



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:11 PM EDT

PDB ID : 6KOO / pdb_00006koo
Title : Mycobacterium tuberculosis initial transcription complex comprising sigma H and 5'-OH RNA of 7 nt
Authors : Li, L.; Zhang, Y.
Deposited on : 2019-08-12
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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:

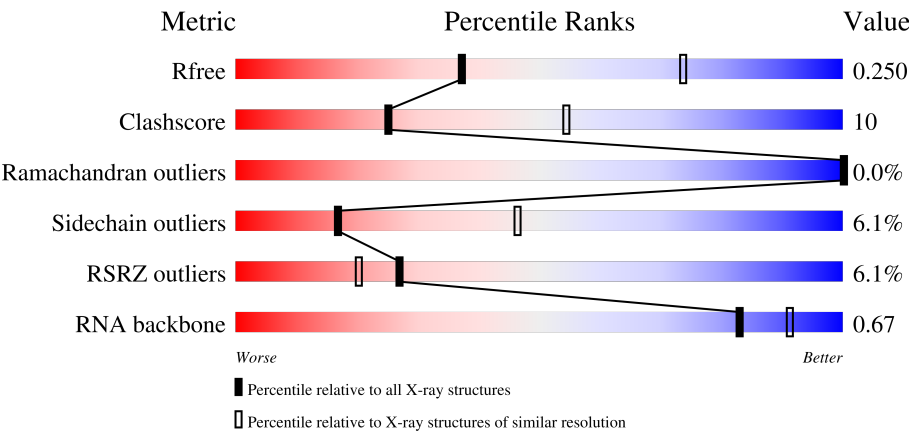
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



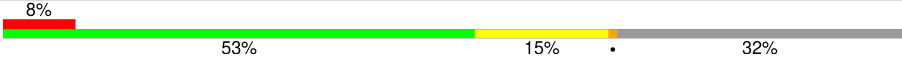
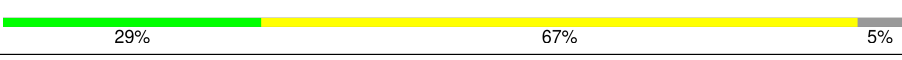
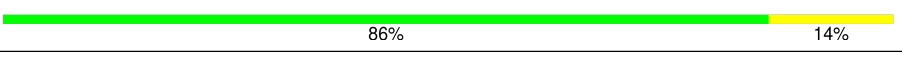
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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 $\leq 5\%$. 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	368	48%10%41% 7%
1	B	368	43%17%38% 7%
2	C	1174	71%24% 6%
3	D	1317	73%21% 4%

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Mol	Chain	Length	Quality of chain
4	E	110	
5	F	218	
6	G	23	
7	H	21	
8	I	7	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 24837 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	217	Total	C	N	O	S	0	0	0
			1646	1035	285	324	2			
1	B	230	Total	C	N	O	S	0	0	0
			1670	1057	283	328	2			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP P9WGZ1
A	-19	GLY	-	expression tag	UNP P9WGZ1
A	-18	HIS	-	expression tag	UNP P9WGZ1
A	-17	HIS	-	expression tag	UNP P9WGZ1
A	-16	HIS	-	expression tag	UNP P9WGZ1
A	-15	HIS	-	expression tag	UNP P9WGZ1
A	-14	HIS	-	expression tag	UNP P9WGZ1
A	-13	HIS	-	expression tag	UNP P9WGZ1
A	-12	HIS	-	expression tag	UNP P9WGZ1
A	-11	HIS	-	expression tag	UNP P9WGZ1
A	-10	HIS	-	expression tag	UNP P9WGZ1
A	-9	HIS	-	expression tag	UNP P9WGZ1
A	-8	SER	-	expression tag	UNP P9WGZ1
A	-7	SER	-	expression tag	UNP P9WGZ1
A	-6	GLY	-	expression tag	UNP P9WGZ1
A	-5	HIS	-	expression tag	UNP P9WGZ1
A	-4	ILE	-	expression tag	UNP P9WGZ1
A	-3	GLU	-	expression tag	UNP P9WGZ1
A	-2	GLY	-	expression tag	UNP P9WGZ1
A	-1	ARG	-	expression tag	UNP P9WGZ1
A	0	HIS	-	expression tag	UNP P9WGZ1
B	-20	MET	-	initiating methionine	UNP P9WGZ1
B	-19	GLY	-	expression tag	UNP P9WGZ1
B	-18	HIS	-	expression tag	UNP P9WGZ1
B	-17	HIS	-	expression tag	UNP P9WGZ1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP P9WGZ1
B	-15	HIS	-	expression tag	UNP P9WGZ1
B	-14	HIS	-	expression tag	UNP P9WGZ1
B	-13	HIS	-	expression tag	UNP P9WGZ1
B	-12	HIS	-	expression tag	UNP P9WGZ1
B	-11	HIS	-	expression tag	UNP P9WGZ1
B	-10	HIS	-	expression tag	UNP P9WGZ1
B	-9	HIS	-	expression tag	UNP P9WGZ1
B	-8	SER	-	expression tag	UNP P9WGZ1
B	-7	SER	-	expression tag	UNP P9WGZ1
B	-6	GLY	-	expression tag	UNP P9WGZ1
B	-5	HIS	-	expression tag	UNP P9WGZ1
B	-4	ILE	-	expression tag	UNP P9WGZ1
B	-3	GLU	-	expression tag	UNP P9WGZ1
B	-2	GLY	-	expression tag	UNP P9WGZ1
B	-1	ARG	-	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	1135	Total	C	N	O	S	0	0	0
			8673	5428	1519	1687	39			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	MET	-	initiating methionine	UNP P9WGY9
C	0	VAL	-	expression tag	UNP P9WGY9

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1258	Total	C	N	O	S	0	0	0
			9763	6118	1766	1838	41			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP P9WGY7
D	1	VAL	-	expression tag	UNP P9WGY7

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	75	Total	C	N	O	0	0	0
			592	378	99	115			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	182	Total	C	N	O	S	0	0	0
			1432	896	251	280	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	GLY	-	expression tag	UNP P9WGH9
F	0	ALA	-	expression tag	UNP P9WGH9

- Molecule 6 is a DNA chain called DNA (5'-D(*TP*TP*GP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	23	Total	C	N	O	P	0	0	0
			475	226	89	138	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	20	Total	C	N	O	P	0	0	0
			412	196	77	120	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	7	Total	C	N	O	P	0	0	0
			142	65	24	47	6			

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

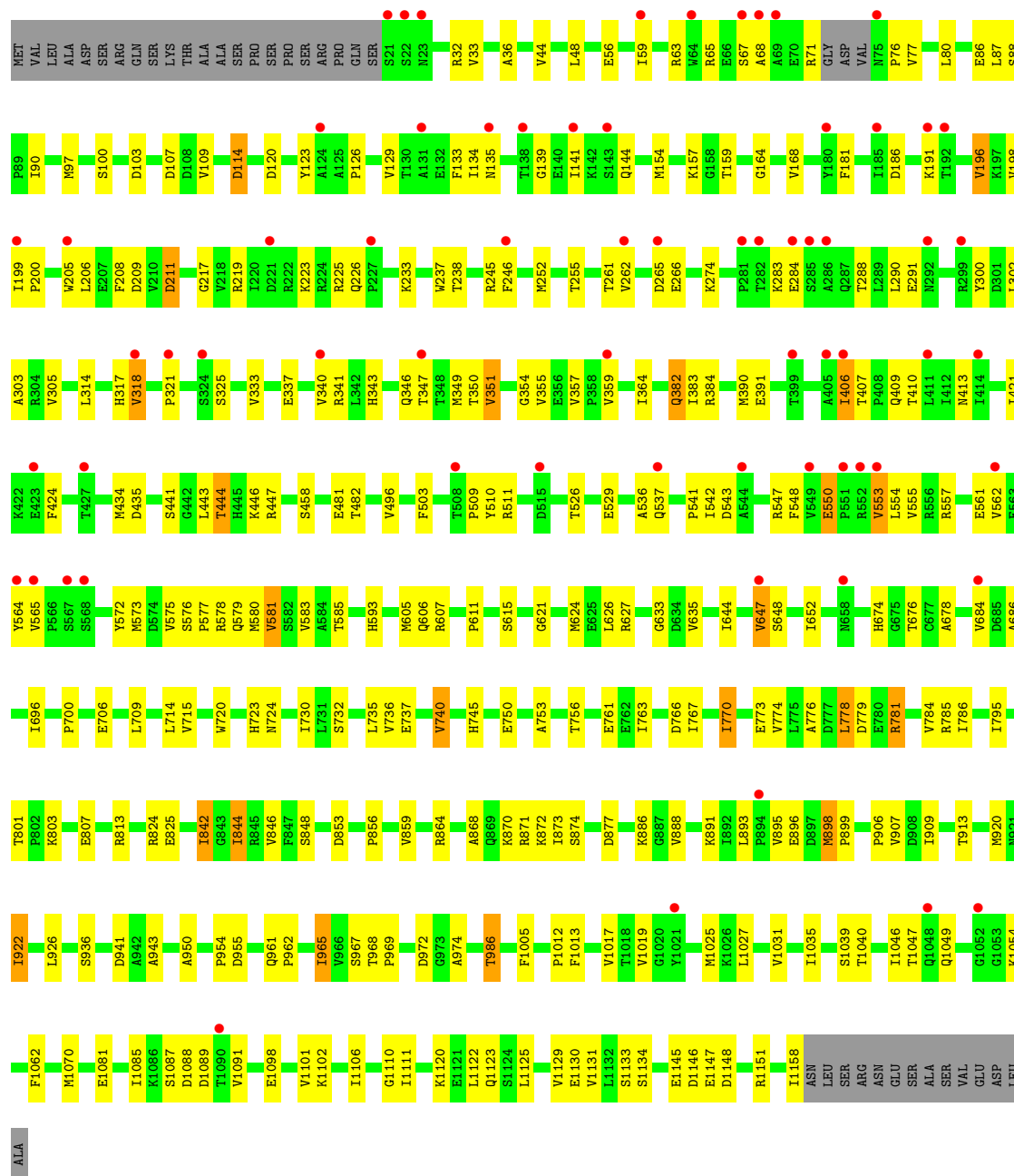
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	Zn	0	0
			2	2		

