



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 11:05 AM EDT

PDB ID : 6DVE / pdb_00006dve
Title : Crystal structure of Mycobacterium tuberculosis transcription initiation complex(ECF selenomethionine-labelled sigma factor L) with 6 nt spacer
Authors : Lin, W.; Das, K.; Feng, Y.; Ebright, R.H.
Deposited on : 2018-06-23
Resolution : 3.81 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

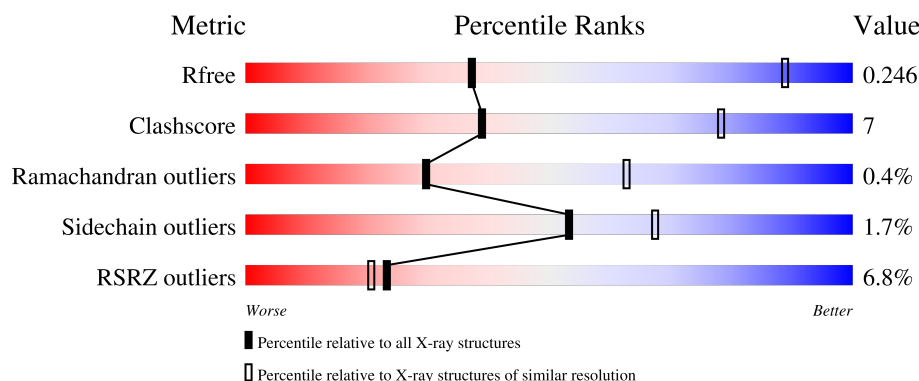
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.81 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	1043 (3.98-3.66)
Clashscore	190562	1075 (3.98-3.66)
Ramachandran outliers	187476	1029 (3.98-3.66)
Sidechain outliers	187428	1024 (3.98-3.66)
RSRZ outliers	180081	1042 (3.98-3.66)

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	
1	B	359	
2	C	1178	
3	D	1316	
4	E	110	

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Mol	Chain	Length	Quality of chain
5	F	177	10% 81% 17%
6	G	12	25% 33% 67%
7	H	24	25% 38% 63%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24785 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	Se	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*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	12	Total	C	N	O	P	0	0	0
			244	117	45	71	11			

- Molecule 7 is a DNA chain called DNA (5'-D(P*CP*GP*TP*GP*TP*GP*AP*GP*TP*AP*AP*CP*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
			490	234	90	143	23			

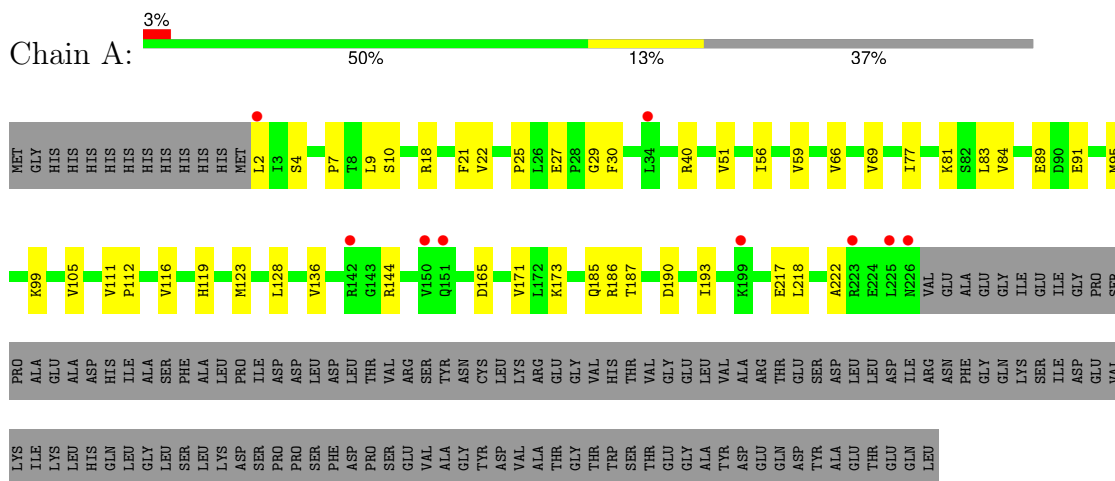
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

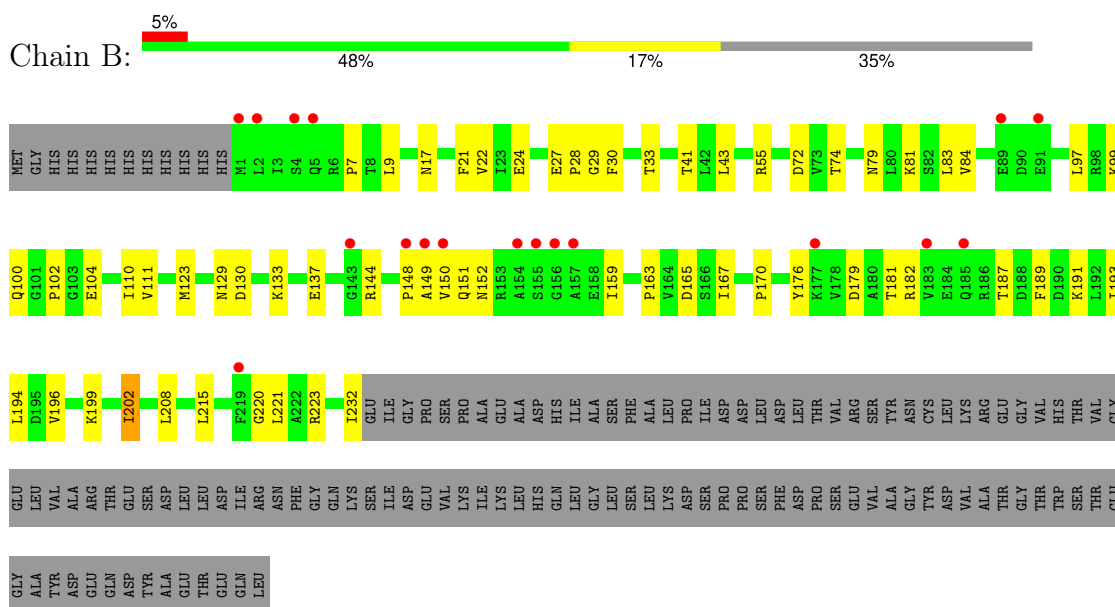
3 Residue-property plots

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.

