Full wwPDB X-ray Structure Validation Report (i)

Jul 16, 2024 – 04:27 PM JST

PDB ID	:	8W8O
Title	:	Thermus thermophilus initiation complex in the half-translocated state
Authors	:	Li, L.; Zhang, Y.
Deposited on	:	2023-09-04
Resolution	:	2.51 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 (i) 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 (1)) were used in the production of this report:

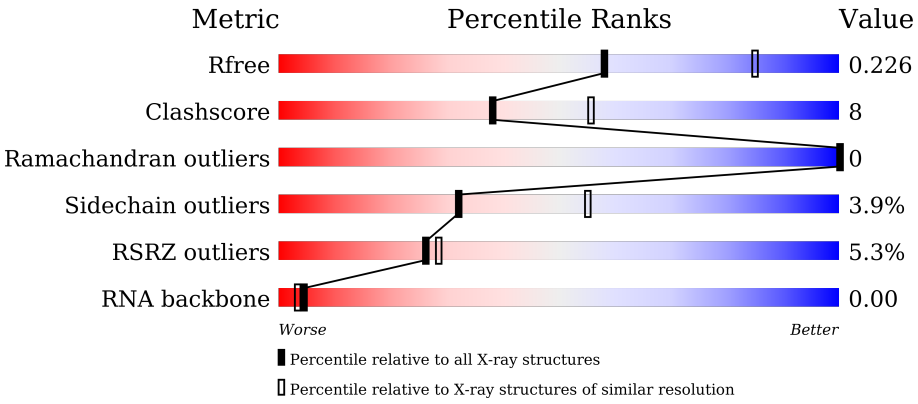
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.51 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)
RNA backbone	3102	1020 (2.86-2.18)

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	315	58% 13% 28%
1	B	315	54% 17% 29%
2	C	1119	81% 17%
3	D	1524	78% 19%

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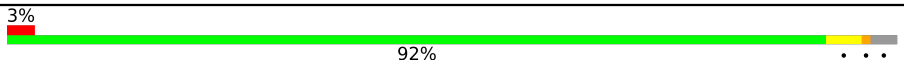
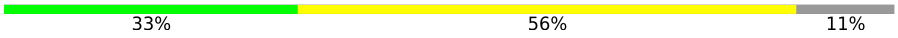
Mol	Chain	Length	Quality of chain
4	E	99	
5	F	443	
6	G	21	
7	H	27	
8	I	3	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 29261 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	228	Total	C	N	O	S	0	0	0
			1792	1144	312	334	2			
1	B	224	Total	C	N	O	S	0	0	0
			1767	1130	307	328	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1107	Total	C	N	O	S	0	0	0
			8728	5523	1560	1621	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1481	Total	C	N	O	S	0	3	0
			11682	7412	2056	2178	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	96	Total	C	N	O	S	0	0	0
			781	497	137	143	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2804	1767	509	524	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	expression tag	UNP Q5SKW1
F	-18	GLY	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	SER	-	expression tag	UNP Q5SKW1
F	-15	HIS	-	expression tag	UNP Q5SKW1
F	-14	HIS	-	expression tag	UNP Q5SKW1
F	-13	HIS	-	expression tag	UNP Q5SKW1
F	-12	HIS	-	expression tag	UNP Q5SKW1
F	-11	HIS	-	expression tag	UNP Q5SKW1
F	-10	HIS	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	SER	-	expression tag	UNP Q5SKW1
F	-7	GLY	-	expression tag	UNP Q5SKW1
F	-6	LEU	-	expression tag	UNP Q5SKW1
F	-5	VAL	-	expression tag	UNP Q5SKW1
F	-4	PRO	-	expression tag	UNP Q5SKW1
F	-3	ARG	-	expression tag	UNP Q5SKW1
F	-2	GLY	-	expression tag	UNP Q5SKW1
F	-1	SER	-	expression tag	UNP Q5SKW1
F	0	HIS	-	expression tag	UNP Q5SKW1

- Molecule 6 is a DNA chain called DNA (21-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	18	Total	C	N	O	P	0	0	0
			369	175	71	106	17			

- Molecule 7 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			

- Molecule 8 is a RNA chain called RNA (5'-(GTP)GA-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	3	Total	C	N	O	P	0	0	0
			77	30	15	27	5			

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Mg 1 1	0	0
9	D	3	Total Mg 3 3	0	0
9	F	1	Total Mg 1 1	0	0
9	I	2	Total Mg 2 2	0	0

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 11 is water.

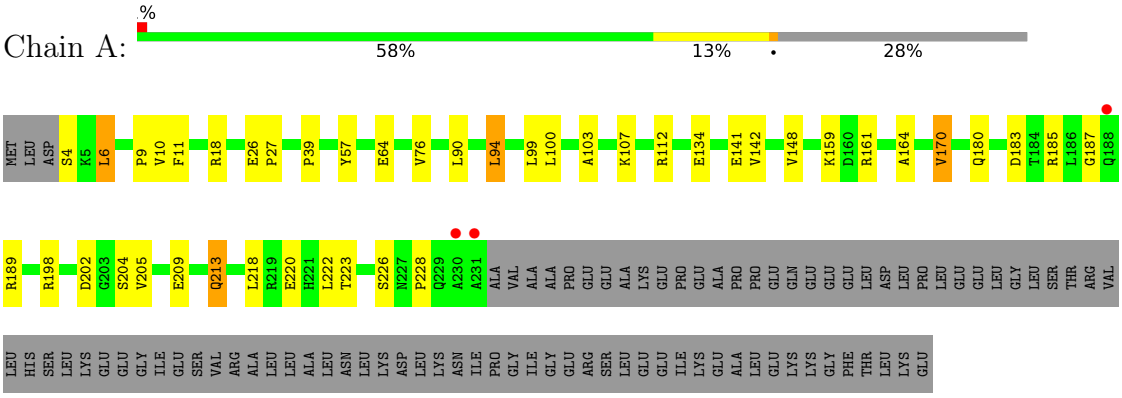
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	44	Total O 44 44	0	0
11	B	29	Total O 29 29	0	0
11	C	270	Total O 270 270	0	0
11	D	304	Total O 304 304	0	0
11	E	32	Total O 32 32	0	0
11	F	37	Total O 37 37	0	0
11	G	14	Total O 14 14	0	0
11	H	5	Total O 5 5	0	0
11	I	22	Total O 22 22	0	0

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.

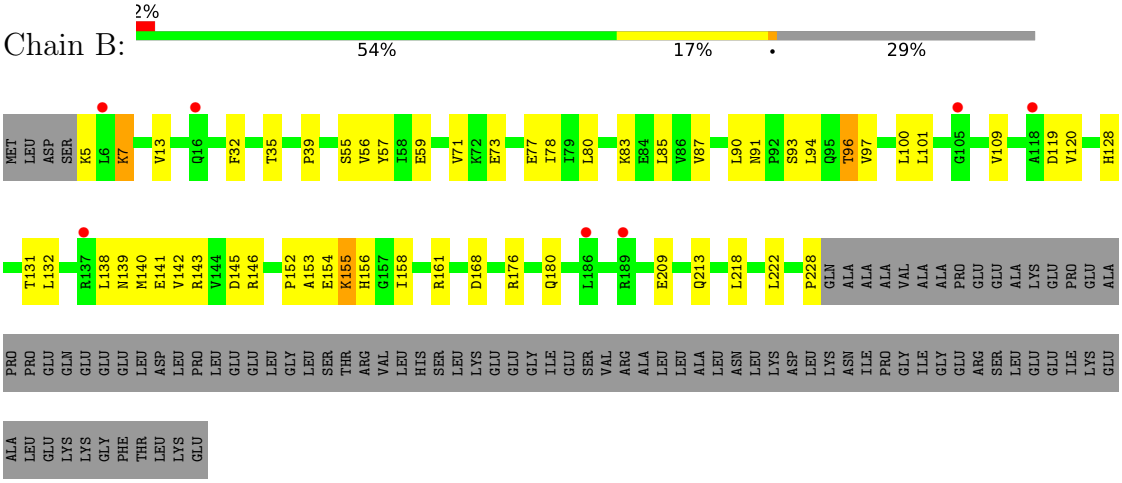
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



