



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 02:49 PM JST

PDB ID : 6JCY
Title : Mycobacterium tuberculosis RNA polymerase transcription initiation open complex with a chimeric ECF sigma factor sigH/E
Authors : Li, L.; Zhang, Y.
Deposited on : 2019-01-30
Resolution : 3.11 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
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

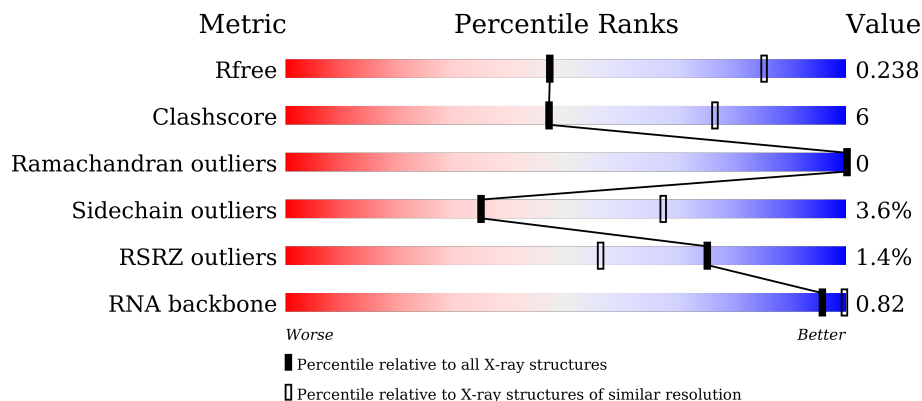
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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.



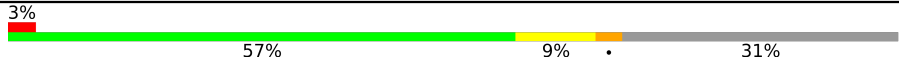

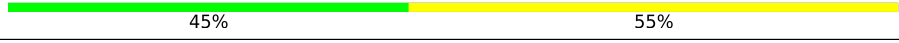
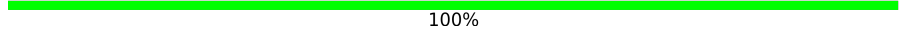
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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	 50% 10% 40%
1	B	368	 50% 12% 37%
2	C	1174	 81% 15% ..
3	D	1317	 79% 16% ..

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Mol	Chain	Length	Quality of chain
4	E	110	
5	F	209	
6	G	23	
7	H	20	
8	I	6	

2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 24729 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
			Total	C	N	O	S			
1	A	221	1673	1054	288	329	2	0	0	0
1	B	231	1719	1085	293	338	3	0	0	0

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
			Total	C	N	O	S			
2	C	1139	8572	5364	1504	1665	39	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	5	MET	-	initiating methionine	UNP P9WGY9
C	6	VAL	-	expression tag	UNP P9WGY9

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1260	9802	6141	1774	1847	40	0	0	0

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
			Total	C	N	O			
4	E	76	594	379	101	114	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	164	1238	774	221	238	5	0	0	0

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
			Total	C	N	O	P			
6	G	23	464	221	84	137	22	0	0	0

- 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*T)-3').

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
8	I	6	122	56	21	40	5	0	0	0

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

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

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

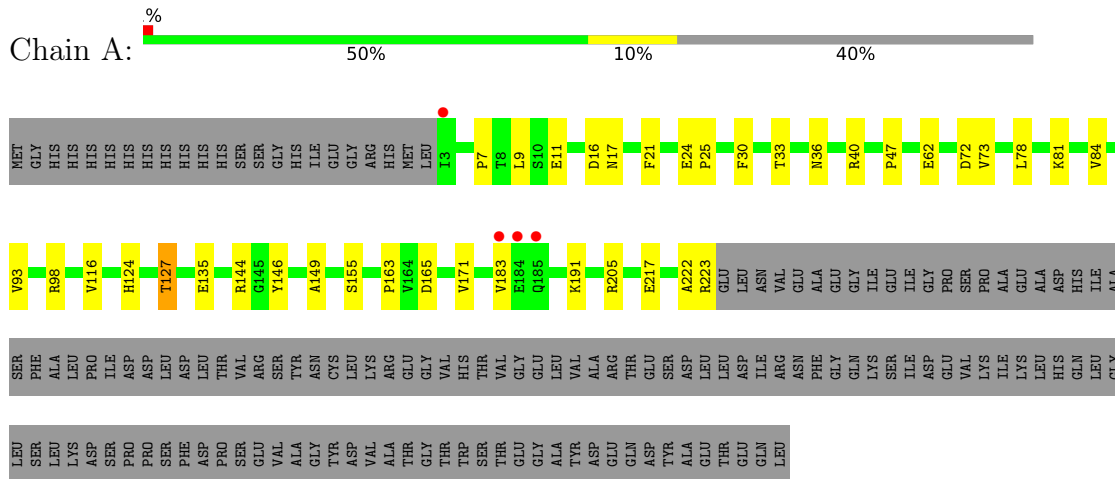
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	11	Total	O	0	0
			11	11		
11	B	9	Total	O	0	0
			9	9		
11	C	37	Total	O	0	0
			37	37		
11	D	58	Total	O	0	0
			58	58		
11	E	2	Total	O	0	0
			2	2		
11	F	5	Total	O	0	0
			5	5		
11	G	1	Total	O	0	0
			1	1		
11	H	6	Total	O	0	0
			6	6		
11	I	1	Total	O	0	0
			1	1		

