Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 12:45 PM EDT

PDB ID	:	6DVE
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:

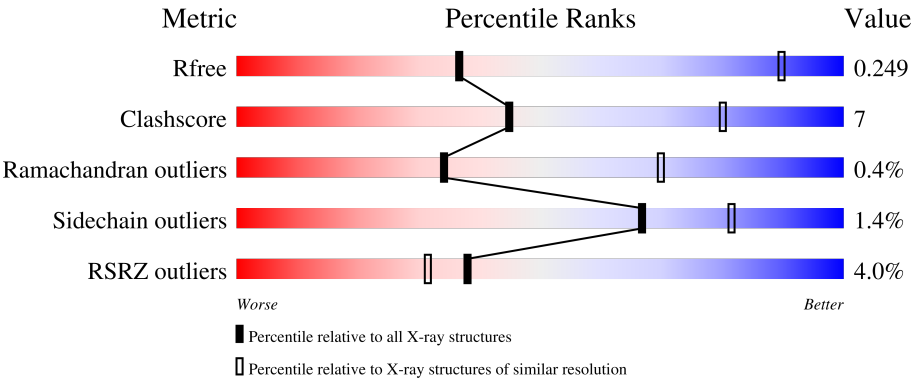
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.81 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.



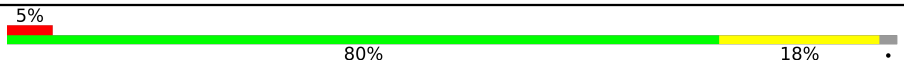
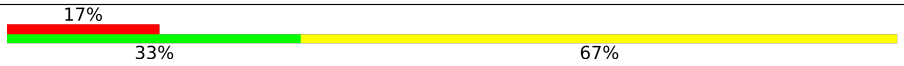
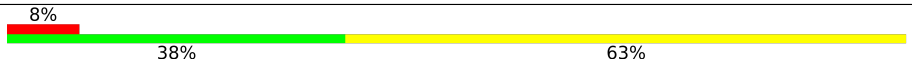
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1231 (4.04-3.60)
Clashscore	141614	1031 (4.02-3.62)
Ramachandran outliers	138981	1261 (4.04-3.60)
Sidechain outliers	138945	1255 (4.04-3.60)
RSRZ outliers	127900	1139 (4.04-3.60)

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 <=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	% 50% 12% 37%
1	B	359	2% 49% 15% 35%
2	C	1178	2% 80% 16% .
3	D	1316	5% 80% 16% .
4	E	110	7% 57% 16% 26%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	177	
6	G	12	
7	H	24	

2 Entry composition (i)

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 (three-letter code: ZN) (formula: Zn).

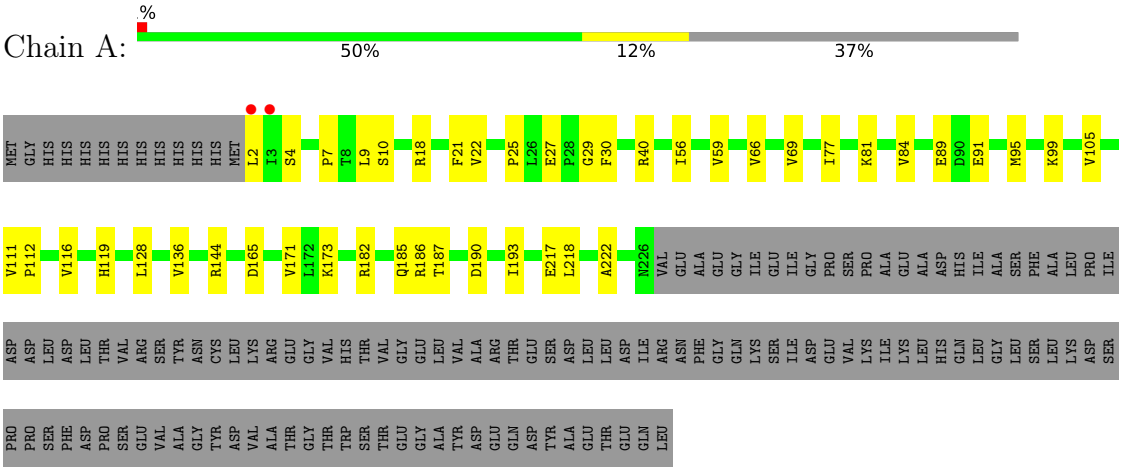
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		

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.

