Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 04:42 PM JST

PDB ID	:	5ZX3
Title	:	Mycobacterium tuberculosis RNA polymerase holoenzyme with ECF sigma factor sigma H
Authors	:	Li, L.; Zhang, Y.
Deposited on	:	2018-05-17
Resolution	:	2.75 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:

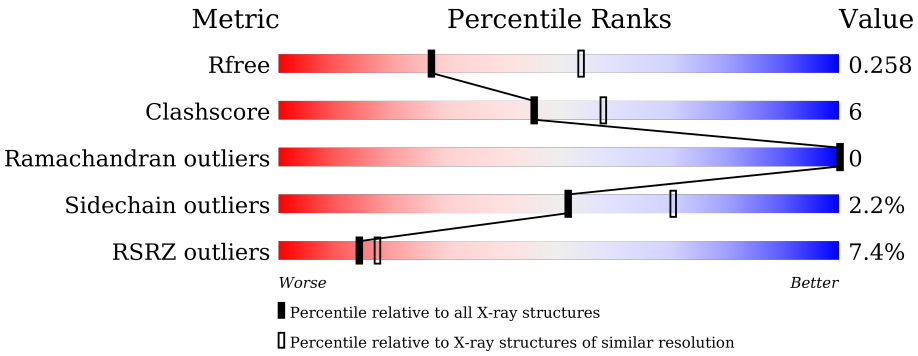
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	368	2% 52% 7% 40%
1	B	368	5% 48% 15% 37%
2	C	1174	9% 79% 15% 6%
3	D	1317	5% 80% 16% 5%
4	E	110	5% 55% 13% 31%
5	F	218	8% 61% 17% 21%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 23311 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	221	Total	C	N	O	S	0	0	0
			1673	1054	288	329	2			
1	B	231	Total	C	N	O	S	0	0	0
			1728	1090	293	342	3			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	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	-	expression tag	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	1105	Total	C	N	O	S	0	0	0
			8188	5112	1443	1596	37			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	5	MET	-	expression tag	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
3	D	1257	Total	C	N	O	S	0	0	0
			9742	6100	1762	1840	40			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	expression tag	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	76	Total	C	N	O	0	0	0
			596	380	101	115			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	173	Total	C	N	O	S	0	0	0
			1329	837	224	263	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 ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is water.

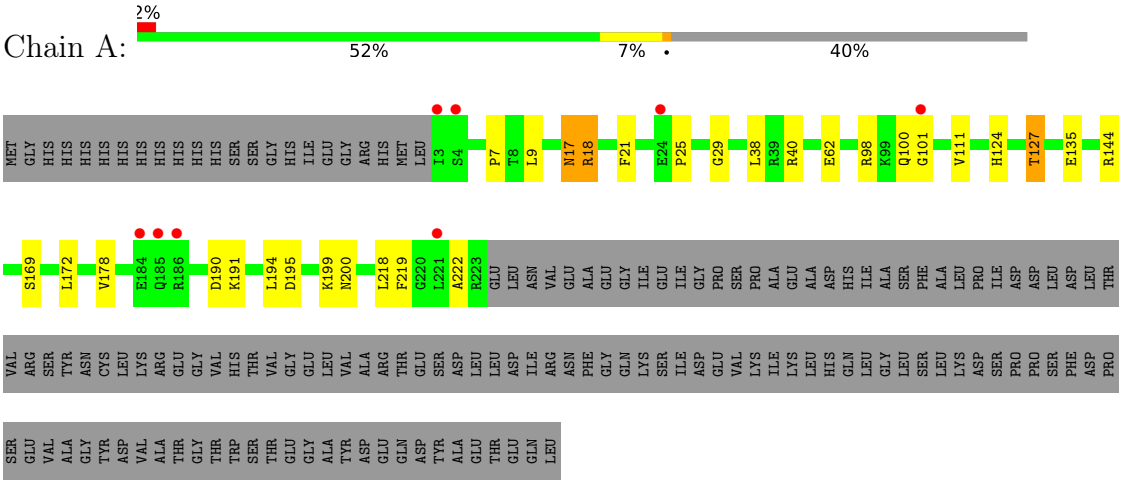
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			1	1		
7	C	29	Total	O	0	0
			29	29		
7	D	22	Total	O	0	0
			22	22		
7	F	1	Total	O	0	0
			1	1		

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.

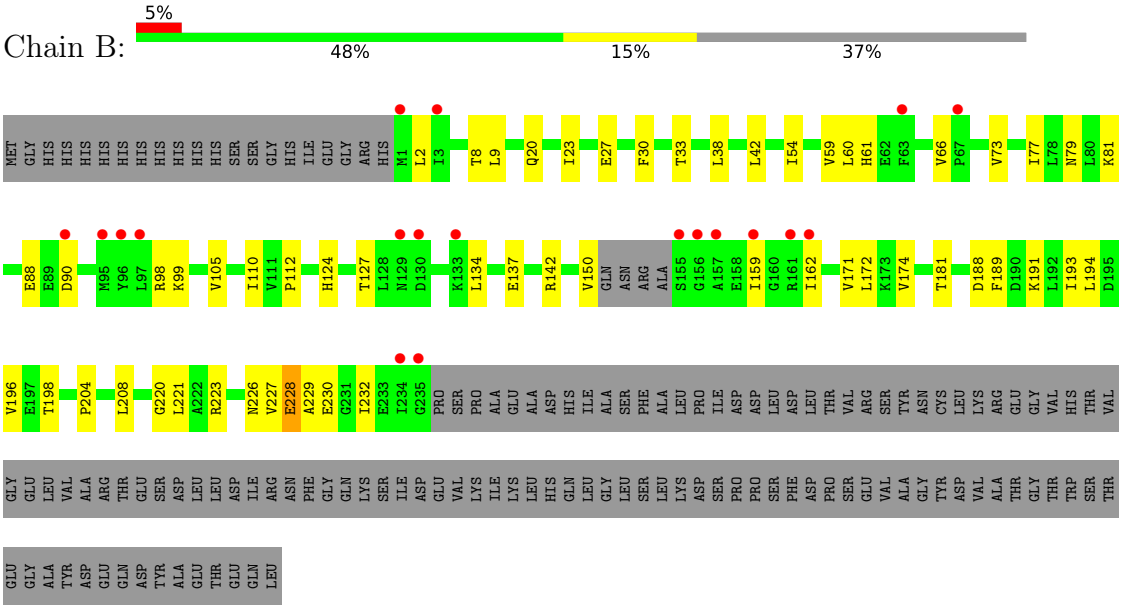
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