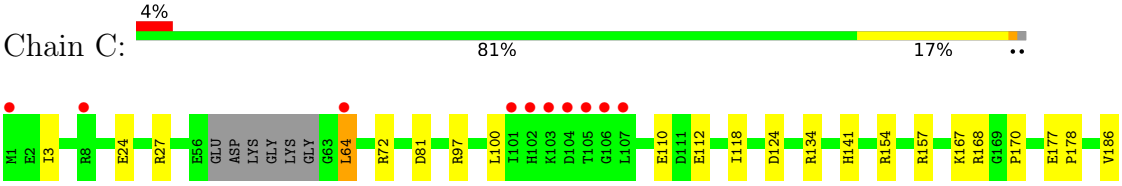
• Molecule 1: DNA-directed RNA polymerase subunit alpha

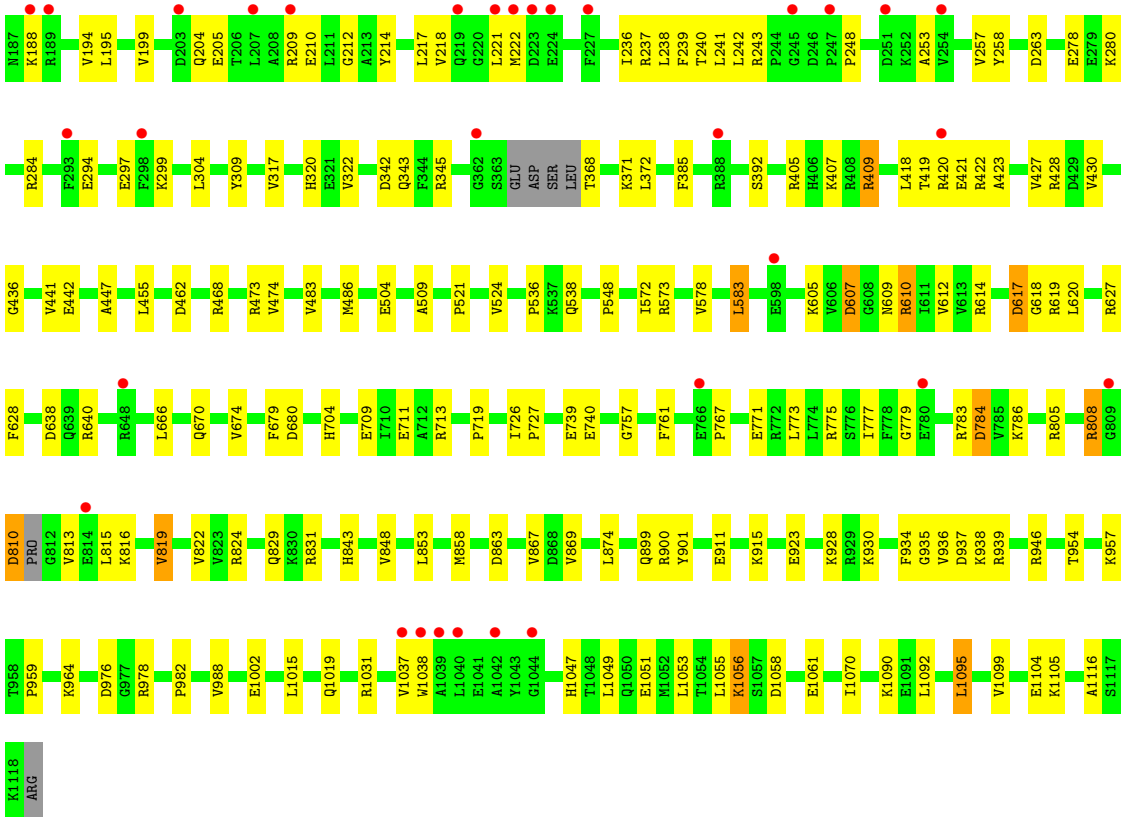
Chain B:



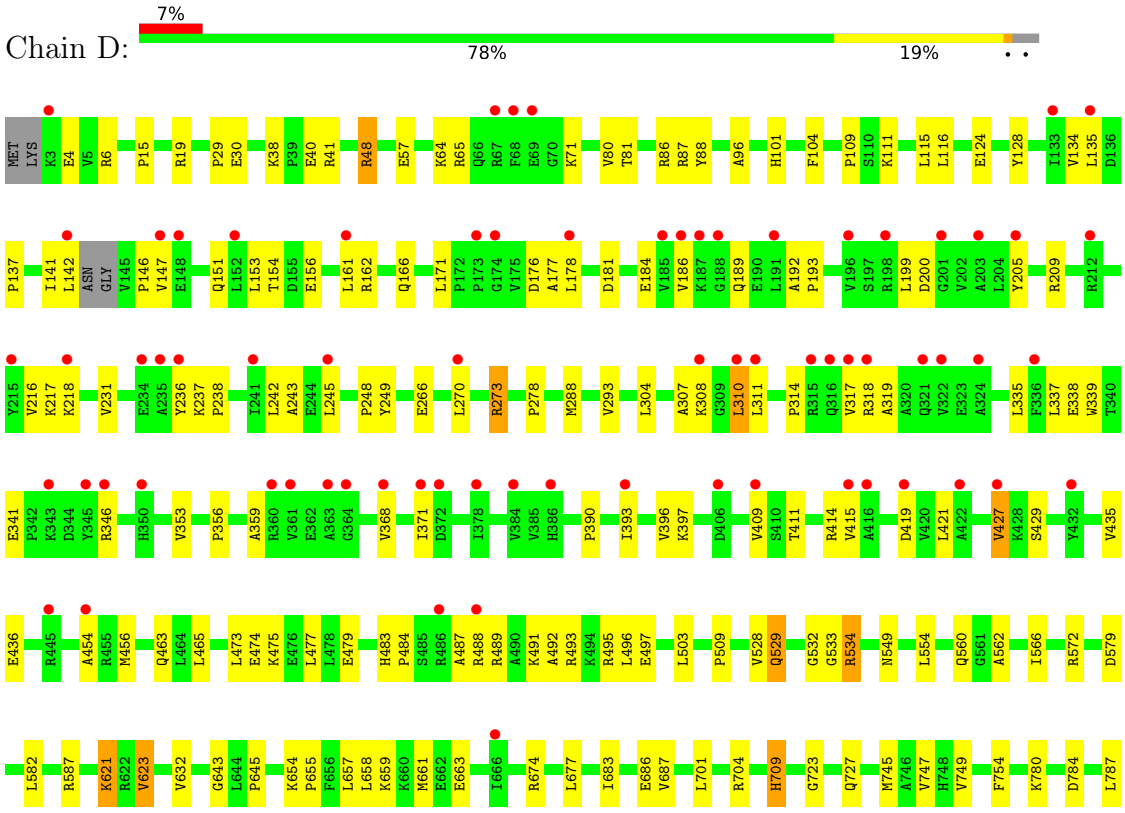
• Molecule 2: DNA-directed RNA polymerase subunit beta

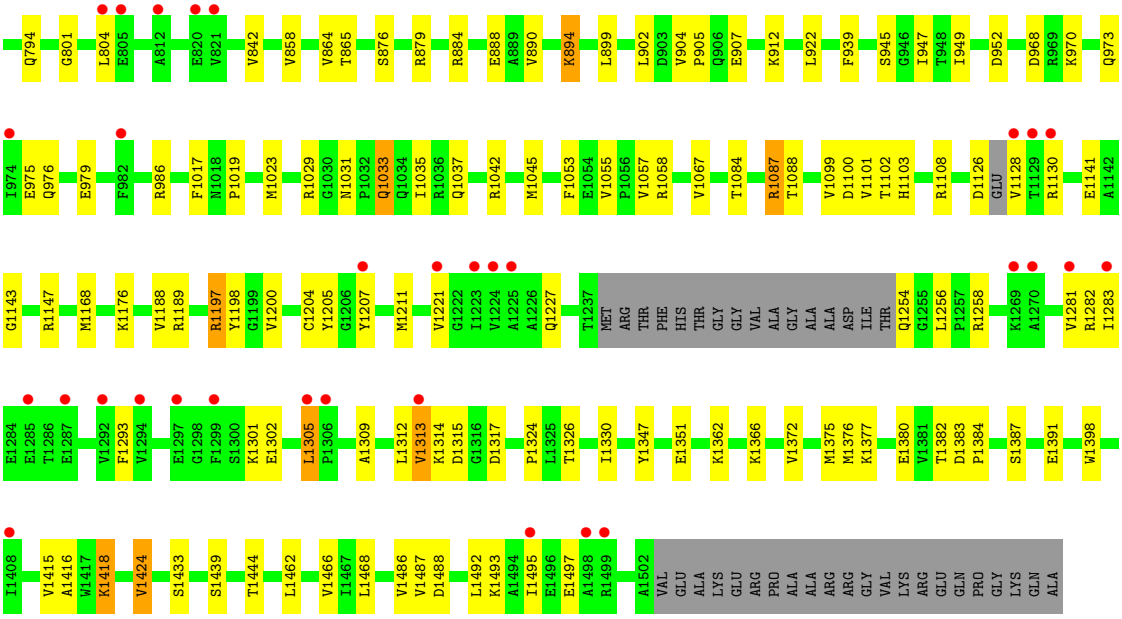
Chain C:



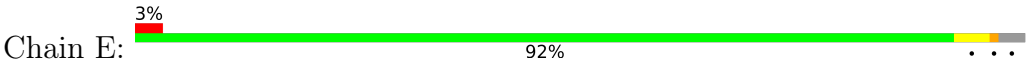


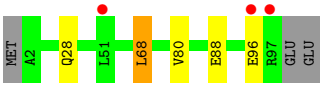
• Molecule 3: DNA-directed RNA polymerase subunit beta'



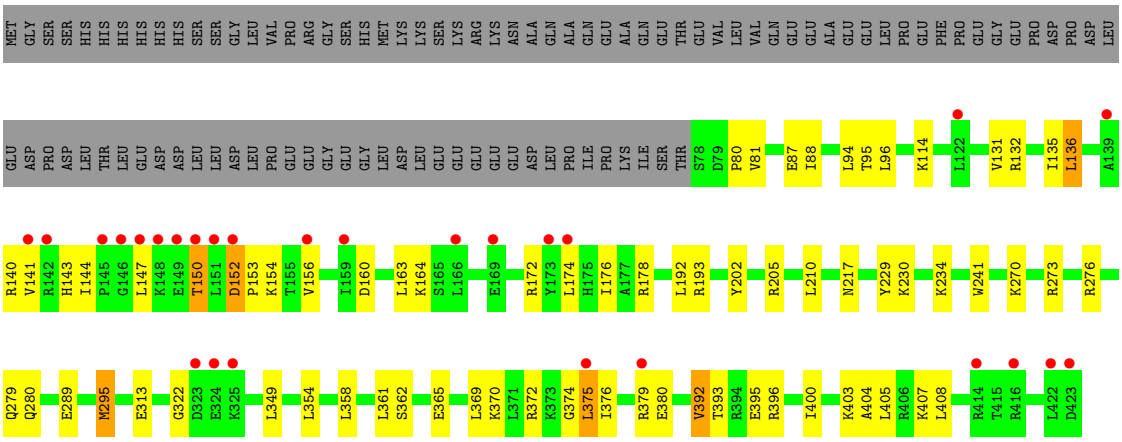


• Molecule 4: DNA-directed RNA polymerase subunit omega

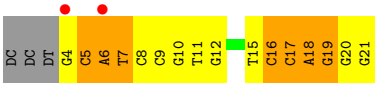




• Molecule 5: RNA polymerase sigma factor SigA



• Molecule 6: DNA (21-MER)



• Molecule 7: DNA (27-MER)

Chain H:

• Molecule 8: RNA (5'-(GTP)GA-3')

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	183.40Å 103.80Å 295.04Å 90.00° 99.19° 90.00°	Depositor
Resolution (Å)	39.88 – 2.51 39.88 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.88-2.51) 99.0 (39.88-2.51)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.187 , 0.226 0.187 , 0.226	Depositor DCC
R_{free} test set	9212 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	51.4	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.012 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l 0.012 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	29261	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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, MG, GTP

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	0.46	0/1824	0.63	0/2480
1	B	0.43	0/1799	0.60	0/2446
2	C	0.47	0/8892	0.63	0/12022
3	D	0.45	0/11895	0.62	0/16084
4	E	0.47	0/795	0.63	0/1071
5	F	0.41	0/2849	0.56	0/3833
6	G	0.93	0/414	1.39	8/638 (1.3%)
7	H	0.96	0/556	1.05	0/858
8	I	0.64	0/50	1.23	1/76 (1.3%)
All	All	0.48	0/29074	0.65	9/39508 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	19	DG	P-O3'-C3'	-9.45	108.36	119.70
6	G	6	DA	P-O3'-C3'	-9.17	108.69	119.70
6	G	18	DA	P-O3'-C3'	-9.04	108.86	119.70
6	G	15	DT	P-O3'-C3'	-8.73	109.23	119.70
6	G	17	DC	P-O3'-C3'	-8.40	109.62	119.70
6	G	16	DC	P-O3'-C3'	-7.99	110.12	119.70
6	G	5	DC	P-O3'-C3'	-6.94	111.37	119.70
6	G	7	DT	P-O3'-C3'	-5.67	112.90	119.70
8	I	6	G	P-O3'-C3'	-5.26	113.39	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1792	0	1844	30	0
1	B	1767	0	1821	39	0
2	C	8728	0	8834	135	0
3	D	11682	0	11899	189	0
4	E	781	0	797	4	0
5	F	2804	0	2873	49	0
6	G	369	0	203	22	0
7	H	495	0	272	14	0
8	I	77	0	33	0	0
9	B	1	0	0	0	0
9	D	3	0	0	0	0
9	F	1	0	0	0	0
9	I	2	0	0	0	0
10	D	2	0	0	0	0
11	A	44	0	0	4	0
11	B	29	0	0	0	0
11	C	270	0	0	9	0
11	D	304	0	0	17	0
11	E	32	0	0	1	0
11	F	37	0	0	3	0
11	G	14	0	0	1	0
11	H	5	0	0	0	0
11	I	22	0	0	0	0
All	All	29261	0	28576	431	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 8.

