



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2023 – 08:08 AM EDT

PDB ID : 3S1N
Title : RNA Polymerase II Initiation Complex with a 5-nt RNA (variant 2)
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on : 2011-05-15
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

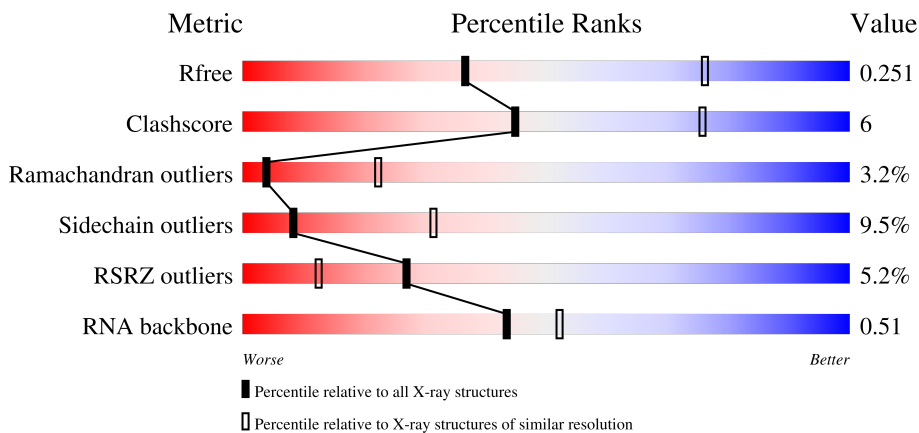
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.



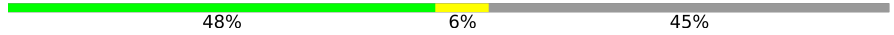




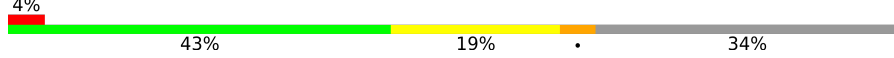


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	
2	B	1224	
3	C	318	
4	E	215	

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

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 28570 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
			Total	C	N	O	S			
1	A	1405	11043	6965	1936	2081	61	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1114	8861	5610	1549	1647	55	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	85	688	439	116	130	3	0	0	0

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

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

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

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

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

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

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

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

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

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

- Molecule 11 is a RNA chain called RNA (5'-R(*AP*GP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
11	R	5	107	49	23	31	4	0	0	0

- Molecule 12 is a DNA chain called DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*CP*GP*AP*TP*GP*CP*TP*CP*TP*CP*GP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
12	T	8	162	77	28	49	8	0	0	0

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

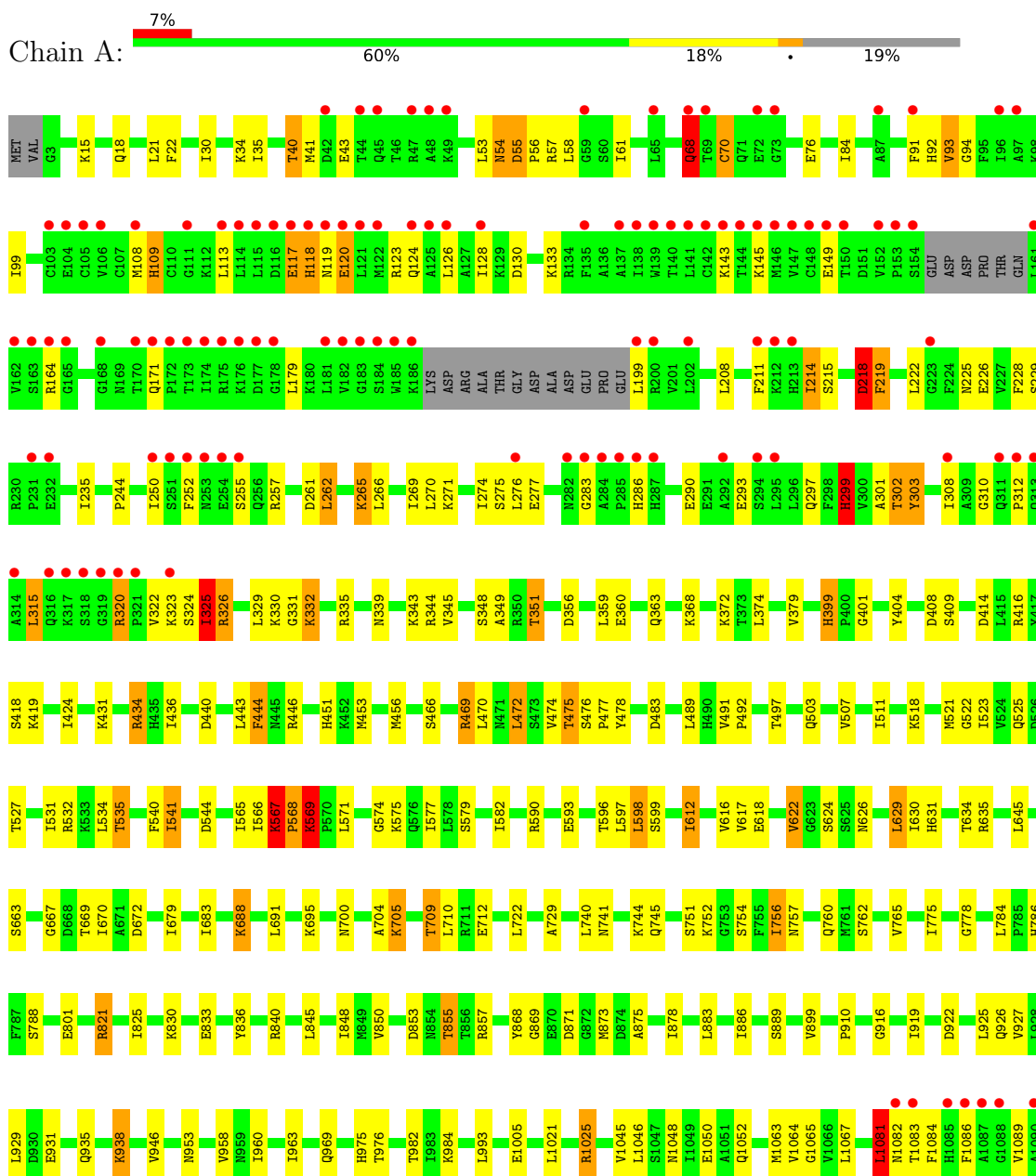
- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

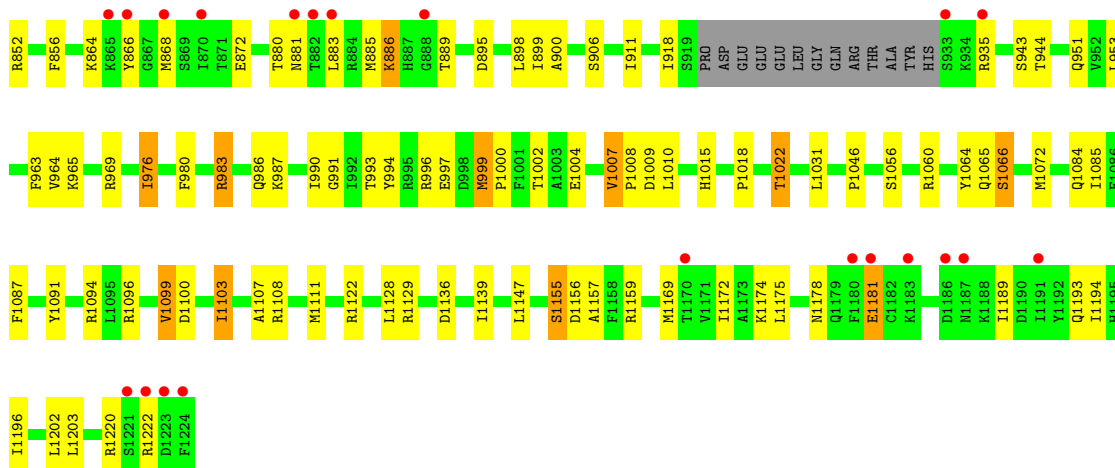
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total 1	Mg 1	0	0

