Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 06:58 PM BST

PDB ID	:	6DVB
Title	:	Crystal structure of Mycobacterium tuberculosis transcription initiation complex(ECF sigma factor L) containing 5nt RNA with 5nt spacer
Authors	:	Lin, W.; Das, K.; Feng, Y.; Ebright, R.H.
Deposited on	:	2018-06-23
Resolution	:	3.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

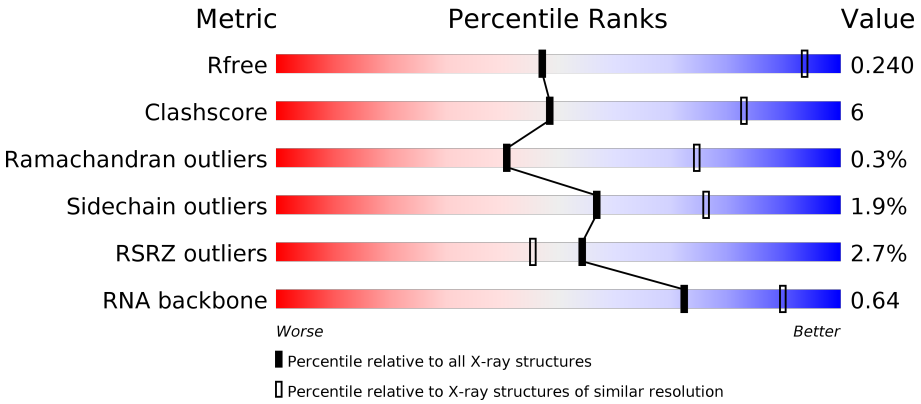
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

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 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 <=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	359	% 53% 10% 37%
1	B	359	% 51% 13% 35%
2	C	1178	% 81% 14%
3	D	1316	4% 80% 16%

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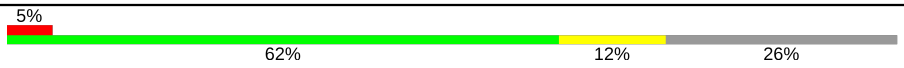
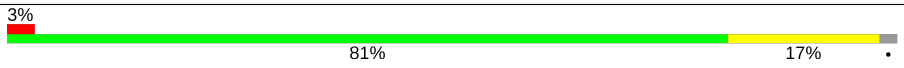
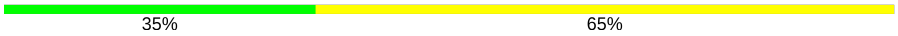
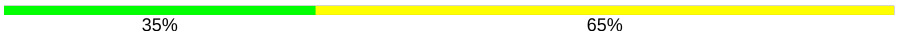
Mol	Chain	Length	Quality of chain
4	E	110	
5	F	177	
6	I	5	
7	G	17	
8	H	23	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 24975 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1716	1080	296	338	2			
1	B	232	Total	C	N	O	S	0	0	0
			1732	1093	296	341	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP P9WGZ1
A	-10	GLY	-	expression tag	UNP P9WGZ1
A	-9	HIS	-	expression tag	UNP P9WGZ1
A	-8	HIS	-	expression tag	UNP P9WGZ1
A	-7	HIS	-	expression tag	UNP P9WGZ1
A	-6	HIS	-	expression tag	UNP P9WGZ1
A	-5	HIS	-	expression tag	UNP P9WGZ1
A	-4	HIS	-	expression tag	UNP P9WGZ1
A	-3	HIS	-	expression tag	UNP P9WGZ1
A	-2	HIS	-	expression tag	UNP P9WGZ1
A	-1	HIS	-	expression tag	UNP P9WGZ1
A	0	HIS	-	expression tag	UNP P9WGZ1
B	-11	MET	-	initiating methionine	UNP P9WGZ1
B	-10	GLY	-	expression tag	UNP P9WGZ1
B	-9	HIS	-	expression tag	UNP P9WGZ1
B	-8	HIS	-	expression tag	UNP P9WGZ1
B	-7	HIS	-	expression tag	UNP P9WGZ1
B	-6	HIS	-	expression tag	UNP P9WGZ1
B	-5	HIS	-	expression tag	UNP P9WGZ1
B	-4	HIS	-	expression tag	UNP P9WGZ1
B	-3	HIS	-	expression tag	UNP P9WGZ1
B	-2	HIS	-	expression tag	UNP P9WGZ1
B	-1	HIS	-	expression tag	UNP P9WGZ1
B	0	HIS	-	expression tag	UNP P9WGZ1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1126	Total	C	N	O	S	0	0	0
			8724	5459	1531	1695	39			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1265	Total	C	N	O	S	0	0	0
			9895	6195	1794	1866	40			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	81	Total	C	N	O	0	0	0
			630	403	106	121			

- Molecule 5 is a protein called ECF RNA polymerase sigma factor SigL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	174	Total	C	N	O	S	0	0	0
			1352	840	256	254	2			

- Molecule 6 is a RNA chain called RNA (5'-R(*CP*UP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	I	5	Total	C	N	O	P	0	0	0
			102	47	18	33	4			

- Molecule 7 is a DNA chain called DNA (5'-D(*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	17	Total	C	N	O	P	0	0	0
			350	166	68	100	16			

- Molecule 8 is a DNA chain called DNA (5'-D(P*CP*GP*TP*GP*TP*CP*AP*GP*TP*AP*GP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	23	Total	C	N	O	P	0	0	0
			472	225	87	138	22			

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

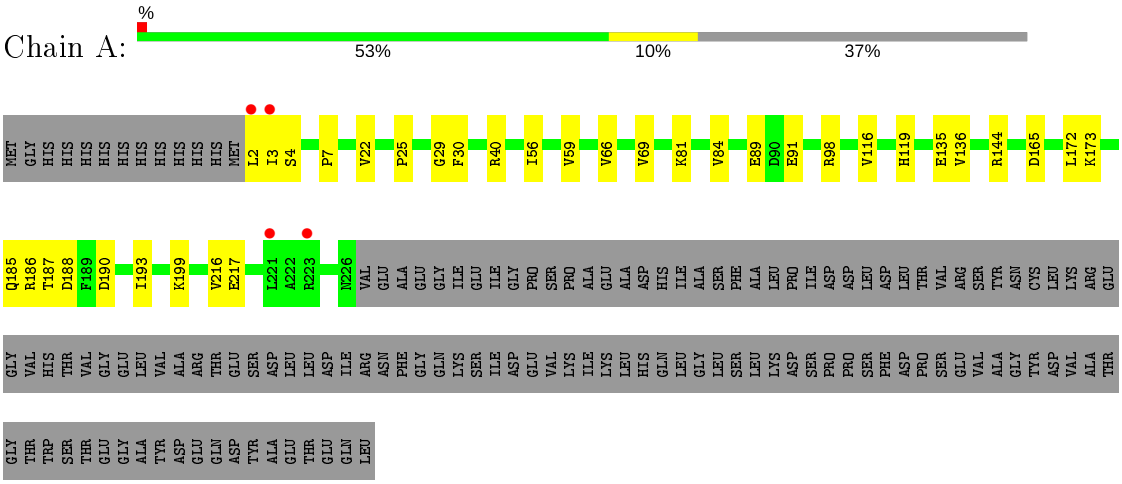
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	2	Total Zn 2 2	0	0

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.