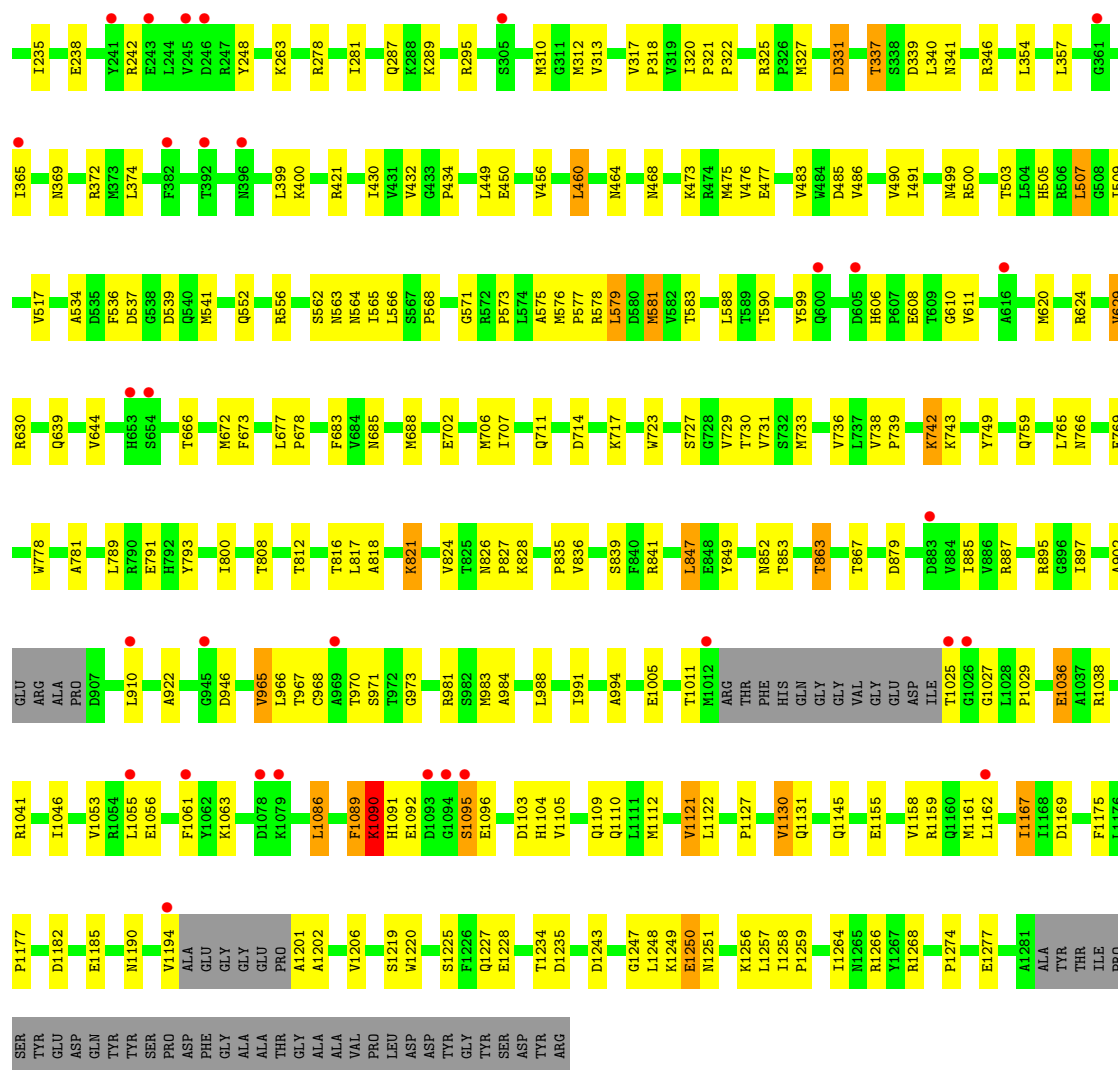
- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	1	Total 1	Mg 1	0	0

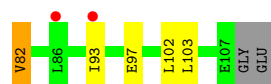
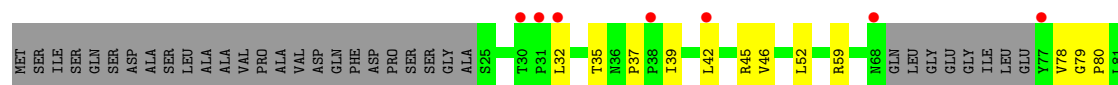
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	C	8	Total 8	O 8	0	0
11	D	12	Total 12	O 12	0	0
11	F	4	Total 4	O 4	0	0
11	H	3	Total 3	O 3	0	0
11	I	2	Total 2	O 2	0	0

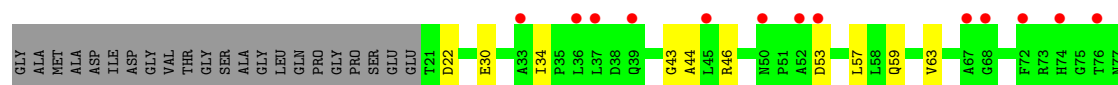


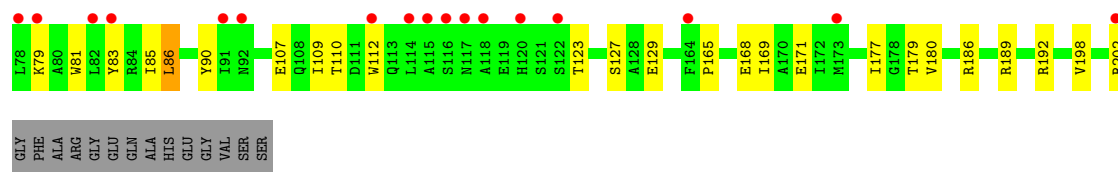


• Molecule 4: DNA-directed RNA polymerase subunit omega

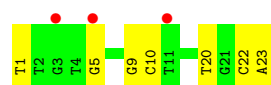


• Molecule 5: ECF RNA polymerase sigma factor SigH

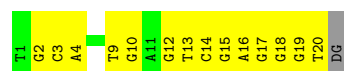
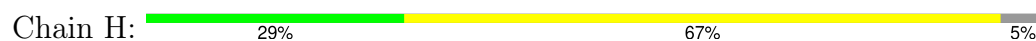




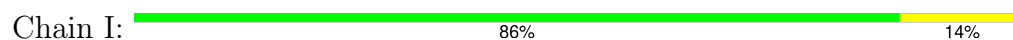
- Molecule 6: DNA (5'-D(*TP*TP*GP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*A)-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	125.03Å 162.31Å 128.48Å 90.00° 117.03° 90.00°	Depositor
Resolution (Å)	31.38 – 2.80 31.38 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.9 (31.38-2.80) 97.4 (31.38-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.206 , 0.248 0.208 , 0.250	Depositor DCC
R_{free} test set	2398 reflections (2.18%)	wwPDB-VP
Wilson B-factor (Å ²)	77.6	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24837	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.24	0/1671	0.48	0/2273
1	B	0.33	0/1695	0.49	1/2314 (0.0%)
2	C	0.33	1/8830 (0.0%)	0.48	0/11988
3	D	0.28	1/9923 (0.0%)	0.46	1/13425 (0.0%)
4	E	0.20	0/604	0.40	0/822
5	F	0.21	0/1460	0.38	0/1983
6	G	0.27	0/533	0.47	0/823
7	H	0.43	0/462	0.50	0/713
8	I	0.28	0/157	0.50	0/242
All	All	0.30	2/25335 (0.0%)	0.47	2/34583 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	77	VAL	C-O	-5.61	1.18	1.23
3	D	1250	GLU	C-O	-5.52	1.17	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	GLU	N-CA-C	8.92	120.42	108.38
3	D	1090	LYS	N-CA-C	5.59	117.01	108.52

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	1646	0	1676	28	0
1	B	1670	0	1651	46	0
2	C	8673	0	8508	187	0
3	D	9763	0	9772	205	0
4	E	592	0	587	11	0
5	F	1432	0	1359	22	0
6	G	475	0	261	6	0
7	H	412	0	227	22	0
8	I	142	0	78	1	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
11	C	8	0	0	0	0
11	D	12	0	0	0	0
11	F	4	0	0	0	0
11	H	3	0	0	0	0
11	I	2	0	0	0	0
All	All	24837	0	24119	476	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 10.

