



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 23, 2024 – 04:12 PM JST

PDB ID : 8Y0C
Title : Crystal structure of FnCas12a in complex with pre-crRNA and 18nt target DNA
Authors : Chen, J.; Liu, L.
Deposited on : 2024-01-22
Resolution : 3.45 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 ⓘ 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)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

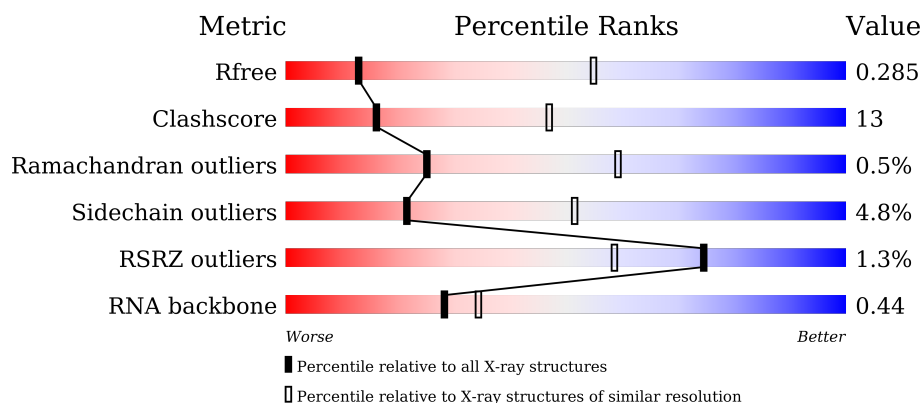
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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}	164625	1597 (3.52-3.40)
Clashscore	180529	1041 (3.50-3.42)
Ramachandran outliers	177936	1026 (3.50-3.42)
Sidechain outliers	177891	1027 (3.50-3.42)
RSRZ outliers	164620	1596 (3.52-3.40)
RNA backbone	3690	1057 (3.92-3.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	58	
2	C	27	
3	D	11	
4	A	1300	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12057 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 RNA chain called RNA (42-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	42	Total	C	N	O	P	0	0	0
			890	400	155	294	41			

- Molecule 2 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	27	Total	C	N	O	P	0	0	0
			550	265	95	163	27			

- Molecule 3 is a DNA chain called DNA (5'-D(P*AP*GP*TP*CP*CP*TP*TP*AP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	11	Total	C	N	O	P	0	0	0
			221	107	34	69	11			

- Molecule 4 is a protein called CRISPR-associated endonuclease Cas12a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1260	Total	C	N	O	S	0	0	0
			10392	6681	1711	1978	22			

There is a discrepancy between the modelled and reference sequences:

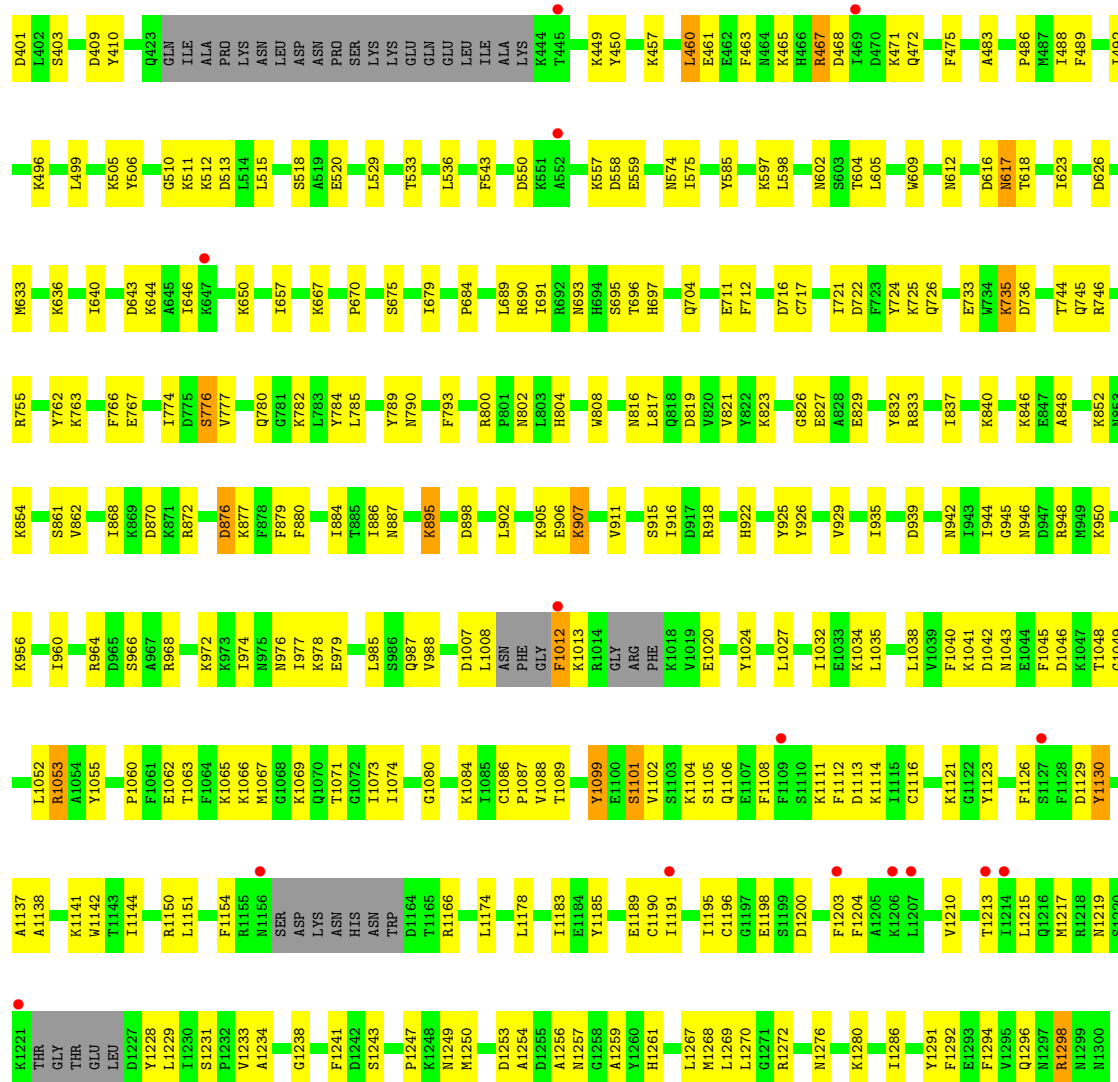
Chain	Residue	Modelled	Actual	Comment	Reference
A	1006	ALA	GLU	conflict	UNP A0Q7Q2