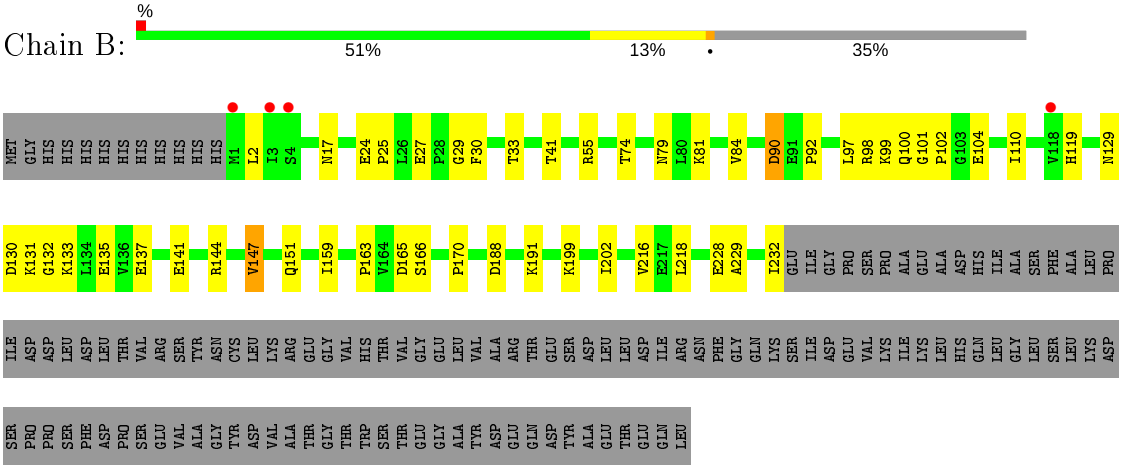
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



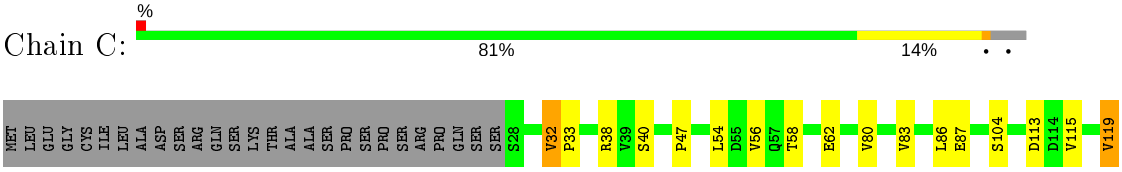
- Molecule 1: DNA-directed RNA polymerase subunit alpha

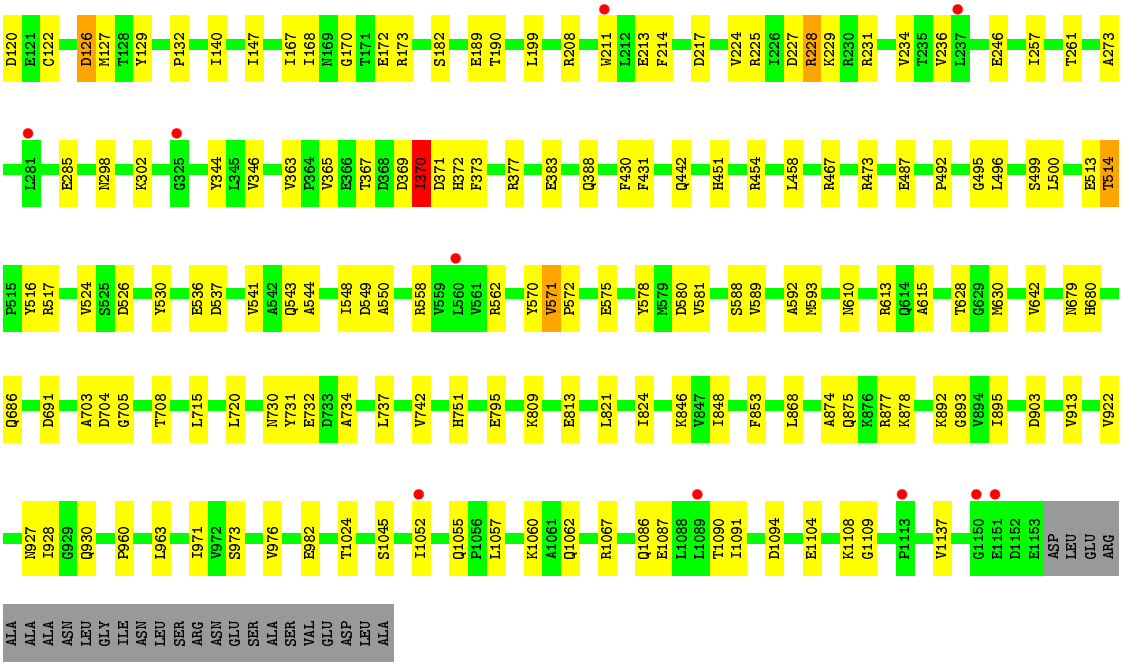
Chain B:



