Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 04:08 AM EDT

PDB ID	:	7MLJ
Title	:	Crystal structure of Thermus thermophilus reiterative transcription complex with 4nt oligo-G RNA
Authors	:	Liu, Y.; Ebright, R.H.
Deposited on	:	2021-04-28
Resolution	:	3.75 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:

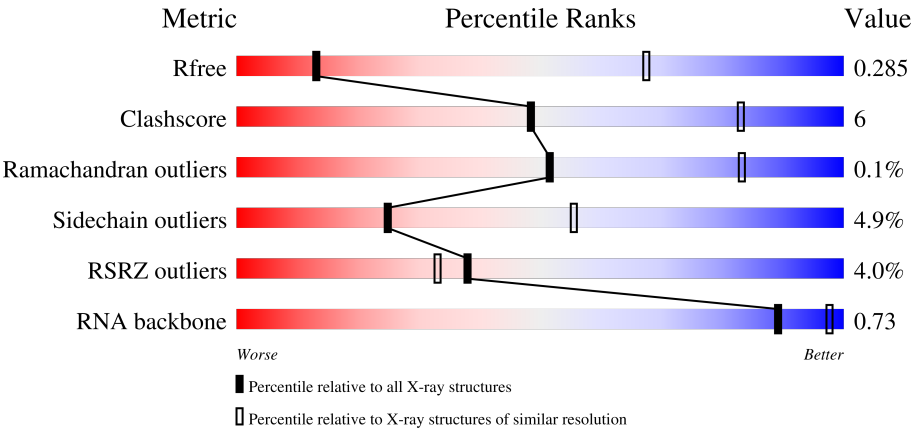
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.75 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	1039 (3.94-3.58)
Clashscore	141614	1051 (3.92-3.60)
Ramachandran outliers	138981	1015 (3.92-3.60)
Sidechain outliers	138945	1011 (3.92-3.60)
RSRZ outliers	127900	1050 (3.96-3.56)
RNA backbone	3102	1035 (4.52-3.00)

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% 59% 13% 28%
1	B	315	57% 12% • 30%
2	C	1119	4% 81% 17% ••
3	D	1524	5% 78% 18% ••

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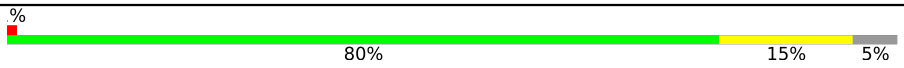
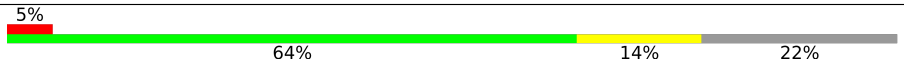
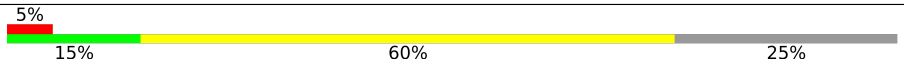
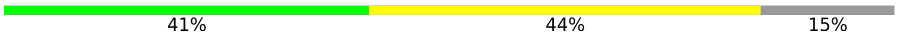
Mol	Chain	Length	Quality of chain
4	E	99	
5	F	443	
6	G	20	
7	I	4	
8	H	27	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	MG	B	2002	-	-	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 28489 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	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	222	Total	C	N	O	S	0	0	0
			1750	1118	304	326	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1486	Total	C	N	O	S	0	0	0
			11738	7441	2067	2195	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	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
			2807	1770	509	524	4			

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(P*CP*AP*TP*CP*CP*GP*TP*GP*CP*CP *CP*TP*GP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	15	Total	C	N	O	P	0	0	0
			304	144	54	91	15			

- Molecule 7 is a RNA chain called RNA (5'-R(P*GP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	4	Total	C	N	O	P	0	0	0
			92	40	20	28	4			

- Molecule 8 is a DNA chain called DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP* GP*CP*TP*GP*GP*CP*AP*CP*GP*GP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	23	Total	C	N	O	P	0	0	0
			478	227	94	135	22			

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

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

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

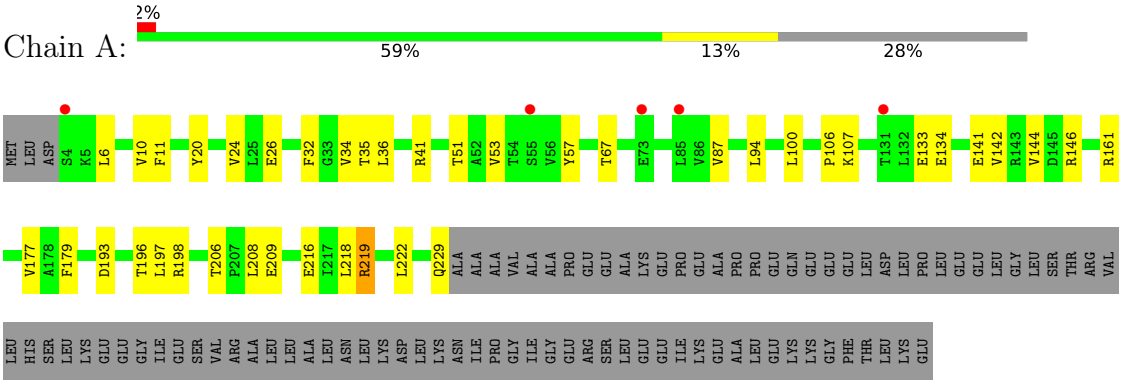
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	2	Total Zn 2 2	0	0

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.

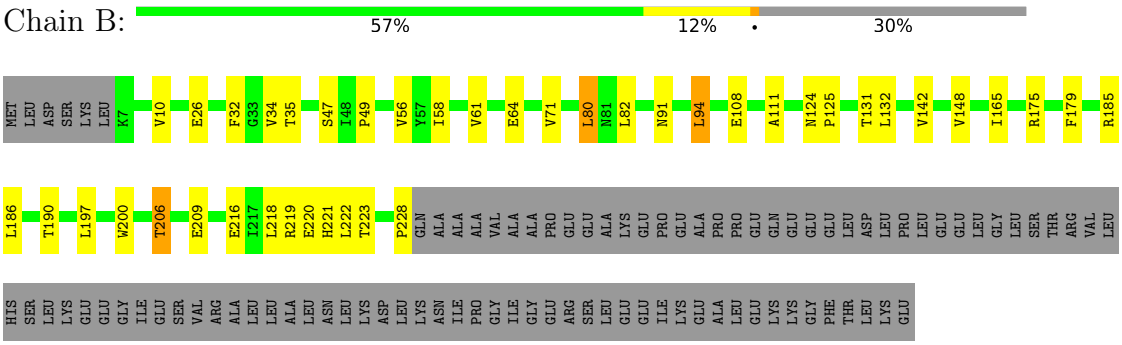
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



