Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 04:32 AM JST

PDB ID	:	6KQF
Title	:	Thermus thermophilus initial transcription complex comprising sigma A and 5'-OH RNA of 5 nt
Authors	:	Zhang, Y.; Li, L.; Ebright, R.H.
Deposited on	:	2019-08-17
Resolution	:	2.45 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:

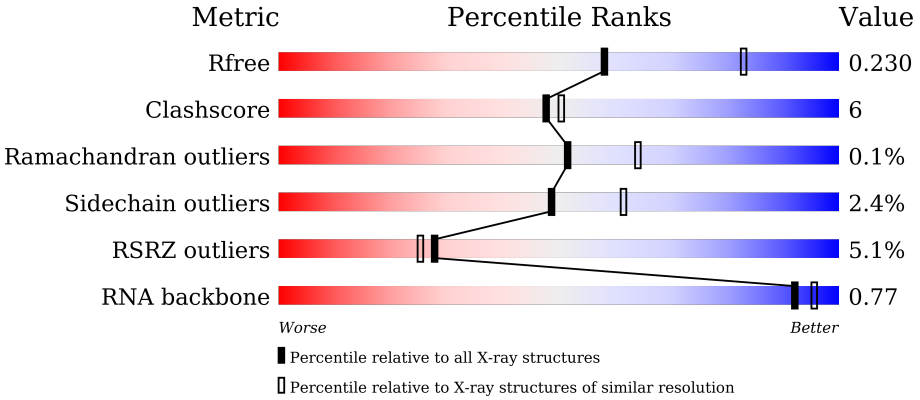
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)
RNA backbone	3102	1001 (2.80-2.12)

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	2% 62% 12% 27%
1	B	315	% 58% 12% 29%
2	C	1119	3% 83% 15% ••
3	D	1524	8% 82% 15% ••

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Mol	Chain	Length	Quality of chain
4	E	99	2% 85% 10% 5%
5	F	443	3% 68% 10% 22%
6	G	21	5% 29% 52% 19%
7	H	27	11% 37% 52% 11%
8	I	5	60% 40%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 29358 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	231	1814	1158	316	338	2	0	1	0
1	B	223	1758	1124	305	327	2	0	0	0

- 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	1112	8786	5559	1567	1636	24	0	3	0

- 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	1486	11759	7458	2070	2195	36	0	3	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	94	761	486	132	139	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	346	2803	1767	508	524	4	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	initiating methionine	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 (5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	G	17	350	166	68	100	16	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
8	I	5	102	47	18	33	4	0	0	0

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

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

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

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

- Molecule 11 is water.

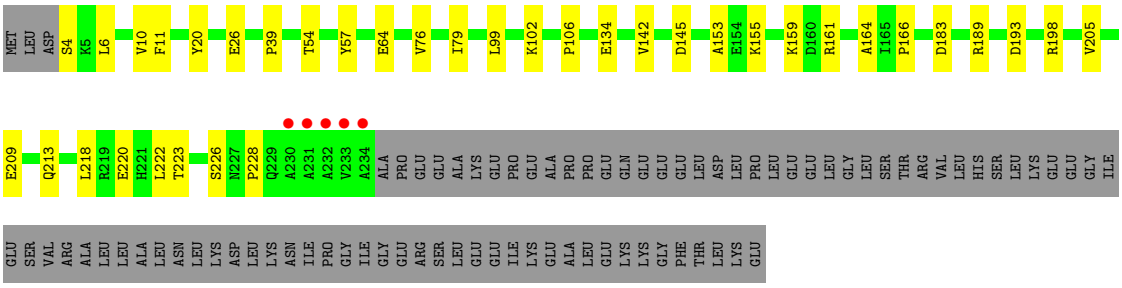
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	38	38	38	0	0
			Total	O		
11	B	25	25	25	0	0
			Total	O		
11	C	246	246	246	0	0
			Total	O		
11	D	310	310	310	0	0
			Total	O		
11	E	30	30	30	0	0
			Total	O		
11	F	46	46	46	0	0
			Total	O		
11	G	16	16	16	0	0
			Total	O		
11	H	8	8	8	0	0
			Total	O		
11	I	5	5	5	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.

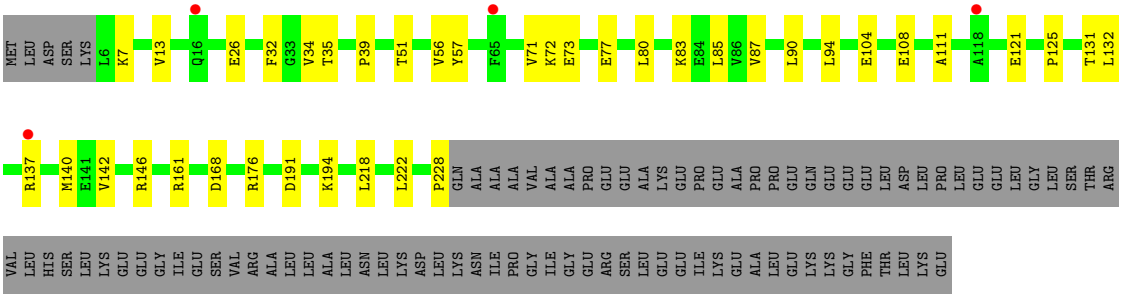
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



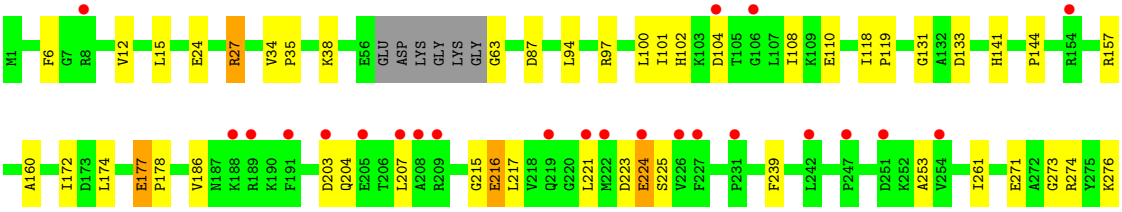
• Molecule 1: DNA-directed RNA polymerase subunit alpha