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Mg	0	0
			2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	O	0	0
			2	2		



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	124.28Å 124.28Å 268.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.22 – 3.45 47.22 – 3.45	Depositor EDS
% Data completeness (in resolution range)	88.9 (47.22-3.45) 88.8 (47.22-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.216 , 0.285 0.217 , 0.285	Depositor DCC
R_{free} test set	1394 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	12057	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	B	0.89	0/995	1.80	36/1548 (2.3%)
2	C	1.15	1/615 (0.2%)	1.17	2/946 (0.2%)
3	D	1.15	1/245 (0.4%)	1.25	1/375 (0.3%)
4	A	0.55	0/10595	0.71	3/14220 (0.0%)
All	All	0.64	2/12450 (0.0%)	0.90	42/17089 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	-3	DT	C3'-O3'	-7.79	1.33	1.44
3	D	0	DC	C3'-O3'	-5.93	1.36	1.44

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	C	C2-N1-C1'	9.34	129.07	118.80
1	B	-10	U	N3-C2-O2	-8.90	115.97	122.20
1	B	4	A	C8-N9-C4	8.30	109.12	105.80
1	B	-11	C	C6-N1-C2	-8.05	117.08	120.30
1	B	-19	A	N1-C6-N6	-7.47	114.12	118.60
1	B	-10	U	P-O3'-C3'	7.45	128.64	119.70
1	B	20	C	N1-C2-O2	7.10	123.16	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	-10	U	N1-C2-O2	7.00	127.70	122.80
1	B	-14	C	C6-N1-C2	-6.78	117.59	120.30
1	B	-14	C	N3-C4-C5	-6.63	119.25	121.90
1	B	20	C	C6-N1-C1'	-6.44	113.07	120.80
1	B	0	G	O4'-C1'-N9	6.39	113.32	108.20
1	B	9	U	N1-C2-O2	-6.18	118.47	122.80
1	B	-17	U	N3-C4-C5	-6.13	110.92	114.60
1	B	18	G	N3-C4-C5	-6.13	125.54	128.60
1	B	20	C	C6-N1-C2	-6.11	117.86	120.30
1	B	-19	A	C5-C6-N6	5.91	128.43	123.70
1	B	-8	U	N1-C2-N3	5.88	118.43	114.90
1	B	7	C	N1-C2-O2	-5.82	115.41	118.90
4	A	460	LEU	CA-CB-CG	5.79	128.62	115.30
1	B	3	A	C2-N3-C4	-5.79	107.70	110.60
1	B	-3	G	C4-N9-C1'	-5.71	119.07	126.50
1	B	-15	U	N1-C2-O2	-5.53	118.93	122.80
1	B	14	U	C6-N1-C2	-5.53	117.68	121.00
1	B	3	A	N1-C6-N6	5.48	121.89	118.60
1	B	20	C	C5-C6-N1	5.42	123.71	121.00
1	B	4	A	N9-C4-C5	-5.41	103.64	105.80
1	B	7	C	N3-C2-O2	5.38	125.67	121.90
3	D	-7	DT	N3-C4-O4	5.36	123.12	119.90
1	B	-3	G	N3-C4-N9	-5.35	122.79	126.00
1	B	-3	G	N3-C4-C5	5.30	131.25	128.60
1	B	-18	A	O5'-P-OP2	5.30	117.06	110.70
1	B	7	C	C5-C6-N1	5.29	123.64	121.00
2	C	-4	DT	N3-C4-O4	5.28	123.06	119.90
1	B	-8	U	C4-C5-C6	5.26	122.85	119.70
1	B	20	C	N3-C2-O2	-5.24	118.23	121.90
1	B	-3	G	C8-N9-C1'	5.22	133.78	127.00
1	B	4	A	C4-C5-C6	-5.20	114.40	117.00
1	B	0	G	N3-C4-C5	-5.10	126.05	128.60
4	A	324	LEU	CA-CB-CG	5.05	126.92	115.30
4	A	617	ASN	C-N-CA	-5.05	109.08	121.70
2	C	-15	DT	O4'-C4'-C3'	-5.03	102.49	104.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	789	TYR	Peptide

