



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:48 PM GMT

PDB ID : 3S2D  
Title : RNA Polymerase II Initiation Complex with a 5-nt RNA containing a 5Br-U  
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.  
Deposited on : 2011-05-16  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

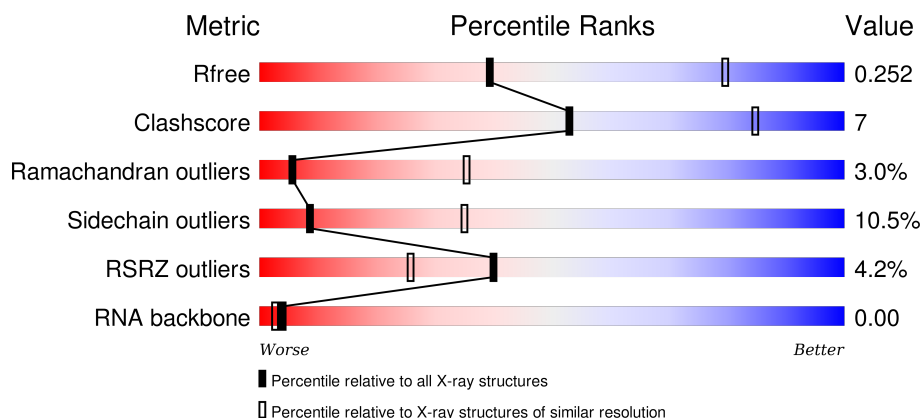
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)
RNA backbone	2183	1079 (3.70-2.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	<div> <div>6%</div> <div> <div></div> <div>59%</div> <div>19%</div> <div>•</div> <div>19%</div> </div> </div>
2	B	1224	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>22%</div> <div>•</div> <div>9%</div> </div> </div>
3	C	318	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>19%</div> <div>•</div> <div>16%</div> </div> </div>
4	E	215	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>14%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	F	155	<div><div></div><div>53%</div><div></div><div>45%</div></div>
6	H	146	<div><div>5%</div><div></div><div>71%</div><div>15%</div><div>5%</div><div>9%</div></div>
7	I	122	<div><div></div><div>81%</div><div></div><div>16%</div><div></div></div>
8	J	70	<div><div></div><div>60%</div><div></div><div>29%</div><div></div><div>7%</div></div>
9	K	120	<div><div>%</div><div></div><div>67%</div><div>28%</div><div></div><div>5%</div></div>
10	L	70	<div><div>%</div><div></div><div>41%</div><div>20%</div><div></div><div>34%</div></div>
11	R	5	<div><div></div><div>40%</div><div></div><div>60%</div></div>
12	T	29	<div><div>7%</div><div></div><div>14%</div><div>17%</div><div>14%</div><div>55%</div></div>

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 28672 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1405	Total	C	N	O	S	0	0	0
			11043	6965	1936	2081	61			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 11 is a RNA chain called RNA (5'-R(\*AP\*GP\*GP\*(5BU)P\*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
11	R	5	Total	Br	C	N	O	P	0	0	0
			109	1	49	22	33	4			

- 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\*CP\*AP\*CP\*CP\*TP\*CP\*GP\*AP\*TP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	13	Total	C	N	O	P	0	0	0
			262	125	46	78	13			

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

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

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

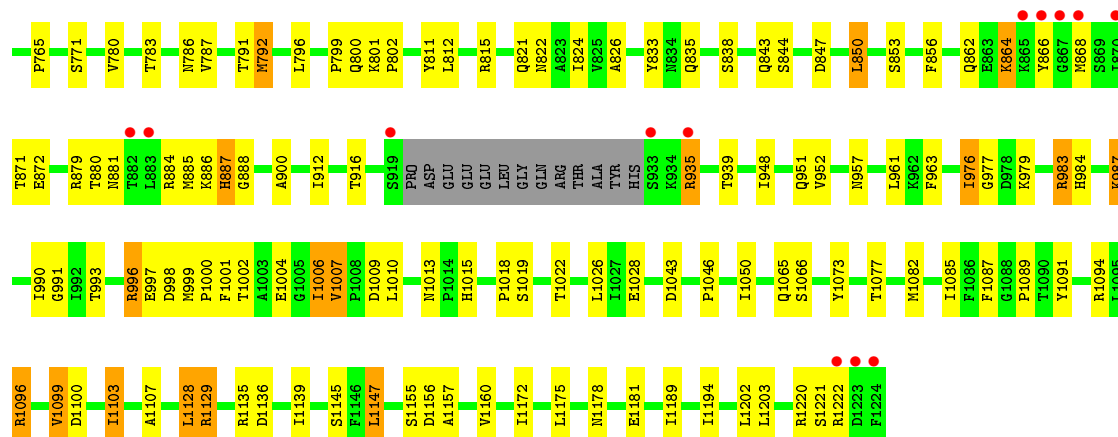
- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

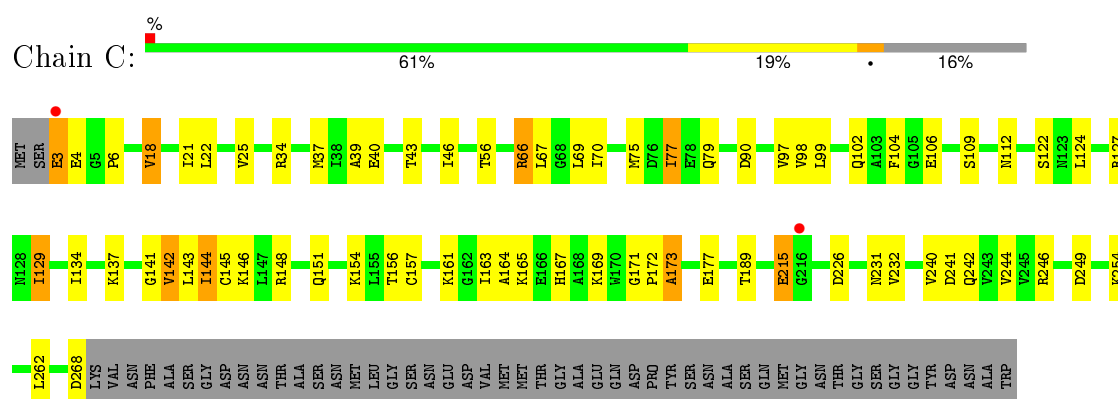




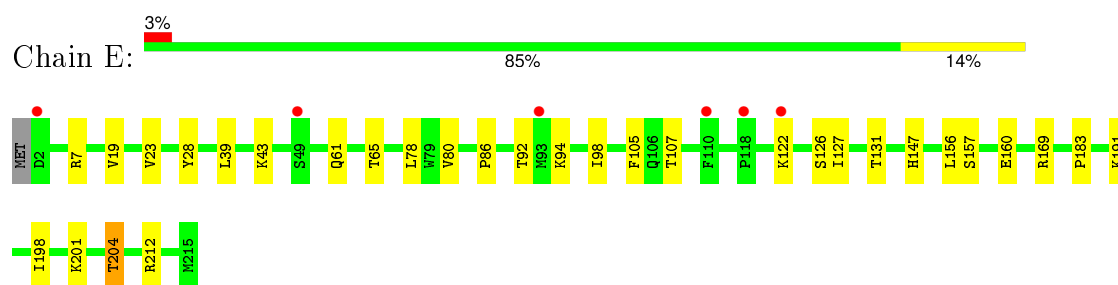




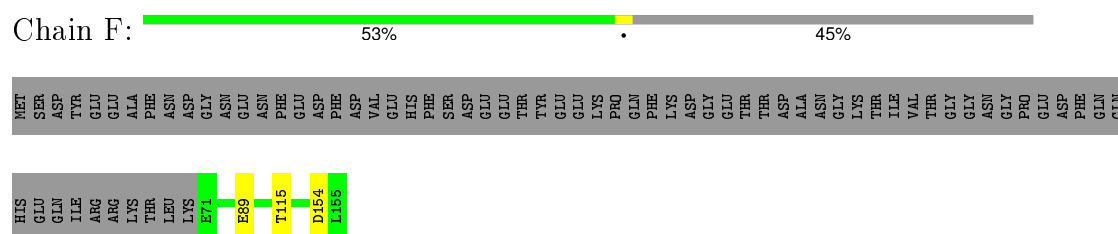
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