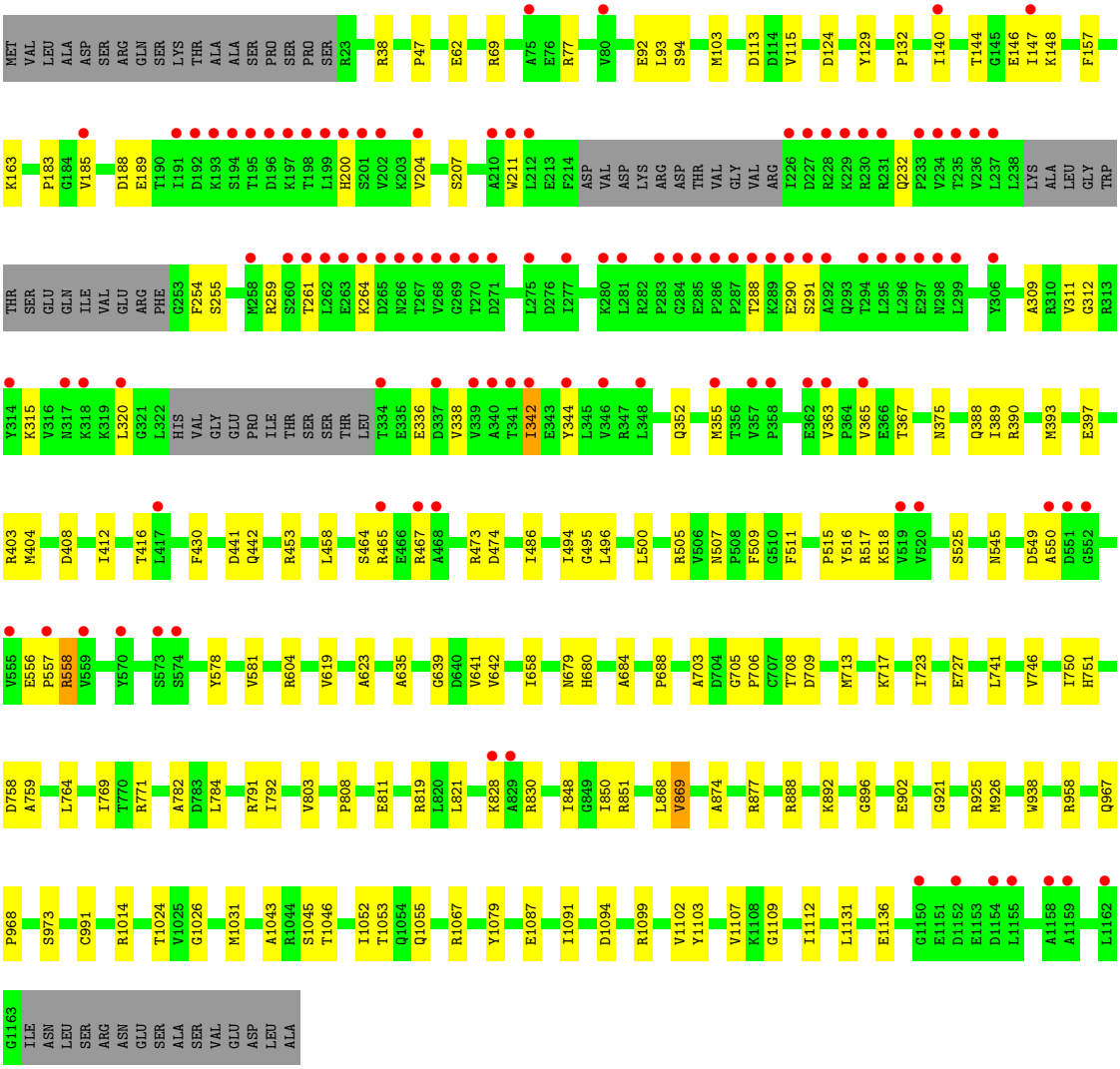
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:

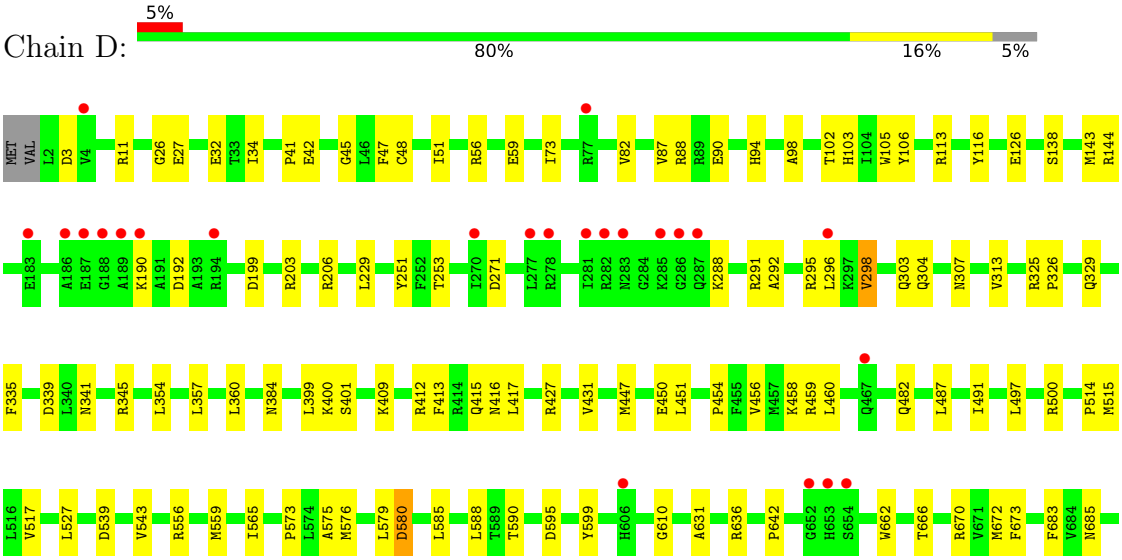


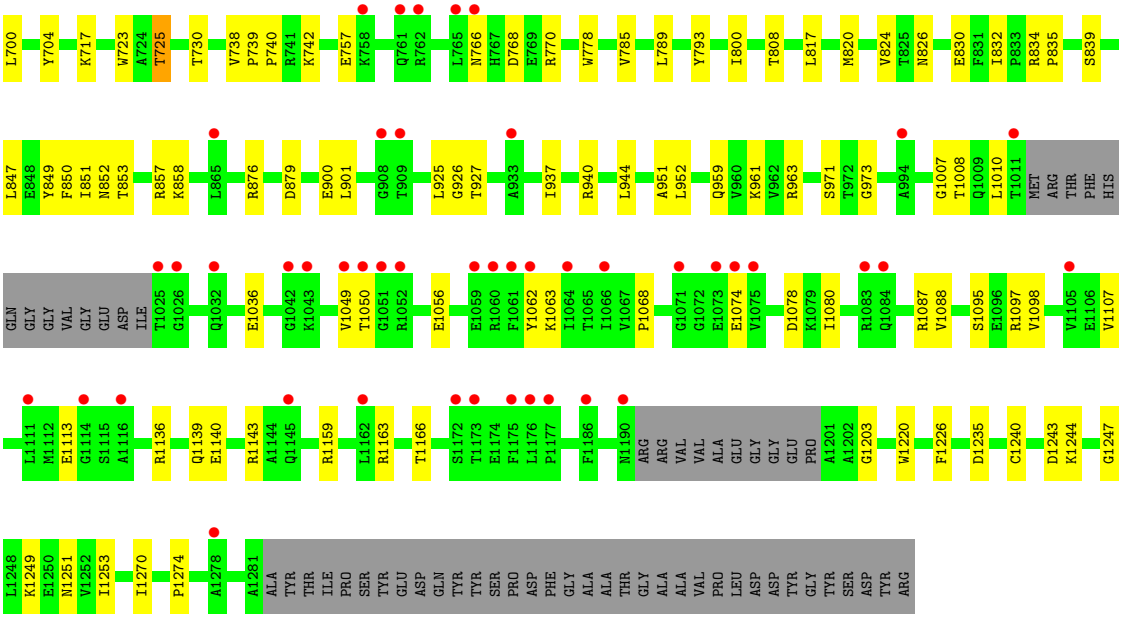
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:

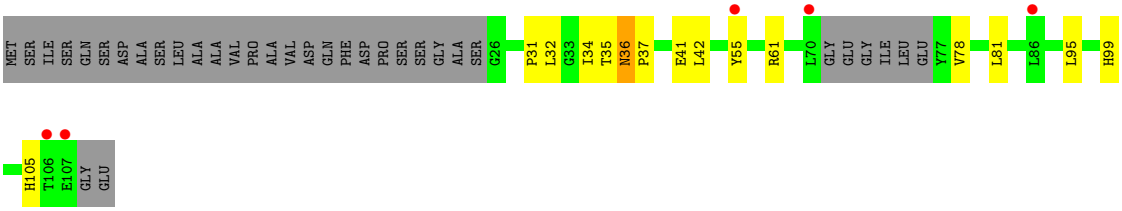


• Molecule 3: DNA-directed RNA polymerase subunit beta'

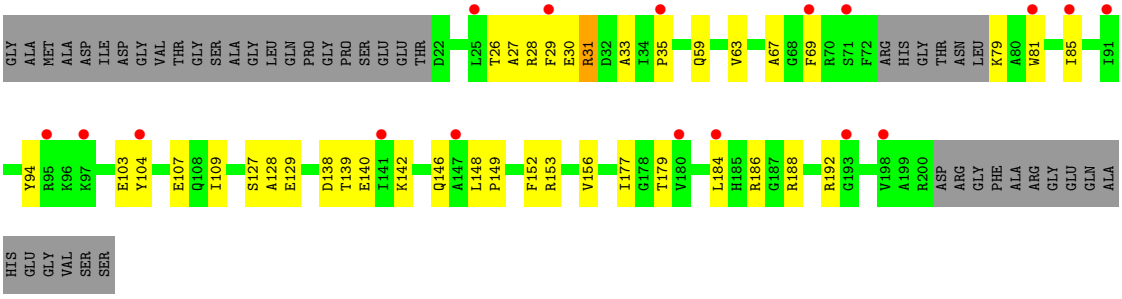




• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: ECF RNA polymerase sigma factor SigH



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	130.57Å 159.79Å 131.44Å 90.00° 118.72° 90.00°	Depositor
Resolution (Å)	41.64 – 2.75 48.35 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.7 (41.64-2.75) 97.7 (48.35-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.218 , 0.258 0.219 , 0.258	Depositor DCC
R_{free} test set	2160 reflections (1.80%)	wwPDB-VP
Wilson B-factor (Å^2)	78.9	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 49.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.002 for -h-l,k,h 0.002 for l,k,-h-l 0.014 for h,-k,-h-l 0.014 for -h-l,-k,l 0.011 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	23311	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.25	0/1699	0.48	0/2313
1	B	0.25	0/1753	0.48	0/2386
2	C	0.26	1/8333 (0.0%)	0.45	0/11331
3	D	0.25	0/9905	0.43	0/13402
4	E	0.25	0/607	0.39	0/826
5	F	0.24	0/1355	0.39	0/1843
All	All	0.25	1/23652 (0.0%)	0.44	0/32101