All (431) 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:1380:GLU:HB3	3:D:1418:LYS:HD3	1.56	0.87
6:G:9:DC:H2'	6:G:10:DG:C8	2.13	0.84
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.65	0.79
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:628:PHE:H	2:C:638:ASP:HB3	1.48	0.78
3:D:456:MET:SD	11:D:1896:HOH:O	2.41	0.78
1:B:152:PRO:HD2	1:B:155:LYS:HG2	1.71	0.72
5:F:370:LYS:HA	5:F:375:LEU:HD12	1.72	0.71
2:C:937:ASP:OD1	2:C:939:ARG:HD3	1.91	0.71
3:D:87:ARG:NH2	11:D:1701:HOH:O	2.25	0.70
3:D:658:LEU:HA	3:D:661:MET:HE3	1.74	0.70
1:A:4:SER:O	1:A:189:ARG:NH2	2.21	0.70
1:B:90:LEU:HD12	1:B:119:ASP:HA	1.75	0.69
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.73	0.69
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.75	0.69
2:C:420:ARG:HG2	2:C:421:GLU:H	1.57	0.69
1:B:100:LEU:HD23	1:B:141:GLU:HG2	1.74	0.68
3:D:317:VAL:HG23	3:D:339:TRP:HB3	1.75	0.68
3:D:134:VAL:HG22	3:D:151:GLN:H	1.59	0.67
2:C:810:ASP:HB2	2:C:813:VAL:HG21	1.77	0.67
3:D:57:GLU:HG3	3:D:64:LYS:HG2	1.75	0.67
1:A:185:ARG:NH2	1:A:187:GLY:O	2.28	0.67
2:C:617:ASP:OD2	2:C:619:ARG:NE	2.27	0.67
2:C:954:THR:HB	2:C:957:LYS:HD2	1.76	0.67
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.77	0.66
5:F:193:ARG:HB2	7:H:6:DT:H1'	1.77	0.66
3:D:1254:GLN:NE2	11:D:1702:HOH:O	2.25	0.66
2:C:97:ARG:NH1	2:C:110:GLU:OE1	2.29	0.65
2:C:134:ARG:NH2	6:G:21:DG:H2"	2.11	0.65
6:G:19:DG:H2"	6:G:20:DG:C8	2.31	0.65
3:D:489:ARG:NH1	3:D:1391:GLU:OE2	2.31	0.64
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.81	0.63
3:D:134:VAL:HG12	3:D:454:ALA:HB2	1.79	0.63
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.79	0.63
5:F:392:VAL:HG13	5:F:396:ARG:HB3	1.80	0.63
3:D:288:MET:HG2	3:D:307:ALA:HB2	1.79	0.63
2:C:428:ARG:NH2	2:C:447:ALA:O	2.31	0.62
3:D:162:ARG:O	3:D:414:ARG:NH1	2.31	0.62
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.81	0.62
3:D:248:PRO:HG3	3:D:308:LYS:HE3	1.81	0.62
2:C:640:ARG:HG3	2:C:640:ARG:HH11	1.64	0.62
3:D:1384:PRO:HA	3:D:1415:VAL:HG13	1.82	0.62
5:F:322:GLY:HA3	6:G:20:DG:H21	1.65	0.61
2:C:194:VAL:HG22	2:C:221:LEU:HD12	1.82	0.61
3:D:199:LEU:HB2	3:D:397:LYS:HE3	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:657:LEU:HG	3:D:661:MET:HE2	1.81	0.61
2:C:170:PRO:HA	7:H:13:DT:O4	2.00	0.61
5:F:152:ASP:OD2	5:F:154:LYS:HB3	1.99	0.61
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.35	0.61
1:B:128:HIS:HE1	1:B:131:THR:HG23	1.66	0.61
3:D:534:ARG:NH2	5:F:313:GLU:O	2.32	0.61
5:F:289:GLU:N	5:F:289:GLU:OE1	2.34	0.61
3:D:1254:GLN:HB2	3:D:1258:ARG:HB2	1.82	0.60
3:D:621:LYS:NZ	11:D:1710:HOH:O	2.33	0.60
2:C:239:PHE:CD1	2:C:253:ALA:HA	2.35	0.60
3:D:1087[A]:ARG:HG3	3:D:1256:LEU:HD23	1.82	0.60
3:D:1101:VAL:HG23	3:D:1102:THR:HG23	1.84	0.60
2:C:420:ARG:HG2	2:C:421:GLU:N	2.17	0.60
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.28	0.59
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.84	0.59
5:F:362:SER:OG	5:F:365:GLU:HG2	2.03	0.59
3:D:178:LEU:HG	3:D:192:ALA:HA	1.84	0.59
2:C:1058:ASP:OD1	3:D:621:LYS:HE2	2.03	0.59
3:D:266:GLU:HB2	3:D:314:PRO:HB3	1.83	0.59
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.84	0.58
1:A:222:LEU:HD11	1:B:218:LEU:HG	1.85	0.58
6:G:10:DG:H2'	6:G:11:DT:C6	2.38	0.58
1:B:32:PHE:HA	1:B:35:THR:HB	1.83	0.58
3:D:181:ASP:HB2	3:D:205:TYR:CD2	2.37	0.58
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.85	0.58
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.36	0.58
5:F:172:ARG:O	5:F:176:ILE:HG12	2.04	0.58
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.86	0.58
1:B:101:LEU:HD21	1:B:109:VAL:HG11	1.86	0.57
2:C:773:LEU:HD23	5:F:354:LEU:HD13	1.86	0.57
3:D:200:ASP:O	3:D:397:LYS:HG2	2.03	0.57
5:F:322:GLY:HA3	6:G:20:DG:N2	2.19	0.57
6:G:11:DT:H4'	6:G:12:DG:OP1	2.04	0.57
11:C:1302:HOH:O	5:F:280:GLN:HG2	2.04	0.57
1:B:156:HIS:ND1	1:B:158:ILE:HG23	2.19	0.57
1:A:159:LYS:HE3	1:A:164:ALA:O	2.04	0.57
3:D:86:ARG:NH1	11:D:1715:HOH:O	2.37	0.57
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.40	0.57
2:C:167:LYS:NZ	11:C:1206:HOH:O	2.37	0.57
2:C:278:GLU:OE2	2:C:284:ARG:NH2	2.37	0.57
1:B:57:TYR:CD1	1:B:161:ARG:HD2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.87	0.57
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.87	0.57
6:G:10:DG:H2"	6:G:11:DT:O5'	2.05	0.56
2:C:628:PHE:H	2:C:638:ASP:CB	2.17	0.56
1:A:209:GLU:O	1:A:213:GLN:HG2	2.06	0.56
3:D:166:GLN:HB2	3:D:396:VAL:HG22	1.87	0.56
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.87	0.56
3:D:142:LEU:HD13	3:D:161:LEU:HD21	1.87	0.55
2:C:212:GLY:HA2	2:C:218:VAL:HG21	1.88	0.55
1:B:143:ARG:NH1	1:B:158:ILE:HD12	2.22	0.55
2:C:605:LYS:HB2	2:C:612:VAL:HB	1.89	0.55
3:D:1126:ASP:OD2	3:D:1130:ARG:NH2	2.27	0.55
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.88	0.55
3:D:236:TYR:CE2	3:D:242:LEU:HD12	2.41	0.55
6:G:18:DA:H2'	6:G:19:DG:C8	2.41	0.55
3:D:156:GLU:CD	3:D:156:GLU:H	2.10	0.55
6:G:21:DG:H2'	6:G:21:DG:N3	2.22	0.55
3:D:1487:VAL:HG11	3:D:1492:LEU:HD13	1.87	0.54
5:F:396:ARG:O	5:F:400:ILE:HG23	2.06	0.54
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.89	0.54
2:C:607:ASP:HB3	2:C:609:ASN:H	1.73	0.54
7:H:10:DA:H2"	7:H:11:DG:C8	2.42	0.54
2:C:294:GLU:HB3	2:C:299:LYS:HE2	1.89	0.54
2:C:409:ARG:NH2	2:C:442:GLU:HG2	2.22	0.54
2:C:64:LEU:HG	2:C:100:LEU:HD21	1.89	0.53
2:C:911:GLU:O	2:C:915:LYS:HG2	2.08	0.53
3:D:421:LEU:HB2	3:D:427:VAL:HG22	1.89	0.53
2:C:236:ILE:O	2:C:240:THR:HG23	2.07	0.53
2:C:727:PRO:HB3	2:C:783:ARG:HD3	1.91	0.53
3:D:493:ARG:O	3:D:497:GLU:HG3	2.08	0.53
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.09	0.53
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.88	0.53
3:D:1087[A]:ARG:NH2	11:D:1720:HOH:O	2.42	0.53
6:G:7:DT:H5"	6:G:7:DT:H6	1.73	0.53
2:C:1047:HIS:HE1	11:D:1841:HOH:O	1.91	0.53
3:D:794:GLN:HB3	11:D:1724:HOH:O	2.09	0.53
3:D:171:LEU:HD11	3:D:393:ILE:HD11	1.91	0.52
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.91	0.52
3:D:1197:ARG:HD2	3:D:1198:TYR:CZ	2.45	0.52
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.92	0.52
6:G:16:DC:H2'	6:G:17:DC:H6	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:16:DC:H2'	6:G:17:DC:C6	2.45	0.52
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.44	0.52
2:C:614:ARG:NH2	2:C:618:GLY:O	2.43	0.52
3:D:171:LEU:HD12	3:D:390:PRO:HG2	1.92	0.52
3:D:709:HIS:HD2	11:D:1994:HOH:O	1.91	0.52
2:C:709:GLU:HG3	2:C:824:ARG:HG2	1.91	0.52
3:D:135:LEU:HD13	3:D:463:GLN:HG2	1.92	0.52
2:C:674:VAL:HG22	2:C:869:VAL:HG22	1.91	0.52
1:A:228:PRO:HB3	1:B:13:VAL:HG21	1.92	0.52
3:D:1058:ARG:HD2	11:D:1897:HOH:O	2.09	0.52
2:C:214:TYR:O	2:C:217:LEU:HD12	2.09	0.51
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.91	0.51
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.76	0.51
5:F:202:TYR:HD2	5:F:205:ARG:HH21	1.58	0.51
2:C:297:GLU:OE1	2:C:299:LYS:NZ	2.42	0.51
3:D:1347:TYR:CZ	3:D:1351:GLU:HG3	2.46	0.51
1:A:10:VAL:HG12	1:A:26:GLU:O	2.11	0.51