- Molecule 2: DNA-directed RNA polymerase subunit beta

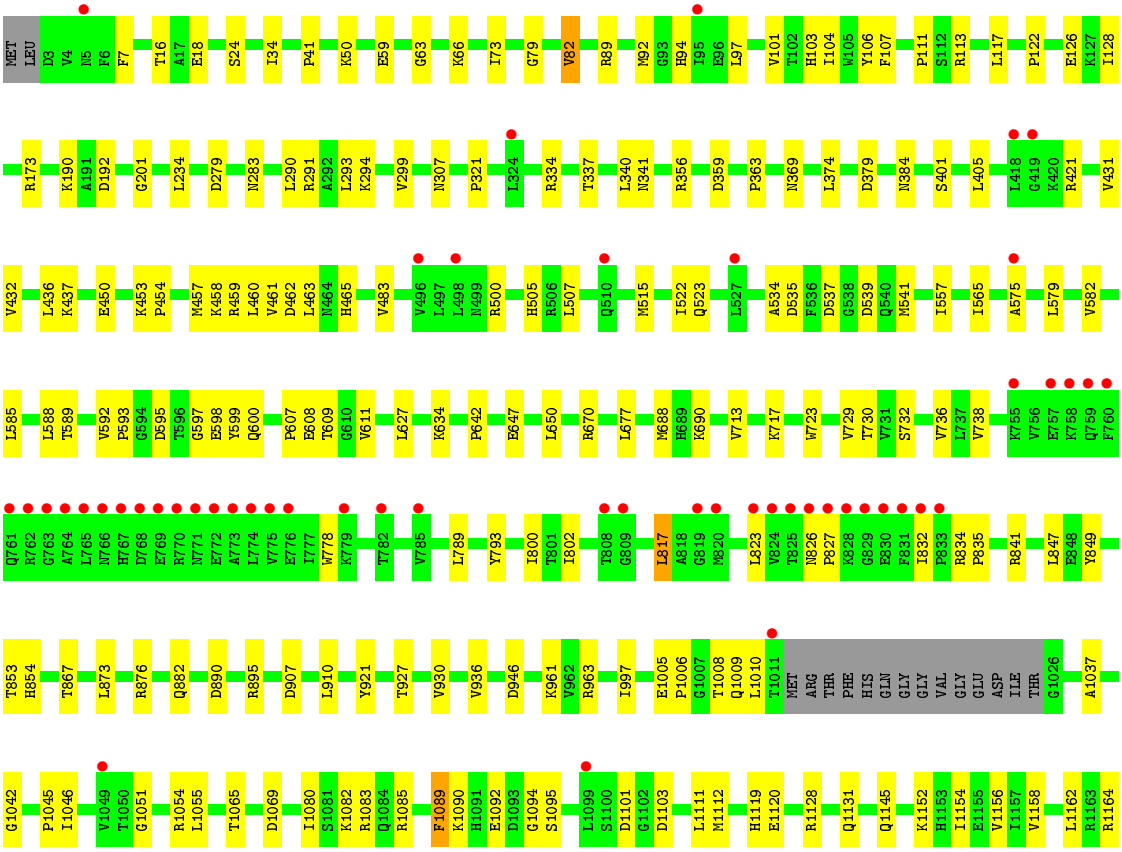
Chain C:

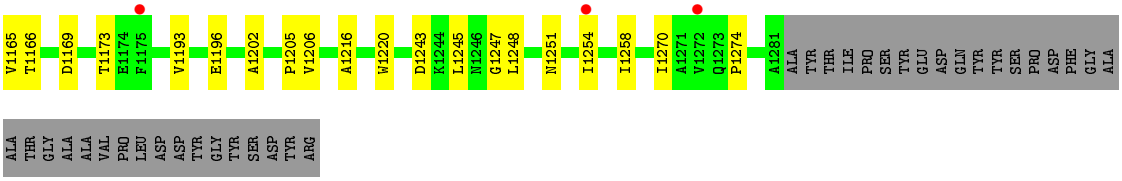




- Molecule 3: DNA-directed RNA polymerase subunit beta'

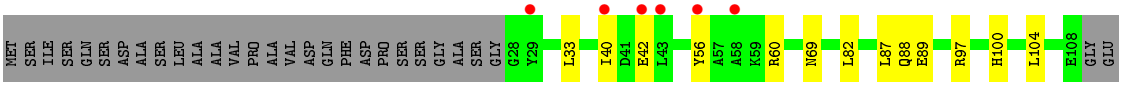
Chain D:





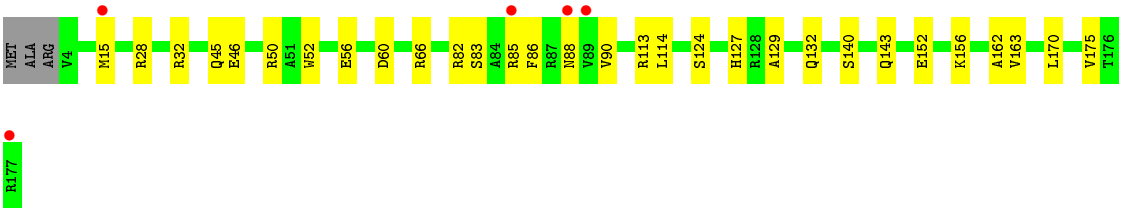
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



• Molecule 5: ECF RNA polymerase sigma factor SigL

Chain F:



• Molecule 6: RNA (5'-R(*CP*UP*CP*GP*A)-3')

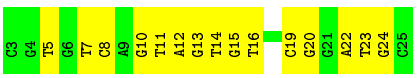
Chain I:

• Molecule 7: DNA (5'-D(*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*G)-3')

Chain G:

• Molecule 8: DNA (5'-D(P*CP*GP*TP*GP*TP*CP*AP*GP*TP*AP*GP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*C)-3')

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	143.66Å 160.58Å 240.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.25 – 3.80 97.80 – 3.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (52.25-3.80) 96.7 (97.80-3.80)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 3.78Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.202 , 0.241 0.200 , 0.240	Depositor DCC
R_{free} test set	2693 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	104.9	Xtriage
Anisotropy	0.822	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 84.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	24975	wwPDB-VP
Average B, all atoms (Å^2)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: ZN

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	0.24	0/1742	0.44	0/2370
1	B	0.24	0/1758	0.44	0/2397
2	C	0.24	0/8883	0.42	0/12043
3	D	0.23	0/10061	0.40	0/13600
4	E	0.23	0/643	0.38	0/877
5	F	0.23	0/1374	0.38	0/1869
6	I	0.13	0/113	0.69	0/174
7	G	0.51	0/393	0.88	0/606
8	H	0.53	0/529	0.96	0/816
All	All	0.25	0/25496	0.44	0/34752