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

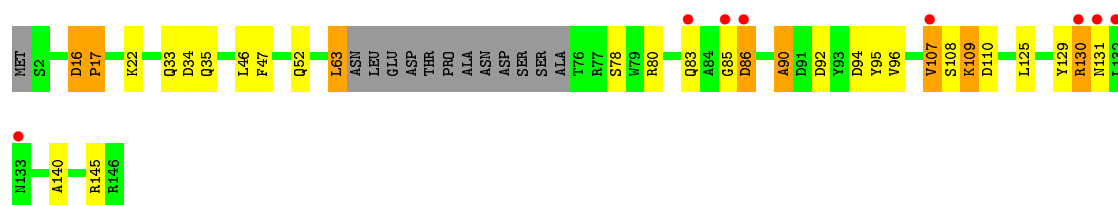


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



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





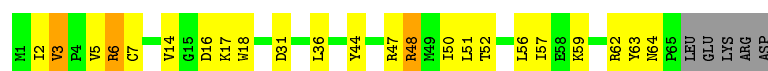
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I: 81% 16%



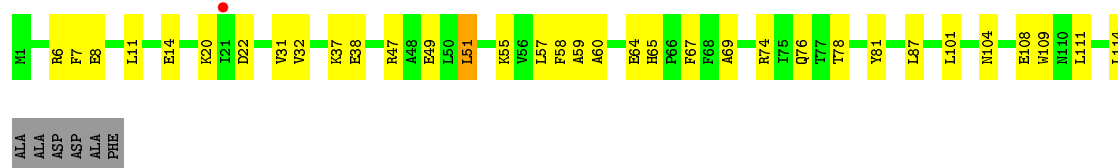
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 60% 29% 7%



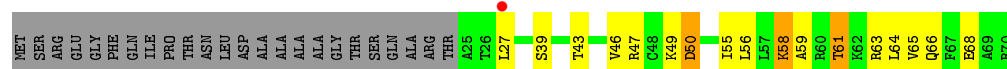
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K: 67% 28% 5%



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

Chain L: 41% 20% 34%



- Molecule 11: RNA (5'-R(\*AP\*GP\*GP\*(5BU)P\*G)-3')

Chain R: 40% 60%



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

Chain T: 7% 14% 14% 55%

DC	DT	DA	DC	DC	DC	DG	DA	DT	DA	DA	DA	DG	DC	DA	DG	DA	C16	G17	A18	T19	C20	A21	C22	C23	T24	C25	G26	A27	T28	DG



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.29Å 220.77Å 192.24Å 90.00° 97.69° 90.00°	Depositor
Resolution (Å)	47.76 – 3.20 47.76 – 3.19	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.76-3.20) 98.5 (47.76-3.19)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.183 , 0.231 0.206 , 0.252	Depositor DCC
$R_{free}$ test set	5317 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.2	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 84.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	2 of 107358 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	28672	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5BU, 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	0.44	0/11241	0.72	1/15199 (0.0%)
2	B	0.46	0/9033	0.74	4/12181 (0.0%)
3	C	0.42	0/2133	0.76	1/2891 (0.0%)
4	E	0.42	0/1788	0.66	0/2406
5	F	0.44	0/700	0.66	0/945
6	H	0.43	0/1086	0.74	0/1470
7	I	0.41	0/989	0.72	0/1331
8	J	0.48	0/541	0.81	0/727
9	K	0.40	0/937	0.65	0/1265
10	L	0.49	0/365	0.84	0/485
11	R	0.99	0/99	1.65	2/154 (1.3%)
12	T	1.08	0/292	1.86	11/447 (2.5%)
All	All	0.46	0/29204	0.76	19/39501 (0.0%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	647	GLY	C-N-CA	7.61	140.72	121.70
12	T	17	DG	O4'-C1'-N9	7.56	113.29	108.00
12	T	24	DT	O4'-C1'-N1	7.48	113.24	108.00
12	T	26	DG	P-O3'-C3'	7.27	128.43	119.70
12	T	22	DC	O4'-C4'-C3'	-7.10	101.66	104.50
3	C	172	PRO	C-N-CA	6.83	138.77	121.70
12	T	17	DG	C1'-O4'-C4'	-6.67	103.43	110.10
2	B	628	THR	C-N-CA	6.03	136.77	121.70
11	R	8	G	C4'-C3'-C2'	-6.00	96.60	102.60
11	R	10	G	O4'-C1'-N9	5.85	112.88	108.20
12	T	23	DC	O4'-C1'-N1	5.85	112.09	108.00
12	T	20	DC	O4'-C1'-N1	5.81	112.07	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	19	DT	C4-C5-C7	5.54	122.33	119.00
12	T	22	DC	C4'-C3'-C2'	-5.40	98.24	103.10
2	B	648	HIS	N-CA-CB	5.33	120.18	110.60
12	T	18	DA	O4'-C1'-N9	5.27	111.69	108.00
2	B	140	ILE	C-N-CA	5.23	134.76	121.70
1	A	1123	GLY	C-N-CA	5.15	134.58	121.70
12	T	21	DA	C4'-C3'-C2'	-5.02	98.58	103.10

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	175	0
2	B	8861	0	8884	143	0
3	C	2095	0	2051	38	0
4	E	1752	0	1776	15	0
5	F	688	0	707	1	0
6	H	1068	0	1040	11	0
7	I	971	0	927	7	0
8	J	532	0	542	18	0
9	K	919	0	929	19	0
10	L	363	0	386	5	0
11	R	109	0	54	1	0
12	T	262	0	147	3	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	28672	0	28576	378	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 7.