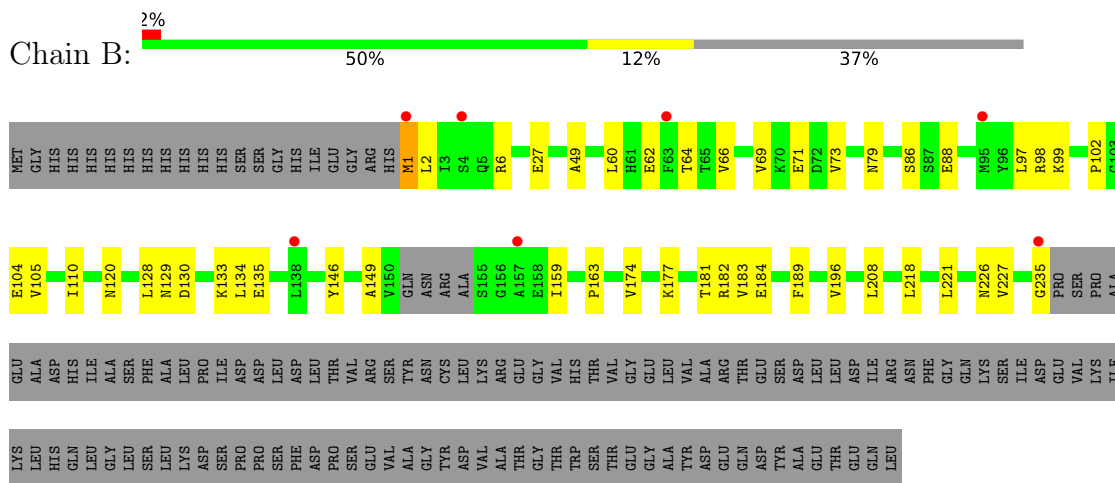
3 Residue-property plots

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.

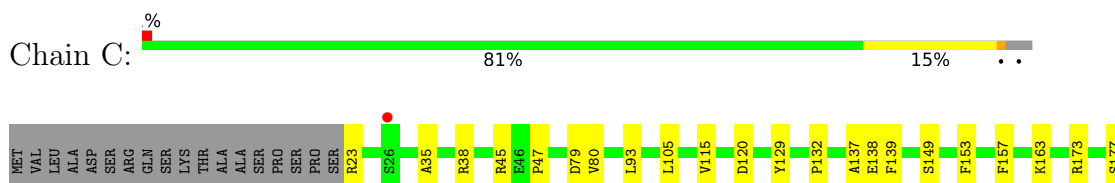
- Molecule 1: DNA-directed RNA polymerase subunit alpha

