



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2018 – 02:25 AM EST

PDB ID : 4C3I
Title : Structure of 14-subunit RNA polymerase I at 3.0 Å resolution, crystal form C2-100
Authors : Fernandez-Tornero, C.; Moreno-Morcillo, M.; Rashid, U.J.; Taylor, N.M.I.; Ruiz, F.M.; Gruene, T.; Legrand, P.; Steuerwald, U.; Muller, C.W.
Deposited on : 2013-08-24
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

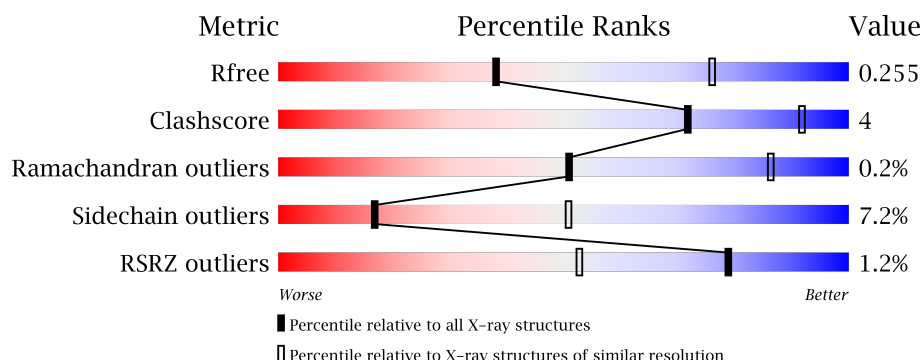
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1664	
2	B	1203	
3	C	335	
4	D	137	
5	E	215	

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Mol	Chain	Length	Quality of chain
6	F	155	
7	G	326	
8	H	146	
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	ZN	J	1070	-	-	-	X
18	MPD	G	1317	-	-	-	X

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 34252 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 I SUBUNIT RPA190.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1484	Total	C	N	O	S	0	0	0
			11695	7388	2031	2213	63			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1176	Total	C	N	O	S	0	0	0
			9322	5898	1629	1745	50			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	304	Total	C	N	O	S	0	0	0
			2418	1536	414	460	8			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	59	Total	C	N	O	0	0	0
			466	292	80	94			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	12	SER	THR	conflict	UNP P50106

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	215	Total	C	N	O	S	0	0	0
			1759	1116	310	321	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			823	522	144	154	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	259	Total	C	N	O	S	0	0	0
			2052	1301	348	398	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	134	Total	C	N	O	S	0	0	0
			1072	676	181	211	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	124	Total	C	N	O	S	0	0	0
			942	584	160	189	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	69	Total	C	N	O	S	0	0	0
			569	362	101	100	6			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUB-UNIT RPAC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	103	Total	C	N	O	S	0	0	0
			810	506	132	167	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	45	Total	C	N	O	S	0	0	0
			359	221	71	63	4			

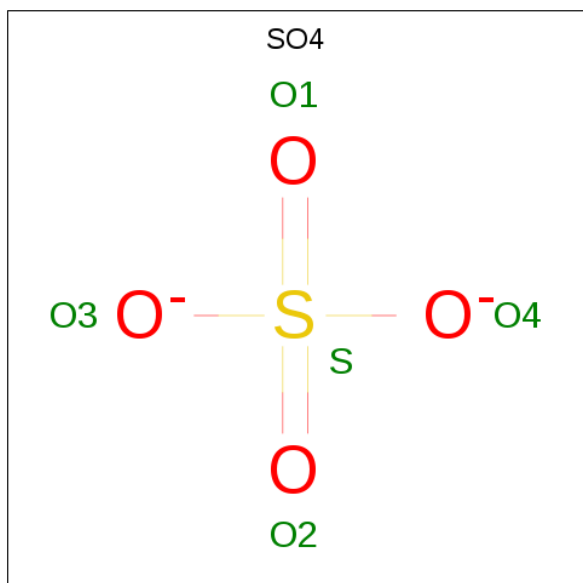
- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	105	Total	C	N	O		0	0	0
			831	528	137	166				

- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	139	Total	C	N	O	S	0	0	0
			1103	706	179	214	4			

- Molecule 15 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	A	1	Total	O	S	0	0
			5	4	1		
15	A	1	Total	O	S	0	0
			5	4	1		
15	K	1	Total	O	S	0	0
			5	4	1		

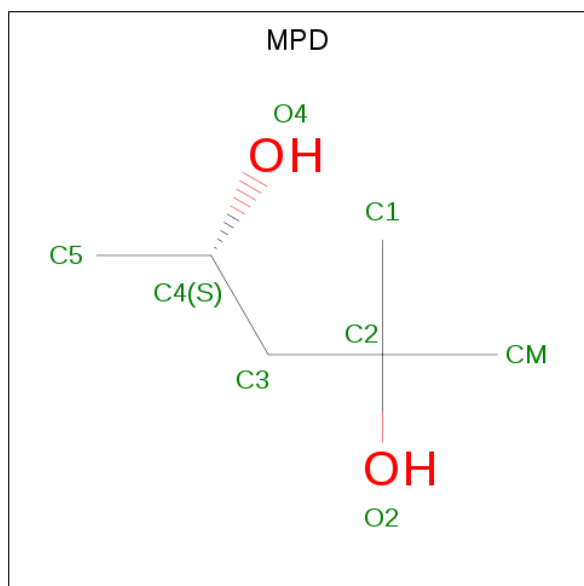
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

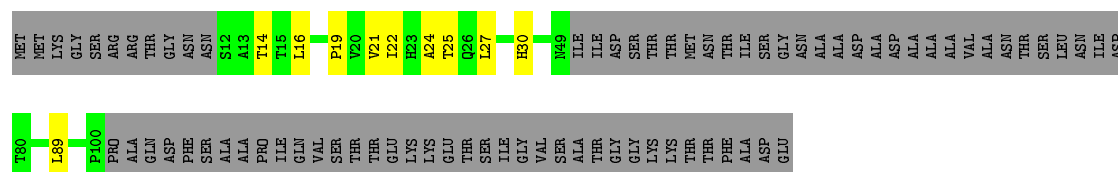
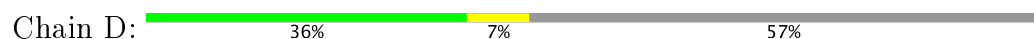
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	B	1	Total	Mg	0	0
			1	1		

- Molecule 18 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).