All (476) 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)
7:H:14:DC:H2'	7:H:15:DG:H5''	1.20	1.11
7:H:14:DC:C2'	7:H:15:DG:H5''	1.96	0.95
3:D:1090:LYS:HG3	3:D:1095:SER:C	1.96	0.90
3:D:1090:LYS:HG3	3:D:1095:SER:O	1.75	0.87
7:H:19:DG:C2'	7:H:20:DT:H5'	2.06	0.86
2:C:606:GLN:HG2	2:C:1025:MET:HE1	1.59	0.85
1:A:40:ARG:HE	1:B:33:THR:HG22	1.43	0.83
2:C:557:ARG:H	2:C:561:GLU:HB3	1.45	0.81
7:H:12:DG:H2''	7:H:13:DT:H5'	1.60	0.80
2:C:537:GLN:HG3	3:D:847:LEU:HD11	1.65	0.79
3:D:1090:LYS:CD	3:D:1091:HIS:H	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:59:ARG:HH22	4:E:79:GLY:HA3	1.47	0.79
2:C:1040:THR:HG22	5:F:127:SER:HB2	1.64	0.78
2:C:553:VAL:O	2:C:564:TYR:HA	1.83	0.78
7:H:16:DA:C2'	7:H:17:DG:H5'	2.15	0.77
3:D:1090:LYS:HD3	3:D:1091:HIS:H	1.50	0.76
3:D:92:MET:HG3	3:D:321:PRO:HD3	1.68	0.75
1:B:151:GLN:HG2	1:B:163:PRO:HG2	1.69	0.75
3:D:113:ARG:NH1	3:D:1235:ASP:OD1	2.22	0.73
3:D:539:ASP:CG	8:I:10:A:O3'	2.33	0.72
3:D:1090:LYS:CB	3:D:1096:GLU:HA	2.20	0.72
7:H:16:DA:H2''	7:H:17:DG:H5'	1.73	0.71
3:D:47:PHE:O	3:D:88:ARG:NH2	2.24	0.71
3:D:1169:ASP:H	3:D:1202:ALA:HB3	1.56	0.70
3:D:1089:PHE:HD1	3:D:1089:PHE:H	1.38	0.70
1:B:69:VAL:HG12	1:B:71:GLU:H	1.56	0.70
2:C:44:VAL:O	2:C:627:ARG:NH2	2.25	0.69
2:C:103:ASP:O	2:C:129:VAL:HA	1.93	0.69
2:C:56:GLU:OE1	2:C:63:ARG:HD3	1.93	0.69
1:B:30:PHE:HA	1:B:33:THR:HG23	1.73	0.69
7:H:19:DG:H2'	7:H:20:DT:H5'	1.74	0.69
2:C:144:GLN:HE22	2:C:409:GLN:HB2	1.57	0.68
2:C:745:HIS:HD2	2:C:871:ARG:HG3	1.57	0.68
2:C:1047:THR:HG23	2:C:1049:GLN:H	1.58	0.68
7:H:19:DG:H2''	7:H:20:DT:H5'	1.76	0.68
3:D:1274:PRO:HG3	4:E:78:VAL:HG11	1.75	0.68
2:C:803:LYS:O	3:D:56:ARG:NH2	2.28	0.67
2:C:913:THR:HG23	3:D:731:VAL:HG23	1.75	0.67
3:D:885:ILE:HG13	3:D:887:ARG:HD3	1.75	0.67
1:B:64:THR:HA	1:B:73:VAL:HB	1.78	0.66
2:C:67:SER:O	2:C:71:ARG:HD3	1.96	0.66
4:E:46:VAL:HG21	4:E:52:LEU:HB2	1.77	0.66
2:C:542:ILE:HG23	2:C:547:ARG:H	1.59	0.66
1:B:97:LEU:HD13	1:B:110:ILE:HG22	1.79	0.65
3:D:365:ILE:HD12	5:F:34:ILE:HD13	1.77	0.65
2:C:893:LEU:HB2	2:C:898:MET:HE1	1.77	0.64
3:D:1247:GLY:HA3	3:D:1250:GLU:OE1	1.97	0.64
2:C:1040:THR:HG21	5:F:129:GLU:H	1.63	0.64
1:A:93:VAL:HG11	1:A:116:VAL:HG11	1.80	0.64
2:C:114:ASP:OD1	2:C:114:ASP:N	2.27	0.64
2:C:341:ARG:HD2	2:C:349:MET:HG3	1.78	0.64
3:D:1219:SER:CB	3:D:1250:GLU:OE2	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1087:SER:HB3	3:D:421:ARG:O	1.98	0.63
7:H:3:DC:H2''	7:H:4:DA:N7	2.14	0.63
3:D:1090:LYS:HD3	3:D:1091:HIS:N	2.14	0.62
1:A:63:PHE:CD1	2:C:842:ILE:HD11	2.34	0.62
7:H:9:DT:H2'	7:H:10:DG:C8	2.34	0.62
5:F:186:ARG:HA	5:F:189:ARG:HD2	1.81	0.62
1:A:222:ALA:HB1	1:B:208:LEU:HG	1.80	0.62
2:C:351:VAL:HG23	2:C:354:GLY:HA3	1.81	0.62
2:C:36:ALA:HB2	2:C:969:PRO:HG2	1.82	0.62
3:D:739:PRO:HG2	3:D:742:LYS:HB2	1.81	0.62
1:B:98:ARG:HA	1:B:134:LEU:O	1.99	0.61
2:C:1035:ILE:O	2:C:1054:LYS:NZ	2.30	0.61
2:C:1130:GLU:OE1	3:D:11:ARG:NH2	2.24	0.61
3:D:981:ARG:HA	3:D:988:LEU:HA	1.83	0.61
3:D:59:GLU:HG2	3:D:66:LYS:HG3	1.82	0.61
3:D:1011:THR:O	3:D:1145:GLN:NE2	2.32	0.60
3:D:1092:GLU:OE2	3:D:1104:HIS:ND1	2.34	0.60
3:D:97:LEU:HD22	3:D:374:LEU:HD21	1.83	0.60
5:F:110:THR:HG22	5:F:112:TRP:H	1.66	0.60
2:C:407:THR:HG23	2:C:409:GLN:H	1.66	0.60
7:H:12:DG:C2'	7:H:13:DT:H5'	2.30	0.60
1:B:228:GLU:HA	1:B:228:GLU:OE1	2.02	0.60
1:A:40:ARG:NE	1:B:33:THR:HG22	2.16	0.60
3:D:629:VAL:HG12	3:D:630:ARG:HG3	1.82	0.60
2:C:1098:GLU:HG2	2:C:1102:LYS:HE2	1.82	0.59
3:D:106:TYR:HB3	3:D:312:MET:HE3	1.83	0.59
2:C:678:ALA:HA	2:C:700:PRO:HG3	1.83	0.59
2:C:926:LEU:HD22	3:D:733:MET:HE3	1.83	0.59
1:A:213:LYS:HD2	1:B:223:ARG:HD2	1.83	0.59
2:C:848:SER:O	2:C:853:ASP:HB2	2.03	0.59
2:C:968:THR:HG23	2:C:974:ALA:H	1.68	0.59
2:C:1120:LYS:HE3	3:D:92:MET:HE2	1.85	0.58
3:D:1248:LEU:HD12	3:D:1249:LYS:N	2.18	0.58
2:C:536:ALA:HA	2:C:555:VAL:HG12	1.86	0.58
2:C:895:VAL:HG13	2:C:906:PRO:HG2	1.86	0.58
2:C:444:THR:OG1	2:C:607:ARG:HD2	2.03	0.58
1:A:57:ASP:HB2	1:A:135:GLU:HB3	1.86	0.57
7:H:19:DG:H2''	7:H:20:DT:C5'	2.33	0.57
2:C:337:GLU:OE2	2:C:341:ARG:NH2	2.36	0.57
3:D:847:LEU:HD12	3:D:847:LEU:H	1.68	0.57
1:A:107:ALA:HB2	1:A:123:MET:HE2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:233:LYS:HZ3	2:C:262:VAL:HA	1.68	0.57
1:A:86:SER:OG	1:A:119:HIS:NE2	2.31	0.57
3:D:1055:LEU:HD11	3:D:1086:LEU:HD21	1.87	0.57
2:C:134:ILE:HG12	2:C:141:ILE:HG12	1.87	0.57
2:C:383:ILE:HG12	2:C:421:ILE:HD11	1.85	0.57
3:D:21:ARG:NE	3:D:96:GLU:OE2	2.29	0.57
3:D:1167:ILE:HG22	3:D:1177:PRO:HA	1.87	0.56
2:C:382:GLN:HG2	2:C:424:PHE:HB2	1.87	0.56
2:C:776:ALA:O	2:C:785:ARG:NH2	2.37	0.56
3:D:339:ASP:HB3	3:D:399:LEU:HB3	1.87	0.56
2:C:407:THR:HG22	2:C:410:THR:HG23	1.86	0.56
1:B:5:GLN:HA	1:B:233:GLU:HG3	1.87	0.56
2:C:856:PRO:HG2	2:C:859:VAL:HG21	1.87	0.56
2:C:32:ARG:HA	2:C:965:ILE:HG22	1.88	0.56
2:C:714:LEU:HD23	2:C:907:VAL:HA	1.87	0.56
4:E:37:PRO:HG2	4:E:42:LEU:HD11	1.88	0.56
2:C:1129:VAL:HG22	3:D:12:ILE:HG23	1.87	0.56
3:D:1227:GLN:HG2	3:D:1228:GLU:HG3	1.87	0.56
2:C:626:LEU:HB2	2:C:706:GLU:HG2	1.89	0.55
3:D:1182:ASP:HB3	3:D:1185:GLU:HG2	1.87	0.55
3:D:1219:SER:HB2	3:D:1250:GLU:OE2	2.06	0.55
2:C:581:VAL:HG13	2:C:585:THR:HB	1.87	0.55
2:C:735:LEU:HA	2:C:740:VAL:HG13	1.87	0.55
3:D:1089:PHE:CD1	3:D:1089:PHE:N	2.72	0.55
1:B:55:ARG:NH2	1:B:159:ILE:O	2.34	0.55
2:C:652:ILE:HD13	2:C:696:ILE:HG22	1.89	0.55
1:B:5:GLN:CB	1:B:234:ILE:H	2.20	0.55
1:B:218:LEU:O	1:B:221:LEU:HB2	2.06	0.55
3:D:86:LYS:O	3:D:89:ARG:HG2	2.06	0.55
2:C:133:PHE:CZ	2:C:406:ILE:HD11	2.42	0.55
3:D:155:MET:HE1	3:D:219:LEU:HD22	1.89	0.55
3:D:565:ILE:H	3:D:706:MET:HE1	1.71	0.55
2:C:593:HIS:HB3	2:C:922:ILE:HD12	1.89	0.55
3:D:103:HIS:HB3	3:D:106:TYR:HD2	1.72	0.55
3:D:12:ILE:HD11	3:D:1220:TRP:CE3	2.42	0.55
3:D:20:ILE:HD13	3:D:318:PRO:HD3	1.89	0.55
3:D:879:ASP:OD1	3:D:1249:LYS:NZ	2.39	0.55
2:C:541:PRO:HG2	2:C:550:GLU:HB2	1.90	0.54
7:H:3:DC:H2"	7:H:4:DA:C8	2.41	0.54
3:D:357:LEU:HD21	5:F:63:VAL:HG22	1.89	0.54
2:C:90:ILE:HD13	2:C:391:GLU:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:557:ARG:N	2:C:561:GLU:HB3	2.21	0.54
2:C:109:VAL:HG11	2:C:123:TYR:CE1	2.42	0.54
3:D:1190:ASN:HD21	3:D:1201:ALA:HB1	1.73	0.54
2:C:1146:ASP:OD1	3:D:71:LYS:NZ	2.40	0.54
3:D:1027:GLY:H	3:D:1029:PRO:HD2	1.73	0.53
1:B:54:ILE:HG22	1:B:138:LEU:HG	1.89	0.53
2:C:510:TYR:HB3	2:C:572:TYR:HB3	1.90	0.53
3:D:62:CYS:N	3:D:78:CYS:SG	2.81	0.53
1:B:34:LEU:HD12	1:B:192:LEU:HD22	1.90	0.53
1:B:123:MET:HE2	1:B:125:ILE:HG22	1.89	0.53
2:C:1046:ILE:HD12	2:C:1046:ILE:H	1.74	0.53
1:B:59:VAL:HG11	1:B:66:VAL:HG22	1.91	0.53
2:C:1062:PHE:HZ	2:C:1070:MET:HE3	1.73	0.53
5:F:110:THR:HG22	5:F:112:TRP:N	2.24	0.53
2:C:750:GLU:OE1	2:C:864:ARG:NH1	2.42	0.53
2:C:961:GLN:HG3	2:C:962:PRO:HD2	1.89	0.53
3:D:12:ILE:HD11	3:D:1220:TRP:CZ3	2.44	0.53
2:C:736:VAL:HG13	2:C:872:LYS:HD2	1.91	0.53
2:C:97:MET:HB2	2:C:133:PHE:HE1	1.74	0.52
2:C:364:ILE:HD12	2:C:364:ILE:H	1.74	0.52
3:D:1090:LYS:HD2	3:D:1091:HIS:H	1.70	0.52
3:D:102:THR:HG22	3:D:313:VAL:HG22	1.90	0.52
2:C:217:GLY:HA3	2:C:225:ARG:HD2	1.92	0.52
3:D:34:ILE:HG22	3:D:41:PRO:HA	1.91	0.52
2:C:68:ALA:HA	2:C:71:ARG:HD3	1.92	0.52
5:F:30:GLU:HA	5:F:34:ILE:HD12	1.92	0.52
3:D:116:TYR:O	3:D:295:ARG:NH1	2.43	0.51
3:D:1248:LEU:HD12	3:D:1248:LEU:C	2.34	0.51
1:A:217:GLU:HG2	1:B:233:GLU:OE1	2.10	0.51
2:C:842:ILE:HG12	2:C:868:ALA:HB2	1.92	0.51