All (378) 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:1123:GLY:HA3	1:A:1124:HIS:HB2	1.59	0.83
1:A:869:GLY:O	4:E:204:THR:HG21	1.79	0.82
8:J:48:ARG:O	8:J:52:THR:HB	1.80	0.82
2:B:1013:ASN:HD21	2:B:1015:HIS:HD2	1.28	0.81
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.45	0.81
3:C:98:VAL:H	3:C:122:SER:HB2	1.44	0.81
1:A:535:THR:HG21	1:A:617:VAL:H	1.46	0.79
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.66	0.78
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.66	0.75
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.68	0.73
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.69	0.73
2:B:345:LYS:HA	2:B:347:LYS:H	1.52	0.73
1:A:855:THR:HG21	1:A:857:ARG:HE	1.55	0.72
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.73	0.71
3:C:142:VAL:H	8:J:16:ASP:HB3	1.57	0.69
2:B:783:THR:HG22	8:J:63:TYR:CE1	2.28	0.68
1:A:469:ARG:NH2	2:B:991:GLY:O	2.26	0.68
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	2.09	0.68
1:A:756:ILE:H	1:A:756:ILE:HD13	1.59	0.67
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.75	0.67
1:A:998:LEU:HD12	1:A:1001:ARG:HG3	1.77	0.66
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.76	0.66
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.76	0.66
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.28	0.66
1:A:399:HIS:O	1:A:401:GLY:N	2.29	0.66
2:B:864:LYS:H	2:B:872:GLU:HB2	1.60	0.66
2:B:654:ARG:H	2:B:657:HIS:HD2	1.44	0.65
1:A:754:SER:H	1:A:757:ASN:HD22	1.45	0.65
4:E:19:VAL:O	4:E:23:VAL:HG23	1.98	0.64
3:C:167:HIS:HD2	3:C:169:LYS:H	1.45	0.63
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.80	0.63
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.80	0.62
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.81	0.62
1:A:567:LYS:HD3	6:H:95:TYR:CE1	2.35	0.62
1:A:269:ILE:HG22	1:A:299:HIS:HB3	1.82	0.62
2:B:996:ARG:HH22	3:C:173:ALA:HB1	1.65	0.61
1:A:453:MET:HB3	1:A:477:PRO:HB3	1.81	0.61
3:C:6:PRO:HB3	3:C:25:VAL:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:LEU:HD11	2:B:811:TYR:O	2.00	0.61
2:B:1002:THR:HG22	2:B:1004:GLU:H	1.65	0.61
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.83	0.61
2:B:864:LYS:HG2	2:B:871:THR:HG23	1.82	0.61
1:A:215:SER:HB3	1:A:218:ASP:HB2	1.82	0.61
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.47	0.60
2:B:1013:ASN:ND2	2:B:1015:HIS:HD2	2.00	0.60
1:A:741:ASN:HD22	1:A:744:LYS:H	1.50	0.60
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.68	0.59
1:A:824:LEU:HD21	2:B:765:PRO:HB3	1.84	0.59
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.85	0.58
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.85	0.58
2:B:801:LYS:O	8:J:52:THR:HG23	2.04	0.58
2:B:1013:ASN:HD21	2:B:1015:HIS:CD2	2.16	0.58
3:C:171:GLY:C	3:C:173:ALA:H	2.07	0.58
1:A:946:VAL:HG22	4:E:201:LYS:HD2	1.86	0.58
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.86	0.57
1:A:265:LYS:HD3	1:A:322:VAL:HG11	1.86	0.57
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.33	0.57
2:B:38:PHE:H	2:B:41:LYS:HB2	1.69	0.57
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.87	0.57
2:B:976:ILE:O	2:B:990:ILE:HB	2.05	0.57
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.86	0.57
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.85	0.57
6:H:125:LEU:HG	6:H:130:ARG:NH1	2.20	0.56
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.69	0.56
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.69	0.56
2:B:744:HIS:HD2	2:B:746:SER:H	1.54	0.56
1:A:786:HIS:HE1	2:B:742:GLU:OE1	1.88	0.56
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.88	0.56
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.86	0.56
1:A:472:LEU:O	1:A:475:THR:HB	2.05	0.56
2:B:843:GLN:HB2	2:B:993:THR:HB	1.88	0.56
1:A:251:SER:HB3	1:A:258:GLY:HA3	1.88	0.56
1:A:483:ASP:HB2	2:B:987:LYS:HG3	1.88	0.56
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.89	0.55
2:B:872:GLU:HG2	2:B:916:THR:HG22	1.88	0.55
1:A:565:ILE:HG12	1:A:567:LYS:NZ	2.22	0.55
9:K:65:HIS:HD2	9:K:67:PHE:H	1.55	0.55
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.89	0.55
1:A:640:GLN:H	1:A:640:GLN:CD	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.89	0.55
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.42	0.54
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.89	0.54
2:B:128:LEU:HB2	2:B:167:ILE:HG22	1.88	0.54
1:A:511:ILE:HA	1:A:521:MET:HE3	1.89	0.54
2:B:706:GLN:O	2:B:710:LEU:HB2	2.07	0.54
1:A:472:LEU:HD21	2:B:835:GLN:HB2	1.89	0.54
11:R:6:A:H61	12:T:24:DT:H3	1.54	0.54
6:H:125:LEU:HG	6:H:130:ARG:HH12	1.73	0.54
3:C:262:LEU:HD11	9:K:87:LEU:HD23	1.89	0.54
1:A:596:THR:C	1:A:598:LEU:H	2.10	0.54
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.38	0.54
1:A:855:THR:CG2	1:A:857:ARG:HE	2.21	0.53
1:A:527:THR:HG21	1:A:650:GLN:HA	1.90	0.53
2:B:884:ARG:HG3	2:B:935:ARG:HE	1.73	0.53
6:H:63:LEU:HB2	6:H:90:ALA:H	1.74	0.53
1:A:579:SER:HA	1:A:582:ILE:HD12	1.90	0.53
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.89	0.53
2:B:241:ARG:HA	2:B:253:THR:HG22	1.89	0.53
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.90	0.53
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.91	0.53
2:B:1129:ARG:HB3	12:T:21:DA:H5"	1.91	0.53
2:B:984:HIS:HB3	2:B:1022:THR:OG1	2.09	0.53
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.92	0.53
2:B:542:MET:HE1	2:B:743:ILE:HB	1.91	0.53
2:B:195:CYS:SG	2:B:783:THR:HB	2.49	0.52
1:A:535:THR:HG21	1:A:617:VAL:N	2.18	0.52
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.91	0.52
1:A:946:VAL:HG13	4:E:201:LYS:HB3	1.92	0.52
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.92	0.52
1:A:404:TYR:HA	1:A:413:ILE:O	2.09	0.52
2:B:1013:ASN:ND2	2:B:1015:HIS:CD2	2.77	0.52
3:C:56:THR:HG21	3:C:145:CYS:SG	2.50	0.52
3:C:102:GLN:HG2	3:C:154:LYS:HG3	1.92	0.52
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.92	0.51
2:B:887:HIS:HA	2:B:888:GLY:C	2.31	0.51
1:A:785:PRO:HG2	2:B:703:ILE:HD12	1.92	0.51
3:C:134:ILE:HG12	3:C:141:GLY:H	1.75	0.51
1:A:704:ALA:HB2	1:A:710:LEU:HA	1.92	0.51
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.93	0.51
1:A:709:THR:HG22	1:A:711:ARG:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:80:ARG:HG2	9:K:57:LEU:HD22	1.92	0.51
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.93	0.51
1:A:1123:GLY:HA3	1:A:1124:HIS:CB	2.37	0.51
2:B:515:HIS:H	2:B:518:HIS:CD2	2.29	0.51
1:A:134:ARG:HD2	1:A:221:SER:O	2.11	0.51
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.76	0.51
2:B:570:VAL:HB	2:B:573:GLN:HG2	1.93	0.50
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.93	0.50
1:A:113:LEU:HD12	1:A:218:ASP:HB3	1.94	0.50
1:A:571:LEU:HD23	6:H:46:LEU:HD11	1.94	0.50
1:A:1422:ARG:HG3	2:B:1220:ARG:HH12	1.75	0.50
1:A:663:SER:HB2	2:B:1085:ILE:HG13	1.94	0.50
1:A:729:ALA:HA	1:A:732:LEU:HD12	1.93	0.50
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.77	0.50
1:A:406:ILE:HD11	1:A:433:GLU:HG3	1.94	0.50
3:C:22:LEU:HG	3:C:25:VAL:HG21	1.94	0.50
2:B:579:ARG:HG3	2:B:623:GLU:HG2	1.93	0.50
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.94	0.50
1:A:1123:GLY:CA	1:A:1124:HIS:HB2	2.38	0.49
9:K:38:GLU:O	9:K:69:ALA:O	2.30	0.49
12:T:19:DT:H2'	12:T:20:DC:C6	2.48	0.49
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.95	0.49
1:A:667:GLY:HA2	1:A:670:ILE:HG12	1.95	0.49
2:B:1009:ASP:OD2	8:J:48:ARG:NH2	2.46	0.49
3:C:165:LYS:O	9:K:6:ARG:NH1	2.46	0.49
3:C:167:HIS:CD2	3:C:169:LYS:H	2.30	0.49
1:A:839:ARG:NH2	1:A:1402:PHE:O	2.44	0.49
1:A:211:PHE:HA	1:A:214:ILE:HD11	1.95	0.49
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.78	0.49
1:A:899:VAL:HB	1:A:929:LEU:HD22	1.95	0.48
3:C:66:ARG:NH2	8:J:3:VAL:O	2.35	0.48
1:A:70:CYS:HB2	2:B:1172:ILE:HG23	1.95	0.48
1:A:531:ILE:O	1:A:535:THR:HB	2.13	0.48
2:B:976:ILE:HG23	2:B:977:GLY:H	1.79	0.48
2:B:69:LEU:HD12	2:B:90:ILE:HB	1.95	0.48
2:B:792:MET:HA	2:B:856:PHE:O	2.14	0.48
1:A:567:LYS:HB3	6:H:96:VAL:H	1.79	0.48
1:A:1086:PHE:HB3	1:A:1092:LYS:HB3	1.96	0.48
1:A:55:ASP:O	1:A:57:ARG:N	2.46	0.48
7:I:26:LEU:HD23	7:I:37:GLU:HA	1.95	0.48
1:A:683:ILE:HG21	1:A:801:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:GLU:HG3	2:B:249:ARG:HH22	1.79	0.47
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.14	0.47
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.94	0.47
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.96	0.47
3:C:70:ILE:HD11	3:C:144:ILE:HD12	1.96	0.47
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.79	0.47
9:K:108:GLU:HA	9:K:111:LEU:HD12	1.96	0.47
1:A:825:ILE:HD12	2:B:512:ARG:HB3	1.96	0.47
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.67	0.47
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.97	0.47
4:E:39:LEU:HG	4:E:43:LYS:HE3	1.96	0.47
1:A:565:ILE:HG22	1:A:569:LYS:O	2.15	0.47
1:A:445:ASN:HB2	1:A:455:MET:HG3	1.96	0.47
4:E:107:THR:HG22	4:E:131:THR:HB	1.97	0.47
4:E:157:SER:HB3	4:E:160:GLU:HG3	1.97	0.47
1:A:115:LEU:HD21	1:A:145:LYS:HE3	1.96	0.47
1:A:356:ASP:HB3	1:A:359:LEU:HB2	1.96	0.47
3:C:3:GLU:HB3	9:K:104:ASN:HD21	1.80	0.47
1:A:1130:GLN:O	1:A:1134:ILE:HG12	2.15	0.47
2:B:345:LYS:HA	2:B:347:LYS:N	2.27	0.47
1:A:357:PRO:HD2	2:B:833:TYR:CE2	2.50	0.47
2:B:428:ILE:HD11	2:B:448:ILE:HG23	1.97	0.47
2:B:754:SER:HB2	2:B:812:LEU:HD11	1.97	0.47
9:K:65:HIS:CD2	9:K:67:PHE:H	2.33	0.46
1:A:535:THR:CG2	1:A:617:VAL:H	2.21	0.46
9:K:51:LEU:HD13	9:K:59:ALA:HB3	1.97	0.46
9:K:55:LYS:HD2	9:K:81:TYR:HD1	1.81	0.46
