	A	618	GLU
1	A	622	VAL
1	A	629	LEU
1	A	634	THR
1	A	645	LEU
1	A	657	LEU
1	A	664	THR
1	A	666	ILE
1	A	670	ILE
1	A	675	THR
1	A	683	ILE
1	A	691	LEU
1	A	738	LYS
1	A	740	LEU
1	A	754	SER
1	A	756	ILE
1	A	768	GLN
1	A	773	LYS
1	A	782	ARG
1	A	821	ARG
1	A	822	GLU
1	A	831	THR
1	A	834	THR
1	A	839	ARG
1	A	846	GLU

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Mol	Chain	Res	Type
1	A	851	HIS
1	A	855	THR
1	A	886	ILE
1	A	896	ARG
1	A	915	SER
1	A	919	ILE
1	A	920	LEU
1	A	929	LEU
1	A	932	GLU
1	A	934	LYS
1	A	941	LYS
1	A	948	VAL
1	A	973	ILE
1	A	983	ILE
1	A	998	LEU
1	A	1001	ARG
1	A	1009	ASN
1	A	1015	VAL
1	A	1019	CYS
1	A	1024	SER
1	A	1029	ARG
1	A	1038	THR
1	A	1040	GLN
1	A	1047	SER
1	A	1062	GLU
1	A	1064	VAL
1	A	1067	LEU
1	A	1080	THR
1	A	1100	ARG
1	A	1116	LEU
1	A	1118	VAL
1	A	1124	HIS
1	A	1133	LEU
1	A	1134	ILE
1	A	1142	THR
1	A	1146	VAL
1	A	1147	THR
1	A	1170	ILE
1	A	1173	HIS
1	A	1174	PHE
1	A	1195	LEU
1	A	1199	ARG

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Mol	Chain	Res	Type
1	A	1208	THR
1	A	1215	ARG
1	A	1218	GLN
1	A	1223	ASP
1	A	1234	GLU
1	A	1237	ILE
1	A	1242	VAL
1	A	1243	VAL
1	A	1255	GLU
1	A	1257	ASP
1	A	1265	ASN
1	A	1288	ASP
1	A	1295	THR
1	A	1297	GLU
1	A	1301	GLU
1	A	1303	GLU
1	A	1315	GLU
1	A	1317	MET
1	A	1325	THR
1	A	1327	ILE
1	A	1334	ASP
1	A	1336	MET
1	A	1341	ILE
1	A	1366	ARG
1	A	1376	THR
1	A	1382	THR
1	A	1383	SER
1	A	1386	ARG
1	A	1387	HIS
1	A	1391	ARG
1	A	1393	ASN
1	A	1400	CYS
1	A	1405	THR
1	A	1418	LEU
1	A	1422	ARG
1	A	1426	GLU
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1451	VAL
1	A	1453	TYR
1	A	1454	MET

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Mol	Chain	Res	Type
2	B	25	ILE
2	B	26	THR
2	B	40	GLU
2	B	44	VAL
2	B	46	GLN
2	B	58	THR
2	B	63	ILE
2	B	91	SER
2	B	101	MET
2	B	102	VAL
2	B	118	ARG
2	B	121	ASN
2	B	122	LEU
2	B	126	SER
2	B	128	LEU
2	B	134	LYS
2	B	178	ASN
2	B	183	GLU
2	B	192	LEU
2	B	212	LEU
2	B	213	ILE
2	B	218	SER
2	B	222	ILE
2	B	240	ILE
2	B	251	ILE
2	B	261	ARG
2	B	262	GLU
2	B	264	SER
2	B	267	ARG
2	B	272	THR
2	B	278	GLN
2	B	299	GLU
2	B	317	CYS
2	B	332	ASP
2	B	337	ARG
2	B	339	THR
2	B	341	LEU
2	B	343	ILE
2	B	344	LYS
2	B	346	GLU
2	B	348	ARG
2	B	350	GLN

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Mol	Chain	Res	Type
2	B	365	THR
2	B	367	LEU
2	B	373	ARG
2	B	385	LEU
2	B	394	ASP
2	B	395	GLN
2	B	396	ASP
2	B	398	ARG
2	B	401	PHE
2	B	408	LEU
2	B	412	LEU
2	B	416	LEU
2	B	423	LYS
2	B	427	ASP
2	B	428	ILE
2	B	434	ARG
2	B	437	GLU
2	B	446	LEU
2	B	452	THR
2	B	453	ILE
2	B	461	LEU
2	B	466	TRP
2	B	470	LYS
2	B	476	ARG
2	B	485	ARG
2	B	498	THR
2	B	510	LYS
2	B	547	VAL
2	B	549	THR
2	B	552	MET
2	B	570	VAL
2	B	574	SER
2	B	582	VAL
2	B	598	GLU
2	B	603	LEU
2	B	604	ARG
2	B	615	MET
2	B	620	ARG
2	B	628	THR
2	B	629	ASP
2	B	642	ASP
2	B	644	GLU