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	B	890	0	449	17	0
2	C	550	0	308	4	0
3	D	221	0	127	7	0
4	A	10392	0	10350	289	1
5	B	2	0	0	0	0
6	A	2	0	0	1	0
All	All	12057	0	11234	301	1

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 13.

All (301) 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)
4:A:371:LYS:HE2	4:A:489:PHE:HB3	1.47	0.93
1:B:19:C:N3	1:B:21:G:N2	2.20	0.89
4:A:518:SER:O	6:A:1401:HOH:O	1.95	0.85
4:A:960:ILE:HG22	4:A:977:ILE:HD12	1.63	0.81
2:C:0:DC:H4'	4:A:827:GLU:HG3	1.63	0.81
4:A:1063:THR:HG22	4:A:1065:LYS:H	1.46	0.79
4:A:1062:GLU:HG2	4:A:1063:THR:H	1.46	0.79
1:B:-15:U:OP1	4:A:833:ARG:NH2	2.16	0.79
4:A:396:ASP:HB3	4:A:398:SER:H	1.47	0.78
4:A:342:LEU:HD22	4:A:347:ASP:HB3	1.64	0.77
4:A:1102:VAL:O	4:A:1106:GLN:HG3	1.85	0.76
4:A:533:THR:CG2	4:A:575:ILE:HD12	2.17	0.75
4:A:895:LYS:HE3	4:A:898:ASP:OD2	1.85	0.75
4:A:1101:SER:HB3	4:A:1104:LYS:HE3	1.67	0.74
4:A:533:THR:HB	4:A:575:ILE:CD1	2.18	0.74
4:A:390:LYS:HB3	4:A:558:ASP:HB2	1.70	0.73
4:A:533:THR:HG22	4:A:575:ILE:HD12	1.69	0.73
4:A:1267:LEU:HD12	4:A:1294:PHE:HZ	1.54	0.73
4:A:944:ILE:HG21	4:A:987:GLN:HG2	1.69	0.73
4:A:643:ASP:HA	4:A:646:ILE:HG12	1.71	0.72
4:A:650:LYS:NZ	4:A:767:GLU:OE2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:373:THR:O	4:A:377:LEU:HD13	1.91	0.70
4:A:55:ASP:OD1	4:A:186:ARG:NH1	2.25	0.70
4:A:618:THR:HG21	4:A:633:MET:O	1.91	0.69
4:A:670:PRO:HG3	4:A:724:TYR:OH	1.92	0.69
4:A:1099:TYR:HE2	4:A:1204:PHE:HB2	1.57	0.68
3:D:O:DC:C2	4:A:667:LYS:HE2	2.28	0.68
4:A:1048:THR:HA	4:A:1053:ARG:HB3	1.74	0.68
4:A:275:GLN:HG2	4:A:332:THR:OG1	1.93	0.68
4:A:964:ARG:HD2	4:A:977:ILE:HD11	1.75	0.68
4:A:289:PHE:CE1	4:A:296:LYS:HB2	2.27	0.68
4:A:1045:PHE:CE2	4:A:1052:LEU:HD13	2.28	0.68
4:A:905:LYS:NZ	4:A:1276:ASN:O	2.28	0.67
4:A:356:TYR:HB3	4:A:496:LYS:HD2	1.77	0.66
4:A:533:THR:HB	4:A:575:ILE:HD11	1.76	0.66
4:A:1154:PHE:HE1	4:A:1166:ARG:HB3	1.60	0.66
4:A:87:LYS:NZ	4:A:213:GLU:OE2	2.27	0.66
4:A:180:LYS:HG3	4:A:181:GLY:N	2.10	0.66
4:A:821:VAL:HG23	4:A:887:ASN:HA	1.77	0.65
4:A:275:GLN:OE1	4:A:330:SER:OG	2.13	0.65
4:A:400:THR:HG23	4:A:410:TYR:HB2	1.78	0.64
4:A:960:ILE:CG2	4:A:977:ILE:HD12	2.28	0.64
4:A:1089:THR:HG21	4:A:1233:VAL:HG12	1.80	0.64
4:A:51:LYS:HD2	4:A:182:PHE:CD1	2.33	0.64
4:A:1189:GLU:OE2	4:A:1189:GLU:N	2.22	0.63
4:A:218:TYR:O	4:A:222:LYS:HG3	1.99	0.62
4:A:722:ASP:O	4:A:726:GLN:HG3	1.98	0.62
4:A:916:ILE:O	4:A:1024:TYR:OH	2.15	0.62
4:A:460:LEU:HD11	4:A:475:PHE:HB2	1.81	0.62
4:A:1086:CYS:HG	4:A:1231:SER:HG	1.21	0.61
4:A:1099:TYR:HE2	4:A:1204:PHE:CB	2.13	0.61
1:B:16:A:O2'	4:A:298:LYS:NZ	2.33	0.61
4:A:243:THR:HG23	4:A:255:GLN:HG3	1.83	0.61
4:A:57:TYR:HB2	4:A:141:TRP:CE3	2.36	0.60
4:A:282:ASN:OD1	4:A:323:VAL:HG13	2.02	0.60