3 Residue-property plots [i](#)

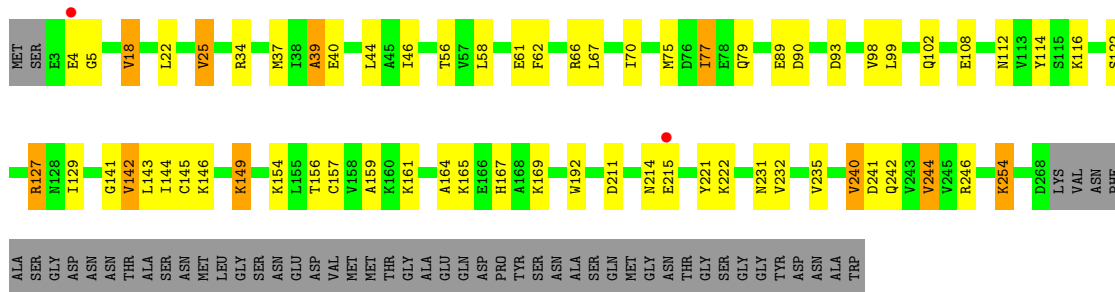
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA-directed RNA polymerase II subunit RPB1

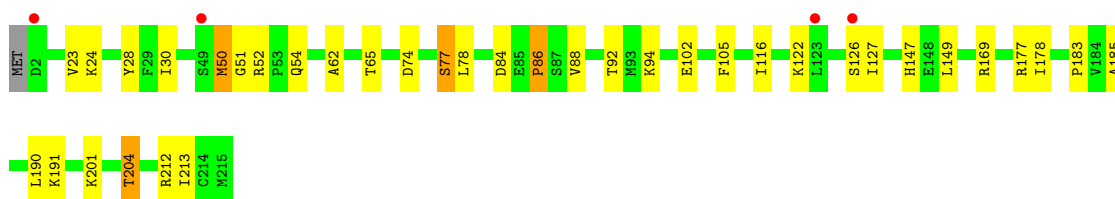
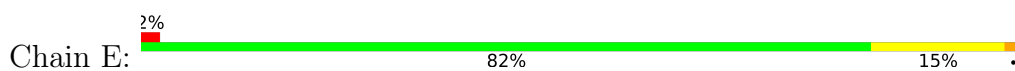




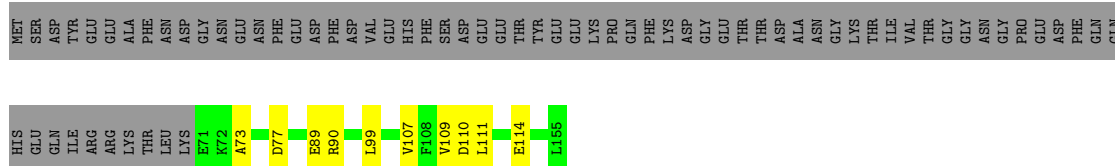
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



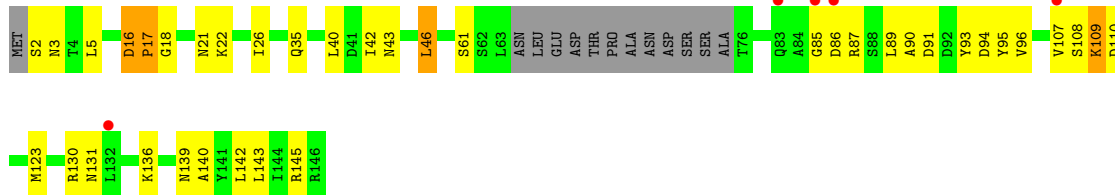
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



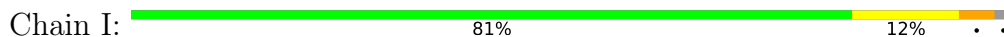
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



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



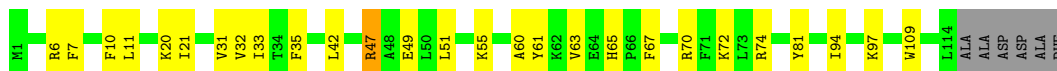
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



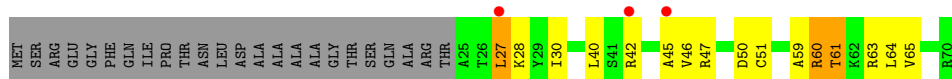
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



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



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



- Molecule 11: RNA (5'-R(*AP*GP*AP*GP*C)-3')



- Molecule 12: DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*C
P*GP*AP*TP*GP*CP*TP*CP*TP*CP*GP*AP*TP*G)-3')



DC	DT	DA	DC	DC	DG	DA	DT	DA	DA	DG	DC	DA	DG	DA	C16	G17	A18	T19	G20	T22	C23	DT	DC	DG	DA	DT	DG
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4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.30Å 221.13Å 191.94Å 90.00° 97.52° 90.00°	Depositor
Resolution (Å)	47.80 – 3.10 47.80 – 3.08	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.80-3.10) 99.0 (47.80-3.08)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.07Å)	Xtrriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.191 , 0.232 0.207 , 0.251	Depositor DCC
R_{free} test set	5960 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	65.5	Xtrriage
Anisotropy	0.740	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28570	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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	A	0.43	0/11241	0.72	3/15199 (0.0%)
2	B	0.43	0/9033	0.71	3/12181 (0.0%)
3	C	0.40	0/2133	0.71	1/2891 (0.0%)
4	E	0.41	0/1788	0.66	0/2406
5	F	0.42	0/700	0.64	0/945
6	H	0.42	0/1086	0.74	0/1470
7	I	0.41	0/989	0.74	0/1331
8	J	0.47	0/541	0.78	0/727
9	K	0.38	0/937	0.62	0/1265
10	L	0.48	0/365	0.82	0/485
11	R	0.92	0/120	1.45	1/186 (0.5%)
12	T	1.15	0/180	1.93	6/275 (2.2%)
All	All	0.44	0/29113	0.73	14/39361 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	22	DT	O4'-C1'-N1	8.29	113.80	108.00
2	B	647	GLY	C-N-CA	8.15	142.07	121.70
1	A	218	ASP	C-N-CA	7.05	139.32	121.70
12	T	19	DT	O4'-C1'-N1	6.59	112.61	108.00
12	T	16	DC	O4'-C1'-N1	6.19	112.33	108.00
1	A	1123	GLY	C-N-CA	5.99	136.68	121.70
2	B	648	HIS	N-CA-CB	5.80	121.05	110.60
1	A	117	GLU	C-N-CA	5.54	135.55	121.70
11	R	10	C	O4'-C1'-N1	5.38	112.50	108.20
3	C	39	ALA	N-CA-C	5.32	125.37	111.00
2	B	140	ILE	C-N-CA	5.26	134.85	121.70
12	T	23	DC	O4'-C1'-N1	5.15	111.60	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	21	DC	O4'-C1'-N1	5.13	111.59	108.00
12	T	19	DT	P-O3'-C3'	5.05	125.76	119.70

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	11043	0	11133	179	0
2	B	8861	0	8884	124	0
3	C	2095	0	2051	33	0
4	E	1752	0	1776	17	0
5	F	688	0	707	4	0
6	H	1068	0	1040	15	0
7	I	971	0	927	12	0
8	J	532	0	542	15	0
9	K	919	0	929	18	0
10	L	363	0	386	3	0
11	R	107	0	56	0	0
12	T	162	0	91	0	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	28570	0	28522	368	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 6.