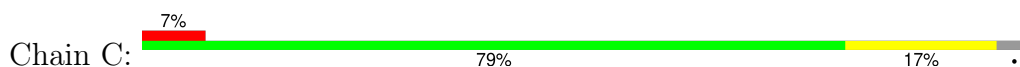
- Molecule 1: DNA-directed RNA polymerase subunit alpha

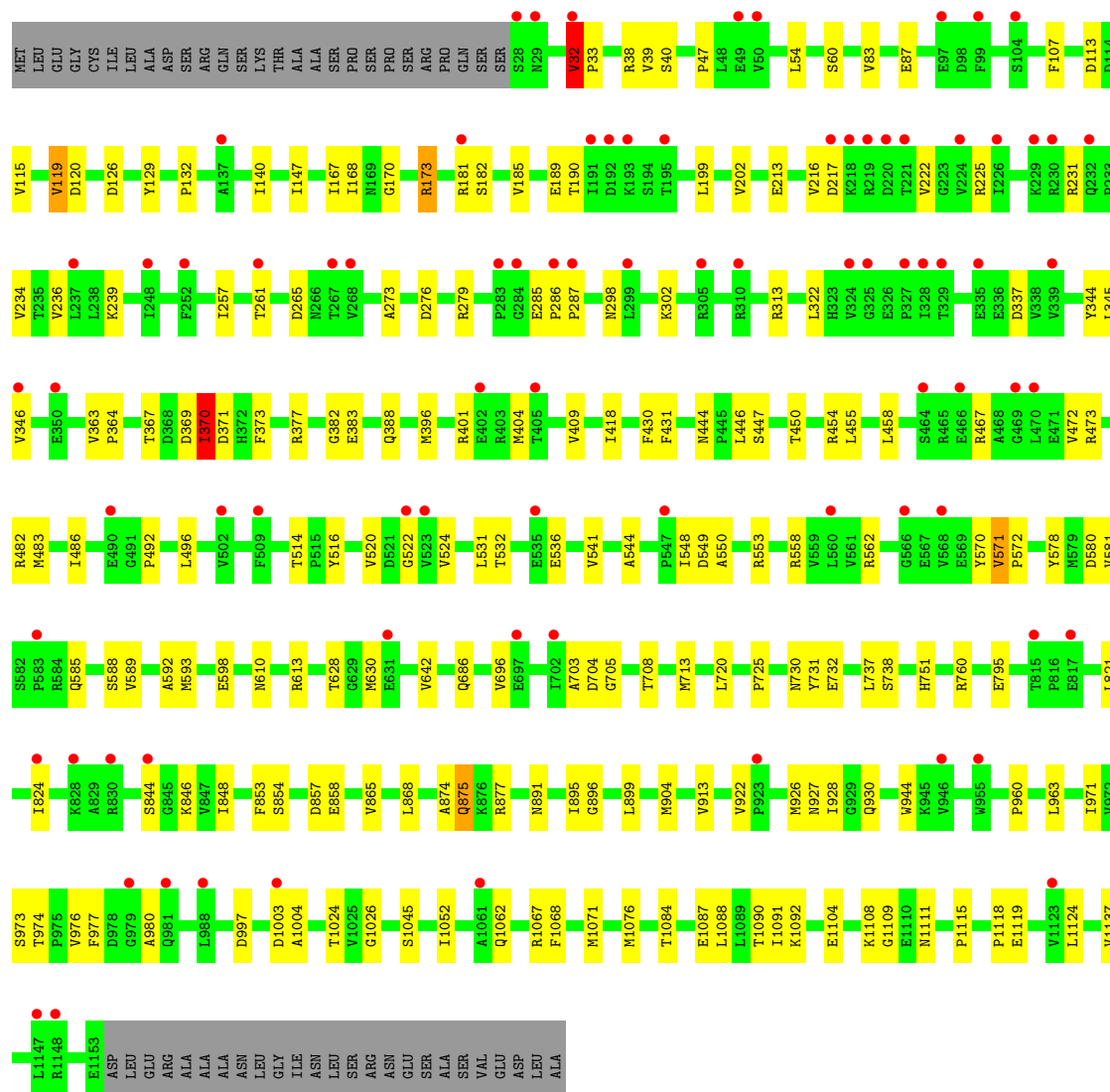


- Molecule 1: DNA-directed RNA polymerase subunit alpha

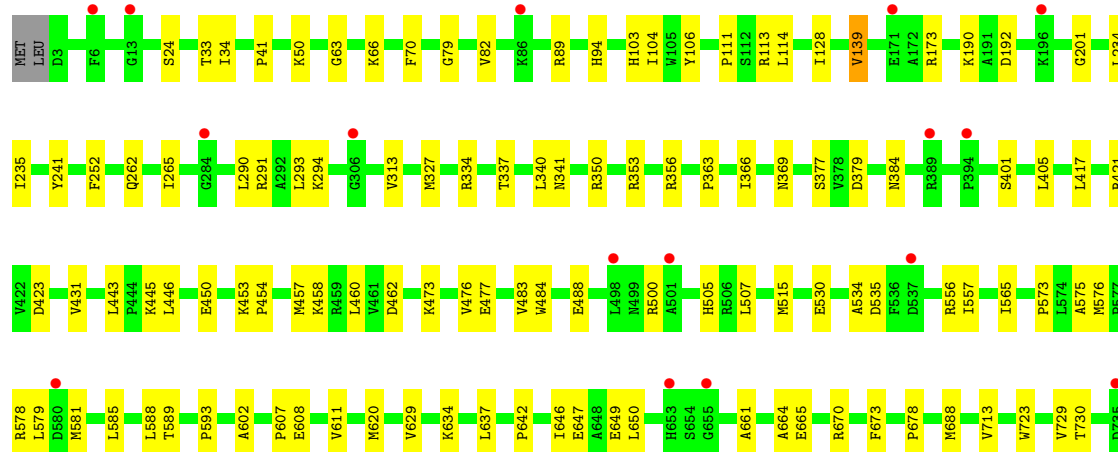
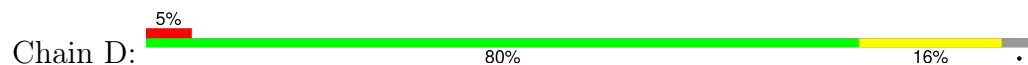


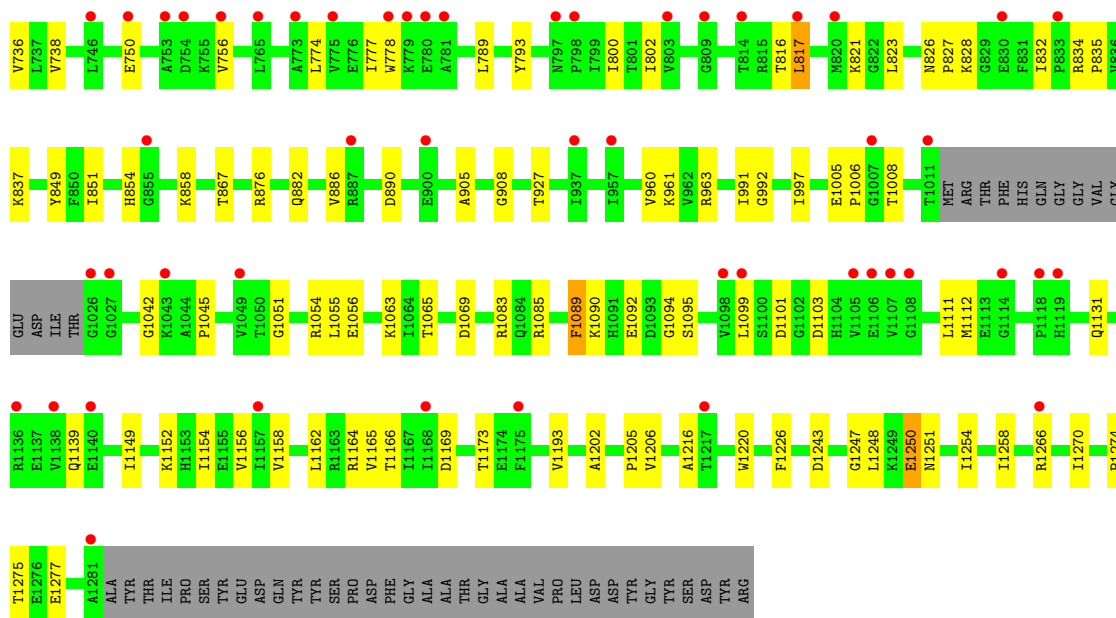
- Molecule 2: DNA-directed RNA polymerase subunit beta