3:C:69:LEU:O	8:J:6:ARG:HD2	2.15	0.46
1:A:752:LYS:HB3	2:B:1018:PRO:HG2	1.98	0.46
2:B:544:CYS:HB2	2:B:634:TYR:CE1	2.50	0.46
2:B:516:ASN:H	2:B:516:ASN:HD22	1.64	0.46
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	1.97	0.46
1:A:512:VAL:HA	1:A:519:PRO:HA	1.97	0.46
1:A:848:ILE:HD12	1:A:864:ILE:HG13	1.98	0.46
2:B:213:ILE:HD12	2:B:497:ARG:HB3	1.98	0.46
4:E:198:ILE:HD13	4:E:212:ARG:HG3	1.96	0.46
2:B:613:VAL:HG22	2:B:628:THR:HA	1.98	0.46
2:B:654:ARG:H	2:B:657:HIS:CD2	2.31	0.45
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.98	0.45
10:L:49:LYS:O	10:L:50:ASP:HB2	2.16	0.45
3:C:77:ILE:HD12	3:C:161:LYS:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:957:ASN:HD22	2:B:961:LEU:HD12	1.80	0.45
1:A:173:THR:HB	1:A:184:SER:HB3	1.97	0.45
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.96	0.45
1:A:306:ASN:HD21	1:A:313:GLN:HB2	1.80	0.45
1:A:456:MET:HG2	1:A:510:GLN:HG3	1.98	0.45
1:A:519:PRO:HD3	1:A:631:HIS:CD2	2.52	0.45
9:K:8:GLU:O	9:K:37:LYS:HD2	2.16	0.45
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.52	0.45
2:B:1100:ASP:HA	2:B:1103:ILE:HD11	1.98	0.45
2:B:36:ALA:HB2	2:B:661:LEU:HD22	1.98	0.45
1:A:349:ALA:HB2	1:A:374:LEU:HD11	1.98	0.45
3:C:46:ILE:HD12	3:C:157:CYS:HB3	1.99	0.45
1:A:821:ARG:HG3	1:A:825:ILE:HD11	1.99	0.45
1:A:1116:LEU:HB3	1:A:1308:THR:HB	1.98	0.45
1:A:1116:LEU:HD12	1:A:1329:THR:HB	1.98	0.45
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.99	0.45
2:B:1043:ASP:O	2:B:1050:ILE:HD13	2.17	0.45
1:A:1266:THR:HA	1:A:1270:ASN:HD22	1.81	0.45
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.99	0.45
3:C:148:ARG:HB3	3:C:151:GLN:HG3	1.99	0.45
1:A:378:GLU:HG2	1:A:388:LEU:HD11	1.99	0.45
1:A:902:LEU:HD23	1:A:921:GLY:HA2	1.99	0.45
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.52	0.45
2:B:578:THR:OG1	2:B:593:PRO:HG3	2.17	0.45
2:B:364:ILE:HD13	2:B:585:VAL:HG13	1.98	0.44
1:A:1102:LYS:HG2	1:A:1106:ASN:ND2	2.32	0.44
1:A:756:ILE:CD1	1:A:756:ILE:H	2.27	0.44
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.99	0.44
7:I:69:PRO:HD2	7:I:85:PHE:O	2.18	0.44
1:A:443:LEU:HD11	1:A:455:MET:HG2	1.99	0.44
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.32	0.44
1:A:666:ILE:HG12	2:B:1026:LEU:HB2	1.99	0.44
1:A:942:PHE:O	1:A:946:VAL:HG23	2.18	0.44
2:B:1082:MET:HA	3:C:189:THR:HA	2.00	0.44
1:A:350:ARG:HD2	2:B:1128:LEU:HD21	2.00	0.44
1:A:821:ARG:O	1:A:825:ILE:HG12	2.17	0.44
1:A:747:VAL:HG21	1:A:758:ILE:HD11	1.99	0.44
3:C:104:PHE:HD2	3:C:106:GLU:HG3	1.82	0.44
1:A:774:ARG:HG3	1:A:797:LYS:HE3	2.00	0.44
10:L:61:THR:HB	10:L:63:ARG:H	1.82	0.44
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:ARG:HG3	2:B:204:ILE:HD13	1.98	0.44
1:A:414:ASP:OD1	1:A:416:ARG:HG2	2.17	0.44
2:B:38:PHE:HA	2:B:42:GLY:H	1.83	0.44
1:A:353:ILE:HG12	1:A:487:MET:HG3	2.00	0.44
2:B:405:ARG:HB3	2:B:631:GLY:HA3	1.98	0.44
6:H:33:GLN:HG3	6:H:129:TYR:OH	2.18	0.44
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.47	0.44
8:J:5:VAL:HG12	8:J:6:ARG:HG3	2.00	0.44
2:B:63:ILE:O	2:B:67:SER:HB3	2.18	0.44
1:A:1138:ILE:HG13	1:A:1282:VAL:HG21	2.00	0.44
1:A:315:LEU:HA	1:A:320:ARG:HB3	2.00	0.44
1:A:329:LEU:HA	1:A:335:ARG:H	1.83	0.43
3:C:164:ALA:HA	3:C:167:HIS:O	2.18	0.43
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.53	0.43
1:A:924:LYS:O	1:A:927:VAL:HG12	2.18	0.43
2:B:356:LEU:HA	2:B:360:PHE:HB3	2.00	0.43
2:B:277:LYS:H	2:B:277:LYS:HG3	1.53	0.43
1:A:567:LYS:CB	1:A:568:PRO:CD	2.96	0.43
8:J:44:TYR:HA	8:J:47:ARG:HB2	2.00	0.43
1:A:1100:ARG:HH21	1:A:1330:ASN:HB2	1.82	0.43
2:B:708:GLU:O	2:B:710:LEU:N	2.52	0.43
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.99	0.43
2:B:800:GLN:HB2	2:B:821:GLN:HA	2.01	0.43
3:C:143:LEU:HD21	3:C:146:LYS:HE3	2.00	0.43
1:A:873:MET:HB3	1:A:878:ILE:HD11	2.00	0.43
9:K:58:PHE:HB3	9:K:76:GLN:HB3	2.01	0.43
2:B:824:ILE:HD13	2:B:1089:PRO:HB3	2.00	0.43
1:A:379:VAL:HG22	1:A:431:LYS:HG2	1.99	0.43
1:A:958:VAL:HG11	1:A:1049:ILE:HG23	2.01	0.43
2:B:695:ALA:HA	2:B:698:GLU:HB2	2.01	0.43
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.33	0.43
2:B:912:ILE:HB	2:B:939:THR:HB	2.00	0.43
2:B:640:VAL:CG1	2:B:649:LYS:HB3	2.49	0.43
2:B:706:GLN:HB2	2:B:710:LEU:HD23	2.01	0.43
3:C:171:GLY:C	3:C:173:ALA:N	2.70	0.43
1:A:456:MET:HE2	1:A:507:VAL:HA	2.01	0.43
3:C:18:VAL:HG23	3:C:232:VAL:HB	2.01	0.43
1:A:1285:MET:HG3	1:A:1307:GLU:OE1	2.19	0.42
1:A:1129:GLU:HA	1:A:1132:LYS:HE3	2.00	0.42
3:C:70:ILE:CD1	3:C:144:ILE:HD12	2.49	0.42
2:B:653:VAL:HG22	2:B:689:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.01	0.42
2:B:29:ASP:HB3	2:B:658:ILE:HG12	2.01	0.42
4:E:61:GLN:HE21	4:E:105:PHE:HE2	1.67	0.42
9:K:7:PHE:HB2	9:K:11:LEU:HD22	2.01	0.42
2:B:762:ASN:ND2	2:B:1022:THR:HA	2.34	0.42
1:A:1308:THR:HG22	1:A:1310:GLY:O	2.19	0.42
1:A:1393:ASN:ND2	1:A:1393:ASN:H	2.16	0.42
3:C:40:GLU:HG2	3:C:163:ILE:HD12	2.00	0.42
2:B:227:LYS:HG2	2:B:236:HIS:CD2	2.55	0.42
2:B:800:GLN:HG3	2:B:821:GLN:HG2	2.02	0.42
1:A:351:THR:HG21	1:A:466:SER:O	2.20	0.42
2:B:1002:THR:HB	2:B:1006:ILE:H	1.84	0.42
1:A:1161:THR:OG1	1:A:1170:ILE:HG13	2.20	0.42
8:J:36:LEU:HD11	8:J:51:LEU:HB2	2.02	0.42
2:B:379:GLY:HA2	2:B:382:ILE:HD12	2.01	0.42
2:B:577:ALA:HB1	2:B:589:VAL:HB	2.02	0.42
1:A:304:MET:HA	1:A:325:ILE:HD12	2.01	0.42
1:A:595:THR:HG21	1:A:604:GLY:HA3	2.02	0.42
2:B:952:VAL:HB	10:L:58:LYS:CB	2.50	0.42
2:B:519:TRP:HZ2	2:B:705:MET:CE	2.32	0.42
2:B:123:THR:HA	2:B:204:ILE:O	2.20	0.42
1:A:741:ASN:HB3	1:A:744:LYS:HB3	2.02	0.42
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	2.01	0.42
2:B:979:LYS:HE3	2:B:987:LYS:HB2	2.02	0.42
1:A:579:SER:HB3	1:A:611:GLN:HA	2.01	0.42
2:B:256:VAL:HG12	2:B:385:LEU:HD22	2.01	0.42
1:A:329:LEU:HD22	2:B:1203:LEU:HD12	2.02	0.42
9:K:32:VAL:HG22	9:K:74:ARG:HG3	2.02	0.42
2:B:999:MET:HB3	2:B:1007:VAL:HG22	2.01	0.41
2:B:638:PHE:CE1	2:B:743:ILE:HA	2.55	0.41
1:A:679:ILE:HG23	1:A:729:ALA:HB1	2.01	0.41
1:A:1208:THR:O	1:A:1212:VAL:HG23	2.19	0.41
3:C:46:ILE:HG23	3:C:157:CYS:HB3	2.01	0.41
2:B:744:HIS:CD2	2:B:746:SER:OG	2.72	0.41
6:H:16:ASP:HA	6:H:17:PRO:HD3	1.91	0.41
2:B:286:PHE:HB3	2:B:297:ILE:HG12	2.02	0.41
2:B:620:ARG:HD2	7:I:68:LEU:HD11	2.02	0.41
4:E:94:LYS:O	4:E:98:ILE:HG12	2.20	0.41
2:B:551:PRO:HB2	2:B:555:ILE:HD11	2.03	0.41
1:A:1426:GLU:HG2	1:A:1426:GLU:H	1.44	0.41
1:A:1152:ILE:HB	7:I:44:TYR:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:HIS:O	2:B:364:ILE:HB	2.19	0.41
2:B:363:HIS:CD2	2:B:585:VAL:HG22	2.53	0.41
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.55	0.41
1:A:1342:GLU:HG3	4:E:198:ILE:HG21	2.03	0.41
1:A:457:ALA:HB2	1:A:501:LEU:HB3	2.03	0.41
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.50	0.41
1:A:444:PHE:HE2	1:A:470:LEU:CD2	2.34	0.41
1:A:1100:ARG:NH2	1:A:1330:ASN:HB2	2.35	0.41
1:A:629:LEU:O	1:A:633:VAL:HG23	2.20	0.41
1:A:731:ARG:HD3	1:A:755:PHE:CZ	2.56	0.41
2:B:291:ILE:HD12	2:B:291:ILE:N	2.36	0.41
1:A:968:GLN:HA	1:A:973:ILE:HD13	2.02	0.41
2:B:1135:ARG:HG3	2:B:1147:LEU:HD21	2.02	0.41
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.61	0.41
3:C:22:LEU:HD11	9:K:101:LEU:HD21	2.01	0.41
2:B:651:LEU:HD11	2:B:707:PRO:HB3	2.03	0.41
1:A:456:MET:HB2	1:A:478:TYR:OH	2.21	0.41
1:A:1191:TRP:HZ3	7:I:43:VAL:HG21	1.85	0.41
1:A:589:GLN:HB3	1:A:961:ARG:HH22	1.86	0.41
1:A:848:ILE:HG21	1:A:1370:LEU:HD11	2.02	0.41
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.54	0.41
1:A:91:PHE:H	1:A:297:GLN:HE22	1.69	0.41
2:B:476:ARG:O	2:B:478:GLY:N	2.54	0.41
1:A:567:LYS:HG3	1:A:568:PRO:HD2	2.03	0.41
1:A:534:LEU:O	1:A:574:GLY:HA3	2.21	0.41
4:E:19:VAL:HG11	4:E:80:VAL:HG11	2.02	0.41
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.53	0.41
1:A:666:ILE:HG12	2:B:1026:LEU:CB	2.51	0.41
1:A:351:THR:HG22	1:A:352:VAL:H	1.84	0.41
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.21	0.41
2:B:515:HIS:CD2	2:B:517:THR:H	2.39	0.41
1:A:709:THR:HB	1:A:712:GLU:HB2	2.02	0.41
2:B:102:VAL:HG23	2:B:112:LEU:HD22	2.02	0.41
1:A:828:ALA:HB2	2:B:530:GLY:HA2	2.02	0.40
1:A:1259:MET:HA	1:A:1262:LYS:HE2	2.03	0.40
1:A:559:VAL:HG13	6:H:78:SER:HA	2.02	0.40
1:A:711:ARG:HG2	7:I:97:MET:HE2	2.03	0.40
1:A:374:LEU:HA	2:B:1107:ALA:HB2	2.03	0.40
2:B:826:ALA:HB2	2:B:1087:PHE:HD1	1.86	0.40
1:A:1327:ILE:O	4:E:147:HIS:HE1	2.04	0.40
1:A:1338:VAL:HG12	1:A:1339:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:ILE:HG23	1:A:567:LYS:CG	2.44	0.40
2:B:708:GLU:H	2:B:708:GLU:HG2	1.63	0.40
1:A:541:ILE:HD11	1:A:577:ILE:HG12	2.03	0.40
8:J:3:VAL:HG21	8:J:18:TRP:HB2	2.04	0.40
8:J:14:VAL:HA	8:J:17:LYS:HD3	2.02	0.40
1:A:18:GLN:HE21	1:A:1418:LEU:HB2	1.87	0.40
1:A:785:PRO:HD2	1:A:786:HIS:CD2	2.57	0.40
2:B:211:VAL:HG21	2:B:483:LEU:HD13	2.03	0.40
1:A:1138:ILE:HG22	1:A:1319:VAL:HG21	2.04	0.40
9:K:7:PHE:O	9:K:11:LEU:HB2	2.22	0.40
1:A:179:LEU:HD11	1:A:298:PHE:HD1	1.87	0.40
1:A:500:GLU:OE2	1:A:1438:THR:HG21	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%)	1234 (88%)	124 (9%)	37 (3%)	6	39
2	B	1096/1224 (90%)	962 (88%)	96 (9%)	38 (4%)	4	31
3	C	264/318 (83%)	239 (90%)	21 (8%)	4 (2%)	13	55
4	E	212/215 (99%)	203 (96%)	7 (3%)	2 (1%)	21	67
5	F	83/155 (54%)	75 (90%)	7 (8%)	1 (1%)	16	60
6	H	129/146 (88%)	103 (80%)	16 (12%)	10 (8%)	1	8
7	I	117/122 (96%)	105 (90%)	11 (9%)	1 (1%)	21	67
8	J	63/70 (90%)	58 (92%)	2 (3%)	3 (5%)	3	22
9	K	112/120 (93%)	107 (96%)	4 (4%)	1 (1%)	21	67
10	L	44/70 (63%)	30 (68%)	7 (16%)	7 (16%)	0	1
All	All	3515/4173 (84%)	3116 (89%)	295 (8%)	104 (3%)	5	35