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	94	SER	C-N	6.00	1.45	1.34

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	23	0
1	B	1728	0	1747	34	0
2	C	8188	0	7786	105	0
3	D	9742	0	9715	134	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	596	0	594	13	0
5	F	1329	0	1231	26	0
6	D	2	0	0	0	0
7	A	1	0	0	0	0
7	C	29	0	0	0	0
7	D	22	0	0	0	0
7	F	1	0	0	0	0
All	All	23311	0	22780	293	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 (293) 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)
2:C:1046:THR:HG22	5:F:127:SER:HB2	1.62	0.79
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.63	0.78
3:D:739:PRO:HG2	3:D:742:LYS:HB2	1.66	0.77
3:D:190:LYS:HD2	3:D:192:ASP:HB3	1.66	0.77
2:C:1024:THR:H	3:D:730:THR:HG21	1.49	0.76
2:C:388:GLN:HG2	2:C:430:PHE:HB2	1.69	0.74
3:D:1274:PRO:HG3	4:E:78:VAL:HG11	1.73	0.70
2:C:782:ALA:O	2:C:791:ARG:NH2	2.25	0.70
5:F:26:THR:O	5:F:29:PHE:HB3	1.92	0.70
3:D:1274:PRO:HB3	4:E:81:LEU:HD11	1.74	0.69
3:D:824:VAL:HG11	3:D:852:ASN:HA	1.77	0.67
1:B:98:ARG:HA	1:B:134:LEU:O	1.94	0.67
3:D:834:ARG:HD3	3:D:835:PRO:HD2	1.77	0.67
2:C:758:ASP:HB3	2:C:868:LEU:HD23	1.77	0.66
3:D:360:LEU:HD21	5:F:67:ALA:HB2	1.78	0.66
3:D:879:ASP:OD2	3:D:1249:LYS:NZ	2.29	0.65
1:A:9:LEU:HD11	1:A:21:PHE:HB3	1.78	0.65
3:D:417:LEU:HD22	3:D:1253:ILE:HG23	1.79	0.64
1:B:90:ASP:OD2	1:B:142:ARG:NH1	2.29	0.63
2:C:458:LEU:HD21	2:C:496:LEU:HD13	1.81	0.63
2:C:93:LEU:HD22	2:C:393:MET:HB3	1.80	0.63
2:C:792:ILE:HG13	2:C:850:ILE:HD12	1.79	0.63
2:C:207:SER:HB3	2:C:309:ALA:HB2	1.81	0.62
3:D:1166:THR:O	3:D:1203:GLY:HA2	1.99	0.62
3:D:971:SER:O	3:D:1163:ARG:NH2	2.33	0.62
2:C:1067:ARG:HH12	3:D:415:GLN:HA	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:876:ARG:NH1	3:D:1036:GLU:OE1	2.33	0.61
2:C:124:ASP:OD1	2:C:851:ARG:NH1	2.33	0.61
3:D:1062:TYR:N	3:D:1080:ILE:O	2.33	0.61
3:D:47:PHE:O	3:D:88:ARG:NH2	2.34	0.61
5:F:28:ARG:O	5:F:31:ARG:HG3	2.01	0.61
3:D:357:LEU:HD21	5:F:63:VAL:HG22	1.82	0.61
1:A:40:ARG:HG3	2:C:902:GLU:HG3	1.83	0.61
2:C:315:LYS:NZ	2:C:375:ASN:OD1	2.34	0.61
2:C:474:ASP:HA	3:D:857:ARG:HG2	1.82	0.61
3:D:326:PRO:HG2	5:F:109:ILE:HD12	1.81	0.61
3:D:456:VAL:O	3:D:460:LEU:HB2	2.01	0.61
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.34	0.61
2:C:635:ALA:HB2	2:C:713:MET:HG2	1.83	0.61
2:C:453:ARG:NH1	2:C:500:LEU:O	2.33	0.60
3:D:113:ARG:NH2	3:D:1235:ASP:OD1	2.34	0.60
3:D:599:TYR:HA	3:D:610:GLY:HA3	1.83	0.60
2:C:1043:ALA:HB2	3:D:447:MET:HG2	1.84	0.60
4:E:31:PRO:HB3	4:E:35:THR:HG23	1.84	0.60
2:C:684:ALA:HA	2:C:706:PRO:HG3	1.84	0.60
1:A:7:PRO:HA	1:A:25:PRO:HG2	1.84	0.60
1:B:226:ASN:OD1	1:B:227:VAL:N	2.36	0.59
2:C:1052:ILE:HG12	3:D:326:PRO:HG3	1.83	0.59
3:D:565:ILE:HG23	3:D:575:ALA:HB3	1.84	0.58
2:C:921:GLY:O	2:C:925:ARG:HG2	2.03	0.58
4:E:36:ASN:CG	4:E:37:PRO:HD3	2.24	0.58
1:A:222:ALA:HA	1:B:9:LEU:HD22	1.85	0.58
3:D:45:GLY:H	3:D:48:CYS:HB2	1.69	0.57
1:A:17:ASN:OD1	1:A:17:ASN:N	2.37	0.57
2:C:62:GLU:OE2	2:C:69:ARG:NH2	2.38	0.57
2:C:1087:GLU:HG3	2:C:1091:ILE:HD11	1.86	0.57
3:D:345:ARG:NH2	5:F:103:GLU:OE1	2.37	0.57
2:C:741:LEU:HA	2:C:746:VAL:HG13	1.86	0.56
3:D:307:ASN:HD21	3:D:1240:CYS:HB2	1.70	0.56
3:D:1139:GLN:HG3	3:D:1143:ARG:HD2	1.86	0.56
2:C:723:ILE:O	3:D:730:THR:HG23	2.05	0.56
1:A:172:LEU:HD13	1:A:199:LYS:HG2	1.87	0.55
3:D:826:ASN:N	3:D:830:GLU:O	2.32	0.55
4:E:36:ASN:OD1	4:E:36:ASN:N	2.37	0.55
5:F:31:ARG:O	5:F:35:PRO:HD2	2.06	0.55
3:D:739:PRO:HD3	3:D:789:LEU:HD13	1.89	0.55
3:D:973:GLY:O	3:D:1159:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:549:ASP:OD1	2:C:550:ALA:N	2.40	0.55
1:A:124:HIS:HE1	1:A:127:THR:HG22	1.72	0.54
1:A:222:ALA:HB1	1:B:208:LEU:HG	1.88	0.54
2:C:255:SER:O	2:C:259:ARG:CB	2.55	0.54
3:D:400:LYS:HG3	5:F:107:GLU:HG3	1.90	0.54
2:C:1109:GLY:HA3	3:D:458:LYS:HE3	1.90	0.54
2:C:474:ASP:OD1	2:C:474:ASP:N	2.41	0.54
3:D:412:ARG:HA	3:D:416:ASN:HB2	1.90	0.54
1:A:169:SER:O	1:A:199:LYS:NZ	2.41	0.53
4:E:32:LEU:O	4:E:35:THR:HG22	2.09	0.53
1:B:99:LYS:HD3	1:B:105:VAL:HG22	1.91	0.53
2:C:557:PRO:HB2	2:C:558:ARG:HD3	1.91	0.53
3:D:876:ARG:HG2	3:D:1226:PHE:HZ	1.74	0.53
2:C:1112:ILE:O	4:E:61:ARG:NH2	2.42	0.53
3:D:1270:ILE:HD13	4:E:55:TYR:HE1	1.74	0.53
2:C:1045:SER:HB3	3:D:450:GLU:O	2.09	0.52
3:D:487:LEU:O	3:D:491:ILE:HG12	2.08	0.52
1:B:77:ILE:HG22	1:B:81:LYS:HE2	1.90	0.52
3:D:491:ILE:HG23	3:D:514:PRO:HG2	1.90	0.52
2:C:486:ILE:HD11	3:D:849:TYR:HE1	1.74	0.52
3:D:384:ASN:HB2	3:D:401:SER:HB3	1.92	0.52
2:C:619:VAL:HG12	2:C:750:ILE:HG13	1.92	0.51
1:A:29:GLY:N	1:A:190:ASP:OD2	2.42	0.51
1:B:124:HIS:HE1	1:B:127:THR:HG23	1.75	0.51
1:B:191:LYS:HE2	1:B:193:ILE:HD11	1.92	0.51
2:C:288:THR:HB	2:C:291:SER:HB3	1.91	0.51
1:B:228:GLU:HG3	1:B:229:ALA:N	2.25	0.51
2:C:442:GLN:HE21	2:C:679:ASN:H	1.58	0.51