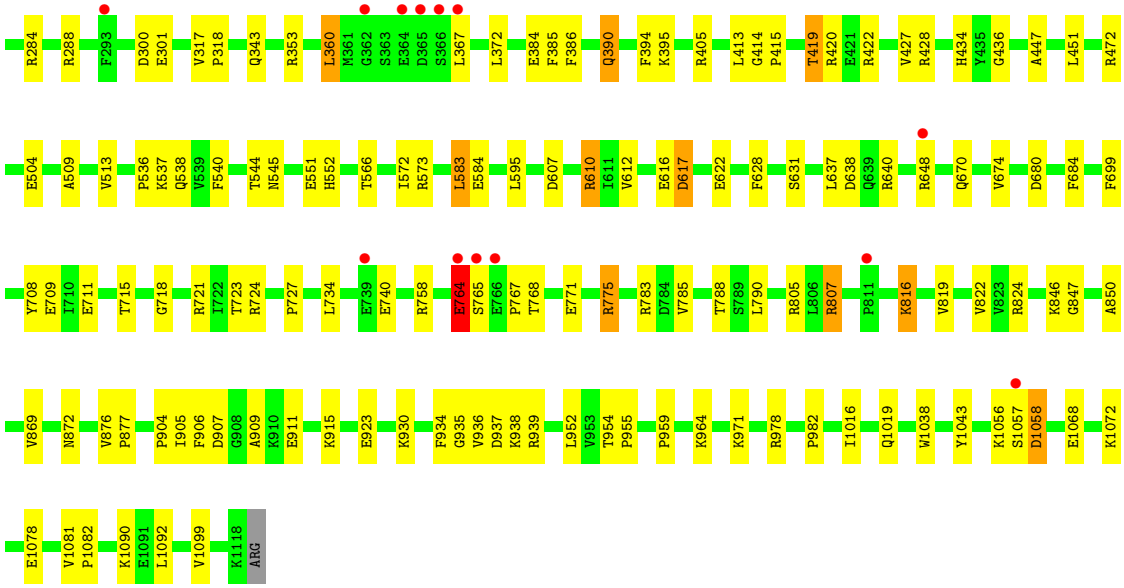
Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit beta

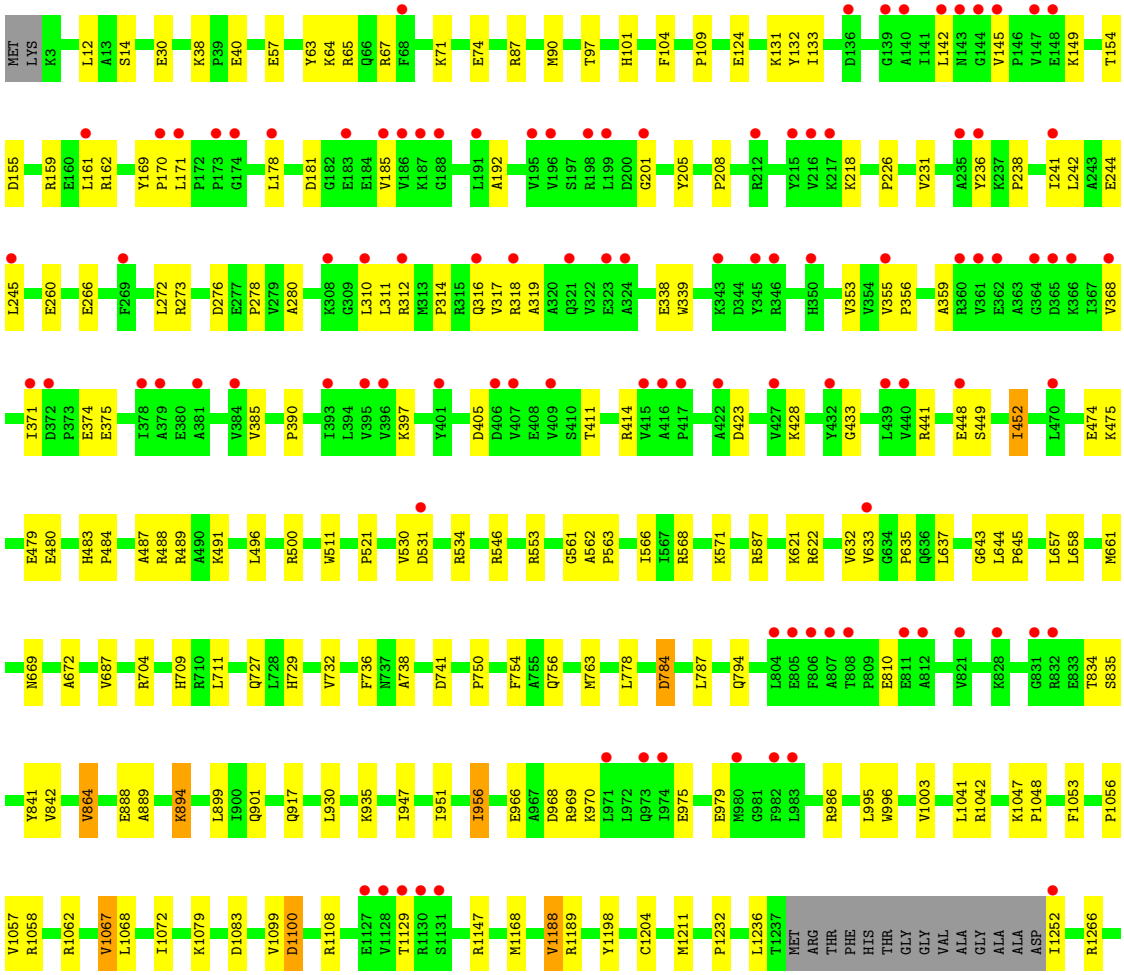
Chain C:

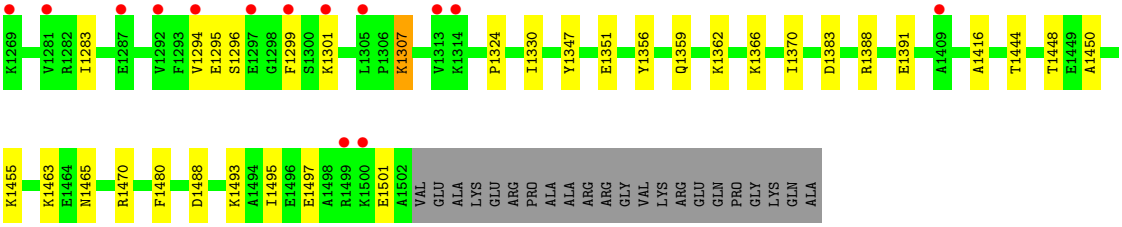




• Molecule 3: DNA-directed RNA polymerase subunit beta'

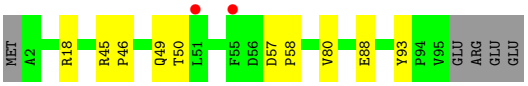
Chain D:





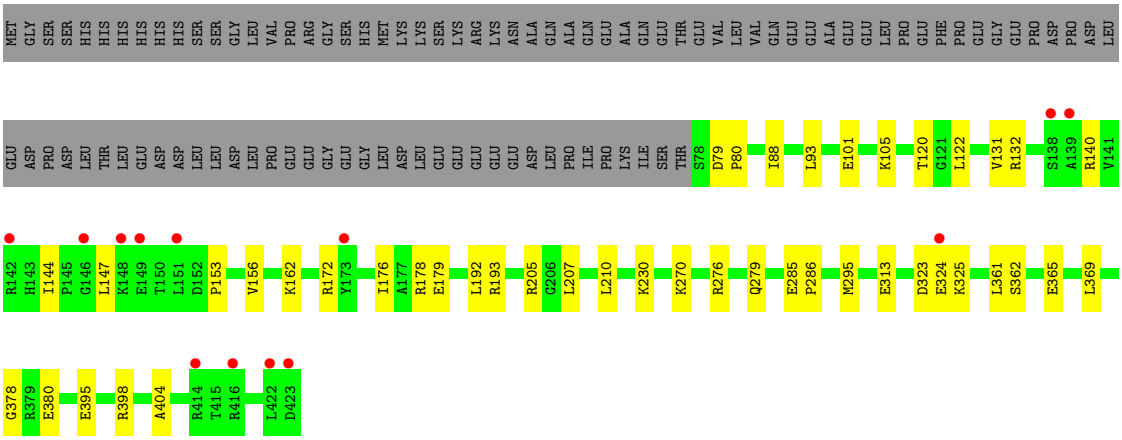
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



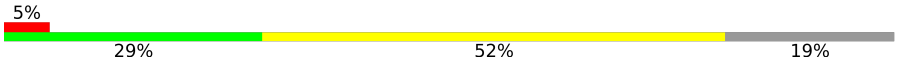
• Molecule 5: RNA polymerase sigma factor SigA

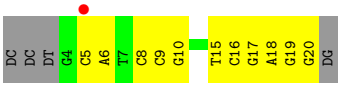
Chain F:



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

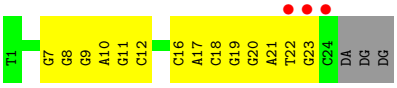
Chain G:





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

Chain H:



• Molecule 8: RNA (5'-R(*CP*UP*CP*GP*A)-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	183.64Å 103.64Å 296.19Å 90.00° 98.95° 90.00°	Depositor
Resolution (Å)	48.85 – 2.45 48.85 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.85-2.45) 99.8 (48.85-2.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.199 , 0.230 0.199 , 0.230	Depositor DCC
R_{free} test set	10041 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	48.9	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.014 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	29358	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.23	0/1849	0.44	0/2515
1	B	0.22	0/1790	0.42	0/2435
2	C	0.27	0/8963	0.45	0/12122
3	D	0.25	0/11975	0.44	0/16189
4	E	0.26	0/775	0.42	0/1045
5	F	0.25	0/2848	0.41	0/3833
6	G	0.45	0/393	0.97	0/606
7	H	0.41	0/556	0.92	0/858
8	I	0.29	0/113	0.76	0/174
All	All	0.26	0/29262	0.47	0/39777