All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	54	ASN
1	A	55	ASP
1	A	250	ILE
1	A	399	HIS
1	A	418	SER
1	A	424	ILE
1	A	567	LYS
1	A	1223	ASP
2	B	250	PHE
2	B	477	ALA
2	B	648	HIS
2	B	708	GLU
2	B	709	ASP
2	B	712	PRO
2	B	731	VAL
2	B	734	HIS
2	B	751	VAL
2	B	850	LEU
2	B	1046	PRO
2	B	1156	ASP
2	B	1181	GLU
3	C	173	ALA
8	J	2	ILE
8	J	6	ARG
10	L	50	ASP
10	L	56	LEU
1	A	118	HIS
1	A	286	HIS
1	A	312	PRO
1	A	324	SER
1	A	332	LYS
1	A	775	ILE
1	A	1123	GLY
1	A	1234	GLU
1	A	1437	GLY
2	B	367	LEU
2	B	465	ASN
2	B	469	GLN
2	B	526	GLU
2	B	629	ASP
2	B	887	HIS

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Mol	Chain	Res	Type
2	B	976	ILE
2	B	1155	SER
3	C	142	VAL
4	E	126	SER
6	H	85	GLY
6	H	131	ASN
10	L	64	LEU
1	A	56	PRO
1	A	68	GLN
1	A	308	ILE
1	A	423	ASP
1	A	1221	LYS
2	B	137	TYR
2	B	139	ALA
2	B	471	LYS
2	B	646	LEU
2	B	879	ARG
2	B	1221	SER
5	F	154	ASP
6	H	90	ALA
6	H	109	LYS
7	I	77	LYS
9	K	64	GLU
10	L	46	VAL
10	L	59	ALA
1	A	214	ILE
1	A	257	ARG
1	A	610	GLY
1	A	672	ASP
1	A	852	TYR
1	A	1083	THR
2	B	248	SER
2	B	478	GLY
2	B	1096	ARG
2	B	1157	ALA
2	B	1178	ASN
3	C	90	ASP
3	C	215	GLU
4	E	86	PRO
6	H	86	ASP
10	L	47	ARG
1	A	35	ILE