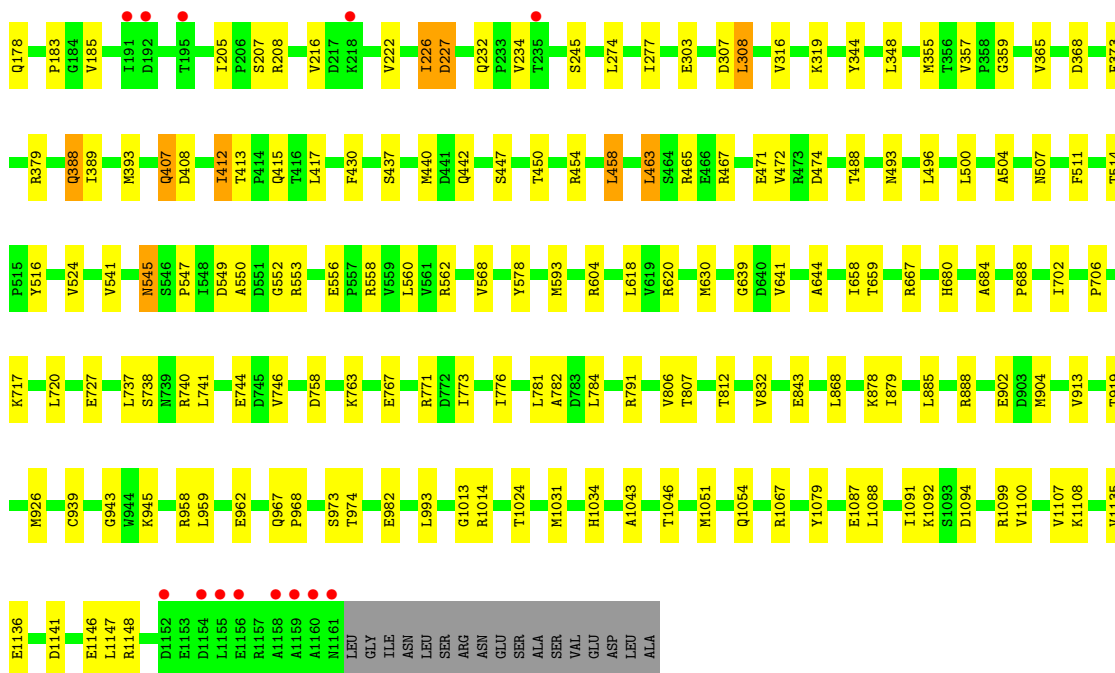


- Molecule 1: DNA-directed RNA polymerase subunit alpha

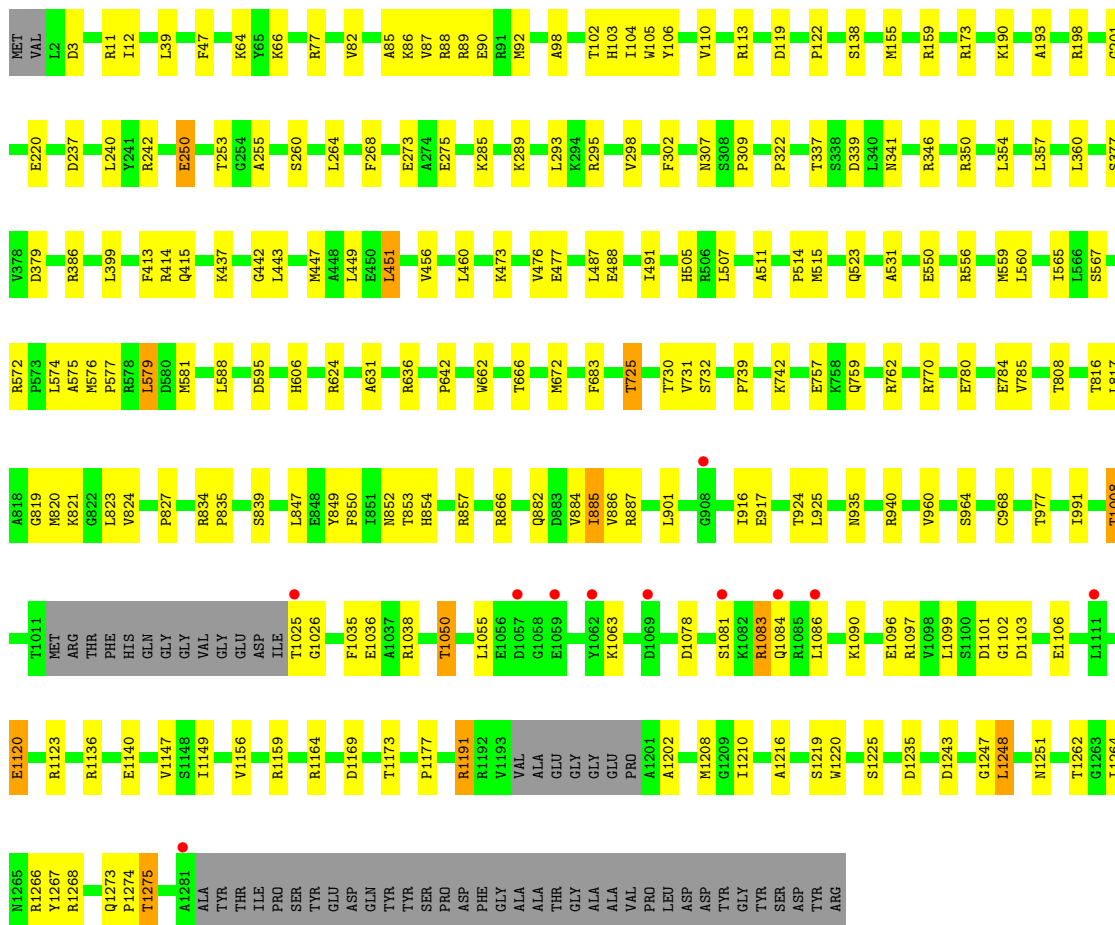
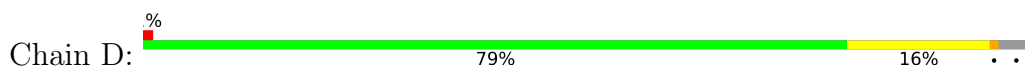


- Molecule 2: DNA-directed RNA polymerase subunit beta





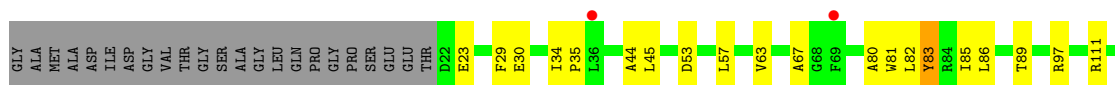
• Molecule 3: DNA-directed RNA polymerase subunit beta'



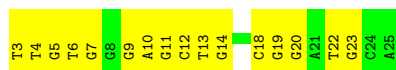
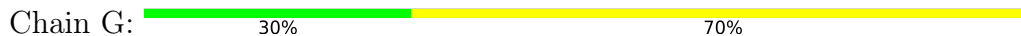
- Molecule 4: DNA-directed RNA polymerase subunit omega



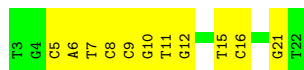
- Molecule 5: ECF RNA polymerase sigma factor SigH, ECF RNA polymerase sigma factor SigE, ECF RNA polymerase sigma factor SigH



- 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*T)-3')



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



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	128.94Å 163.00Å 129.31Å 90.00° 117.81° 90.00°	Depositor
Resolution (Å)	48.77 – 3.11 49.05 – 3.11	Depositor EDS
% Data completeness (in resolution range)	92.5 (48.77-3.11) 92.6 (49.05-3.11)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.195 , 0.238 0.195 , 0.238	Depositor DCC
R_{free} test set	2376 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	92.6	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.012 for -h-l,k,h 0.012 for l,k,-h-l 0.026 for h,-k,-h-l 0.027 for -h-l,-k,l 0.025 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24729	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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, 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	0.26	0/1699	0.47	0/2313
1	B	0.25	0/1744	0.46	0/2375
2	C	0.27	0/8730	0.45	0/11869
3	D	0.26	0/9966	0.43	0/13479
4	E	0.25	0/605	0.41	0/823
5	F	0.24	0/1263	0.39	0/1722
6	G	0.62	0/520	0.98	0/802
7	H	0.58	0/462	0.92	0/713
8	I	0.32	0/135	0.88	0/208
All	All	0.28	0/25124	0.48	0/34304