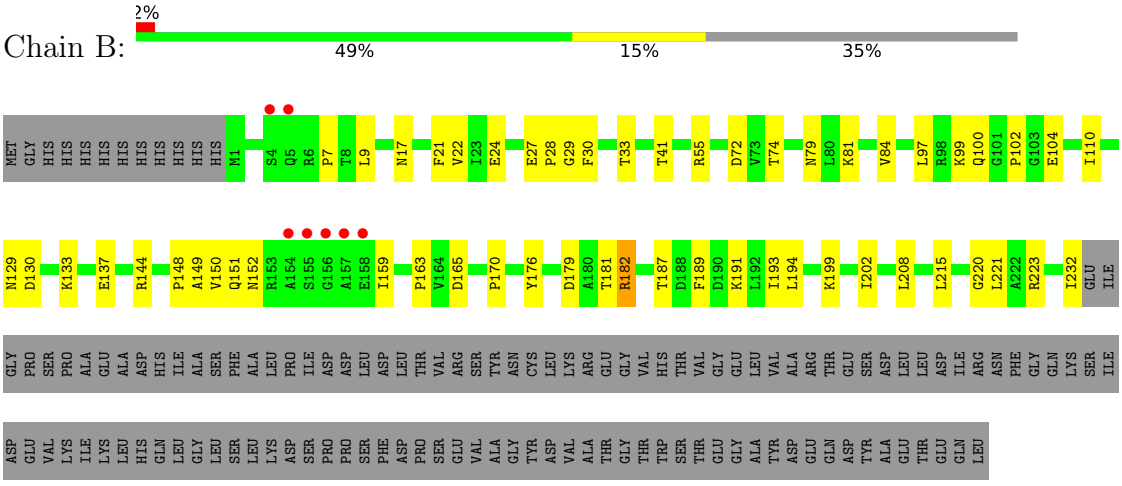
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



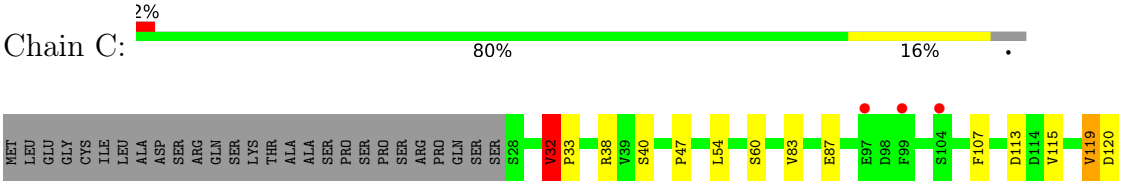
• Molecule 1: DNA-directed RNA polymerase subunit alpha

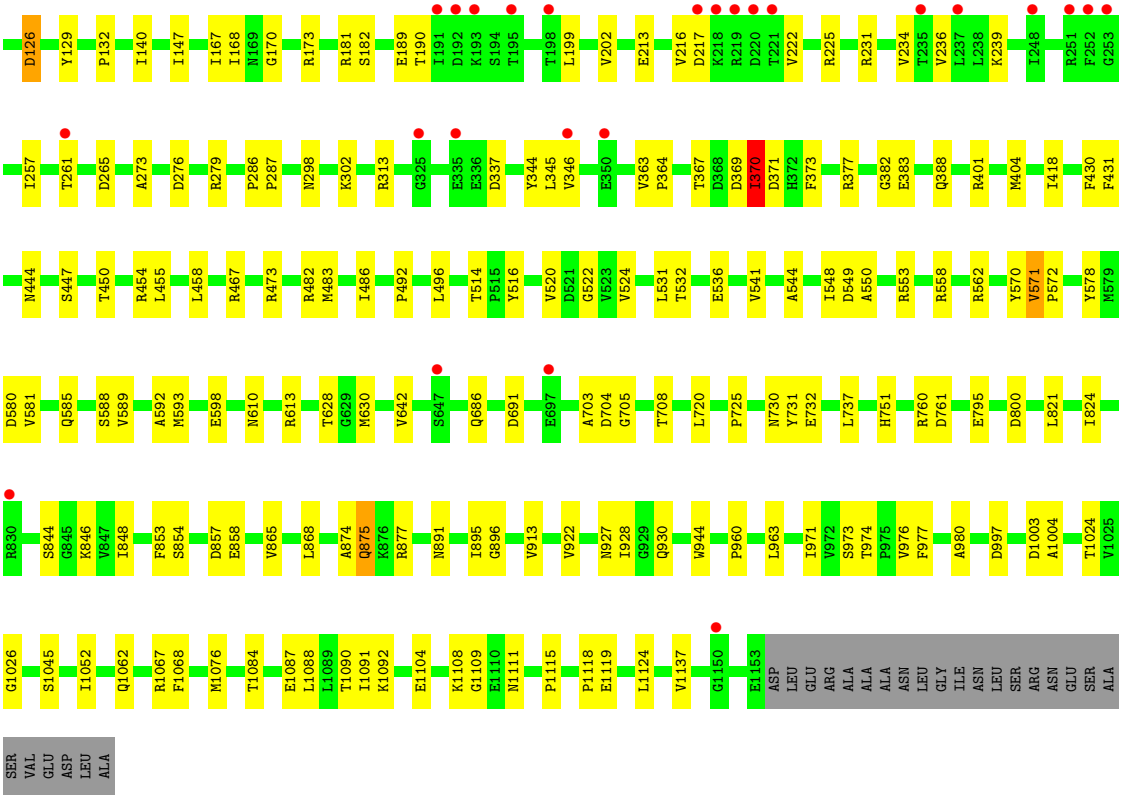
Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit beta