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

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	1716	0	1756	26	0
1	B	1732	0	1754	31	0
2	C	8724	0	8651	109	0
3	D	9895	0	9953	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	630	0	622	11	0
5	F	1352	0	1346	20	0
6	I	102	0	56	1	0
7	G	350	0	192	9	0
8	H	472	0	261	14	0
9	D	2	0	0	0	0
All	All	24975	0	24591	296	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 (296) 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)
3:D:334:ARG:HD3	5:F:90:VAL:HG21	1.55	0.87
2:C:558:ARG:HB3	2:C:570:TYR:HB3	1.67	0.76
1:A:4:SER:HB3	1:B:144:ARG:HH12	1.50	0.76
2:C:1024:THR:H	3:D:730:THR:HG21	1.49	0.75
3:D:832:ILE:HG22	3:D:834:ARG:H	1.53	0.74
2:C:593:MET:HA	2:C:628:THR:HG21	1.69	0.74
3:D:454:PRO:HA	3:D:457:MET:HE2	1.71	0.72
3:D:827:PRO:HD3	3:D:854:HIS:HB3	1.72	0.72
3:D:1090:LYS:HE2	3:D:1103:ASP:HA	1.71	0.72
1:B:90:ASP:OD1	1:B:90:ASP:N	2.23	0.71
3:D:1055:LEU:H	3:D:1101:ASP:HB3	1.56	0.71
2:C:541:VAL:HG12	2:C:578:TYR:HB2	1.73	0.70
1:B:84:VAL:HG12	1:B:199:LYS:HD2	1.73	0.70
1:B:81:LYS:HD3	1:B:165:ASP:HB2	1.73	0.69
3:D:337:THR:OG1	3:D:341:ASN:ND2	2.26	0.68
3:D:1090:LYS:HB3	3:D:1092:GLU:HG2	1.75	0.67
3:D:363:PRO:HG2	5:F:15:MET:HG3	1.77	0.67
3:D:1248:LEU:HD22	3:D:1258:ILE:HB	1.77	0.66
2:C:458:LEU:HD21	2:C:496:LEU:HD13	1.78	0.66
5:F:50:ARG:NH1	8:H:5:DT:O4	2.30	0.65
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.28	0.64
1:B:100:GLN:HG3	1:B:133:LYS:HB2	1.78	0.64
2:C:285:GLU:OE1	8:H:10:DG:N2	2.30	0.64
3:D:1173:THR:HG22	3:D:1193:VAL:HG21	1.79	0.64
2:C:1104:GLU:OE1	5:F:113:ARG:NH1	2.32	0.63
2:C:47:PRO:HG2	2:C:581:VAL:HG13	1.79	0.62
3:D:882:GLN:HG3	3:D:997:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:GLU:HB2	1:B:191:LYS:HG3	1.80	0.62
2:C:113:ASP:HB3	2:C:132:PRO:HG2	1.80	0.62
3:D:1045:PRO:HG2	3:D:1111:LEU:HB2	1.81	0.62
7:G:11:DT:H2'	7:G:12:DG:C8	2.35	0.61
1:A:186:ARG:HG3	1:A:187:THR:HG23	1.83	0.61
2:C:536:GLU:OE2	2:C:562:ARG:NH2	2.33	0.61
2:C:104:SER:HB3	2:C:140:ILE:HB	1.83	0.60
3:D:50:LYS:HE2	3:D:79:GLY:HA3	1.82	0.60
2:C:371:ASP:OD1	8:H:15:DG:N2	2.31	0.60
2:C:372:HIS:NE2	2:C:537:ASP:OD2	2.35	0.60
3:D:356:ARG:NH2	5:F:46:GLU:OE2	2.34	0.59
2:C:234:VAL:HG12	2:C:261:THR:HG21	1.84	0.59
1:A:22:VAL:HG12	1:A:193:ILE:HG12	1.83	0.59
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.36	0.59
3:D:1051:GLY:HA2	3:D:1069:ASP:HB2	1.83	0.59
2:C:628:THR:HG23	2:C:630:MET:H	1.68	0.58
2:C:928:ILE:HD11	3:D:817:LEU:HD11	1.84	0.58
5:F:124:SER:OG	5:F:127:HIS:ND1	2.33	0.58
1:A:56:ILE:HG12	1:A:136:VAL:HG22	1.85	0.58
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.86	0.58
3:D:1085:ARG:HA	3:D:1112:MET:HA	1.86	0.58
2:C:213:GLU:OE1	2:C:225:ARG:NH1	2.36	0.58
3:D:460:LEU:HD11	3:D:483:VAL:HG12	1.86	0.58
2:C:83:VAL:HG13	2:C:87:GLU:HB2	1.86	0.57
3:D:793:TYR:HB3	3:D:800:ILE:HG13	1.87	0.57
1:B:92:PRO:HB3	1:B:141:GLU:HG2	1.87	0.57
2:C:454:ARG:HH12	2:C:487:GLU:HG2	1.70	0.57
3:D:291:ARG:NH2	8:H:24:DG:O6	2.37	0.56
3:D:1092:GLU:HG3	3:D:1094:GLY:H	1.70	0.56
1:A:40:ARG:NH1	1:B:29:GLY:O	2.39	0.56
1:A:144:ARG:NH2	1:B:27:GLU:OE2	2.39	0.56
2:C:571:VAL:HG22	2:C:572:PRO:HD2	1.88	0.55
3:D:1131:GLN:HE21	3:D:1162:LEU:HD12	1.72	0.55
2:C:217:ASP:OD2	2:C:231:ARG:NH2	2.40	0.54
3:D:34:ILE:HA	3:D:41:PRO:HA	1.88	0.54
3:D:436:LEU:HD11	3:D:523:GLN:HB3	1.89	0.54
3:D:1169:ASP:H	3:D:1202:ALA:HB3	1.72	0.54
2:C:285:GLU:OE2	8:H:10:DG:N1	2.40	0.54
1:B:129:ASN:OD1	1:B:130:ASP:N	2.39	0.54
1:B:102:PRO:HB3	1:B:130:ASP:HA	1.90	0.54