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 (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	1814	0	1869	26	0
1	B	1758	0	1808	24	0
2	C	8786	0	8891	109	0
3	D	11759	0	12002	149	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	761	0	778	5	0
5	F	2803	0	2871	28	0
6	G	350	0	192	20	0
7	H	495	0	272	27	0
8	I	102	0	55	4	0
9	B	1	0	0	0	0
9	D	2	0	0	0	0
9	F	1	0	0	0	0
10	D	2	0	0	0	0
11	A	38	0	0	0	0
11	B	25	0	0	0	0
11	C	246	0	0	3	0
11	D	310	0	0	10	0
11	E	30	0	0	0	0
11	F	46	0	0	0	0
11	G	16	0	0	1	0
11	H	8	0	0	1	0
11	I	5	0	0	0	0
All	All	29358	0	28738	346	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 (346) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:21:DA:H2"	7:H:22:DT:H5"	1.34	1.06
6:G:19:DG:H2"	6:G:20:DG:H5'	1.40	1.04
6:G:15:DT:H2'	6:G:16:DC:C6	1.94	1.00
7:H:21:DA:H2"	7:H:22:DT:C5'	1.93	0.99
6:G:19:DG:C2'	6:G:20:DG:H5'	2.03	0.89
7:H:21:DA:C2'	7:H:22:DT:H5"	2.05	0.87
2:C:63:GLY:HA3	2:C:100:LEU:HD21	1.63	0.78
6:G:18:DA:N7	11:G:101:HOH:O	2.21	0.73
3:D:241:ILE:HA	3:D:312:ARG:HG2	1.72	0.71
2:C:628:PHE:H	2:C:638:ASP:HB3	1.56	0.70
3:D:87:ARG:NH2	11:D:2103:HOH:O	2.24	0.70
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.73	0.70
7:H:10:DA:H2'	7:H:11:DG:C8	2.27	0.69
2:C:24:GLU:OE2	2:C:27:ARG:NH2	2.26	0.68
3:D:704:ARG:HD2	3:D:738:ALA:HB2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.75	0.67
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.26	0.67
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.75	0.67
3:D:65:ARG:NH1	5:F:378:GLY:O	2.27	0.66
7:H:20:DG:H2'	7:H:21:DA:C8	2.31	0.66
2:C:617:ASP:OD1	2:C:617:ASP:N	2.29	0.65
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.78	0.65
3:D:661:MET:SD	11:D:2364:HOH:O	2.54	0.65
2:C:216:GLU:O	2:C:216:GLU:HG3	1.96	0.65
2:C:758:ARG:HH21	2:C:788:THR:HB	1.62	0.65
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.30	0.64
2:C:390:GLN:HB3	2:C:415:PRO:HD3	1.80	0.64
2:C:428:ARG:NH2	2:C:447:ALA:O	2.30	0.64
2:C:97:ARG:NH1	2:C:110:GLU:OE1	2.31	0.64
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.31	0.64
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.31	0.63
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.80	0.63
2:C:631:SER:HB3	2:C:637:LEU:HD13	1.80	0.63
2:C:215:GLY:O	2:C:216:GLU:HB3	1.99	0.63
3:D:109:PRO:HB3	7:H:21:DA:H5"	1.81	0.62
3:D:894:LYS:H	3:D:894:LYS:HD3	1.64	0.62
3:D:530:VAL:HG12	3:D:531:ASP:H	1.64	0.62
7:H:12:DC:O5'	7:H:12:DC:H6	1.81	0.62
6:G:9:DC:O2	7:H:19:DG:N2	2.23	0.62
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.82	0.62
3:D:57:GLU:HG3	3:D:64:LYS:HG2	1.82	0.62
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.79	0.62
2:C:904:PRO:HB2	2:C:907:ASP:HB3	1.82	0.62
3:D:1495:ILE:HD13	4:E:80:VAL:HG21	1.81	0.61
3:D:272:LEU:HB2	3:D:280:ALA:HB3	1.83	0.61
2:C:1019:GLN:HG2	2:C:1058:ASP:HB3	1.81	0.60
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.83	0.60
3:D:711:LEU:HD13	3:D:778:LEU:HD23	1.83	0.60
7:H:20:DG:H2"	7:H:21:DA:O4'	2.01	0.60
3:D:1465:ASN:OD1	3:D:1470:ARG:NH1	2.34	0.60
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.83	0.59
6:G:18:DA:H2'	6:G:19:DG:C8	2.37	0.59
2:C:805:ARG:O	2:C:807[A]:ARG:NH2	2.34	0.59
2:C:207:LEU:HD13	2:C:221:LEU:HD21	1.85	0.58
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.86	0.58
3:D:546:ARG:NH2	11:D:2107:HOH:O	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:657:LEU:HG	3:D:661:MET:HE2	1.84	0.58
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.87	0.57
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.87	0.57
3:D:561:GLY:HA3	5:F:132:ARG:HD3	1.86	0.57
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.87	0.57
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.86	0.57
6:G:5:DC:H1'	6:G:6:DA:OP2	2.04	0.57
7:H:21:DA:C1'	7:H:22:DT:H5"	2.34	0.57
6:G:15:DT:C4	6:G:16:DC:N4	2.73	0.56
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.88	0.56
2:C:536:PRO:HB3	3:D:1067:VAL:HG11	1.87	0.56
1:B:94:LEU:O	1:B:146:ARG:NH2	2.39	0.56
3:D:966:GLU:O	3:D:969:ARG:HG2	2.06	0.56
3:D:1470:ARG:NH1	11:D:2113:HOH:O	2.39	0.56
3:D:162:ARG:O	3:D:414:ARG:NH1	2.36	0.55
6:G:8:DC:N3	7:H:20:DG:N2	2.51	0.55
2:C:684:PHE:HB3	3:D:633:VAL:HG21	1.89	0.55
6:G:16:DC:H2'	6:G:17:DG:C8	2.42	0.55
1:A:4:SER:O	1:A:189:ARG:NH2	2.37	0.55
3:D:317:VAL:HG23	3:D:339:TRP:HB3	1.88	0.55
3:D:562:ALA:O	5:F:140:ARG:NH1	2.27	0.55
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.89	0.54
3:D:1048:PRO:O	3:D:1079:LYS:NZ	2.34	0.54
2:C:906:PHE:CG	3:D:1067:VAL:HG12	2.43	0.54
3:D:553:ARG:NH2	11:D:2118:HOH:O	2.40	0.54
3:D:97:THR:HG21	3:D:571:LYS:HG2	1.90	0.54
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.90	0.54
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.88	0.54
2:C:1057:SER:HB2	3:D:622:ARG:O	2.07	0.54
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.90	0.54
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.90	0.53
6:G:8:DC:C4	6:G:9:DC:N4	2.76	0.53
3:D:1488:ASP:OD1	3:D:1488:ASP:N	2.38	0.53
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.89	0.53
7:H:19:DG:H2"	7:H:20:DG:O5'	2.08	0.53
3:D:489:ARG:NH1	3:D:1391:GLU:OE2	2.39	0.53
2:C:727:PRO:HB3	2:C:783:ARG:HD3	1.90	0.53
3:D:1450:ALA:HA	3:D:1455:LYS:HE3	1.90	0.53
3:D:633:VAL:HG13	3:D:635:PRO:HD3	1.91	0.53
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.90	0.52
2:C:405:ARG:NH2	11:C:1212:HOH:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:405:ARG:HD3	2:C:566:THR:HG21	1.91	0.52
1:A:99:LEU:HB2	1:A:142:VAL:HG22	1.90	0.52
2:C:367:LEU:HD13	2:C:372:LEU:HD21	1.90	0.52
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.92	0.52
3:D:1236:LEU:HA	3:D:1359:GLN:HG3	1.90	0.52
3:D:411:THR:O	5:F:178:ARG:NH1	2.43	0.52
2:C:612:VAL:HG22	2:C:622:GLU:HG3	1.92	0.51
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.46	0.51
6:G:10:DG:N2	7:H:18:DC:O2	2.43	0.51
7:H:22:DT:H2"	7:H:23:DG:C8	2.45	0.51
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.93	0.51
1:A:209:GLU:O	1:A:213:GLN:HG2	2.10	0.51
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.92	0.51
2:C:923:GLU:OE2	2:C:964:LYS:NZ	2.42	0.51
7:H:16:DC:H2"	7:H:17:DA:C8	2.46	0.51
2:C:133:ASP:HB3	2:C:395:LYS:HD2	1.92	0.51
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.11	0.51
2:C:905:ILE:HG13	2:C:905:ILE:O	2.11	0.51
3:D:750:PRO:HG2	3:D:756:GLN:NE2	2.26	0.51
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.92	0.51
2:C:846:LYS:NZ	8:I:5:A:OP1	2.38	0.51
3:D:1100:ASP:OD2	3:D:1463:LYS:NZ	2.41	0.51
2:C:94:LEU:HD22	2:C:118:ILE:HD11	1.93	0.50
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.44	0.50
3:D:500:ARG:NH1	3:D:1388:ARG:O	2.42	0.50
2:C:911:GLU:O	2:C:915:LYS:HG2	2.12	0.50
3:D:956:ILE:HD11	3:D:1062:ARG:HG2	1.94	0.50
5:F:80:PRO:HB2	5:F:210:LEU:HD11	1.92	0.50
1:A:193:ASP:OD1	2:C:938:LYS:NZ	2.41	0.50
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.93	0.50
1:B:90:LEU:HD21	1:B:121:GLU:HB2	1.93	0.50
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.94	0.50
1:B:51:THR:OG1	1:B:87:VAL:O	2.29	0.50
3:D:405:ASP:HB3	3:D:423:ASP:HA	1.93	0.50
6:G:8:DC:C2	7:H:20:DG:N2	2.79	0.50
1:B:57:TYR:CD1	1:B:161:ARG:HD2	2.47	0.49
3:D:968:ASP:OD1	3:D:1058:ARG:NH2	2.45	0.49
3:D:704:ARG:CD	3:D:738:ALA:HB2	2.41	0.49
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.94	0.49
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.27	0.49
3:D:704:ARG:HD3	3:D:736:PHE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:276:ARG:O	5:F:279:GLN:HG3	2.12	0.49
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.95	0.49
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.95	0.49
3:D:1232:PRO:HG2	3:D:1356:TYR:HE1	1.77	0.49
5:F:395:GLU:OE2	5:F:398:ARG:NH2	2.46	0.49
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.94	0.49
5:F:144:ILE:HB	5:F:147:LEU:HD13	1.94	0.49
5:F:323:ASP:OD1	5:F:325:LYS:N	2.45	0.49
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.48	0.49
2:C:144:PRO:HB2	2:C:273:GLY:HA3	1.95	0.49
2:C:390:GLN:HG2	2:C:414:GLY:HA2	1.94	0.49
2:C:930:LYS:HE3	2:C:935:GLY:HA2	1.94	0.49
3:D:841:TYR:HB2	3:D:864:VAL:HG22	1.94	0.49
2:C:223:ASP:OD1	2:C:225:SER:OG	2.30	0.48
2:C:427:VAL:HG23	2:C:428:ARG:HG3	1.95	0.48
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.93	0.48
2:C:1016:ILE:O	3:D:87:ARG:NH1	2.44	0.48
3:D:834:THR:OG1	3:D:835:SER:N	2.45	0.48
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.94	0.48
2:C:768:THR:OG1	2:C:771:GLU:OE1	2.31	0.48
3:D:534:ARG:NH2	5:F:313:GLU:O	2.46	0.48
5:F:93:LEU:HD21	5:F:193:ARG:HD2	1.95	0.48
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.95	0.48
2:C:816:LYS:HG3	2:C:819:VAL:HG21	1.95	0.48
3:D:621:LYS:NZ	11:D:2130:HOH:O	2.46	0.48
1:B:104:GLU:OE2	1:B:137:ARG:NH1	2.47	0.48
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.95	0.48
2:C:724:ARG:NH2	2:C:734:LEU:O	2.47	0.48
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.13	0.48
3:D:1444:THR:O	3:D:1448:THR:HG23	2.13	0.48