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Mol	Chain	Res	Type
2	B	658	ILE
2	B	696	GLU
2	B	708	GLU
2	B	709	ASP
2	B	722	ASP
2	B	730	ARG
2	B	734	HIS
2	B	766	ARG
2	B	786	ASN
2	B	790	ASP
2	B	797	TYR
2	B	806	THR
2	B	835	GLN
2	B	837	ASP
2	B	844	SER
2	B	871	THR
2	B	874	PHE
2	B	878	GLN
2	B	882	THR
2	B	895	ASP
2	B	904	ARG
2	B	934	LYS
2	B	942	ARG
2	B	944	THR
2	B	945	GLU
2	B	946	ASN
2	B	953	LEU
2	B	954	VAL
2	B	956	THR
2	B	964	VAL
2	B	970	THR
2	B	973	ILE
2	B	975	GLN
2	B	976	ILE
2	B	986	GLN
2	B	987	LYS
2	B	997	GLU
2	B	999	MET
2	B	1006	ILE
2	B	1007	VAL
2	B	1028	GLU
2	B	1031	LEU

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Mol	Chain	Res	Type
2	B	1045	SER
2	B	1065	GLN
2	B	1072	MET
2	B	1084	GLN
2	B	1098	MET
2	B	1106	ARG
2	B	1112	GLN
2	B	1113	VAL
2	B	1117	GLN
2	B	1123	SER
2	B	1128	LEU
2	B	1133	MET
2	B	1135	ARG
2	B	1137	CYS
2	B	1138	MET
2	B	1148	LYS
2	B	1150	ARG
2	B	1156	ASP
2	B	1160	VAL
2	B	1175	LEU
2	B	1176	ASN
2	B	1179	GLN
2	B	1183	LYS
2	B	1195	HIS
2	B	1202	LEU
2	B	1210	MET
2	B	1212	ILE
3	C	11	ARG
3	C	12	GLU
3	C	16	ASP
3	C	22	LEU
3	C	23	SER
3	C	25	VAL
3	C	26	ASP
3	C	57	VAL
3	C	62	PHE
3	C	78	GLU
3	C	80	LEU
3	C	89	GLU
3	C	102	GLN
3	C	119	VAL
3	C	125	MET

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Mol	Chain	Res	Type
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	148	ARG
3	C	154	LYS
3	C	195	GLN
3	C	197	SER
3	C	211	ASP
3	C	215	GLU
3	C	226	ASP
3	C	238	ILE
3	C	240	VAL
3	C	245	VAL
3	C	260	LEU
3	C	262	LEU
3	C	263	THR
3	C	264	GLN
3	C	265	MET
3	C	268	ASP
4	D	5	THR
4	D	9	GLN
4	D	18	VAL
4	D	19	GLU
4	D	27	LEU
4	D	32	GLU
4	D	35	LEU
4	D	38	ILE
4	D	41	GLN
4	D	43	GLU
4	D	47	LEU
4	D	52	LEU
4	D	65	GLU
4	D	67	ARG
4	D	75	LYS
4	D	123	LEU
4	D	126	ILE
4	D	133	THR
4	D	134	THR
4	D	137	ASN
4	D	139	LYS
4	D	156	ASP
4	D	182	SER

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Mol	Chain	Res	Type
4	D	187	THR
4	D	197	SER
4	D	201	LYS
4	D	204	ASP
4	D	213	GLU
5	E	14	ARG
5	E	31	THR
5	E	41	ASP
5	E	45	LYS
5	E	46	TYR
5	E	60	PHE
5	E	69	ILE
5	E	84	ASP
5	E	92	THR
5	E	115	ASN
5	E	127	ILE
5	E	131	THR
5	E	140	LEU
5	E	165	LEU
5	E	175	LEU
5	E	182	ASP
5	E	184	VAL
5	E	190	LEU
5	E	191	LYS
5	E	192	ARG
6	F	72	LYS
6	F	79	ARG
6	F	82	THR
6	F	86	THR
6	F	90	ARG
6	F	103	MET
6	F	109	VAL
6	F	115	THR
6	F	118	LEU
6	F	155	LEU
7	G	5	LYS
7	G	7	LEU
7	G	11	ILE
7	G	13	LEU
7	G	22	MET
7	G	26	LEU
7	G	28	THR

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Mol	Chain	Res	Type
7	G	60	ARG
7	G	64	THR
7	G	65	ASP
7	G	90	THR
7	G	93	SER
7	G	114	LEU
7	G	118	ASP
7	G	122	ASN
7	G	133	SER
7	G	141	SER
7	G	143	ILE
7	G	151	ILE
7	G	152	SER
7	G	164	LYS
8	H	12	VAL
8	H	14	GLU
8	H	23	VAL
8	H	26	ILE
8	H	35	GLN
8	H	42	ILE
8	H	76	THR
8	H	78	SER
8	H	86	ASP
8	H	89	LEU
8	H	91	ASP
8	H	107	VAL
8	H	112	ILE
8	H	130	ARG
8	H	135	LEU
8	H	146	ARG
9	I	8	ARG
9	I	31	THR
9	I	43	VAL
9	I	50	THR
9	I	55	THR
9	I	83	ASN
9	I	94	ASP
9	I	104	LEU
9	I	106	CYS
9	I	109	ILE
9	I	118	ARG
9	I	120	GLN