2:C:237:ARG:O	2:C:241:LEU:HG	2.10	0.51
3:D:411:THR:HG23	3:D:436:GLU:HA	1.93	0.51
6:G:20:DG:H5'	6:G:21:DG:C6	2.45	0.51
3:D:894:LYS:H	3:D:894:LYS:HD2	1.74	0.51
3:D:15:PRO:O	3:D:19:ARG:HG3	2.11	0.50
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.93	0.50
5:F:132:ARG:HG2	5:F:136:LEU:HD22	1.94	0.50
7:H:23:DG:H2"	7:H:24:DC:H5"	1.93	0.50
2:C:194:VAL:HG23	11:C:1221:HOH:O	2.11	0.50
3:D:645:PRO:HB3	3:D:723:GLY:O	2.11	0.50
3:D:30:GLU:OE1	3:D:40:GLU:HG2	2.12	0.50
3:D:904:VAL:HG12	3:D:905:PRO:HD2	1.93	0.50
2:C:436:GLY:HA2	2:C:538:GLN:O	2.12	0.50
2:C:680:ASP:OD2	2:C:978:ARG:NH2	2.45	0.50
2:C:816:LYS:O	2:C:819:VAL:HG13	2.12	0.50
3:D:109:PRO:HB3	7:H:21:DA:OP1	2.12	0.50
3:D:1084:THR:O	3:D:1088:THR:HG23	2.11	0.50
3:D:562:ALA:O	5:F:140:ARG:NH1	2.45	0.49
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.94	0.49
1:A:180:GLN:NE2	2:C:935:GLY:O	2.46	0.49
2:C:368:THR:HG23	2:C:371:LYS:HD2	1.95	0.49
5:F:276:ARG:O	5:F:279:GLN:HG3	2.12	0.49
1:B:78:ILE:HG21	1:B:140:MET:HE1	1.93	0.49
2:C:462:ASP:HB3	2:C:468:ARG:CD	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:317:VAL:HG22	2:C:320:HIS:HD1	1.78	0.49
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.95	0.49
2:C:548:PRO:O	2:C:843:HIS:HE1	1.94	0.49
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.45	0.49
2:C:1056:LYS:HB3	3:D:623:VAL:HG22	1.95	0.49
3:D:319:ALA:HA	3:D:337:LEU:HD23	1.95	0.49
2:C:923:GLU:OE2	2:C:964:LYS:NZ	2.45	0.49
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.95	0.49
3:D:1197:ARG:HD2	3:D:1198:TYR:CE2	2.48	0.49
1:B:94:LEU:HD21	1:B:97:VAL:HG22	1.95	0.49
7:H:9:DG:H2"	7:H:10:DA:C8	2.48	0.49
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.27	0.48
3:D:1019:PRO:HG3	11:D:1858:HOH:O	2.12	0.48
3:D:1033:GLN:O	3:D:1037:GLN:HG3	2.13	0.48
2:C:195:LEU:O	2:C:199:VAL:HG23	2.13	0.48
3:D:1017:PHE:HE1	11:D:1724:HOH:O	1.95	0.48
5:F:229:TYR:CZ	5:F:230:LYS:HD3	2.48	0.48
1:B:91:ASN:ND2	1:B:93:SER:HB2	2.27	0.48
2:C:775:ARG:O	2:C:779:GLY:N	2.43	0.48
3:D:1035:ILE:HD11	11:D:1828:HOH:O	2.13	0.48
2:C:342:ASP:OD1	2:C:345:ARG:NH1	2.46	0.48
3:D:483:HIS:CE1	3:D:488:ARG:HD3	2.48	0.48
3:D:654:LYS:HD3	3:D:674[A]:ARG:NH1	2.29	0.48
1:A:220:GLU:O	1:A:223:THR:HB	2.14	0.48
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.94	0.48
3:D:209:ARG:O	3:D:346:ARG:HD3	2.12	0.48
5:F:372:ARG:O	5:F:380:GLU:HB2	2.14	0.48
1:A:94:LEU:HD12	11:A:416:HOH:O	2.13	0.48
2:C:1056:LYS:NZ	3:D:749:VAL:O	2.46	0.48
5:F:135:ILE:HD11	5:F:178:ARG:HB3	1.95	0.48
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.94	0.48
1:B:155:LYS:N	1:B:155:LYS:HD3	2.29	0.48
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.96	0.48
1:A:11:PHE:O	1:B:228:PRO:HA	2.14	0.47
1:B:97:VAL:HG21	1:B:120:VAL:HG21	1.96	0.47
2:C:3:ILE:HD13	2:C:900:ARG:HB2	1.95	0.47
3:D:71:LYS:O	3:D:80:VAL:HG12	2.14	0.47
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.95	0.47
2:C:810:ASP:HB2	2:C:813:VAL:CG2	2.43	0.47
5:F:152:ASP:OD1	5:F:154:LYS:HD3	2.15	0.47
5:F:393:THR:HG22	5:F:395:GLU:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:GLU:HB2	1:B:139:ASN:HB3	1.97	0.47
3:D:1283:ILE:HG13	3:D:1315:ASP:OD2	2.13	0.47
3:D:1305:LEU:HD13	3:D:1309:ALA:HB3	1.96	0.47
1:A:170:VAL:HG13	11:A:439:HOH:O	2.14	0.47
3:D:353:VAL:HG22	3:D:368:VAL:HG22	1.96	0.47
1:B:7:LYS:HB2	1:B:7:LYS:HE3	1.68	0.47
2:C:1051:GLU:HG2	2:C:1055:LEU:HD12	1.96	0.47
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.65	0.47
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.97	0.47
5:F:270:LYS:HG2	5:F:295:MET:HE1	1.96	0.47
2:C:858:MET:HG2	2:C:867:VAL:O	2.13	0.47
2:C:946:ARG:HG3	11:C:1417:HOH:O	2.15	0.47
2:C:1015:LEU:HD11	3:D:528:VAL:HG11	1.96	0.47
2:C:1053:LEU:HA	3:D:621:LYS:HD2	1.97	0.47
1:A:202:ASP:OD1	1:A:204:SER:HB3	2.15	0.47
2:C:1031:ARG:NH2	11:C:1213:HOH:O	2.47	0.47
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.96	0.47
3:D:487:ALA:O	3:D:491:LYS:HG2	2.15	0.47
3:D:1197:ARG:HG2	3:D:1398:TRP:CE2	2.50	0.47
1:A:112:ARG:HD3	11:A:405:HOH:O	2.14	0.47
3:D:237:LYS:HA	3:D:318:ARG:HG3	1.97	0.47
2:C:419:THR:HG21	2:C:422:ARG:NH2	2.30	0.46
2:C:767:PRO:HB3	2:C:771:GLU:OE1	2.15	0.46
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.97	0.46
2:C:134:ARG:HH21	6:G:21:DG:H2"	1.78	0.46
2:C:420:ARG:C	2:C:422:ARG:H	2.19	0.46
3:D:137:PRO:HB3	3:D:147:VAL:HG12	1.98	0.46
5:F:141:VAL:HG22	11:F:606:HOH:O	2.15	0.46
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.97	0.46
2:C:719:PRO:HD2	2:C:761:PHE:CE2	2.51	0.46
3:D:686:GLU:CD	3:D:686:GLU:H	2.19	0.46
3:D:968:ASP:OD2	3:D:1058:ARG:NH2	2.42	0.46
3:D:111:LYS:HE2	11:D:1822:HOH:O	2.15	0.46
6:G:21:DG:N2	11:G:101:HOH:O	2.48	0.46
2:C:627:ARG:NH2	11:C:1203:HOH:O	2.31	0.46
2:C:72:ARG:NH2	2:C:112:GLU:OE1	2.39	0.46
2:C:808:ARG:HB2	11:C:1439:HOH:O	2.15	0.46
3:D:128:TYR:OH	3:D:579:ASP:OD2	2.27	0.46
3:D:134:VAL:CG2	3:D:151:GLN:H	2.26	0.46
1:A:39:PRO:HG3	1:B:39:PRO:CG	2.41	0.46
2:C:243:ARG:NH1	7:H:9:DG:O6	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.98	0.46
3:D:975:GLU:O	3:D:979:GLU:HG2	2.16	0.46
1:A:226:SER:O	1:A:228:PRO:HD3	2.16	0.46
2:C:1116:ALA:HB2	3:D:88:TYR:HB3	1.98	0.46
3:D:65:ARG:HA	3:D:65:ARG:HD3	1.74	0.45
3:D:529:GLN:HG3	3:D:533:GLY:HA2	1.97	0.45
3:D:801:GLY:O	3:D:804:LEU:HG	2.15	0.45
3:D:1309:ALA:HB1	3:D:1326:THR:HG23	1.98	0.45
5:F:241:TRP:CE2	7:H:1:DT:H4'	2.52	0.45
1:B:153:ALA:HA	1:B:156:HIS:NE2	2.31	0.45
2:C:719:PRO:HD2	2:C:761:PHE:HE2	1.81	0.45
2:C:928:LYS:HE3	2:C:928:LYS:HB2	1.78	0.45
2:C:976:ASP:OD1	2:C:978:ARG:HD3	2.16	0.45
3:D:116:LEU:HD11	3:D:465:LEU:HG	1.99	0.45
5:F:370:LYS:HB3	5:F:376:ILE:HG12	1.97	0.45
6:G:4:DG:C4'	6:G:5:DC:H5'	2.46	0.45
6:G:8:DC:H2"	6:G:9:DC:H5"	1.99	0.45
3:D:1053:PHE:CE2	3:D:1055:VAL:HG22	2.51	0.45
1:B:132:LEU:HD21	1:B:138:LEU:HB2	1.97	0.45
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.98	0.45
7:H:16:DC:H2"	7:H:17:DA:C8	2.51	0.45
1:A:100:LEU:HD22	1:A:141:GLU:HG2	1.98	0.45
2:C:24:GLU:OE2	2:C:27:ARG:NH1	2.49	0.45
3:D:879:ARG:HD3	3:D:902:LEU:O	2.16	0.45
2:C:418:LEU:HD21	7:H:14:DG:C8	2.51	0.45
3:D:1197:ARG:HG2	3:D:1398:TRP:CZ2	2.52	0.45
3:D:1281:VAL:HG11	3:D:1313:VAL:HG13	1.99	0.45
5:F:370:LYS:HB3	5:F:376:ILE:CG1	2.47	0.45
1:A:183:ASP:HA	2:C:938:LYS:HE3	1.98	0.45
2:C:210:GLU:HG2	2:C:304:LEU:HD21	1.99	0.45
5:F:365:GLU:OE2	5:F:407:LYS:NZ	2.47	0.45
1:A:99:LEU:HB2	1:A:142:VAL:HG22	1.98	0.45
6:G:9:DC:H2"	6:G:10:DG:O5'	2.15	0.45
2:C:157:ARG:HA	2:C:157:ARG:HD3	1.75	0.44
2:C:899:GLN:HG3	2:C:901:TYR:CZ	2.52	0.44
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	2.00	0.44
3:D:1383:ASP:HB3	3:D:1416:ALA:HB3	1.98	0.44
2:C:238:LEU:HD12	2:C:241:LEU:HD11	1.99	0.44
2:C:423:ALA:HB3	2:C:428:ARG:HH11	1.82	0.44
2:C:627:ARG:HA	2:C:638:ASP:HB2	1.98	0.44
2:C:1095:LEU:CD1	3:D:582:LEU:HD22	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:176:ASP:OD1	3:D:177:ALA:N	2.44	0.44
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.99	0.44