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	1673	0	1707	24	0
1	B	1719	0	1737	28	0
2	C	8572	0	8294	113	0
3	D	9802	0	9817	130	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	594	0	589	9	0
5	F	1238	0	1131	21	0
6	G	464	0	256	16	0
7	H	412	0	227	8	0
8	I	122	0	66	0	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
11	A	11	0	0	1	0
11	B	9	0	0	0	0
11	C	37	0	0	1	0
11	D	58	0	0	1	0
11	E	2	0	0	0	0
11	F	5	0	0	0	0
11	G	1	0	0	0	0
11	H	6	0	0	0	0
11	I	1	0	0	0	0
All	All	24729	0	23824	298	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (298) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:PRO:HA	1:A:25:PRO:HG2	1.55	0.89
1:B:62:GLU:HG3	1:B:64:THR:HG22	1.65	0.78
3:D:882:GLN:HB2	3:D:1248:LEU:HD11	1.67	0.75
3:D:1274:PRO:HG3	4:E:78:VAL:HG11	1.70	0.72
1:A:24:GLU:HG2	1:A:191:LYS:HG3	1.70	0.71
2:C:388:GLN:HG2	2:C:430:PHE:HB2	1.72	0.71
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.72	0.70
1:B:6:ARG:HH21	1:B:235:GLY:H	1.39	0.70
1:B:79:ASN:HB3	3:D:636:ARG:HH12	1.57	0.69
3:D:565:ILE:HG23	3:D:575:ALA:HB3	1.73	0.69
2:C:684:ALA:HA	2:C:706:PRO:HG3	1.75	0.69
2:C:1024:THR:H	3:D:730:THR:HG21	1.56	0.68
2:C:157:PHE:HE1	2:C:389:ILE:HD11	1.58	0.68
2:C:38:ARG:HG2	2:C:973:SER:HB2	1.76	0.67
1:A:47:PRO:HB3	1:B:1:MET:HB3	1.76	0.67
4:E:36:ASN:OD1	4:E:36:ASN:N	2.27	0.67
3:D:113:ARG:NH2	3:D:1235:ASP:OD1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:293:LEU:HD21	3:D:1177:PRO:HG2	1.78	0.66
4:E:46:VAL:HG21	4:E:52:LEU:HB2	1.80	0.64
2:C:207:SER:H	2:C:308:LEU:HA	1.64	0.63
2:C:463:LEU:HD21	2:C:472:VAL:HG11	1.80	0.63
2:C:782:ALA:O	2:C:791:ARG:NH2	2.31	0.62
2:C:758:ASP:HB3	2:C:868:LEU:HD23	1.82	0.62
3:D:1050:THR:HG23	3:D:1106:GLU:HA	1.81	0.62
2:C:442:GLN:H	2:C:680:HIS:CD2	2.18	0.62
3:D:47:PHE:O	3:D:88:ARG:NH2	2.33	0.62
2:C:458:LEU:HD11	2:C:496:LEU:HD13	1.82	0.61
3:D:1191:ARG:O	3:D:1191:ARG:NE	2.33	0.61
3:D:190:LYS:HD2	3:D:193:ALA:H	1.64	0.61
5:F:163:ILE:HG23	5:F:164:MET:HG3	1.83	0.61
6:G:10:DA:H2''	6:G:11:DG:O4'	2.01	0.61
1:B:183:VAL:HG13	1:B:184:GLU:H	1.66	0.61
2:C:741:LEU:HA	2:C:746:VAL:HG13	1.83	0.61
3:D:138:SER:HG	3:D:253:THR:HG1	1.48	0.60
1:B:226:ASN:OD1	1:B:227:VAL:N	2.33	0.60
3:D:556:ARG:NH2	4:E:34:ILE:O	2.33	0.60
3:D:1101:ASP:OD1	3:D:1102:GLY:N	2.36	0.59
1:A:9:LEU:HD11	1:A:21:PHE:HB3	1.83	0.59
2:C:1100:VAL:HG11	5:F:122:ILE:HD11	1.83	0.59
1:B:99:LYS:HD3	1:B:105:VAL:HG22	1.84	0.58
2:C:658:ILE:HD13	2:C:702:ILE:HG22	1.84	0.58
2:C:767:GLU:HG2	2:C:807:THR:HG22	1.84	0.58
2:C:773:ILE:HB	2:C:776:ILE:HD12	1.86	0.57
3:D:1273:GLN:HG2	3:D:1274:PRO:HD2	1.87	0.57
2:C:763:LYS:HE2	3:D:39:LEU:HB2	1.87	0.57
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.37	0.57
5:F:166:THR:HB	5:F:170:THR:HB	1.86	0.57
7:H:11:DT:H2'	7:H:12:DG:C8	2.40	0.57
3:D:824:VAL:HG11	3:D:852:ASN:HA	1.86	0.56
6:G:6:DT:H2''	6:G:7:DG:C8	2.40	0.56
2:C:1087:GLU:HG3	2:C:1091:ILE:HD11	1.86	0.56
6:G:11:DG:H2''	6:G:12:DC:O4'	2.06	0.56
3:D:449:LEU:HD11	3:D:476:VAL:HG13	1.87	0.56
1:B:69:VAL:HG12	1:B:128:LEU:HD23	1.88	0.56
3:D:1090:LYS:HG2	3:D:1096:GLU:HB2	1.86	0.56
2:C:185:VAL:HG23	2:C:316:VAL:HG12	1.87	0.56
1:B:97:LEU:HB2	1:B:110:ILE:HG13	1.88	0.55
1:A:93:VAL:HG11	1:A:116:VAL:HG21	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ARG:NH2	1:B:27:GLU:OE2	2.40	0.55
3:D:173:ARG:HH21	3:D:201:GLY:HA2	1.70	0.55
3:D:823:LEU:HD23	3:D:835:PRO:HB3	1.89	0.55
2:C:1135:VAL:HG22	3:D:12:ILE:HG13	1.88	0.55
1:A:40:ARG:HE	2:C:902:GLU:HG3	1.71	0.55
1:B:146:TYR:O	3:D:624:ARG:NE	2.40	0.55
3:D:86:LYS:O	3:D:89:ARG:HG2	2.06	0.55
3:D:357:LEU:HD21	5:F:63:VAL:HG22	1.89	0.55
1:A:40:ARG:HD2	2:C:902:GLU:HB2	1.89	0.55
2:C:1136:GLU:OE1	3:D:11:ARG:NH2	2.39	0.54
1:B:60:LEU:HB2	1:B:159:ILE:HG12	1.89	0.54
2:C:208:ARG:N	2:C:307:ASP:O	2.33	0.54
2:C:442:GLN:H	2:C:680:HIS:HD2	1.55	0.54
2:C:467:ARG:NH1	6:G:13:DT:OP1	2.40	0.54
3:D:1081:SER:HB2	3:D:1084:GLN:HG3	1.87	0.54
2:C:407:GLN:HB3	2:C:412:ILE:HG22	1.89	0.54
3:D:1097:ARG:NH1	3:D:1103:ASP:OD2	2.39	0.54
3:D:1120:GLU:HG3	3:D:1123:ARG:HH21	1.72	0.54
3:D:1262:THR:HB	4:E:54:ILE:HD11	1.88	0.54
2:C:771:ARG:NH1	2:C:784:LEU:O	2.41	0.54
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.34	0.54
2:C:474:ASP:HA	3:D:857:ARG:HG2	1.90	0.53
3:D:1035:PHE:HB3	3:D:1210:ILE:HD13	1.90	0.53
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.91	0.53
3:D:785:VAL:HG21	3:D:820:MET:HG2	1.91	0.53
3:D:386:ARG:NH2	7:H:11:DT:OP1	2.41	0.53
2:C:178:GLN:OE1	2:C:379:ARG:NH2	2.36	0.53
2:C:344:TYR:HA	2:C:355:MET:HE1	1.91	0.52
2:C:541:VAL:HG13	2:C:562:ARG:HB2	1.91	0.52
2:C:1054:GLN:HG3	2:C:1099:ARG:HH22	1.73	0.52
2:C:1146:GLU:OE1	2:C:1148:ARG:NH2	2.42	0.52
2:C:524:VAL:N	2:C:552:GLY:O	2.39	0.52
3:D:268:PHE:CZ	3:D:273:GLU:HG3	2.45	0.52
2:C:79:ASP:OD1	2:C:80:VAL:N	2.43	0.52
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.92	0.52