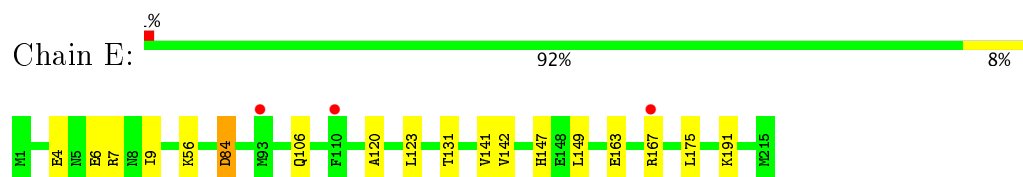


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	G	1	Total	C	O	0	0
			8	6	2		

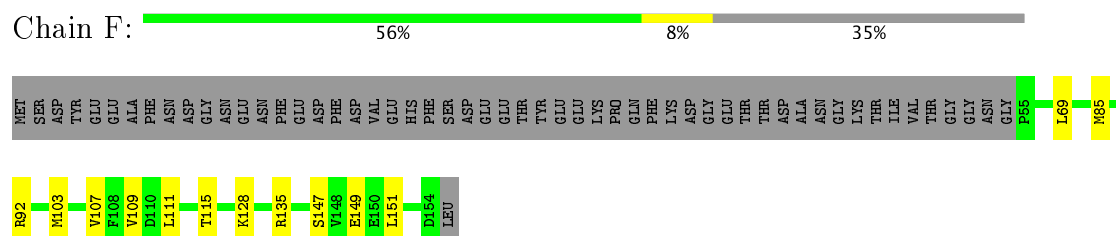
Chain B: 80% 17% ..



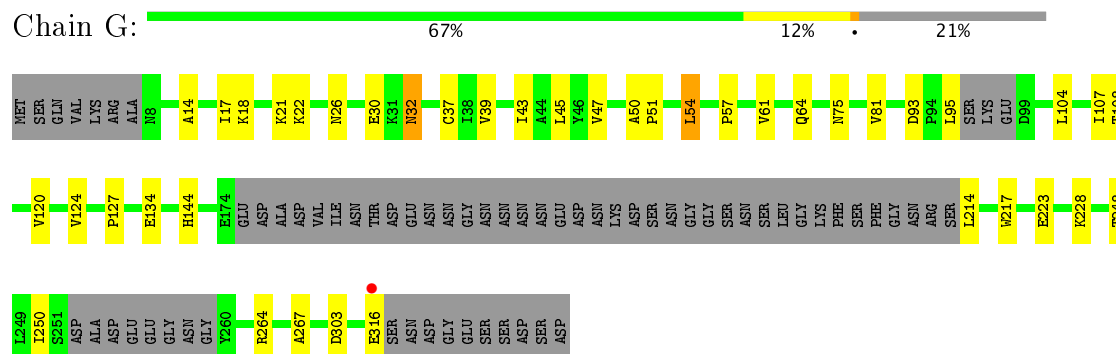
- Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1



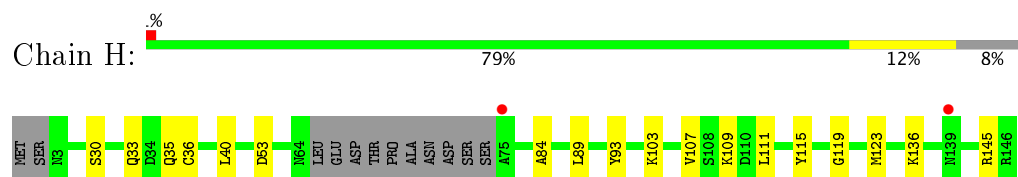
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2



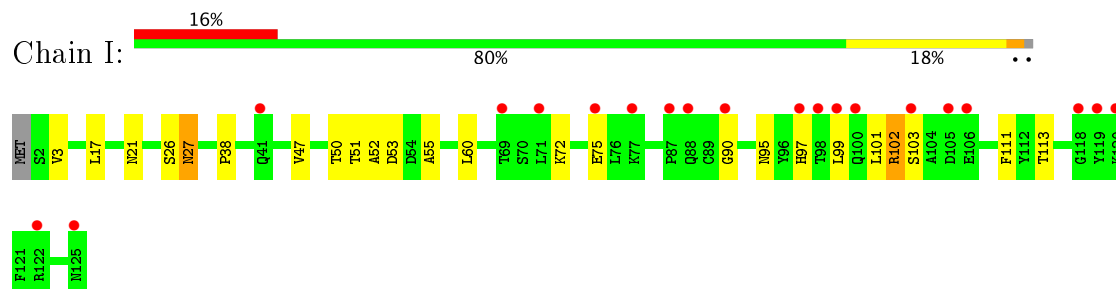
- Molecule 7: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43



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



- Molecule 9: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12



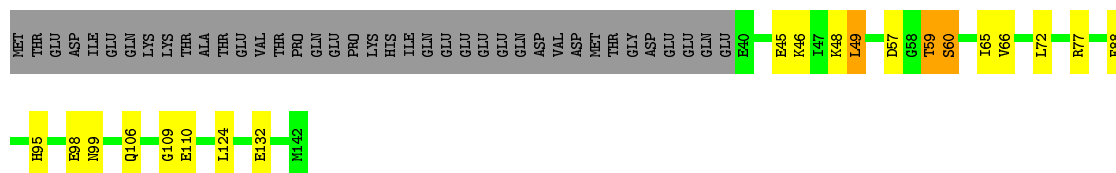
- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5





- Molecule 11: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2

Chain K:  58% 12% 0% 27%



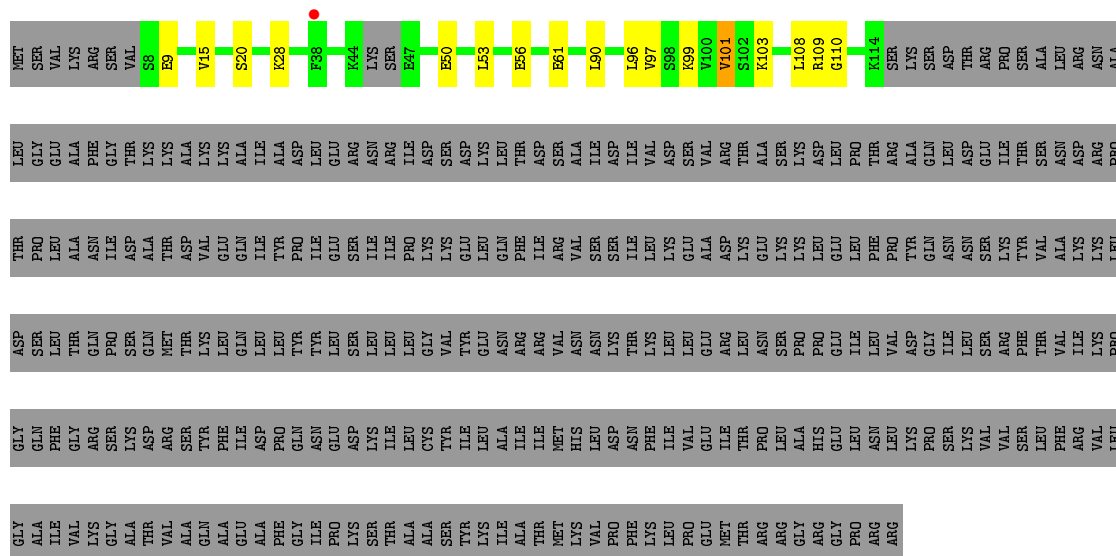
- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L: 57% 7% 36%