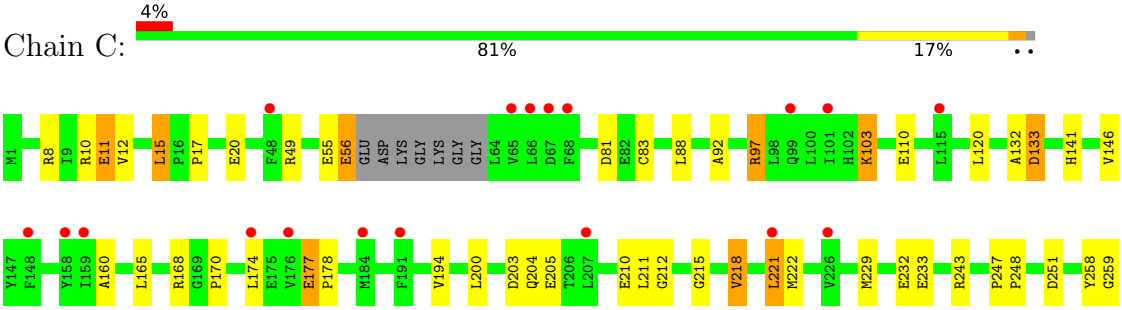
• Molecule 1: DNA-directed RNA polymerase subunit alpha

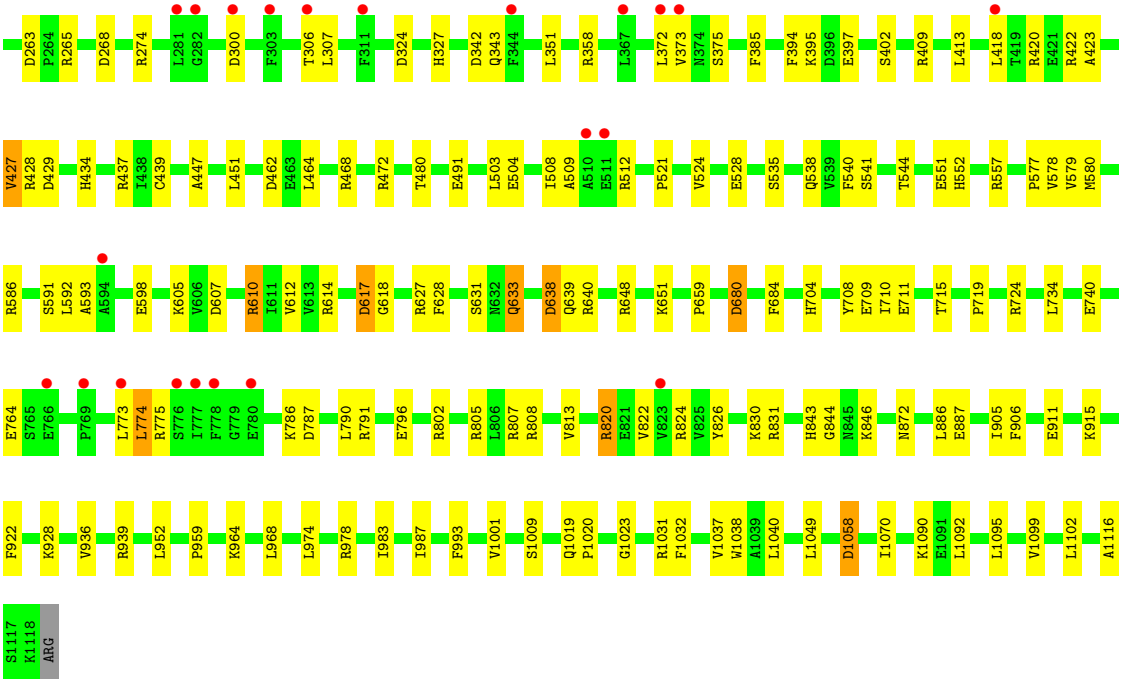
Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit beta

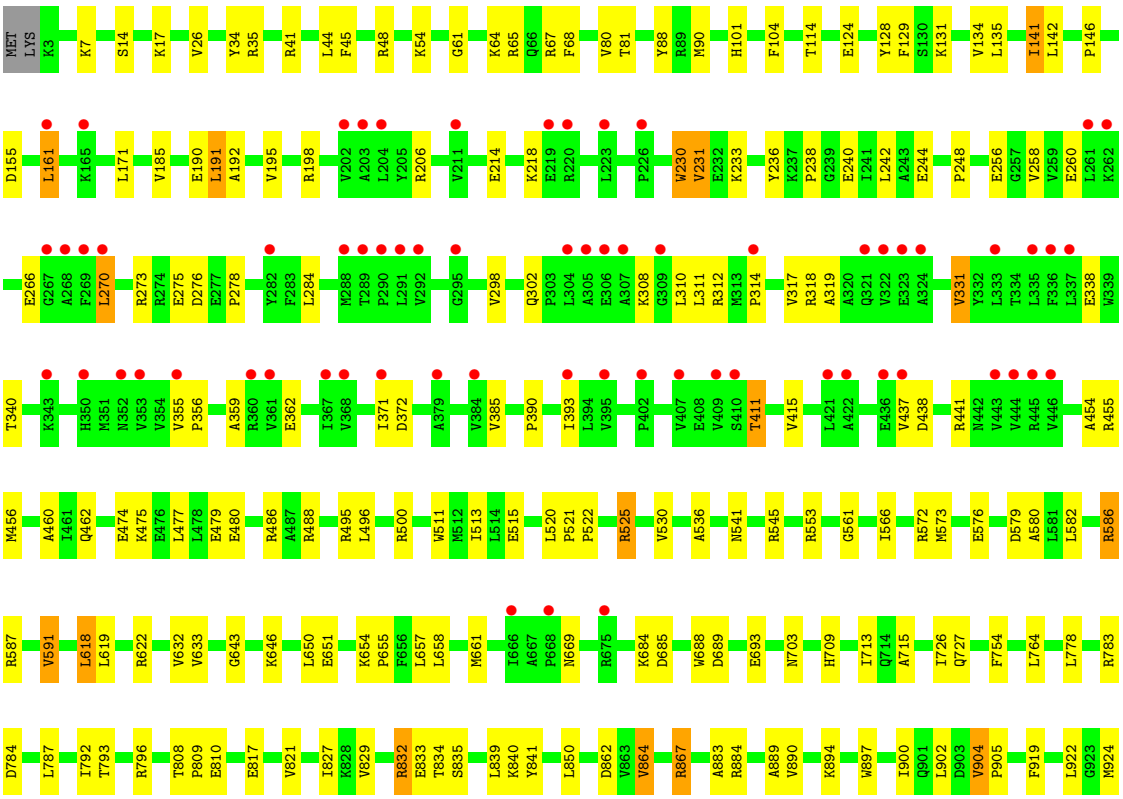
Chain C:

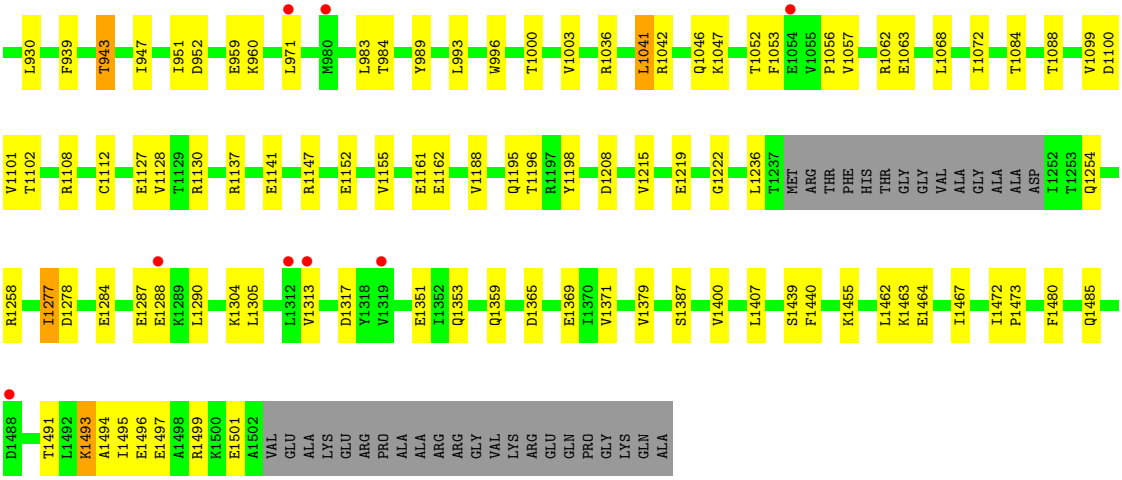




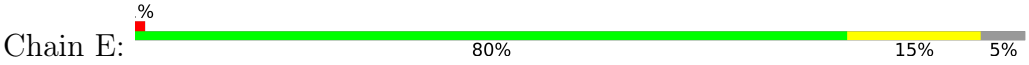
• Molecule 3: DNA-directed RNA polymerase subunit beta'

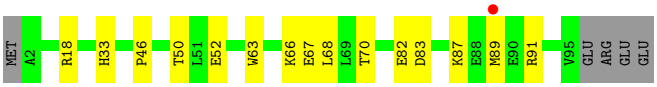
Chain D:



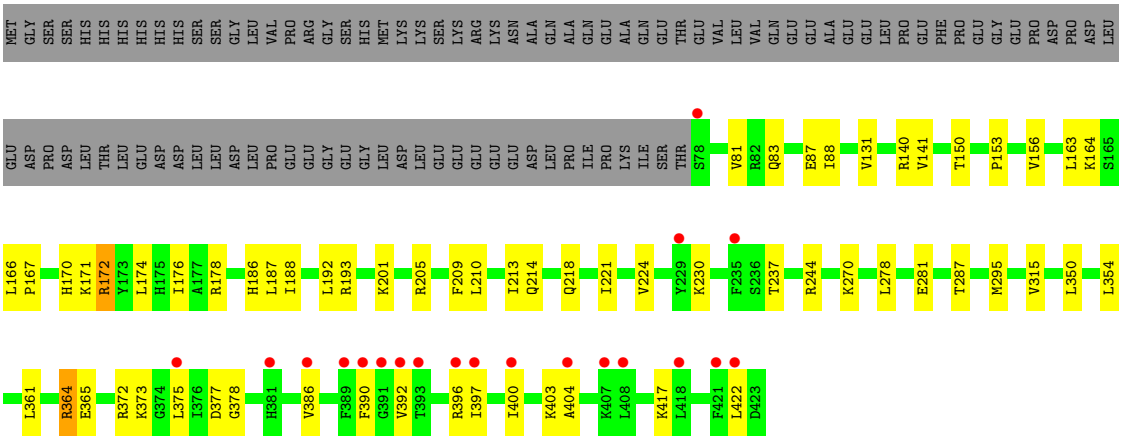


• Molecule 4: DNA-directed RNA polymerase subunit omega

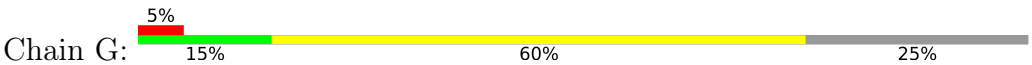




• Molecule 5: RNA polymerase sigma factor SigA



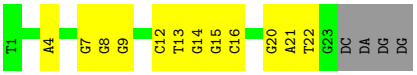
• Molecule 6: DNA (5'-D(P*CP*AP*TP*CP*CP*GP*TP*GP*CP*CP*CP*TP*GP*AP*G)-3')



• Molecule 7: RNA (5'-R(P*GP*GP*GP*G)-3')

• Molecule 8: DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*GP*CP*AP*CP*GP*GP*AP*TP*G)-3')

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	186.31Å 104.66Å 298.41Å 90.00° 98.12° 90.00°	Depositor
Resolution (Å)	46.21 – 3.75 49.32 – 3.75	Depositor EDS
% Data completeness (in resolution range)	97.1 (46.21-3.75) 97.5 (49.32-3.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.265 , 0.283 0.265 , 0.285	Depositor DCC
R_{free} test set	2009 reflections (3.51%)	wwPDB-VP
Wilson B-factor (Å^2)	106.3	Xtriage
Anisotropy	0.807	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 80.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	28489	wwPDB-VP
Average B, all atoms (Å^2)	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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

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	0/1814	0.51	0/2466
1	B	0.25	0/1782	0.52	0/2424
2	C	0.25	0/8937	0.52	0/12087
3	D	0.25	0/11944	0.50	0/16149
4	E	0.24	0/775	0.47	0/1045
5	F	0.24	0/2852	0.49	0/3837
6	G	0.58	0/339	0.93	0/520
7	I	0.36	0/103	1.04	0/160
8	H	0.53	0/538	0.90	0/831
All	All	0.26	0/29084	0.53	0/39519