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Mol	Chain	Res	Type
1	A	958	VAL
2	B	531	GLN
2	B	881	ASN
6	H	83	GLN
6	H	140	ALA
8	J	64	ASN
10	L	39	SER
1	A	310	GLY
1	A	404	TYR
2	B	563	MET
2	B	792	MET
2	B	1099	VAL
6	H	17	PRO
6	H	108	SER
1	A	78	PRO
1	A	331	GLY
1	A	400	PRO
1	A	1384	VAL
6	H	107	VAL
2	B	647	GLY

### 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	1225/1520 (81%)	1083 (88%)	142 (12%)	7	30
2	B	967/1061 (91%)	866 (90%)	101 (10%)	9	35
3	C	234/274 (85%)	209 (89%)	25 (11%)	8	34
4	E	196/197 (100%)	186 (95%)	10 (5%)	29	70
5	F	75/137 (55%)	74 (99%)	1 (1%)	76	92
6	H	117/128 (91%)	103 (88%)	14 (12%)	6	28
7	I	113/116 (97%)	103 (91%)	10 (9%)	12	45
8	J	60/65 (92%)	52 (87%)	8 (13%)	5	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	K	99/102 (97%)	91 (92%)	8 (8%)	15	51
10	L	40/57 (70%)	32 (80%)	8 (20%)	1	8
All	All	3126/3657 (86%)	2799 (90%)	327 (10%)	8	35

All (327) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	30	ILE
1	A	40	THR
1	A	41	MET
1	A	43	GLU
1	A	58	LEU
1	A	61	ILE
1	A	65	LEU
1	A	69	THR
1	A	70	CYS
1	A	88	LYS
1	A	90	VAL
1	A	93	VAL
1	A	126	LEU
1	A	130	ASP
1	A	133	LYS
1	A	143	LYS
1	A	144	THR
1	A	171	GLN
1	A	204	THR
1	A	222	LEU
1	A	225	ASN
1	A	252	PHE
1	A	254	GLU
1	A	270	LEU
1	A	282	ASN
1	A	298	PHE
1	A	303	TYR
1	A	308	ILE
1	A	320	ARG
1	A	323	LYS
1	A	325	ILE
1	A	330	LYS
1	A	335	ARG

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Mol	Chain	Res	Type
1	A	344	ARG
1	A	351	THR
1	A	354	SER
1	A	368	LYS
1	A	389	THR
1	A	407	ARG
1	A	408	ASP
1	A	434	ARG
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	455	MET
1	A	470	LEU
1	A	475	THR
1	A	476	SER
1	A	496	GLU
1	A	498	ARG
1	A	527	THR
1	A	532	ARG
1	A	535	THR
1	A	541	ILE
1	A	544	ASP
1	A	571	LEU
1	A	590	ARG
1	A	595	THR
1	A	598	LEU
1	A	603	ASN
1	A	612	ILE
1	A	618	GLU
1	A	622	VAL
1	A	625	SER
1	A	629	LEU
1	A	634	THR
1	A	637	LYS
1	A	640	GLN
1	A	666	ILE
1	A	672	ASP
1	A	688	LYS
1	A	695	LYS
1	A	702	LEU
1	A	705	LYS