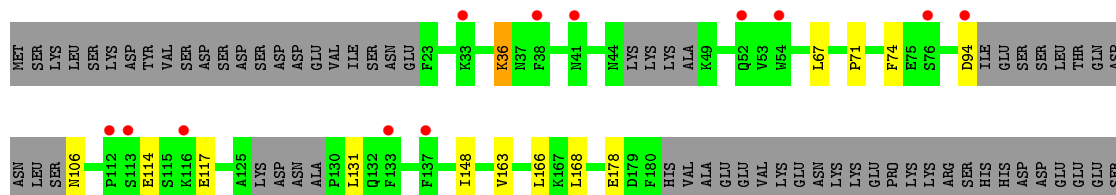
- Molecule 13: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49

Chain M: 21% . 75%



- Molecule 14: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34

Chain N: 



SER
GLU
LYS
LYS
LYS
LYS
LYS
LYS
GLU
LYS
ARG
GLU
LYS
ARG
GLU
LYS
LYS
ASP
LYS
LYS
ASP
LYS
LYS
LYS
LYS
LYS
HIS
ARG
ASP

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	400.53Å 140.22Å 122.89Å 90.00° 100.14° 90.00°	Depositor
Resolution (Å)	84.00 – 3.00 84.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (84.00-3.00) 99.1 (84.00-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.199 , 0.231 0.218 , 0.255	Depositor DCC
R_{free} test set	6608 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	93.9	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 66.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	34252	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: MG, MPD, ZN, SO4

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	0.39	0/11907	0.58	0/16088
2	B	0.39	0/9527	0.59	0/12879
3	C	0.39	0/2469	0.61	0/3347
4	D	0.39	0/472	0.53	0/639
5	E	0.40	0/1795	0.55	0/2416
6	F	0.39	0/838	0.54	0/1129
7	G	0.39	0/2094	0.58	0/2843
8	H	0.39	0/1090	0.57	0/1476
9	I	0.40	0/955	0.55	0/1288
10	J	0.40	0/578	0.62	0/775
11	K	0.39	0/821	0.60	0/1108
12	L	0.38	0/361	0.60	0/478
13	M	0.38	0/846	0.52	0/1136
14	N	0.37	0/1124	0.52	0/1512
All	All	0.39	0/34877	0.58	0/47114

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	11695	0	11764	116	0
2	B	9322	0	9187	93	0
3	C	2418	0	2401	24	0
4	D	466	0	466	3	0
5	E	1759	0	1788	7	0
6	F	823	0	841	7	0
7	G	2052	0	2016	17	0
8	H	1072	0	1042	7	0
9	I	942	0	935	7	0
10	J	569	0	585	12	0
11	K	810	0	801	11	0
12	L	359	0	381	1	0
13	M	831	0	820	10	0
14	N	1103	0	1106	6	0
15	A	10	0	0	0	0
15	K	5	0	0	0	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	B	1	0	0	0	0
18	G	8	0	14	2	0
All	All	34252	0	34147	270	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 4.