All (368) 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)
1:A:535:THR:HG21	1:A:617:VAL:H	1.29	0.96
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.48	0.94
2:B:801:LYS:O	8:J:52:THR:HG23	1.76	0.86
2:B:345:LYS:HA	2:B:347:LYS:H	1.44	0.83
1:A:1376:THR:HG23	4:E:212:ARG:HH22	1.47	0.80
1:A:565:ILE:HG23	1:A:567:LYS:HG3	1.63	0.78
1:A:1123:GLY:HA3	1:A:1124:HIS:HB2	1.66	0.77
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.67	0.76
1:A:754:SER:H	1:A:757:ASN:HD22	1.34	0.75
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	2.00	0.75
2:B:515:HIS:HD2	2:B:517:THR:H	1.31	0.75
2:B:744:HIS:HD2	2:B:746:SER:H	1.33	0.75
1:A:218:ASP:H	1:A:219:PHE:HB3	1.52	0.74
1:A:444:PHE:HE2	1:A:470:LEU:HD23	1.52	0.74
1:A:535:THR:CG2	1:A:617:VAL:H	1.99	0.74
1:A:215:SER:HB3	1:A:218:ASP:HB2	1.70	0.74
1:A:869:GLY:O	4:E:204:THR:HG21	1.88	0.72
1:A:315:LEU:HA	1:A:320:ARG:HB3	1.72	0.72
1:A:756:ILE:HD13	1:A:756:ILE:H	1.53	0.72
1:A:469:ARG:NH2	2:B:991:GLY:O	2.24	0.70
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.27	0.70
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.20	0.70
2:B:654:ARG:H	2:B:657:HIS:HD2	1.39	0.69
1:A:531:ILE:O	1:A:535:THR:HB	1.93	0.69
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.75	0.68
2:B:839:MET:HE2	2:B:980:PHE:HB2	1.75	0.67
1:A:219:PHE:H	1:A:222:LEU:HG	1.60	0.67
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.59	0.67
1:A:368:LYS:HD3	1:A:372:LYS:HE3	1.76	0.66
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.78	0.65
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.77	0.65
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.79	0.65
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.79	0.64
1:A:1123:GLY:CA	1:A:1124:HIS:HB2	2.27	0.64
1:A:855:THR:HG21	1:A:857:ARG:HE	1.63	0.63
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.80	0.63
1:A:741:ASN:HD22	1:A:744:LYS:H	1.45	0.63
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.80	0.63
1:A:786:HIS:HE1	2:B:742:GLU:OE1	1.82	0.62
2:B:515:HIS:H	2:B:518:HIS:CD2	2.17	0.62
3:C:167:HIS:HD2	3:C:169:LYS:H	1.44	0.62
2:B:864:LYS:H	2:B:872:GLU:HB2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1072:MET:HG3	2:B:1085:ILE:HB	1.80	0.62
2:B:43:LEU:HD11	2:B:811:TYR:O	2.00	0.62
1:A:667:GLY:HA2	1:A:670:ILE:HD12	1.82	0.61
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.82	0.61
3:C:66:ARG:NH2	8:J:3:VAL:O	2.31	0.61
1:A:1329:THR:HG22	1:A:1331:SER:H	1.66	0.61
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.48	0.61
1:A:40:THR:HG23	1:A:54:ASN:HD21	1.67	0.60
2:B:1002:THR:HG22	2:B:1004:GLU:H	1.65	0.60
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.33	0.60
1:A:53:LEU:HG	1:A:54:ASN:HD22	1.66	0.60
1:A:399:HIS:O	1:A:401:GLY:N	2.32	0.60
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.84	0.59
3:C:102:GLN:HG2	3:C:154:LYS:HG3	1.84	0.59
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.85	0.59
2:B:346:GLU:HA	2:B:349:ILE:HD12	1.84	0.59
1:A:535:THR:HG21	1:A:617:VAL:N	2.10	0.58
1:A:532:ARG:HH12	1:A:745:GLN:HE21	1.51	0.58
1:A:1105:LEU:HB3	1:A:1384:VAL:HG22	1.86	0.58
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.36	0.58
1:A:567:LYS:HB3	6:H:95:TYR:HA	1.84	0.58
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.86	0.58
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.86	0.58
1:A:825:ILE:HD12	2:B:512:ARG:HB3	1.84	0.57
1:A:709:THR:HB	1:A:712:GLU:H	1.70	0.57
3:C:56:THR:HG22	3:C:58:LEU:H	1.70	0.57
9:K:65:HIS:HD2	9:K:67:PHE:H	1.51	0.57
3:C:93:ASP:O	3:C:127:ARG:NH2	2.36	0.57
9:K:21:ILE:HG12	9:K:33:ILE:HG12	1.87	0.57
1:A:1086:PHE:HB3	1:A:1092:LYS:HB3	1.87	0.57
2:B:839:MET:CE	2:B:980:PHE:HB2	2.35	0.56
9:K:49:GLU:HG3	9:K:94:ILE:HG13	1.87	0.56
1:A:567:LYS:HZ3	6:H:43:ASN:HB3	1.70	0.56
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.87	0.56
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.87	0.56
7:I:111:THR:HG23	7:I:113:ASP:H	1.71	0.56
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.87	0.55
1:A:1317:MET:HA	1:A:1322:ILE:HD11	1.88	0.55
3:C:165:LYS:O	9:K:6:ARG:NH1	2.40	0.55
1:A:91:PHE:HE1	1:A:99:ILE:HG21	1.71	0.55
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:62:ALA:HB3	4:E:78:LEU:HB3	1.87	0.55
2:B:486:TYR:OH	2:B:1096:ARG:HB3	2.07	0.55
2:B:424:LEU:O	2:B:428:ILE:HG12	2.06	0.55
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.89	0.55
3:C:221:TYR:HB3	6:H:46:LEU:HD22	1.89	0.54
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.90	0.54
1:A:120:GLU:HA	1:A:123:ARG:HB2	1.90	0.54
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.54	0.54
2:B:275:TYR:HB2	2:B:355:ILE:HD11	1.89	0.54
1:A:208:LEU:HD23	1:A:235:ILE:HD11	1.88	0.54
2:B:651:LEU:HD21	2:B:741:CYS:HB3	1.88	0.54
1:A:596:THR:C	1:A:598:LEU:H	2.10	0.54
1:A:567:LYS:HB3	6:H:96:VAL:H	1.73	0.54
2:B:516:ASN:H	2:B:516:ASN:HD22	1.56	0.54
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.89	0.54
4:E:178:ILE:HB	4:E:212:ARG:HD3	1.88	0.54
8:J:28:ASP:HB3	8:J:30:LEU:HD12	1.89	0.53
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.72	0.53
6:H:2:SER:HB3	6:H:3:ASN:HB2	1.90	0.53
1:A:669:THR:O	1:A:762:SER:HB3	2.09	0.53
1:A:1064:VAL:HG12	1:A:1370:LEU:HD22	1.90	0.53
6:H:2:SER:N	6:H:61:SER:HG	2.06	0.53
1:A:700:ASN:HD22	7:I:115:LYS:HB2	1.73	0.53
1:A:756:ILE:H	1:A:756:ILE:CD1	2.22	0.53
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.91	0.52
1:A:935:GLN:HE22	1:A:938:LYS:HD3	1.73	0.52
2:B:284:ILE:HG21	2:B:333:PHE:HD2	1.74	0.52
2:B:640:VAL:CG1	2:B:649:LYS:HB3	2.40	0.52
3:C:108:GLU:HA	3:C:149:LYS:HG2	1.91	0.52
2:B:1009:ASP:OD2	8:J:48:ARG:NH2	2.43	0.52
3:C:22:LEU:HG	3:C:25:VAL:HG21	1.90	0.52
1:A:1123:GLY:HA3	1:A:1124:HIS:CB	2.38	0.52
8:J:1:MET:N	8:J:57:ILE:H	2.08	0.52
1:A:265:LYS:HG2	1:A:303:TYR:HB2	1.92	0.52
2:B:515:HIS:CD2	2:B:517:THR:H	2.20	0.52
10:L:59:ALA:O	10:L:60:ARG:HB3	2.10	0.52
2:B:302:CYS:HA	2:B:310:MET:HE3	1.91	0.52
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.91	0.52
4:E:88:VAL:HB	4:E:116:ILE:HD13	1.92	0.52
1:A:351:THR:HG21	1:A:466:SER:O	2.11	0.51
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ASP:HB3	1:A:359:LEU:HB2	1.93	0.51
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.76	0.51
1:A:57:ARG:HA	1:A:68:GLN:HB3	1.91	0.51
1:A:544:ASP:HB2	9:K:47:ARG:HH21	1.74	0.51
1:A:626:ASN:O	1:A:631:HIS:CD2	2.63	0.51
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.92	0.51
1:A:269:ILE:HG22	1:A:299:HIS:HB2	1.93	0.51
1:A:541:ILE:HD11	1:A:577:ILE:HG12	1.93	0.51
7:I:50:THR:HG22	7:I:52:ILE:H	1.76	0.51
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.94	0.50
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.93	0.50
7:I:10:CYS:HB3	7:I:12:ASN:HD22	1.76	0.50
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.44	0.50
1:A:456:MET:HE2	1:A:507:VAL:HA	1.93	0.50
2:B:241:ARG:HA	2:B:253:THR:HG22	1.93	0.50
1:A:567:LYS:O	1:A:569:LYS:N	2.45	0.50
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.92	0.50
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.65	0.50
1:A:262:LEU:HD11	1:A:325:ILE:HG12	1.94	0.50
4:E:50:MET:HG2	4:E:52:ARG:HH11	1.76	0.50
1:A:218:ASP:N	1:A:219:PHE:HB3	2.22	0.49
1:A:472:LEU:O	1:A:475:THR:HB	2.12	0.49
1:A:503:GLN:NE2	5:F:90:ARG:HH22	2.11	0.49
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.94	0.49
1:A:1081:LEU:HD23	1:A:1083:THR:HB	1.93	0.49
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.93	0.49
2:B:797:TYR:O	8:J:1:MET:HG2	2.13	0.49
1:A:379:VAL:HG22	1:A:431:LYS:HG2	1.93	0.49
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.47	0.49
7:I:50:THR:H	7:I:92:ARG:HH22	1.60	0.49
1:A:117:GLU:H	1:A:118:HIS:HB2	1.77	0.49
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.94	0.49
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.28	0.49
1:A:225:ASN:HD22	1:A:228:PHE:H	1.60	0.49
1:A:1191:TRP:HZ3	7:I:43:VAL:HG21	1.77	0.49
1:A:91:PHE:HB2	1:A:297:GLN:HE22	1.77	0.49
1:A:349:ALA:HB2	1:A:374:LEU:HD11	1.94	0.49
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.13	0.49
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.77	0.49
2:B:345:LYS:HA	2:B:347:LYS:N	2.22	0.48
3:C:77:ILE:HD12	3:C:161:LYS:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:638:PHE:CE1	2:B:743:ILE:HA	2.48	0.48
4:E:147:HIS:CD2	4:E:149:LEU:H	2.31	0.48
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.28	0.48
1:A:299:HIS:HA	1:A:302:THR:HG22	1.96	0.48
3:C:98:VAL:H	3:C:122:SER:HB2	1.78	0.48
3:C:114:TYR:HB2	3:C:116:LYS:HG2	1.94	0.48
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.96	0.48
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.96	0.48
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.95	0.48
1:A:626:ASN:O	1:A:631:HIS:HD2	1.97	0.48
7:I:62:ILE:HG12	7:I:84:VAL:HG11	1.95	0.48
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.95	0.48
1:A:575:LYS:HD3	1:A:612:ILE:HD11	1.96	0.48
1:A:117:GLU:N	1:A:118:HIS:HB2	2.29	0.47
1:A:567:LYS:HE3	6:H:46:LEU:HD12	1.95	0.47
1:A:1138:ILE:HG22	1:A:1319:VAL:HG21	1.96	0.47
6:H:109:LYS:HG3	6:H:110:ASP:H	1.78	0.47
1:A:705:LYS:HE3	1:A:705:LYS:H	1.78	0.47
1:A:855:THR:CG2	1:A:857:ARG:HE	2.26	0.47
1:A:356:ASP:OD2	9:K:65:HIS:HE1	1.98	0.47