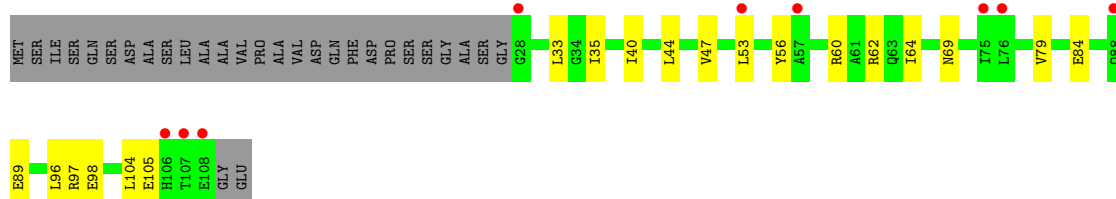


- Molecule 3: DNA-directed RNA polymerase subunit beta'

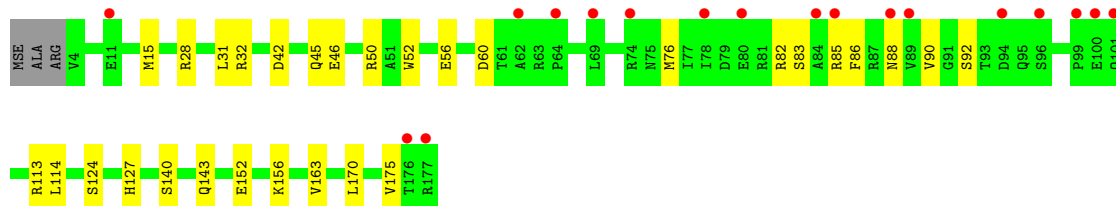
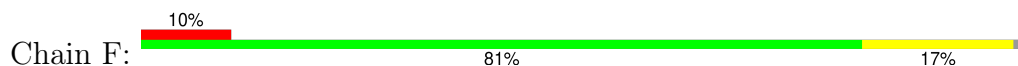




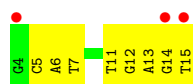
- Molecule 4: DNA-directed RNA polymerase subunit omega



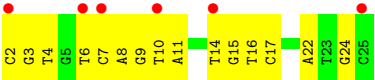
- Molecule 5: ECF RNA polymerase sigma factor SigL



- Molecule 6: DNA (5'-D(*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*T)-3')



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	142.76Å 160.61Å 240.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.68 – 3.81 46.68 – 3.81	Depositor EDS
% Data completeness (in resolution range)	58.5 (46.68-3.81) 74.9 (46.68-3.81)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.200 , 0.248 0.198 , 0.246	Depositor DCC
R_{free} test set	2000 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	1.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 68.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	24785	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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	0.31	0/2370
1	B	0.12	0/1758	0.34	0/2397
2	C	0.10	0/8883	0.31	0/12043
3	D	0.11	0/10061	0.31	0/13600
4	E	0.11	0/643	0.30	0/877
5	F	0.13	0/1372	0.34	0/1863
6	G	0.20	0/273	0.43	0/420
7	H	0.26	0/549	0.50	0/846
All	All	0.11	0/25281	0.32	0/34416