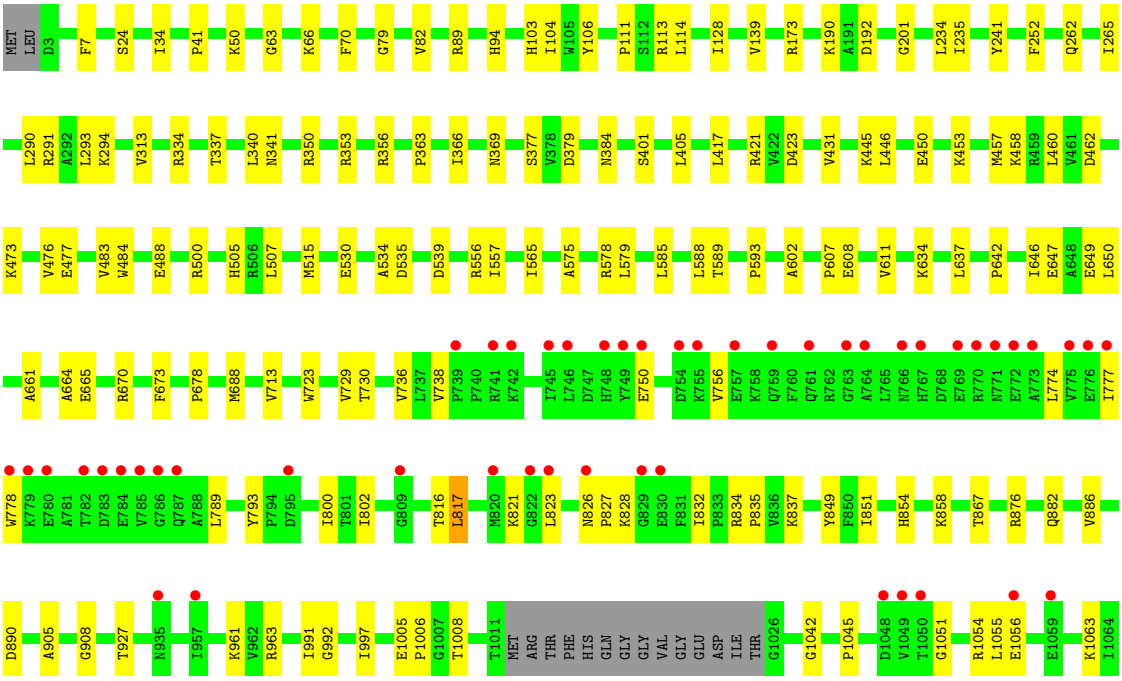
Chain C:

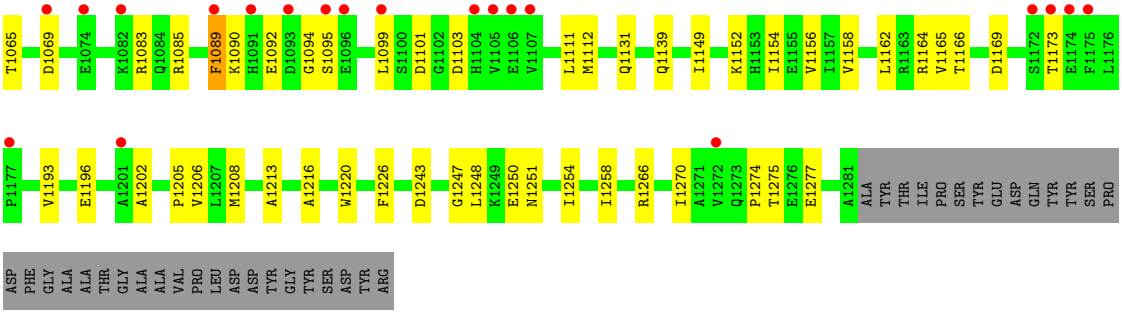




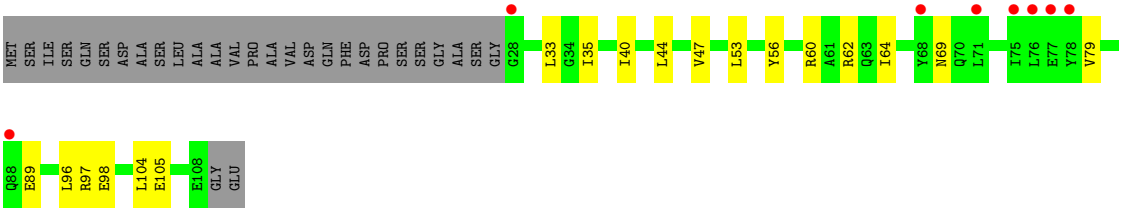
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:

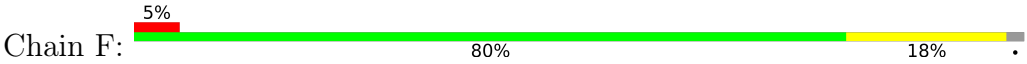


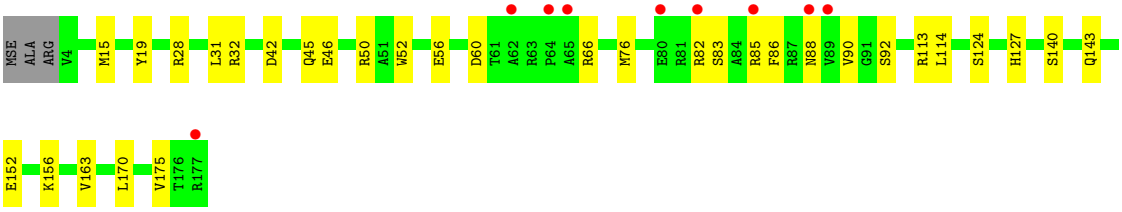


• Molecule 4: DNA-directed RNA polymerase subunit omega

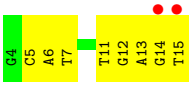


• Molecule 5: ECF RNA polymerase sigma factor SigL

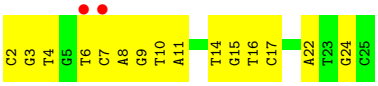




• Molecule 6: DNA (5'-D(*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*T)-3')



• 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 (i)

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 50.13 – 3.81	Depositor EDS
% Data completeness (in resolution range)	58.5 (46.68-3.81) 75.0 (50.13-3.81)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.200 , 0.248 0.200 , 0.249	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)	0.24 , 48.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.83	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.*