4:A:602:ASN:ND2	4:A:616:ASP:O	2.18	0.60
4:A:1195:ILE:HG22	4:A:1203:PHE:CZ	2.37	0.59
4:A:64:GLU:OE2	4:A:118:LYS:HD2	2.02	0.59
4:A:1067:MET:HG3	4:A:1071:THR:HG22	1.84	0.59
4:A:1267:LEU:HD12	4:A:1294:PHE:CZ	2.36	0.59
4:A:467:ARG:HH11	4:A:472:GLN:HA	1.67	0.59
4:A:145:SER:HB3	4:A:150:ILE:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:837:ILE:HD11	4:A:870:ASP:HB2	1.85	0.59
4:A:1292:PHE:O	4:A:1296:GLN:HB2	2.03	0.59
4:A:693:ASN:HA	4:A:704:GLN:HB2	1.85	0.58
4:A:1130:TYR:HB3	4:A:1138:ALA:HB1	1.84	0.58
1:B:-2:A:OP2	4:A:1041:LYS:HE3	2.03	0.58
4:A:121:ASN:HA	4:A:124:ASN:HD21	1.68	0.58
4:A:282:ASN:CG	4:A:323:VAL:HG13	2.23	0.58
4:A:27:THR:HG21	4:A:785:LEU:H	1.68	0.58
4:A:640:ILE:HD11	4:A:782:LYS:HB3	1.86	0.58
1:B:-17:U:H2'	4:A:872:ARG:HD3	1.86	0.57
4:A:160:THR:OG1	4:A:161:ASP:N	2.37	0.57
4:A:520:GLU:HG3	4:A:972:LYS:HG2	1.86	0.57
4:A:125:GLN:HA	4:A:176:THR:HG21	1.86	0.57
4:A:1247:PRO:HB2	4:A:1249:ASN:OD1	2.05	0.57
4:A:380:ASP:HB3	4:A:386:LEU:CD2	2.35	0.57
4:A:381:LEU:HD23	4:A:386:LEU:HB2	1.87	0.57
4:A:623:ILE:HG13	4:A:657:ILE:HD11	1.87	0.57
4:A:717:CYS:O	4:A:721:ILE:HG13	2.05	0.57
4:A:722:ASP:OD2	4:A:744:THR:HG21	2.05	0.57
4:A:371:LYS:HE2	4:A:489:PHE:CB	2.30	0.56
4:A:774:ILE:O	4:A:777:VAL:HG12	2.05	0.56
4:A:352:MET:CE	4:A:499:LEU:HD21	2.35	0.56
4:A:612:ASN:ND2	4:A:733:GLU:OE1	2.33	0.56
4:A:945:GLY:CA	4:A:946:ASN:HB2	2.34	0.56
4:A:1210:VAL:HA	4:A:1213:THR:HG22	1.87	0.56
4:A:690:ARG:NH2	4:A:716:ASP:OD1	2.36	0.56
4:A:1144:ILE:HD12	4:A:1215:LEU:HD21	1.87	0.56
4:A:20:GLU:OE2	4:A:877:LYS:HD3	2.06	0.55
4:A:776:SER:O	4:A:780:GLN:HG3	2.06	0.55
4:A:61:PHE:CE1	4:A:65:ILE:HD13	2.42	0.55
4:A:235:LYS:CE	4:A:259:SER:HA	2.37	0.55
4:A:657:ILE:HG13	4:A:766:PHE:CE1	2.41	0.55
4:A:1045:PHE:CZ	4:A:1052:LEU:HD13	2.42	0.54
4:A:925:TYR:CZ	4:A:1256:ALA:HB2	2.43	0.54
4:A:113:ILE:CD1	4:A:190:TYR:HB3	2.38	0.54
4:A:240:GLU:HB3	4:A:241:GLU:OE2	2.08	0.54
4:A:1130:TYR:CD1	4:A:1138:ALA:HB1	2.43	0.54
4:A:121:ASN:HA	4:A:124:ASN:ND2	2.22	0.54
4:A:604:THR:O	4:A:617:ASN:HA	2.08	0.54
4:A:1067:MET:SD	4:A:1071:THR:HG21	2.48	0.54
4:A:356:TYR:CZ	4:A:529:LEU:HD22	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:-11:DA:H2'	2:C:-10:DA:C8	2.43	0.54
4:A:877:LYS:HB2	4:A:879:PHE:CE2	2.42	0.54
4:A:457:LYS:O	4:A:461:GLU:HB2	2.08	0.53
4:A:1229:LEU:HB2	4:A:1254:ALA:HB2	1.91	0.53
4:A:170:LYS:O	4:A:173:LYS:HG3	2.09	0.53
4:A:922:HIS:HA	4:A:942:ASN:HD21	1.73	0.53
4:A:343:GLU:O	4:A:512:LYS:HD2	2.09	0.53
4:A:1086:CYS:SG	4:A:1231:SER:OG	2.49	0.53
4:A:926:TYR:CE2	4:A:939:ASP:HB3	2.43	0.53
4:A:1269:LEU:CD1	4:A:1286:ILE:HD11	2.39	0.53
4:A:906:GLU:HG3	4:A:907:LYS:HD3	1.90	0.53
4:A:1228:TYR:HB2	4:A:1243:SER:OG	2.09	0.52
4:A:275:GLN:OE1	4:A:326:LYS:HB2	2.08	0.52