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	32	0
1	B	1732	0	1754	39	0
2	C	8724	0	8651	118	0
3	D	9895	0	9953	138	0
4	E	630	0	622	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1352	0	1346	23	0
6	G	244	0	137	7	0
7	H	490	0	272	19	0
8	D	2	0	0	0	0
All	All	24785	0	24491	336	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (336) 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	1.52	0.90
1:A:40:ARG:HE	1:B:33:THR:HG22	1.42	0.84
6:G:11:DT:H2'	6:G:12:DG:C8	2.16	0.80
7:H:2:DC:H2'	7:H:3:DG:C8	2.18	0.78
2:C:1024:THR:H	3:D:730:THR:HG21	1.50	0.76
1:B:81:LYS:HD3	1:B:165:ASP:HB2	1.66	0.76
1:B:182:ARG:HB3	1:B:187:THR:HA	1.68	0.74
3:D:454:PRO:HA	3:D:457:MET:HE2	1.70	0.74
1:B:84:VAL:HG12	1:B:199:LYS:HD2	1.71	0.73
2:C:928:ILE:HD11	3:D:817:LEU:HD11	1.71	0.72
3:D:1090:LYS:HB3	3:D:1092:GLU:HG2	1.72	0.72
3:D:832:ILE:HG22	3:D:834:ARG:H	1.55	0.71
2:C:541:VAL:HG12	2:C:578:TYR:HB2	1.72	0.71
7:H:6:DT:H2''	7:H:7:DC:H5'	1.71	0.71
2:C:593:MET:HA	2:C:628:THR:HG21	1.71	0.70
3:D:1173:THR:HG22	3:D:1193:VAL:HG21	1.73	0.70
3:D:1090:LYS:HE2	3:D:1103:ASP:HA	1.74	0.69
7:H:10:DT:H2'	7:H:11:DA:C8	2.28	0.68
2:C:32:VAL:HG13	2:C:33:PRO:HD3	1.75	0.68
2:C:558:ARG:HB3	2:C:570:TYR:HB3	1.76	0.68
3:D:337:THR:OG1	3:D:341:ASN:ND2	2.27	0.67
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.78	0.65
2:C:1087:GLU:HG3	2:C:1091:ILE:HD11	1.76	0.65
2:C:213:GLU:OE1	2:C:225:ARG:NH1	2.28	0.65
2:C:458:LEU:HD21	2:C:496:LEU:HD13	1.78	0.65
6:G:6:DA:H1'	6:G:7:DT:H5'	1.78	0.65
2:C:899:LEU:HB2	2:C:904:MET:HE1	1.79	0.65
3:D:1045:PRO:HG2	3:D:1111:LEU:HB2	1.79	0.65
1:B:181:THR:O	1:B:189:PHE:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1248:LEU:HD22	3:D:1258:ILE:HB	1.78	0.64
1:A:89:GLU:HB3	1:A:91:GLU:HG2	1.79	0.63
2:C:536:GLU:OE2	2:C:562:ARG:NH2	2.32	0.63
5:F:124:SER:HG	5:F:127:HIS:HD1	1.44	0.63
3:D:50:LYS:HE2	3:D:79:GLY:HA3	1.81	0.63
1:B:100:GLN:HG3	1:B:133:LYS:HB2	1.80	0.62
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.25	0.62
3:D:1051:GLY:HA2	3:D:1069:ASP:HB2	1.82	0.62
2:C:168:ILE:HB	2:C:173:ARG:HD2	1.82	0.62
3:D:363:PRO:HG2	5:F:15:MSE:HG3	1.80	0.61
5:F:50:ARG:NH1	7:H:4:DT:O4	2.33	0.61
6:G:12:DG:H2'	6:G:13:DA:C8	2.36	0.61
3:D:458:LYS:NZ	3:D:462:ASP:OD2	2.34	0.61
1:A:56:ILE:HB	1:A:59:VAL:HG22	1.84	0.60
3:D:34:ILE:HA	3:D:41:PRO:HA	1.83	0.60
3:D:453:LYS:HG3	3:D:476:VAL:HG11	1.83	0.60
2:C:47:PRO:HG2	2:C:581:VAL:HG13	1.83	0.59
3:D:356:ARG:NH2	5:F:46:GLU:OE2	2.36	0.59
2:C:571:VAL:HG22	2:C:572:PRO:HD2	1.83	0.59
2:C:686:GLN:HA	2:C:705:GLY:HA2	1.85	0.58
2:C:731:TYR:HE1	3:D:579:LEU:HB2	1.67	0.58
2:C:234:VAL:HG12	2:C:261:THR:HG21	1.85	0.58
1:A:56:ILE:HG12	1:A:136:VAL:HG22	1.85	0.58
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.37	0.57
2:C:1003:ASP:OD1	2:C:1004:ALA:N	2.37	0.57
2:C:824:ILE:HA	5:F:163:VAL:HG13	1.86	0.57
2:C:473:ARG:NH2	2:C:492:PRO:O	2.38	0.57
2:C:1084:THR:O	2:C:1088:LEU:HG	2.04	0.57
6:G:11:DT:H2'	6:G:12:DG:H8	1.70	0.57
2:C:854:SER:HB3	2:C:857:ASP:HB2	1.87	0.57
3:D:190:LYS:HE3	3:D:192:ASP:HB3	1.86	0.57
1:B:55:ARG:NH2	1:B:137:GLU:OE1	2.31	0.57
2:C:524:VAL:HG21	2:C:548:ILE:HD13	1.84	0.57
3:D:291:ARG:NH2	7:H:24:DG:O6	2.33	0.57
3:D:1045:PRO:HB2	3:D:1111:LEU:HD12	1.87	0.57
2:C:181:ARG:NH1	7:H:15:DG:OP2	2.37	0.56
6:G:5:DC:H2''	6:G:6:DA:C8	2.39	0.56
1:B:152:ASN:HB2	1:B:163:PRO:HB3	1.87	0.56
3:D:473:LYS:NZ	3:D:477:GLU:OE2	2.39	0.56
3:D:589:THR:HG22	3:D:670:ARG:HG2	1.86	0.56
3:D:832:ILE:HG13	3:D:851:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1165:VAL:HG12	3:D:1205:PRO:HA	1.88	0.56
7:H:16:DT:H2'	7:H:17:DC:C6	2.40	0.56
2:C:467:ARG:NH1	7:H:14:DT:O2	2.39	0.56
2:C:628:THR:HG23	2:C:630:MET:H	1.70	0.56
5:F:32:ARG:HD3	7:H:9:DG:H4'	1.88	0.56
1:A:186:ARG:HG3	1:A:187:THR:HG23	1.88	0.56
3:D:1275:THR:HB	4:E:105:GLU:HG3	1.87	0.56
3:D:1085:ARG:HA	3:D:1112:MET:HA	1.89	0.55
3:D:1139:GLN:NE2	3:D:1149:ILE:O	2.38	0.55
2:C:450:THR:HG22	2:C:454:ARG:HE	1.70	0.55
2:C:1104:GLU:OE1	5:F:113:ARG:NH1	2.40	0.55
3:D:500:ARG:HD2	3:D:534:ALA:HB2	1.86	0.55
3:D:63:GLY:HA2	3:D:66:LYS:HE2	1.89	0.55
3:D:882:GLN:HG3	3:D:997:ILE:HD11	1.88	0.55
3:D:1083:ARG:HD2	3:D:1112:MET:HE3	1.89	0.55
3:D:1131:GLN:HE21	3:D:1162:LEU:HD12	1.72	0.55
3:D:589:THR:HG21	3:D:688:MET:HG2	1.88	0.55
1:B:97:LEU:HB2	1:B:110:ILE:HG13	1.90	0.54
1:B:102:PRO:HB3	1:B:130:ASP:HA	1.89	0.54
3:D:111:PRO:O	3:D:113:ARG:NH1	2.36	0.54
3:D:340:LEU:HD11	3:D:405:LEU:HD11	1.88	0.54
1:B:129:ASN:OD1	1:B:130:ASP:N	2.37	0.54
1:B:148:PRO:HD2	1:B:151:GLN:HG3	1.89	0.54
2:C:377:ARG:NH2	2:C:383:GLU:OE1	2.38	0.54
3:D:369:ASN:ND2	5:F:45:GLN:OE1	2.39	0.54
1:A:4:SER:HB3	1:B:144:ARG:HH12	1.73	0.53
2:C:257:ILE:HD11	2:C:346:VAL:HG23	1.90	0.53
2:C:40:SER:HA	2:C:973:SER:HB2	1.90	0.53
2:C:401:ARG:HA	2:C:404:MET:HE2	1.90	0.53
3:D:530:GLU:HB2	3:D:578:ARG:HD2	1.89	0.53
1:A:4:SER:HB3	1:B:144:ARG:NH1	2.23	0.53
2:C:944:TRP:NE1	2:C:963:LEU:O	2.25	0.53
7:H:14:DT:H4'	7:H:15:DG:O5'	2.09	0.52
3:D:460:LEU:HD11	3:D:483:VAL:HG12	1.92	0.52
3:D:173:ARG:HH21	3:D:201:GLY:HA2	1.74	0.52
2:C:795:GLU:HG2	2:C:846:LYS:HG2	1.91	0.52
3:D:1092:GLU:HG3	3:D:1094:GLY:H	1.75	0.52
1:A:7:PRO:HG2	1:B:221:LEU:HD11	1.92	0.52
2:C:455:LEU:HD12	2:C:483:MET:HG3	1.92	0.52
