



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:30 PM UTC

PDB ID : 6DVC / pdb_00006dvc
Title : Crystal structure of Mycobacterium tuberculosis transcription initiation complex(ECF sigma factor L) containing 5nt RNA with 6nt spacer
Authors : Lin, W.; Das, K.; Feng, Y.; Ebright, R.H.
Deposited on : 2018-06-23
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

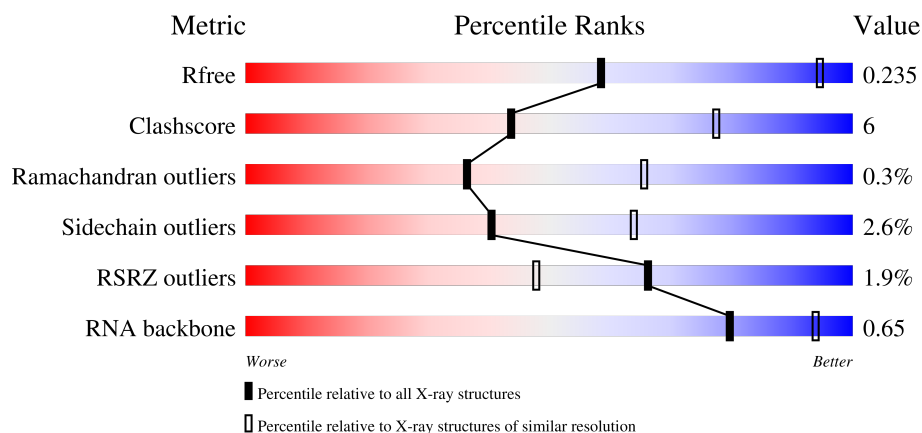
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.



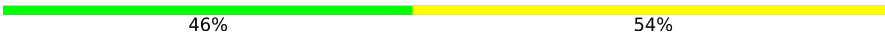
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	359	49% 13% • 37%
1	B	359	3% 47% 16% • 35%
2	C	1178	2% 80% 15% •
3	D	1316	% 82% 13% •

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Mol	Chain	Length	Quality of chain
4	E	110	 4% 57% 16% 26%
5	F	177	 5% 83% 15% •
6	G	17	 41% 59%
7	H	24	 46% 54%
8	I	5	 80% 20%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 24983 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	1264	Total	C	N	O	S	0	0	0
			9884	6189	1790	1865	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 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
6	G	17	Total	C	N	O	P	0	0	0
			350	166	68	100	16			

- Molecule 7 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
7	H	24	Total	C	N	O	P	0	0	0
			491	234	90	144	23			

- Molecule 8 is a RNA chain called RNA (5'-R(*CP*UP*CP*GP*A)-3').

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

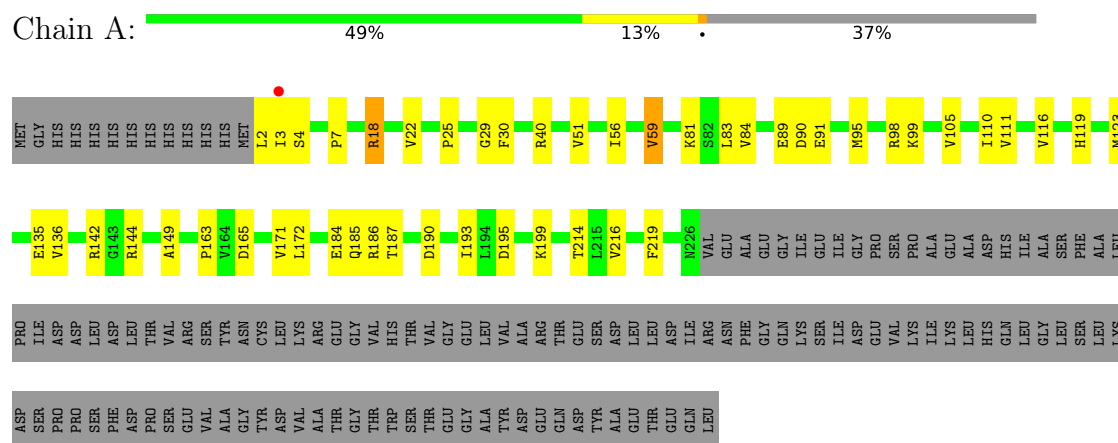
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

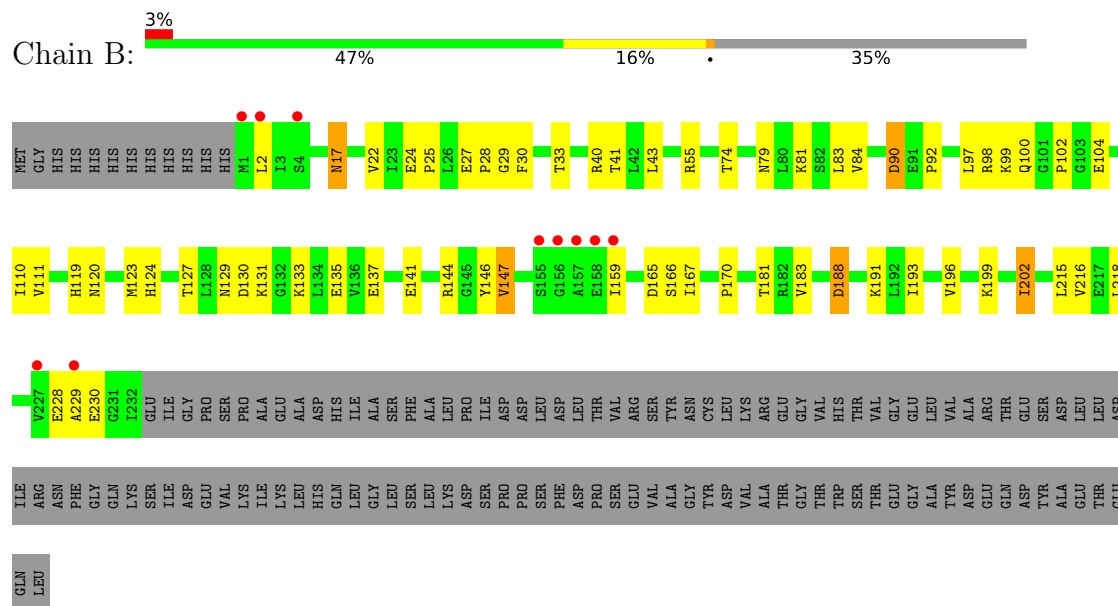
3 Residue-property plots

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.