3:D:666:THR:HG21	3:D:683:PHE:CE1	2.45	0.52
1:A:7:PRO:HB2	1:B:221:LEU:HD11	1.92	0.52
3:D:339:ASP:HB3	3:D:399:LEU:HB3	1.91	0.52
2:C:568:VAL:HG11	3:D:847:LEU:HD13	1.93	0.51
2:C:23:ARG:NH1	2:C:35:ALA:O	2.41	0.51
3:D:834:ARG:HD3	3:D:835:PRO:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1024:THR:OG1	3:D:732:SER:OG	2.28	0.51
7:H:5:DC:H2''	7:H:6:DA:C8	2.45	0.51
3:D:1169:ASP:H	3:D:1202:ALA:HB3	1.76	0.51
2:C:593:MET:HG2	2:C:630:MET:HB3	1.92	0.51
2:C:919:THR:HG23	3:D:731:VAL:HG23	1.93	0.51
3:D:350:ARG:HH11	3:D:377:SER:HB3	1.76	0.51
1:B:49:ALA:HB3	1:B:86:SER:HA	1.93	0.51
2:C:1043:ALA:HB2	3:D:447:MET:HG3	1.93	0.51
3:D:456:VAL:O	3:D:460:LEU:HB2	2.10	0.50
2:C:644:ALA:HB2	2:C:702:ILE:HD11	1.93	0.50
2:C:1051:MET:HA	5:F:114:ALA:HB2	1.91	0.50
2:C:806:VAL:HB	2:C:832:VAL:HB	1.94	0.50
1:A:149:ALA:HB1	1:A:163:PRO:HB2	1.93	0.50
1:A:222:ALA:HB1	1:B:208:LEU:HG	1.94	0.50
3:D:1219:SER:OG	3:D:1243:ASP:OD2	2.20	0.50
1:A:146:TYR:OH	2:C:878:LYS:NZ	2.45	0.49
3:D:588:LEU:HD11	3:D:672:MET:HE3	1.93	0.49
2:C:157:PHE:CE1	2:C:389:ILE:HD11	2.43	0.49
5:F:81:TRP:HE1	6:G:3:DT:H3'	1.77	0.49
5:F:136:LEU:HA	5:F:144:ARG:HD3	1.93	0.49
3:D:507:LEU:HB3	3:D:531:ALA:HB1	1.95	0.49
2:C:727:GLU:H	3:D:725:THR:HG21	1.77	0.49
3:D:198:ARG:NH1	11:D:2102:HOH:O	2.45	0.49
2:C:216:VAL:HG12	2:C:222:VAL:HG22	1.93	0.49
5:F:117:PRO:HG2	5:F:122:ILE:HG22	1.94	0.49
1:A:36:ASN:O	1:A:40:ARG:HG2	2.13	0.49
1:A:124:HIS:CE1	1:A:127:THR:HG22	2.47	0.49
1:B:99:LYS:NZ	1:B:104:GLU:O	2.44	0.49
7:H:10:DG:C8	7:H:11:DT:H72	2.47	0.49
2:C:945:LYS:HB2	2:C:993:LEU:HD21	1.95	0.49
3:D:487:LEU:O	3:D:491:ILE:HG12	2.14	0.48
3:D:1063:LYS:HE2	3:D:1078:ASP:HB2	1.94	0.48
3:D:250:GLU:CD	3:D:250:GLU:H	2.16	0.48
3:D:850:PHE:O	3:D:853:THR:OG1	2.31	0.48
1:A:40:ARG:HD3	2:C:1013:GLY:O	2.13	0.48
2:C:1108:LYS:NZ	5:F:123:TYR:OH	2.46	0.48
3:D:595:ASP:HB3	3:D:631:ALA:HB2	1.96	0.48
1:B:182:ARG:NH2	3:D:488:GLU:OE1	2.47	0.48
3:D:85:ALA:O	3:D:88:ARG:HB2	2.14	0.48
3:D:739:PRO:HG2	3:D:742:LYS:HB2	1.96	0.48
3:D:1275:THR:HG23	4:E:104:GLU:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ASP:OD2	2:C:878:LYS:NZ	2.37	0.48
2:C:226:ILE:HG22	2:C:227:ASP:OD1	2.14	0.48
1:B:149:ALA:HB1	1:B:163:PRO:HB2	1.95	0.47
2:C:138:GLU:HA	2:C:149:SER:HA	1.97	0.47
3:D:886:VAL:HB	3:D:991:ILE:O	2.14	0.47
3:D:1081:SER:HB3	3:D:1083:ARG:HG3	1.97	0.47
3:D:346:ARG:NH2	5:F:53:ASP:OD1	2.46	0.47
3:D:47:PHE:HB3	3:D:88:ARG:HH22	1.80	0.47
3:D:1147:VAL:HG12	3:D:1149:ILE:HG13	1.97	0.47
2:C:516:TYR:HB3	2:C:578:TYR:HB3	1.95	0.47
3:D:3:ASP:OD1	3:D:3:ASP:N	2.47	0.46
3:D:103:HIS:ND1	3:D:105:TRP:HB2	2.31	0.46
5:F:82:LEU:HA	5:F:85:ILE:HD12	1.98	0.46
2:C:1067:ARG:HH12	3:D:415:GLN:HA	1.81	0.46
3:D:1036:GLU:HB3	3:D:1038:ARG:HG3	1.98	0.46
3:D:119:ASP:HB2	3:D:295:ARG:NH1	2.31	0.46
2:C:720:LEU:HD23	2:C:913:VAL:HA	1.97	0.46
3:D:757:GLU:OE2	3:D:770:ARG:NH1	2.49	0.46
3:D:924:THR:OG1	3:D:977:THR:O	2.26	0.46
2:C:120:ASP:OD1	2:C:120:ASP:N	2.37	0.46
3:D:925:LEU:HB3	3:D:940:ARG:HA	1.97	0.46
1:B:120:ASN:N	1:B:120:ASN:OD1	2.48	0.46
2:C:412:ILE:HB	2:C:417:LEU:HD21	1.97	0.46
3:D:780:GLU:O	3:D:784:GLU:HG2	2.16	0.46
2:C:173:ARG:NH1	2:C:437:SER:O	2.49	0.46
2:C:413:THR:HG23	2:C:415:GLN:H	1.80	0.46
3:D:155:MET:O	3:D:159:ARG:HG3	2.15	0.46
3:D:285:LYS:HA	3:D:289:LYS:HD2	1.97	0.46
3:D:98:ALA:HB3	3:D:354:LEU:HD23	1.98	0.45
7:H:15:DT:H2'	7:H:16:DC:C6	2.51	0.45
2:C:781:LEU:HD22	2:C:784:LEU:HD22	1.98	0.45
1:A:81:LYS:HE3	1:A:165:ASP:HB2	1.96	0.45
2:C:303:GLU:H	2:C:303:GLU:CD	2.19	0.45
3:D:576:MET:HG2	3:D:577:PRO:HD2	1.99	0.45
2:C:549:ASP:OD1	2:C:550:ALA:N	2.49	0.45
5:F:30:GLU:HA	5:F:34:ILE:HD13	1.98	0.45
1:B:71:GLU:OE1	1:B:71:GLU:N	2.49	0.45
2:C:1088:LEU:HD23	2:C:1092:LYS:HD2	1.98	0.45
2:C:1079:TYR:CD2	3:D:559:MET:HG2	2.52	0.45
2:C:132:PRO:HB3	2:C:153:PHE:HE1	1.81	0.45
5:F:118:ASN:O	5:F:122:ILE:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:255:ALA:HB3	3:D:260:SER:HB3	1.99	0.45
3:D:849:TYR:O	3:D:853:THR:HG23	2.17	0.45
1:B:174:VAL:HG22	1:B:196:VAL:HG12	1.99	0.44
2:C:163:LYS:HD2	2:C:639:GLY:HA3	1.99	0.44
3:D:264:LEU:O	3:D:268:PHE:HB2	2.17	0.44
3:D:866:ARG:NH1	3:D:1008:THR:O	2.50	0.44
3:D:968:CYS:HB3	3:D:1159:ARG:HH12	1.82	0.44
5:F:34:ILE:N	5:F:35:PRO:HD2	2.33	0.44
2:C:727:GLU:H	3:D:725:THR:CG2	2.31	0.44
6:G:13:DT:H4'	6:G:14:DG:H3'	1.99	0.44
2:C:737:LEU:HD11	2:C:885:LEU:HD11	1.99	0.44
3:D:1055:LEU:N	3:D:1101:ASP:OD2	2.44	0.44
3:D:511:ALA:HB3	3:D:560:LEU:HA	1.98	0.44
1:A:40:ARG:NH2	2:C:1014:ARG:HA	2.33	0.44
2:C:465:ARG:NH1	2:C:493:ASN:OD1	2.50	0.44
3:D:47:PHE:CD1	3:D:322:PRO:HB3	2.53	0.44
3:D:103:HIS:HB3	3:D:106:TYR:HD2	1.82	0.44
1:B:177:LYS:HE3	1:B:177:LYS:HB2	1.78	0.44
3:D:901:LEU:O	3:D:916:ILE:HD11	2.18	0.44
2:C:115:VAL:HG11	2:C:129:TYR:CE1	2.53	0.44
3:D:66:LYS:HB3	3:D:66:LYS:HE2	1.81	0.44
5:F:111:ARG:NH2	7:H:21:DG:O6	2.51	0.44