2:C:738:SER:HA	2:C:904:MET:HE3	1.90	0.52
3:D:1056:GLU:HB2	3:D:1063:LYS:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1275:THR:O	3:D:1277:GLU:N	2.38	0.52
1:B:17:ASN:OD1	1:B:17:ASN:N	2.43	0.52
2:C:369:ASP:C	2:C:371:ASP:H	2.18	0.52
2:C:1067:ARG:HA	3:D:421:ARG:HA	1.92	0.52
1:A:217:GLU:HG2	1:B:232:ILE:HD12	1.91	0.52
2:C:190:THR:HG23	2:C:199:LEU:HB2	1.92	0.52
2:C:217:ASP:OD2	2:C:231:ARG:NH2	2.43	0.52
2:C:113:ASP:HB3	2:C:132:PRO:HG2	1.92	0.51
2:C:821:LEU:HA	2:C:824:ILE:HG12	1.91	0.51
2:C:1052:ILE:O	3:D:89:ARG:NH1	2.43	0.51
1:A:69:VAL:HG12	1:A:128:LEU:HG	1.93	0.51
3:D:789:LEU:HD22	3:D:793:TYR:HE2	1.75	0.51
3:D:826:ASN:HA	3:D:854:HIS:HB3	1.92	0.51
3:D:337:THR:O	5:F:92:SER:HA	2.11	0.51
2:C:83:VAL:HG13	2:C:87:GLU:HB2	1.91	0.51
2:C:720:LEU:HD23	2:C:913:VAL:HA	1.93	0.51
3:D:1169:ASP:H	3:D:1202:ALA:HB3	1.76	0.51
3:D:1220:TRP:CD1	3:D:1243:ASP:HB2	2.46	0.50
2:C:369:ASP:O	2:C:370:ILE:HG12	2.11	0.50
2:C:344:TYR:OH	2:C:364:PRO:O	2.25	0.50
2:C:1119:GLU:OE2	3:D:89:ARG:NH2	2.45	0.50
1:A:9:LEU:HD11	1:A:21:PHE:HB3	1.94	0.50
2:C:446:LEU:HD13	2:C:593:MET:HE1	1.94	0.50
2:C:1045:SER:HB3	3:D:450:GLU:O	2.12	0.50
3:D:585:LEU:O	3:D:589:THR:OG1	2.27	0.49
3:D:826:ASN:HD21	3:D:828:LYS:HE2	1.75	0.49
1:B:99:LYS:NZ	1:B:104:GLU:O	2.42	0.49
3:D:890:ASP:OD1	3:D:963:ARG:NH2	2.39	0.49
1:B:24:GLU:HB2	1:B:191:LYS:HG3	1.93	0.49
3:D:585:LEU:HD13	3:D:673:PHE:HE2	1.78	0.49
1:A:22:VAL:HG12	1:A:193:ILE:HG12	1.94	0.49
3:D:366:ILE:HD11	5:F:15:MSE:HE2	1.95	0.49
4:E:89:GLU:OE2	4:E:97:ARG:NH1	2.45	0.49
1:A:217:GLU:HG2	1:B:232:ILE:HG23	1.95	0.49
3:D:827:PRO:HD3	3:D:854:HIS:CD2	2.47	0.49
3:D:826:ASN:HB3	3:D:832:ILE:HD11	1.95	0.49
5:F:31:LEU:HD21	7:H:10:DT:C2	2.48	0.49
7:H:14:DT:H2"	7:H:15:DG:H5"	1.94	0.49
3:D:729:VAL:HG11	3:D:802:ILE:HD11	1.95	0.49
3:D:1274:PRO:HG3	4:E:79:VAL:HG21	1.95	0.48
2:C:926:MET:HE1	3:D:817:LEU:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1087:GLU:HG2	2:C:1092:LYS:HG3	1.95	0.48
2:C:189:GLU:HB2	2:C:367:THR:HG21	1.95	0.48
2:C:216:VAL:HG22	2:C:222:VAL:HG22	1.93	0.48
2:C:1090:THR:OG1	2:C:1115:PRO:HB3	2.13	0.48
3:D:1270:ILE:HD13	4:E:56:TYR:HE2	1.78	0.48
6:G:14:DG:H2'	6:G:15:DT:C6	2.47	0.48
2:C:119:VAL:HG23	2:C:167:ILE:HD11	1.96	0.48
1:A:7:PRO:HA	1:A:25:PRO:HD2	1.95	0.48
2:C:38:ARG:HA	2:C:971:ILE:HG13	1.96	0.47
2:C:313:ARG:HH22	2:C:337:ASP:CG	2.21	0.47
2:C:610:ASN:OD1	2:C:613:ARG:NH1	2.47	0.47
5:F:140:SER:HB3	5:F:143:GLN:HG3	1.96	0.47
2:C:592:ALA:HA	2:C:976:VAL:HG21	1.96	0.47
1:B:9:LEU:HD11	1:B:21:PHE:HB3	1.96	0.47
2:C:120:ASP:OD1	2:C:120:ASP:N	2.46	0.47
2:C:522:GLY:O	2:C:553:ARG:HA	2.13	0.47
1:B:179:ASP:HB2	1:B:191:LYS:HE2	1.96	0.47
3:D:634:LYS:HG2	3:D:665:GLU:HG2	1.96	0.47
3:D:1247:GLY:H	3:D:1251:ASN:ND2	2.11	0.47
1:B:83:LEU:HB2	1:B:123:MET:HE1	1.96	0.47
2:C:202:VAL:HG21	2:C:345:LEU:HB2	1.96	0.47
2:C:891:ASN:OD1	2:C:891:ASN:N	2.47	0.47
3:D:505:HIS:CD2	3:D:507:LEU:HB2	2.49	0.47
4:E:64:ILE:HD11	4:E:98:GLU:OE2	2.15	0.47
2:C:444:ASN:O	2:C:447:SER:OG	2.27	0.47
2:C:1090:THR:OG1	2:C:1091:ILE:N	2.47	0.47
3:D:1054:ARG:HD3	3:D:1065:THR:HB	1.97	0.47
3:D:1055:LEU:H	3:D:1101:ASP:HB3	1.80	0.47
3:D:1154:ILE:O	3:D:1158:VAL:HG23	2.15	0.47
1:B:182:ARG:NH2	3:D:488:GLU:HG2	2.30	0.46
3:D:778:TRP:CD2	3:D:835:PRO:HG3	2.50	0.46
1:B:149:ALA:C	1:B:151:GLN:H	2.24	0.46
2:C:298:ASN:HA	2:C:302:LYS:HB2	1.97	0.46
3:D:556:ARG:NH1	4:E:35:ILE:O	2.48	0.46
2:C:642:VAL:HB	2:C:703:ALA:HB3	1.97	0.46
2:C:1045:SER:O	3:D:423:ASP:HB3	2.16	0.46
3:D:756:VAL:HG21	3:D:777:ILE:HD11	1.98	0.46
1:A:77:ILE:O	1:A:81:LYS:HG3	2.15	0.46
2:C:725:PRO:HA	2:C:730:ASN:HD21	1.80	0.46
3:D:827:PRO:O	3:D:858:LYS:NZ	2.38	0.46
5:F:170:LEU:HD22	5:F:175:VAL:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:848:ILE:HD13	2:C:874:ALA:HB2	1.96	0.46
1:A:222:ALA:HB1	1:B:208:LEU:HG	1.98	0.46
3:D:876:ARG:HG2	3:D:1226:PHE:HZ	1.81	0.46
3:D:453:LYS:O	3:D:457:MET:HG3	2.16	0.46
1:A:27:GLU:OE2	1:B:144:ARG:NH2	2.46	0.45
2:C:236:VAL:HG13	2:C:273:ALA:HB1	1.97	0.45
3:D:294:LYS:NZ	7:H:22:DA:O5'	2.49	0.45
1:A:144:ARG:NH2	1:B:27:GLU:OE2	2.49	0.45
5:F:28:ARG:NE	7:H:9:DG:H21	2.14	0.45
1:A:99:LYS:HG2	1:A:105:VAL:HG22	1.99	0.45
2:C:704:ASP:HB2	2:C:708:THR:HB	1.98	0.45
1:A:29:GLY:N	1:A:190:ASP:OD2	2.41	0.45
2:C:60:SER:OG	2:C:382:GLY:N	2.34	0.45
2:C:126:ASP:HA	2:C:170:GLY:HA3	1.99	0.45
2:C:396:MET:HE3	2:C:396:MET:HB2	1.88	0.45
1:A:83:LEU:HA	1:A:123:MET:HE1	1.97	0.45
2:C:446:LEU:HB2	2:C:713:MET:HE2	1.99	0.45
2:C:486:ILE:HD11	3:D:849:TYR:HE2	1.81	0.45
3:D:384:ASN:H	3:D:401:SER:HB3	1.82	0.45
1:B:220:GLY:HA2	1:B:223:ARG:HB3	1.99	0.45
2:C:396:MET:HE1	2:C:418:ILE:HG23	1.99	0.44
3:D:103:HIS:HB3	3:D:106:TYR:HD2	1.82	0.44
1:A:185:GLN:HG2	1:A:186:ARG:H	1.80	0.44
3:D:557:ILE:HG23	4:E:40:ILE:HD11	2.00	0.44
1:A:30:PHE:HE1	1:B:41:THR:HA	1.81	0.44
3:D:262:GLN:HB2	3:D:313:VAL:HG11	1.97	0.44
3:D:128:ILE:HD11	3:D:234:LEU:HD11	2.00	0.44
3:D:736:VAL:HG13	3:D:817:LEU:HD23	1.99	0.44
3:D:1166:THR:HB	3:D:1206:VAL:HG21	2.00	0.44
2:C:544:ALA:HB2	2:C:580:ASP:HB2	1.99	0.44
2:C:927:ASN:O	2:C:930:GLN:HG2	2.18	0.44
5:F:88:ASN:O	5:F:90:VAL:N	2.50	0.44
1:A:95:MET:HG2	1:A:112:PRO:HA	1.99	0.44
2:C:549:ASP:OD1	2:C:550:ALA:N	2.50	0.44
2:C:1090:THR:HG22	2:C:1118:PRO:HG3	1.99	0.44