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1782	0	1834	23	0
1	B	1750	0	1797	24	0
2	C	8770	0	8874	113	0
3	D	11738	0	11971	154	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	761	0	778	12	0
5	F	2807	0	2882	40	0
6	G	304	0	169	9	0
7	I	92	0	44	2	0
8	H	478	0	260	18	0
9	B	2	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
All	All	28489	0	28609	344	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 (344) 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:1491:THR:HG21	4:E:89:MET:HG2	1.63	0.79
2:C:773:LEU:HB2	5:F:375:LEU:HD11	1.67	0.77
1:B:206:THR:HG22	1:B:209:GLU:H	1.52	0.74
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.69	0.74
2:C:422:ARG:HA	8:H:16:DC:H5'	1.68	0.74
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.72	0.71
3:D:61:GLY:O	3:D:64:LYS:NZ	2.23	0.70
1:A:94:LEU:O	1:A:146:ARG:NH1	2.25	0.70
8:H:14:DG:H8	8:H:14:DG:H5"	1.57	0.69
2:C:17:PRO:HB2	2:C:20:GLU:HB3	1.74	0.68
8:H:21:DA:H2"	8:H:22:DT:H5'	1.74	0.68
2:C:170:PRO:HA	8:H:14:DG:H22	1.59	0.67
2:C:55:GLU:O	2:C:56:GLU:HB3	1.95	0.67
2:C:983:ILE:HG21	2:C:987:ILE:HD11	1.78	0.66
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.78	0.66
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.78	0.65
8:H:21:DA:H2'	8:H:22:DT:C6	2.32	0.65
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.79	0.65
3:D:1108:ARG:NH1	3:D:1198:TYR:O	2.30	0.64
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.79	0.64
3:D:124:GLU:OE2	3:D:587:ARG:NH1	2.31	0.63
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.81	0.63
2:C:905:ILE:HG23	2:C:906:PHE:HD2	1.62	0.63
8:H:12:DC:H2"	8:H:13:DT:H5'	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:397:ILE:HD12	5:F:400:ILE:HD11	1.81	0.62
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.80	0.62
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.82	0.62
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.81	0.61
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.82	0.61
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.81	0.61
5:F:193:ARG:HB3	8:H:7:DG:H5"	1.82	0.61
2:C:628:PHE:H	2:C:638:ASP:HB2	1.65	0.60
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.81	0.60
6:G:14:DC:H2'	6:G:15:DC:C6	2.35	0.60
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.84	0.60
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.84	0.60
2:C:97:ARG:NH1	2:C:110:GLU:OE2	2.34	0.60
3:D:1236:LEU:HA	3:D:1359:GLN:HG3	1.84	0.59
2:C:1116:ALA:HB2	3:D:88:TYR:HB3	1.84	0.59
2:C:774:LEU:HD23	5:F:354:LEU:HD21	1.83	0.59
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.84	0.59
3:D:1101:VAL:HG13	3:D:1102:THR:HG23	1.84	0.59
5:F:187:LEU:HD23	5:F:224:VAL:HG13	1.83	0.59
2:C:210:GLU:HB3	2:C:211:LEU:HD12	1.83	0.59
3:D:65:ARG:NH1	5:F:378:GLY:O	2.36	0.58
2:C:605:LYS:HB2	2:C:612:VAL:HB	1.85	0.58
3:D:832:ARG:HD2	3:D:833:GLU:H	1.67	0.58
2:C:591:SER:O	2:C:593:ALA:N	2.34	0.58
3:D:520:LEU:O	3:D:525:ARG:NH1	2.37	0.58
3:D:1100:ASP:OD1	3:D:1463:LYS:NZ	2.27	0.58
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.84	0.58
6:G:15:DC:H2'	6:G:16:DC:C6	2.39	0.58
2:C:774:LEU:HG	5:F:350:LEU:HD11	1.86	0.58
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.33	0.58
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.85	0.58
2:C:1019:GLN:HG2	2:C:1058:ASP:HB3	1.85	0.57
3:D:480:GLU:OE2	3:D:488:ARG:NH1	2.37	0.57
1:B:91:ASN:HB3	1:B:94:LEU:HB2	1.87	0.57
2:C:212:GLY:HA2	2:C:218:VAL:HG21	1.85	0.57
3:D:1353:GLN:NE2	3:D:1365:ASP:OD1	2.37	0.57
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.85	0.57
3:D:520:LEU:HD23	3:D:525:ARG:HG2	1.85	0.57
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.86	0.56
3:D:371:ILE:HG23	5:F:230:LYS:HD2	1.87	0.56
3:D:586:ARG:NH2	6:G:10:DC:OP1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:617:ASP:OD1	2:C:617:ASP:N	2.39	0.56
3:D:134:VAL:HG12	3:D:454:ALA:HB2	1.88	0.56
3:D:41:ARG:HG3	3:D:48:ARG:HE	1.71	0.55
3:D:834:THR:OG1	3:D:835:SER:N	2.38	0.55
2:C:420:ARG:NH2	7:I:1:G:OP2	2.39	0.54
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.89	0.54
2:C:397:GLU:HG3	2:C:631:SER:HB2	1.88	0.54
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.87	0.54
3:D:462:GLN:HB2	3:D:513:ILE:HG21	1.90	0.54
2:C:259:GLY:HA2	2:C:263:ASP:HB2	1.90	0.54
3:D:959:GLU:N	3:D:959:GLU:OE1	2.40	0.54
3:D:618:LEU:HG	3:D:1467:ILE:HG23	1.90	0.54
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.90	0.53
3:D:809:PRO:HB3	3:D:839:LEU:HD13	1.90	0.53
3:D:1491:THR:O	3:D:1495:ILE:HG13	2.08	0.53
2:C:577:PRO:HG2	2:C:580:MET:HG2	1.90	0.53
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.91	0.53
2:C:243:ARG:NH2	8:H:9:DG:O6	2.39	0.53
3:D:850:LEU:HD12	3:D:884:ARG:NH2	2.24	0.53
2:C:221:LEU:HD11	2:C:307:LEU:HD21	1.90	0.52
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.91	0.52
3:D:477:LEU:HB2	3:D:496:LEU:HD13	1.91	0.52
3:D:1208:ASP:HB2	3:D:1215:VAL:HA	1.92	0.52
5:F:188:ILE:HD13	5:F:221:ILE:HG12	1.92	0.52
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.42	0.52
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.91	0.52
2:C:194:VAL:HG22	2:C:221:LEU:HD23	1.92	0.51
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.90	0.51
3:D:142:LEU:HB2	3:D:161:LEU:HD11	1.92	0.51
1:B:220:GLU:O	1:B:223:THR:OG1	2.25	0.51
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.76	0.51
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.93	0.51
3:D:1046:GLN:N	3:D:1046:GLN:OE1	2.42	0.51
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.92	0.51
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.92	0.50
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.93	0.50
1:A:32:PHE:HE1	1:B:47:SER:HG	1.59	0.50
1:A:206:THR:HG22	1:A:208:LEU:H	1.76	0.50
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.12	0.50
3:D:960:LYS:NZ	3:D:1063:GLU:OE2	2.40	0.50
1:A:32:PHE:HA	1:A:35:THR:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LEU:HD11	1:B:221:HIS:HB3	1.94	0.50
3:D:462:GLN:NE2	3:D:515:GLU:OE2	2.39	0.50
1:A:53:VAL:HG22	1:A:144:VAL:HG22	1.94	0.50
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.94	0.50
2:C:593:ALA:HB1	2:C:659:PRO:HD2	1.94	0.49
3:D:1147:ARG:NH2	3:D:1369:GLU:OE1	2.43	0.49
1:A:216:GLU:OE2	1:A:219:ARG:NH1	2.46	0.49
1:A:218:LEU:HG	1:B:222:LEU:HD11	1.93	0.49
3:D:233:LYS:NZ	3:D:240:GLU:OE2	2.29	0.49
3:D:821:VAL:HG11	3:D:827:ILE:HD12	1.95	0.49
2:C:15:LEU:O	2:C:586:ARG:NH2	2.41	0.49
3:D:244:GLU:HG3	3:D:310:LEU:HG	1.94	0.49
3:D:128:TYR:OH	3:D:579:ASP:OD2	2.24	0.49
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.27	0.49
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.95	0.49
3:D:784:ASP:HB2	3:D:939:PHE:HE1	1.78	0.49
3:D:657:LEU:HG	3:D:661:MET:HE2	1.95	0.48
2:C:1023:GLY:HA2	6:G:18:DG:OP2	2.12	0.48
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.94	0.48
3:D:1258:ARG:HH21	3:D:1351:GLU:HG2	1.77	0.48
2:C:168:ARG:HD3	2:C:268:ASP:HB3	1.94	0.48
2:C:203:ASP:OD1	2:C:204:GLN:N	2.43	0.48
2:C:614:ARG:NH1	2:C:618:GLY:O	2.46	0.48
3:D:1003:VAL:HG21	3:D:1041:LEU:HG	1.95	0.48
5:F:392:VAL:HB	5:F:396:ARG:HG2	1.94	0.48
6:G:9:DC:H1'	6:G:10:DC:H5'	1.94	0.48
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.96	0.48
8:H:20:DG:H2"	8:H:21:DA:C8	2.49	0.48
2:C:1031:ARG:HG2	6:G:16:DC:H5"	1.95	0.48
3:D:231:VAL:O	3:D:236:TYR:OH	2.31	0.48
2:C:719:PRO:HB3	2:C:820:ARG:NE	2.28	0.48
3:D:34:TYR:CZ	3:D:35:ARG:HG3	2.48	0.48
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.95	0.48
5:F:400:ILE:HG22	5:F:403:LYS:HE2	1.96	0.48
6:G:12:DT:H2'	6:G:13:DG:C8	2.49	0.47
3:D:141:ILE:HA	3:D:146:PRO:HA	1.96	0.47
3:D:475:LYS:O	3:D:479:GLU:HG2	2.15	0.47
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.95	0.47
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.14	0.47
3:D:1102:THR:HG21	3:D:1371:VAL:HG22	1.95	0.47
2:C:557:ARG:HG3	2:C:844:GLY:HA3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:171:LEU:HD22	3:D:390:PRO:HG2	1.95	0.47
2:C:773:LEU:HD23	5:F:354:LEU:HD22	1.96	0.47
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.45	0.47
3:D:191:LEU:HB3	3:D:393:ILE:HD12	1.97	0.47
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.97	0.47
3:D:897:TRP:CH2	3:D:902:LEU:HD22	2.50	0.47
1:B:124:ASN:OD1	1:B:124:ASN:N	2.48	0.47
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.80	0.47
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.96	0.47
8:H:13:DT:O2	8:H:13:DT:O4'	2.29	0.47
3:D:230:TRP:CD1	3:D:331:VAL:HG21	2.50	0.47
8:H:14:DG:H5"	8:H:14:DG:C8	2.45	0.47
2:C:351:LEU:HD12	2:C:375:SER:HA	1.97	0.46
3:D:841:TYR:HB2	3:D:864:VAL:HG22	1.96	0.46
1:A:20:TYR:OH	1:A:198:ARG:HD2	2.16	0.46
1:B:64:GLU:HA	1:B:165:ILE:HD13	1.96	0.46
3:D:1494:ALA:HB1	4:E:91:ARG:HH22	1.80	0.46