[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	0.23	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	0.24	0/10061	0.40	0/13600
4	E	0.24	0/643	0.38	0/877
5	F	0.24	0/1372	0.40	0/1863
6	G	0.59	0/273	0.96	0/420
7	H	0.60	0/549	0.98	0/846
All	All	0.26	0/25281	0.45	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	31	0
1	B	1732	0	1754	37	0
2	C	8724	0	8651	111	0
3	D	9895	0	9953	131	0
4	E	630	0	622	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1352	0	1346	22	0
6	G	244	0	137	6	0
7	H	490	0	272	18	0
8	D	2	0	0	0	0
All	All	24785	0	24491	320	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 (320) 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
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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
3:D:1056:GLU:HB2	3:D:1063:LYS:HG3	1.91	0.52
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:1067:ARG:HA	3:D:421:ARG:HA	1.92	0.52
3:D:473:LYS:NZ	3:D:477:GLU:OE2	2.39	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:38:ARG:HA	2:C:971:ILE:HG13	1.96	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
2:C:369:ASP:C	2:C:371:ASP:H	2.18	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
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
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
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
2:C:401:ARG:HA	2:C:404:MET:HE2	1.98	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:313:ARG:HH22	2:C:337:ASP:CG	2.21	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
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
2:C:514:THR:HG1	2:C:585:GLN:NE2	2.18	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:1005:GLU:HB3	3:D:1006:PRO:HD3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ALA:C	1:B:151:GLN:H	2.24	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
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:514:THR:HG1	2:C:585:GLN:HE21	1.67	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
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
3:D:1208:MET:HE3	3:D:1213:ALA:HB2	2.03	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
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
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
3:D:294:LYS:HB2	3:D:294:LYS:HE3	1.88	0.40
3:D:991:ILE:HD12	3:D:1266:ARG:HH12	1.87	0.40
3:D:1101:ASP:N	3:D:1101:ASP:OD1	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	12	48
2	C	1124/1178 (95%)	1076 (96%)	43 (4%)	5 (0%)	34	70
3	D	1261/1316 (96%)	1200 (95%)	57 (4%)	4 (0%)	41	74
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%)	34	70

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	607	PRO
2	C	732	GLU
2	C	520	VAL
1	B	7	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%)	190 (98%)	4 (2%)	53	73
1	B	191/308 (62%)	189 (99%)	2 (1%)	76	86
2	C	950/998 (95%)	935 (98%)	15 (2%)	62	79
3	D	1050/1095 (96%)	1040 (99%)	10 (1%)	76	86
4	E	66/90 (73%)	66 (100%)	0	100	100
5	F	134/133 (101%)	128 (96%)	6 (4%)	27	57
All	All	2585/2932 (88%)	2548 (99%)	37 (1%)	67	81

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	111	VAL
1	A	171	VAL
1	A	182	ARG
1	B	79	ASN
1	B	182	ARG
2	C	32	VAL
2	C	54	LEU
2	C	119	VAL
2	C	126	ASP
2	C	363	VAL
2	C	370	ILE
2	C	373	PHE
2	C	571	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	691	ASP
2	C	761	ASP
2	C	800	ASP
2	C	858	GLU
2	C	875	GLN
2	C	1062	GLN
2	C	1137	VAL
3	D	7	PHE
3	D	70	PHE
3	D	82	VAL
3	D	515	MET
3	D	535	ASP
3	D	539	ASP
3	D	650	LEU
3	D	738	VAL
3	D	817	LEU
3	D	1196	GLU
5	F	19	TYR
5	F	56	GLU
5	F	60	ASP
5	F	66	ARG
5	F	85	ARG
5	F	86	PHE