3:D:1042:GLY:O	3:D:1083:ARG:NH2	2.48	0.44
2:C:588:SER:OG	2:C:589:VAL:N	2.51	0.44
2:C:760:ARG:HG2	2:C:865:VAL:HG22	2.00	0.44
2:C:168:ILE:HG12	2:C:431:PHE:HB3	2.00	0.44
3:D:646:ILE:O	3:D:649:GLU:HG3	2.18	0.43
4:E:47:VAL:HG23	4:E:56:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:235:ILE:HD12	3:D:241:TYR:HD1	1.83	0.43
3:D:588:LEU:HD23	3:D:723:TRP:CD1	2.54	0.43
2:C:32:VAL:H	2:C:33:PRO:HD3	1.84	0.43
7:H:14:DT:H6	7:H:14:DT:H2'	1.63	0.43
1:B:30:PHE:HA	1:B:33:THR:HG23	1.99	0.43
2:C:516:TYR:HD2	2:C:531:LEU:HD13	1.83	0.43
2:C:737:LEU:HG	2:C:895:ILE:HD12	1.99	0.43
3:D:823:LEU:HD23	3:D:835:PRO:HB3	2.00	0.43
1:A:218:LEU:HD12	1:A:218:LEU:HA	1.84	0.43
3:D:24:SER:HB2	3:D:94:HIS:HB3	2.00	0.43
3:D:1089:PHE:HA	3:D:1095:SER:HA	1.99	0.43
2:C:388:GLN:HG3	2:C:430:PHE:HB2	1.99	0.43
3:D:445:LYS:HB3	3:D:484:TRP:CZ3	2.54	0.43
1:A:10:SER:HB3	1:A:22:VAL:HG23	2.00	0.43
2:C:960:PRO:HD2	2:C:963:LEU:HD22	1.99	0.43
3:D:793:TYR:HB3	3:D:800:ILE:HG13	2.01	0.43
3:D:867:THR:HG22	3:D:1008:THR:HG23	2.01	0.43
2:C:107:PHE:HE1	2:C:418:ILE:HD11	1.83	0.43
3:D:139:VAL:HA	3:D:252:PHE:HA	2.01	0.43
1:B:28:PRO:HA	1:B:29:GLY:HA2	1.48	0.43
1:B:72:ASP:OD1	1:B:72:ASP:N	2.52	0.43
1:B:74:THR:HG21	3:D:608:GLU:HB2	2.00	0.43
1:A:84:VAL:HG13	1:A:119:HIS:HB2	2.01	0.42
2:C:239:LYS:NZ	2:C:265:ASP:OD2	2.50	0.42
2:C:514:THR:OG1	2:C:585:GLN:NE2	2.47	0.42
7:H:7:DC:H2'	7:H:8:DA:C8	2.54	0.42
3:D:575:ALA:O	3:D:713:VAL:HG21	2.18	0.42
3:D:637:LEU:O	3:D:661:ALA:HA	2.19	0.42
1:B:22:VAL:HG12	1:B:193:ILE:HG12	2.01	0.42
3:D:1250:GLU:O	3:D:1254:ILE:HG12	2.19	0.42
7:H:9:DG:H2''	7:H:10:DT:OP1	2.19	0.42
1:A:112:PRO:HB2	1:A:116:VAL:HG23	2.01	0.42
1:B:170:PRO:HB2	1:B:202:ILE:HD11	2.01	0.42
1:B:176:TYR:HB3	1:B:194:LEU:HD23	2.02	0.42
2:C:974:THR:HG23	2:C:980:ALA:H	1.84	0.42
5:F:152:GLU:HG3	5:F:156:LYS:HE3	2.02	0.42
2:C:896:GLY:HA2	3:D:431:VAL:HG13	2.00	0.42
3:D:290:LEU:HA	3:D:293:LEU:HD12	2.02	0.42
3:D:789:LEU:HD22	3:D:793:TYR:CE2	2.54	0.42
1:A:173:LYS:HE3	1:A:173:LYS:HB2	1.93	0.42
2:C:751:HIS:CD2	2:C:877:ARG:HD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1068:PHE:HZ	2:C:1076:MET:HG2	1.84	0.42
3:D:350:ARG:HD2	3:D:377:SER:OG	2.20	0.42
5:F:82:ARG:HB3	5:F:83:SER:H	1.65	0.42
2:C:276:ASP:O	2:C:279:ARG:HG2	2.20	0.42
2:C:558:ARG:HA	2:C:571:VAL:O	2.19	0.42
1:B:41:THR:HG21	1:B:215:LEU:HG	2.01	0.42
2:C:32:VAL:H	2:C:33:PRO:CD	2.33	0.42
2:C:286:PRO:HA	2:C:287:PRO:HD3	1.92	0.42
4:E:47:VAL:HG11	4:E:53:LEU:HB2	2.01	0.42
2:C:182:SER:HB2	2:C:377:ARG:HB2	2.01	0.42
3:D:573:PRO:HB2	3:D:576:MET:HE2	2.01	0.42
3:D:1005:GLU:HB3	3:D:1006:PRO:HD3	2.01	0.42
2:C:1124:LEU:HD22	3:D:417:LEU:HD11	2.02	0.42
3:D:353:ARG:HH22	5:F:42:ASP:HB3	1.85	0.42
3:D:565:ILE:HG23	3:D:575:ALA:HB3	2.02	0.42
3:D:816:THR:HG23	3:D:821:LYS:HA	2.02	0.42
3:D:927:THR:HB	3:D:961:LYS:HB3	2.02	0.42
1:B:167:ILE:HG23	3:D:620:MET:HE1	2.03	0.41
2:C:720:LEU:HD12	2:C:1026:GLY:O	2.20	0.41
2:C:844:SER:O	2:C:875:GLN:HB3	2.19	0.41
2:C:853:PHE:HD2	2:C:868:LEU:HD23	1.85	0.41
3:D:750:GLU:OE1	3:D:837:LYS:NZ	2.48	0.41
3:D:774:LEU:HD23	3:D:777:ILE:HD12	2.02	0.41
4:E:33:LEU:H	4:E:33:LEU:HD23	1.84	0.41
2:C:1108:LYS:HE3	5:F:114:LEU:HD22	2.02	0.41
3:D:446:LEU:HD12	3:D:446:LEU:H	1.85	0.41
1:A:18:ARG:NH2	2:C:997:ASP:OD1	2.53	0.41
2:C:140:ILE:HA	2:C:147:ILE:HG12	2.02	0.41
2:C:1109:GLY:O	4:E:69:ASN:ND2	2.51	0.41
3:D:1099:LEU:HD23	3:D:1099:LEU:HA	1.91	0.41
4:E:60:ARG:HG2	4:E:104:LEU:HD11	2.02	0.41
2:C:115:VAL:HG11	2:C:129:TYR:CZ	2.55	0.41
2:C:1111:ASN:HB3	4:E:62:ARG:NH1	2.35	0.41
3:D:1152:LYS:O	3:D:1156:VAL:HG23	2.20	0.41
5:F:76:MSE:HE3	5:F:76:MSE:HB2	1.98	0.41
2:C:285:GLU:CD	7:H:9:DG:H1	2.28	0.41
3:D:363:PRO:HD3	5:F:52:TRP:CE2	2.55	0.41
3:D:905:ALA:HB3	3:D:908:GLY:O	2.21	0.41
1:A:81:LYS:NZ	1:A:165:ASP:HB2	2.35	0.41
2:C:482:ARG:NH2	2:C:532:THR:O	2.53	0.41
3:D:578:ARG:H	3:D:581:MET:HE3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1045:PRO:HG3	3:D:1112:MET:HE2	2.03	0.41
2:C:213:GLU:HG3	2:C:225:ARG:HB2	2.03	0.41
2:C:598:GLU:HB3	2:C:977:PHE:HD2	1.85	0.41
3:D:602:ALA:HB2	3:D:608:GLU:HG3	2.02	0.41
3:D:611:VAL:HG22	3:D:634:LYS:HB2	2.03	0.41
4:E:96:LEU:HD12	4:E:96:LEU:HA	1.91	0.41
5:F:88:ASN:C	5:F:90:VAL:H	2.28	0.41
3:D:114:LEU:HD21	3:D:265:ILE:HD11	2.03	0.41
3:D:634:LYS:HA	3:D:664:ALA:O	2.21	0.41
3:D:886:VAL:O	3:D:992:GLY:N	2.54	0.40
4:E:44:LEU:HA	4:E:47:VAL:HG12	2.03	0.40
2:C:1071:MET:HE3	6:G:15:DT:H5'	2.02	0.40
3:D:294:LYS:HB2	3:D:294:LYS:HE3	1.88	0.40
3:D:33:THR:HB	3:D:327:MET:HE1	2.04	0.40
3:D:991:ILE:HD12	3:D:1266:ARG:HH12	1.87	0.40
3:D:1101:ASP:OD1	3:D:1101:ASP:N	2.55	0.40
1:A:66:VAL:O	1:A:69:VAL:HG22	2.22	0.40
3:D:111:PRO:HB3	7:H:22:DA:H5''	2.02	0.40
3:D:642:PRO:HG2	3:D:647:GLU:HB2	2.02	0.40
3:D:789:LEU:HD23	3:D:789:LEU:HA	1.90	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%)	211 (95%)	12 (5%)	0	100	100
1	B	230/359 (64%)	208 (90%)	19 (8%)	3 (1%)	9	39
2	C	1124/1178 (95%)	1076 (96%)	43 (4%)	5 (0%)	30	63
3	D	1261/1316 (96%)	1200 (95%)	57 (4%)	4 (0%)	36	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	79/110 (72%)	75 (95%)	4 (5%)	0	100	100
5	F	172/177 (97%)	166 (96%)	6 (4%)	0	100	100
All	All	3089/3499 (88%)	2936 (95%)	141 (5%)	12 (0%)	30	63