4:A:91:ASP:O	4:A:94:LEU:HB2	2.10	0.52
3:D:-4:DT:OP1	4:A:176:THR:OG1	2.26	0.52
3:D:0:DC:O2	4:A:667:LYS:HE2	2.09	0.52
4:A:533:THR:HB	4:A:575:ILE:HD12	1.92	0.52
1:B:-8:U:O4	4:A:861:SER:HB3	2.10	0.52
4:A:512:LYS:HA	4:A:585:TYR:OH	2.09	0.52
4:A:1183:ILE:HD11	4:A:1198:GLU:OE2	2.09	0.52
4:A:1121:LYS:HB3	4:A:1123:TYR:CE1	2.46	0.51
4:A:146:LYS:HE2	4:A:163:ASP:OD1	2.11	0.51
4:A:381:LEU:HD11	4:A:391:ILE:HD13	1.92	0.51
4:A:916:ILE:HA	4:A:925:TYR:O	2.10	0.51
4:A:964:ARG:HD2	4:A:977:ILE:CD1	2.39	0.51
4:A:229:ILE:HG13	4:A:231:TYR:CE1	2.46	0.51
4:A:533:THR:CB	4:A:575:ILE:HD12	2.41	0.51
4:A:11:TYR:CE1	4:A:1060:PRO:HG3	2.46	0.50
4:A:911:VAL:CG2	4:A:1270:LEU:HD11	2.41	0.50
4:A:166:LEU:O	4:A:170:LYS:HD3	2.11	0.50
4:A:27:THR:HG21	4:A:785:LEU:N	2.26	0.50
4:A:1112:PHE:CE1	4:A:1126:PHE:HB3	2.46	0.50
4:A:1269:LEU:HD13	4:A:1286:ILE:HD11	1.94	0.50
4:A:675:SER:O	4:A:679:ILE:N	2.43	0.50
4:A:876:ASP:OD1	4:A:876:ASP:N	2.43	0.49
1:B:-1:U:O4	4:A:802:ASN:HB3	2.12	0.49
4:A:840:LYS:O	4:A:868:ILE:HG23	2.12	0.49
4:A:1234:ALA:HB1	4:A:1238:GLY:HA2	1.94	0.49
4:A:380:ASP:HB3	4:A:386:LEU:HD23	1.94	0.49
4:A:684:PRO:HB2	4:A:689:LEU:HD22	1.94	0.49
4:A:1195:ILE:HG22	4:A:1203:PHE:HZ	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:21:LEU:HD21	4:A:880:PHE:HB2	1.95	0.49
4:A:48:LYS:O	4:A:52:GLN:HG3	2.12	0.49
4:A:461:GLU:O	4:A:465:LYS:HG3	2.12	0.49
4:A:945:GLY:HA2	4:A:946:ASN:HB2	1.94	0.49
4:A:1007:ASP:O	4:A:1008:LEU:HG	2.13	0.49
4:A:85:LYS:HE3	4:A:94:LEU:HD21	1.95	0.49
4:A:985:LEU:HD22	4:A:1027:LEU:HB2	1.94	0.49
4:A:1032:ILE:HG12	4:A:1074:ILE:HD12	1.94	0.49
4:A:1043:ASN:HD22	4:A:1049:GLY:HA3	1.77	0.48
4:A:213:GLU:O	4:A:217:LYS:HG3	2.12	0.48
4:A:113:ILE:HD11	4:A:190:TYR:HB3	1.95	0.48
4:A:1012:PHE:HB2	4:A:1080:GLY:HA2	1.95	0.48
1:B:-11:C:H5'	4:A:852:LYS:HD2	1.96	0.48
4:A:382:LYS:HE3	4:A:483:ALA:CB	2.42	0.48
4:A:1151:LEU:HB2	4:A:1219:ASN:HB3	1.94	0.48
4:A:34:ARG:HH12	4:A:636:LYS:HE3	1.78	0.48
1:B:21:G:H1'	1:B:22:U:H5''	1.96	0.47
4:A:657:ILE:HG13	4:A:766:PHE:HE1	1.78	0.47
4:A:293:GLU:OE2	4:A:297:ARG:NH1	2.44	0.47
4:A:345:ASP:HB3	4:A:506:TYR:HB3	1.96	0.47
4:A:725:LYS:HE3	4:A:744:THR:HG22	1.96	0.47
4:A:925:TYR:CD2	4:A:926:TYR:N	2.82	0.47
4:A:159:ILE:HA	4:A:164:GLU:OE1	2.15	0.47
4:A:711:GLU:HG2	4:A:712:PHE:H	1.79	0.47
4:A:976:ASN:C	4:A:977:ILE:HD13	2.35	0.47
4:A:1088:VAL:HG23	4:A:1089:THR:HG23	1.97	0.47
4:A:1113:ASP:O	4:A:1114:LYS:HG2	2.14	0.47
4:A:308:SER:OG	4:A:313:ASP:O	2.24	0.47
4:A:275:GLN:HG3	4:A:275:GLN:O	2.14	0.47
4:A:762:TYR:CZ	4:A:823:LYS:HG2	2.50	0.47
4:A:386:LEU:HD13	4:A:386:LEU:HA	1.78	0.47
4:A:403:SER:OG	4:A:409:ASP:O	2.31	0.46
4:A:697:HIS:CD2	4:A:697:HIS:H	2.33	0.46
4:A:1111:LYS:HE3	4:A:1111:LYS:HB2	1.58	0.46