2:B:953:LEU:O	2:B:964:VAL:HG23	2.15	0.47
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.79	0.47
7:I:102:VAL:HG22	7:I:109:ILE:HG12	1.95	0.47
1:A:821:ARG:O	1:A:825:ILE:HG12	2.15	0.47
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.48	0.47
2:B:849:GLY:O	2:B:852:ARG:HB2	2.15	0.47
1:A:15:LYS:HB3	2:B:1220:ARG:HG3	1.96	0.47
1:A:266:LEU:HA	1:A:269:ILE:HG12	1.95	0.47
1:A:345:VAL:HG12	2:B:1155:SER:HB2	1.96	0.47
1:A:451:HIS:HB3	1:A:453:MET:H	1.80	0.47
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.50	0.47
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.97	0.47
1:A:219:PHE:HZ	1:A:226:GLU:HA	1.80	0.46
1:A:492:PRO:HB3	1:A:497:THR:HG22	1.96	0.46
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.98	0.46
2:B:516:ASN:H	2:B:516:ASN:ND2	2.12	0.46
2:B:899:ILE:HD12	2:B:911:ILE:HG22	1.96	0.46
3:C:221:TYR:HD1	3:C:222:LYS:HG2	1.81	0.46
1:A:360:GLU:HB2	1:A:363:GLN:HG3	1.97	0.46
2:B:783:THR:HG22	8:J:63:TYR:CE1	2.47	0.46
2:B:1100:ASP:HA	2:B:1103:ILE:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.98	0.46
2:B:1100:ASP:HA	2:B:1103:ILE:HD11	1.98	0.46
1:A:663:SER:HB2	2:B:1085:ILE:HG13	1.98	0.46
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.98	0.46
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.98	0.46
1:A:444:PHE:CE2	1:A:470:LEU:HD23	2.40	0.46
1:A:511:ILE:HA	1:A:521:MET:HE3	1.98	0.46
4:E:185:ALA:HA	4:E:190:LEU:HD12	1.98	0.46
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.97	0.46
2:B:806:THR:HG22	2:B:808:ALA:H	1.81	0.46
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.48	0.46
3:C:46:ILE:HA	3:C:159:ALA:HA	1.98	0.46
9:K:7:PHE:O	9:K:11:LEU:HB2	2.16	0.46
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.49	0.46
1:A:569:LYS:HD2	3:C:221:TYR:HB2	1.98	0.46
1:A:211:PHE:HA	1:A:214:ILE:HD11	1.99	0.45
1:A:414:ASP:OD1	1:A:416:ARG:HG2	2.16	0.45
2:B:620:ARG:HD2	7:I:68:LEU:HD11	1.99	0.45
4:E:147:HIS:HD2	4:E:149:LEU:H	1.64	0.45
1:A:752:LYS:HB3	2:B:1018:PRO:HG2	1.99	0.45
2:B:1060:ARG:HA	2:B:1064:TYR:O	2.16	0.45
2:B:1099:VAL:O	2:B:1103:ILE:HG13	2.16	0.45
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.82	0.45
2:B:980:PHE:CE2	2:B:1094:ARG:HD3	2.50	0.45
4:E:24:LYS:HB3	4:E:30:ILE:HB	1.98	0.45
1:A:575:LYS:HB3	1:A:612:ILE:HG13	1.97	0.45
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.98	0.45
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.98	0.45
3:C:142:VAL:H	8:J:16:ASP:HB3	1.81	0.45
1:A:120:GLU:HG2	1:A:124:GLN:HE21	1.80	0.45
1:A:453:MET:HB3	1:A:477:PRO:HB3	1.97	0.45
2:B:118:ARG:HG3	2:B:204:ILE:HD13	1.98	0.45
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.82	0.45
2:B:466:TRP:HB3	2:B:475:SER:HB2	1.98	0.45
9:K:49:GLU:HG3	9:K:94:ILE:CG1	2.47	0.45
1:A:374:LEU:HA	2:B:1107:ALA:HB2	1.99	0.45
1:A:935:GLN:NE2	1:A:938:LYS:HD3	2.31	0.45
4:E:77:SER:HB2	4:E:105:PHE:CD2	2.52	0.45
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.98	0.45
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.98	0.45
1:A:1021:LEU:HD11	1:A:1025:ARG:HH11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:LEU:HD11	2:B:170:LEU:HB2	1.99	0.45
10:L:61:THR:HB	10:L:63:ARG:H	1.82	0.45
1:A:540:PHE:HB3	1:A:571:LEU:HG	1.98	0.45
2:B:745:PRO:O	2:B:748:ILE:HG12	2.17	0.45
2:B:724:ASP:HB3	2:B:727:LYS:HD2	1.98	0.44
2:B:864:LYS:HB3	2:B:872:GLU:H	1.81	0.44
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.52	0.44
4:E:147:HIS:CD2	4:E:149:LEU:HB2	2.52	0.44
1:A:544:ASP:HB2	9:K:47:ARG:NH2	2.32	0.44
1:A:70:CYS:HB2	2:B:1172:ILE:HG23	1.99	0.44
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.82	0.44
7:I:47:GLU:OE1	7:I:50:THR:HG23	2.17	0.44
1:A:58:LEU:HD23	1:A:244:PRO:HD3	1.98	0.44
1:A:760:GLN:HG2	1:A:765:VAL:HA	1.99	0.44
2:B:211:VAL:O	2:B:480:SER:HA	2.17	0.44
2:B:706:GLN:O	2:B:710:LEU:HB2	2.16	0.44
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.83	0.44
2:B:986:GLN:HE21	2:B:1022:THR:HG21	1.83	0.44
3:C:143:LEU:HD21	3:C:146:LYS:HE3	2.00	0.44
8:J:48:ARG:O	8:J:52:THR:HB	2.17	0.44
1:A:596:THR:O	1:A:598:LEU:N	2.51	0.44
1:A:92:HIS:HD2	1:A:94:GLY:H	1.66	0.44
1:A:850:VAL:HG23	1:A:1064:VAL:HG21	1.99	0.44
2:B:994:TYR:HD1	2:B:999:MET:HE3	1.82	0.44
3:C:18:VAL:HG22	3:C:240:VAL:HB	2.00	0.44
1:A:55:ASP:O	1:A:57:ARG:N	2.51	0.44
1:A:567:LYS:HZ3	6:H:95:TYR:HE1	1.65	0.44
1:A:899:VAL:HB	1:A:929:LEU:HD22	2.00	0.44
1:A:1128:GLN:HG2	1:A:1132:LYS:HE3	2.00	0.44
3:C:18:VAL:HG23	3:C:232:VAL:HB	2.00	0.44
3:C:242:GLN:NE2	3:C:246:ARG:HE	2.13	0.44
8:J:17:LYS:HD3	8:J:41:LEU:HD21	1.99	0.44
2:B:898:LEU:HD21	2:B:964:VAL:HG11	2.00	0.43
9:K:32:VAL:HG22	9:K:74:ARG:HG3	2.00	0.43
1:A:21:LEU:HD12	1:A:229:SER:HB2	2.00	0.43
3:C:62:PHE:O	3:C:66:ARG:HG3	2.19	0.43
1:A:324:SER:O	1:A:326:ARG:N	2.43	0.43
1:A:946:VAL:HG22	4:E:201:LYS:HD2	1.99	0.43
2:B:476:ARG:O	2:B:478:GLY:N	2.51	0.43
3:C:37:MET:HE2	3:C:244:VAL:HA	1.99	0.43
1:A:704:ALA:HB2	1:A:710:LEU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:MET:O	1:A:109:HIS:HB2	2.19	0.43
1:A:534:LEU:O	1:A:574:GLY:HA3	2.18	0.43
2:B:822:ASN:ND2	8:J:52:THR:HG21	2.32	0.43
1:A:1154:TYR:CE1	7:I:18:GLU:HG3	2.53	0.43
6:H:16:ASP:HA	6:H:17:PRO:HD3	1.88	0.43
1:A:525:GLN:HB3	2:B:835:GLN:HG2	2.01	0.43
2:B:219:ALA:HB2	2:B:405:ARG:HG2	2.00	0.43
3:C:67:LEU:HA	3:C:70:ILE:HD12	2.00	0.43
1:A:1193:LEU:HB3	1:A:1240:CYS:HB2	2.00	0.43
1:A:483:ASP:O	2:B:987:LYS:HE2	2.18	0.43
2:B:640:VAL:HG12	2:B:649:LYS:HB3	2.00	0.43
4:E:77:SER:HB2	4:E:105:PHE:HD2	1.83	0.42
1:A:535:THR:HG23	1:A:616:VAL:HA	2.01	0.42
6:H:93:TYR:HA	6:H:145:ARG:HB3	2.02	0.42
9:K:7:PHE:HA	9:K:10:PHE:CZ	2.54	0.42
1:A:265:LYS:HD3	1:A:322:VAL:HG21	2.01	0.42
1:A:1388:GLY:O	1:A:1391:ARG:HG3	2.20	0.42
2:B:918:ILE:HG13	2:B:935:ARG:HD2	2.00	0.42
9:K:61:TYR:HA	9:K:72:LYS:O	2.19	0.42
1:A:751:SER:HB2	2:B:1015:HIS:CE1	2.55	0.42
1:A:830:LYS:HE2	1:A:1082:ASN:HD22	1.85	0.42
9:K:55:LYS:HB2	9:K:81:TYR:CD1	2.54	0.42
2:B:851:PHE:O	2:B:1094:ARG:NH1	2.52	0.42
1:A:778:GLY:HA3	2:B:516:ASN:ND2	2.35	0.42
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.54	0.42
2:B:706:GLN:H	2:B:710:LEU:HG	1.84	0.42
6:H:40:LEU:HD13	6:H:123:MET:HG3	2.01	0.42
1:A:688:LYS:HD3	1:A:688:LYS:HA	1.96	0.42
1:A:1266:THR:HA	1:A:1270:ASN:HD22	1.85	0.42
1:A:629:LEU:HD13	1:A:645:LEU:HD21	2.02	0.42
1:A:963:ILE:HG22	1:A:1045:VAL:HG22	2.00	0.42
1:A:518:LYS:HE2	1:A:624:SER:O	2.19	0.41
1:A:579:SER:HA	1:A:582:ILE:HD12	2.01	0.41
1:A:1089:VAL:HB	1:A:1092:LYS:HD3	2.01	0.41
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	2.01	0.41
2:B:566:LEU:HD11	2:B:586:TRP:CE2	2.54	0.41
1:A:446:ARG:HD3	1:A:478:TYR:O	2.20	0.41
2:B:69:LEU:HD12	2:B:90:ILE:HB	2.01	0.41
2:B:363:HIS:CD2	2:B:585:VAL:HG22	2.56	0.41
2:B:758:PHE:CZ	2:B:1031:LEU:HD22	2.55	0.41
2:B:944:THR:HG21	2:B:1122:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:ILE:HB	2:B:141:ASP:HB2	2.03	0.41
1:A:348:SER:HA	1:A:489:LEU:O	2.20	0.41
1:A:1156:PRO:HA	1:A:1190:PRO:HB3	2.03	0.41
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	2.02	0.41
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.17	0.41
1:A:982:THR:HG22	1:A:984:LYS:H	1.86	0.41
2:B:634:TYR:CD1	2:B:692:TYR:HB3	2.56	0.41
2:B:983:ARG:HH11	2:B:983:ARG:HB2	1.86	0.41
6:H:89:LEU:C	6:H:91:ASP:H	2.23	0.41
1:A:683:ILE:HG21	1:A:801:GLU:HG3	2.03	0.41
1:A:845:LEU:O	1:A:1065:GLY:HA3	2.20	0.41
1:A:1138:ILE:HG13	1:A:1282:VAL:HG21	2.03	0.41
3:C:254:LYS:HD3	9:K:42:LEU:HD13	2.02	0.41
2:B:181:LEU:HD22	2:B:189:LEU:HD23	2.03	0.41
2:B:758:PHE:HZ	2:B:1031:LEU:HD22	1.85	0.41
1:A:274:ILE:HA	1:A:277:GLU:HB2	2.03	0.41
1:A:290:GLU:HA	1:A:293:GLU:HB2	2.03	0.41
2:B:1103:ILE:HG13	2:B:1103:ILE:H	1.66	0.41
3:C:39:ALA:HA	3:C:164:ALA:HB3	2.01	0.41
5:F:111:LEU:HD23	5:F:114:GLU:O	2.20	0.41
1:A:567:LYS:NZ	6:H:46:LEU:HB2	2.36	0.41
2:B:619:ILE:H	2:B:619:ILE:HG12	1.78	0.41
2:B:841:MET:O	2:B:993:THR:HA	2.21	0.40
2:B:1172:ILE:HG22	2:B:1174:LYS:HG3	2.03	0.40
1:A:883:LEU:O	1:A:886:ILE:HG22	2.21	0.40
2:B:408:LEU:HD11	2:B:545:ILE:HD12	2.02	0.40
3:C:44:LEU:HD22	3:C:129:ILE:HG13	2.03	0.40
1:A:993:LEU:HD22	1:A:1046:LEU:HG	2.04	0.40
2:B:976:ILE:O	2:B:990:ILE:HB	2.20	0.40
1:A:522:GLY:HA2	1:A:630:ILE:HD13	2.03	0.40
1:A:871:ASP:HB3	4:E:204:THR:HG23	2.03	0.40
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.62	0.40
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.02	0.40
2:B:356:LEU:HA	2:B:360:PHE:HB3	2.04	0.40
6:H:96:VAL:HG13	6:H:143:LEU:HG	2.03	0.40
1:A:145:LYS:HB3	1:A:171:GLN:HE22	1.86	0.40
1:A:326:ARG:HG2	1:A:1406:VAL:HG21	2.04	0.40
5:F:107:VAL:HG12	5:F:109:VAL:H	1.86	0.40
9:K:35:PHE:O	9:K:70:ARG:HA	2.21	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	1395/1733 (80%)	1237 (89%)	112 (8%)	46 (3%)	4	21
2	B	1096/1224 (90%)	966 (88%)	94 (9%)	36 (3%)	4	21
3	C	264/318 (83%)	247 (94%)	11 (4%)	6 (2%)	6	28
4	E	212/215 (99%)	201 (95%)	7 (3%)	4 (2%)	8	33
5	F	83/155 (54%)	74 (89%)	8 (10%)	1 (1%)	13	44
6	H	129/146 (88%)	99 (77%)	22 (17%)	8 (6%)	1	9
7	I	117/122 (96%)	101 (86%)	14 (12%)	2 (2%)	9	36
8	J	63/70 (90%)	59 (94%)	2 (3%)	2 (3%)	4	22
9	K	112/120 (93%)	109 (97%)	3 (3%)	0	100	100
10	L	44/70 (63%)	31 (70%)	6 (14%)	7 (16%)	0	0
All	All	3515/4173 (84%)	3124 (89%)	279 (8%)	112 (3%)	4	22