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	159	ILE
2	C	370	ILE
3	D	678	PRO
1	B	150	VAL
3	D	593	PRO
3	D	1089	PHE
2	C	32	VAL
2	C	922	VAL
3	D	607	PRO
2	C	732	GLU
2	C	520	VAL
1	B	7	PRO

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%)	190 (98%)	4 (2%)	47	64
1	B	191/308 (62%)	186 (97%)	5 (3%)	40	60
2	C	950/998 (95%)	932 (98%)	18 (2%)	50	66
3	D	1050/1095 (96%)	1038 (99%)	12 (1%)	65	73
4	E	66/90 (73%)	65 (98%)	1 (2%)	57	69
5	F	134/133 (101%)	130 (97%)	4 (3%)	36	57
All	All	2585/2932 (88%)	2541 (98%)	44 (2%)	53	67

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	51	VAL
1	A	111	VAL
1	A	171	VAL
1	B	43	LEU
1	B	79	ASN
1	B	111	VAL
1	B	196	VAL
1	B	202	ILE
2	C	32	VAL
2	C	39	VAL
2	C	54	LEU
2	C	119	VAL
2	C	173	ARG
2	C	185	VAL
2	C	322	LEU
2	C	363	VAL
2	C	370	ILE
2	C	373	PHE
2	C	409	VAL
2	C	472	VAL
2	C	571	VAL
2	C	696	VAL
2	C	858	GLU
2	C	875	GLN
2	C	1062	GLN
2	C	1137	VAL
3	D	70	PHE
3	D	82	VAL
3	D	139	VAL
3	D	443	LEU
3	D	515	MET
3	D	535	ASP
3	D	629	VAL
3	D	650	LEU
3	D	738	VAL
3	D	817	LEU
3	D	960	VAL
3	D	1250	GLU
4	E	84	GLU
5	F	56	GLU
5	F	60	ASP
5	F	85	ARG

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Mol	Chain	Res	Type
5	F	86	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	142	ASN
2	C	349	HIS
2	C	386	GLN
2	C	685	ASN
2	C	700	GLN
2	C	755	HIS
2	C	918	ASN
2	C	1054	GLN
3	D	262	GLN
3	D	564	ASN
3	D	687	GLN
3	D	767	HIS
3	D	1109	GLN
3	D	1269	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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, 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%)	0.34	9 (4%) 42 30	17, 47, 117, 159	0
1	B	232/359 (64%)	0.63	18 (7%) 19 18	23, 68, 131, 190	0
2	C	1126/1178 (95%)	0.54	83 (7%) 20 19	10, 58, 145, 190	0
3	D	1265/1316 (96%)	0.57	66 (5%) 33 25	9, 70, 174, 237	0
4	E	81/110 (73%)	0.94	9 (11%) 10 13	50, 83, 153, 208	0
5	F	172/177 (97%)	0.81	18 (10%) 11 14	34, 86, 160, 190	0
6	G	12/12 (100%)	1.44	3 (25%) 2 3	109, 142, 163, 165	0
7	H	24/24 (100%)	1.49	6 (25%) 2 3	113, 153, 212, 257	0
All	All	3137/3535 (88%)	0.58	212 (6%) 23 21	9, 66, 163, 257	0