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Mol	Chain	Res	Type
1	A	710	LEU
1	A	716	ASP
1	A	722	LEU
1	A	731	ARG
1	A	740	LEU
1	A	756	ILE
1	A	771	GLU
1	A	788	SER
1	A	801	GLU
1	A	806	ARG
1	A	821	ARG
1	A	826	ASP
1	A	847	ASP
1	A	855	THR
1	A	885	THR
1	A	908	LEU
1	A	920	LEU
1	A	925	LEU
1	A	932	GLU
1	A	938	LYS
1	A	953	ASN
1	A	969	GLN
1	A	988	LEU
1	A	1005	GLU
1	A	1015	VAL
1	A	1022	LEU
1	A	1025	ARG
1	A	1029	ARG
1	A	1064	VAL
1	A	1067	LEU
1	A	1081	LEU
1	A	1084	PHE
1	A	1110	ASN
1	A	1113	THR
1	A	1161	THR
1	A	1168	GLU
1	A	1176	LEU
1	A	1187	GLN
1	A	1195	LEU
1	A	1230	GLU
1	A	1233	ASP
1	A	1237	ILE

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Mol	Chain	Res	Type
1	A	1257	ASP
1	A	1261	LYS
1	A	1264	GLU
1	A	1267	MET
1	A	1269	GLU
1	A	1277	GLU
1	A	1280	GLU
1	A	1288	ASP
1	A	1297	GLU
1	A	1299	VAL
1	A	1303	GLU
1	A	1309	ASP
1	A	1333	ILE
1	A	1334	ASP
1	A	1351	GLU
1	A	1354	ASN
1	A	1364	ASN
1	A	1366	ARG
1	A	1382	THR
1	A	1391	ARG
1	A	1393	ASN
1	A	1398	MET
1	A	1403	GLU
1	A	1426	GLU
2	B	22	SER
2	B	25	ILE
2	B	40	GLU
2	B	45	SER
2	B	46	GLN
2	B	63	ILE
2	B	65	GLU
2	B	66	ASP
2	B	68	THR
2	B	101	MET
2	B	134	LYS
2	B	135	ARG
2	B	167	ILE
2	B	175	ARG
2	B	208	SER
2	B	217	ARG
2	B	234	ILE
2	B	240	ILE

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Mol	Chain	Res	Type
2	B	276	ILE
2	B	277	LYS
2	B	282	ILE
2	B	311	LEU
2	B	355	ILE
2	B	365	THR
2	B	393	LYS
2	B	394	ASP
2	B	396	ASP
2	B	404	LYS
2	B	413	LEU
2	B	424	LEU
2	B	437	GLU
2	B	451	LYS
2	B	461	LEU
2	B	468	GLU
2	B	471	LYS
2	B	479	VAL
2	B	480	SER
2	B	485	ARG
2	B	487	THR
2	B	493	SER
2	B	531	GLN
2	B	547	VAL
2	B	555	ILE
2	B	574	SER
2	B	591	ARG
2	B	604	ARG
2	B	616	ILE
2	B	644	GLU
2	B	645	SER
2	B	653	VAL
2	B	655	LYS
2	B	658	ILE
2	B	696	GLU
2	B	762	ASN
2	B	780	VAL
2	B	786	ASN
2	B	787	VAL
2	B	791	THR
2	B	815	ARG
2	B	838	SER

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Mol	Chain	Res	Type
2	B	844	SER
2	B	850	LEU
2	B	853	SER
2	B	862	GLN
2	B	864	LYS
2	B	866	TYR
2	B	868	MET
2	B	880	THR
2	B	885	MET
2	B	886	LYS
2	B	935	ARG
2	B	948	ILE
2	B	951	GLN
2	B	963	PHE
2	B	983	ARG
2	B	987	LYS
2	B	996	ARG
2	B	997	GLU
2	B	998	ASP
2	B	1006	ILE
2	B	1007	VAL
2	B	1010	LEU
2	B	1019	SER
2	B	1028	GLU
2	B	1065	GLN
2	B	1066	SER
2	B	1077	THR
2	B	1094	ARG
2	B	1096	ARG
2	B	1099	VAL
2	B	1103	ILE
2	B	1128	LEU
2	B	1129	ARG
2	B	1145	SER
2	B	1147	LEU
2	B	1160	VAL
2	B	1175	LEU
2	B	1189	ILE
2	B	1194	ILE
2	B	1202	LEU
2	B	1222	ARG
3	C	3	GLU

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Mol	Chain	Res	Type
3	C	4	GLU
3	C	18	VAL
3	C	21	ILE
3	C	34	ARG
3	C	37	MET
3	C	43	THR
3	C	66	ARG
3	C	75	MET
3	C	77	ILE
3	C	79	GLN
3	C	109	SER
3	C	124	LEU
3	C	127	ARG
3	C	129	ILE
3	C	137	LYS
3	C	144	ILE
3	C	156	THR
3	C	215	GLU
3	C	226	ASP
3	C	240	VAL
3	C	244	VAL
3	C	249	ASP
3	C	254	LYS
3	C	268	ASP
4	E	7	ARG
4	E	65	THR
4	E	78	LEU
4	E	92	THR
4	E	122	LYS
4	E	127	ILE
4	E	156	LEU
4	E	169	ARG
4	E	191	LYS
4	E	204	THR
5	F	115	THR
6	H	16	ASP
6	H	22	LYS
6	H	34	ASP
6	H	35	GLN
6	H	52	GLN
6	H	63	LEU
6	H	86	ASP

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Mol	Chain	Res	Type
6	H	92	ASP
6	H	94	ASP
6	H	107	VAL
6	H	109	LYS
6	H	110	ASP
6	H	130	ARG
6	H	145	ARG
7	I	35	VAL
7	I	52	ILE
7	I	61	ASP
7	I	66	PRO
7	I	70	ARG
7	I	84	VAL
7	I	87	GLN
7	I	106	CYS
7	I	111	THR
7	I	119	THR
8	J	3	VAL
8	J	7	CYS
8	J	31	ASP
8	J	48	ARG
8	J	56	LEU
8	J	57	ILE
8	J	59	LYS
8	J	62	ARG
9	K	14	GLU
9	K	20	LYS
9	K	22	ASP
9	K	31	VAL
9	K	49	GLU
9	K	51	LEU
9	K	78	THR
9	K	114	LEU
10	L	27	LEU
10	L	43	THR
10	L	55	ILE
10	L	58	LYS
10	L	61	THR
10	L	65	VAL
10	L	66	GLN
10	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	18	GLN
1	A	54	ASN
1	A	92	HIS
1	A	225	ASN
1	A	297	GLN
1	A	339	ASN
1	A	358	ASN
1	A	503	GLN
1	A	517	ASN
1	A	545	GLN
1	A	626	ASN
1	A	631	HIS
1	A	741	ASN
1	A	742	ASN
1	A	745	GLN
1	A	757	ASN
1	A	786	HIS
1	A	926	GLN
1	A	1130	GLN
1	A	1140	HIS
1	A	1171	GLN
1	A	1258	HIS
1	A	1270	ASN
1	A	1364	ASN
1	A	1393	ASN
2	B	46	GLN
2	B	121	ASN
2	B	255	GLN
2	B	363	HIS
2	B	499	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	657	HIS
2	B	734	HIS
2	B	744	HIS
2	B	762	ASN
2	B	957	ASN
2	B	984	HIS
2	B	1013	ASN
2	B	1015	HIS

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Mol	Chain	Res	Type
2	B	1025	HIS
2	B	1084	GLN
2	B	1161	HIS
2	B	1211	ASN
3	C	73	GLN
3	C	112	ASN
3	C	167	HIS
3	C	242	GLN
6	H	35	GLN
6	H	131	ASN
7	I	90	GLN
9	K	65	HIS
9	K	104	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	5/5 (100%)	4 (80%)	1 (20%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	7	G
11	R	8	G
11	R	9	5BU
11	R	10	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	R	6	A