2:C:721:ARG:HH22	2:C:785:VAL:HG11	1.79	0.48
3:D:226:PRO:HG2	3:D:245:LEU:HD11	1.96	0.47
3:D:371:ILE:HG23	5:F:230:LYS:HD2	1.95	0.47
3:D:487:ALA:O	3:D:491:LYS:HG2	2.14	0.47
7:H:17:DA:N9	7:H:18:DC:C5	2.83	0.47
2:C:271:GLU:OE1	2:C:288:ARG:NH1	2.42	0.47
2:C:537:LYS:NZ	11:C:1224:HOH:O	2.47	0.47
2:C:764:GLU:H	2:C:764:GLU:HG3	1.42	0.47
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.78	0.47
3:D:637:LEU:HD11	3:D:727:GLN:HB3	1.96	0.47
3:D:975:GLU:O	3:D:979:GLU:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:794:GLN:HB3	11:D:2101:HOH:O	2.15	0.47
1:B:73:GLU:HB3	1:B:77:GLU:HB3	1.96	0.47
2:C:203:ASP:OD1	2:C:204:GLN:N	2.48	0.47
2:C:971:LYS:NZ	11:C:1215:HOH:O	2.42	0.47
3:D:658:LEU:HA	3:D:661:MET:HE3	1.96	0.47
2:C:572:ILE:HG13	2:C:573:ARG:HG3	1.96	0.47
3:D:231:VAL:O	3:D:236:TYR:OH	2.32	0.47
3:D:131:LYS:NZ	3:D:154:THR:HG22	2.30	0.47
6:G:16:DC:H2'	6:G:17:DG:H8	1.79	0.46
7:H:20:DG:C2'	7:H:21:DA:C8	2.96	0.46
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.50	0.46
3:D:1266:ARG:NE	7:H:18:DC:OP1	2.49	0.46
1:B:191:ASP:OD1	1:B:191:ASP:N	2.41	0.46
3:D:1383:ASP:HB3	3:D:1416:ALA:HB3	1.98	0.46
5:F:270:LYS:HG2	5:F:295:MET:HE1	1.97	0.46
2:C:101:ILE:HG12	2:C:108:ILE:HG12	1.98	0.46
2:C:224:GLU:CD	2:C:224:GLU:H	2.19	0.46
7:H:21:DA:C2'	7:H:22:DT:C5'	2.77	0.46
2:C:674:VAL:HG12	2:C:869:VAL:HB	1.96	0.46
3:D:169:TYR:HA	3:D:170:PRO:HD3	1.82	0.46
5:F:172:ARG:O	5:F:176:ILE:HG12	2.15	0.46
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.98	0.46
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.97	0.46
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.98	0.46
3:D:1168:MET:HE3	3:D:1168:MET:HA	1.98	0.46
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.98	0.45
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.49	0.45
1:A:64:GLU:HG3	1:A:79:ILE:HD12	1.97	0.45
2:C:680:ASP:OD2	2:C:978:ARG:NH2	2.49	0.45
3:D:244:GLU:HG3	3:D:310:LEU:HG	1.97	0.45
2:C:436:GLY:HA2	2:C:538:GLN:O	2.17	0.45
2:C:616:GLU:OE1	2:C:648:ARG:NH1	2.49	0.45
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.52	0.45
3:D:1362:LYS:HD3	11:D:2349:HOH:O	2.16	0.45
1:A:20:TYR:OH	1:A:198:ARG:HD2	2.17	0.45
1:A:183:ASP:HA	2:C:938:LYS:HE3	1.98	0.45
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.98	0.45
3:D:178:LEU:HG	3:D:192:ALA:HA	1.97	0.45
7:H:9:DG:C2	7:H:10:DA:C2	3.04	0.45
3:D:729:HIS:O	3:D:732:VAL:HG22	2.17	0.45
5:F:362:SER:OG	5:F:365:GLU:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:GLU:O	1:A:223:THR:HB	2.17	0.45
5:F:101:GLU:HG2	5:F:105:LYS:HE2	1.98	0.45
1:B:140:MET:HB3	1:B:140:MET:HE2	1.90	0.45
2:C:1068:GLU:OE2	2:C:1072:LYS:NZ	2.50	0.44
3:D:1307:LYS:H	3:D:1307:LYS:HG3	1.53	0.44
7:H:11:DG:OP2	11:H:101:HOH:O	2.21	0.44
3:D:1366:LYS:O	3:D:1370:ILE:HG12	2.17	0.44
7:H:20:DG:H2"	7:H:21:DA:C5'	2.47	0.44
2:C:670:GLN:HG2	2:C:699:PHE:CD2	2.52	0.44
3:D:181:ASP:HB2	3:D:205:TYR:CD2	2.52	0.44
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.52	0.44
2:C:394:PHE:CE2	6:G:20:DG:H5"	2.52	0.44
3:D:970:LYS:HD3	3:D:995:LEU:HD13	1.99	0.44
6:G:15:DT:H2'	6:G:16:DC:H6	1.69	0.44
2:C:420:ARG:C	2:C:422:ARG:H	2.20	0.44
5:F:105:LYS:HD3	5:F:179:GLU:HG2	1.99	0.44
7:H:17:DA:C5	7:H:18:DC:N4	2.85	0.44
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	2.00	0.44
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.53	0.44
3:D:132:TYR:OH	3:D:568:ARG:NH1	2.51	0.44
3:D:142:LEU:HB2	3:D:161:LEU:HD21	1.99	0.44
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.99	0.43
6:G:15:DT:O2	8:I:5:A:C2	2.72	0.43
1:A:159:LYS:HE3	1:A:164:ALA:O	2.18	0.43
2:C:300:ASP:OD1	2:C:301:GLU:N	2.52	0.43
2:C:343:GLN:HG3	2:C:385:PHE:HB2	2.00	0.43
3:D:1347:TYR:CZ	3:D:1351:GLU:HG3	2.54	0.43
3:D:374:GLU:HG2	3:D:375:GLU:HG3	2.00	0.43
3:D:901:GLN:NE2	11:D:2128:HOH:O	2.45	0.43
4:E:57:ASP:HA	4:E:58:PRO:HD3	1.87	0.43
2:C:15:LEU:HD11	2:C:583:LEU:HD11	2.00	0.43
2:C:35:PRO:HG2	2:C:38:LYS:HD2	1.99	0.43
2:C:177:GLU:HG3	2:C:178:PRO:HD2	2.00	0.43
3:D:185:VAL:N	3:D:201:GLY:O	2.51	0.43
3:D:1463:LYS:HB3	3:D:1463:LYS:HE2	1.81	0.43
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.18	0.43
1:B:32:PHE:HA	1:B:35:THR:HB	2.01	0.43
3:D:30:GLU:OE1	3:D:40:GLU:HG2	2.18	0.43
3:D:1283:ILE:H	3:D:1283:ILE:HG13	1.59	0.43
1:A:10:VAL:HG12	1:A:26:GLU:O	2.19	0.43
2:C:872:ASN:ND2	3:D:784:ASP:OD2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1057:SER:CB	3:D:622:ARG:O	2.67	0.43
3:D:1003:VAL:HG21	3:D:1041:LEU:HG	2.01	0.43
3:D:644:LEU:HD12	3:D:645:PRO:HD2	2.01	0.43
2:C:584:GLU:OE2	2:C:584:GLU:N	2.49	0.42
3:D:1296:SER:HB3	3:D:1299:PHE:HB2	2.01	0.42
1:A:102:LYS:HE3	1:A:102:LYS:HB2	1.87	0.42
5:F:279:GLN:HB3	5:F:286:PRO:HD3	2.01	0.42
2:C:239:PHE:CD1	2:C:253:ALA:HA	2.54	0.42
3:D:38:LYS:HA	3:D:38:LYS:HD3	1.92	0.42
3:D:318:ARG:NH1	3:D:338:GLU:OE1	2.52	0.42
2:C:715:THR:OG1	2:C:718:GLY:O	2.23	0.42
2:C:850:ALA:HB1	3:D:633:VAL:HG12	2.00	0.42
3:D:1047:LYS:HG2	3:D:1053[A]:PHE:CE2	2.55	0.42
1:A:153:ALA:HB1	1:A:166:PRO:HB2	2.02	0.42
1:A:155:LYS:HA	1:A:155:LYS:HD2	1.83	0.42
5:F:193:ARG:NH1	7:H:7:DG:N7	2.67	0.42
6:G:15:DT:O2	8:I:5:A:H2	2.03	0.42
2:C:87:ASP:HA	2:C:131:GLY:HA3	2.02	0.42
2:C:419:THR:HG23	2:C:422:ARG:HG3	2.00	0.42
2:C:540:PHE:HB3	2:C:544:THR:HB	2.02	0.42
2:C:1090:LYS:HD3	2:C:1090:LYS:HA	1.77	0.42
3:D:12:LEU:HD23	3:D:12:LEU:HA	1.79	0.42
1:A:39:PRO:CG	1:B:39:PRO:HG3	2.46	0.42
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.55	0.42
1:B:111:ALA:HB3	1:B:125:PRO:HA	2.02	0.42
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.84	0.42
2:C:765:SER:O	2:C:767:PRO:HD3	2.19	0.42
2:C:905:ILE:O	2:C:906:PHE:HB2	2.20	0.42
2:C:708:TYR:HB3	2:C:790:LEU:HD21	2.00	0.42
3:D:428:LYS:HB3	3:D:428:LYS:HE2	1.87	0.42
4:E:45:ARG:HA	4:E:46:PRO:HD3	1.93	0.42
7:H:22:DT:H4'	7:H:23:DG:OP1	2.19	0.42
1:B:80:LEU:HD21	3:D:842:VAL:HG12	2.01	0.41
1:B:108:GLU:HG2	1:B:131:THR:HG22	2.02	0.41
2:C:157:ARG:HA	2:C:157:ARG:HD3	1.86	0.41
3:D:483:HIS:CE1	3:D:488:ARG:HD3	2.55	0.41
3:D:669:ASN:ND2	3:D:672:ALA:H	2.18	0.41
2:C:102[A]:HIS:CE1	2:C:104:ASP:HB2	2.55	0.41
2:C:420:ARG:HE	2:C:420:ARG:HB2	1.62	0.41
3:D:433:GLY:HA2	3:D:449:SER:H	1.85	0.41
3:D:475:LYS:O	3:D:479:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1211:MET:HB2	3:D:1211:MET:HE3	1.98	0.41
1:A:11:PHE:O	1:B:228:PRO:HA	2.20	0.41
1:A:54:THR:HG21	1:A:145:ASP:HB2	2.02	0.41
3:D:935:LYS:HE2	3:D:935:LYS:HB3	1.87	0.41
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.55	0.41
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	2.03	0.41
5:F:207:LEU:HD23	5:F:207:LEU:HA	1.90	0.41
2:C:1081:VAL:HA	2:C:1082:PRO:HD2	1.90	0.41
6:G:19:DG:H1	8:I:1:C:H42	1.67	0.41
1:A:226:SER:O	1:A:228:PRO:HD3	2.21	0.41
3:D:316:GLN:NE2	11:D:2148:HOH:O	2.52	0.41
2:C:119:PRO:HG2	2:C:386:PHE:CD2	2.56	0.41
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.56	0.41
3:D:161:LEU:HB3	3:D:452:ILE:HD11	2.02	0.41
3:D:951:ILE:HG13	3:D:1062:ARG:HD2	2.02	0.41
1:B:85:LEU:HG	1:B:87:VAL:HG23	2.03	0.41
2:C:847:GLY:HA2	3:D:741:ASP:HA	2.01	0.41
3:D:63:TYR:OH	3:D:74:GLU:OE2	2.31	0.41
3:D:353:VAL:HG22	3:D:368:VAL:HG22	2.03	0.41
3:D:397:LYS:O	3:D:448:GLU:HG2	2.20	0.41
2:C:6:PHE:CD1	2:C:909:ALA:HB2	2.55	0.41
3:D:480:GLU:OE2	3:D:488:ARG:NH2	2.54	0.41
5:F:79:ASP:OD2	7:H:8:DG:N1	2.38	0.41
3:D:90:MET:SD	3:D:521:PRO:HD3	2.62	0.40
3:D:236:TYR:CE1	3:D:242:LEU:HD12	2.56	0.40
3:D:643:GLY:CA	3:D:727:GLN:HB2	2.48	0.40
1:A:228:PRO:HB3	1:B:13:VAL:HG21	2.03	0.40
3:D:452:ILE:H	3:D:452:ILE:HG13	1.65	0.40
6:G:15:DT:C2'	6:G:16:DC:O4'	2.69	0.40
2:C:63:GLY:N	2:C:367:LEU:HD12	2.35	0.40
2:C:317:VAL:HA	2:C:318:PRO:HD3	1.92	0.40
2:C:771:GLU:O	2:C:775:ARG:HB2	2.22	0.40
2:C:954:THR:HA	2:C:955:PRO:HD3	1.92	0.40
3:D:155:ASP:OD2	3:D:159:ARG:NH1	2.53	0.40
3:D:171:LEU:HD23	3:D:171:LEU:HA	1.85	0.40
2:C:34:VAL:HA	2:C:35:PRO:HD2	1.92	0.40
2:C:360:LEU:HD12	2:C:360:LEU:HA	1.86	0.40
2:C:551:GLU:HG2	2:C:552:HIS:CD2	2.57	0.40
2:C:876:VAL:H	2:C:877:PRO:HD2	1.87	0.40
3:D:208:PRO:HA	3:D:390:PRO:HA	2.02	0.40
3:D:1294:VAL:HB	3:D:1301:LYS:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.83	0.40
2:C:850:ALA:HB1	3:D:632:VAL:HG13	2.03	0.40
3:D:889:ALA:HB1	3:D:930:LEU:HA	2.02	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	230/315 (73%)	230 (100%)	0	0	100	100
1	B	221/315 (70%)	215 (97%)	6 (3%)	0	100	100
2	C	1111/1119 (99%)	1082 (97%)	28 (2%)	1 (0%)	51	64
3	D	1485/1524 (97%)	1445 (97%)	39 (3%)	1 (0%)	51	64
4	E	92/99 (93%)	89 (97%)	3 (3%)	0	100	100
5	F	344/443 (78%)	339 (98%)	5 (2%)	0	100	100
All	All	3483/3815 (91%)	3400 (98%)	81 (2%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	764	GLU
3	D	563	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	201/273 (74%)	199 (99%)	2 (1%)	76	84
1	B	196/273 (72%)	193 (98%)	3 (2%)	65	76
2	C	938/941 (100%)	906 (97%)	32 (3%)	37	48
3	D	1256/1279 (98%)	1231 (98%)	25 (2%)	55	67
4	E	83/88 (94%)	80 (96%)	3 (4%)	35	46
5	F	300/388 (77%)	294 (98%)	6 (2%)	55	67
All	All	2974/3242 (92%)	2903 (98%)	71 (2%)	49	61