3:D:273:ARG:NH1	3:D:278:PRO:HB3	2.33	0.44
3:D:288:MET:HE2	3:D:288:MET:HB3	1.90	0.44
3:D:419:ASP:H	3:D:429:SER:HB3	1.82	0.44
1:B:176:ARG:HD3	11:D:1707:HOH:O	2.18	0.44
3:D:141:ILE:HA	3:D:146:PRO:HA	1.98	0.44
6:G:6:DA:H2'	6:G:7:DT:H71	2.00	0.44
3:D:192:ALA:HB1	3:D:193:PRO:HD2	1.98	0.44
3:D:780:LYS:HE3	3:D:912:LYS:HD3	1.99	0.44
1:B:73:GLU:HB3	1:B:77:GLU:HB3	1.99	0.44
2:C:863:ASP:N	11:C:1202:HOH:O	2.25	0.44
3:D:236:TYR:CZ	3:D:242:LEU:HD12	2.53	0.44
2:C:578:VAL:HA	2:C:900:ARG:HG2	2.00	0.44
2:C:739:GLU:HG2	2:C:740:GLU:N	2.32	0.44
2:C:205:GLU:O	2:C:209:ARG:HG2	2.18	0.43
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.53	0.43
3:D:949:ILE:HD11	3:D:1023:MET:HE1	2.00	0.43
1:B:154:GLU:CD	1:B:154:GLU:H	2.20	0.43
1:A:103:ALA:HB1	1:A:107:LYS:HD3	2.00	0.43
2:C:679:PHE:CE2	2:C:853:LEU:HD11	2.54	0.43
2:C:1019:GLN:NE2	3:D:621:LYS:HE3	2.33	0.43
3:D:1143:GLY:O	3:D:1147:ARG:HD2	2.18	0.43
5:F:88:ILE:CD1	5:F:192:LEU:HB3	2.49	0.43
2:C:988:VAL:HG21	3:D:949:ILE:O	2.18	0.43
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.53	0.43
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.52	0.43
3:D:572:ARG:NH2	5:F:87:GLU:OE2	2.50	0.43
3:D:1031:ASN:O	3:D:1035:ILE:HG12	2.18	0.43
3:D:1176:LYS:HE2	3:D:1176:LYS:HB3	1.64	0.43
2:C:134:ARG:NH1	2:C:392:SER:O	2.51	0.43
6:G:6:DA:H61	7:H:22:DT:H3	1.66	0.43
1:B:7:LYS:H	1:B:7:LYS:HG3	1.58	0.43
2:C:930:LYS:HA	2:C:930:LYS:HD2	1.91	0.43
3:D:184:GLU:OE1	3:D:184:GLU:N	2.50	0.43
2:C:81:ASP:OD1	2:C:81:ASP:N	2.52	0.43
2:C:280:LYS:HE3	2:C:309:TYR:CZ	2.54	0.43
2:C:726:ILE:HD11	2:C:757:GLY:HA3	2.01	0.43
3:D:704:ARG:HB2	3:D:745:MET:CE	2.49	0.43
5:F:143:HIS:CE1	5:F:150:THR:HA	2.54	0.43
5:F:80:PRO:HB2	5:F:210:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:374:GLY:HA2	5:F:379:ARG:O	2.19	0.43
1:A:6:LEU:HD21	1:A:27:PRO:HG2	2.00	0.43
3:D:29:PRO:HG3	3:D:549:ASN:OD1	2.19	0.43
3:D:477:LEU:HD22	3:D:492:ALA:HA	2.00	0.43
3:D:864:VAL:CG1	3:D:865:THR:N	2.82	0.43
3:D:1101:VAL:HG21	3:D:1424:VAL:HG22	2.01	0.43
5:F:276:ARG:HD3	11:F:620:HOH:O	2.19	0.43
2:C:853:LEU:HB2	2:C:858:MET:CE	2.47	0.42
3:D:231:VAL:HG23	3:D:243:ALA:HA	2.01	0.42
2:C:124:ASP:OD2	2:C:407:LYS:NZ	2.42	0.42
2:C:240:THR:HG22	2:C:248:PRO:HG3	2.01	0.42
3:D:1282:ARG:HA	3:D:1315:ASP:OD1	2.19	0.42
3:D:245:LEU:HD13	3:D:249:TYR:HB3	2.01	0.42
3:D:701:LEU:O	3:D:747:VAL:HA	2.20	0.42
3:D:1495:ILE:HD13	4:E:80:VAL:HG21	2.01	0.42
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.54	0.42
2:C:473:ARG:HG3	2:C:474:VAL:N	2.35	0.42
3:D:1168:MET:HE3	3:D:1168:MET:HA	2.00	0.42
1:B:96:THR:HB	1:B:145:ASP:OD1	2.18	0.42
1:B:209:GLU:O	1:B:213:GLN:HG3	2.19	0.42
2:C:784:ASP:OD1	2:C:784:ASP:N	2.34	0.42
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.55	0.42
3:D:310:LEU:HD13	3:D:310:LEU:HA	1.79	0.42
3:D:904:VAL:CG1	3:D:905:PRO:HD2	2.49	0.42
2:C:317:VAL:HG22	2:C:320:HIS:ND1	2.34	0.42
2:C:1053:LEU:HD11	3:D:1466:VAL:HG13	2.01	0.42
3:D:473:LEU:HD21	3:D:495:ARG:HH21	1.84	0.42
3:D:876:SER:OG	3:D:879:ARG:HG3	2.20	0.42
1:B:85:LEU:HG	1:B:87:VAL:HG23	2.02	0.42
3:D:270:LEU:HD13	3:D:304:LEU:HD13	2.01	0.42
3:D:1293:PHE:HA	3:D:1301:LYS:O	2.19	0.42
1:A:18:ARG:NH1	11:A:402:HOH:O	2.38	0.42
2:C:536:PRO:HB3	3:D:1067:VAL:CG2	2.50	0.42
2:C:874:LEU:O	3:D:1029:ARG:HG3	2.20	0.42
3:D:970:LYS:O	3:D:973:GLN:HB3	2.19	0.42
3:D:4:GLU:OE2	3:D:6:ARG:HD3	2.20	0.42
4:E:68:LEU:HD12	4:E:68:LEU:HA	1.86	0.42
2:C:422:ARG:HD3	7:H:15:DT:C6	2.54	0.41
3:D:199:LEU:HB2	3:D:397:LYS:CE	2.49	0.41
3:D:784:ASP:HB2	3:D:939:PHE:CE1	2.55	0.41
3:D:968:ASP:CG	3:D:1058:ARG:HH22	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1087[A]:ARG:HG3	3:D:1256:LEU:CD2	2.47	0.41
3:D:1141:GLU:HB2	3:D:1362:LYS:HZ1	1.85	0.41
5:F:131:VAL:HG13	5:F:178:ARG:HD3	2.02	0.41
5:F:144:ILE:HB	5:F:147:LEU:HD13	2.01	0.41
2:C:777:ILE:HD11	5:F:408:LEU:HD13	2.01	0.41
3:D:48:ARG:NH1	11:D:1745:HOH:O	2.52	0.41
3:D:654:LYS:HD3	3:D:674[A]:ARG:HH12	1.85	0.41
5:F:273:ARG:HG2	5:F:276:ARG:NH1	2.35	0.41
2:C:258:TYR:O	2:C:263:ASP:N	2.53	0.41
3:D:475:LYS:O	3:D:479:GLU:HG2	2.20	0.41
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	2.03	0.41
3:D:1382:THR:HG23	3:D:1418:LYS:HD2	2.02	0.41
5:F:160:ASP:OD2	5:F:164:LYS:HE2	2.20	0.41
2:C:420:ARG:HE	2:C:420:ARG:HB3	1.58	0.41
3:D:677:LEU:HD21	3:D:687:VAL:HG21	2.02	0.41
3:D:709:HIS:HA	3:D:1227:GLN:HB3	2.01	0.41
3:D:884:ARG:NH2	11:D:1707:HOH:O	2.29	0.41
3:D:115:LEU:CD1	3:D:509:PRO:HB3	2.51	0.41
3:D:205:TYR:CE1	3:D:390:PRO:HG3	2.56	0.41
5:F:217:ASN:OD1	11:F:601:HOH:O	2.21	0.41
5:F:234:LYS:HE2	5:F:234:LYS:HB3	1.88	0.41
1:B:94:LEU:O	1:B:146:ARG:NH2	2.39	0.41
2:C:188:LYS:HB2	2:C:188:LYS:HE2	1.85	0.41
3:D:1384:PRO:O	3:D:1387:SER:OG	2.29	0.41
4:E:28:GLN:NE2	11:E:101:HOH:O	2.39	0.41
2:C:154:ARG:NH1	2:C:178:PRO:HG3	2.36	0.41
2:C:583:LEU:HD23	2:C:583:LEU:HA	1.63	0.41
3:D:154:THR:H	3:D:154:THR:HG23	1.67	0.41
3:D:1205:TYR:CZ	3:D:1366:LYS:HE3	2.54	0.41
3:D:1314:LYS:HG2	3:D:1317:ASP:OD2	2.21	0.41
2:C:572:ILE:HG13	2:C:573:ARG:HG3	2.02	0.41
2:C:1002:GLU:HB2	11:C:1276:HOH:O	2.20	0.41
3:D:41:ARG:HG3	3:D:48:ARG:HH21	1.86	0.41
3:D:945:SER:OG	3:D:947:ILE:HG12	2.21	0.41
2:C:614:ARG:NH1	2:C:620:LEU:HD13	2.36	0.41
3:D:217:LYS:HE3	3:D:341:GLU:OE1	2.20	0.41
3:D:566:ILE:HD11	5:F:192:LEU:HD21	2.03	0.41
3:D:902:LEU:O	3:D:902:LEU:HG	2.20	0.41
7:H:9:DG:H2"	7:H:10:DA:N7	2.36	0.41
2:C:521:PRO:HG2	3:D:1053:PHE:CZ	2.56	0.41
2:C:607:ASP:HB3	2:C:610:ARG:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	2.02	0.41
2:C:1104:GLU:OE2	2:C:1105:LYS:HG3	2.22	0.40
3:D:371:ILE:HD12	5:F:230:LYS:HA	2.03	0.40
5:F:114:LYS:HA	5:F:114:LYS:HD3	1.86	0.40
2:C:713:ARG:HD3	3:D:532:GLY:HA2	2.03	0.40
2:C:1070:ILE:CG2	3:D:655:PRO:HB2	2.52	0.40
3:D:109:PRO:HD3	7:H:20:DG:H5"	2.02	0.40
3:D:186:VAL:O	3:D:189:GLN:HB3	2.20	0.40
3:D:1103:HIS:O	3:D:1462:LEU:HG	2.20	0.40
3:D:1211:MET:HB2	3:D:1211:MET:HE3	2.01	0.40
6:G:6:DA:H2'	6:G:7:DT:C6	2.56	0.40
1:A:9:PRO:HB3	1:A:27:PRO:O	2.22	0.40
2:C:204:GLN:HG3	2:C:222:MET:SD	2.61	0.40
2:C:468:ARG:HA	2:C:486:MET:O	2.21	0.40
3:D:409:VAL:HG23	3:D:435:VAL:HG11	2.03	0.40
3:D:659:LYS:HE3	3:D:663:GLU:OE2	2.21	0.40
3:D:38:LYS:HD3	3:D:38:LYS:HA	1.93	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	226/315 (72%)	225 (100%)	1 (0%)	0	100	100
1	B	222/315 (70%)	214 (96%)	8 (4%)	0	100	100
2	C	1099/1119 (98%)	1066 (97%)	33 (3%)	0	100	100
3	D	1476/1524 (97%)	1440 (98%)	36 (2%)	0	100	100
4	E	94/99 (95%)	92 (98%)	2 (2%)	0	100	100
5	F	344/443 (78%)	336 (98%)	8 (2%)	0	100	100
All	All	3461/3815 (91%)	3373 (98%)	88 (2%)	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	199/273 (73%)	191 (96%)	8 (4%)	31	54
1	B	197/273 (72%)	191 (97%)	6 (3%)	41	66
2	C	929/941 (99%)	893 (96%)	36 (4%)	32	55
3	D	1242/1279 (97%)	1190 (96%)	52 (4%)	30	51
4	E	85/88 (97%)	83 (98%)	2 (2%)	49	73
5	F	300/388 (77%)	286 (95%)	14 (5%)	26	46
All	All	2952/3242 (91%)	2834 (96%)	118 (4%)	32	54