All (270) 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:712:ILE:H	11:K:106:GLN:HE22	1.22	0.88
2:B:99:VAL:HG21	2:B:417:ILE:HD11	1.55	0.87
2:B:16:PHE:HD2	2:B:978:ALA:HB2	1.51	0.75
1:A:86:TYR:H	1:A:431:GLN:HE22	1.36	0.72
1:A:824:THR:HG23	2:B:1023:ARG:HB2	1.71	0.71
3:C:222:VAL:HG21	3:C:225:ALA:HB2	1.73	0.71
1:A:432:ASN:HD21	1:A:444:GLN:H	1.38	0.70
1:A:1023:LEU:HB3	1:A:1190:SER:HB3	1.74	0.68
3:C:229:LEU:HB3	3:C:293:ARG:HG2	1.76	0.67
3:C:70:ILE:HG23	3:C:74:GLU:HB2	1.77	0.67
2:B:524:SER:HB3	2:B:528:LEU:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:72:LYS:HB2	9:I:75:GLU:HB2	1.80	0.64
2:B:558:VAL:HA	2:B:561:ILE:HD12	1.80	0.62
1:A:713:VAL:H	1:A:738:ASN:HD21	1.47	0.62
2:B:190:ILE:HD13	2:B:190:ILE:H	1.63	0.62
1:A:1038:ILE:HB	1:A:1047:GLN:HB2	1.82	0.62
1:A:913:PRO:HB3	1:A:926:GLN:HE22	1.63	0.62
1:A:701:ARG:H	1:A:706:HIS:HD2	1.46	0.61
2:B:749:THR:O	10:J:52:THR:HG23	2.01	0.61
1:A:785:GLN:HB3	1:A:793:ILE:HG22	1.83	0.60
2:B:748:GLN:HB3	10:J:52:THR:HG22	1.85	0.59
10:J:48:ARG:O	10:J:52:THR:HB	2.02	0.59
2:B:211:ARG:HH22	2:B:243:GLN:HE22	1.49	0.59
13:M:61:GLU:HB3	13:M:101:VAL:HG23	1.84	0.59
2:B:52:LEU:HG	2:B:61:LEU:HD13	1.84	0.59
5:E:147:HIS:HD2	5:E:149:LEU:H	1.50	0.59
3:C:275:VAL:HG21	3:C:293:ARG:HH21	1.66	0.58
2:B:839:LYS:HG3	2:B:857:PRO:HD2	1.86	0.58
1:A:332:GLN:HE22	1:A:350:VAL:H	1.51	0.58
1:A:1660:VAL:HB	7:G:57:PRO:HG3	1.85	0.57
1:A:527:PRO:HG2	1:A:547:ILE:HA	1.85	0.57
1:A:15:ASP:HB2	2:B:1197:ARG:HB3	1.85	0.57
1:A:727:THR:HG22	1:A:730:GLN:HG3	1.85	0.57
1:A:1051:GLY:HA3	1:A:1580:ARG:HG2	1.85	0.57
2:B:786:ALA:HB1	2:B:928:SER:HB2	1.86	0.57
11:K:88:PHE:HB3	11:K:106:GLN:HB2	1.86	0.57
1:A:943:ILE:HG12	2:B:960:ILE:HD11	1.87	0.56
2:B:1090:ASP:HA	2:B:1094:ASN:HB2	1.86	0.56
2:B:840:LEU:HD21	2:B:857:PRO:HB2	1.87	0.56
1:A:952:LEU:HD21	1:A:1000:MET:HB3	1.85	0.56
1:A:581:ILE:HD11	1:A:605:VAL:HG21	1.87	0.56
2:B:791:LYS:O	2:B:795:GLU:HG2	2.06	0.56
2:B:1045:GLN:HB3	2:B:1063:ARG:HG3	1.88	0.55
3:C:92:ILE:HG12	10:J:2:ILE:HD11	1.88	0.55
3:C:232:GLN:HE21	3:C:234:ASN:HD21	1.55	0.55
11:K:46:LYS:HA	11:K:66:VAL:HG22	1.88	0.55
2:B:721:MET:HG3	2:B:1036:LEU:HD21	1.89	0.55
3:C:91:VAL:HG11	10:J:60:PHE:HB3	1.89	0.55
1:A:677:GLY:HA3	1:A:786:TYR:OH	2.07	0.54
1:A:970:LYS:HE2	2:B:685:VAL:HG21	1.89	0.54
2:B:857:PRO:HB3	2:B:871:ILE:HD13	1.89	0.54
2:B:748:GLN:HB2	2:B:769:PHE:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:108:THR:HG22	18:G:1317:MPD:H31	1.89	0.54
1:A:1316:VAL:HG21	1:A:1498:ILE:HA	1.90	0.54
13:M:9:GLU:HG2	14:N:71:PRO:HB3	1.89	0.54
2:B:908:ARG:HD2	3:C:95:GLU:HG2	1.89	0.54
1:A:1657:LEU:HD11	6:F:135:ARG:HB2	1.89	0.54
1:A:676:ALA:HB2	1:A:821:ILE:HD13	1.90	0.54
1:A:438:ILE:HG23	2:B:1192:MET:HG2	1.90	0.54
1:A:701:ARG:H	1:A:706:HIS:CD2	2.24	0.54
1:A:438:ILE:HA	1:A:456:VAL:HG22	1.89	0.54
10:J:2:ILE:HG23	10:J:57:ILE:HG21	1.90	0.54
7:G:134:GLU:HB3	7:G:228:LYS:HE2	1.89	0.53
1:A:1596:LEU:HD22	1:A:1602:GLY:HA2	1.90	0.53
2:B:323:ARG:HH22	2:B:351:GLN:HE22	1.56	0.53
7:G:81:VAL:HA	7:G:124:VAL:HG12	1.90	0.53
2:B:282:HIS:HD2	13:M:99:LYS:HD2	1.73	0.53
1:A:1056:ASP:HB3	1:A:1059:LYS:HD3	1.91	0.53
7:G:50:ALA:H	7:G:64:GLN:HE22	1.56	0.53
1:A:1501:ILE:HG23	1:A:1504:ILE:HB	1.91	0.52
2:B:979:GLN:HG2	2:B:996:PHE:HE1	1.73	0.52
13:M:28:LYS:HD2	14:N:106:ASN:HB2	1.90	0.52
1:A:1062:HIS:HA	1:A:1065:GLN:HB2	1.90	0.52
3:C:58:ASN:HA	3:C:296:ASN:HB3	1.90	0.52
9:I:95:ASN:HB2	9:I:113:THR:HB	1.90	0.52
2:B:123:PRO:HG2	2:B:172:LEU:HD11	1.92	0.52
5:E:131:THR:HG21	5:E:191:LYS:HE2	1.91	0.52
7:G:108:THR:HA	18:G:1317:MPD:H4	1.92	0.52
1:A:1478:ALA:HB1	9:I:21:ASN:HB3	1.92	0.51
2:B:646:HIS:H	2:B:646:HIS:CD2	2.28	0.51
1:A:1229:ALA:CB	1:A:1597:ALA:HB2	2.41	0.51
2:B:726:MET:HG3	2:B:742:TYR:HB3	1.93	0.51
1:A:588:LEU:HB2	1:A:636:HIS:HB2	1.91	0.51
3:C:216:HIS:HD2	3:C:218:LYS:H	1.59	0.51
1:A:712:ILE:N	11:K:106:GLN:HE22	2.01	0.51
1:A:518:GLU:HG3	6:F:115:THR:HG21	1.93	0.50
2:B:293:ILE:HG12	2:B:302:LEU:HD23	1.91	0.50
1:A:1239:THR:HB	1:A:1542:THR:HB	1.92	0.50
13:M:53:LEU:HB2	13:M:96:LEU:HD22	1.93	0.50
1:A:381:SER:HB2	1:A:453:ILE:HG23	1.94	0.50
1:A:1039:ARG:HD2	1:A:1045:LEU:HA	1.94	0.50
7:G:51:PRO:HA	7:G:54:LEU:HD13	1.95	0.49
2:B:574:SER:HB2	13:M:97:VAL:HG11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:861:VAL:HG21	1:A:892:LEU:HA	1.94	0.49
1:A:836:THR:HG23	1:A:839:GLY:H	1.78	0.49
1:A:986:PHE:HB2	2:B:960:ILE:HD12	1.95	0.49
3:C:195:LYS:HB3	10:J:61:LEU:HD11	1.94	0.49
1:A:1348:VAL:HG11	2:B:270:LEU:HD12	1.94	0.49
2:B:731:VAL:HG21	10:J:59:LYS:HG2	1.93	0.49
1:A:1038:ILE:HD12	1:A:1185:VAL:HG21	1.94	0.49
2:B:129:ARG:HA	2:B:888:ILE:HG21	1.95	0.49
1:A:918:LYS:HE2	1:A:922:CYS:HB3	1.93	0.49
7:G:18:LYS:HA	7:G:21:LYS:HD2	1.95	0.49
13:M:109:ARG:HG3	13:M:110:GLY:H	1.77	0.49
2:B:252:TYR:HB2	2:B:381:LEU:HD21	1.94	0.48
2:B:740:LYS:HA	2:B:804:TYR:O	2.13	0.48
2:B:110:ASN:HB3	2:B:118:GLU:HG2	1.95	0.48
1:A:496:GLY:HA3	1:A:615:ARG:HB2	1.94	0.48
2:B:823:GLN:HG2	2:B:863:ASP:HB3	1.94	0.48
3:C:113:LEU:HD11	3:C:132:ILE:HD12	1.94	0.48
3:C:192:LEU:HD21	3:C:195:LYS:HE3	1.95	0.48
1:A:1196:PRO:HB2	1:A:1575:ILE:HG21	1.96	0.48
1:A:727:THR:H	1:A:730:GLN:HE21	1.61	0.48
11:K:95:HIS:HB3	11:K:98:GLU:HG2	1.96	0.48
1:A:502:ALA:HA	1:A:581:ILE:CG2	2.43	0.48
2:B:375:LEU:HA	2:B:378:ILE:HD12	1.96	0.48
7:G:47:VAL:HG21	7:G:61:VAL:HG13	1.96	0.48
2:B:700:LEU:HA	2:B:703:LEU:HD12	1.96	0.48
1:A:1610:PHE:CD2	1:A:1632:GLU:HG2	2.49	0.48
1:A:538:ASN:HA	1:A:575:LYS:HG2	1.96	0.48
2:B:103:SER:HB3	2:B:138:LEU:HB2	1.95	0.48
2:B:916:LYS:HB3	2:B:1036:LEU:HD12	1.95	0.48
11:K:57:ASP:HB2	11:K:59:THR:H	1.79	0.47
1:A:126:GLN:HB3	1:A:343:PRO:HD3	1.96	0.47
2:B:480:GLN:HE21	2:B:508:PHE:H	1.61	0.47
8:H:103:LYS:HB3	8:H:115:TYR:HB2	1.96	0.47
1:A:952:LEU:HD23	1:A:1004:GLU:HG3	1.95	0.47
6:F:128:LYS:HD2	6:F:149:GLU:HA	1.97	0.47
2:B:656:LEU:HB3	14:N:148:ILE:HG12	1.97	0.47
5:E:56:LYS:HE2	5:E:84:ASP:H	1.80	0.47
8:H:107:VAL:O	8:H:111:LEU:HB2	2.15	0.47
1:A:37:VAL:HG12	1:A:49:LEU:HB2	1.95	0.47
1:A:1634:LEU:HD13	1:A:1643:VAL:HG11	1.96	0.47
1:A:536:ILE:HD11	1:A:575:LYS:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:LEU:HA	1:A:882:ILE:HD12	1.97	0.47
2:B:362:LEU:HD22	2:B:369:ASP:HB3	1.97	0.47
5:E:4:GLU:HG2	5:E:7:ARG:HH12	1.80	0.47
1:A:438:ILE:HD12	2:B:1192:MET:HA	1.98	0.46
1:A:862:THR:OG1	1:A:878:ARG:HB3	2.15	0.46
7:G:14:ALA:HA	7:G:17:ILE:HD12	1.97	0.46
1:A:1275:THR:HG23	1:A:1289:SER:HB2	1.97	0.46
1:A:1640:ARG:HH11	1:A:1648:ASN:HB3	1.78	0.46
1:A:671:GLN:HE22	2:B:784:ASP:HB2	1.80	0.46