1:B:228:GLU:HG2	1:B:229:ALA:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:473:ARG:NH2	2:C:492:PRO:O	2.40	0.54
1:A:89:GLU:HB3	1:A:91:GLU:HG2	1.90	0.54
2:C:182:SER:HB2	2:C:377:ARG:HB2	1.89	0.54
3:D:173:ARG:HH21	3:D:201:GLY:HA2	1.73	0.54
3:D:1042:GLY:O	3:D:1083:ARG:NH2	2.39	0.53
3:D:1045:PRO:HB2	3:D:1111:LEU:HD12	1.90	0.53
2:C:1087:GLU:HG3	2:C:1091:ILE:HD11	1.90	0.53
2:C:960:PRO:HD2	2:C:963:LEU:HD22	1.89	0.53
7:G:12:DG:H2'	7:G:13:DA:C8	2.43	0.53
3:D:611:VAL:HG22	3:D:634:LYS:HB2	1.90	0.53
2:C:848:ILE:HD13	2:C:874:ALA:HB2	1.91	0.53
3:D:1165:VAL:HG12	3:D:1205:PRO:HA	1.91	0.53
3:D:789:LEU:HD22	3:D:793:TYR:HE2	1.73	0.53
1:B:99:LYS:NZ	1:B:104:GLU:O	2.37	0.53
2:C:32:VAL:HG13	2:C:33:PRO:HD3	1.90	0.53
2:C:731:TYR:HB3	3:D:432:VAL:HG21	1.90	0.53
1:A:56:ILE:HB	1:A:59:VAL:HG22	1.90	0.53
1:B:102:PRO:HD3	1:B:131:LYS:H	1.73	0.52
2:C:190:THR:HG23	2:C:199:LEU:HB2	1.91	0.52
3:D:1270:ILE:HD13	4:E:56:TYR:HE2	1.74	0.52
2:C:524:VAL:HG21	2:C:548:ILE:HD13	1.91	0.52
3:D:778:TRP:CD2	3:D:835:PRO:HG3	2.45	0.52
2:C:592:ALA:HA	2:C:976:VAL:HG21	1.92	0.52
2:C:168:ILE:HB	2:C:173:ARG:HD2	1.92	0.52
2:C:824:ILE:HA	5:F:163:VAL:HG13	1.91	0.52
3:D:500:ARG:HD2	3:D:534:ALA:HB2	1.92	0.52
3:D:867:THR:HG22	3:D:1008:THR:HG23	1.91	0.52
4:E:42:GLU:OE1	4:E:100:HIS:NE2	2.36	0.52
3:D:369:ASN:ND2	5:F:45:GLN:OE1	2.39	0.52
7:G:14:DG:H8	7:G:14:DG:H5'	1.75	0.52
7:G:20:DG:H5"	7:G:20:DG:H8	1.75	0.52
2:C:451:HIS:HA	2:C:454:ARG:HG2	1.91	0.51
3:D:1220:TRP:CD1	3:D:1243:ASP:HB2	2.45	0.51
2:C:257:ILE:HD11	2:C:346:VAL:HG23	1.91	0.51
3:D:826:ASN:HB3	3:D:832:ILE:HD11	1.92	0.51
1:A:216:VAL:HG13	1:B:216:VAL:HG13	1.92	0.51
2:C:610:ASN:OD1	2:C:613:ARG:NH1	2.43	0.51
1:B:84:VAL:HG23	1:B:119:HIS:HB2	1.92	0.50
3:D:437:LYS:HG3	4:E:33:LEU:HD11	1.94	0.50
5:F:124:SER:HG	5:F:127:HIS:HD1	1.59	0.50
3:D:589:THR:HG22	3:D:670:ARG:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:505:HIS:CD2	3:D:507:LEU:HB2	2.47	0.50
1:A:7:PRO:HA	1:A:25:PRO:HD2	1.93	0.50
3:D:895:ARG:HD2	3:D:1128:ARG:HH22	1.77	0.50
3:D:500:ARG:NH2	6:I:7:A:O2'	2.44	0.49
1:B:17:ASN:OD1	1:B:17:ASN:N	2.43	0.49
3:D:600:GLN:HB2	3:D:609:THR:HB	1.93	0.49
3:D:729:VAL:HG11	3:D:802:ILE:HD11	1.95	0.49
2:C:1086:GLN:O	2:C:1090:THR:OG1	2.27	0.49
2:C:377:ARG:NH2	2:C:383:GLU:OE1	2.41	0.49
2:C:549:ASP:OD1	2:C:550:ALA:N	2.46	0.49
2:C:751:HIS:CD2	2:C:877:ARG:HD2	2.48	0.49
2:C:853:PHE:HD2	2:C:868:LEU:HD23	1.77	0.49
3:D:585:LEU:O	3:D:589:THR:OG1	2.30	0.49
3:D:384:ASN:H	3:D:401:SER:HB3	1.78	0.49
2:C:298:ASN:HA	2:C:302:LYS:HB2	1.95	0.49
2:C:704:ASP:HB2	2:C:708:THR:HB	1.94	0.49
7:G:5:DC:H2"	7:G:6:DA:C8	2.48	0.48
2:C:442:GLN:HB2	2:C:679:ASN:HB2	1.95	0.48
2:C:795:GLU:HG2	2:C:846:LYS:HG2	1.94	0.48
1:B:97:LEU:HB2	1:B:110:ILE:HG13	1.94	0.48
3:D:122:PRO:HG2	8:H:23:DT:H3'	1.96	0.48
3:D:458:LYS:NZ	3:D:462:ASP:OD2	2.44	0.48
4:E:89:GLU:OE2	4:E:97:ARG:NH1	2.47	0.48
1:B:55:ARG:NH2	1:B:137:GLU:OE1	2.45	0.48
2:C:32:VAL:H	2:C:33:PRO:HD3	1.78	0.48
3:D:1166:THR:HB	3:D:1206:VAL:HG21	1.96	0.48
1:B:170:PRO:HB2	1:B:202:ILE:HD11	1.96	0.48
2:C:454:ARG:HH11	2:C:499:SER:HB2	1.79	0.48
2:C:1052:ILE:O	3:D:89:ARG:NH1	2.47	0.48
2:C:544:ALA:HB2	2:C:580:ASP:HB2	1.96	0.48
2:C:892:LYS:HG3	3:D:537:ASP:HB2	1.95	0.48
1:B:147:VAL:HG13	1:B:166:SER:HB2	1.95	0.48
2:C:227:ASP:OD1	8:H:13:DG:N2	2.45	0.48
2:C:168:ILE:HG12	2:C:431:PHE:HB3	1.96	0.48
3:D:565:ILE:HG23	3:D:575:ALA:HB3	1.96	0.48
3:D:103:HIS:HB3	3:D:106:TYR:HD2	1.78	0.47
3:D:107:PHE:HZ	3:D:126:GLU:HG2	1.79	0.47