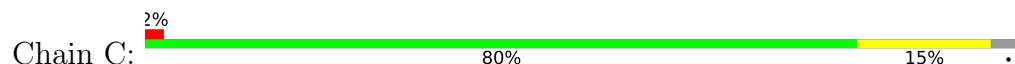
• Molecule 1: DNA-directed RNA polymerase subunit alpha

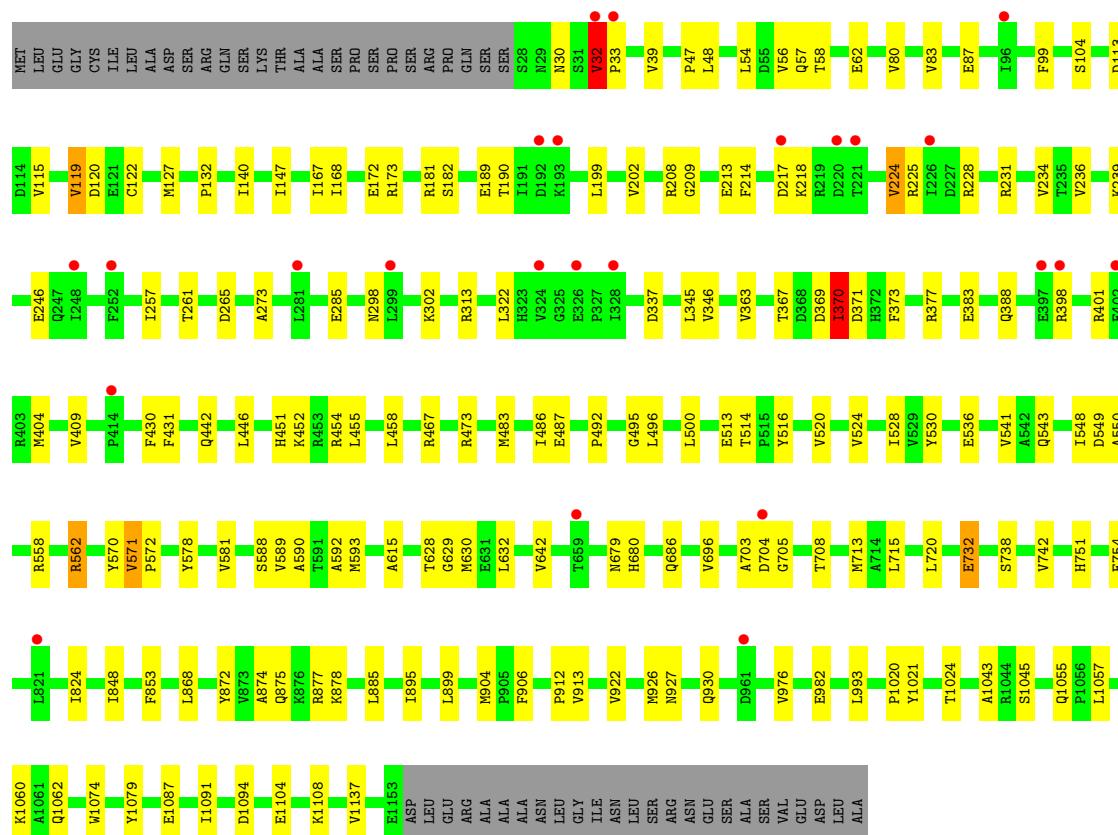


• Molecule 1: DNA-directed RNA polymerase subunit alpha

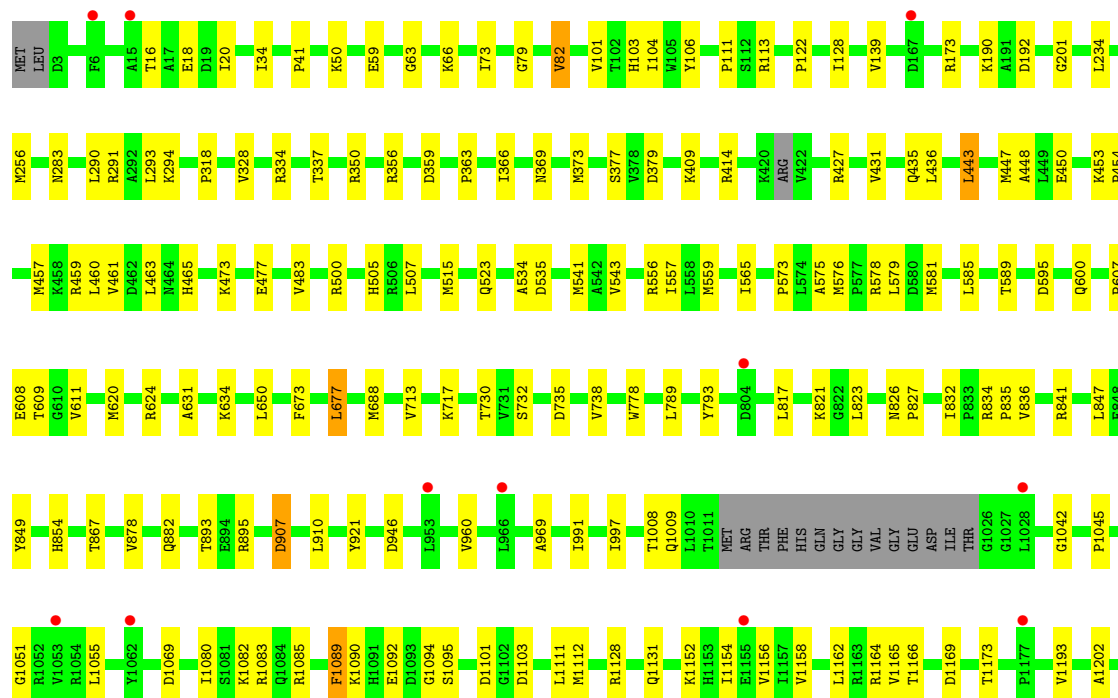
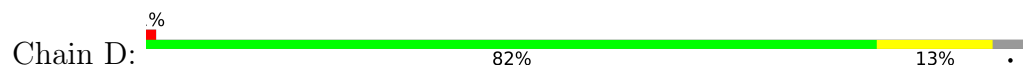