2:C:49:ARG:CZ	2:C:49:ARG:HB3	2.45	0.46
3:D:619:LEU:HD11	3:D:1439:SER:HB2	1.98	0.46
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.49	0.46
5:F:166:LEU:HD13	5:F:170:HIS:HB3	1.97	0.46
1:B:216:GLU:OE2	1:B:219:ARG:NH2	2.43	0.46
2:C:200:LEU:HD13	2:C:300:ASP:HB2	1.98	0.46
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.16	0.46
8:H:12:DC:C2'	8:H:13:DT:H5'	2.44	0.46
4:E:52:GLU:OE1	4:E:52:GLU:N	2.44	0.46
2:C:578:VAL:HG23	2:C:579:VAL:HG23	1.97	0.46
2:C:764:GLU:OE2	3:D:54:LYS:HE2	2.16	0.46
2:C:422:ARG:NH1	8:H:14:DG:H5'	2.31	0.46
3:D:129:PHE:O	5:F:83:GLN:NE2	2.49	0.46
5:F:237:THR:OG1	8:H:4:DA:H2'	2.15	0.46
4:E:83:ASP:O	4:E:87:LYS:HG2	2.16	0.46
3:D:1000:THR:HG23	3:D:1036:ARG:HD2	1.97	0.46
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.97	0.45
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.49	0.45
3:D:1485:GLN:NE2	4:E:82:GLU:OE1	2.46	0.45
5:F:397:ILE:HA	5:F:400:ILE:HG12	1.97	0.45
2:C:627:ARG:NE	2:C:639:GLN:O	2.49	0.45
3:D:455:ARG:HB2	3:D:460:ALA:HB2	1.98	0.45
6:G:7:DA:C8	6:G:8:DT:H72	2.51	0.45
2:C:427:VAL:HG22	8:H:15:DG:N2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:684:PHE:HB3	3:D:633:VAL:HG21	1.98	0.45
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.97	0.45
5:F:167:PRO:O	5:F:171:LYS:N	2.49	0.45
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.98	0.45
5:F:188:ILE:HG12	5:F:224:VAL:HG21	1.99	0.45
2:C:420:ARG:HD3	2:C:447:ALA:HB1	1.98	0.45
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.99	0.45
1:B:175:ARG:N	1:B:200:TRP:O	2.45	0.45
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.52	0.45
3:D:1462:LEU:HD23	3:D:1473:PRO:HD2	1.98	0.45
5:F:172:ARG:O	5:F:176:ILE:HG12	2.17	0.45
6:G:19:DA:H2"	6:G:20:DG:C8	2.52	0.45
2:C:740:GLU:HB3	2:C:805:ARG:NH1	2.31	0.45
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.98	0.45
3:D:270:LEU:HD12	3:D:284:LEU:HD11	1.99	0.45
3:D:784:ASP:HB2	3:D:939:PHE:CE1	2.52	0.45
4:E:83:ASP:OD1	4:E:83:ASP:N	2.49	0.45
3:D:703:ASN:HB2	3:D:713:ILE:HG12	1.99	0.45
2:C:1009:SER:HB3	3:D:651:GLU:O	2.17	0.44
3:D:658:LEU:HA	3:D:661:MET:HE3	1.98	0.44
2:C:886:LEU:HD21	3:D:951:ILE:HG12	1.98	0.44
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.52	0.44
3:D:1495:ILE:HG22	3:D:1499:ARG:HD2	1.99	0.44
2:C:10:ARG:NH1	2:C:12:VAL:HG12	2.32	0.44
3:D:26:VAL:HG11	3:D:44:LEU:HD23	2.00	0.44
3:D:248:PRO:HG3	3:D:308:LYS:HG3	1.99	0.44
3:D:536:ALA:HA	5:F:315:VAL:O	2.16	0.44
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.99	0.44
2:C:168:ARG:NH2	2:C:265:ARG:O	2.51	0.44
3:D:131:LYS:O	3:D:456:MET:HG2	2.18	0.44
2:C:437:ARG:NH2	2:C:491:GLU:OE1	2.45	0.44
2:C:1095:LEU:HD23	3:D:582:LEU:HD22	2.00	0.44
3:D:632:VAL:N	3:D:726:ILE:O	2.51	0.44
3:D:1464:GLU:OE1	3:D:1464:GLU:N	2.43	0.44
4:E:67:GLU:O	4:E:70:THR:OG1	2.28	0.44
1:A:107:LYS:HE3	1:A:107:LYS:HB2	1.84	0.44
1:A:206:THR:HB	1:A:209:GLU:HG3	2.00	0.44
2:C:872:ASN:ND2	3:D:784:ASP:OD2	2.42	0.44
5:F:164:LYS:HA	5:F:171:LYS:HE3	2.00	0.44
1:A:51:THR:OG1	1:A:87:VAL:O	2.26	0.44
1:B:58:ILE:HB	1:B:61:VAL:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.79	0.44
3:D:411:THR:HB	3:D:437:VAL:H	1.82	0.44
3:D:889:ALA:HB1	3:D:930:LEU:HA	2.00	0.44
4:E:66:LYS:O	4:E:70:THR:HG23	2.18	0.44
1:B:185:ARG:HB3	1:B:190:THR:HG23	2.00	0.43
3:D:114:THR:HG23	3:D:495:ARG:HG2	2.00	0.43
3:D:646:LYS:HB3	3:D:688:TRP:CZ3	2.53	0.43
3:D:654:LYS:O	3:D:658:LEU:HG	2.18	0.43
3:D:1152:GLU:HG3	3:D:1161:GLU:HA	2.00	0.43
1:A:100:LEU:HD23	1:A:141:GLU:HG2	2.00	0.43
2:C:218:VAL:O	2:C:222:MET:HG2	2.18	0.43
3:D:1462:LEU:HD22	3:D:1472:ILE:HB	2.00	0.43
3:D:561:GLY:HA2	5:F:140:ARG:HH11	1.83	0.43
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.53	0.43
3:D:939:PHE:O	3:D:943:THR:HG22	2.17	0.43
4:E:33:HIS:CE1	4:E:89:MET:HB3	2.53	0.43
3:D:17:LYS:HE3	3:D:17:LYS:HB2	1.72	0.43
3:D:573:MET:SD	5:F:210:LEU:HB3	2.58	0.43
5:F:278:LEU:HA	5:F:281:GLU:HG2	2.00	0.43
8:H:14:DG:C8	8:H:14:DG:OP2	2.70	0.43
2:C:351:LEU:HD11	2:C:373:VAL:HG13	2.01	0.43
3:D:185:VAL:HG11	3:D:191:LEU:HD11	2.00	0.43
3:D:580:ALA:HB1	3:D:591:VAL:HG11	2.00	0.43
5:F:373:LYS:HA	5:F:373:LYS:HD3	1.67	0.43
2:C:11:GLU:H	2:C:11:GLU:HG2	1.54	0.43
2:C:724:ARG:NH2	2:C:734:LEU:O	2.52	0.43
3:D:236:TYR:H	3:D:319:ALA:HB3	1.84	0.43
1:A:41:ARG:HA	1:A:177:VAL:HG11	2.01	0.43
2:C:605:LYS:HB3	2:C:610:ARG:NH1	2.33	0.43
3:D:314:PRO:HB2	3:D:317:VAL:HG12	2.00	0.43
3:D:438:ASP:OD2	3:D:441:ARG:NH1	2.52	0.43
5:F:372:ARG:HG2	5:F:386:VAL:HG21	2.01	0.43
3:D:808:THR:HB	3:D:810:GLU:HG2	2.00	0.43
5:F:201:LYS:NZ	5:F:244:ARG:HH12	2.17	0.43
2:C:503:LEU:HD23	2:C:508:ILE:HA	2.01	0.42
3:D:829:VAL:HG21	3:D:839:LEU:HD11	2.01	0.42
3:D:840:LYS:HE3	3:D:841:TYR:CZ	2.53	0.42
2:C:843:HIS:NE2	2:C:887:GLU:OE1	2.46	0.42
2:C:911:GLU:O	2:C:915:LYS:HG2	2.20	0.42
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	2.01	0.42
3:D:572:ARG:NH2	5:F:87:GLU:OE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1463:LYS:HE2	3:D:1463:LYS:HB3	1.86	0.42
2:C:165:LEU:HB2	2:C:168:ARG:HG3	2.00	0.42
2:C:258:TYR:O	2:C:263:ASP:N	2.53	0.42
3:D:1102:THR:O	3:D:1222:GLY:HA3	2.18	0.42
3:D:1387:SER:HB3	3:D:1407:LEU:HD11	2.01	0.42
1:A:11:PHE:O	1:B:228:PRO:HA	2.18	0.42
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.54	0.42
2:C:423:ALA:O	2:C:428:ARG:NH1	2.53	0.42
2:C:680:ASP:H	3:D:943:THR:HB	1.84	0.42
2:C:160:ALA:HB3	2:C:174:LEU:HB2	2.00	0.42
2:C:146:VAL:HG11	2:C:306:THR:HG22	2.00	0.42
2:C:540:PHE:HB3	2:C:544:THR:HB	2.01	0.42
3:D:689:ASP:O	3:D:693:GLU:HG3	2.19	0.42
3:D:1277:ILE:HG22	3:D:1278:ASP:H	1.83	0.42
5:F:364:ARG:HG2	5:F:390:PHE:CE1	2.55	0.42
1:A:36:LEU:HD23	1:A:36:LEU:HA	1.91	0.42
3:D:684:LYS:HE2	3:D:684:LYS:HB3	1.91	0.42
3:D:355:VAL:HG13	3:D:359:ALA:HB3	2.01	0.42
1:A:10:VAL:HG22	1:A:26:GLU:O	2.20	0.41
1:B:80:LEU:HB3	3:D:867:ARG:NH1	2.35	0.41
2:C:524:VAL:HG13	2:C:528:GLU:HB2	2.02	0.41
3:D:787:LEU:HD21	3:D:947:ILE:HG21	2.01	0.41
3:D:883:ALA:HA	3:D:900:ILE:HD13	2.02	0.41
4:E:46:PRO:HD2	4:E:63:TRP:CE2	2.55	0.41
1:B:32:PHE:HA	1:B:35:THR:HB	2.02	0.41
2:C:397:GLU:N	2:C:633:GLN:OE1	2.40	0.41
2:C:83:CYS:HA	2:C:88:LEU:HB2	2.02	0.41
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.55	0.41
3:D:541:ASN:O	3:D:545:ARG:HG3	2.20	0.41
1:B:10:VAL:HG22	1:B:26:GLU:O	2.21	0.41
1:B:179:PHE:HB3	1:B:197:LEU:HD13	2.02	0.41
2:C:103:LYS:H	2:C:103:LYS:HG3	1.60	0.41
3:D:214:GLU:HB3	3:D:340:THR:HB	2.02	0.41
5:F:209:PHE:CZ	5:F:213:ILE:HD11	2.55	0.41
2:C:12:VAL:HG21	2:C:472:ARG:HD3	2.02	0.41
2:C:133:ASP:HB3	2:C:395:LYS:HD2	2.03	0.41
3:D:1047:LYS:HG2	3:D:1053:PHE:CZ	2.55	0.41
2:C:551:GLU:HG2	2:C:552:HIS:CD2	2.56	0.41
2:C:598:GLU:O	2:C:651:LYS:HG3	2.21	0.41
2:C:1020:PRO:HD2	3:D:622:ARG:O	2.20	0.41
3:D:258:VAL:HG12	3:D:273:ARG:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:553:ARG:HD3	5:F:214:GLN:HB3	2.03	0.41
1:A:133:GLU:HG2	1:A:134:GLU:N	2.35	0.41
2:C:132:ALA:HB1	2:C:394:PHE:HE1	1.84	0.41
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.76	0.41
3:D:685:ASP:HA	3:D:688:TRP:HD1	1.86	0.41
3:D:919:PHE:CE2	3:D:924:MET:HG2	2.55	0.41
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.53	0.41
5:F:270:LYS:HG2	5:F:295:MET:HE1	2.01	0.41
8:H:7:DG:H5'	8:H:7:DG:H8	1.86	0.41
1:B:111:ALA:HB3	1:B:125:PRO:HA	2.03	0.41
2:C:1032:PHE:HZ	2:C:1040:LEU:HG	1.86	0.41
3:D:1112:CYS:HB3	3:D:1196:THR:OG1	2.21	0.41
2:C:229:MET:HB2	2:C:233:GLU:HB2	2.02	0.40
2:C:439:CYS:HB2	2:C:541:SER:HB3	2.03	0.40
2:C:846:LYS:NZ	7:I:4:G:OP1	2.44	0.40
3:D:45:PHE:CD1	3:D:522:PRO:HB3	2.56	0.40
4:E:68:LEU:HD12	4:E:68:LEU:HA	1.92	0.40
2:C:684:PHE:HE1	3:D:783:ARG:HB2	1.87	0.40
2:C:708:TYR:OH	2:C:796:GLU:OE1	2.28	0.40
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.57	0.40
2:C:974:LEU:HD12	2:C:974:LEU:HA	1.96	0.40
3:D:90:MET:SD	3:D:521:PRO:HD3	2.61	0.40
3:D:206:ARG:HA	3:D:206:ARG:HH11	1.86	0.40
3:D:298:VAL:HG12	3:D:302:GLN:NE2	2.35	0.40
3:D:796:ARG:NH1	3:D:862:ASP:OD1	2.54	0.40
3:D:989:TYR:CZ	3:D:993:LEU:HD11	2.57	0.40
3:D:1046:GLN:HA	3:D:1052:THR:HA	2.04	0.40
3:D:792:ILE:HG13	3:D:793:THR:HG23	2.03	0.40
3:D:890:VAL:HB	3:D:922:LEU:HD13	2.03	0.40
5:F:81:VAL:HB	8:H:8:DG:N1	2.37	0.40
2:C:535:SER:O	2:C:538:GLN:HG2	2.21	0.40
2:C:1070:ILE:CG2	3:D:655:PRO:HB2	2.52	0.40
3:D:1084:THR:O	3:D:1088:THR:HG23	2.21	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	224/315 (71%)	219 (98%)	5 (2%)	0	100 100
1	B	220/315 (70%)	215 (98%)	5 (2%)	0	100 100
2	C	1107/1119 (99%)	1082 (98%)	23 (2%)	2 (0%)	47 78
3	D	1482/1524 (97%)	1449 (98%)	31 (2%)	2 (0%)	51 83
4	E	92/99 (93%)	91 (99%)	1 (1%)	0	100 100
5	F	344/443 (78%)	338 (98%)	6 (2%)	0	100 100
All	All	3469/3815 (91%)	3394 (98%)	71 (2%)	4 (0%)	51 83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	592	LEU
3	D	1440	PHE
2	C	215	GLY
3	D	530	VAL