2:C:1094:ASP:HA	2:C:1099:ARG:HH21	1.83	0.43
3:D:413:PHE:CD1	3:D:1225:SER:HB3	2.53	0.43
3:D:1025:THR:OG1	3:D:1026:GLY:N	2.49	0.43
3:D:437:LYS:HA	3:D:437:LYS:HD3	1.81	0.43
3:D:491:ILE:HG23	3:D:514:PRO:HG2	1.99	0.43
3:D:1220:TRP:CD1	3:D:1243:ASP:HB2	2.53	0.43
3:D:1264:ILE:HD11	3:D:1267:TYR:CE2	2.54	0.43
2:C:245:SER:HB3	11:C:1235:HOH:O	2.18	0.43
2:C:507:ASN:N	2:C:511:PHE:O	2.45	0.43
1:A:223:ARG:HD3	11:A:407:HOH:O	2.18	0.43
2:C:139:PHE:CZ	2:C:412:ILE:HD11	2.53	0.43
2:C:888:ARG:HG2	2:C:1031:MET:HE3	2.00	0.43
3:D:819:GLY:O	3:D:839:SER:HB3	2.18	0.43
3:D:885:ILE:HG12	3:D:887:ARG:NH1	2.33	0.43
6:G:19:DG:H2''	6:G:20:DG:C8	2.54	0.43
3:D:337:THR:HB	3:D:341:ASN:HD22	1.83	0.43
3:D:572:ARG:HH21	3:D:917:GLU:HG2	1.82	0.43
2:C:549:ASP:HB3	2:C:553:ARG:H	1.84	0.43
3:D:642:PRO:HG3	3:D:662:TRP:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:816:THR:HG23	3:D:821:LYS:HA	1.99	0.43
3:D:991:ILE:HG13	3:D:1266:ARG:NH1	2.34	0.43
5:F:44:ALA:HB2	5:F:86:LEU:HD11	2.00	0.43
6:G:22:DT:H1'	6:G:23:DG:H5'	1.99	0.43
1:B:66:VAL:HG23	1:B:73:VAL:HG22	2.00	0.43
3:D:935:ASN:OD1	3:D:935:ASN:N	2.50	0.43
2:C:183:PRO:HA	2:C:205:ILE:O	2.19	0.42
2:C:472:VAL:HG22	6:G:14:DG:C2	2.54	0.42
3:D:1136:ARG:O	3:D:1140:GLU:HG2	2.18	0.42
1:A:78:LEU:HD21	2:C:620:ARG:CZ	2.49	0.42
2:C:740:ARG:NH1	2:C:744:GLU:OE1	2.52	0.42
1:B:1:MET:HG3	1:B:2:LEU:HD12	2.00	0.42
2:C:93:LEU:HD22	2:C:393:MET:HB3	2.01	0.42
3:D:473:LYS:HE2	3:D:477:GLU:OE2	2.19	0.42
2:C:222:VAL:HG12	2:C:234:VAL:HG21	2.01	0.42
2:C:355:MET:HB2	2:C:355:MET:HE2	1.77	0.42
3:D:122:PRO:CG	6:G:22:DT:H3'	2.50	0.42
1:A:11:GLU:OE2	1:A:205:ARG:NH2	2.51	0.42
2:C:105:LEU:HD11	2:C:137:ALA:HB1	2.01	0.42
2:C:467:ARG:HB3	6:G:14:DG:H2''	2.02	0.42
2:C:507:ASN:HB2	2:C:511:PHE:O	2.19	0.42
2:C:545:ASN:O	2:C:545:ASN:ND2	2.50	0.42
2:C:547:PRO:CG	2:C:556:GLU:HG2	2.50	0.42
3:D:64:LYS:HD2	3:D:77:ARG:HD3	2.02	0.42
1:B:133:LYS:NZ	1:B:135:GLU:HB2	2.35	0.42
3:D:242:ARG:HD3	3:D:242:ARG:HA	1.92	0.42
4:E:65:ASP:O	4:E:69:GLN:HG2	2.19	0.42
2:C:967:GLN:HG3	2:C:968:PRO:HD2	2.02	0.41
2:C:562:ARG:HD3	3:D:847:LEU:HD21	2.01	0.41
3:D:884:VAL:HG11	3:D:1156:VAL:HG13	2.01	0.41
2:C:45:ARG:O	2:C:47:PRO:HD3	2.20	0.41
3:D:87:VAL:HA	3:D:90:GLU:HG2	2.01	0.41
3:D:92:MET:HB2	3:D:92:MET:HE2	1.89	0.41
3:D:360:LEU:HD21	5:F:67:ALA:HB2	2.02	0.41
7:H:7:DT:H2''	7:H:8:DC:C6	2.55	0.41
2:C:618:LEU:HD12	2:C:717:LYS:HE3	2.02	0.41
2:C:939:CYS:O	2:C:943:GLY:N	2.51	0.41
3:D:759:GLN:HG2	3:D:762:ARG:NH2	2.35	0.41
1:A:98:ARG:HG3	1:A:135:GLU:HG3	2.01	0.41
3:D:827:PRO:HG3	3:D:854:HIS:HD2	1.86	0.41
5:F:81:TRP:O	5:F:85:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:357:VAL:O	2:C:359:GLY:N	2.53	0.41
3:D:302:PHE:CE1	3:D:309:PRO:HA	2.55	0.41
3:D:567:SER:HB2	3:D:574:LEU:HG	2.02	0.41
2:C:348:LEU:HD13	2:C:365:VAL:HG12	2.02	0.41
2:C:738:SER:HB2	2:C:904:MET:HG3	2.02	0.41
2:C:1043:ALA:HB1	3:D:451:LEU:HD13	2.02	0.41
1:A:62:GLU:O	1:A:73:VAL:HB	2.20	0.41
1:B:98:ARG:HA	1:B:134:LEU:O	2.21	0.41
2:C:408:ASP:O	2:C:412:ILE:HG23	2.21	0.41
2:C:440:MET:HG2	2:C:442:GLN:HG3	2.03	0.41
3:D:550:GLU:HG3	4:E:57:ALA:HB1	2.01	0.41
2:C:227:ASP:OD1	2:C:227:ASP:N	2.40	0.41
2:C:274:LEU:HA	2:C:277:ILE:HG22	2.03	0.41
2:C:959:LEU:HA	2:C:959:LEU:HD23	1.83	0.41
3:D:579:LEU:HD23	3:D:808:THR:HB	2.02	0.41
3:D:1086:LEU:HD23	3:D:1099:LEU:HB3	2.02	0.41
3:D:159:ARG:HH12	3:D:220:GLU:HB2	1.85	0.40
3:D:237:ASP:HB3	3:D:240:LEU:HB3	2.03	0.40
5:F:80:ALA:HA	6:G:7:DG:O6	2.21	0.40
7:H:9:DC:H2''	7:H:10:DG:C8	2.56	0.40
2:C:500:LEU:HG	2:C:504:ALA:HB3	2.03	0.40
2:C:680:HIS:O	2:C:1034:HIS:HE1	2.04	0.40
6:G:4:DT:H2''	6:G:5:DG:O5'	2.21	0.40
1:A:24:GLU:HB2	1:A:25:PRO:HD3	2.03	0.40
1:B:181:THR:O	1:B:189:PHE:HB2	2.21	0.40
2:C:319:LYS:HE2	2:C:368:ASP:OD2	2.21	0.40
2:C:879:ILE:HD12	2:C:879:ILE:HA	1.88	0.40
5:F:83:TYR:HB3	6:G:7:DG:C6	2.55	0.40
6:G:9:DG:H2''	6:G:10:DA:C8	2.57	0.40
2:C:547:PRO:HG3	2:C:556:GLU:HG2	2.03	0.40
2:C:926:MET:HE1	3:D:817:LEU:HA	2.04	0.40
6:G:18:DC:H2''	6:G:19:DG:C8	2.57	0.40
1:B:102:PRO:HB3	1:B:130:ASP:HA	2.04	0.40
3:D:1262:THR:HG23	4:E:50:TYR:HD1	1.86	0.40
5:F:57:LEU:HD11	5:F:89:THR:HG23	2.03	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	219/368 (60%)	211 (96%)	8 (4%)	0	100	100
1	B	227/368 (62%)	213 (94%)	14 (6%)	0	100	100
2	C	1137/1174 (97%)	1091 (96%)	46 (4%)	0	100	100
3	D	1254/1317 (95%)	1218 (97%)	36 (3%)	0	100	100
4	E	72/110 (66%)	69 (96%)	3 (4%)	0	100	100
5	F	162/209 (78%)	159 (98%)	3 (2%)	0	100	100
All	All	3071/3546 (87%)	2961 (96%)	110 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	188/315 (60%)	177 (94%)	11 (6%)	19	50
1	B	189/315 (60%)	185 (98%)	4 (2%)	53	79
2	C	897/995 (90%)	863 (96%)	34 (4%)	33	66
3	D	1032/1096 (94%)	1003 (97%)	29 (3%)	43	73
4	E	63/90 (70%)	58 (92%)	5 (8%)	12	40
5	F	115/167 (69%)	108 (94%)	7 (6%)	18	49
All	All	2484/2978 (83%)	2394 (96%)	90 (4%)	35	67