4:A:138:LEU:HD23	4:A:142:LEU:HD13	1.96	0.46
4:A:390:LYS:CB	4:A:558:ASP:HB2	2.40	0.46
4:A:964:ARG:HD2	4:A:977:ILE:CG1	2.45	0.46
4:A:964:ARG:O	4:A:968:ARG:HG3	2.15	0.46
4:A:51:LYS:HB3	4:A:182:PHE:CE1	2.51	0.46
4:A:598:LEU:HD21	4:A:832:TYR:HB2	1.97	0.46
4:A:902:LEU:HD23	4:A:902:LEU:HA	1.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:72:SER:O	4:A:75:LEU:HB2	2.16	0.46
4:A:968:ARG:HG2	4:A:974:ILE:HD13	1.98	0.46
4:A:1052:LEU:HD23	4:A:1053:ARG:HH12	1.81	0.46
4:A:1087:PRO:HG2	4:A:1241:PHE:CE2	2.51	0.46
4:A:244:PHE:HB3	4:A:271:ASN:ND2	2.31	0.46
4:A:210:LYS:HE3	4:A:325:PHE:CE2	2.51	0.45
4:A:618:THR:HG22	4:A:618:THR:O	2.15	0.45
4:A:1062:GLU:HG2	4:A:1063:THR:N	2.24	0.45
3:D:-4:DT:H2''	3:D:-3:DT:H5''	1.98	0.45
4:A:142:LEU:HD23	4:A:166:LEU:HD13	1.97	0.45
1:B:-1:U:OP1	4:A:1034:LYS:HD3	2.16	0.45
4:A:1174:LEU:HG	4:A:1210:VAL:HG11	1.97	0.45
4:A:191:SER:HB3	4:A:195:ILE:HD11	1.98	0.45
4:A:848:ALA:HA	4:A:862:VAL:HG12	1.98	0.45
4:A:280:LYS:O	4:A:284:ILE:HG13	2.17	0.45
4:A:460:LEU:HA	4:A:463:PHE:HB3	1.99	0.45
4:A:1178:LEU:HD12	4:A:1185:TYR:CD2	2.51	0.45
4:A:337:PHE:HE2	4:A:339:ILE:HD13	1.81	0.44
4:A:1038:LEU:HB3	4:A:1055:TYR:HB2	1.98	0.44
4:A:27:THR:HG22	4:A:784:TYR:HA	1.99	0.44
4:A:85:LYS:O	4:A:89:SER:HB2	2.17	0.44
4:A:488:ILE:HD12	4:A:536:LEU:HD13	1.99	0.44
4:A:725:LYS:CE	4:A:744:THR:HG22	2.47	0.44
4:A:375:SER:HA	4:A:486:PRO:HG3	1.99	0.44
4:A:956:LYS:O	4:A:960:ILE:HG13	2.17	0.44
4:A:58:HIS:O	4:A:62:ILE:HG13	2.18	0.44
4:A:130:ALA:HB2	4:A:136:SER:HB2	1.99	0.44
4:A:609:TRP:CD1	4:A:826:GLY:HA2	2.53	0.44
4:A:1129:ASP:HB2	4:A:1141:LYS:HG2	1.99	0.44
4:A:1200:ASP:HB3	4:A:1203:PHE:HB3	1.99	0.44
4:A:202:ARG:O	4:A:206:ASP:HB2	2.17	0.44
4:A:27:THR:O	4:A:31:ILE:HG13	2.17	0.43
4:A:49:LYS:HD3	4:A:168:ILE:HD13	2.00	0.43
4:A:369:SER:OG	4:A:372:GLU:HG3	2.19	0.43
1:B:-8:U:H5	4:A:862:VAL:O	2.00	0.43
1:B:-5:U:H6	1:B:-5:U:O5'	2.01	0.43
4:A:50:ALA:O	4:A:54:ILE:HG13	2.19	0.43
4:A:468:ASP:O	4:A:472:GLN:HB3	2.18	0.43
4:A:915:SER:OG	4:A:1259:ALA:O	2.24	0.43
4:A:944:ILE:CD1	4:A:988:VAL:HG12	2.48	0.43
4:A:918:ARG:HH21	4:A:1020:GLU:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1104:LYS:H	4:A:1104:LYS:HG3	1.62	0.43
4:A:65:ILE:O	4:A:69:VAL:HG23	2.18	0.43
4:A:249:LYS:HD3	4:A:250:THR:HG23	2.01	0.43
4:A:763:LYS:HB3	4:A:763:LYS:HE2	1.55	0.43
4:A:1063:THR:HB	4:A:1066:LYS:H	1.83	0.43
1:B:7:C:H2'	1:B:8:A:C8	2.53	0.43
4:A:1183:ILE:HG21	4:A:1191:ILE:HG23	1.99	0.43
4:A:1217:MET:O	4:A:1229:LEU:HA	2.18	0.43
4:A:60:PHE:CD2	4:A:141:TRP:NE1	2.86	0.43
4:A:120:LYS:HG3	4:A:121:ASN:N	2.33	0.43
4:A:300:ILE:O	4:A:304:ILE:HG13	2.19	0.43
4:A:394:LYS:HD2	4:A:396:ASP:CG	2.39	0.43
4:A:208:LEU:HB3	4:A:209:PRO:HD3	2.01	0.43
4:A:290:VAL:HG21	4:A:297:ARG:NH1	2.34	0.43