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	205	VAL
1	B	7	LYS
1	B	34	VAL
1	B	72	LYS
2	C	27	ARG
2	C	141	HIS
2	C	177	GLU
2	C	216	GLU
2	C	217	LEU
2	C	224	GLU
2	C	261	ILE
2	C	274	ARG
2	C	276	LYS
2	C	284	ARG
2	C	353	ARG
2	C	360	LEU
2	C	384	GLU
2	C	390	GLN
2	C	419	THR
2	C	434	HIS
2	C	513	VAL
2	C	583	LEU
2	C	595	LEU
2	C	610	ARG
2	C	617	ASP
2	C	640	ARG
2	C	723	THR

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Mol	Chain	Res	Type
2	C	764	GLU
2	C	775	ARG
2	C	807[A]	ARG
2	C	807[B]	ARG
2	C	816	LYS
2	C	952	LEU
2	C	1056	LYS
2	C	1058	ASP
2	C	1078	GLU
3	D	67	ARG
3	D	71	LYS
3	D	133	ILE
3	D	145	VAL
3	D	149	LYS
3	D	276	ASP
3	D	452	ILE
3	D	687	VAL
3	D	709	HIS
3	D	754	PHE
3	D	784	ASP
3	D	810	GLU
3	D	864	VAL
3	D	894	LYS
3	D	956	ILE
3	D	986	ARG
3	D	1067	VAL
3	D	1083	ASP
3	D	1100	ASP
3	D	1129	THR
3	D	1188	VAL
3	D	1252	ILE
3	D	1295	GLU
3	D	1307	LYS
3	D	1501	GLU
4	E	49	GLN
4	E	50	THR
4	E	93	TYR
5	F	88	ILE
5	F	162	LYS
5	F	205	ARG
5	F	324	GLU
5	F	369	LEU