2:C:229:LYS:NZ	8:H:11:DT:O4	2.40	0.47
2:C:1060:LYS:N	7:G:18:DA:OP1	2.47	0.47
2:C:120:ASP:N	2:C:120:ASP:OD1	2.47	0.47
2:C:514:THR:HG23	2:C:516:TYR:HE2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:GLU:HG2	1:B:232:ILE:HD12	1.97	0.47
2:C:140:ILE:HA	2:C:147:ILE:HG12	1.95	0.47
2:C:731:TYR:HE1	3:D:579:LEU:HB2	1.79	0.47
3:D:907:ASP:N	3:D:907:ASP:OD1	2.43	0.47
3:D:557:ILE:HG23	4:E:40:ILE:HD11	1.95	0.47
3:D:789:LEU:HD22	3:D:793:TYR:CE2	2.50	0.47
1:A:188:ASP:OD2	1:B:151:GLN:NE2	2.38	0.47
1:A:30:PHE:HE1	1:B:41:THR:HA	1.78	0.47
3:D:128:ILE:HD11	3:D:234:LEU:HD11	1.96	0.47
2:C:686:GLN:HA	2:C:705:GLY:HA2	1.96	0.47
2:C:369:ASP:O	2:C:370:ILE:HG12	2.14	0.47
3:D:340:LEU:HD11	3:D:405:LEU:HD11	1.96	0.47
8:H:11:DT:H2'	8:H:12:DA:C8	2.49	0.47
2:C:642:VAL:HB	2:C:703:ALA:HB3	1.96	0.47
3:D:59:GLU:HG2	3:D:66:LYS:HD3	1.97	0.47
1:B:101:GLY:N	1:B:132:GLY:O	2.47	0.46
3:D:290:LEU:HA	3:D:293:LEU:HD12	1.97	0.46
2:C:369:ASP:C	2:C:371:ASP:H	2.18	0.46
5:F:129:ALA:HA	5:F:132:GLN:HG2	1.98	0.46
1:A:40:ARG:HB3	1:A:40:ARG:HE	1.60	0.46
3:D:92:MET:SD	3:D:321:PRO:HD3	2.56	0.46
7:G:14:DG:H2'	7:G:15:DT:C6	2.50	0.46
2:C:513:GLU:HB3	2:C:530:TYR:HB3	1.97	0.46
3:D:834:ARG:HD2	3:D:835:PRO:HD2	1.98	0.46
1:A:98:ARG:HG3	1:A:135:GLU:HG3	1.98	0.46
1:A:3:ILE:HA	1:A:3:ILE:HD12	1.85	0.46
3:D:1089:PHE:HA	3:D:1095:SER:HA	1.98	0.46
2:C:473:ARG:HB3	2:C:495:GLY:HA3	1.98	0.45
3:D:117:LEU:HD12	3:D:299:VAL:HG22	1.98	0.45
2:C:189:GLU:HB2	2:C:367:THR:HG21	1.98	0.45
3:D:1046:ILE:HD11	3:D:1120:GLU:HB3	1.98	0.45
3:D:294:LYS:NZ	8:H:22:DA:O5'	2.50	0.45
3:D:1274:PRO:HB3	4:E:82:LEU:HD11	1.98	0.45
2:C:228:ARG:O	2:C:228:ARG:HG3	2.15	0.45
2:C:742:VAL:HG13	2:C:878:LYS:HD3	1.99	0.45
3:D:111:PRO:O	3:D:113:ARG:NH1	2.47	0.45
3:D:16:THR:HG22	3:D:18:GLU:H	1.81	0.45
2:C:38:ARG:HA	2:C:971:ILE:HG13	1.99	0.45
3:D:1247:GLY:H	3:D:1251:ASN:ND2	2.15	0.45
3:D:63:GLY:HA2	3:D:66:LYS:HE2	1.99	0.45
5:F:152:GLU:HG3	5:F:156:LYS:HE3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ARG:NE	1:B:33:THR:HG22	2.31	0.45
2:C:388:GLN:HG3	2:C:430:PHE:HB2	1.99	0.45
2:C:927:ASN:O	2:C:930:GLN:HG2	2.16	0.45
3:D:190:LYS:HE3	3:D:192:ASP:HB3	1.99	0.45
3:D:717:LYS:HE2	3:D:717:LYS:HB3	1.84	0.45
3:D:890:ASP:OD1	3:D:963:ARG:NH2	2.37	0.45
5:F:170:LEU:HD22	5:F:175:VAL:HG21	1.98	0.45
2:C:467:ARG:NE	8:H:16:DT:OP2	2.49	0.45
2:C:40:SER:HA	2:C:973:SER:HB2	1.99	0.44
1:A:81:LYS:NZ	1:A:165:ASP:HB2	2.32	0.44
3:D:736:VAL:HG13	3:D:817:LEU:HD23	1.99	0.44
1:B:30:PHE:HA	1:B:33:THR:HG23	2.00	0.44
2:C:730:ASN:HA	2:C:734:ALA:HB3	1.99	0.44
3:D:453:LYS:O	3:D:457:MET:HG3	2.17	0.44
1:B:98:ARG:HG2	1:B:135:GLU:HG2	2.00	0.44
2:C:236:VAL:HG13	2:C:273:ALA:HB1	1.99	0.44
2:C:56:VAL:HG21	2:C:500:LEU:HD22	1.99	0.44
2:C:1045:SER:HB3	3:D:450:GLU:O	2.18	0.44
4:E:33:LEU:H	4:E:33:LEU:HD23	1.83	0.44
2:C:543:GLN:HG3	3:D:847:LEU:HD13	1.98	0.44
2:C:809:LYS:HE2	2:C:813:GLU:HB2	1.99	0.44
3:D:642:PRO:HG2	3:D:647:GLU:HB2	2.00	0.44
5:F:140:SER:HB3	5:F:143:GLN:HG3	1.99	0.44
1:A:185:GLN:HG2	1:A:186:ARG:H	1.83	0.44
2:C:720:LEU:HD23	2:C:913:VAL:HA	1.99	0.44
2:C:893:GLY:HA2	3:D:537:ASP:HA	2.00	0.44
3:D:1245:LEU:HD13	3:D:1254:ILE:HD13	1.99	0.44
5:F:88:ASN:O	5:F:90:VAL:N	2.51	0.44
2:C:172:GLU:OE1	2:C:442:GLN:NE2	2.51	0.43
3:D:1152:LYS:O	3:D:1156:VAL:HG23	2.18	0.43
2:C:211:TRP:CZ3	8:H:14:DT:H2'	2.53	0.43
2:C:615:ALA:HB3	2:C:715:LEU:HD22	2.00	0.43
8:H:7:DT:H2"	8:H:8:DC:OP1	2.17	0.43
3:D:823:LEU:HD23	3:D:835:PRO:HB3	2.01	0.43
2:C:119:VAL:HG23	2:C:167:ILE:HD11	2.01	0.43
3:D:290:LEU:HD23	3:D:293:LEU:HD12	2.01	0.43