1:B:54:ILE:HA	1:B:137:GLU:O	2.10	0.50
2:C:1046:THR:HG21	5:F:129:GLU:H	1.76	0.50
2:C:1091:ILE:HD12	2:C:1102:VAL:HG21	1.93	0.50
3:D:98:ALA:HB3	3:D:354:LEU:HD23	1.94	0.50
5:F:27:ALA:O	5:F:30:GLU:HB2	2.12	0.50
2:C:792:ILE:HD12	2:C:792:ILE:H	1.76	0.50
3:D:56:ARG:NH1	3:D:59:GLU:OE2	2.44	0.50
3:D:778:TRP:CD2	3:D:835:PRO:HG3	2.47	0.50
3:D:1049:VAL:HA	3:D:1107:VAL:HG22	1.93	0.50
1:B:66:VAL:HG23	1:B:73:VAL:HG22	1.94	0.50
2:C:115:VAL:HG11	2:C:129:TYR:CE1	2.47	0.50
3:D:1270:ILE:HD13	4:E:55:TYR:CE1	2.47	0.50
2:C:473:ARG:O	3:D:857:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1244:LYS:NZ	3:D:1244:LYS:H	2.09	0.50
2:C:717:LYS:HG3	2:C:746:VAL:HG23	1.94	0.50
3:D:482:GLN:OE1	3:D:482:GLN:N	2.41	0.50
3:D:103:HIS:HB3	3:D:106:TYR:HD2	1.77	0.49
4:E:42:LEU:HD13	4:E:95:LEU:HD22	1.93	0.49
2:C:403:ARG:NH1	2:C:416:THR:O	2.46	0.49
3:D:666:THR:HG21	3:D:683:PHE:CE1	2.48	0.49
2:C:1136:GLU:OE1	3:D:11:ARG:NH2	2.40	0.49
3:D:271:ASP:OD1	3:D:303:GLN:NE2	2.40	0.49
3:D:670:ARG:NH1	3:D:685:ASN:OD1	2.39	0.49
2:C:183:PRO:HB2	2:C:312:GLY:HA3	1.95	0.48
3:D:1136:ARG:O	3:D:1140:GLU:HG2	2.12	0.48
2:C:967:GLN:HG3	2:C:968:PRO:HD2	1.95	0.48
3:D:138:SER:OG	3:D:253:THR:OG1	2.27	0.48
2:C:355:MET:N	2:C:363:VAL:O	2.46	0.48
2:C:888:ARG:HG2	2:C:1031:MET:HE3	1.94	0.48
3:D:901:LEU:HD11	3:D:952:LEU:HD13	1.95	0.48
2:C:1053:THR:HG23	2:C:1055:GLN:H	1.78	0.48
1:A:40:ARG:HH11	2:C:1014:ARG:HA	1.79	0.48
5:F:152:PHE:HE2	5:F:186:ARG:HB2	1.78	0.48
2:C:77:ARG:HH11	2:C:505:ARG:HH12	1.61	0.48
2:C:464:SER:HB2	2:C:467:ARG:HG3	1.95	0.48
3:D:116:TYR:O	3:D:295:ARG:NH1	2.47	0.48
3:D:925:LEU:HB3	3:D:940:ARG:HA	1.95	0.48
1:A:38:LEU:HD13	1:A:194:LEU:HD22	1.96	0.47
2:C:558:ARG:H	2:C:558:ARG:HH11	1.62	0.47
2:C:473:ARG:HB3	2:C:495:GLY:HA3	1.97	0.47
2:C:926:MET:HE1	3:D:817:LEU:HA	1.97	0.47
2:C:113:ASP:HB3	2:C:132:PRO:HD2	1.96	0.47
5:F:149:PRO:HG2	5:F:152:PHE:CD1	2.50	0.47
2:C:771:ARG:NH1	2:C:784:LEU:O	2.48	0.47
3:D:447:MET:HB3	3:D:447:MET:HE2	1.71	0.47
1:A:124:HIS:CE1	1:A:127:THR:HG22	2.48	0.47
1:B:30:PHE:HA	1:B:33:THR:OG1	2.15	0.47
3:D:700:LEU:O	3:D:704:TYR:HB2	2.15	0.47
2:C:727:GLU:H	3:D:725:THR:CG2	2.27	0.47
3:D:144:ARG:NH2	3:D:229:LEU:O	2.44	0.47
2:C:311:VAL:HG13	2:C:509:PHE:HB3	1.97	0.46
1:B:181:THR:O	1:B:189:PHE:HB2	2.15	0.46
2:C:408:ASP:O	2:C:412:ILE:HG23	2.16	0.46
2:C:507:ASN:HB2	2:C:511:PHE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:338:VAL:O	2:C:342:ILE:HG12	2.15	0.46
3:D:409:LYS:O	3:D:415:GLN:HG3	2.15	0.46
3:D:1244:LYS:H	3:D:1244:LYS:HZ3	1.63	0.46
3:D:876:ARG:HG2	3:D:1226:PHE:CZ	2.51	0.46
1:B:223:ARG:HH12	1:B:227:VAL:HA	1.81	0.46
1:B:8:THR:O	1:B:23:ILE:HA	2.16	0.46
1:A:18:ARG:NH1	1:A:195:ASP:OD2	2.49	0.46
3:D:595:ASP:HB3	3:D:631:ALA:HB2	1.98	0.46
2:C:1079:TYR:CD2	3:D:559:MET:HG2	2.51	0.46
3:D:1095:SER:OG	3:D:1097:ARG:NH2	2.49	0.46
3:D:573:PRO:HG2	3:D:576:MET:HE2	1.98	0.45
1:A:219:PHE:HE1	1:B:38:LEU:HG	1.80	0.45
2:C:473:ARG:HD3	2:C:494:ILE:O	2.17	0.45
2:C:803:VAL:HG11	2:C:869:VAL:HG11	1.98	0.45
1:A:100:GLN:HG3	1:A:101:GLY:N	2.32	0.45
3:D:1068:PRO:HD3	3:D:1074:GLU:HA	1.98	0.45
3:D:102:THR:HG22	3:D:313:VAL:HG22	1.99	0.45
1:B:124:HIS:CE1	1:B:127:THR:HG23	2.52	0.45
2:C:623:ALA:HB2	2:C:709:ASP:HB3	1.98	0.45
3:D:32:GLU:HB3	3:D:42:GLU:HG3	1.97	0.45
2:C:352:GLN:O	2:C:365:VAL:HB	2.17	0.45
2:C:441:ASP:HA	2:C:680:HIS:NE2	2.32	0.45
3:D:515:MET:HB3	3:D:515:MET:HE2	1.57	0.45
2:C:556:GLU:OE1	2:C:558:ARG:NH1	2.41	0.45
3:D:1078:ASP:OD1	3:D:1078:ASP:N	2.48	0.45
4:E:41:GLU:OE1	4:E:99:HIS:NE2	2.45	0.45
2:C:38:ARG:HG2	2:C:973:SER:HB2	1.98	0.45
3:D:116:TYR:HB3	3:D:298:VAL:HG11	1.99	0.45
3:D:413:PHE:HA	3:D:417:LEU:HD12	1.98	0.45
2:C:759:ALA:HB2	2:C:769:ILE:HG13	1.99	0.45
2:C:848:ILE:HD13	2:C:874:ALA:HB2	1.99	0.45
3:D:3:ASP:OD1	3:D:3:ASP:N	2.48	0.45
3:D:143:MET:HG2	3:D:251:TYR:CE2	2.52	0.44
5:F:188:ARG:O	5:F:192:ARG:HG3	2.17	0.44
1:A:7:PRO:HB2	1:B:221:LEU:HD11	2.00	0.44
2:C:77:ARG:NH1	2:C:505:ARG:HH12	2.15	0.44
3:D:757:GLU:OE1	3:D:770:ARG:NH1	2.44	0.44
2:C:896:GLY:HA2	3:D:431:VAL:HB	2.00	0.44
5:F:29:PHE:HB2	5:F:69:PHE:CE2	2.52	0.44
2:C:1103:TYR:CE2	3:D:454:PRO:HG3	2.52	0.44
3:D:766:ASN:O	3:D:770:ARG:N	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ARG:NH1	2:C:1014:ARG:HA	2.32	0.44
2:C:140:ILE:HG13	2:C:147:ILE:HG12	1.99	0.44
3:D:585:LEU:HD13	3:D:673:PHE:HE1	1.82	0.44
3:D:1166:THR:O	3:D:1203:GLY:CA	2.65	0.44
3:D:26:GLY:HA3	3:D:51:ILE:HG22	2.00	0.44
3:D:292:ALA:O	3:D:296:LEU:HB2	2.18	0.44
3:D:527:LEU:HD22	3:D:575:ALA:O	2.18	0.44
1:B:59:VAL:HG11	1:B:66:VAL:HG22	2.00	0.43
1:B:79:ASN:HB3	3:D:636:ARG:HH12	1.83	0.43
3:D:1087:ARG:HA	3:D:1113:GLU:HG2	2.00	0.43
3:D:793:TYR:HB3	3:D:800:ILE:HG13	2.00	0.43
1:B:230:GLU:O	1:B:232:ILE:HG13	2.18	0.43
3:D:500:ARG:NH1	3:D:539:ASP:OD2	2.51	0.43