4:E:80:PRO:HB3	4:E:93:ILE:HG21	1.91	0.51
2:C:181:PHE:CD2	2:C:196:VAL:HB	2.46	0.51
2:C:723:HIS:CD2	2:C:891:LYS:HD2	2.46	0.51
1:B:95:MET:HG2	1:B:113:PRO:HD2	1.91	0.51
2:C:481:GLU:OE2	2:C:607:ARG:NH2	2.41	0.51
2:C:786:ILE:HG13	2:C:844:ILE:HD12	1.92	0.51
7:H:2:DG:H2''	7:H:3:DC:O5'	2.11	0.51
3:D:1025:THR:HA	3:D:1041:ARG:HD2	1.93	0.51
3:D:1248:LEU:HA	3:D:1259:PRO:HD2	1.92	0.51
2:C:724:ASN:HB3	2:C:730:ILE:HG13	1.92	0.51
3:D:1090:LYS:HB2	3:D:1096:GLU:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:226:PHE:CE1	3:D:248:TYR:HB3	2.46	0.50
3:D:430:ILE:HD11	3:D:539:ASP:HB2	1.94	0.50
3:D:702:GLU:HG3	3:D:946:ASP:HB2	1.93	0.50
3:D:1225:SER:OG	3:D:1249:LYS:HE3	2.10	0.50
2:C:511:ARG:HD3	2:C:573:MET:HE2	1.93	0.50
2:C:80:LEU:HD21	2:C:383:ILE:HD13	1.94	0.50
2:C:577:PRO:C	2:C:579:GLN:H	2.18	0.50
3:D:1056:GLU:HB2	3:D:1063:LYS:HB3	1.93	0.50
3:D:1219:SER:OG	3:D:1250:GLU:OE2	2.30	0.50
2:C:955:ASP:N	2:C:955:ASP:OD1	2.43	0.50
2:C:186:ASP:N	2:C:191:LYS:O	2.43	0.50
3:D:331:ASP:OD1	3:D:331:ASP:N	2.44	0.50
3:D:184:LEU:HD11	3:D:197:VAL:HG21	1.94	0.49
3:D:666:THR:HG21	3:D:683:PHE:CE1	2.47	0.49
2:C:626:LEU:HA	2:C:706:GLU:HA	1.93	0.49
2:C:709:LEU:HB2	2:C:1025:MET:HE2	1.95	0.49
4:E:32:LEU:O	4:E:35:THR:HG22	2.12	0.49
2:C:305:VAL:HG12	2:C:503:PHE:HB3	1.92	0.49
3:D:67:ARG:HH12	3:D:69:ARG:HH21	1.59	0.49
3:D:114:LEU:HG	3:D:312:MET:HE2	1.95	0.49
2:C:252:MET:HA	2:C:255:THR:HG22	1.94	0.49
2:C:898:MET:HG2	2:C:907:VAL:O	2.12	0.49
2:C:893:LEU:HB2	2:C:898:MET:CE	2.43	0.49
2:C:1133:SER:OG	2:C:1134:SER:N	2.45	0.49
3:D:973:GLY:O	3:D:1159:ARG:NH2	2.45	0.49
3:D:562:SER:HA	3:D:565:ILE:HD11	1.94	0.49
4:E:82:VAL:HG22	4:E:102:LEU:HD22	1.93	0.49
2:C:157:LYS:HD2	2:C:633:GLY:HA3	1.95	0.49
7:H:18:DG:H2'	7:H:19:DG:H5'	1.95	0.49
6:G:9:DG:H2'	6:G:10:DC:O4'	2.13	0.49
1:B:94:THR:O	1:B:113:PRO:HG3	2.11	0.49
3:D:173:ARG:NE	3:D:204:GLU:OE2	2.41	0.49
3:D:499:ASN:HB2	3:D:509:ILE:HG12	1.95	0.49
5:F:43:GLY:HA2	5:F:46:ARG:HD3	1.95	0.49
2:C:107:ASP:HB3	2:C:126:PRO:HD2	1.94	0.48
1:A:84:VAL:HG13	1:A:119:HIS:HB2	1.96	0.48
1:B:146:TYR:O	3:D:624:ARG:NE	2.46	0.48
2:C:803:LYS:HG2	2:C:807:GLU:HB2	1.95	0.48
2:C:922:ILE:HG12	3:D:817:LEU:HD11	1.95	0.48
3:D:1053:VAL:HG12	3:D:1103:ASP:O	2.13	0.48
3:D:812:THR:O	3:D:816:THR:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:922:ALA:HA	3:D:981:ARG:HD3	1.95	0.48
2:C:1089:ASP:OD2	2:C:1110:GLY:N	2.46	0.48
2:C:1148:ASP:OD1	2:C:1148:ASP:N	2.47	0.48
3:D:966:LEU:HD22	3:D:1131:GLN:HB3	1.96	0.48
3:D:1158:VAL:HA	3:D:1161:MET:HE2	1.95	0.48
3:D:1257:LEU:HD12	3:D:1268:ARG:HE	1.78	0.48
2:C:135:ASN:O	2:C:139:GLY:N	2.47	0.48
2:C:219:ARG:HG3	2:C:223:LYS:O	2.14	0.48
2:C:874:SER:N	2:C:877:ASP:OD2	2.47	0.47
1:B:102:PRO:HA	1:B:128:LEU:O	2.13	0.47
3:D:78:CYS:HB3	3:D:80:VAL:HG23	1.95	0.47
3:D:67:ARG:NH1	3:D:69:ARG:HH21	2.12	0.47
3:D:337:THR:HG22	3:D:341:ASN:HD22	1.80	0.47
3:D:563:ASN:ND2	4:E:39:ILE:HD12	2.29	0.47
3:D:588:LEU:HD11	3:D:672:MET:HE3	1.96	0.47
3:D:759:GLN:HG2	3:D:765:LEU:HG	1.96	0.47
3:D:793:TYR:HB3	3:D:800:ILE:HG13	1.97	0.47
1:A:95:MET:HE2	1:A:112:PRO:HB3	1.96	0.47
2:C:576:SER:OG	2:C:577:PRO:O	2.30	0.47
2:C:786:ILE:HD12	2:C:786:ILE:H	1.79	0.47
3:D:885:ILE:HG22	3:D:994:ALA:HA	1.97	0.47
1:B:100:GLN:HA	1:B:133:LYS:HA	1.95	0.47
2:C:778:LEU:HD12	2:C:784:VAL:HA	1.96	0.47
2:C:1039:SER:HB3	3:D:450:GLU:O	2.15	0.47
3:D:581:MET:HE3	3:D:717:LYS:HG3	1.96	0.47
1:B:102:PRO:HD3	1:B:130:ASP:HA	1.96	0.47
1:B:172:LEU:HD13	1:B:199:LYS:HG3	1.97	0.47
2:C:593:HIS:HB3	2:C:922:ILE:CD1	2.45	0.47
2:C:888:VAL:HG22	3:D:536:PHE:O	2.14	0.47
2:C:899:PRO:HB3	2:C:1013:PHE:HE2	1.80	0.47
7:H:16:DA:N6	7:H:17:DG:O6	2.48	0.47
2:C:71:ARG:HG2	2:C:71:ARG:HH11	1.79	0.47
1:A:219:PHE:CE1	1:B:215:LEU:HD13	2.50	0.46
3:D:460:LEU:HD21	3:D:483:VAL:HG12	1.97	0.46
3:D:568:PRO:HB3	3:D:984:ALA:HB2	1.97	0.46
3:D:1131:GLN:HG3	3:D:1162:LEU:HD12	1.97	0.46
3:D:1264:ILE:HG22	3:D:1266:ARG:H	1.80	0.46
3:D:577:PRO:HB3	3:D:581:MET:HB3	1.97	0.46
3:D:588:LEU:HD13	3:D:723:TRP:CE2	2.51	0.46
2:C:1062:PHE:CZ	2:C:1070:MET:HE3	2.51	0.46
3:D:902:ALA:HB1	3:D:910:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:196:VAL:HG13	2:C:208:PHE:HB2	1.97	0.46
2:C:198:VAL:HB	2:C:206:LEU:HB3	1.96	0.46
3:D:400:LYS:HG3	5:F:107:GLU:HG3	1.97	0.46
3:D:863:THR:O	3:D:867:THR:HG22	2.16	0.46
2:C:302:LEU:O	2:C:325:SER:HB2	2.16	0.46
2:C:577:PRO:O	2:C:578:ARG:HG2	2.15	0.46
2:C:647:VAL:HG21	2:C:684:VAL:HG23	1.98	0.46
5:F:198:VAL:O	5:F:202:ARG:N	2.44	0.46
2:C:86:GLU:OE1	2:C:384:ARG:NH2	2.49	0.46
2:C:205:TRP:CH2	6:G:10:DC:H2'	2.51	0.46
2:C:337:GLU:HA	2:C:340:VAL:HG22	1.98	0.46
3:D:468:ASN:OD1	3:D:468:ASN:N	2.48	0.46
3:D:1090:LYS:CD	3:D:1091:HIS:N	2.72	0.46
1:B:72:ASP:OD1	1:B:73:VAL:N	2.48	0.46
3:D:73:ILE:O	3:D:82:VAL:HG12	2.16	0.46
3:D:1167:ILE:HD13	3:D:1175:PHE:HB3	1.98	0.46
5:F:44:ALA:HB2	5:F:86:LEU:HD11	1.98	0.46
3:D:571:GLY:HA2	3:D:983:MET:O	2.16	0.46
2:C:435:ASP:HA	2:C:674:HIS:NE2	2.31	0.46
2:C:941:ASP:C	2:C:943:ALA:H	2.24	0.46
3:D:346:ARG:NH2	5:F:53:ASP:OD1	2.40	0.46
3:D:1110:GLN:NE2	3:D:1112:MET:O	2.36	0.46
1:B:51:VAL:HA	1:B:139:VAL:O	2.16	0.45
1:B:110:ILE:HD11	1:B:118:VAL:HG21	1.98	0.45
2:C:144:GLN:NE2	2:C:409:GLN:HB2	2.28	0.45
3:D:666:THR:HG22	3:D:685:ASN:OD1	2.15	0.45
3:D:500:ARG:HD2	3:D:534:ALA:HB2	1.98	0.45
3:D:507:LEU:HD11	3:D:564:ASN:HB3	1.98	0.45
3:D:573:PRO:HG2	3:D:576:MET:HE2	1.97	0.45
3:D:1277:GLU:CD	3:D:1277:GLU:H	2.22	0.45
7:H:16:DA:C6	7:H:17:DG:C6	3.04	0.45
1:B:235:GLY:HA2	1:B:236:PRO:HD3	1.83	0.45
2:C:390:MET:HG3	2:C:413:ASN:O	2.17	0.45
2:C:611:PRO:HD2	2:C:676:THR:HB	1.99	0.45
3:D:579:LEU:HD23	3:D:808:THR:HB	1.98	0.45
7:H:19:DG:H5''	7:H:19:DG:H8	1.82	0.45
3:D:1127:PRO:HA	3:D:1130:VAL:HG23	1.97	0.45
2:C:346:GLN:O	2:C:359:VAL:HB	2.16	0.45
3:D:67:ARG:HG3	3:D:69:ARG:H	1.80	0.45
3:D:1248:LEU:HB2	3:D:1258:ILE:HB	1.99	0.45
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:599:TYR:CE1	3:D:608:GLU:HB2	2.52	0.45
3:D:778:TRP:CD2	3:D:835:PRO:HG3	2.52	0.45
2:C:168:VAL:HG23	2:C:434:MET:HB2	1.99	0.45
2:C:226:GLN:HG3	2:C:274:LYS:HD3	1.99	0.45
2:C:317:HIS:HB3	2:C:321:PRO:HG2	1.98	0.45
2:C:318:VAL:HG21	2:C:355:VAL:HG21	1.98	0.45
3:D:566:LEU:HA	3:D:573:PRO:HA	1.98	0.45
3:D:599:TYR:HA	3:D:610:GLY:HA3	1.99	0.45
3:D:749:TYR:CG	3:D:781:ALA:HB2	2.52	0.45
3:D:1220:TRP:CD1	3:D:1243:ASP:HB2	2.52	0.45
4:E:59:ARG:NH2	4:E:79:GLY:HA3	2.22	0.45
3:D:766:ASN:HB3	3:D:769:GLU:HG3	1.99	0.45
1:A:215:LEU:HD13	1:B:219:PHE:CE1	2.52	0.44
3:D:105:TRP:HB3	3:D:1234:THR:HG22	1.98	0.44
3:D:369:ASN:OD1	3:D:372:ARG:NH2	2.50	0.44
2:C:543:ASP:OD1	2:C:543:ASP:N	2.49	0.44
3:D:707:ILE:O	3:D:711:GLN:HG3	2.17	0.44
3:D:727:SER:OG	3:D:729:VAL:HG22	2.18	0.44
2:C:621:GLY:O	2:C:967:SER:HA	2.18	0.44
3:D:565:ILE:HG23	3:D:575:ALA:HB3	2.00	0.44
3:D:824:VAL:HG11	3:D:852:ASN:HA	1.99	0.44
3:D:1274:PRO:HA	4:E:103:LEU:HA	1.99	0.44
2:C:246:PHE:HB3	2:C:252:MET:HG3	1.98	0.44
1:A:205:ARG:HG3	1:B:225:LEU:HD13	2.00	0.44
2:C:1017:VAL:HA	3:D:730:THR:HG21	2.00	0.44
5:F:168:GLU:O	5:F:171:GLU:HG2	2.18	0.44
2:C:526:THR:HG22	2:C:529:GLU:OE2	2.16	0.44
2:C:1081:GLU:HG3	2:C:1085:ILE:HD11	1.99	0.44
3:D:677:LEU:HB3	3:D:678:PRO:HD2	1.99	0.44
3:D:1105:VAL:HG13	3:D:1109:GLN:HB3	2.00	0.44
2:C:715:VAL:HG23	2:C:909:ILE:HG23	1.99	0.44