3:D:873:LEU:HA	3:D:876:ARG:HE	1.84	0.43
2:C:517:ARG:NH2	2:C:526:ASP:OD1	2.51	0.43
3:D:1010:LEU:HD23	3:D:1145:GLN:HG3	2.00	0.43
3:D:24:SER:HB2	3:D:94:HIS:HB3	2.01	0.43
2:C:982:GLU:HG3	3:D:841:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:32:VAL:H	2:C:33:PRO:CD	2.32	0.43
3:D:1101:ASP:OD1	3:D:1101:ASP:N	2.52	0.43
3:D:1080:ILE:HG22	3:D:1082:LYS:H	1.83	0.43
3:D:1131:GLN:HG2	3:D:1158:VAL:HG12	2.01	0.43
1:B:74:THR:HG21	3:D:608:GLU:HB2	2.01	0.42
1:A:84:VAL:HG13	1:A:119:HIS:HB2	2.01	0.42
1:A:144:ARG:HH12	1:B:2:LEU:HB2	1.84	0.42
3:D:431:VAL:N	3:D:522:ILE:O	2.47	0.42
3:D:592:VAL:HB	3:D:595:ASP:HB2	2.01	0.42
3:D:463:LEU:HB2	3:D:465:HIS:HD2	1.84	0.42
3:D:598:GLU:HG2	3:D:599:TYR:H	1.83	0.42
1:A:29:GLY:N	1:A:190:ASP:OD2	2.48	0.42
1:A:40:ARG:NH2	2:C:903:ASP:OD1	2.53	0.42
3:D:582:VAL:HG21	3:D:690:LYS:HB2	2.02	0.42
3:D:363:PRO:HD3	5:F:52:TRP:CE2	2.54	0.42
2:C:1067:ARG:NH1	7:G:16:DC:OP1	2.52	0.42
2:C:115:VAL:HG11	2:C:129:TYR:CZ	2.55	0.42
2:C:731:TYR:CE1	3:D:579:LEU:HB2	2.54	0.42
3:D:930:VAL:HG22	3:D:936:VAL:HG12	2.01	0.42
3:D:73:ILE:O	3:D:82:VAL:HG22	2.20	0.42
3:D:921:TYR:HE1	3:D:946:ASP:HA	1.84	0.42
5:F:170:LEU:HD13	5:F:175:VAL:HG11	2.00	0.42
4:E:87:LEU:HG	4:E:88:GLN:HG3	2.01	0.42
2:C:1108:LYS:HE3	5:F:114:LEU:HD22	2.01	0.42
3:D:1154:ILE:O	3:D:1158:VAL:HG23	2.20	0.42
5:F:127:HIS:HB3	5:F:162:ALA:HB2	2.02	0.42
1:B:24:GLU:HA	1:B:25:PRO:HA	1.75	0.41
2:C:1109:GLY:O	4:E:69:ASN:ND2	2.50	0.41
3:D:589:THR:HG21	3:D:688:MET:HG2	2.01	0.41
5:F:28:ARG:O	5:F:32:ARG:HG3	2.19	0.41
2:C:58:THR:O	2:C:62:GLU:HG3	2.20	0.41
3:D:849:TYR:O	3:D:853:THR:HG23	2.19	0.41
3:D:927:THR:HB	3:D:961:LYS:HB3	2.02	0.41
7:G:18:DA:H2'	7:G:19:DG:C8	2.54	0.41
2:C:122:CYS:HA	2:C:127:MET:HG3	2.03	0.41
2:C:454:ARG:NH1	2:C:499:SER:HB2	2.34	0.41
2:C:572:PRO:HG2	2:C:575:GLU:HB2	2.02	0.41
1:A:66:VAL:O	1:A:69:VAL:HG22	2.20	0.41
2:C:1055:GLN:HG2	2:C:1094:ASP:HB3	2.02	0.41
2:C:344:TYR:CZ	2:C:365:VAL:HA	2.55	0.41
2:C:442:GLN:H	2:C:680:HIS:CD2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:737:LEU:HG	2:C:895:ILE:HD12	2.02	0.41
3:D:1037:ALA:O	3:D:1119:HIS:NE2	2.54	0.41
2:C:588:SER:OG	2:C:589:VAL:N	2.54	0.41
2:C:821:LEU:HA	2:C:824:ILE:HG12	2.01	0.41
2:C:86:LEU:HA	2:C:86:LEU:HD23	1.91	0.41
4:E:60:ARG:HG2	4:E:104:LEU:HD11	2.01	0.41
1:A:173:LYS:HE3	1:A:173:LYS:HB2	1.83	0.41
3:D:1054:ARG:HD3	3:D:1065:THR:HB	2.03	0.41
3:D:431:VAL:O	3:D:523:GLN:HA	2.20	0.41
3:D:588:LEU:HD23	3:D:723:TRP:CD1	2.56	0.41
3:D:97:LEU:HD22	3:D:374:LEU:HD21	2.03	0.40
2:C:126:ASP:HA	2:C:170:GLY:HA3	2.02	0.40
2:C:214:PHE:CD1	2:C:224:VAL:HB	2.57	0.40
3:D:597:GLY:HA3	3:D:627:LEU:HA	2.03	0.40
3:D:575:ALA:O	3:D:713:VAL:HG21	2.22	0.40
2:C:1024:THR:OG1	3:D:732:SER:HB2	2.21	0.40
5:F:82:ARG:HB3	5:F:83:SER:H	1.69	0.40
1:A:172:LEU:HB2	1:A:199:LYS:HG2	2.03	0.40
3:D:500:ARG:HB2	3:D:541:MET:HG2	2.02	0.40
2:C:1067:ARG:HA	3:D:421:ARG:HA	2.04	0.40
3:D:1005:GLU:HB3	3:D:1006:PRO:HD3	2.04	0.40
8:H:19:DC:H2"	8:H:20:DG:C8	2.56	0.40
3:D:1270:ILE:HG21	4:E:56:TYR:CE2	2.57	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	223/359 (62%)	217 (97%)	6 (3%)	0	100	100
1	B	230/359 (64%)	212 (92%)	17 (7%)	1 (0%)	34	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	C	1124/1178 (95%)	1074 (96%)	46 (4%)	4 (0%)	34 70
3	D	1261/1316 (96%)	1200 (95%)	58 (5%)	3 (0%)	47 79
4	E	79/110 (72%)	76 (96%)	3 (4%)	0	100 100
5	F	172/177 (97%)	168 (98%)	4 (2%)	0	100 100
All	All	3089/3499 (88%)	2947 (95%)	134 (4%)	8 (0%)	41 74