1:A:1038:ILE:HD11	1:A:1050:TYR:HB2	1.96	0.46
1:A:19:LEU:HG	2:B:1195:ARG:HB2	1.98	0.46
3:C:333:ILE:HG22	11:K:49:LEU:HB2	1.97	0.46
1:A:1288:ARG:HB2	1:A:1476:LEU:HB2	1.98	0.46
1:A:32:ILE:HG21	1:A:49:LEU:HD13	1.96	0.46
1:A:1112:PRO:HD2	1:A:1115:LYS:HB2	1.97	0.46
2:B:880:ALA:HB2	2:B:907:ILE:HG13	1.98	0.46
3:C:229:LEU:HD23	3:C:293:ARG:HB3	1.97	0.46
3:C:334:THR:HB	11:K:48:LYS:HG3	1.98	0.46
1:A:1263:LEU:HD22	1:A:1267:ILE:HD11	1.98	0.46
1:A:700:ILE:HD11	1:A:735:VAL:HA	1.97	0.46
2:B:721:MET:O	2:B:725:THR:HG23	2.16	0.46
1:A:986:PHE:CB	2:B:960:ILE:HD12	2.46	0.46
3:C:110:PRO:C	3:C:112:MET:H	2.20	0.45
1:A:537:GLN:HB2	1:A:578:TYR:HE1	1.81	0.45
2:B:977:ILE:HD13	14:N:163:VAL:HG21	1.99	0.45
3:C:236:LEU:HD11	3:C:290:LYS:HG3	1.98	0.45
1:A:1658:ALA:HB2	7:G:107:ILE:HD11	1.98	0.45
2:B:143:TRP:HB3	2:B:152:LEU:HB2	1.99	0.45
1:A:1032:VAL:HG21	1:A:1179:ILE:HG12	1.99	0.45
3:C:229:LEU:HD21	3:C:295:ARG:HA	1.99	0.45
2:B:1097:ASP:OD2	2:B:1181:VAL:HG22	2.17	0.45
1:A:456:VAL:HG21	2:B:1192:MET:HG3	1.99	0.45
2:B:13:THR:HG21	2:B:977:ILE:HB	1.99	0.45
2:B:65:VAL:HA	2:B:68:ILE:HG12	1.97	0.45
2:B:940:GLU:OE2	3:C:228:ARG:HB2	2.18	0.45
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.99	0.45
1:A:1261:VAL:HG11	1:A:1308:VAL:HG21	1.99	0.44
1:A:692:TYR:O	1:A:696:ILE:HG12	2.17	0.44
10:J:32:GLU:H	10:J:32:GLU:HG2	1.53	0.44
1:A:862:THR:HG21	1:A:875:LEU:HD12	1.99	0.44
9:I:27:ASN:HA	9:I:38:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:ILE:HD11	1:A:1174:TYR:CE2	2.52	0.44
7:G:30:GLU:HG2	7:G:32:ASN:HB2	1.99	0.44
1:A:1029:GLY:HA3	1:A:1041:ALA:HB2	1.99	0.44
1:A:1655:ASP:HB2	6:F:135:ARG:HB3	2.00	0.44
5:E:120:ALA:HA	5:E:123:LEU:HD12	2.01	0.43
2:B:748:GLN:HB3	10:J:52:THR:CG2	2.47	0.43
13:M:9:GLU:HA	14:N:71:PRO:HA	2.00	0.43
1:A:233:CYS:HB3	1:A:236:CYS:O	2.18	0.43
1:A:727:THR:HG21	8:H:119:GLY:O	2.18	0.43
2:B:251:HIS:HE1	2:B:261:ARG:HD2	1.84	0.43
2:B:953:ALA:O	2:B:957:ARG:HG2	2.19	0.43
5:E:141:VAL:HG12	5:E:142:VAL:HG23	2.00	0.43
1:A:657:TYR:HA	1:A:667:ARG:HG3	2.01	0.43
8:H:40:LEU:HB2	8:H:123:MET:HG3	1.99	0.43
1:A:387:SER:HA	1:A:390:LEU:HD12	2.01	0.43
2:B:403:LEU:HD21	2:B:408:LEU:HD13	2.00	0.43
1:A:385:LEU:HD13	1:A:437:PHE:HA	2.00	0.43
1:A:885:ASP:HB3	1:A:888:LYS:HB2	2.01	0.43
2:B:15:ASP:HA	2:B:978:ALA:HB3	2.00	0.43
9:I:97:HIS:HB3	9:I:111:PHE:HB2	2.01	0.43
1:A:739:VAL:HG11	1:A:812:VAL:HG21	2.00	0.43
2:B:19:LEU:HD11	10:J:26:GLN:HG2	2.00	0.43
2:B:211:ARG:HH22	2:B:243:GLN:NE2	2.16	0.43
2:B:612:LYS:HD3	2:B:626:ILE:HD11	2.01	0.42
2:B:14:ALA:HB1	2:B:755:ASN:HD21	1.84	0.42
2:B:249:VAL:HB	2:B:261:ARG:HB3	2.01	0.42
4:D:19:PRO:HG2	4:D:22:ILE:HD11	2.01	0.42
6:F:107:VAL:HG12	6:F:109:VAL:H	1.84	0.42
1:A:396:ILE:HG12	1:A:426:ALA:HB1	2.01	0.42
11:K:46:LYS:O	11:K:65:ILE:HA	2.20	0.42
1:A:827:THR:HG21	2:B:1026:ILE:HA	2.02	0.42
7:G:264:ARG:H	7:G:267:ALA:HB3	1.84	0.42
1:A:591:ARG:HB2	1:A:633:MET:HG2	2.02	0.42
1:A:966:LEU:HB2	1:A:969:PHE:HD2	1.85	0.42
2:B:936:MET:HG3	2:B:937:PRO:HD2	2.01	0.42
2:B:788:ILE:HB	2:B:948:ILE:HB	2.02	0.42
1:A:502:ALA:HA	1:A:581:ILE:HG22	2.01	0.42
2:B:190:ILE:HD11	2:B:496:PHE:HE2	1.85	0.42
1:A:1238:MET:HB2	1:A:1521:THR:HB	2.01	0.42
1:A:536:ILE:HG23	1:A:544:VAL:HB	2.02	0.42
1:A:912:VAL:HA	1:A:913:PRO:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:VAL:HG21	2:B:1040:VAL:HG23	2.02	0.42
2:B:301:PHE:O	2:B:305:ARG:HG2	2.19	0.42
4:D:30:HIS:HA	7:G:39:VAL:HG23	2.00	0.42
4:D:24:ALA:HA	7:G:43:ILE:HG22	2.02	0.42
12:L:29:TYR:HD2	12:L:39:SER:HA	1.85	0.42
11:K:60:SER:HB3	11:K:106:GLN:HG2	2.02	0.42
1:A:1014:SER:HA	1:A:1223:ARG:HH22	1.84	0.41
1:A:1053:ASP:HB2	1:A:1174:TYR:OH	2.20	0.41
1:A:1550:LEU:HD12	1:A:1555:VAL:HA	2.02	0.41
6:F:85:MET:HB2	6:F:151:LEU:HB3	2.01	0.41
9:I:52:ALA:HB3	9:I:55:ALA:HB2	2.02	0.41
1:A:7:VAL:HG21	2:B:1177:ALA:HB2	2.02	0.41
1:A:966:LEU:HD23	2:B:522:PRO:HB3	2.02	0.41
1:A:646:GLU:HB3	2:B:1084:THR:OG1	2.20	0.41
2:B:526:GLY:HA2	2:B:696:ILE:HA	2.02	0.41
2:B:600:GLN:HA	2:B:603:ILE:HD12	2.02	0.41
2:B:561:ILE:HG12	2:B:620:LEU:HD12	2.01	0.41
3:C:252:PRO:HD2	3:C:255:VAL:HG21	2.02	0.41
9:I:102:ARG:HB3	9:I:103:SER:H	1.77	0.41
1:A:990:ILE:HD12	1:A:995:TYR:HA	2.03	0.41
2:B:201:LYS:HD3	2:B:465:LEU:O	2.20	0.41
2:B:44:PRO:O	2:B:48:SER:HB2	2.20	0.41
2:B:207:ILE:HB	2:B:505:ARG:HA	2.02	0.41
1:A:1654:PHE:CE2	6:F:92:ARG:HD3	2.56	0.41
7:G:26:ASN:ND2	7:G:37:CYS:HA	2.35	0.41
8:H:93:TYR:HA	8:H:145:ARG:HG3	2.03	0.41
1:A:970:LYS:HG2	1:A:971:PRO:HD2	2.02	0.41
1:A:636:HIS:HD2	2:B:1091:ARG:HH21	1.68	0.41
3:C:187:ALA:HB1	3:C:306:GLY:HA3	2.02	0.41
5:E:6:GLU:HA	5:E:9:ILE:HD12	2.02	0.41
7:G:45:LEU:HD11	7:G:120:VAL:HG12	2.02	0.41
2:B:1079:LEU:O	2:B:1084:THR:HG22	2.21	0.41
3:C:80:ALA:HA	3:C:208:CYS:HA	2.03	0.41
1:A:124:LEU:HD21	1:A:189:VAL:HA	2.01	0.41
8:H:35:GLN:HB3	8:H:111:LEU:HD21	2.01	0.41
1:A:1229:ALA:HB2	1:A:1597:ALA:HB2	2.03	0.41
13:M:20:SER:HB3	14:N:36:LYS:HB2	2.02	0.41
1:A:1272:VAL:HG11	1:A:1485:MET:HB3	2.03	0.41
1:A:1459:LYS:HB2	1:A:1473:LYS:HB2	2.03	0.41
1:A:399:LEU:HD11	1:A:422:ARG:HB3	2.02	0.41
1:A:98:LEU:HD13	1:A:320:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:15:VAL:HG12	13:M:90:LEU:HB2	2.03	0.41
2:B:61:LEU:HD21	2:B:413:LEU:HD13	2.02	0.40
8:H:30:SER:HB3	8:H:36:CYS:HB3	2.03	0.40
1:A:1626:VAL:HG21	2:B:1194:ILE:HG12	2.03	0.40
1:A:755:ILE:HG12	1:A:930:LEU:HB3	2.03	0.40
2:B:1084:THR:HG23	2:B:1084:THR:O	2.21	0.40
3:C:65:ASN:HA	3:C:227:TYR:HE2	1.86	0.40
1:A:1613:MET:HE3	1:A:1622:LEU:HD13	2.02	0.40
1:A:857:ALA:HB2	1:A:899:LYS:HD2	2.03	0.40
2:B:218:ILE:HG12	2:B:391:PRO:HG3	2.03	0.40
11:K:109:GLY:O	11:K:110:GLU:HG2	2.21	0.40
2:B:737:SER:HA	2:B:806:THR:HG21	2.04	0.40
2:B:49:PHE:O	2:B:52:LEU:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	1466/1664 (88%)	1393 (95%)	71 (5%)	2 (0%)	55	89
2	B	1166/1203 (97%)	1094 (94%)	70 (6%)	2 (0%)	51	86
3	C	300/335 (90%)	284 (95%)	16 (5%)	0	100	100
4	D	55/137 (40%)	52 (94%)	3 (6%)	0	100	100
5	E	213/215 (99%)	202 (95%)	11 (5%)	0	100	100
6	F	98/155 (63%)	96 (98%)	2 (2%)	0	100	100
7	G	251/326 (77%)	234 (93%)	16 (6%)	1 (0%)	38	78
8	H	130/146 (89%)	119 (92%)	10 (8%)	1 (1%)	22	64
9	I	122/125 (98%)	109 (89%)	11 (9%)	2 (2%)	11	46
10	J	67/70 (96%)	62 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	101/142 (71%)	96 (95%)	5 (5%)	0	100	100
12	L	43/70 (61%)	39 (91%)	4 (9%)	0	100	100
13	M	101/415 (24%)	93 (92%)	8 (8%)	0	100	100
14	N	131/233 (56%)	123 (94%)	8 (6%)	0	100	100
All	All	4244/5236 (81%)	3996 (94%)	240 (6%)	8 (0%)	51	86