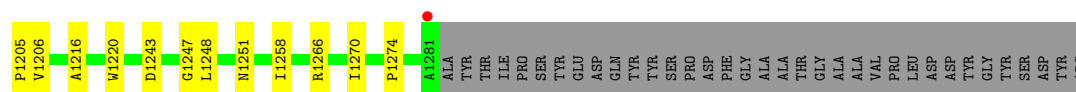
• Molecule 2: DNA-directed RNA polymerase subunit beta



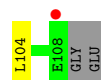
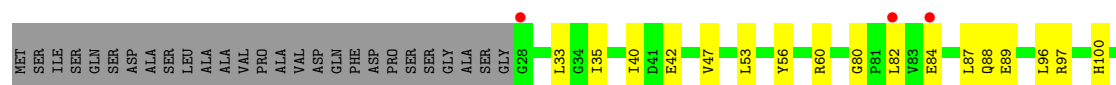


• Molecule 3: DNA-directed RNA polymerase subunit beta'

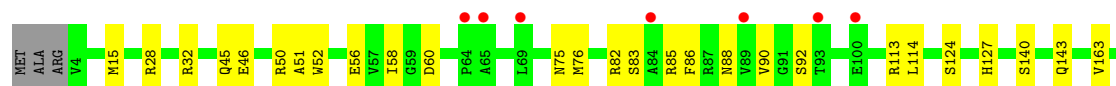
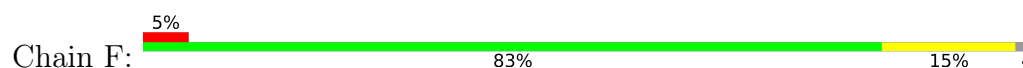




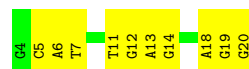
- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: ECF RNA polymerase sigma factor SigL



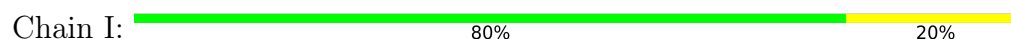
- Molecule 6: DNA (5'-D(*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*G)-3')



- Molecule 7: DNA (5'-D(P*CP*GP*TP*GP*TP*CP*AP*GP*TP*AP*GP*TP*GP*TP*CP*A P*CP*GP*GP*AP*TP*GP*C)-3')



- Molecule 8: RNA (5'-R(*CP*UP*CP*GP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	146.32Å 161.52Å 240.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.92 – 3.30 92.92 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (92.92-3.30) 99.4 (92.92-3.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.198 , 0.235 0.196 , 0.235	Depositor DCC
R_{free} test set	4270 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	91.3	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 84.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24983	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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

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	0.10	0/1742	0.30	0/2370
1	B	0.10	0/1758	0.30	0/2397
2	C	0.10	0/8883	0.30	0/12043
3	D	0.09	0/10049	0.28	0/13583
4	E	0.09	0/643	0.27	0/877
5	F	0.10	0/1374	0.28	0/1869
6	G	0.18	0/393	0.38	0/606
7	H	0.21	0/550	0.45	0/848
8	I	0.07	0/113	0.21	0/174
All	All	0.10	0/25505	0.30	0/34767