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	192	ASP	7.7
1	B	155	SER	7.2
3	D	1049	VAL	6.4
5	F	89	VAL	5.8
3	D	1281	ALA	5.2
1	B	154	ALA	4.9
1	B	156	GLY	4.8
2	C	979	GLY	4.7
2	C	237	LEU	4.6
3	D	773	ALA	4.2
4	E	108	GLU	4.2
3	D	394	PRO	4.1
3	D	1011	THR	4.0
5	F	88	ASN	4.0
1	B	150	VAL	3.9
1	B	157	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
3	D	1106	GLU	3.9
4	E	57	ALA	3.9
3	D	1026	GLY	3.7
4	E	28	GLY	3.7
2	C	217	ASP	3.7
2	C	29	ASN	3.7
7	H	6	DT	3.7
1	A	2	LEU	3.6
2	C	466	GLU	3.6
2	C	325	GLY	3.5
2	C	218	LYS	3.5
2	C	28	SER	3.5
3	D	820	MET	3.5
2	C	252	PHE	3.5
3	D	746	LEU	3.4
6	G	14	DG	3.4
3	D	13	GLY	3.4
1	B	5	GLN	3.4
2	C	219	ARG	3.4
4	E	76	LEU	3.3
2	C	817	GLU	3.3
2	C	1061	ALA	3.3
3	D	580	ASP	3.3
6	G	15	DT	3.2
7	H	7	DC	3.2
2	C	299	LEU	3.2
1	B	183	VAL	3.2
3	D	1105	VAL	3.2
2	C	191	ILE	3.1
2	C	195	THR	3.1
2	C	193	LYS	3.1
2	C	324	VAL	3.1
3	D	775	VAL	3.1
1	A	150	VAL	3.1
2	C	464	SER	3.1
3	D	817	LEU	3.1
2	C	560	LEU	3.1
2	C	284	GLY	3.0
2	C	283	PRO	3.0
2	C	469	GLY	3.0
2	C	923	PRO	3.0
3	D	1138	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
3	D	803	VAL	3.0
2	C	402	GLU	2.9
1	B	1	MET	2.9
1	B	4	SER	2.9
1	B	143	GLY	2.9
2	C	329	THR	2.9
1	B	89	GLU	2.9
3	D	1136	ARG	2.9
5	F	85	ARG	2.9
1	B	185	GLN	2.9
2	C	339	VAL	2.9
2	C	220	ASP	2.9
2	C	104	SER	2.9
3	D	1007	GLY	2.9
1	B	149	ALA	2.9
2	C	815	THR	2.8
1	A	223	ARG	2.8
2	C	268	VAL	2.8
5	F	84	ALA	2.8
3	D	6	PHE	2.8
1	B	148	PRO	2.8
2	C	327	PRO	2.8
1	B	2	LEU	2.8
3	D	756	VAL	2.8
3	D	750	GLU	2.8
3	D	780	GLU	2.7
4	E	107	THR	2.7
3	D	171	GLU	2.7
2	C	1148	ARG	2.7
2	C	702	ILE	2.7
4	E	106	HIS	2.7
2	C	946	VAL	2.7
2	C	328	ILE	2.7
3	D	1099	LEU	2.7
2	C	981	GLN	2.6
3	D	937	ILE	2.6
5	F	101	GLN	2.6
1	A	34	LEU	2.6
2	C	535	GLU	2.6
1	A	226	ASN	2.6
3	D	284	GLY	2.6
3	D	1107	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	305	ARG	2.6
2	C	248	ILE	2.6
7	H	2	DC	2.6
3	D	809	GLY	2.6
2	C	99	PHE	2.6
4	E	88	GLN	2.6
2	C	522	GLY	2.6
2	C	566	GLY	2.6
2	C	267	THR	2.5
1	A	225	LEU	2.5
3	D	1118	PRO	2.5
2	C	221	THR	2.5
1	B	91	GLU	2.5
2	C	1123	VAL	2.5
5	F	100	GLU	2.5
5	F	78	ILE	2.5
2	C	523	VAL	2.5
2	C	568	VAL	2.5
3	D	1098	VAL	2.5
7	H	10	DT	2.5
2	C	509	PHE	2.5
7	H	25	DC	2.5
2	C	224	VAL	2.5
1	A	151	GLN	2.4
2	C	50	VAL	2.4
3	D	779	LYS	2.4
2	C	49	GLU	2.4
2	C	830	ARG	2.4
2	C	547	PRO	2.4
5	F	176	THR	2.4
4	E	75	ILE	2.4
3	D	735	ASP	2.4
2	C	697	GLU	2.4
5	F	99	PRO	2.4
1	A	142	ARG	2.4
2	C	310	ARG	2.4
5	F	94	ASP	2.4
5	F	62	ALA	2.4
1	A	199	LYS	2.4
2	C	828	LYS	2.4
2	C	405	THR	2.3
2	C	97	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	230	ARG	2.3
3	D	1266	ARG	2.3
2	C	261	THR	2.3
2	C	955	TRP	2.3
3	D	86	LYS	2.3
5	F	177	ARG	2.3
2	C	335	GLU	2.3
5	F	80	GLU	2.3
7	H	14	DT	2.3
3	D	1168	ILE	2.3
3	D	1175	PHE	2.3
2	C	137	ALA	2.3
3	D	196	LYS	2.3
6	G	4	DG	2.3
2	C	988	LEU	2.2
3	D	1027	GLY	2.2
2	C	470	LEU	2.2
3	D	814	THR	2.2
3	D	389	ARG	2.2
3	D	778	TRP	2.2
3	D	1043	LYS	2.2
2	C	1147	LEU	2.2
4	E	53	LEU	2.2
5	F	74	ARG	2.2
3	D	798	PRO	2.2
3	D	1108	GLY	2.2
3	D	1140	GLU	2.2
3	D	1217	THR	2.2
1	B	177	LYS	2.2
2	C	229	LYS	2.2
2	C	1003	ASP	2.2
3	D	537	ASP	2.2
3	D	753	ALA	2.2
3	D	765	LEU	2.2
2	C	32	VAL	2.2
2	C	583	PRO	2.2
3	D	957	ILE	2.2
3	D	653	HIS	2.2
5	F	69	LEU	2.2
2	C	346	VAL	2.2
3	D	306	GLY	2.2
3	D	830	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
5	F	64	PRO	2.2
3	D	498	LEU	2.2
5	F	96	SER	2.1
2	C	824	ILE	2.1
3	D	1157	ILE	2.1
3	D	855	GLY	2.1
3	D	887	ARG	2.1
1	B	219	PHE	2.1
2	C	631	GLU	2.1
3	D	781	ALA	2.1
3	D	797	ASN	2.1
2	C	232	GLN	2.1
2	C	502	VAL	2.1
3	D	1119	HIS	2.1
3	D	655	GLY	2.1
2	C	287	PRO	2.1
2	C	844	SER	2.1
2	C	286	PRO	2.1
3	D	833	PRO	2.1
2	C	490	GLU	2.1
5	F	11	GLU	2.1
3	D	754	ASP	2.1
3	D	900	GLU	2.0
3	D	1114	GLY	2.0
2	C	181	ARG	2.0
2	C	226	ILE	2.0
2	C	350	GLU	2.0
3	D	501	ALA	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
8	ZN	D	2002	1/1	0.97	0.05	82,82,82,82	0
8	ZN	D	2001	1/1	1.00	0.04	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.