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Mol	Chain	Res	Type
5	F	380	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	434	HIS
3	D	66	GLN
3	D	669	ASN
3	D	976	GLN
3	D	1172	HIS
5	F	83	GLN
5	F	218	GLN
5	F	381	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	4/5 (80%)	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 6 ligands modelled in this entry, 6 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	231/315 (73%)	-0.07	5 (2%) 62 58	41, 58, 85, 127	0
1	B	223/315 (70%)	0.07	4 (1%) 68 65	44, 69, 96, 111	0
2	C	1112/1119 (99%)	0.08	36 (3%) 47 44	27, 50, 105, 130	0
3	D	1486/1524 (97%)	0.34	118 (7%) 12 9	26, 58, 115, 137	1 (0%)
4	E	94/99 (94%)	-0.32	2 (2%) 63 60	32, 50, 86, 106	0
5	F	346/443 (78%)	0.16	13 (3%) 40 37	38, 67, 107, 131	0
6	G	17/21 (80%)	0.02	1 (5%) 22 19	55, 71, 156, 162	0
7	H	24/27 (88%)	-0.05	3 (12%) 3 2	68, 93, 155, 175	0
8	I	5/5 (100%)	-0.24	0 100 100	46, 48, 62, 74	0
All	All	3538/3868 (91%)	0.18	182 (5%) 28 25	26, 58, 112, 175	1 (0%)