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	28	0
1	B	1732	0	1754	40	0
2	C	8724	0	8651	109	0
3	D	9884	0	9939	114	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	630	0	622	13	0
5	F	1352	0	1346	23	0
6	G	350	0	192	9	0
7	H	491	0	272	22	0
8	I	102	0	56	1	0
9	D	2	0	0	0	0
All	All	24983	0	24588	300	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 (300) 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:40:ARG:HE	1:B:33:THR:HG22	1.32	0.93
2:C:467:ARG:HG3	7:H:16:DT:H5'	1.63	0.79
1:A:95:MET:HE3	1:A:110:ILE:HG21	1.65	0.79
2:C:593:MET:HA	2:C:628:THR:HG21	1.68	0.74
1:A:4:SER:HB3	1:B:144:ARG:HH12	1.52	0.74
3:D:363:PRO:HG2	5:F:15:MET:HG3	1.70	0.74
3:D:832:ILE:HG22	3:D:834:ARG:H	1.54	0.73
2:C:1024:THR:H	3:D:730:THR:HG21	1.53	0.72
2:C:32:VAL:HG13	2:C:33:PRO:HD3	1.71	0.71
3:D:1090:LYS:HE2	3:D:1103:ASP:HA	1.71	0.71
5:F:50:ARG:NH1	7:H:4:DT:O4	2.25	0.70
2:C:558:ARG:HB3	2:C:570:TYR:HB3	1.74	0.70
3:D:1090:LYS:HB3	3:D:1092:GLU:HG2	1.74	0.69
2:C:467:ARG:NH1	7:H:14:DT:OP1	2.26	0.69
1:B:84:VAL:HG12	1:B:199:LYS:HD2	1.74	0.68
2:C:541:VAL:HG12	2:C:578:TYR:HB2	1.76	0.68
1:B:90:ASP:OD1	1:B:90:ASP:N	2.26	0.67
3:D:907:ASP:OD1	3:D:907:ASP:N	2.20	0.67
3:D:454:PRO:HA	3:D:457:MET:HE2	1.77	0.66
5:F:75:ASN:ND2	7:H:4:DT:O2	2.28	0.66
3:D:50:LYS:HE2	3:D:79:GLY:HA3	1.77	0.66
2:C:113:ASP:HB3	2:C:132:PRO:HG2	1.76	0.66
2:C:899:LEU:HB2	2:C:904:MET:HE1	1.79	0.65
2:C:1087:GLU:HG3	2:C:1091:ILE:HD11	1.79	0.64
2:C:536:GLU:OE2	2:C:562:ARG:NH2	2.29	0.64
3:D:557:ILE:HG23	4:E:40:ILE:HD11	1.79	0.64
1:A:144:ARG:NH2	1:B:27:GLU:OE2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1055:LEU:H	3:D:1101:ASP:HB3	1.63	0.63
2:C:458:LEU:HD21	2:C:496:LEU:HD13	1.81	0.63
3:D:366:ILE:HD11	5:F:15:MET:HE2	1.81	0.62
2:C:401:ARG:HA	2:C:404:MET:HE2	1.82	0.61
3:D:1248:LEU:HD22	3:D:1258:ILE:HB	1.81	0.61
3:D:291:ARG:NH2	7:H:24:DG:O6	2.33	0.61
3:D:1045:PRO:HG2	3:D:1111:LEU:HB2	1.83	0.61
1:A:186:ARG:HG3	1:A:187:THR:HG23	1.83	0.60
2:C:104:SER:HB3	2:C:140:ILE:HB	1.83	0.60
2:C:30:ASN:ND2	2:C:629:GLY:O	2.34	0.60
3:D:111:PRO:O	3:D:113:ARG:NH1	2.33	0.60
3:D:1173:THR:HG22	3:D:1193:VAL:HG21	1.82	0.60
3:D:500:ARG:HD2	3:D:534:ALA:HB2	1.84	0.59
2:C:181:ARG:NH1	7:H:15:DG:OP2	2.36	0.58
2:C:168:ILE:HG12	2:C:431:PHE:HB3	1.85	0.58
1:B:55:ARG:NH2	1:B:137:GLU:OE1	2.36	0.58
1:A:40:ARG:NE	1:B:33:THR:HG22	2.13	0.58
2:C:571:VAL:HG22	2:C:572:PRO:HD2	1.86	0.58
2:C:982:GLU:HG3	3:D:841:ARG:HH12	1.69	0.57
1:B:24:GLU:HB2	1:B:191:LYS:HG3	1.86	0.57
2:C:590:ALA:HA	2:C:593:MET:HE3	1.85	0.57
3:D:356:ARG:NH2	5:F:46:GLU:OE2	2.37	0.57
3:D:1051:GLY:HA2	3:D:1069:ASP:HB2	1.85	0.57
3:D:1085:ARG:HA	3:D:1112:MET:HA	1.87	0.57
2:C:926:MET:HE1	3:D:817:LEU:HA	1.87	0.57
3:D:826:ASN:HB3	3:D:832:ILE:HD11	1.87	0.56
6:G:11:DT:H2'	6:G:12:DG:C8	2.40	0.56
2:C:285:GLU:OE1	7:H:9:DG:N2	2.37	0.56
2:C:182:SER:HB2	2:C:377:ARG:HB2	1.86	0.56
2:C:628:THR:HG23	2:C:630:MET:H	1.70	0.56
3:D:611:VAL:HG22	3:D:634:LYS:HB2	1.86	0.56
3:D:827:PRO:HD3	3:D:854:HIS:HB3	1.88	0.56
5:F:140:SER:HB3	5:F:143:GLN:HG3	1.87	0.56
1:B:17:ASN:OD1	1:B:17:ASN:N	2.38	0.56
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.89	0.55
2:C:83:VAL:HG13	2:C:87:GLU:HB2	1.89	0.55
2:C:234:VAL:HG12	2:C:261:THR:HG21	1.87	0.55
1:A:7:PRO:HA	1:A:25:PRO:HD2	1.89	0.55
1:B:100:GLN:HG3	1:B:133:LYS:HB2	1.88	0.55
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.40	0.55
2:C:473:ARG:NH2	2:C:492:PRO:O	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:HA	1:A:123:MET:HE1	1.89	0.54
2:C:47:PRO:HG2	2:C:581:VAL:HG13	1.89	0.54
2:C:524:VAL:HG21	2:C:548:ILE:HD13	1.89	0.54
3:D:334:ARG:HD3	5:F:90:VAL:HG21	1.88	0.54
3:D:173:ARG:HH21	3:D:201:GLY:HA2	1.73	0.54
3:D:505:HIS:CD2	3:D:507:LEU:HB2	2.43	0.54
3:D:34:ILE:HA	3:D:41:PRO:HA	1.88	0.54
2:C:377:ARG:NH2	2:C:383:GLU:OE1	2.38	0.54
3:D:1092:GLU:HG3	3:D:1094:GLY:H	1.72	0.53
3:D:1165:VAL:HG12	3:D:1205:PRO:HA	1.90	0.53
7:H:14:DT:H4'	7:H:15:DG:O5'	2.09	0.53
3:D:1083:ARG:HD2	3:D:1112:MET:HE3	1.90	0.53
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.29	0.53
3:D:867:THR:HG22	3:D:1008:THR:HG23	1.90	0.53
1:B:84:VAL:HG23	1:B:119:HIS:HB2	1.90	0.53
1:B:92:PRO:HB3	1:B:141:GLU:HG2	1.91	0.52
1:B:81:LYS:HD3	1:B:165:ASP:HB2	1.91	0.52
2:C:228:ARG:HD3	7:H:14:DT:H73	1.90	0.52
3:D:1131:GLN:HE21	3:D:1162:LEU:HD12	1.74	0.52
2:C:467:ARG:HG2	7:H:15:DG:H2''	1.91	0.52
4:E:60:ARG:NH2	4:E:80:GLY:O	2.43	0.52
1:A:89:GLU:HB3	1:A:91:GLU:HG2	1.92	0.52
2:C:257:ILE:HD11	2:C:346:VAL:HG23	1.90	0.52
3:D:122:PRO:HG2	7:H:23:DT:H3'	1.91	0.51
4:E:87:LEU:HG	4:E:88:GLN:HG3	1.91	0.51
2:C:168:ILE:HB	2:C:173:ARG:HD2	1.93	0.51
3:D:573:PRO:HB2	3:D:576:MET:HE2	1.92	0.51