3:D:57:ASP:HB3	3:D:58:TRP:CD1	2.53	0.44
3:D:278:ARG:O	3:D:281:ILE:HG13	2.17	0.44
7:H:13:DT:H2'	7:H:14:DC:C6	2.53	0.44
1:B:170:PRO:HB2	1:B:202:ILE:HD11	2.00	0.44
2:C:200:PRO:HG3	2:C:300:TYR:CE2	2.53	0.44
2:C:950:ALA:O	2:C:954:PRO:HD2	2.18	0.44
3:D:159:ARG:HH12	3:D:220:GLU:HB2	1.83	0.44
1:A:144:ARG:NH1	1:B:2:LEU:O	2.50	0.43
2:C:351:VAL:H	2:C:354:GLY:HA3	1.83	0.43
3:D:460:LEU:HD12	3:D:486:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:81:TRP:NE1	6:G:1:DT:H2'	2.32	0.43
1:A:11:GLU:HG2	1:A:12:ASP:N	2.34	0.43
2:C:211:ASP:OD1	2:C:211:ASP:N	2.51	0.43
3:D:895:ARG:HB2	3:D:967:THR:HB	2.00	0.43
1:A:110:ILE:O	1:A:112:PRO:HD3	2.18	0.43
1:A:112:PRO:HB2	1:A:116:VAL:HG22	1.99	0.43
1:A:146:TYR:CD2	2:C:737:GLU:HG2	2.54	0.43
2:C:120:ASP:HA	2:C:164:GLY:HA3	1.99	0.43
2:C:196:VAL:CG1	2:C:208:PHE:HB2	2.48	0.43
3:D:61:TYR:HB3	3:D:78:CYS:SG	2.58	0.43
3:D:500:ARG:HB2	3:D:541:MET:HG2	2.01	0.43
4:E:97:GLU:HB3	4:E:103:LEU:HD22	2.00	0.43
5:F:59:GLN:O	5:F:63:VAL:HG23	2.18	0.43
5:F:79:LYS:HE2	6:G:5:DG:C8	2.53	0.43
5:F:177:ILE:HD12	5:F:177:ILE:H	1.82	0.43
1:B:107:ALA:HB3	1:B:121:PRO:HA	2.01	0.43
2:C:36:ALA:HA	2:C:972:ASP:O	2.18	0.43
2:C:542:ILE:HG22	2:C:543:ASP:O	2.19	0.43
2:C:886:LYS:HE3	3:D:537:ASP:HB2	2.01	0.43
2:C:1070:MET:HE1	3:D:509:ILE:HG21	1.99	0.43
3:D:739:PRO:HD3	3:D:789:LEU:HD13	1.99	0.43
3:D:1112:MET:HE2	3:D:1112:MET:HB2	1.83	0.43
2:C:1098:GLU:OE2	2:C:1151:ARG:NH2	2.52	0.43
3:D:1251:ASN:OD1	3:D:1256:LYS:HD2	2.18	0.43
1:B:79:ASN:O	1:B:123:MET:HE1	2.19	0.43
2:C:481:GLU:OE2	2:C:607:ARG:HD3	2.18	0.43
3:D:325:ARG:HD2	3:D:341:ASN:OD1	2.18	0.43
3:D:968:CYS:SG	3:D:970:THR:HG23	2.59	0.43
2:C:32:ARG:CZ	2:C:965:ILE:HG23	2.49	0.43
2:C:288:THR:O	2:C:291:GLU:HG2	2.18	0.43
2:C:732:SER:HA	2:C:898:MET:CE	2.49	0.43
2:C:1111:ILE:HD13	3:D:3:ASP:HB2	2.00	0.43
3:D:581:MET:HG2	3:D:717:LYS:HA	2.00	0.43
2:C:435:ASP:HA	2:C:674:HIS:CD2	2.53	0.43
3:D:473:LYS:O	3:D:477:GLU:HG3	2.19	0.43
1:A:62:GLU:OE2	2:C:870:LYS:NZ	2.39	0.43
3:D:608:GLU:CD	3:D:608:GLU:H	2.27	0.43
2:C:97:MET:HB2	2:C:133:PHE:CE1	2.51	0.43
2:C:303:ALA:HB3	2:C:305:VAL:HG22	2.00	0.43
2:C:88:SER:HB2	2:C:100:SER:HA	2.01	0.42
2:C:237:TRP:CZ2	2:C:333:VAL:HG21	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:509:PRO:HB2	2:C:575:VAL:HG11	2.01	0.42
3:D:98:ALA:HB3	3:D:354:LEU:HD23	2.01	0.42
3:D:849:TYR:O	3:D:853:THR:HG23	2.19	0.42
7:H:15:DG:C5'	7:H:15:DG:H8	2.32	0.42
1:A:61:HIS:HE1	1:A:63:PHE:O	2.03	0.42
2:C:314:LEU:O	2:C:357:VAL:HG21	2.19	0.42
2:C:644:ILE:HG22	2:C:686:ALA:HA	2.00	0.42
2:C:735:LEU:HD22	2:C:740:VAL:HG21	2.00	0.42
3:D:327:MET:HG3	3:D:337:THR:HG23	2.01	0.42
1:A:11:GLU:OE2	1:A:205:ARG:HD3	2.19	0.42
2:C:1123:GLN:OE1	3:D:92:MET:HE1	2.19	0.42
3:D:281:ILE:O	3:D:289:LYS:NZ	2.45	0.42
2:C:541:PRO:HD2	2:C:550:GLU:OE2	2.19	0.42
2:C:786:ILE:HG13	2:C:844:ILE:CD1	2.49	0.42
1:B:78:LEU:HD21	3:D:611:VAL:HG23	2.01	0.42
3:D:449:LEU:HD11	3:D:476:VAL:HG13	2.01	0.42
2:C:314:LEU:C	2:C:357:VAL:HG21	2.45	0.42
3:D:1122:LEU:HA	3:D:1130:VAL:CG2	2.49	0.42
1:B:66:VAL:HG23	1:B:73:VAL:HG22	2.02	0.42
2:C:496:VAL:HG23	2:C:581:VAL:O	2.19	0.42
2:C:761:GLU:OE2	2:C:801:THR:OG1	2.32	0.42
3:D:357:LEU:CD2	5:F:63:VAL:HG22	2.49	0.42
2:C:217:GLY:HA3	2:C:225:ARG:CG	2.50	0.42
3:D:238:GLU:O	3:D:242:ARG:HG2	2.20	0.42
3:D:475:MET:HE3	3:D:475:MET:HB2	1.96	0.42
1:A:40:ARG:HG2	2:C:896:GLU:HB2	2.02	0.42
2:C:795:ILE:HD12	2:C:795:ILE:H	1.84	0.42
2:C:873:ILE:HD12	2:C:873:ILE:HA	1.96	0.42
3:D:30:LYS:HE3	3:D:32:GLU:OE1	2.20	0.42
3:D:552:GLN:O	3:D:556:ARG:HG3	2.20	0.42
3:D:1046:ILE:HG22	3:D:1110:GLN:HA	2.01	0.42
5:F:81:TRP:O	5:F:85:ILE:HG13	2.20	0.42
2:C:48:LEU:CD2	2:C:446:LYS:HD2	2.50	0.41
2:C:605:MET:HE1	2:C:886:LYS:HD3	2.02	0.41
2:C:779:ASP:OD1	2:C:781:ARG:HG3	2.20	0.41
2:C:1122:LEU:HD13	2:C:1129:VAL:HG21	2.02	0.41
3:D:432:VAL:HG13	3:D:434:PRO:HD3	2.01	0.41
3:D:505:HIS:CD2	3:D:1005:GLU:HG3	2.55	0.41
1:A:199:LYS:O	1:A:200:ASN:HB2	2.18	0.41
2:C:920:MET:HE1	3:D:817:LEU:HA	2.02	0.41
3:D:66:LYS:HB2	3:D:66:LYS:HE3	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:263:LYS:HD3	3:D:263:LYS:HA	1.94	0.41
3:D:1036:GLU:HB3	3:D:1038:ARG:HG3	2.02	0.41
5:F:57:LEU:HD11	5:F:90:TYR:HB2	2.02	0.41
3:D:131:PHE:HB2	3:D:372:ARG:NH1	2.35	0.41
3:D:155:MET:CE	3:D:219:LEU:HB3	2.50	0.41
3:D:320:ILE:HG21	3:D:340:LEU:HD23	2.03	0.41
3:D:673:PHE:CE2	3:D:688:MET:HG3	2.56	0.41
3:D:12:ILE:HG21	3:D:12:ILE:HD13	1.85	0.41
3:D:1122:LEU:HD13	3:D:1130:VAL:HG21	2.02	0.41
5:F:165:PRO:O	5:F:169:ILE:HG13	2.20	0.41
1:B:128:LEU:HD21	1:B:134:LEU:HG	2.02	0.41
3:D:52:PHE:CD1	3:D:322:PRO:HD3	2.55	0.41
3:D:97:LEU:HD11	3:D:317:VAL:HG23	2.02	0.41
3:D:122:PRO:HG2	6:G:20:DT:H3'	2.01	0.41
2:C:154:MET:HA	2:C:159:THR:O	2.21	0.41
2:C:807:GLU:OE1	3:D:56:ARG:NH2	2.54	0.41
3:D:1227:GLN:HG3	7:H:10:DG:H5'	2.03	0.41
7:H:19:DG:C2'	7:H:20:DT:C5'	2.85	0.41
1:B:30:PHE:O	1:B:34:LEU:HG	2.19	0.41
1:B:101:GLY:N	1:B:132:GLY:O	2.52	0.41
1:B:227:VAL:O	1:B:228:GLU:CG	2.69	0.41
2:C:80:LEU:HA	2:C:80:LEU:HD23	1.80	0.41
2:C:245:ARG:NH2	2:C:351:VAL:HG12	2.35	0.41
3:D:736:VAL:HG12	3:D:818:ALA:HB2	2.03	0.41
3:D:817:LEU:O	3:D:839:SER:HB2	2.20	0.41
3:D:1121:VAL:HG22	3:D:1130:VAL:HG13	2.02	0.41
3:D:965:VAL:HG22	3:D:1155:GLU:HB3	2.03	0.41
6:G:22:DC:H2''	6:G:23:DA:N7	2.35	0.41
1:A:62:GLU:O	1:A:73:VAL:HB	2.20	0.41
2:C:265:ASP:HB2	2:C:283:LYS:HG3	2.03	0.41
2:C:577:PRO:C	2:C:579:GLN:N	2.78	0.41
3:D:64:LYS:HE3	3:D:65:TYR:OH	2.21	0.41
3:D:1090:LYS:HB3	3:D:1096:GLU:HA	2.02	0.41
3:D:1122:LEU:HA	3:D:1130:VAL:HG22	2.03	0.41
2:C:246:PHE:CD2	2:C:252:MET:HE2	2.56	0.41
1:A:88:GLU:HG2	1:A:115:GLY:O	2.21	0.40
2:C:583:VAL:HG13	2:C:624:MET:HE2	2.03	0.40
3:D:71:LYS:HB2	3:D:71:LYS:HE3	1.71	0.40
3:D:826:ASN:HB3	3:D:828:LYS:H	1.86	0.40
1:B:169:SER:HB3	3:D:620:MET:HE1	2.02	0.40
2:C:767:ILE:HG21	2:C:770:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:936:SER:OG	2:C:986:THR:HG23	2.21	0.40
2:C:1125:LEU:HD13	3:D:105:TRP:CZ2	2.56	0.40
1:B:170:PRO:HA	1:B:199:LYS:HE3	2.04	0.40
2:C:443:LEU:O	2:C:447:ARG:HG3	2.22	0.40
2:C:720:TRP:HE1	2:C:899:PRO:HD3	1.86	0.40
2:C:753:ALA:HB2	2:C:763:ILE:HG13	2.02	0.40
2:C:1005:PHE:HA	2:C:1012:PRO:HA	2.03	0.40
1:A:175:THR:HG22	1:A:195:ASP:HB3	2.04	0.40
3:D:736:VAL:O	3:D:841:ARG:NE	2.52	0.40
3:D:826:ASN:OD1	3:D:827:PRO:HD2	2.21	0.40
2:C:261:THR:HB	2:C:266:GLU:OE1	2.21	0.40
2:C:580:MET:HG3	2:C:581:VAL:HG23	2.03	0.40
3:D:310:MET:HE3	3:D:310:MET:HB3	1.89	0.40
3:D:821:LYS:HB3	3:D:836:VAL:HB	2.04	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	213/368 (58%)	208 (98%)	5 (2%)	0	100	100
1	B	224/368 (61%)	211 (94%)	13 (6%)	0	100	100
2	C	1131/1174 (96%)	1082 (96%)	48 (4%)	1 (0%)	48	77
3	D	1250/1317 (95%)	1211 (97%)	39 (3%)	0	100	100
4	E	71/110 (64%)	68 (96%)	3 (4%)	0	100	100
5	F	180/218 (83%)	177 (98%)	3 (2%)	0	100	100
All	All	3069/3555 (86%)	2957 (96%)	111 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	76	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	185/315 (59%)	177 (96%)	8 (4%)	26	60
1	B	177/315 (56%)	159 (90%)	18 (10%)	7	23
2	C	929/995 (93%)	866 (93%)	63 (7%)	14	42
3	D	1026/1096 (94%)	972 (95%)	54 (5%)	20	52
4	E	64/90 (71%)	62 (97%)	2 (3%)	35	70
5	F	143/175 (82%)	135 (94%)	8 (6%)	19	50
All	All	2524/2986 (84%)	2371 (94%)	153 (6%)	17	46