2:C:163:LYS:HE3	2:C:639:GLY:O	2.18	0.43
2:C:261:THR:HG23	2:C:264:LYS:HZ1	1.84	0.43
3:D:900:GLU:OE2	3:D:959:GLN:NE2	2.40	0.43
3:D:925:LEU:HD13	3:D:944:LEU:HD21	2.00	0.43
2:C:189:GLU:HA	2:C:200:HIS:HA	2.01	0.43
3:D:927:THR:HG23	3:D:961:LYS:HD3	2.01	0.43
4:E:55:TYR:CZ	4:E:105:HIS:HB2	2.53	0.43
5:F:138:ASP:C	5:F:140:GLU:H	2.22	0.43
2:C:764:LEU:HB2	2:C:808:PRO:HB2	1.99	0.43
5:F:153:ARG:HA	5:F:156:VAL:HG22	2.00	0.43
2:C:157:PHE:HE1	2:C:389:ILE:HD11	1.83	0.43
2:C:1131:LEU:HD13	3:D:105:TRP:CH2	2.53	0.43
3:D:850:PHE:O	3:D:853:THR:OG1	2.34	0.43
2:C:188:ASP:HA	2:C:367:THR:HG23	1.99	0.43
2:C:516:TYR:HB3	2:C:578:TYR:HB3	2.01	0.43
2:C:705:GLY:N	2:C:708:THR:OG1	2.52	0.43
3:D:1007:GLY:HA2	3:D:1010:LEU:HD13	2.01	0.43
3:D:325:ARG:HD2	3:D:341:ASN:OD1	2.19	0.43
3:D:579:LEU:HD23	3:D:808:THR:HB	2.00	0.43
3:D:1088:VAL:HG22	3:D:1098:VAL:HG22	2.01	0.43
1:B:171:VAL:HA	1:B:198:THR:HA	2.00	0.42
3:D:817:LEU:O	3:D:839:SER:HB2	2.19	0.42
5:F:29:PHE:O	5:F:33:ALA:N	2.46	0.42
5:F:81:TRP:CZ2	5:F:85:ILE:HD11	2.53	0.42
1:A:178:VAL:HA	1:A:191:LYS:O	2.19	0.42
1:B:20:GLN:HA	1:B:194:LEU:O	2.20	0.42
2:C:515:PRO:HG2	2:C:581:VAL:HG21	2.01	0.42
2:C:1094:ASP:OD1	2:C:1094:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:344:TYR:CZ	2:C:365:VAL:HA	2.55	0.42
2:C:545:ASN:O	2:C:545:ASN:ND2	2.53	0.42
2:C:828:LYS:HG2	2:C:830:ARG:H	1.84	0.42
1:B:188:ASP:OD1	1:B:188:ASP:N	2.43	0.42
1:B:220:GLY:HA2	1:B:223:ARG:HB3	2.01	0.42
2:C:47:PRO:HG3	2:C:517:ARG:HD2	2.02	0.42
3:D:329:GLN:HB3	3:D:335:PHE:CE2	2.55	0.42
3:D:1056:GLU:HB2	3:D:1063:LYS:HB3	2.01	0.42
3:D:203:ARG:HG3	3:D:206:ARG:HH12	1.85	0.42
3:D:588:LEU:HD11	3:D:672:MET:HE3	2.02	0.42
3:D:1220:TRP:CD1	3:D:1243:ASP:HB2	2.53	0.42
1:B:42:LEU:HD21	1:B:208:LEU:HA	2.02	0.42
3:D:832:ILE:HD12	3:D:851:ILE:HG23	2.01	0.42
3:D:580:ASP:OD1	3:D:580:ASP:N	2.51	0.42
5:F:184:LEU:HA	5:F:184:LEU:HD23	1.82	0.42
2:C:254:PHE:CG	2:C:255:SER:N	2.88	0.41
2:C:518:LYS:O	2:C:525:SER:OG	2.26	0.41
2:C:811:GLU:O	2:C:819:ARG:NH1	2.53	0.41
3:D:785:VAL:HG21	3:D:820:MET:SD	2.60	0.41
5:F:59:GLN:O	5:F:63:VAL:HG23	2.20	0.41
2:C:92:GLU:OE2	2:C:390:ARG:NH2	2.53	0.41
1:A:144:ARG:HH12	1:B:2:LEU:HB2	1.84	0.41
1:B:174:VAL:HG13	1:B:196:VAL:HG12	2.02	0.41
2:C:938:TRP:HB2	2:C:1026:GLY:HA2	2.02	0.41
2:C:1099:ARG:HD3	5:F:128:ALA:HB2	2.03	0.41
3:D:339:ASP:HB3	3:D:399:LEU:HB3	2.02	0.41
3:D:937:ILE:HD11	3:D:951:ALA:HB1	2.02	0.41
3:D:739:PRO:HA	3:D:740:PRO:HD3	1.89	0.41
5:F:177:ILE:H	5:F:177:ILE:HG13	1.71	0.41
2:C:751:HIS:CD2	2:C:877:ARG:HD2	2.56	0.41
3:D:717:LYS:HE2	3:D:717:LYS:HB3	1.96	0.41
3:D:847:LEU:HD23	3:D:847:LEU:HA	1.87	0.41
3:D:926:GLY:HA2	3:D:963:ARG:HG3	2.03	0.41
2:C:1103:TYR:OH	5:F:129:GLU:OE2	2.38	0.41
3:D:288:LYS:HA	3:D:291:ARG:HD2	2.02	0.41
3:D:642:PRO:HG3	3:D:662:TRP:CE2	2.55	0.41
3:D:26:GLY:HA3	3:D:51:ILE:CG2	2.51	0.41
3:D:87:VAL:HA	3:D:90:GLU:HG2	2.03	0.41
1:A:144:ARG:NH2	1:B:27:GLU:OE2	2.54	0.41
1:B:110:ILE:O	1:B:112:PRO:HD3	2.21	0.41
2:C:148:LYS:HA	2:C:148:LYS:HZ3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:642:VAL:HB	2:C:703:ALA:HB3	2.03	0.41
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.94	0.40
2:C:93:LEU:HD11	2:C:397:GLU:HB2	2.02	0.40
3:D:27:GLU:HB2	3:D:94:HIS:CE1	2.56	0.40
5:F:142:LYS:HE2	5:F:146:GLN:NE2	2.37	0.40
1:A:98:ARG:HG3	1:A:135:GLU:HG3	2.03	0.40
2:C:103:MET:HE1	2:C:404:MET:O	2.22	0.40
3:D:556:ARG:NE	4:E:34:ILE:HG23	2.37	0.40
3:D:588:LEU:HD13	3:D:723:TRP:CE2	2.55	0.40
1:B:61:HIS:NE2	1:B:159:ILE:HD13	2.36	0.40
3:D:459:ARG:HA	3:D:459:ARG:HD2	1.90	0.40
3:D:497:LEU:O	3:D:543:VAL:HA	2.21	0.40
3:D:1050:THR:OG1	3:D:1107:VAL:HG23	2.21	0.40
1:B:223:ARG:HH22	1:B:227:VAL:HG13	1.85	0.40
2:C:185:VAL:HG22	2:C:204:VAL:HG22	2.03	0.40
3:D:34:ILE:HG22	3:D:41:PRO:HA	2.03	0.40
3:D:288:LYS:HE2	3:D:288:LYS:HB3	1.85	0.40
3:D:527:LEU:HA	3:D:527:LEU:HD23	1.89	0.40
3:D:666:THR:HG22	3:D:685:ASN:OD1	2.22	0.40
5:F:138:ASP:O	5:F:139:THR:OG1	2.35	0.40
1:B:196:VAL:HG23	1:B:204:PRO:HB3	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	219/368 (60%)	213 (97%)	6 (3%)	0	100	100
1	B	227/368 (62%)	216 (95%)	11 (5%)	0	100	100
2	C	1097/1174 (93%)	1070 (98%)	27 (2%)	0	100	100
3	D	1251/1317 (95%)	1231 (98%)	20 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	72/110 (66%)	71 (99%)	1 (1%)	0	100	100
5	F	169/218 (78%)	162 (96%)	7 (4%)	0	100	100
All	All	3035/3555 (85%)	2963 (98%)	72 (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	188/315 (60%)	182 (97%)	6 (3%)	39	59
1	B	191/315 (61%)	185 (97%)	6 (3%)	40	60
2	C	830/995 (83%)	812 (98%)	18 (2%)	52	70
3	D	1020/1096 (93%)	1004 (98%)	16 (2%)	62	77
4	E	64/90 (71%)	63 (98%)	1 (2%)	62	77
5	F	128/175 (73%)	122 (95%)	6 (5%)	26	45
All	All	2421/2986 (81%)	2368 (98%)	53 (2%)	52	70