1:A:56:ILE:HG12	1:A:136:VAL:HG22	1.93	0.51
1:B:228:GLU:HG2	1:B:229:ALA:H	1.75	0.51
3:D:128:ILE:HD11	3:D:234:LEU:HD11	1.92	0.51
3:D:1045:PRO:HB2	3:D:1111:LEU:HD12	1.93	0.51
2:C:369:ASP:C	2:C:371:ASP:H	2.18	0.51
2:C:217:ASP:OD2	2:C:231:ARG:NH2	2.44	0.51
3:D:1270:ILE:HD13	4:E:56:TYR:HE2	1.75	0.51
3:D:1274:PRO:HB3	4:E:82:LEU:HD11	1.92	0.51
3:D:369:ASN:ND2	5:F:45:GLN:OE1	2.39	0.50
2:C:853:PHE:HD2	2:C:868:LEU:HD23	1.76	0.50
3:D:1042:GLY:O	3:D:1083:ARG:NH2	2.43	0.50
2:C:140:ILE:HA	2:C:147:ILE:HG12	1.92	0.50
2:C:172:GLU:OE1	2:C:442:GLN:NE2	2.45	0.50
1:A:22:VAL:HG12	1:A:193:ILE:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:443:LEU:HD13	3:D:448:ALA:HB2	1.93	0.50
6:G:20:DG:H5''	6:G:20:DG:H8	1.77	0.50
1:B:102:PRO:HB3	1:B:130:ASP:HA	1.93	0.50
3:D:460:LEU:HD11	3:D:483:VAL:HG12	1.94	0.49
1:B:147:VAL:HG13	1:B:166:SER:HB2	1.92	0.49
3:D:778:TRP:CD2	3:D:835:PRO:HG3	2.47	0.49
1:B:74:THR:HG21	3:D:608:GLU:HB2	1.95	0.49
4:E:42:GLU:OE1	4:E:100:HIS:NE2	2.37	0.49
6:G:5:DC:H2''	6:G:6:DA:N7	2.27	0.49
2:C:33:PRO:HG2	2:C:632:LEU:HD21	1.94	0.49
2:C:446:LEU:HD13	2:C:593:MET:HE1	1.93	0.49
1:A:56:ILE:HB	1:A:59:VAL:HG22	1.94	0.49
2:C:120:ASP:OD1	2:C:120:ASP:N	2.46	0.49
3:D:600:GLN:HB2	3:D:609:THR:HB	1.94	0.49
2:C:213:GLU:OE1	2:C:225:ARG:NH1	2.46	0.49
3:D:1166:THR:HB	3:D:1206:VAL:HG21	1.95	0.49
2:C:824:ILE:HG22	5:F:163:VAL:HG13	1.94	0.48
2:C:592:ALA:HA	2:C:976:VAL:HG21	1.95	0.48
3:D:565:ILE:HG23	3:D:575:ALA:HB3	1.95	0.48
1:A:3:ILE:HG13	1:A:4:SER:H	1.79	0.48
2:C:99:PHE:HB3	7:H:7:DC:H1'	1.95	0.48
3:D:789:LEU:HD22	3:D:793:TYR:HE2	1.79	0.48
6:G:19:DG:H1	8:I:3:C:H42	1.61	0.48
1:A:30:PHE:HE1	1:B:41:THR:HA	1.79	0.48
1:A:214:THR:OG1	1:B:230:GLU:HG3	2.13	0.48
2:C:738:SER:HA	2:C:904:MET:HE3	1.95	0.48
2:C:742:VAL:HG13	2:C:878:LYS:HD3	1.96	0.48
3:D:63:GLY:HA2	3:D:66:LYS:HE2	1.96	0.48
3:D:1169:ASP:H	3:D:1202:ALA:HB3	1.77	0.48
2:C:298:ASN:HA	2:C:302:LYS:HB2	1.96	0.48
5:F:124:SER:OG	5:F:127:HIS:ND1	2.33	0.48
1:B:167:ILE:HG23	3:D:620:MET:HE1	1.94	0.47
1:A:216:VAL:HG13	1:B:216:VAL:HG13	1.96	0.47
5:F:46:GLU:HB3	5:F:76:MET:HE1	1.95	0.47
1:B:170:PRO:HB2	1:B:202:ILE:HD11	1.96	0.47
3:D:59:GLU:HG2	3:D:66:LYS:HD3	1.96	0.47
3:D:190:LYS:HE3	3:D:192:ASP:HB3	1.95	0.47
4:E:33:LEU:HD23	4:E:33:LEU:H	1.80	0.47
1:B:129:ASN:OD1	1:B:130:ASP:N	2.44	0.47
4:E:89:GLU:OE2	4:E:97:ARG:NH1	2.47	0.47
2:C:982:GLU:HG3	3:D:841:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:337:THR:O	5:F:92:SER:HA	2.14	0.47
2:C:190:THR:HG23	2:C:199:LEU:HB2	1.96	0.47
2:C:848:ILE:HD13	2:C:874:ALA:HB2	1.96	0.47
3:D:334:ARG:CD	5:F:90:VAL:HG21	2.45	0.46
2:C:754:GLU:HG3	2:C:872:TYR:HE2	1.80	0.46
3:D:578:ARG:H	3:D:581:MET:HE3	1.81	0.46
1:A:98:ARG:HG3	1:A:135:GLU:HG3	1.97	0.46
6:G:14:DG:H8	6:G:14:DG:H5'	1.81	0.46
3:D:556:ARG:HG3	4:E:35:ILE:HD11	1.97	0.46
3:D:821:LYS:HB3	3:D:836:VAL:HB	1.96	0.46
2:C:189:GLU:HB2	2:C:367:THR:HG21	1.98	0.46
2:C:1055:GLN:HG2	2:C:1094:ASP:HB3	1.98	0.46
3:D:585:LEU:HD13	3:D:673:PHE:HE2	1.79	0.46
2:C:218:LYS:NZ	6:G:7:DT:OP2	2.47	0.46
2:C:398:ARG:HH12	5:F:32:ARG:HB2	1.80	0.46
2:C:1045:SER:HB3	3:D:450:GLU:O	2.16	0.46
2:C:454:ARG:HH12	2:C:487:GLU:HG2	1.80	0.46
3:D:16:THR:HG22	3:D:18:GLU:H	1.81	0.46
1:B:98:ARG:HG2	1:B:135:GLU:HG2	1.98	0.46
2:C:442:GLN:HB2	2:C:679:ASN:HB2	1.97	0.46
2:C:751:HIS:CD2	2:C:877:ARG:HD2	2.51	0.46
3:D:895:ARG:HD2	3:D:1128:ARG:HH22	1.81	0.46
2:C:642:VAL:HB	2:C:703:ALA:HB3	1.97	0.46
1:A:144:ARG:HH12	1:B:2:LEU:HB2	1.81	0.45
3:D:463:LEU:HB2	3:D:465:HIS:HD2	1.81	0.45
3:D:677:LEU:H	3:D:677:LEU:HG	1.55	0.45
6:G:5:DC:H2''	6:G:6:DA:C8	2.51	0.45
7:H:7:DC:OP1	7:H:7:DC:H4'	2.15	0.45
1:B:124:HIS:HE1	1:B:127:THR:HG23	1.82	0.45
2:C:549:ASP:OD1	2:C:550:ALA:N	2.50	0.45
3:D:447:MET:HE1	3:D:543:VAL:HG21	1.99	0.45
6:G:12:DG:H2'	6:G:13:DA:C8	2.52	0.45
7:H:9:DG:N3	7:H:9:DG:H2'	2.32	0.45
1:A:185:GLN:HG2	1:A:186:ARG:H	1.81	0.45
1:B:146:TYR:O	3:D:624:ARG:NE	2.50	0.45
2:C:1104:GLU:OE1	5:F:113:ARG:NH1	2.50	0.45
1:B:188:ASP:OD1	1:B:188:ASP:N	2.48	0.45
5:F:88:ASN:O	5:F:90:VAL:N	2.49	0.45
3:D:290:LEU:HD23	3:D:293:LEU:HD12	1.98	0.45
3:D:882:GLN:HG3	3:D:997:ILE:HD11	1.98	0.45
2:C:122:CYS:HA	2:C:127:MET:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:369:ASP:O	2:C:370:ILE:HG12	2.15	0.45
2:C:513:GLU:HB3	2:C:530:TYR:HB3	1.98	0.45
3:D:436:LEU:HD11	3:D:523:GLN:HB3	1.98	0.44
2:C:927:ASN:O	2:C:930:GLN:HG2	2.16	0.44
1:B:102:PRO:HD3	1:B:131:LYS:H	1.82	0.44
3:D:500:ARG:HB2	3:D:541:MET:HG2	1.98	0.44
3:D:732:SER:HB3	3:D:735:ASP:OD1	2.18	0.44
7:H:6:DT:H3'	7:H:7:DC:H5''	1.99	0.44
2:C:1043:ALA:HB2	3:D:447:MET:HG2	1.99	0.44
2:C:1108:LYS:HE3	5:F:114:LEU:HD22	1.99	0.44