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	GLY
2	B	532	HIS
2	B	1154	ASP
1	A	1338	ARG
8	H	84	ALA
9	I	26	SER
7	G	127	PRO
9	I	90	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	1306/1465 (89%)	1234 (94%)	72 (6%)	25	63
2	B	1024/1053 (97%)	926 (90%)	98 (10%)	10	36
3	C	269/296 (91%)	244 (91%)	25 (9%)	10	38
4	D	56/116 (48%)	50 (89%)	6 (11%)	8	29
5	E	197/197 (100%)	192 (98%)	5 (2%)	53	84
6	F	90/137 (66%)	86 (96%)	4 (4%)	33	72
7	G	234/291 (80%)	219 (94%)	15 (6%)	20	57
8	H	116/128 (91%)	111 (96%)	5 (4%)	33	72
9	I	109/110 (99%)	98 (90%)	11 (10%)	9	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	64/65 (98%)	57 (89%)	7 (11%)	7	29
11	K	93/130 (72%)	84 (90%)	9 (10%)	9	35
12	L	40/57 (70%)	37 (92%)	3 (8%)	16	49
13	M	94/371 (25%)	89 (95%)	5 (5%)	26	65
14	N	128/220 (58%)	118 (92%)	10 (8%)	15	47
All	All	3820/4636 (82%)	3545 (93%)	275 (7%)	17	51