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	ALA	10.2
3	D	144	GLY	8.3
1	A	233	VAL	6.0
2	C	365	ASP	5.7
3	D	1128	VAL	5.4
3	D	1130	ARG	5.2
1	A	234	ALA	5.2
3	D	173	PRO	5.1
5	F	146	GLY	5.0
3	D	201	GLY	4.7
2	C	811	PRO	4.5
3	D	409	VAL	4.5
2	C	362	GLY	4.3
3	D	1294	VAL	4.3
3	D	1129	THR	4.3

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Mol	Chain	Res	Type	RSRZ
3	D	360	ARG	4.1
3	D	1299	PHE	4.1
3	D	147	VAL	4.0
3	D	422	ALA	4.0
5	F	422	LEU	4.0
3	D	142	LEU	4.0
3	D	371	ILE	4.0
3	D	191	LEU	3.9
3	D	364	GLY	3.8
3	D	804	LEU	3.7
3	D	821	VAL	3.7
4	E	55	PHE	3.6
7	H	24	DC	3.6
2	C	104	ASP	3.6
3	D	245	LEU	3.5
1	A	230	ALA	3.5
3	D	361	VAL	3.5
2	C	364	GLU	3.5
3	D	1127	GLU	3.5
3	D	416	ALA	3.5
3	D	161	LEU	3.4
3	D	470	LEU	3.4
1	A	231	ALA	3.4
3	D	381	ALA	3.4
3	D	974	ILE	3.4
2	C	221	LEU	3.4
4	E	51	LEU	3.4
3	D	982	PHE	3.3
3	D	980	MET	3.3
3	D	186	VAL	3.3
3	D	316	GLN	3.3
5	F	139	ALA	3.2
3	D	310	LEU	3.2
2	C	764	GLU	3.1
3	D	406	ASP	3.1
3	D	312	ARG	3.1
2	C	1057	SER	3.1
1	B	118	ALA	3.1
3	D	1305	LEU	3.1
3	D	368	VAL	3.1
3	D	321	GLN	3.0
3	D	393	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
3	D	68	PHE	2.9
5	F	414	ARG	2.9
3	D	812	ALA	2.9
3	D	1313	VAL	2.9
2	C	191	PHE	2.9
3	D	811	GLU	2.8
3	D	427	VAL	2.8
1	B	16	GLN	2.8
3	D	1252	ILE	2.8
3	D	1297	GLU	2.8
5	F	423	ASP	2.8
2	C	189	ARG	2.8
2	C	227	PHE	2.8
3	D	440	VAL	2.8
3	D	148	GLU	2.8
5	F	142	ARG	2.8
3	D	372	ASP	2.8
2	C	766	GLU	2.7
3	D	432	TYR	2.7
3	D	395	VAL	2.7
3	D	140	ALA	2.7
2	C	219	GLN	2.7
5	F	138	SER	2.7
2	C	106	GLY	2.7
3	D	174	GLY	2.7
2	C	226	VAL	2.7
2	C	208	ALA	2.7
3	D	235	ALA	2.7
5	F	149	GLU	2.7
3	D	136	ASP	2.7
5	F	148	LYS	2.6
2	C	367	LEU	2.6
3	D	216	VAL	2.6
3	D	143	ASN	2.6
3	D	362	GLU	2.6
3	D	805	GLU	2.6
2	C	8	ARG	2.6
3	D	185	VAL	2.6
3	D	139	GLY	2.6
3	D	1269	LYS	2.6
3	D	1314	LYS	2.6
2	C	739	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	417	PRO	2.5
2	C	251	ASP	2.5
2	C	293	PHE	2.5
2	C	188	LYS	2.5
3	D	241	ILE	2.5
3	D	1499	ARG	2.5
2	C	207	LEU	2.5
2	C	242	LEU	2.5
3	D	178	LEU	2.5
3	D	396	VAL	2.5
3	D	318	ARG	2.4
3	D	1301	LYS	2.4
3	D	183	GLU	2.4
2	C	222	MET	2.4
2	C	247	PRO	2.4
2	C	648	ARG	2.4
3	D	195	VAL	2.4
3	D	199	LEU	2.4
3	D	439	LEU	2.4
3	D	187	LYS	2.4
3	D	832	ARG	2.4
3	D	983	LEU	2.4
3	D	198	ARG	2.4
3	D	1292	VAL	2.4
3	D	145	VAL	2.4
3	D	350	HIS	2.4
5	F	416	ARG	2.4
2	C	366	SER	2.4
2	C	254	VAL	2.3
3	D	355	VAL	2.3
5	F	173	TYR	2.3
3	D	1131	SER	2.3
3	D	171	LEU	2.3
3	D	308	LYS	2.3
3	D	196	VAL	2.3
3	D	633	VAL	2.3
2	C	205	GLU	2.3
3	D	1287	GLU	2.3
3	D	365	ASP	2.3
2	C	154	ARG	2.3
3	D	973	GLN	2.3
2	C	209	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	346	ARG	2.2
2	C	203	ASP	2.2
3	D	531	ASP	2.2
3	D	448	GLU	2.2
3	D	343	LYS	2.2
5	F	151	LEU	2.2
2	C	224	GLU	2.2
3	D	345	TYR	2.2
3	D	366	LYS	2.2
2	C	765	SER	2.2
3	D	379	ALA	2.2
3	D	1281	VAL	2.2
3	D	808	THR	2.2
3	D	828	LYS	2.2
3	D	831	GLY	2.2
3	D	407	VAL	2.2
3	D	415	VAL	2.2
1	B	65	PHE	2.2
7	H	23	DG	2.2
3	D	1409	ALA	2.1
3	D	971	LEU	2.1
7	H	22	DT	2.1
3	D	215	TYR	2.1
3	D	1500	LYS	2.1
3	D	170	PRO	2.1
3	D	212	ARG	2.1
3	D	384	VAL	2.1
3	D	401	TYR	2.1
3	D	807	ALA	2.1
2	C	231	PRO	2.1
3	D	269	PHE	2.1
3	D	323	GLU	2.1
6	G	5	DC	2.1
3	D	217	LYS	2.1
3	D	188	GLY	2.0
3	D	806	PHE	2.0
5	F	324	GLU	2.0
3	D	378	ILE	2.0
1	B	137	ARG	2.0
3	D	324	ALA	2.0
3	D	236	TYR	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(Å^2)	Q<0.9
9	MG	B	2001	1/1	0.90	0.12	64,64,64,64	0
9	MG	F	2001	1/1	0.93	0.06	52,52,52,52	0
9	MG	D	2004	1/1	0.96	0.08	74,74,74,74	0
9	MG	D	2003	1/1	0.96	0.17	37,37,37,37	0
10	ZN	D	2002	1/1	0.99	0.08	71,71,71,71	0
10	ZN	D	2001	1/1	1.00	0.14	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.