2:C:313:ARG:HH22	2:C:337:ASP:CG	2.26	0.44
2:C:686:GLN:HA	2:C:705:GLY:HA2	1.99	0.44
2:C:704:ASP:HB2	2:C:708:THR:HB	1.98	0.44
3:D:595:ASP:HB3	3:D:631:ALA:HB2	1.99	0.44
1:B:30:PHE:HA	1:B:33:THR:HG23	2.00	0.44
2:C:853:PHE:HB2	2:C:868:LEU:HB3	1.99	0.44
4:E:96:LEU:HD12	4:E:96:LEU:HA	1.85	0.44
1:A:29:GLY:N	1:A:190:ASP:OD2	2.44	0.44
1:B:99:LYS:NZ	1:B:104:GLU:O	2.46	0.44
3:D:823:LEU:HD23	3:D:835:PRO:HB3	2.00	0.44
7:H:14:DT:H2''	7:H:15:DG:H5''	1.99	0.44
1:B:28:PRO:HA	1:B:29:GLY:HA2	1.48	0.43
1:B:24:GLU:HA	1:B:25:PRO:HA	1.75	0.43
7:H:10:DT:H2'	7:H:11:DA:C8	2.53	0.43
1:A:81:LYS:NZ	1:A:165:ASP:HB2	2.34	0.43
2:C:1074:TRP:CE2	3:D:878:VAL:HG11	2.53	0.43
2:C:1079:TYR:CD2	3:D:559:MET:HG2	2.54	0.43
3:D:453:LYS:O	3:D:457:MET:HG3	2.18	0.43
2:C:236:VAL:HG13	2:C:273:ALA:HB1	2.00	0.43
2:C:446:LEU:HB2	2:C:713:MET:HE2	1.99	0.43
1:A:172:LEU:HB2	1:A:199:LYS:HG2	2.00	0.43
2:C:56:VAL:HG21	2:C:500:LEU:HD22	2.01	0.43
3:D:435:GLN:OE1	3:D:435:GLN:N	2.39	0.43
3:D:991:ILE:HD12	3:D:1266:ARG:HH12	1.83	0.43
3:D:1220:TRP:CD1	3:D:1243:ASP:HB2	2.54	0.43
3:D:20:ILE:HG23	3:D:318:PRO:HB3	2.00	0.43
4:E:47:VAL:HG11	4:E:53:LEU:HB2	2.01	0.43
3:D:103:HIS:HB3	3:D:106:TYR:HD2	1.84	0.42
1:A:90:ASP:OD1	1:A:142:ARG:HD3	2.19	0.42
2:C:732:GLU:HB3	3:D:579:LEU:HD12	2.01	0.42
3:D:1152:LYS:O	3:D:1156:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ARG:HD3	1:B:40:ARG:HA	1.88	0.42
1:B:83:LEU:HB2	1:B:123:MET:HE1	2.01	0.42
2:C:228:ARG:O	2:C:228:ARG:HG3	2.18	0.42
2:C:486:ILE:HD11	3:D:849:TYR:HE2	1.84	0.42
3:D:290:LEU:HA	3:D:293:LEU:HD12	2.01	0.42
3:D:893:THR:HG21	3:D:969:ALA:HB3	2.02	0.42
5:F:51:ALA:HB1	5:F:58:ILE:HD11	2.02	0.42
2:C:239:LYS:NZ	2:C:265:ASP:OD2	2.53	0.42
2:C:543:GLN:HG3	3:D:847:LEU:HD13	2.00	0.42
3:D:921:TYR:HE1	3:D:946:ASP:HA	1.85	0.42
3:D:1080:ILE:HG22	3:D:1082:LYS:H	1.83	0.42
1:A:219:PHE:CD1	1:B:215:LEU:HD13	2.55	0.42
2:C:48:LEU:HB2	2:C:528:ILE:HD13	2.00	0.42
3:D:111:PRO:HB3	7:H:22:DA:H5''	2.02	0.42
7:H:14:DT:H5'	7:H:15:DG:OP1	2.19	0.42
1:B:84:VAL:HG22	1:B:120:ASN:CG	2.45	0.42
2:C:473:ARG:HB3	2:C:495:GLY:HA3	2.02	0.42
5:F:88:ASN:C	5:F:90:VAL:H	2.27	0.42
2:C:209:GLY:O	7:H:13:DC:N4	2.53	0.42
3:D:1101:ASP:OD1	3:D:1101:ASP:N	2.52	0.42
3:D:1154:ILE:O	3:D:1158:VAL:HG23	2.20	0.42
2:C:119:VAL:HG23	2:C:167:ILE:HD11	2.02	0.41
2:C:516:TYR:HB3	2:C:578:TYR:HB3	2.02	0.41
1:A:84:VAL:HG13	1:A:119:HIS:HB2	2.02	0.41
3:D:473:LYS:NZ	3:D:477:GLU:OE2	2.51	0.41
2:C:202:VAL:HG21	2:C:345:LEU:HB2	2.03	0.41
2:C:214:PHE:CD1	2:C:224:VAL:HB	2.55	0.41
2:C:904:MET:HG2	2:C:913:VAL:O	2.21	0.41
1:B:97:LEU:HB2	1:B:110:ILE:HG13	2.02	0.41
2:C:442:GLN:H	2:C:680:HIS:CD2	2.39	0.41
2:C:451:HIS:HA	2:C:454:ARG:HG2	2.02	0.41
2:C:885:LEU:HG	2:C:895:ILE:HD11	2.03	0.41
2:C:1060:LYS:N	6:G:18:DA:OP1	2.51	0.41
3:D:369:ASN:O	3:D:373:MET:HG3	2.21	0.41
3:D:1274:PRO:HA	4:E:104:LEU:HD23	2.03	0.41
1:A:149:ALA:HB1	1:A:163:PRO:HB2	2.03	0.41
2:C:285:GLU:OE2	7:H:9:DG:N1	2.53	0.41
3:D:73:ILE:O	3:D:82:VAL:HG22	2.21	0.41
3:D:575:ALA:O	3:D:713:VAL:HG21	2.20	0.41
5:F:32:ARG:HD2	7:H:9:DG:O3'	2.20	0.41
2:C:32:VAL:H	2:C:33:PRO:CD	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:455:LEU:HD12	2:C:483:MET:HG3	2.03	0.41
3:D:409:LYS:HG2	3:D:414:ARG:CZ	2.51	0.41
3:D:579:LEU:HD23	3:D:579:LEU:HA	1.94	0.41
2:C:388:GLN:HG3	2:C:430:PHE:HB2	2.03	0.41
2:C:720:LEU:HD23	2:C:913:VAL:HA	2.03	0.41
2:C:899:LEU:HB2	2:C:904:MET:CE	2.48	0.41
3:D:294:LYS:HB2	3:D:294:LYS:HE3	1.79	0.41
3:D:789:LEU:HD22	3:D:793:TYR:CE2	2.55	0.41
3:D:363:PRO:HD3	5:F:52:TRP:CE2	2.56	0.41
2:C:57:GLN:HG3	2:C:452:LYS:HB3	2.03	0.41
2:C:615:ALA:HB3	2:C:715:LEU:HD22	2.02	0.41
1:A:99:LYS:HG2	1:A:105:VAL:HG22	2.03	0.41
2:C:588:SER:OG	2:C:589:VAL:N	2.54	0.41
2:C:906:PHE:HA	2:C:912:PRO:HA	2.02	0.41
3:D:589:THR:HG21	3:D:688:MET:HG2	2.02	0.41
3:D:717:LYS:HE2	3:D:717:LYS:HB3	1.93	0.41
5:F:28:ARG:O	5:F:32:ARG:HG3	2.21	0.41
3:D:350:ARG:HD2	3:D:377:SER:OG	2.21	0.40
3:D:1089:PHE:HA	3:D:1095:SER:HA	2.03	0.40
2:C:58:THR:O	2:C:62:GLU:HG3	2.22	0.40
1:A:18:ARG:NH1	1:A:195:ASP:OD2	2.54	0.40
1:B:28:PRO:HG3	1:B:188:ASP:C	2.47	0.40
2:C:377:ARG:HH22	2:C:383:GLU:CD	2.29	0.40
1:B:22:VAL:HG12	1:B:193:ILE:HG12	2.02	0.40
2:C:1020:PRO:HB2	2:C:1021:TYR:CD2	2.56	0.40
3:D:1270:ILE:HG21	4:E:56:TYR:CE2	2.56	0.40
5:F:82:ARG:HB3	5:F:83:SER:H	1.71	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%)	5 (2%)	1 (0%)	30	60
1	B	230/359 (64%)	213 (93%)	16 (7%)	1 (0%)	30	60
2	C	1124/1178 (95%)	1071 (95%)	48 (4%)	5 (0%)	30	60
3	D	1258/1316 (96%)	1205 (96%)	51 (4%)	2 (0%)	43	71
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	3086/3499 (88%)	2950 (96%)	127 (4%)	9 (0%)	36	65