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	90	LEU
1	A	94	LEU
1	A	134	GLU
1	A	148	VAL
1	A	170	VAL
1	A	205	VAL
1	A	213	GLN
1	B	5	LYS
1	B	7	LYS
1	B	55	SER
1	B	96	THR
1	B	155	LYS
1	B	180	GLN
2	C	64	LEU
2	C	118	ILE
2	C	141	HIS
2	C	168	ARG
2	C	177	GLU

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Mol	Chain	Res	Type
2	C	186	VAL
2	C	242	LEU
2	C	257	VAL
2	C	322	VAL
2	C	372	LEU
2	C	405	ARG
2	C	409	ARG
2	C	427	VAL
2	C	430	VAL
2	C	441	VAL
2	C	455	LEU
2	C	483	VAL
2	C	524	VAL
2	C	583	LEU
2	C	607	ASP
2	C	610	ARG
2	C	617	ASP
2	C	666	LEU
2	C	670	GLN
2	C	784	ASP
2	C	786	LYS
2	C	805	ARG
2	C	808	ARG
2	C	810	ASP
2	C	815	LEU
2	C	819	VAL
2	C	829	GLN
2	C	848	VAL
2	C	1056	LYS
2	C	1061	GLU
2	C	1095	LEU
3	D	48	ARG
3	D	81	THR
3	D	153	LEU
3	D	216	VAL
3	D	273	ARG
3	D	293	VAL
3	D	310	LEU
3	D	335	LEU
3	D	415	VAL
3	D	427	VAL
3	D	503	LEU