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASP
1	A	17	ASN
1	A	30	PHE
1	A	33	THR
1	A	72	ASP
1	A	84	VAL
1	A	127	THR
1	A	155	SER
1	A	171	VAL
1	A	183	VAL
1	A	217	GLU
1	B	1	MET
1	B	88	GLU
1	B	129	ASN
1	B	218	LEU
2	C	177	SER
2	C	226	ILE
2	C	227	ASP
2	C	232	GLN
2	C	308	LEU
2	C	373	PHE
2	C	388	GLN
2	C	407	GLN
2	C	412	ILE
2	C	447	SER
2	C	450	THR
2	C	454	ARG
2	C	458	LEU
2	C	463	LEU
2	C	471	GLU
2	C	488	THR
2	C	514	THR
2	C	545	ASN
2	C	558	ARG
2	C	560	LEU
2	C	604	ARG
2	C	641	VAL
2	C	659	THR
2	C	667	ARG
2	C	812	THR
2	C	843	GLU
2	C	958	ARG

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Mol	Chain	Res	Type
2	C	962	GLU
2	C	974	THR
2	C	982	GLU
2	C	1046	THR
2	C	1107	VAL
2	C	1141	ASP
2	C	1147	LEU
3	D	82	VAL
3	D	102	THR
3	D	110	VAL
3	D	250	GLU
3	D	275	GLU
3	D	298	VAL
3	D	307	ASN
3	D	414	ARG
3	D	443	LEU
3	D	451	LEU
3	D	505	HIS
3	D	515	MET
3	D	579	LEU
3	D	581	MET
3	D	606	HIS
3	D	725	THR
3	D	885	ILE
3	D	960	VAL
3	D	964	SER
3	D	1008	THR
3	D	1050	THR
3	D	1083	ARG
3	D	1120	GLU
3	D	1173	THR
3	D	1191	ARG
3	D	1208	MET
3	D	1248	LEU
3	D	1268	ARG
3	D	1275	THR
4	E	34	ILE
4	E	36	ASN
4	E	46	VAL
4	E	55	TYR
4	E	92	SER
5	F	23	GLU