4:A:1257:ASN:OD1	4:A:1261:HIS:CE1	2.72	0.43
4:A:1253:ASP:OD2	4:A:1253:ASP:N	2.52	0.42
3:D:-3:DT:OP1	4:A:124:ASN:HB2	2.19	0.42
4:A:449:LYS:NZ	4:A:550:ASP:HB2	2.34	0.42
4:A:394:LYS:HD2	4:A:396:ASP:OD1	2.19	0.42
4:A:511:LYS:HE2	4:A:513:ASP:OD2	2.19	0.42
1:B:7:C:H6	1:B:7:C:O5'	2.02	0.42
4:A:61:PHE:HD1	4:A:118:LYS:HD3	1.84	0.42
4:A:1035:LEU:HD13	4:A:1073:ILE:HD11	2.01	0.42
4:A:233:GLN:O	4:A:237:ASP:N	2.49	0.42
4:A:390:LYS:HA	4:A:390:LYS:HD3	1.89	0.42
4:A:1268:MET:HE1	4:A:1291:TYR:HD1	1.83	0.42
4:A:49:LYS:HB3	4:A:159:ILE:HD11	2.02	0.42
4:A:1272:ARG:HH22	4:A:1286:ILE:HA	1.85	0.42
4:A:1032:ILE:CG1	4:A:1074:ILE:HD12	2.50	0.42
4:A:1154:PHE:CE1	4:A:1166:ARG:HB3	2.47	0.42
3:D:-3:DT:OP1	4:A:125:GLN:N	2.30	0.42
4:A:816:ASN:HD22	4:A:817:LEU:CD1	2.33	0.42
1:B:-3:G:OP1	4:A:1041:LYS:HD2	2.20	0.42
4:A:17:LEU:HD13	4:A:808:TRP:HB2	2.02	0.42
4:A:131:LYS:HG3	4:A:132:LYS:HE3	2.02	0.42
4:A:356:TYR:OH	4:A:529:LEU:HD22	2.20	0.41
4:A:691:ILE:HG23	4:A:696:THR:OG1	2.19	0.41
4:A:1108:PHE:HA	4:A:1111:LYS:HE3	2.01	0.41
1:B:5:G:H2'	1:B:6:U:O4'	2.20	0.41
2:C:-16:DT:H2'	2:C:-15:DT:C6	2.55	0.41
4:A:370:ILE:O	4:A:374:LEU:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:505:LYS:HE3	4:A:506:TYR:CE2	2.55	0.41
4:A:394:LYS:HG2	4:A:450:TYR:CE1	2.56	0.41
4:A:1142:TRP:CH2	4:A:1296:GLN:HG2	2.54	0.41
1:B:10:U:H2'	1:B:11:U:C6	2.56	0.41
3:D:-8:DG:C8	3:D:-7:DT:H72	2.55	0.41
4:A:235:LYS:O	4:A:239:ALA:HB2	2.20	0.41
4:A:249:LYS:CB	4:A:265:GLU:HG2	2.51	0.41
4:A:968:ARG:HG2	4:A:974:ILE:CD1	2.50	0.41
4:A:557:LYS:HE3	4:A:559:GLU:OE2	2.20	0.41
4:A:597:LYS:HD2	4:A:829:GLU:HG2	2.03	0.41
4:A:244:PHE:CZ	4:A:272:TYR:HE1	2.38	0.41
4:A:790:ASN:H	4:A:793:PHE:HD1	1.68	0.41
4:A:978:LYS:HE3	4:A:979:GLU:OE2	2.21	0.41
4:A:17:LEU:HD11	4:A:884:ILE:HD13	2.02	0.41
4:A:735:LYS:H	4:A:735:LYS:HG2	1.58	0.41
4:A:925:TYR:HD2	4:A:926:TYR:N	2.19	0.41
4:A:929:VAL:HG12	4:A:935:ILE:HG12	2.03	0.41
4:A:27:THR:CG2	4:A:785:LEU:H	2.33	0.40
4:A:249:LYS:HB2	4:A:265:GLU:HG2	2.03	0.40
4:A:391:ILE:HD11	4:A:543:PHE:CE2	2.55	0.40
4:A:884:ILE:HG13	4:A:886:ILE:HD11	2.02	0.40
4:A:1116:CYS:HA	4:A:1190:CYS:HA	2.04	0.40
4:A:94:LEU:HD23	4:A:94:LEU:HA	1.86	0.40
4:A:109:ILE:O	4:A:113:ILE:HG23	2.21	0.40
4:A:488:ILE:O	4:A:492:ILE:HG13	2.21	0.40
4:A:1071:THR:O	4:A:1071:THR:OG1	2.29	0.40
2:C:-2:DC:H2'	2:C:-1:DT:C6	2.57	0.40
4:A:75:LEU:HA	4:A:75:LEU:HD23	1.88	0.40
4:A:471:LYS:HB2	4:A:471:LYS:HE3	1.95	0.40
4:A:762:TYR:CE1	4:A:823:LYS:HG2	2.56	0.40
4:A:1040:PHE:C	4:A:1042:ASP:H	2.23	0.40
4:A:1294:PHE:O	4:A:1298:ARG:HG2	2.21	0.40
4:A:54:ILE:HD13	4:A:54:ILE:HG21	1.84	0.40
4:A:73:GLU:OE1	4:A:267:ALA:HB2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:72:SER:OG	4:A:1046:ASP:OD1[5_454]	2.11	0.09