All (275) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	39	ASP
1	A	113	VAL
1	A	129	LEU
1	A	136	LEU
1	A	177	LEU
1	A	195	LYS
1	A	199	ASP
1	A	211	THR
1	A	270	ILE
1	A	274	MET
1	A	325	ASP
1	A	345	LEU
1	A	361	VAL
1	A	373	LEU
1	A	398	ASP
1	A	399	LEU
1	A	403	LEU
1	A	406	LEU
1	A	413	LEU
1	A	518	GLU
1	A	536	ILE
1	A	562	LEU
1	A	572	THR
1	A	586	VAL
1	A	587	VAL
1	A	621	THR
1	A	684	ASP
1	A	685	SER
1	A	743	ASP

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Mol	Chain	Res	Type
1	A	747	ILE
1	A	831	ASP
1	A	840	ASN
1	A	844	THR
1	A	862	THR
1	A	878	ARG
1	A	952	LEU
1	A	960	MET
1	A	1065	GLN
1	A	1089	LEU
1	A	1164	LYS
1	A	1171	GLN
1	A	1175	MET
1	A	1179	ILE
1	A	1183	GLU
1	A	1193	VAL
1	A	1202	LEU
1	A	1205	PHE
1	A	1217	LEU
1	A	1242	ILE
1	A	1248	ASP
1	A	1252	ASP
1	A	1263	LEU
1	A	1268	ASP
1	A	1273	THR
1	A	1313	LEU
1	A	1343	ASP
1	A	1474	LEU
1	A	1475	GLU
1	A	1481	GLU
1	A	1501	ILE
1	A	1502	PRO
1	A	1505	ASP
1	A	1531	ASP
1	A	1533	GLU
1	A	1550	LEU
1	A	1552	THR
1	A	1592	GLN
1	A	1609	SER
1	A	1628	ASP
1	A	1629	ASN
1	A	1649	VAL

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Mol	Chain	Res	Type
2	B	13	THR
2	B	15	ASP
2	B	17	ARG
2	B	19	LEU
2	B	22	GLU
2	B	27	ASN
2	B	35	PHE
2	B	52	LEU
2	B	54	GLU
2	B	60	LEU
2	B	73	ILE
2	B	101	GLN
2	B	108	MET
2	B	139	LEU
2	B	150	GLU
2	B	156	ARG
2	B	168	ASN
2	B	186	GLU
2	B	190	ILE
2	B	202	LEU
2	B	206	LEU
2	B	212	ASN
2	B	217	ILE
2	B	234	ILE
2	B	250	LEU
2	B	265	ARG
2	B	268	GLU
2	B	274	VAL
2	B	276	ILE
2	B	304	ASP
2	B	306	LEU
2	B	316	ARG
2	B	332	ASP
2	B	356	ARG
2	B	364	LYS
2	B	373	MET
2	B	374	LEU
2	B	381	LEU
2	B	413	LEU
2	B	431	ASP
2	B	438	ILE
2	B	441	LYS

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Mol	Chain	Res	Type
2	B	455	GLU
2	B	471	VAL
2	B	479	GLN
2	B	480	GLN
2	B	481	VAL
2	B	485	THR
2	B	519	LYS
2	B	542	LEU
2	B	550	ARG
2	B	588	ILE
2	B	617	THR
2	B	640	LEU
2	B	646	HIS
2	B	684	ASN
2	B	692	THR
2	B	721	MET
2	B	743	ARG
2	B	752	VAL
2	B	782	ASP
2	B	787	MET
2	B	789	ILE
2	B	794	ASP
2	B	821	ILE
2	B	832	TRP
2	B	835	GLU
2	B	840	LEU
2	B	842	GLU
2	B	848	ILE
2	B	859	CYS
2	B	873	THR
2	B	887	LEU
2	B	888	ILE
2	B	896	GLN
2	B	897	GLU
2	B	898	LEU
2	B	933	THR
2	B	940	GLU
2	B	944	GLN
2	B	956	SER
2	B	965	GLU
2	B	967	LEU
2	B	977	ILE

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Mol	Chain	Res	Type
2	B	994	ASP
2	B	1000	LEU
2	B	1020	GLU
2	B	1033	TYR
2	B	1037	ARG
2	B	1041	ASN
2	B	1042	ASP
2	B	1065	ARG
2	B	1076	ARG
2	B	1110	ILE
2	B	1123	ILE
2	B	1157	GLN
2	B	1181	VAL
2	B	1201	GLU
3	C	30	GLU
3	C	39	ASP
3	C	46	SER
3	C	47	LEU
3	C	81	GLU
3	C	89	THR
3	C	97	LEU
3	C	106	LEU
3	C	117	ASP
3	C	120	LEU
3	C	151	THR
3	C	181	ASP
3	C	182	CYS
3	C	188	ASP
3	C	209	ILE
3	C	224	THR
3	C	229	LEU
3	C	235	ILE
3	C	240	LYS
3	C	259	ASP
3	C	277	ARG
3	C	291	LEU
3	C	303	GLU
3	C	331	CYS
3	C	334	THR
4	D	14	THR
4	D	16	LEU
4	D	21	VAL

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Mol	Chain	Res	Type
4	D	25	THR
4	D	27	LEU
4	D	89	LEU
5	E	84	ASP
5	E	106	GLN
5	E	163	GLU
5	E	167	ARG
5	E	175	LEU
6	F	69	LEU
6	F	103	MET
6	F	111	LEU
6	F	147	SER
7	G	22	LYS
7	G	32	ASN
7	G	54	LEU
7	G	75	ASN
7	G	93	ASP
7	G	95	LEU
7	G	104	LEU
7	G	144	HIS
7	G	214	LEU
7	G	217	TRP
7	G	223	GLU
7	G	248	THR
7	G	250	ILE
7	G	303	ASP
7	G	316	GLU
8	H	33	GLN
8	H	53	ASP
8	H	89	LEU
8	H	109	LYS
8	H	136	LYS
9	I	3	VAL
9	I	17	LEU
9	I	27	ASN
9	I	47	VAL
9	I	50	THR
9	I	51	THR
9	I	53	ASP
9	I	60	LEU
9	I	99	LEU
9	I	101	LEU

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Mol	Chain	Res	Type
9	I	102	ARG
10	J	2	ILE
10	J	14	VAL
10	J	26	GLN
10	J	32	GLU
10	J	47	ARG
10	J	48	ARG
10	J	68	LYS
11	K	45	GLU
11	K	49	LEU
11	K	59	THR
11	K	60	SER
11	K	72	LEU
11	K	77	ARG
11	K	99	ASN
11	K	124	LEU
11	K	132	GLU
12	L	27	LEU
12	L	38	LEU
12	L	62	LYS
13	M	50	GLU
13	M	56	GLU
13	M	101	VAL
13	M	103	LYS
13	M	108	LEU
14	N	36	LYS
14	N	67	LEU
14	N	74	PHE
14	N	94	ASP
14	N	114	GLU
14	N	117	GLU
14	N	131	LEU
14	N	166	LEU
14	N	168	LEU
14	N	178	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	GLN
1	A	332	GLN
1	A	431	GLN