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%)	192 (96%)	7 (4%)	36 63
1	B	195/273 (71%)	190 (97%)	5 (3%)	46 70
2	C	936/941 (100%)	885 (95%)	51 (5%)	22 54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	D	1253/1279 (98%)	1185 (95%)	68 (5%)	22 54
4	E	83/88 (94%)	82 (99%)	1 (1%)	71 84
5	F	301/388 (78%)	289 (96%)	12 (4%)	31 60
All	All	2967/3242 (92%)	2823 (95%)	144 (5%)	25 55

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	34	VAL
1	A	67	THR
1	A	142	VAL
1	A	193	ASP
1	A	219	ARG
1	A	229	GLN
1	B	34	VAL
1	B	80	LEU
1	B	94	LEU
1	B	186	LEU
1	B	206	THR
2	C	8	ARG
2	C	11	GLU
2	C	15	LEU
2	C	56	GLU
2	C	81	ASP
2	C	97	ARG
2	C	103	LYS
2	C	133	ASP
2	C	141	HIS
2	C	177	GLU
2	C	205	GLU
2	C	218	VAL
2	C	221	LEU
2	C	232	GLU
2	C	251	ASP
2	C	274	ARG
2	C	342	ASP
2	C	358	ARG
2	C	372	LEU
2	C	402	SER
2	C	409	ARG