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	51	VAL
1	A	52	THR
1	A	59	VAL
1	A	69	VAL
1	A	116	VAL
1	A	171	VAL
1	A	213	LYS
1	B	33	THR
1	B	34	LEU
1	B	59	VAL
1	B	75	GLU
1	B	88	GLU
1	B	91	GLU
1	B	94	THR
1	B	110	ILE
1	B	111	VAL
1	B	116	VAL

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Mol	Chain	Res	Type
1	B	150	VAL
1	B	172	LEU
1	B	181	THR
1	B	202	ILE
1	B	214	THR
1	B	226	ASN
1	B	227	VAL
1	B	228	GLU
2	C	33	VAL
2	C	59	ILE
2	C	65	ARG
2	C	87	LEU
2	C	114	ASP
2	C	196	VAL
2	C	199	ILE
2	C	209	ASP
2	C	211	ASP
2	C	238	THR
2	C	284	GLU
2	C	290	LEU
2	C	318	VAL
2	C	343	HIS
2	C	347	THR
2	C	350	THR
2	C	351	VAL
2	C	382	GLN
2	C	406	ILE
2	C	441	SER
2	C	444	THR
2	C	458	SER
2	C	482	THR
2	C	548	PHE
2	C	550	GLU
2	C	553	VAL
2	C	554	LEU
2	C	562	VAL
2	C	565	VAL
2	C	581	VAL
2	C	615	SER
2	C	635	VAL
2	C	647	VAL
2	C	648	SER