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Mol	Chain	Res	Type
1	A	432	ASN
1	A	580	HIS
1	A	590	ASN
1	A	592	GLN
1	A	636	HIS
1	A	671	GLN
1	A	693	GLN
1	A	706	HIS
1	A	730	GLN
1	A	738	ASN
1	A	798	HIS
1	A	926	GLN
1	A	1026	GLN
1	A	1036	ASN
1	A	1113	HIS
1	A	1128	ASN
1	A	1599	ASN
2	B	146	ASN
2	B	151	ASN
2	B	166	GLN
2	B	212	ASN
2	B	243	GLN
2	B	251	HIS
2	B	282	HIS
2	B	351	GLN
2	B	361	HIS
2	B	400	GLN
2	B	480	GLN
2	B	646	HIS
2	B	686	HIS
2	B	695	ASN
2	B	724	GLN
2	B	755	ASN
2	B	896	GLN
2	B	975	HIS
2	B	987	ASN
2	B	999	GLN
2	B	1041	ASN
2	B	1053	ASN
2	B	1114	GLN
3	C	130	ASN
3	C	232	GLN

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Mol	Chain	Res	Type
4	D	30	HIS
5	E	147	HIS
5	E	179	GLN
7	G	20	HIS
7	G	32	ASN
7	G	64	GLN
7	G	65	HIS
7	G	140	GLN
7	G	150	HIS
8	H	35	GLN
9	I	21	ASN
9	I	97	HIS
10	J	64	ASN
11	K	106	GLN
13	M	16	GLN
14	N	132	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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
15	SO4	A	2664	-	4,4,4	0.17	0	6,6,6	0.05	0
15	SO4	A	2665	-	4,4,4	0.17	0	6,6,6	0.08	0
18	MPD	G	1317	-	7,7,7	0.55	0	9,10,10	0.57	0
15	SO4	K	1143	-	4,4,4	0.16	0	6,6,6	0.09	0

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
15	SO4	A	2664	-	-	0/0/0/0	0/0/0/0
15	SO4	A	2665	-	-	0/0/0/0	0/0/0/0
18	MPD	G	1317	-	-	0/5/5/5	0/0/0/0
15	SO4	K	1143	-	-	0/0/0/0	0/0/0/0

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	G	1317	MPD	2	0

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1484/1664 (89%)	-0.26	6 (0%) 92 77	62, 98, 156, 225	0
2	B	1176/1203 (97%)	-0.26	3 (0%) 93 82	60, 107, 142, 176	0
3	C	304/335 (90%)	-0.26	5 (1%) 72 44	93, 122, 160, 197	0
4	D	59/137 (43%)	-0.38	0 100 100	82, 124, 147, 158	0
5	E	215/215 (100%)	-0.26	3 (1%) 75 49	78, 136, 183, 202	0
6	F	100/155 (64%)	-0.49	0 100 100	69, 86, 125, 142	0
7	G	259/326 (79%)	-0.22	1 (0%) 92 77	71, 121, 196, 231	0
8	H	134/146 (91%)	-0.18	2 (1%) 74 47	94, 123, 152, 165	0
9	I	124/125 (99%)	0.78	20 (16%) 2 1	116, 187, 215, 228	0
10	J	69/70 (98%)	-0.12	0 100 100	94, 112, 141, 161	0
11	K	103/142 (72%)	-0.53	0 100 100	82, 106, 136, 171	0
12	L	45/70 (64%)	-0.46	0 100 100	107, 128, 149, 153	0
13	M	105/415 (25%)	-0.02	1 (0%) 82 58	137, 229, 262, 267	0
14	N	139/233 (59%)	0.16	12 (8%) 11 4	111, 249, 267, 276	0
All	All	4316/5236 (82%)	-0.22	53 (1%) 79 53	60, 111, 202, 276	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	98	THR	8.2
9	I	99	LEU	7.0
9	I	118	GLY	6.9
9	I	105	ASP	6.0
9	I	87	PRO	5.1
9	I	120	LYS	5.1
9	I	103	SER	4.9
1	A	1340	THR	4.8

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Mol	Chain	Res	Type	RSRZ
14	N	113	SER	4.5
9	I	119	TYR	4.2
9	I	122	ARG	3.8
14	N	54	TRP	3.7
9	I	77	LYS	3.4
3	C	174	ARG	3.3
3	C	264	GLU	3.3
14	N	76	SER	3.3
9	I	100	GLN	3.2
9	I	97	HIS	3.2
2	B	894	LYS	3.1
2	B	830	ASP	3.1
9	I	90	GLY	3.0
8	H	75	ALA	2.8
13	M	38	PHE	2.8
14	N	33	LYS	2.8
14	N	94	ASP	2.8
1	A	375	GLU	2.7
3	C	286	ALA	2.7
9	I	75	GLU	2.7
14	N	52	GLN	2.5
14	N	116	LYS	2.5
3	C	261	GLY	2.5
2	B	895	PHE	2.5
14	N	41	ASN	2.4
1	A	1476	LEU	2.4
7	G	316	GLU	2.4
1	A	1013	THR	2.4
9	I	71	LEU	2.4
5	E	110	PHE	2.4
5	E	93	MET	2.4
14	N	38	PHE	2.3
8	H	139	ASN	2.3
14	N	112	PRO	2.3
1	A	264	ASN	2.3
5	E	167	ARG	2.3
1	A	1513	GLU	2.2
14	N	133	PHE	2.2
9	I	69	THR	2.2
9	I	88	GLN	2.1
14	N	137	PHE	2.1
3	C	270	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
9	I	41	GLN	2.1
9	I	125	ASN	2.1
9	I	106	GLU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
18	MPD	G	1317	8/8	0.86	0.37	7.53	99,101,103,104	0
16	ZN	J	1070	1/1	1.00	0.23	2.94	104,104,104,104	0
16	ZN	B	2205	1/1	1.00	0.17	0.12	79,79,79,79	0
16	ZN	L	1071	1/1	0.99	0.11	-0.15	125,125,125,125	0
16	ZN	A	2666	1/1	0.99	0.14	-0.58	108,108,108,108	0
16	ZN	A	2667	1/1	0.99	0.14	-0.64	95,95,95,95	0
16	ZN	I	1126	1/1	0.99	0.12	-0.81	138,138,138,138	0
16	ZN	I	1127	1/1	0.87	0.11	-1.75	153,153,153,153	0
15	SO4	A	2664	5/5	0.87	0.12	-	177,177,178,180	0
15	SO4	A	2665	5/5	0.86	0.20	-	166,167,168,168	0
17	MG	B	2204	1/1	0.92	0.90	-	89,89,89,89	0
15	SO4	K	1143	5/5	0.96	0.13	-	147,147,149,149	0

6.5 Other polymers [i](#)

There are no such residues in this entry.