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
11	5BU	R	9	11,12	13,22,23	2.87	3 (23%)	14,32,35	4.64	5 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	5BU	R	9	11,12	-	0/3/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	9	5BU	C6-N1	3.24	1.39	1.35
11	R	9	5BU	C4-N3	3.42	1.39	1.33
11	R	9	5BU	C4-C5	8.83	1.49	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	9	5BU	C5-C4-N3	-9.15	114.23	124.00
11	R	9	5BU	O3'-C3'-C4'	-2.32	104.10	111.05
11	R	9	5BU	O4'-C4'-C3'	-2.25	100.62	105.15
11	R	9	5BU	C5-C6-N1	2.34	124.38	119.79
11	R	9	5BU	C4-N3-C2	13.79	127.17	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1405/1733 (81%)	0.11	98 (6%) 19 11	42, 85, 175, 219	0
2	B	1114/1224 (91%)	-0.05	34 (3%) 52 38	37, 78, 147, 189	0
3	C	266/318 (83%)	-0.26	2 (0%) 87 80	49, 75, 114, 155	0
4	E	214/215 (99%)	0.01	6 (2%) 56 42	61, 115, 162, 175	0
5	F	85/155 (54%)	-0.29	0 100 100	66, 96, 133, 152	0
6	H	133/146 (91%)	0.33	8 (6%) 25 14	80, 119, 154, 166	0
7	I	119/122 (97%)	-0.25	0 100 100	55, 93, 129, 142	0
8	J	65/70 (92%)	-0.27	0 100 100	49, 67, 102, 117	0
9	K	114/120 (95%)	-0.22	1 (0%) 85 78	51, 77, 104, 120	0
10	L	46/70 (65%)	0.11	1 (2%) 65 50	61, 116, 143, 158	0
11	R	4/5 (80%)	-0.51	0 100 100	78, 91, 109, 113	0
12	T	13/29 (44%)	0.69	2 (15%) 3 2	84, 115, 174, 181	0
All	All	3578/4207 (85%)	-0.00	152 (4%) 40 26	37, 84, 162, 219	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	8.7
1	A	1087	ALA	8.2
1	A	255	SER	7.0
12	T	28	DT	6.8
6	H	85	GLY	6.6
1	A	1085	HIS	6.2
2	B	883	LEU	6.1
6	H	86	ASP	6.0
1	A	318	SER	5.9
1	A	141	LEU	5.6
1	A	1091	SER	5.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	317	LYS	5.4
1	A	182	VAL	5.4
1	A	69	THR	5.2
1	A	173	THR	5.1
2	B	474	SER	5.1
1	A	1123	GLY	5.1
1	A	319	GLY	5.0
1	A	183	GLY	5.0
1	A	144	THR	4.9
2	B	1224	PHE	4.8
1	A	45	GLN	4.8
1	A	87	ALA	4.5
1	A	1086	PHE	4.4
1	A	103	CYS	4.3
1	A	177	ASP	4.3
1	A	176	LYS	4.3
10	L	27	LEU	4.3
1	A	49	LYS	4.3
1	A	1083	THR	4.2
1	A	186	LYS	4.2
1	A	314	ALA	4.2
1	A	146	MET	4.2
2	B	472	ALA	4.2
1	A	116	ASP	4.2
1	A	174	ILE	4.2
1	A	42	ASP	4.2
1	A	1088	GLY	4.2
1	A	1082	ASN	4.1
2	B	1223	ASP	4.0
1	A	257	ARG	4.0
2	B	933	SER	3.9
1	A	1175	SER	3.8
2	B	865	LYS	3.7
1	A	254	GLU	3.7
1	A	139	TRP	3.6
1	A	115	LEU	3.6
2	B	136	THR	3.6
2	B	882	THR	3.6
2	B	469	GLN	3.6
1	A	316	GLN	3.5
2	B	468	GLU	3.4
1	A	147	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
4	E	2	ASP	3.4
1	A	140	THR	3.4
1	A	142	CYS	3.4
1	A	1090	ALA	3.3
1	A	175	ARG	3.3
6	H	83	GLN	3.3
1	A	199	LEU	3.3
2	B	866	TYR	3.3
6	H	132	LEU	3.3
4	E	110	PHE	3.2
1	A	105	CYS	3.2
1	A	149	GLU	3.2
1	A	1254	ALA	3.2
1	A	118	HIS	3.2
1	A	1256	GLU	3.2
1	A	171	GLN	3.2
1	A	145	LYS	3.2
1	A	251	SER	3.1
1	A	143	LYS	3.1
1	A	313	GLN	3.1
1	A	286	HIS	3.1
2	B	470	LYS	3.0
1	A	44	THR	3.0
4	E	118	PRO	3.0
6	H	130	ARG	3.0
1	A	153	PRO	3.0
1	A	1084	PHE	3.0
1	A	168	GLY	2.9
1	A	1002	GLY	2.9
1	A	122	MET	2.9
2	B	870	ILE	2.8
1	A	152	VAL	2.8
1	A	285	PRO	2.8
2	B	429	PHE	2.8
2	B	66	ASP	2.8
1	A	137	ALA	2.8
2	B	473	MET	2.8
2	B	709	ASP	2.8
2	B	471	LYS	2.8
2	B	1222	ARG	2.8
1	A	258	GLY	2.7
6	H	131	ASN	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	154	SER	2.7
2	B	475	SER	2.6
1	A	283	GLY	2.6
1	A	250	ILE	2.6
4	E	93	MET	2.6
1	A	295	LEU	2.5
2	B	89	GLU	2.5
2	B	868	MET	2.5
1	A	114	LEU	2.5
1	A	200	ARG	2.5
1	A	1089	VAL	2.5
1	A	1124	HIS	2.5
1	A	121	LEU	2.5
1	A	1092	LYS	2.5
9	K	21	ILE	2.4
1	A	323	LYS	2.4
4	E	122	LYS	2.4
1	A	181	LEU	2.4
2	B	140	ILE	2.4
1	A	135	PHE	2.4
1	A	212	LYS	2.4
2	B	935	ARG	2.4
2	B	919	SER	2.4
1	A	124	GLN	2.4
6	H	107	VAL	2.4
1	A	320	ARG	2.4
12	T	27	DA	2.4
1	A	256	GLN	2.3
3	C	216	GLY	2.3
1	A	163	SER	2.3
1	A	253	ASN	2.3
1	A	1258	HIS	2.3
2	B	135	ARG	2.3
1	A	1108	ALA	2.2
1	A	1257	ASP	2.2
3	C	3	GLU	2.2
6	H	133	ASN	2.2
1	A	311	GLN	2.2
4	E	49	SER	2.2
1	A	214	ILE	2.2
1	A	120	GLU	2.2
1	A	104	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	250	PHE	2.1
2	B	647	GLY	2.1
1	A	430	TRP	2.1
1	A	288	ALA	2.1
1	A	294	SER	2.1
2	B	645	SER	2.1
2	B	246	LYS	2.1
2	B	867	GLY	2.1
1	A	148	CYS	2.1
1	A	138	ILE	2.1
1	A	210	ILE	2.1
1	A	161	LEU	2.1
1	A	975	HIS	2.0
2	B	420	LEU	2.0
2	B	431	TYR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
11	5BU	R	9	21/22	0.95	0.16	-	77,80,90,102	1

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
13	ZN	I	203	1/1	0.97	0.10	-0.85	87,87,87,87	0
13	ZN	I	204	1/1	0.99	0.11	-1.00	66,66,66,66	0
13	ZN	B	1307	1/1	0.96	0.10	-1.02	149,149,149,149	0
13	ZN	C	319	1/1	0.98	0.12	-1.10	67,67,67,67	0
13	ZN	J	101	1/1	0.99	0.18	-1.29	58,58,58,58	0
13	ZN	L	105	1/1	0.98	0.08	-1.39	102,102,102,102	0
13	ZN	A	1734	1/1	0.64	0.13	-1.57	300,300,300,300	0
13	ZN	A	1735	1/1	0.89	0.09	-2.19	135,135,135,135	0
14	MG	A	2001	1/1	0.98	0.14	-	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.