5.3 Torsion angles

5.3.1 Protein backbone

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
4	A	1246/1300 (96%)	1185 (95%)	55 (4%)	6 (0%)	25 59

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	574	ASN
4	A	160	THR
4	A	626	ASP
4	A	1013	LYS
4	A	1137	ALA
4	A	510	GLY

5.3.2 Protein sidechains

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
4	A	1144/1183 (97%)	1089 (95%)	55 (5%)	21 51

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	1	MET
4	A	39	ASP
4	A	64	GLU
4	A	67	SER
4	A	72	SER

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Mol	Chain	Res	Type
4	A	85	LYS
4	A	115	ASP
4	A	131	LYS
4	A	136	SER
4	A	137	ASP
4	A	151	GLU
4	A	202	ARG
4	A	252	GLU
4	A	265	GLU
4	A	272	TYR
4	A	289	PHE
4	A	298	LYS
4	A	352	MET
4	A	398	SER
4	A	401	ASP
4	A	467	ARG
4	A	515	LEU
4	A	605	LEU
4	A	644	LYS
4	A	695	SER
4	A	735	LYS
4	A	736	ASP
4	A	745	GLN
4	A	746	ARG
4	A	755	ARG
4	A	776	SER
4	A	800	ARG
4	A	804	HIS
4	A	819	ASP
4	A	846	LYS
4	A	854	LYS
4	A	876	ASP
4	A	895	LYS
4	A	907	LYS
4	A	948	ARG
4	A	950	LYS
4	A	966	SER
4	A	1012	PHE
4	A	1053	ARG
4	A	1069	LYS
4	A	1084	LYS
4	A	1099	TYR

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Mol	Chain	Res	Type
4	A	1101	SER
4	A	1105	SER
4	A	1130	TYR
4	A	1150	ARG
4	A	1196	CYS
4	A	1250	MET
4	A	1280	LYS
4	A	1298	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	77	GLN
4	A	617	ASN
4	A	697	HIS
4	A	843	HIS
4	A	901	ASN
4	A	1043	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	41/58 (70%)	6 (14%)	2 (4%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	-10	U
1	B	-9	G
1	B	-7	U
1	B	-6	G
1	B	21	G
1	B	22	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	-10	U
1	B	0	G

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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	B	42/58 (72%)	-0.74	0 100 100	19, 27, 101, 139	0
2	C	27/27 (100%)	-0.63	0 100 100	21, 39, 70, 98	0
3	D	11/11 (100%)	-0.61	0 100 100	33, 38, 78, 95	0
4	A	1260/1300 (96%)	-0.20	18 (1%) 73 57	14, 44, 112, 152	0
All	All	1340/1396 (95%)	-0.23	18 (1%) 74 59	14, 43, 112, 152	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	1207	LEU	5.3
4	A	1203	PHE	3.7
4	A	1213	THR	2.9
4	A	1214	ILE	2.9
4	A	298	LYS	2.7
4	A	1206	LYS	2.6
4	A	1109	PHE	2.5
4	A	1156	ASN	2.5
4	A	1191	ILE	2.5
4	A	112	TYR	2.4
4	A	1221	LYS	2.3
4	A	1127	SER	2.3
4	A	647	LYS	2.3
4	A	552	ALA	2.3
4	A	469	ILE	2.2
4	A	445	THR	2.2
4	A	1012	PHE	2.1
4	A	381	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MG	B	101	1/1	0.95	0.28	2,2,2,2	0
5	MG	B	102	1/1	0.96	0.20	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.