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Mol	Chain	Res	Type
2	C	740	VAL
2	C	756	THR
2	C	766	ASP
2	C	770	ILE
2	C	773	GLU
2	C	774	VAL
2	C	778	LEU
2	C	781	ARG
2	C	813	ARG
2	C	824	ARG
2	C	825	GLU
2	C	842	ILE
2	C	844	ILE
2	C	846	VAL
2	C	898	MET
2	C	922	ILE
2	C	965	ILE
2	C	986	THR
2	C	1019	VAL
2	C	1027	LEU
2	C	1031	VAL
2	C	1088	ASP
2	C	1091	VAL
2	C	1101	VAL
2	C	1106	ILE
2	C	1131	VAL
2	C	1145	GLU
2	C	1147	GLU
2	C	1158	ILE
3	D	4	VAL
3	D	12	ILE
3	D	92	MET
3	D	101	VAL
3	D	117	LEU
3	D	148	LEU
3	D	150	THR
3	D	177	LEU
3	D	181	LEU
3	D	235	ILE
3	D	287	GLN
3	D	331	ASP
3	D	337	THR

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Mol	Chain	Res	Type
3	D	456	VAL
3	D	460	LEU
3	D	464	ASN
3	D	485	ASP
3	D	490	VAL
3	D	491	ILE
3	D	503	THR
3	D	507	LEU
3	D	517	VAL
3	D	578	ARG
3	D	579	LEU
3	D	581	MET
3	D	583	THR
3	D	590	THR
3	D	606	HIS
3	D	629	VAL
3	D	639	GLN
3	D	644	VAL
3	D	714	ASP
3	D	738	VAL
3	D	742	LYS
3	D	743	LYS
3	D	791	GLU
3	D	821	LYS
3	D	847	LEU
3	D	863	THR
3	D	897	ILE
3	D	965	VAL
3	D	971	SER
3	D	991	ILE
3	D	1036	GLU
3	D	1061	PHE
3	D	1086	LEU
3	D	1089	PHE
3	D	1090	LYS
3	D	1095	SER
3	D	1121	VAL
3	D	1130	VAL
3	D	1167	ILE
3	D	1194	VAL
3	D	1206	VAL
4	E	45	ARG