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Mol	Chain	Res	Type
10	J	9	SER
10	J	13	VAL
10	J	14	VAL
10	J	16	ASP
10	J	20	SER
10	J	23	ASN
10	J	28	ASP
10	J	30	LEU
10	J	31	ASP
10	J	34	THR
10	J	41	LEU
10	J	42	LYS
10	J	43	ARG
10	J	48	ARG
10	J	57	ILE
11	K	6	ARG
11	K	9	LEU
11	K	11	LEU
11	K	20	LYS
11	K	21	ILE
11	K	25	THR
11	K	31	VAL
11	K	33	ILE
11	K	47	ARG
11	K	51	LEU
11	K	78	THR
11	K	91	CYS
11	K	101	LEU
11	K	103	THR
11	K	107	THR
11	K	108	GLU
11	K	114	LEU
12	L	27	LEU
12	L	34	CYS
12	L	38	LEU
12	L	50	ASP
12	L	51	CYS
12	L	55	ILE
12	L	58	LYS
12	L	61	THR
12	L	64	LEU
12	L	65	VAL

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Mol	Chain	Res	Type
12	L	68	GLU
12	L	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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	$\# Z > 2$
14	BRU	T	22	14	19,21,22	1.87	3 (15%)	22,30,33	4.08	6 (27%)

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
14	BRU	T	22	14	-	0/5/21/22	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	22	BRU	C4-C5	5.85	1.50	1.39
14	T	22	BRU	C6-N1	3.42	1.42	1.34
14	T	22	BRU	BR-C5	2.48	1.96	1.90

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	22	BRU	C6-N1-C2	-15.92	117.89	122.41
14	T	22	BRU	C5-C6-N1	6.34	123.85	119.67
14	T	22	BRU	N3-C2-N1	5.79	120.80	115.97
14	T	22	BRU	O4'-C1'-N1	4.26	115.69	107.68
14	T	22	BRU	BR-C5-C4	3.33	126.17	120.11
14	T	22	BRU	C2'-C1'-N1	2.48	120.52	114.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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.

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	1422/1732 (82%)	0.03	4 (0%) 91 83	64, 116, 174, 247	0
2	B	1115/1224 (91%)	0.09	5 (0%) 90 79	67, 130, 191, 222	0
3	C	266/318 (83%)	0.01	0 100 100	90, 119, 163, 183	0
4	D	178/221 (80%)	0.06	0 100 100	102, 135, 182, 198	0
5	E	214/215 (99%)	0.03	2 (0%) 81 62	90, 151, 199, 208	0
6	F	84/155 (54%)	-0.06	0 100 100	70, 95, 126, 149	0
7	G	171/171 (100%)	0.15	0 100 100	87, 116, 155, 179	0
8	H	133/146 (91%)	0.38	0 100 100	122, 161, 195, 205	0
9	I	119/122 (97%)	0.12	3 (2%) 54 36	123, 158, 192, 214	0
10	J	65/70 (92%)	-0.09	0 100 100	97, 115, 153, 166	0
11	K	115/120 (95%)	0.01	0 100 100	83, 115, 163, 181	0
12	L	46/70 (65%)	0.15	2 (4%) 34 23	103, 159, 184, 191	0
13	N	11/15 (73%)	0.51	0 100 100	203, 219, 272, 273	0
14	T	17/27 (62%)	0.56	0 100 100	170, 216, 267, 270	0
All	All	3956/4606 (85%)	0.07	16 (0%) 90 79	64, 125, 189, 273	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	93	MET	3.4
9	I	120	GLN	3.0
1	A	194	ALA	2.9
1	A	1455	PRO	2.7
2	B	864	LYS	2.6
2	B	733	HIS	2.5
9	I	117	LYS	2.5
5	E	123	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	340	ALA	2.4
2	B	708	GLU	2.3
12	L	25	ALA	2.2
9	I	119	THR	2.1
1	A	155	GLU	2.1
1	A	254	GLU	2.1
12	L	26	THR	2.0
2	B	865	LYS	2.0

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

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
14	BRU	T	22	20/21	0.29	2.69	221,231,236,237	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
16	MG	A	2458	1/1	0.29	2.39	106,106,106,106	0
15	ZN	B	2225	1/1	0.22	0.53	92,92,92,92	0
15	ZN	I	1121	1/1	0.11	-0.40	126,126,126,126	0
15	ZN	J	1066	1/1	0.24	-0.59	90,90,90,90	0
15	ZN	A	2457	1/1	0.15	-0.93	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
15	ZN	C	1269	1/1	0.10	-1.05	88,88,88,88	0
15	ZN	L	1071	1/1	0.08	-1.39	164,164,164,164	0
15	ZN	I	1122	1/1	0.04	-1.53	197,197,197,197	0
15	ZN	A	2456	1/1	0.06	-2.34	146,146,146,146	0

6.5 Other polymers ⓘ

There are no such residues in this entry.