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Mol	Chain	Res	Type
2	C	418	LEU
2	C	427	VAL
2	C	429	ASP
2	C	434	HIS
2	C	464	LEU
2	C	480	THR
2	C	512	ARG
2	C	610	ARG
2	C	617	ASP
2	C	633	GLN
2	C	638	ASP
2	C	640	ARG
2	C	648	ARG
2	C	680	ASP
2	C	715	THR
2	C	774	LEU
2	C	775	ARG
2	C	786	LYS
2	C	807	ARG
2	C	808	ARG
2	C	813	VAL
2	C	820	ARG
2	C	830	LYS
2	C	928	LYS
2	C	939	ARG
2	C	952	LEU
2	C	968	LEU
2	C	978	ARG
2	C	1001	VAL
2	C	1058	ASP
3	D	67	ARG
3	D	68	PHE
3	D	80	VAL
3	D	81	THR
3	D	135	LEU
3	D	141	ILE
3	D	155	ASP
3	D	161	LEU
3	D	190	GLU
3	D	191	LEU
3	D	198	ARG
3	D	230	TRP

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Mol	Chain	Res	Type
3	D	231	VAL
3	D	256	GLU
3	D	270	LEU
3	D	275	GLU
3	D	276	ASP
3	D	312	ARG
3	D	331	VAL
3	D	362	GLU
3	D	372	ASP
3	D	411	THR
3	D	415	VAL
3	D	486	ARG
3	D	500	ARG
3	D	525	ARG
3	D	576	GLU
3	D	586	ARG
3	D	591	VAL
3	D	618	LEU
3	D	650	LEU
3	D	669	ASN
3	D	709	HIS
3	D	754	PHE
3	D	778	LEU
3	D	817	GLU
3	D	832	ARG
3	D	864	VAL
3	D	867	ARG
3	D	894	LYS
3	D	904	VAL
3	D	943	THR
3	D	971	LEU
3	D	983	LEU
3	D	984	THR
3	D	1041	LEU
3	D	1062	ARG
3	D	1127	GLU
3	D	1128	VAL
3	D	1130	ARG
3	D	1155	VAL
3	D	1162	GLU
3	D	1188	VAL
3	D	1195	GLN