All (112) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	55	ASP
1	A	109	HIS
1	A	325	ILE
1	A	567	LYS
1	A	1223	ASP
2	B	139	ALA
2	B	367	LEU
2	B	469	GLN
2	B	477	ALA
2	B	648	HIS
2	B	712	PRO
2	B	751	VAL
2	B	880	THR

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Mol	Chain	Res	Type
2	B	1046	PRO
2	B	1156	ASP
3	C	4	GLU
4	E	77	SER
6	H	85	GLY
6	H	109	LYS
6	H	131	ASN
6	H	140	ALA
8	J	2	ILE
10	L	28	LYS
10	L	46	VAL
10	L	50	ASP
10	L	60	ARG
1	A	40	THR
1	A	219	PHE
1	A	286	HIS
1	A	299	HIS
1	A	409	SER
1	A	418	SER
1	A	569	LYS
1	A	597	LEU
1	A	1081	LEU
1	A	1123	GLY
1	A	1124	HIS
1	A	1437	GLY
2	B	137	TYR
2	B	707	PRO
2	B	709	ASP
2	B	850	LEU
2	B	881	ASN
2	B	883	LEU
2	B	1066	SER
3	C	5	GLY
3	C	141	GLY
4	E	86	PRO
6	H	90	ALA
10	L	64	LEU
1	A	68	GLN
1	A	76	GLU
1	A	118	HIS
1	A	250	ILE
1	A	312	PRO