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	18	ARG
1	A	62	GLU
1	A	111	VAL
1	A	127	THR
1	A	200	ASN
1	B	60	LEU
1	B	88	GLU
1	B	150	VAL
1	B	162	ILE
1	B	172	LEU
1	B	228	GLU

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Mol	Chain	Res	Type
2	C	144	THR
2	C	146	GLU
2	C	211	TRP
2	C	232	GLN
2	C	290	GLU
2	C	320	LEU
2	C	336	GLU
2	C	342	ILE
2	C	465	ARG
2	C	558	ARG
2	C	604	ARG
2	C	641	VAL
2	C	821	LEU
2	C	869	VAL
2	C	892	LYS
2	C	958	ARG
2	C	991	CYS
2	C	1107	VAL
3	D	73	ILE
3	D	82	VAL
3	D	126	GLU
3	D	199	ASP
3	D	298	VAL
3	D	304	GLN
3	D	427	ARG
3	D	451	LEU
3	D	517	VAL
3	D	580	ASP
3	D	590	THR
3	D	725	THR
3	D	738	VAL
3	D	768	ASP
3	D	858	LYS
3	D	1008	THR
4	E	36	ASN
5	F	31	ARG
5	F	79	LYS
5	F	94	TYR
5	F	104	TYR
5	F	148	LEU
5	F	179	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
2	C	442	GLN
2	C	543	GLN
2	C	1129	GLN
3	D	761	GLN
3	D	1227	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	221/368 (60%)	0.05	8 (3%) 42 51	57, 75, 117, 149	0
1	B	231/368 (62%)	0.37	19 (8%) 11 14	65, 100, 138, 153	0
2	C	1105/1174 (94%)	0.52	109 (9%) 7 8	49, 74, 172, 200	0
3	D	1257/1317 (95%)	0.26	70 (5%) 24 29	50, 83, 139, 164	0
4	E	76/110 (69%)	0.37	5 (6%) 18 21	79, 98, 121, 127	0
5	F	173/218 (79%)	0.70	17 (9%) 7 8	56, 119, 141, 151	0
All	All	3063/3555 (86%)	0.38	228 (7%) 14 17	49, 83, 149, 200	0

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	286	GLY	8.5
2	C	287	PRO	8.1
2	C	288	THR	7.3
2	C	283	PRO	7.3
3	D	285	LYS	7.1
3	D	1025	THR	7.0
2	C	296	LEU	6.8
3	D	287	GLN	6.7
2	C	268	VAL	6.6
2	C	346	VAL	6.4
2	C	211	TRP	6.2
2	C	284	GLY	6.0
3	D	653	HIS	5.9
1	B	1	MET	5.7
2	C	269	GLY	5.7
2	C	262	LEU	5.6
2	C	341	THR	5.5
3	D	652	GLY	5.4
2	C	267	THR	5.3