All (9) 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
2	C	32	VAL
3	D	607	PRO
1	A	184	GLU
2	C	520	VAL
2	C	922	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/308 (63%)	187 (96%)	7 (4%)	31	58
1	B	191/308 (62%)	179 (94%)	12 (6%)	16	44
2	C	950/998 (95%)	927 (98%)	23 (2%)	43	65
3	D	1049/1095 (96%)	1028 (98%)	21 (2%)	48	68
4	E	66/90 (73%)	65 (98%)	1 (2%)	57	72
5	F	134/136 (98%)	130 (97%)	4 (3%)	36	61
All	All	2584/2935 (88%)	2516 (97%)	68 (3%)	40	64

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	18	ARG
1	A	51	VAL
1	A	59	VAL
1	A	111	VAL
1	A	116	VAL
1	A	171	VAL
1	B	17	ASN
1	B	43	LEU
1	B	79	ASN
1	B	90	ASP
1	B	111	VAL
1	B	147	VAL
1	B	181	THR
1	B	183	VAL
1	B	188	ASP
1	B	196	VAL
1	B	202	ILE
1	B	218	LEU
2	C	32	VAL
2	C	39	VAL
2	C	54	LEU
2	C	80	VAL
2	C	115	VAL
2	C	119	VAL
2	C	208	ARG
2	C	224	VAL
2	C	246	GLU
2	C	322	LEU
2	C	363	VAL
2	C	370	ILE
2	C	373	PHE
2	C	409	VAL
2	C	514	THR
2	C	562	ARG
2	C	571	VAL
2	C	696	VAL
2	C	875	GLN
2	C	993	LEU
2	C	1057	LEU
2	C	1062	GLN
2	C	1137	VAL