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Mol	Chain	Res	Type
3	D	1219	GLU
3	D	1277	ILE
3	D	1284	GLU
3	D	1287	GLU
3	D	1288	GLU
3	D	1290	LEU
3	D	1304	LYS
3	D	1305	LEU
3	D	1313	VAL
3	D	1317	ASP
3	D	1455	LYS
3	D	1493	LYS
3	D	1496	GLU
3	D	1501	GLU
4	E	50	THR
5	F	88	ILE
5	F	141	VAL
5	F	150	THR
5	F	172	ARG
5	F	186	HIS
5	F	205	ARG
5	F	218	GLN
5	F	287	THR
5	F	364	ARG
5	F	377	ASP
5	F	417	LYS
5	F	422	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	350	HIS
3	D	1172	HIS
3	D	1195	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	I	3/4 (75%)	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 7 ligands modelled in this entry, 7 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	226/315 (71%)	-0.07	5 (2%) 62 56	113, 141, 165, 179	0
1	B	222/315 (70%)	-0.18	0 100 100	105, 148, 179, 195	0
2	C	1111/1119 (99%)	0.23	40 (3%) 42 37	83, 151, 200, 219	0
3	D	1486/1524 (97%)	0.26	74 (4%) 28 26	90, 142, 197, 245	1 (0%)
4	E	94/99 (94%)	-0.04	1 (1%) 80 77	123, 166, 198, 211	0
5	F	346/443 (78%)	0.26	20 (5%) 23 19	112, 160, 213, 223	0
6	G	15/20 (75%)	-0.27	1 (6%) 17 14	130, 168, 224, 224	0
7	I	4/4 (100%)	1.32	0 100 100	155, 174, 199, 203	0
8	H	23/27 (85%)	0.10	0 100 100	168, 198, 281, 298	0
All	All	3527/3866 (91%)	0.19	141 (3%) 38 33	83, 149, 201, 298	1 (0%)

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	367	ILE	7.7
3	D	289	THR	6.9
3	D	305	ALA	6.8
3	D	322	VAL	6.5
3	D	355	VAL	6.5
3	D	409	VAL	6.0
3	D	337	LEU	5.9
2	C	776	SER	5.9
3	D	269	PHE	5.7
3	D	445	ARG	5.5
3	D	368	VAL	5.4
3	D	203	ALA	5.4
2	C	66	LEU	5.2
3	D	444	VAL	5.0
3	D	324	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
3	D	220	ARG	4.7
5	F	404	ALA	4.3
2	C	777	ILE	4.3
3	D	290	PRO	4.1
5	F	381	HIS	4.1
3	D	335	LEU	4.0
5	F	390	PHE	3.9
3	D	262	LYS	3.8
3	D	321	GLN	3.8
5	F	400	ILE	3.8
1	A	131	THR	3.8
3	D	268	ALA	3.8
3	D	353	VAL	3.8
2	C	773	LEU	3.8
3	D	282	TYR	3.8
2	C	68	PHE	3.7
3	D	1488	ASP	3.7
1	A	4	SER	3.7
3	D	352	ASN	3.7
3	D	1054	GLU	3.6
3	D	291	LEU	3.5
2	C	174	LEU	3.4
3	D	219	GLU	3.4
5	F	421	PHE	3.4
3	D	384	VAL	3.3
2	C	823	VAL	3.3
2	C	221	LEU	3.2
5	F	386	VAL	3.2
3	D	306	GLU	3.2
5	F	422	LEU	3.2
3	D	393	ILE	3.1
2	C	372	LEU	3.1
3	D	165	LYS	3.0
5	F	407	LYS	3.0
3	D	1288	GLU	2.9
2	C	48	PHE	2.9
3	D	443	VAL	2.9
5	F	397	ILE	2.9
5	F	391	GLY	2.8
5	F	408	LEU	2.8
3	D	360	ARG	2.8
2	C	367	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	207	LEU	2.8
3	D	202	VAL	2.8
3	D	421	LEU	2.8
5	F	229	TYR	2.7
3	D	304	LEU	2.7
2	C	306	THR	2.7
2	C	159	ILE	2.7
3	D	323	GLU	2.7
5	F	389	PHE	2.6
3	D	211	VAL	2.6
2	C	99	GLN	2.6
3	D	407	VAL	2.6
5	F	418	LEU	2.6
3	D	1312	LEU	2.6
2	C	766	GLU	2.6
3	D	223	LEU	2.6
5	F	375	LEU	2.6
5	F	235	PHE	2.5
2	C	344	PHE	2.5
3	D	295	GLY	2.5
3	D	350	HIS	2.5
3	D	267	GLY	2.5
3	D	307	ALA	2.5
3	D	371	ILE	2.5
3	D	314	PRO	2.5
3	D	343	LYS	2.4
2	C	511	GLU	2.4
2	C	148	PHE	2.4
1	A	73	GLU	2.4
3	D	422	ALA	2.4
2	C	158	TYR	2.4
2	C	778	PHE	2.4
3	D	675	ARG	2.4
2	C	281	LEU	2.4
3	D	292	VAL	2.4
5	F	392	VAL	2.4
2	C	65	VAL	2.3
2	C	115	LEU	2.3
3	D	436	GLU	2.3
6	G	20	DG	2.3
3	D	336	PHE	2.3
1	A	55	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	510	ALA	2.3
3	D	666	ILE	2.3
3	D	446	VAL	2.3
3	D	1319	VAL	2.3
3	D	402	PRO	2.3
2	C	594	ALA	2.2
3	D	288	MET	2.2
2	C	780	GLU	2.2
2	C	176	VAL	2.2
4	E	89	MET	2.2
5	F	78	SER	2.2
3	D	261	LEU	2.2
3	D	437	VAL	2.2
3	D	226	PRO	2.2
3	D	980	MET	2.2
3	D	1313	VAL	2.2
5	F	396	ARG	2.2
3	D	204	LEU	2.2
2	C	226	VAL	2.2
2	C	769	PRO	2.2
3	D	333	LEU	2.2
2	C	303	PHE	2.2
3	D	361	VAL	2.2
2	C	373	VAL	2.1
3	D	668	PRO	2.1
2	C	101	ILE	2.1
3	D	971	LEU	2.1
3	D	309	GLY	2.1
2	C	282	GLY	2.1
3	D	270	LEU	2.1
2	C	300	ASP	2.1
5	F	393	THR	2.1
1	A	85	LEU	2.1
2	C	191	PHE	2.0
3	D	161	LEU	2.0
2	C	184	MET	2.0
3	D	410	SER	2.0
2	C	67	ASP	2.0
3	D	379	ALA	2.0
2	C	418	LEU	2.0
3	D	395	VAL	2.0
2	C	311	PHE	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	2002	1/1	0.74	0.48	92,92,92,92	0
9	MG	B	2001	1/1	0.83	0.38	139,139,139,139	0
10	ZN	D	2002	1/1	0.90	0.06	197,197,197,197	0
9	MG	F	2001	1/1	0.91	0.08	147,147,147,147	0
9	MG	D	2004	1/1	0.91	0.27	149,149,149,149	0
10	ZN	D	2001	1/1	0.95	0.22	123,123,123,123	0
9	MG	D	2003	1/1	0.98	0.40	98,98,98,98	0

6.5 Other polymers (i)

There are no such residues in this entry.