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Mol	Chain	Res	Type
3	D	529	GLN
3	D	534	ARG
3	D	560	GLN
3	D	621	LYS
3	D	623	VAL
3	D	632	VAL
3	D	683	ILE
3	D	709	HIS
3	D	754	PHE
3	D	858	VAL
3	D	894	LYS
3	D	899	LEU
3	D	907	GLU
3	D	976	GLN
3	D	986	ARG
3	D	1033	GLN
3	D	1045[A]	MET
3	D	1045[B]	MET
3	D	1087[A]	ARG
3	D	1087[B]	ARG
3	D	1100	ASP
3	D	1128	VAL
3	D	1188	VAL
3	D	1197	ARG
3	D	1200	VAL
3	D	1207	TYR
3	D	1221	VAL
3	D	1302	GLU
3	D	1305	LEU
3	D	1312	LEU
3	D	1313	VAL
3	D	1376	MET
3	D	1377	LYS
3	D	1418	LYS
3	D	1424	VAL
3	D	1433	SER
3	D	1439	SER
3	D	1444	THR
3	D	1468	LEU
3	D	1486	VAL
3	D	1488	ASP
4	E	68	LEU

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Mol	Chain	Res	Type
4	E	96	GLU
5	F	81	VAL
5	F	94	LEU
5	F	95	THR
5	F	96	LEU
5	F	136	LEU
5	F	150	THR
5	F	152	ASP
5	F	295	MET
5	F	349	LEU
5	F	358	LEU
5	F	369	LEU
5	F	375	LEU
5	F	392	VAL
5	F	405	LEU

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

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	1/3 (33%)	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 9 ligands modelled in this entry, 9 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	228/315 (72%)	-0.24	3 (1%) 77 79	43, 58, 81, 99	0
1	B	224/315 (71%)	0.10	7 (3%) 49 53	46, 68, 95, 116	0
2	C	1107/1119 (98%)	0.06	42 (3%) 40 44	31, 52, 109, 134	0
3	D	1481/1524 (97%)	0.31	104 (7%) 16 17	31, 59, 116, 142	0
4	E	96/99 (96%)	-0.12	3 (3%) 49 53	36, 52, 98, 110	0
5	F	346/443 (78%)	0.28	27 (7%) 13 13	42, 71, 111, 128	0
6	G	18/21 (85%)	0.07	2 (11%) 5 5	50, 77, 165, 166	0
7	H	24/27 (88%)	-0.28	0 100 100	70, 85, 134, 166	0
8	I	2/3 (66%)	-0.96	0 100 100	43, 43, 43, 43	0
All	All	3526/3866 (91%)	0.16	188 (5%) 26 28	31, 59, 112, 166	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1499	ARG	4.8
3	D	173	PRO	4.8
3	D	310	LEU	4.7
3	D	422	ALA	4.6
3	D	1283	ILE	4.5
5	F	147	LEU	4.5
5	F	325	LYS	4.5
2	C	107	LEU	4.2
5	F	142	ARG	4.1
3	D	316	GLN	4.1
3	D	68	PHE	4.1
3	D	308	LYS	4.1
2	C	106	GLY	4.0
3	D	322	VAL	4.0
5	F	148	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
2	C	1	MET	4.0
2	C	221	LEU	4.0
3	D	371	ILE	4.0
5	F	150	THR	3.9
2	C	648	ARG	3.9
2	C	189	ARG	3.9
1	A	231	ALA	3.8
3	D	1129	THR	3.8
3	D	1294	VAL	3.7
2	C	104	ASP	3.7
3	D	1130	ARG	3.7
3	D	241	ILE	3.7
3	D	235	ALA	3.7
3	D	318	ARG	3.6
5	F	146	GLY	3.6
3	D	821	VAL	3.6
3	D	1305	LEU	3.6
2	C	362	GLY	3.6
3	D	406	ASP	3.6
3	D	1287	GLU	3.5
3	D	196	VAL	3.5
3	D	1207	TYR	3.4
1	A	188	GLN	3.4
3	D	186	VAL	3.4
3	D	152	LEU	3.4
5	F	122	LEU	3.3
3	D	1306	PRO	3.3
5	F	149	GLU	3.3
3	D	1408	ILE	3.3
3	D	1495	ILE	3.3
3	D	409	VAL	3.3
3	D	805	GLU	3.3
4	E	97	ARG	3.2
3	D	1297	GLU	3.2
3	D	185	VAL	3.2
3	D	212	ARG	3.2
5	F	423	ASP	3.1
5	F	145	PRO	3.1
5	F	422	LEU	3.1
3	D	393	ILE	3.0
5	F	173	TYR	3.0
2	C	227	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
3	D	1128	VAL	2.9
3	D	142	LEU	2.9
3	D	345	TYR	2.9
3	D	384	VAL	2.9
5	F	152	ASP	2.9
3	D	1281	VAL	2.9
3	D	133	ILE	2.9
3	D	378	ILE	2.9
3	D	198	ARG	2.9
1	B	16	GLN	2.9
3	D	205	TYR	2.9
3	D	236	TYR	2.9
2	C	251	ASP	2.8
3	D	1269	LYS	2.8
3	D	336	PHE	2.8
3	D	1299	PHE	2.8
2	C	420	ARG	2.8
5	F	414	ARG	2.8
2	C	1037	VAL	2.8
3	D	350	HIS	2.8
3	D	218	LYS	2.8
5	F	151	LEU	2.8
3	D	188	GLY	2.8
5	F	323	ASP	2.8
3	D	245	LEU	2.8
3	D	360	ARG	2.7
3	D	488	ARG	2.7
3	D	372	ASP	2.7
3	D	201	GLY	2.7
2	C	8	ARG	2.7
2	C	293	PHE	2.7
3	D	178	LEU	2.7
2	C	222	MET	2.7
1	B	105	GLY	2.7
3	D	368	VAL	2.7
4	E	51	LEU	2.7
3	D	1225	ALA	2.7
3	D	364	GLY	2.7
1	B	6	LEU	2.7
3	D	69	GLU	2.6
2	C	224	GLU	2.6
4	E	96	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	982	PHE	2.6
2	C	1042	ALA	2.5
3	D	361	VAL	2.5
3	D	454	ALA	2.5
3	D	67	ARG	2.5
2	C	254	VAL	2.5
3	D	346	ARG	2.5
3	D	161	LEU	2.5
2	C	101	ILE	2.5
3	D	187	LYS	2.5
1	A	230	ALA	2.5
3	D	416	ALA	2.5
3	D	666	ILE	2.5
5	F	159	ILE	2.4
3	D	174	GLY	2.4
2	C	219	GLN	2.4
2	C	64	LEU	2.4
3	D	203	ALA	2.4
3	D	191	LEU	2.4
5	F	174	LEU	2.4
3	D	804	LEU	2.4
5	F	139	ALA	2.4
2	C	388	ARG	2.4
6	G	4	DG	2.4
3	D	135	LEU	2.4
3	D	321	GLN	2.4
5	F	324	GLU	2.3
3	D	147	VAL	2.3
3	D	315	ARG	2.3
6	G	6	DA	2.3
3	D	363	ALA	2.3
5	F	416	ARG	2.3
2	C	103	LYS	2.3
3	D	3	LYS	2.3
3	D	148	GLU	2.3
3	D	317	VAL	2.3
2	C	1044	GLY	2.3
5	F	141	VAL	2.3
1	B	118	ALA	2.3
2	C	1040	LEU	2.3
2	C	780	GLU	2.3
2	C	298	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	1221	VAL	2.2
3	D	812	ALA	2.2
1	B	186	LEU	2.2
2	C	1038	TRP	2.2
5	F	375	LEU	2.2
3	D	974	ILE	2.2
3	D	415	VAL	2.2
3	D	1285	GLU	2.2
3	D	820	GLU	2.2
3	D	386	HIS	2.2
2	C	223	ASP	2.2
3	D	419	ASP	2.1
2	C	207	LEU	2.1
5	F	166	LEU	2.1
3	D	324	ALA	2.1
3	D	1224	VAL	2.1
3	D	1498	ALA	2.1
2	C	105	THR	2.1
2	C	814	GLU	2.1
2	C	188	LYS	2.1
2	C	209	ARG	2.1
3	D	1270	ALA	2.1
3	D	1223	ILE	2.1
1	B	137	ARG	2.1
2	C	766	GLU	2.1
2	C	1039	ALA	2.1
3	D	215	TYR	2.1
3	D	234	GLU	2.1
3	D	1292	VAL	2.1
2	C	102	HIS	2.1
3	D	311	LEU	2.1
3	D	343	LYS	2.1
2	C	203	ASP	2.0
3	D	1313	VAL	2.0
3	D	270	LEU	2.0
5	F	379	ARG	2.0
2	C	598	GLU	2.0
5	F	169	GLU	2.0
2	C	809	GLY	2.0
1	B	189	ARG	2.0
3	D	432	TYR	2.0
3	D	427	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
5	F	156	VAL	2.0
2	C	245	GLY	2.0
3	D	445	ARG	2.0
3	D	486	ARG	2.0
2	C	247	PRO	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
9	MG	B	2001	1/1	0.90	0.14	73,73,73,73	0
9	MG	D	1605	1/1	0.90	0.10	56,56,56,56	0
9	MG	I	102	1/1	0.92	0.10	44,44,44,44	0
9	MG	D	1604	1/1	0.95	0.09	64,64,64,64	0
9	MG	F	501	1/1	0.96	0.07	56,56,56,56	0
9	MG	I	101	1/1	0.98	0.11	43,43,43,43	0
9	MG	D	1603	1/1	0.99	0.16	33,33,33,33	0
10	ZN	D	1602	1/1	0.99	0.09	76,76,76,76	0
10	ZN	D	1601	1/1	1.00	0.14	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.