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Mol	Chain	Res	Type	RSRZ
2	C	291	SER	5.3
3	D	933	ALA	5.2
2	C	292	ALA	5.1
5	F	141	ILE	5.0
2	C	552	GLY	5.0
1	A	3	ILE	4.8
2	C	212	LEU	4.8
2	C	551	ASP	4.8
3	D	1026	GLY	4.7
2	C	340	ALA	4.7
2	C	334	THR	4.7
2	C	261	THR	4.6
1	A	186	ARG	4.6
2	C	235	THR	4.6
1	A	184	GLU	4.5
3	D	1111	LEU	4.5
2	C	289	LYS	4.5
3	D	281	ILE	4.4
2	C	194	SER	4.4
5	F	95	ARG	4.4
3	D	761	GLN	4.4
2	C	201	SER	4.3
5	F	25	LEU	4.3
2	C	231	ARG	4.3
2	C	337	ASP	4.3
2	C	829	ALA	4.3
2	C	342	ILE	4.3
3	D	188	GLY	4.2
4	E	107	GLU	4.2
3	D	1176	LEU	4.2
2	C	198	THR	4.1
2	C	192	ASP	4.1
2	C	1162	LEU	4.1
2	C	295	LEU	4.0
3	D	1042	GLY	4.0
3	D	1084	GLN	4.0
1	B	157	ALA	4.0
2	C	1150	GLY	4.0
2	C	468	ALA	3.9
2	C	559	VAL	3.9
3	D	1049	VAL	3.8
1	B	235	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
2	C	195	THR	3.8
2	C	237	LEU	3.8
3	D	1186	PHE	3.8
2	C	557	PRO	3.8
2	C	1159	ALA	3.7
3	D	1061	PHE	3.7
2	C	298	ASN	3.7
2	C	227	ASP	3.7
1	B	96	TYR	3.6
3	D	1075	VAL	3.6
2	C	1152	ASP	3.6
2	C	297	GLU	3.6
3	D	282	ARG	3.6
5	F	69	PHE	3.6
3	D	762	ARG	3.6
1	B	234	ILE	3.5
2	C	202	VAL	3.5
2	C	277	ILE	3.5
2	C	465	ARG	3.5
3	D	277	LEU	3.4
3	D	1066	ILE	3.4
5	F	104	TYR	3.4
3	D	1105	VAL	3.4
1	B	155	SER	3.4
2	C	1158	ALA	3.4
3	D	190	LYS	3.3
3	D	908	GLY	3.3
2	C	358	PRO	3.3
2	C	271	ASP	3.3
4	E	70	LEU	3.3
2	C	574	SER	3.3
1	B	63	PHE	3.3
2	C	344	TYR	3.3
4	E	106	THR	3.3
2	C	299	LEU	3.3
2	C	320	LEU	3.2
2	C	147	ILE	3.2
5	F	91	ILE	3.2
3	D	1073	GLU	3.2
2	C	236	VAL	3.2
3	D	1011	THR	3.2
2	C	80	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
2	C	357	VAL	3.2
2	C	294	THR	3.1
2	C	280	LYS	3.1
2	C	75	ALA	3.1
5	F	29	PHE	3.1
2	C	260	SER	3.0
2	C	828	LYS	3.0
2	C	200	HIS	3.0
2	C	270	THR	3.0
2	C	348	LEU	3.0
4	E	55	TYR	2.9
3	D	1071	GLY	2.9
3	D	186	ALA	2.9
5	F	35	PRO	2.9
1	B	130	ASP	2.9
2	C	234	VAL	2.9
1	A	185	GLN	2.9
2	C	226	ILE	2.9
3	D	1059	GLU	2.9
5	F	81	TRP	2.9
2	C	191	ILE	2.8
2	C	285	GLU	2.8
3	D	1060	ARG	2.8
2	C	570	TYR	2.8
3	D	1083	ARG	2.8
1	B	90	ASP	2.8
2	C	204	VAL	2.7
3	D	189	ALA	2.7
2	C	573	SER	2.7
5	F	198	VAL	2.7
2	C	196	ASP	2.7
3	D	1043	LYS	2.7
5	F	193	GLY	2.7
3	D	1173	THR	2.7
2	C	140	ILE	2.7
2	C	363	VAL	2.7
5	F	180	VAL	2.6
3	D	909	THR	2.6
1	B	133	LYS	2.6
2	C	417	LEU	2.6
3	D	270	ILE	2.6
3	D	1114	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	183	GLU	2.6
3	D	1116	ALA	2.6
2	C	266	ASN	2.6
3	D	1190	ASN	2.6
2	C	317	ASN	2.6
3	D	283	ASN	2.6
2	C	290	GLU	2.5
2	C	263	GLU	2.5
2	C	550	ALA	2.5
3	D	278	ARG	2.5
3	D	765	LEU	2.5
3	D	758	LYS	2.5
3	D	654	SER	2.5
2	C	210	ALA	2.4
2	C	1154	ASP	2.4
2	C	365	VAL	2.4
3	D	467	GLN	2.4
3	D	1278	ALA	2.4
2	C	230	ARG	2.4
1	A	4	SER	2.4
2	C	1155	LEU	2.4
3	D	296	LEU	2.4
2	C	339	VAL	2.4
1	B	97	LEU	2.4
4	E	86	LEU	2.4
5	F	71	SER	2.4
3	D	1175	PHE	2.4
2	C	265	ASP	2.4
2	C	555	VAL	2.4
3	D	1062	TYR	2.3
2	C	275	LEU	2.3
2	C	193	LYS	2.3
3	D	1064	ILE	2.3
2	C	281	LEU	2.3
1	B	156	GLY	2.3
2	C	286	PRO	2.3
2	C	229	LYS	2.3
3	D	1052	ARG	2.3
3	D	994	ALA	2.3
2	C	306	TYR	2.3
5	F	85	ILE	2.3
1	A	24	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	194	ARG	2.3
2	C	314	TYR	2.3
1	B	159	ILE	2.3
1	B	162	ILE	2.3
3	D	1177	PRO	2.3
3	D	4	VAL	2.3
3	D	865	LEU	2.2
2	C	467	ARG	2.2
1	B	129	ASN	2.2
3	D	1162	LEU	2.2
3	D	1145	GLN	2.2
3	D	1074	GLU	2.2
3	D	606	HIS	2.2
2	C	519	VAL	2.2
2	C	233	PRO	2.2
3	D	766	ASN	2.2
2	C	199	LEU	2.2
5	F	97	LYS	2.2
3	D	1051	GLY	2.2
2	C	264	LYS	2.2
1	B	67	PRO	2.2
2	C	318	LYS	2.1
3	D	1032	GLN	2.1
1	B	95	MET	2.1
1	B	3	ILE	2.1
2	C	185	VAL	2.1
5	F	147	ALA	2.1
3	D	1050	THR	2.1
3	D	77	ARG	2.1
1	A	101	GLY	2.1
2	C	362	GLU	2.1
2	C	520	VAL	2.1
2	C	258	MET	2.1
2	C	355	MET	2.1
5	F	184	LEU	2.0
2	C	197	LYS	2.0
1	A	221	LEU	2.0
1	B	161	ARG	2.0
3	D	187	GLU	2.0
3	D	1172	SER	2.0
2	C	228	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	ZN	D	2001	1/1	0.95	0.18	89,89,89,89	0
6	ZN	D	2002	1/1	0.98	0.15	87,87,87,87	0

6.5 Other polymers (i)

There are no such residues in this entry.