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Mol	Chain	Res	Type
4	E	82	VAL
5	F	22	ASP
5	F	83	TYR
5	F	86	LEU
5	F	109	ILE
5	F	123	THR
5	F	179	THR
5	F	180	VAL
5	F	192	ARG

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	144	GLN
2	C	260	ASN
2	C	597	ASN
2	C	1048	GLN
2	C	1060	GLN
3	D	415	GLN
3	D	505	HIS
3	D	854	HIS
3	D	935	ASN
3	D	1160	GLN
4	E	68	ASN
5	F	59	GLN
5	F	100	GLN
5	F	120	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	6/7 (85%)	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 ⓘ

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 3 ligands modelled in this entry, 3 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	217/368 (58%)	0.27	2 (0%) 81 74	53, 75, 108, 128	0
1	B	230/368 (62%)	0.88	25 (10%) 10 8	75, 112, 147, 156	0
2	C	1135/1174 (96%)	0.41	67 (5%) 28 21	47, 75, 147, 169	0
3	D	1258/1317 (95%)	0.37	56 (4%) 38 30	48, 78, 122, 153	0
4	E	75/110 (68%)	0.76	9 (12%) 9 6	73, 99, 138, 175	0
5	F	182/218 (83%)	1.00	30 (16%) 4 3	32, 103, 132, 147	12 (6%)
6	G	23/23 (100%)	0.58	3 (13%) 7 6	87, 105, 148, 161	3 (13%)
7	H	20/21 (95%)	-0.15	0 100 100	54, 78, 136, 137	0
8	I	7/7 (100%)	-0.68	0 100 100	53, 54, 81, 87	0
All	All	3147/3606 (87%)	0.46	192 (6%) 27 20	32, 81, 138, 175	15 (0%)

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	114	LEU	6.4
5	F	68	GLY	5.7
3	D	201	GLY	5.4
5	F	45	LEU	5.2
1	B	236	PRO	5.1
1	B	183	VAL	5.0
2	C	1052	GLY	4.5
3	D	243	GLU	4.5
2	C	75	ASN	4.5
3	D	87	VAL	4.5
1	B	87	SER	4.4
1	B	2	LEU	4.4
3	D	59	GLU	4.1
1	B	201	SER	4.1
5	F	36	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
5	F	50	ASN	4.0
3	D	197	VAL	3.9
5	F	117	ASN	3.9
5	F	116	SER	3.9
4	E	30	THR	3.9
5	F	78	LEU	3.7
1	B	61	HIS	3.7
3	D	65	TYR	3.7
3	D	246	ASP	3.6
5	F	79	LYS	3.6
2	C	192	THR	3.6
3	D	910	LEU	3.6
5	F	118	ALA	3.5
5	F	82	LEU	3.5
3	D	605	ASP	3.5
3	D	189	ALA	3.5
3	D	969	ALA	3.5
2	C	406	ILE	3.4
2	C	321	PRO	3.4
2	C	1090	THR	3.4
2	C	552	ARG	3.4
5	F	72	PHE	3.4
4	E	31	PRO	3.3
2	C	894	PRO	3.3
1	B	151	GLN	3.3
2	C	21	SER	3.1
3	D	245	VAL	3.1
5	F	91	ILE	3.1
3	D	17	ALA	3.1
6	G	3	DG	3.1
1	B	58	GLY	3.1
5	F	67	ALA	3.1
3	D	1095	SER	3.1
3	D	18	GLU	3.1
2	C	227	PRO	3.1
4	E	32	LEU	3.1
3	D	4	VAL	3.0
5	F	39	GLN	3.0
2	C	69	ALA	3.0
3	D	654	SER	3.0
3	D	205	MET	3.0
3	D	1093	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
2	C	553	VAL	2.9
3	D	60	CYS	2.9
2	C	64	TRP	2.9
2	C	68	ALA	2.9
3	D	184	LEU	2.9
1	B	186	ARG	2.8
5	F	112	TRP	2.8
3	D	155	MET	2.8
2	C	562	VAL	2.8
5	F	120	HIS	2.8
2	C	67	SER	2.8
3	D	1026	GLY	2.8
4	E	38	PRO	2.7
1	B	60	LEU	2.7
3	D	1055	LEU	2.7
1	B	156	GLY	2.7
2	C	414	ILE	2.7
5	F	37	LEU	2.7
1	B	179	ASP	2.7
1	B	188	ASP	2.7
2	C	515	ASP	2.7
2	C	567	SER	2.6
2	C	23	ASN	2.6
2	C	185	ILE	2.6
1	B	157	ALA	2.6
2	C	180	TYR	2.6
1	B	59	VAL	2.6
3	D	216	LEU	2.6
3	D	1025	THR	2.6
2	C	59	ILE	2.6
2	C	647	VAL	2.6
5	F	74	HIS	2.6
1	B	160	GLY	2.6
2	C	564	TYR	2.6
2	C	262	VAL	2.6
2	C	284	GLU	2.6
1	B	125	ILE	2.5
2	C	684	VAL	2.5
3	D	1061	PHE	2.5
2	C	292	ASN	2.5
2	C	285	SER	2.5
2	C	347	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	324	SER	2.5
2	C	281	PRO	2.5
3	D	1012	MET	2.5
3	D	1194	VAL	2.5
2	C	299	ARG	2.5
2	C	508	THR	2.5
2	C	658	ASN	2.5
1	B	1	MET	2.4
3	D	190	LYS	2.4
2	C	205	TRP	2.4
2	C	1048	GLN	2.4
1	A	182	ARG	2.4
2	C	143	SER	2.4
2	C	411	LEU	2.4
2	C	551	PRO	2.4
5	F	164	PHE	2.4
2	C	423	GLU	2.4
1	B	86	SER	2.4
2	C	22	SER	2.4
2	C	138	THR	2.4
4	E	93	ILE	2.4
1	B	150	VAL	2.3
3	D	210	ASP	2.3
1	B	95	MET	2.3
5	F	173	MET	2.3
3	D	73	ILE	2.3
3	D	1094	GLY	2.3
3	D	6	PHE	2.3
1	B	134	LEU	2.3
3	D	177	LEU	2.3
3	D	61	TYR	2.3
3	D	616	ALA	2.3
2	C	221	ASP	2.3
2	C	265	ASP	2.3
3	D	600	GLN	2.3
2	C	568	SER	2.3
2	C	359	VAL	2.3
3	D	361	GLY	2.3
2	C	246	PHE	2.3
2	C	199	ILE	2.3
2	C	282	THR	2.3
5	F	76	THR	2.3

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Mol	Chain	Res	Type	RSRZ
4	E	77	TYR	2.3
2	C	135	ASN	2.2
3	D	396	ASN	2.2
3	D	181	LEU	2.2
2	C	141	ILE	2.2
3	D	51	ILE	2.2
3	D	392	THR	2.2
2	C	565	VAL	2.2
2	C	544	ALA	2.2
4	E	68	ASN	2.2
3	D	1078	ASP	2.2
3	D	305	SER	2.2
5	F	122	SER	2.2
2	C	131	ALA	2.2
4	E	42	LEU	2.2
3	D	241	TYR	2.2
3	D	1162	LEU	2.2
5	F	92	ASN	2.2
3	D	382	PHE	2.2
6	G	5	DG	2.2
2	C	340	VAL	2.1
4	E	86	LEU	2.1
6	G	11	DT	2.1
5	F	33	ALA	2.1
5	F	52	ALA	2.1
1	A	99	LYS	2.1
3	D	883	ASP	2.1
2	C	427	THR	2.1
3	D	150	THR	2.1
2	C	286	ALA	2.1
5	F	202	ARG	2.1
3	D	146	ASN	2.1
3	D	945	GLY	2.1
2	C	1021	TYR	2.1
2	C	549	VAL	2.1
3	D	1079	LYS	2.1
2	C	405	ALA	2.1
5	F	115	ALA	2.1
2	C	191	LYS	2.0
2	C	537	GLN	2.0
1	B	139	VAL	2.0
1	B	158	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
3	D	123	LYS	2.0
3	D	653	HIS	2.0
3	D	365	ILE	2.0
2	C	124	ALA	2.0
2	C	399	THR	2.0
1	B	57	ASP	2.0
5	F	53	ASP	2.0
5	F	83	TYR	2.0
2	C	318	VAL	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
10	MG	D	2003	1/1	0.88	0.11	54,54,54,54	0
9	ZN	D	2002	1/1	0.99	0.03	105,105,105,105	0
9	ZN	D	2001	1/1	0.99	0.02	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.