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Mol	Chain	Res	Type
1	A	332	LYS
1	A	922	ASP
1	A	1221	LYS
2	B	138	GLU
2	B	526	GLU
2	B	563	MET
2	B	792	MET
2	B	886	LYS
3	C	90	ASP
4	E	126	SER
6	H	108	SER
8	J	6	ARG
1	A	214	ILE
1	A	255	SER
1	A	275	SER
1	A	424	ILE
1	A	775	ILE
1	A	1278	ASN
2	B	478	GLY
2	B	646	LEU
2	B	647	GLY
2	B	708	GLU
2	B	943	SER
2	B	1155	SER
2	B	1181	GLU
3	C	142	VAL
7	I	3	THR
7	I	77	LYS
1	A	257	ARG
1	A	593	GLU
1	A	958	VAL
1	A	975	HIS
2	B	364	ILE
2	B	447	ALA
2	B	592	ASN
2	B	1157	ALA
2	B	1169	MET
3	C	214	ASN
5	F	73	ALA
6	H	17	PRO
10	L	27	LEU
10	L	45	ALA

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Mol	Chain	Res	Type
1	A	35	ILE
1	A	56	PRO
1	A	119	ASN
1	A	399	HIS
1	A	404	TYR
2	B	1108	ARG
1	A	283	GLY
1	A	310	GLY
6	H	18	GLY
1	A	331	GLY
1	A	568	PRO
2	B	976	ILE
1	A	599	SER
4	E	51	GLY

5.3.2 Protein sidechains [i](#)

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	1225/1520 (81%)	1098 (90%)	127 (10%)	7 27
2	B	967/1061 (91%)	881 (91%)	86 (9%)	9 34
3	C	234/274 (85%)	215 (92%)	19 (8%)	11 39
4	E	196/197 (100%)	180 (92%)	16 (8%)	11 38
5	F	75/137 (55%)	72 (96%)	3 (4%)	31 65
6	H	117/128 (91%)	101 (86%)	16 (14%)	3 16
7	I	113/116 (97%)	106 (94%)	7 (6%)	18 49
8	J	60/65 (92%)	50 (83%)	10 (17%)	2 9
9	K	99/102 (97%)	93 (94%)	6 (6%)	18 49
10	L	40/57 (70%)	32 (80%)	8 (20%)	1 5
All	All	3126/3657 (86%)	2828 (90%)	298 (10%)	8 31

All (298) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	22	PHE
1	A	30	ILE
1	A	34	LYS
1	A	41	MET
1	A	43	GLU
1	A	61	ILE
1	A	68	GLN
1	A	70	CYS
1	A	84	ILE
1	A	93	VAL
1	A	113	LEU
1	A	120	GLU
1	A	126	LEU
1	A	128	ILE
1	A	143	LYS
1	A	149	GLU
1	A	164	ARG
1	A	179	LEU
1	A	199	LEU
1	A	218	ASP
1	A	252	PHE
1	A	261	ASP
1	A	262	LEU
1	A	265	LYS
1	A	270	LEU
1	A	271	LYS
1	A	276	LEU
1	A	299	HIS
1	A	302	THR
1	A	303	TYR
1	A	308	ILE
1	A	315	LEU
1	A	320	ARG
1	A	323	LYS
1	A	325	ILE
1	A	326	ARG
1	A	329	LEU
1	A	330	LYS
1	A	332	LYS
1	A	343	LYS
1	A	344	ARG
1	A	351	THR