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	159	ILE
2	C	370	ILE
2	C	732	GLU
3	D	1089	PHE
3	D	593	PRO
2	C	32	VAL
2	C	922	VAL
3	D	607	PRO

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	194/308 (63%)	192 (99%)	2 (1%)	76 86
1	B	191/308 (62%)	185 (97%)	6 (3%)	40 65
2	C	950/998 (95%)	933 (98%)	17 (2%)	59 77
3	D	1050/1095 (96%)	1031 (98%)	19 (2%)	59 77
4	E	66/90 (73%)	66 (100%)	0	100 100
5	F	134/136 (98%)	129 (96%)	5 (4%)	34 62
All	All	2585/2935 (88%)	2536 (98%)	49 (2%)	57 76

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	116	VAL
1	B	79	ASN
1	B	90	ASP
1	B	147	VAL
1	B	163	PRO
1	B	188	ASP
1	B	218	LEU
2	C	54	LEU
2	C	80	VAL
2	C	119	VAL
2	C	126	ASP
2	C	208	ARG
2	C	228	ARG
2	C	246	GLU
2	C	363	VAL
2	C	370	ILE
2	C	373	PHE
2	C	514	THR
2	C	571	VAL
2	C	691	ASP
2	C	875	GLN
2	C	1057	LEU
2	C	1062	GLN
2	C	1137	VAL
3	D	7	PHE
3	D	82	VAL
3	D	101	VAL
3	D	279	ASP
3	D	283	ASN
3	D	307	ASN
3	D	359	ASP
3	D	459	ARG
3	D	461	VAL
3	D	515	MET
3	D	535	ASP
3	D	539	ASP
3	D	650	LEU
3	D	677	LEU
3	D	738	VAL
3	D	817	LEU
3	D	910	LEU
3	D	1009	GLN

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Mol	Chain	Res	Type
3	D	1196	GLU
5	F	56	GLU
5	F	60	ASP
5	F	66	ARG
5	F	85	ARG
5	F	86	PHE

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

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	I	4/5 (80%)	0	0

There are no RNA backbone outliers to report.

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 2 ligands modelled in this entry, 2 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^{th} 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	225/359 (62%)	0.07	4 (1%) 68 61	68, 100, 163, 181	0
1	B	232/359 (64%)	0.21	4 (1%) 70 62	79, 122, 175, 204	0
2	C	1126/1178 (95%)	0.08	10 (0%) 84 79	67, 113, 189, 225	0
3	D	1265/1316 (96%)	0.25	55 (4%) 35 30	61, 119, 219, 257	0
4	E	81/110 (73%)	0.61	6 (7%) 14 11	106, 137, 188, 214	0
5	F	174/177 (98%)	0.06	5 (2%) 51 42	90, 134, 196, 232	0
6	I	5/5 (100%)	0.10	0 100 100	100, 101, 123, 140	0
7	G	17/17 (100%)	-0.29	0 100 100	100, 127, 184, 192	0
8	H	23/23 (100%)	0.02	0 100 100	134, 180, 237, 242	0
All	All	3148/3544 (88%)	0.17	84 (2%) 54 45	61, 118, 204, 257	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	825	THR	9.3
3	D	771	ASN	7.3
3	D	830	GLU	6.1
2	C	1150	GLY	5.4
3	D	761	GLN	5.0
5	F	177	ARG	4.4
3	D	829	GLY	4.4
3	D	820	MET	4.4
3	D	826	ASN	4.4
3	D	828	LYS	4.0
3	D	769	GLU	4.0
3	D	770	ARG	4.0
2	C	1151	GLU	4.0
3	D	764	ALA	3.8
3	D	809	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
3	D	773	ALA	3.6
3	D	1175	PHE	3.6
3	D	767	HIS	3.5
3	D	772	GLU	3.3
3	D	833	PRO	3.2
1	B	1	MET	3.2
3	D	765	LEU	3.1
3	D	824	VAL	3.0
3	D	760	PHE	3.0
3	D	832	ILE	3.0
3	D	763	GLY	3.0
3	D	827	PRO	3.0
3	D	1099	LEU	3.0
3	D	774	LEU	2.9
3	D	755	LYS	2.9
3	D	5	ASN	2.9
4	E	43	LEU	2.9
2	C	211	TRP	2.8
1	A	221	LEU	2.8
3	D	776	GLU	2.8
5	F	89	VAL	2.8
3	D	418	LEU	2.8
3	D	759	GLN	2.7
3	D	775	VAL	2.6
3	D	782	THR	2.6
4	E	56	TYR	2.6
3	D	766	ASN	2.5
1	A	2	LEU	2.5
3	D	757	GLU	2.5
5	F	88	ASN	2.5
1	A	223	ARG	2.5
1	A	3	ILE	2.5
2	C	237	LEU	2.4
3	D	831	PHE	2.4
3	D	510	GLN	2.4
3	D	498	LEU	2.4
3	D	819	GLY	2.4
3	D	1049	VAL	2.3
4	E	29	TYR	2.3
4	E	40	ILE	2.3
3	D	1011	THR	2.3
5	F	85	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	527	LEU	2.3
3	D	779	LYS	2.3
1	B	3	ILE	2.3
3	D	762	ARG	2.3
1	B	4	SER	2.2
3	D	823	LEU	2.2
4	E	58	ALA	2.2
3	D	808	THR	2.2
2	C	560	LEU	2.2
3	D	1254	ILE	2.2
4	E	42	GLU	2.1
3	D	324	LEU	2.1
3	D	768	ASP	2.1
3	D	575	ALA	2.1
1	B	118	VAL	2.1
2	C	1052	ILE	2.1
3	D	95	ILE	2.1
3	D	1272	VAL	2.1
3	D	785	VAL	2.1
2	C	1089	LEU	2.1
3	D	419	GLY	2.1
3	D	496	VAL	2.1
2	C	1113	PRO	2.0
2	C	281	LEU	2.0
3	D	758	LYS	2.0
5	F	15	MET	2.0
2	C	325	GLY	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, 95^{th} 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
9	ZN	D	2001	1/1	0.99	0.22	147,147,147,147	0
9	ZN	D	2002	1/1	0.99	0.17	144,144,144,144	0

6.5 Other polymers (i)

There are no such residues in this entry.