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Mol	Chain	Res	Type
3	D	82	VAL
3	D	101	VAL
3	D	139	VAL
3	D	256	MET
3	D	283	ASN
3	D	328	VAL
3	D	359	ASP
3	D	427	ARG
3	D	431	VAL
3	D	443	LEU
3	D	459	ARG
3	D	461	VAL
3	D	515	MET
3	D	535	ASP
3	D	650	LEU
3	D	677	LEU
3	D	738	VAL
3	D	907	ASP
3	D	910	LEU
3	D	960	VAL
3	D	1009	GLN
4	E	84	GLU
5	F	56	GLU
5	F	60	ASP
5	F	85	ARG
5	F	86	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	37	ASN
2	C	142	ASN
2	C	200	HIS
2	C	375	ASN
2	C	386	GLN
2	C	419	ASN
2	C	700	GLN
2	C	755	HIS
2	C	941	HIS
2	C	1054	GLN
2	C	1066	GLN
3	D	145	HIS

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Mol	Chain	Res	Type
3	D	262	GLN
3	D	283	ASN
3	D	564	ASN
3	D	767	HIS
3	D	1109	GLN
3	D	1153	HIS
5	F	122	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	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 oligosaccharides 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 [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	225/359 (62%)	-0.06	1 (0%) 88 79	48, 74, 136, 172	0
1	B	232/359 (64%)	0.27	10 (4%) 40 25	62, 95, 148, 179	0
2	C	1126/1178 (95%)	0.06	24 (2%) 63 44	44, 85, 156, 184	0
3	D	1264/1316 (96%)	0.04	12 (0%) 81 65	42, 90, 176, 221	0
4	E	81/110 (73%)	0.30	4 (4%) 35 23	68, 97, 172, 188	0
5	F	174/177 (98%)	0.10	8 (4%) 37 25	60, 101, 168, 190	0
6	G	17/17 (100%)	0.07	0 100 100	77, 88, 163, 163	0
7	H	24/24 (100%)	0.49	0 100 100	100, 150, 211, 215	0
8	I	5/5 (100%)	-0.36	0 100 100	74, 75, 90, 117	0
All	All	3148/3545 (88%)	0.07	59 (1%) 66 48	42, 89, 164, 221	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	402	GLU	5.1
2	C	192	ASP	4.1
1	B	157	ALA	3.9
1	B	4	SER	3.8
2	C	326	GLU	3.2
2	C	32	VAL	3.2
5	F	65	ALA	3.0
4	E	108	GLU	2.9
3	D	1281	ALA	2.9
3	D	6	PHE	2.9
5	F	93	THR	2.8
3	D	1028	LEU	2.7
3	D	1155	GLU	2.6
2	C	226	ILE	2.6
1	B	159	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	398	ARG	2.5
3	D	953	LEU	2.5
3	D	804	ASP	2.5
2	C	414	PRO	2.5
1	B	2	LEU	2.5
5	F	172	GLU	2.5
1	B	1	MET	2.5
5	F	84	ALA	2.4
2	C	397	GLU	2.4
2	C	217	ASP	2.4
3	D	1177	PRO	2.4
4	E	28	GLY	2.4
5	F	89	VAL	2.4
3	D	15	ALA	2.4
2	C	328	ILE	2.4
1	B	158	GLU	2.4
2	C	193	LYS	2.3
2	C	252	PHE	2.3
2	C	961	ASP	2.3
2	C	281	LEU	2.2
2	C	659	THR	2.2
1	A	3	ILE	2.2
1	B	229	ALA	2.2
2	C	299	LEU	2.2
2	C	221	THR	2.2
3	D	167	ASP	2.2
2	C	96	ILE	2.2
2	C	248	ILE	2.1
2	C	33	PRO	2.1
2	C	821	LEU	2.1
4	E	82	LEU	2.1
2	C	704	ASP	2.1
4	E	84	GLU	2.1
3	D	1053	VAL	2.1
1	B	156	GLY	2.1
5	F	64	PRO	2.1
2	C	324	VAL	2.1
2	C	220	ASP	2.1
3	D	966	LEU	2.0
3	D	1062	TYR	2.0
1	B	155	SER	2.0
1	B	227	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
5	F	100	GLU	2.0
5	F	69	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	ZN	D	2001	1/1	0.99	0.03	100,100,100,100	0
9	ZN	D	2002	1/1	0.99	0.04	105,105,105,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.