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Mol	Chain	Res	Type
1	A	408	ASP
1	A	419	LYS
1	A	434	ARG
1	A	443	LEU
1	A	444	PHE
1	A	469	ARG
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	527	THR
1	A	535	THR
1	A	541	ILE
1	A	566	ILE
1	A	567	LYS
1	A	569	LYS
1	A	590	ARG
1	A	598	LEU
1	A	612	ILE
1	A	618	GLU
1	A	622	VAL
1	A	629	LEU
1	A	634	THR
1	A	635	ARG
1	A	672	ASP
1	A	688	LYS
1	A	691	LEU
1	A	695	LYS
1	A	705	LYS
1	A	709	THR
1	A	722	LEU
1	A	740	LEU
1	A	756	ILE
1	A	788	SER
1	A	821	ARG
1	A	833	GLU
1	A	848	ILE
1	A	855	THR
1	A	919	ILE
1	A	925	LEU
1	A	926	GLN
1	A	927	VAL

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Mol	Chain	Res	Type
1	A	931	GLU
1	A	938	LYS
1	A	953	ASN
1	A	960	ILE
1	A	969	GLN
1	A	976	THR
1	A	1005	GLU
1	A	1025	ARG
1	A	1048	ASN
1	A	1050	GLU
1	A	1052	GLN
1	A	1067	LEU
1	A	1081	LEU
1	A	1084	PHE
1	A	1094	VAL
1	A	1102	LYS
1	A	1109	LYS
1	A	1110	ASN
1	A	1116	LEU
1	A	1142	THR
1	A	1170	ILE
1	A	1176	LEU
1	A	1206	ASP
1	A	1208	THR
1	A	1221	LYS
1	A	1234	GLU
1	A	1237	ILE
1	A	1264	GLU
1	A	1280	GLU
1	A	1293	SER
1	A	1297	GLU
1	A	1309	ASP
1	A	1354	ASN
1	A	1366	ARG
1	A	1376	THR
1	A	1385	THR
1	A	1391	ARG
1	A	1393	ASN
1	A	1398	MET
1	A	1400	CYS
1	A	1426	GLU
1	A	1445	ILE

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Mol	Chain	Res	Type
2	B	25	ILE
2	B	45	SER
2	B	46	GLN
2	B	58	THR
2	B	63	ILE
2	B	89	GLU
2	B	102	VAL
2	B	134	LYS
2	B	135	ARG
2	B	175	ARG
2	B	199	MET
2	B	223	VAL
2	B	225	VAL
2	B	233	PRO
2	B	234	ILE
2	B	261	ARG
2	B	262	GLU
2	B	299	GLU
2	B	305	VAL
2	B	312	GLU
2	B	323	VAL
2	B	355	ILE
2	B	357	GLN
2	B	365	THR
2	B	366	GLN
2	B	384	ARG
2	B	393	LYS
2	B	396	ASP
2	B	426	LYS
2	B	431	TYR
2	B	437	GLU
2	B	451	LYS
2	B	471	LYS
2	B	485	ARG
2	B	516	ASN
2	B	531	GLN
2	B	547	VAL
2	B	555	ILE
2	B	578	THR
2	B	616	ILE
2	B	644	GLU
2	B	646	LEU

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Mol	Chain	Res	Type
2	B	653	VAL
2	B	706	GLN
2	B	708	GLU
2	B	709	ASP
2	B	710	LEU
2	B	762	ASN
2	B	786	ASN
2	B	788	ARG
2	B	791	THR
2	B	796	LEU
2	B	815	ARG
2	B	825	VAL
2	B	866	TYR
2	B	868	MET
2	B	885	MET
2	B	886	LYS
2	B	889	THR
2	B	895	ASP
2	B	906	SER
2	B	951	GLN
2	B	963	PHE
2	B	965	LYS
2	B	983	ARG
2	B	996	ARG
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1022	THR
2	B	1065	GLN
2	B	1099	VAL
2	B	1103	ILE
2	B	1111	MET
2	B	1128	LEU
2	B	1129	ARG
2	B	1147	LEU
2	B	1175	LEU
2	B	1178	ASN
2	B	1181	GLU
2	B	1189	ILE
2	B	1194	ILE
2	B	1196	ILE
2	B	1202	LEU

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Mol	Chain	Res	Type
2	B	1203	LEU
2	B	1222	ARG
3	C	18	VAL
3	C	25	VAL
3	C	34	ARG
3	C	40	GLU
3	C	75	MET
3	C	77	ILE
3	C	79	GLN
3	C	89	GLU
3	C	127	ARG
3	C	145	CYS
3	C	149	LYS
3	C	156	THR
3	C	211	ASP
3	C	215	GLU
3	C	231	ASN
3	C	235	VAL
3	C	240	VAL
3	C	244	VAL
3	C	254	LYS
4	E	50	MET
4	E	54	GLN
4	E	65	THR
4	E	74	ASP
4	E	84	ASP
4	E	86	PRO
4	E	92	THR
4	E	94	LYS
4	E	102	GLU
4	E	122	LYS
4	E	127	ILE
4	E	169	ARG
4	E	177	ARG
4	E	191	LYS
4	E	204	THR
4	E	213	ILE
5	F	77	ASP
5	F	99	LEU
5	F	110	ASP
6	H	5	LEU
6	H	16	ASP

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Mol	Chain	Res	Type
6	H	21	ASN
6	H	22	LYS
6	H	26	ILE
6	H	35	GLN
6	H	42	ILE
6	H	46	LEU
6	H	86	ASP
6	H	87	ARG
6	H	94	ASP
6	H	107	VAL
6	H	130	ARG
6	H	136	LYS
6	H	139	ASN
6	H	142	LEU
7	I	35	VAL
7	I	50	THR
7	I	52	ILE
7	I	77	LYS
7	I	84	VAL
7	I	111	THR
7	I	117	LYS
8	J	2	ILE
8	J	3	VAL
8	J	7	CYS
8	J	22	LEU
8	J	28	ASP
8	J	31	ASP
8	J	37	SER
8	J	48	ARG
8	J	59	LYS
8	J	62	ARG
9	K	20	LYS
9	K	31	VAL
9	K	47	ARG
9	K	51	LEU
9	K	63	VAL
9	K	97	LYS
10	L	27	LEU
10	L	30	ILE
10	L	40	LEU
10	L	42	ARG
10	L	47	ARG

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Mol	Chain	Res	Type
10	L	51	CYS
10	L	61	THR
10	L	65	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	68	GLN
1	A	118	HIS
1	A	124	GLN
1	A	171	GLN
1	A	225	ASN
1	A	256	GLN
1	A	306	ASN
1	A	339	ASN
1	A	503	GLN
1	A	515	GLN
1	A	517	ASN
1	A	545	GLN
1	A	626	ASN
1	A	631	HIS
1	A	700	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	851	HIS
1	A	935	GLN
1	A	996	ASN
1	A	1082	ASN
1	A	1203	ASN
1	A	1258	HIS
1	A	1270	ASN
1	A	1364	ASN
1	A	1432	GLN
2	B	121	ASN
2	B	215	GLN
2	B	325	GLN
2	B	363	HIS
2	B	366	GLN