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Mol	Chain	Res	Type
5	F	29	PHE
5	F	45	LEU
5	F	83	TYR
5	F	97	ARG
5	F	122	ILE
5	F	125	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	680	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	5/6 (83%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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

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	221/368 (60%)	-0.27	4 (1%) 68 47	66, 83, 133, 168	0
1	B	231/368 (62%)	0.03	7 (3%) 50 27	85, 125, 155, 162	0
2	C	1139/1174 (97%)	-0.16	14 (1%) 79 61	54, 88, 147, 170	0
3	D	1260/1317 (95%)	-0.24	11 (0%) 84 69	59, 95, 146, 178	0
4	E	76/110 (69%)	-0.02	3 (3%) 39 20	90, 117, 139, 145	0
5	F	164/209 (78%)	0.21	6 (3%) 41 21	81, 136, 160, 165	0
6	G	23/23 (100%)	-0.19	0 100 100	93, 134, 158, 165	1 (4%)
7	H	20/20 (100%)	-0.54	0 100 100	67, 88, 148, 149	0
8	I	6/6 (100%)	-0.35	0 100 100	60, 62, 72, 87	0
All	All	3140/3595 (87%)	-0.17	45 (1%) 75 56	54, 97, 150, 178	1 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1160	ALA	5.7
3	D	1281	ALA	5.6
4	E	70	LEU	5.5
2	C	1159	ALA	4.7
2	C	1155	LEU	4.4
2	C	1156	GLU	4.3
2	C	1154	ASP	4.1
2	C	1161	ASN	3.9
1	B	157	ALA	3.9
2	C	1158	ALA	3.8
1	A	184	GLU	3.7
2	C	191	ILE	3.7
1	B	63	PHE	3.4
3	D	1059	GLU	3.4
3	D	908	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
5	F	133	GLN	3.3
2	C	1152	ASP	3.3
5	F	151	ASP	3.2
3	D	1086	LEU	3.1
5	F	146	ALA	3.0
3	D	1057	ASP	3.0
1	B	4	SER	2.8
2	C	235	THR	2.8
5	F	145	MET	2.7
2	C	218	LYS	2.6
4	E	27	GLY	2.6
2	C	195	THR	2.6
1	A	3	ILE	2.5
3	D	1084	GLN	2.5
1	B	138	LEU	2.5
3	D	1062	TYR	2.4
3	D	1111	LEU	2.4
1	B	1	MET	2.3
1	A	185	GLN	2.3
2	C	192	ASP	2.3
2	C	26	SER	2.2
1	B	235	GLY	2.2
5	F	36	LEU	2.2
1	B	95	MET	2.1
1	A	183	VAL	2.1
5	F	69	PHE	2.1
4	E	26	GLY	2.0
3	D	1025	THR	2.0
3	D	1069	ASP	2.0
3	D	1081	SER	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, 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(\AA^2)	Q<0.9
10	MG	D	2003	1/1	0.89	0.13	59,59,59,59	0
9	ZN	D	2002	1/1	0.98	0.13	123,123,123,123	0
9	ZN	D	2001	1/1	0.99	0.17	99,99,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.