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

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 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 (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, 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%)	-0.42	2 (0%) 84 78	17, 47, 117, 159	0
1	B	232/359 (64%)	-0.16	7 (3%) 50 39	23, 68, 131, 190	0
2	C	1126/1178 (95%)	-0.29	28 (2%) 57 48	10, 58, 145, 190	0
3	D	1265/1316 (96%)	-0.12	69 (5%) 25 21	9, 70, 174, 237	0
4	E	81/110 (73%)	0.48	8 (9%) 7 6	50, 83, 153, 208	0
5	F	172/177 (97%)	0.19	9 (5%) 27 23	34, 86, 160, 190	0
6	G	12/12 (100%)	0.14	2 (16%) 1 2	109, 142, 163, 165	0
7	H	24/24 (100%)	0.74	2 (8%) 11 9	113, 153, 212, 257	0
All	All	3137/3535 (88%)	-0.17	127 (4%) 38 31	9, 66, 163, 257	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1099	LEU	6.3
5	F	177	ARG	5.7
3	D	1105	VAL	5.2
7	H	6	DT	4.9
3	D	1106	GLU	4.8
1	B	155	SER	4.8
3	D	1049	VAL	4.7
2	C	218	LYS	4.6
3	D	1175	PHE	4.4
2	C	192	ASP	4.1
3	D	820	MET	4.1
3	D	779	LYS	4.0
2	C	237	LEU	4.0
4	E	75	ILE	3.9
3	D	1174	GLU	3.9
1	B	4	SER	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	780	GLU	3.7
2	C	220	ASP	3.6
2	C	252	PHE	3.6
1	B	156	GLY	3.5
1	A	2	LEU	3.5
3	D	783	ASP	3.4
2	C	219	ARG	3.4
2	C	261	THR	3.3
4	E	88	GLN	3.3
1	B	5	GLN	3.2
3	D	769	GLU	3.2
2	C	248	ILE	3.2
3	D	755	LYS	3.2
3	D	1056	GLU	3.2
2	C	221	THR	3.1
4	E	76	LEU	3.1
4	E	77	GLU	3.1
5	F	64	PRO	3.1
3	D	1093	ASP	3.1
3	D	771	ASN	3.1
1	B	154	ALA	3.0
3	D	829	GLY	3.0
2	C	217	ASP	3.0
3	D	1173	THR	3.0
3	D	773	ALA	3.0
5	F	62	ALA	3.0
3	D	746	LEU	3.0
2	C	99	PHE	3.0
3	D	957	ILE	3.0
3	D	1059	GLU	2.9
3	D	759	GLN	2.9
5	F	88	ASN	2.9
3	D	1107	VAL	2.9
4	E	68	TYR	2.9
1	B	157	ALA	2.9
3	D	809	GLY	2.8
3	D	763	GLY	2.8
3	D	750	GLU	2.8
3	D	742	LYS	2.8
3	D	822	GLY	2.7
3	D	830	GLU	2.7
2	C	104	SER	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	195	THR	2.7
3	D	787	GLN	2.7
3	D	778	TRP	2.7
2	C	830	ARG	2.6
2	C	697	GLU	2.6
2	C	335	GLU	2.6
3	D	767	HIS	2.6
3	D	775	VAL	2.6
2	C	235	THR	2.6
4	E	71	LEU	2.5
3	D	782	THR	2.5
3	D	1172	SER	2.5
4	E	28	GLY	2.5
3	D	754	ASP	2.5
7	H	7	DC	2.5
3	D	784	GLU	2.5
3	D	766	ASN	2.5
2	C	191	ILE	2.5
5	F	89	VAL	2.4
2	C	325	GLY	2.4
2	C	193	LYS	2.4
3	D	786	GLY	2.4
3	D	757	GLU	2.4
6	G	14	DG	2.4
3	D	741	ARG	2.4
3	D	826	ASN	2.3
1	A	3	ILE	2.3
3	D	745	ILE	2.3
3	D	1272	VAL	2.3
2	C	346	VAL	2.3
3	D	776	GLU	2.3
3	D	749	TYR	2.3
3	D	770	ARG	2.3
3	D	1050	THR	2.3
3	D	823	LEU	2.3
1	B	158	GLU	2.2
3	D	1089	PHE	2.2
3	D	1069	ASP	2.2
3	D	761	GLN	2.2
2	C	253	GLY	2.2
3	D	772	GLU	2.2
3	D	739	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	1104	HIS	2.2
2	C	647	SER	2.2
3	D	1095	SER	2.2
3	D	785	VAL	2.2
3	D	764	ALA	2.2
3	D	1082	LYS	2.2
3	D	1048	ASP	2.2
2	C	97	GLU	2.2
2	C	198	THR	2.2
6	G	15	DT	2.2
4	E	78	TYR	2.1
3	D	777	ILE	2.1
2	C	251	ARG	2.1
3	D	795	ASP	2.1
5	F	80	GLU	2.1
3	D	1074	GLU	2.1
3	D	935	ASN	2.1
3	D	1096	GLU	2.1
3	D	1177	PRO	2.1
5	F	82	ARG	2.1
2	C	1150	GLY	2.1
3	D	1201	ALA	2.0
2	C	350	GLU	2.0
3	D	748	HIS	2.0
3	D	1091	HIS	2.0
5	F	65	ALA	2.0
5	F	85	ARG	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
8	ZN	D	2002	1/1	0.98	0.08	82,82,82,82	0
8	ZN	D	2001	1/1	0.99	0.10	57,57,57,57	0

6.5 Other polymers (i)

There are no such residues in this entry.