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Mol	Chain	Res	Type
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	531	GLN
2	B	657	HIS
2	B	744	HIS
2	B	762	ASN
2	B	984	HIS
2	B	986	GLN
2	B	1015	HIS
2	B	1025	HIS
2	B	1084	GLN
2	B	1141	HIS
2	B	1161	HIS
3	C	17	ASN
3	C	73	GLN
3	C	112	ASN
3	C	167	HIS
3	C	231	ASN
3	C	242	GLN
4	E	147	HIS
6	H	131	ASN
6	H	139	ASN
7	I	12	ASN
7	I	46	HIS
7	I	89	GLN
8	J	64	ASN
9	K	65	HIS
9	K	76	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	4/5 (80%)	1 (25%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	7	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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	1405/1733 (81%)	0.20	127 (9%) 9 3	42, 82, 183, 220	0
2	B	1114/1224 (91%)	-0.05	41 (3%) 41 21	39, 77, 146, 186	0
3	C	266/318 (83%)	-0.31	2 (0%) 86 72	46, 72, 108, 145	0
4	E	214/215 (99%)	0.00	4 (1%) 66 46	52, 112, 155, 167	0
5	F	85/155 (54%)	-0.31	0 100 100	60, 90, 128, 150	0
6	H	133/146 (91%)	0.28	5 (3%) 40 20	72, 113, 146, 159	0
7	I	119/122 (97%)	-0.30	0 100 100	55, 84, 120, 131	0
8	J	65/70 (92%)	-0.31	0 100 100	46, 66, 98, 109	0
9	K	114/120 (95%)	-0.21	0 100 100	44, 74, 100, 118	0
10	L	46/70 (65%)	0.08	3 (6%) 18 8	53, 108, 135, 156	0
11	R	5/5 (100%)	0.87	1 (20%) 1 0	170, 176, 182, 183	0
12	T	8/29 (27%)	0.91	2 (25%) 0 0	158, 164, 180, 181	0
All	All	3574/4207 (84%)	0.03	185 (5%) 27 12	39, 82, 167, 220	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	8.4
1	A	317	LYS	7.7
1	A	318	SER	6.5
1	A	183	GLY	6.5
6	H	85	GLY	6.4
1	A	316	GLN	6.4
1	A	319	GLY	6.2
1	A	144	THR	6.0
1	A	44	THR	6.0
1	A	69	THR	5.8
1	A	255	SER	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	87	ALA	5.7
1	A	1175	SER	5.7
2	B	1223	ASP	5.6
1	A	125	ALA	5.5
1	A	182	VAL	5.5
2	B	883	LEU	5.3
2	B	474	SER	5.2
1	A	141	LEU	5.1
1	A	253	ASN	5.0
1	A	121	LEU	5.0
1	A	171	GLN	4.9
2	B	1224	PHE	4.8
1	A	1087	ALA	4.8
1	A	118	HIS	4.7
6	H	86	ASP	4.7
1	A	1085	HIS	4.6
1	A	147	VAL	4.6
1	A	173	THR	4.5
1	A	138	ILE	4.5
1	A	314	ALA	4.4
1	A	146	MET	4.4
2	B	469	GLN	4.3
1	A	45	GLN	4.3
2	B	865	LYS	4.3
2	B	1222	ARG	4.2
1	A	73	GLY	4.2
1	A	49	LYS	4.2
1	A	250	ILE	4.2
2	B	472	ALA	4.0
1	A	176	LYS	4.0
1	A	181	LEU	4.0
1	A	282	ASN	3.9
1	A	1125	ALA	3.9
1	A	142	CYS	3.9
1	A	143	LYS	3.9
1	A	122	MET	3.9
1	A	174	ILE	3.9
1	A	177	ASP	3.8
1	A	178	GLY	3.8
1	A	139	TRP	3.8
1	A	1256	GLU	3.7
1	A	163	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	186	LYS	3.7
1	A	199	LEU	3.7
1	A	124	GLN	3.6
1	A	286	HIS	3.6
1	A	1086	PHE	3.6
1	A	115	LEU	3.6
4	E	126	SER	3.6
1	A	184	SER	3.5
1	A	287	HIS	3.5
1	A	116	ASP	3.4
1	A	254	GLU	3.4
2	B	933	SER	3.4
2	B	250	PHE	3.4
1	A	313	GLN	3.4
1	A	294	SER	3.4
2	B	866	TYR	3.4
2	B	136	THR	3.4
2	B	473	MET	3.4
1	A	113	LEU	3.4
1	A	1083	THR	3.4
1	A	311	GLN	3.4
1	A	170	THR	3.4
1	A	152	VAL	3.3
1	A	105	CYS	3.2
1	A	320	ARG	3.2
1	A	295	LEU	3.2
1	A	140	THR	3.2
1	A	149	GLU	3.1
1	A	175	ARG	3.1
1	A	72	GLU	3.1
1	A	96	ILE	3.1
2	B	468	GLU	3.1
2	B	935	ARG	3.1
1	A	283	GLY	3.1
1	A	172	PRO	3.0
1	A	1123	GLY	3.0
1	A	117	GLU	3.0
1	A	164	ARG	3.0
1	A	161	LEU	3.0
1	A	285	PRO	3.0
1	A	1082	ASN	3.0
2	B	1191	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
6	H	132	LEU	3.0
2	B	709	ASP	2.9
1	A	154	SER	2.9
1	A	137	ALA	2.9
1	A	252	PHE	2.9
1	A	251	SER	2.9
1	A	1090	ALA	2.9
10	L	45	ALA	2.9
1	A	97	ALA	2.8
1	A	1088	GLY	2.8
2	B	870	ILE	2.8
1	A	42	ASP	2.8
2	B	1181	GLU	2.8
1	A	200	ARG	2.8
2	B	470	LYS	2.8
10	L	42	ARG	2.8
1	A	108	MET	2.8
1	A	308	ILE	2.7
2	B	471	LYS	2.7
2	B	433	GLN	2.7
1	A	1091	SER	2.7
6	H	83	GLN	2.6
3	C	215	GLU	2.6
2	B	106	ASP	2.6
4	E	2	ASP	2.6
1	A	211	PHE	2.6
1	A	168	GLY	2.6
1	A	292	ALA	2.6
1	A	312	PRO	2.6
11	R	6	A	2.6
1	A	185	TRP	2.6
2	B	430	ARG	2.6
2	B	1186	ASP	2.6
1	A	162	VAL	2.5
1	A	323	LYS	2.5
12	T	19	DT	2.5
2	B	1183	LYS	2.5
2	B	1170	THR	2.5
1	A	145	LYS	2.5
1	A	150	THR	2.5
1	A	165	GLY	2.5
1	A	1254	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	89	GLU	2.5
1	A	153	PRO	2.5
2	B	420	LEU	2.5
6	H	107	VAL	2.5
1	A	148	CYS	2.4
2	B	1187	ASN	2.4
2	B	868	MET	2.4
1	A	284	ALA	2.4
1	A	321	PRO	2.4
2	B	429	PHE	2.4
1	A	119	ASN	2.4
1	A	213	HIS	2.4
2	B	1221	SER	2.4
1	A	128	ILE	2.4
4	E	123	LEU	2.3
1	A	111	GLY	2.3
1	A	91	PHE	2.3
1	A	114	LEU	2.3
1	A	223	GLY	2.3
2	B	881	ASN	2.3
12	T	17	DG	2.3
10	L	27	LEU	2.2
1	A	276	LEU	2.2
1	A	68	GLN	2.2
1	A	104	GLU	2.2
1	A	1092	LYS	2.2
1	A	212	LYS	2.2
1	A	202	LEU	2.2
2	B	882	THR	2.2
2	B	888	GLY	2.2
1	A	48	ALA	2.2
2	B	1180	PHE	2.2
1	A	59	GLY	2.2
1	A	232	GLU	2.2
1	A	231	PRO	2.1
1	A	65	LEU	2.1
1	A	106	VAL	2.1
1	A	103	CYS	2.1
1	A	47	ARG	2.1
1	A	135	PHE	2.1
1	A	126	LEU	2.1
2	B	477	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	248	SER	2.1
2	B	475	SER	2.1
3	C	4	GLU	2.1
1	A	120	GLU	2.0
2	B	66	ASP	2.0
4	E	49	SER	2.0

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

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(Å ²)	Q<0.9
13	ZN	A	1734	1/1	0.57	0.25	300,300,300,300	0
13	ZN	B	1307	1/1	0.81	0.07	159,159,159,159	0
13	ZN	A	1735	1/1	0.89	0.07	146,146,146,146	0
13	ZN	I	203	1/1	0.96	0.09	94,94,94,94	0
14	MG	A	2001	1/1	0.97	0.11	42,42,42,42	0
13	ZN	J	101	1/1	0.99	0.19	57,57,57,57	0
13	ZN	L	105	1/1	0.99	0.08	102,102,102,102	0
13	ZN	I	204	1/1	0.99	0.12	63,63,63,63	0
13	ZN	C	319	1/1	1.00	0.10	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.