



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:35 AM UTC

PDB ID : 6M0X / pdb_00006m0x
Title : Crystal structure of Streptococcus thermophilus Cas9 in complex with AGGA PAM
Authors : Zhang, Y.; Zhang, H.; Xu, X.; Wang, Y.; Chen, W.; Wang, Y.; Wu, Z.; Tang, N.; Wang, Y.; Zhao, S.; Gan, J.; Ji, Q.
Deposited on : 2020-02-23
Resolution : 2.56 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

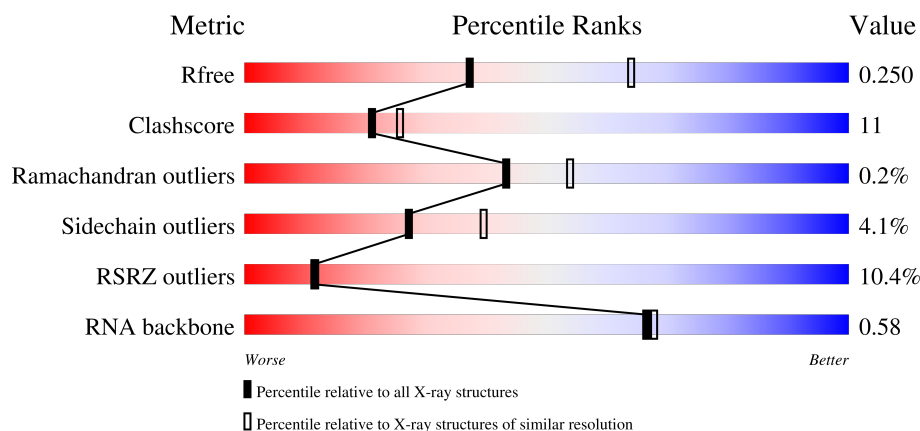
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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}	180053	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)
RNA backbone	3983	1013 (2.80-2.32)

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	A	1122	10% 65% 25% 8%
2	B	71	68% 30%
3	C	28	4% 68% 32%
4	D	8	88% 12%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10523 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 CRISPR-associated endonuclease Cas9 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1032	Total	C	N	O	S	0	0	0
			8229	5213	1433	1566	17			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q03LF7
A	1	GLY	-	expression tag	UNP Q03LF7
A	599	ALA	HIS	engineered mutation	UNP Q03LF7

- Molecule 2 is a RNA chain called RNA (71-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	71	Total	C	N	O	P	0	0	0
			1500	670	271	488	71			

- Molecule 3 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	28	Total	C	N	O	P	0	0	0
			561	272	91	171	27			

- Molecule 4 is a DNA chain called DNA (5'-D(*AP*AP*AP*GP*GP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	8	Total	C	N	O	P	0	0	0
			166	79	38	42	7			

- Molecule 5 is BARIUM ION (CCD ID: BA) (formula: Ba).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total 6	Ba 6	0	0
5	B	6	Total 6	Ba 6	0	0
5	C	1	Total 1	Ba 1	0	0
5	D	1	Total 1	Ba 1	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

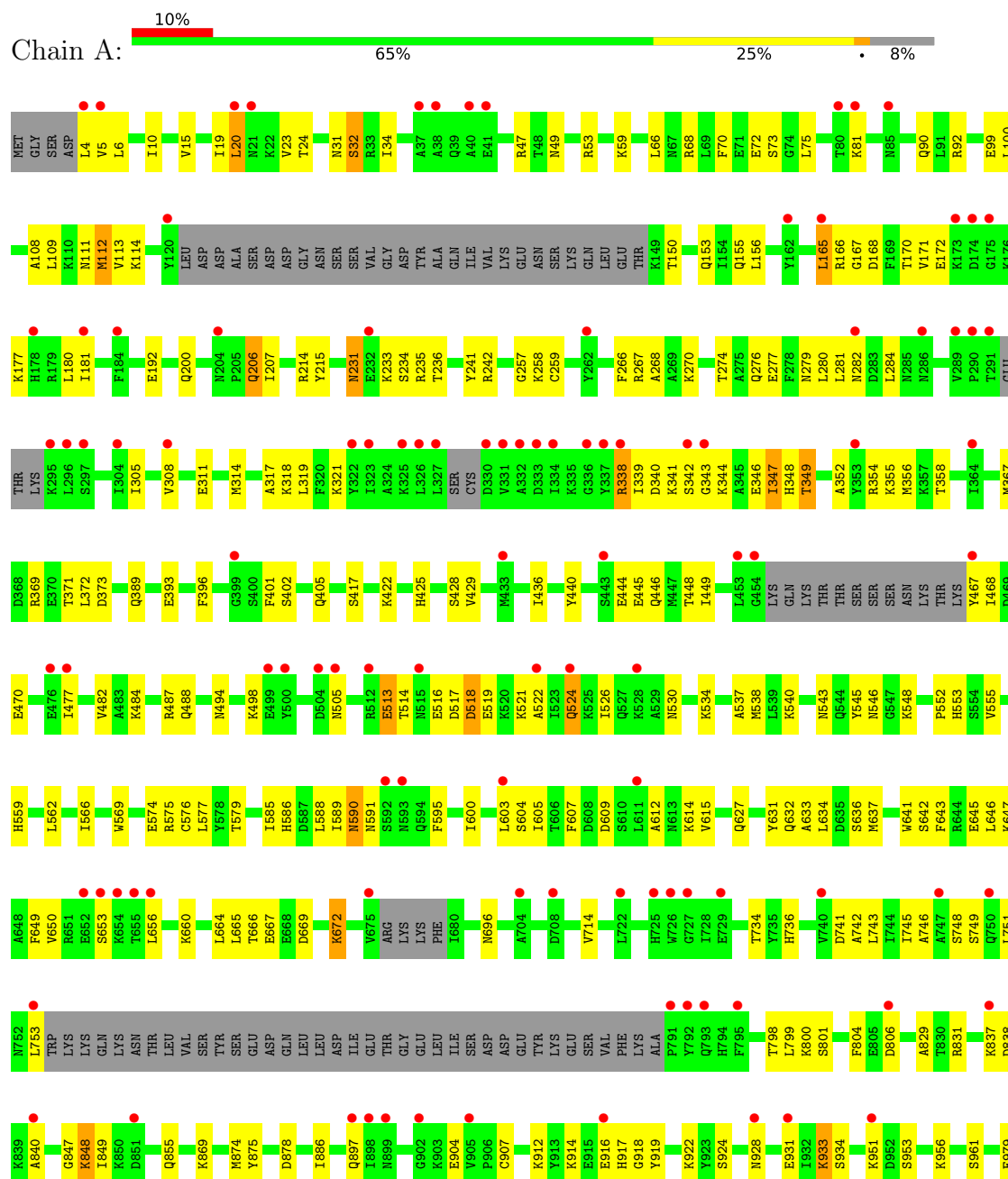
- Molecule 7 is water.

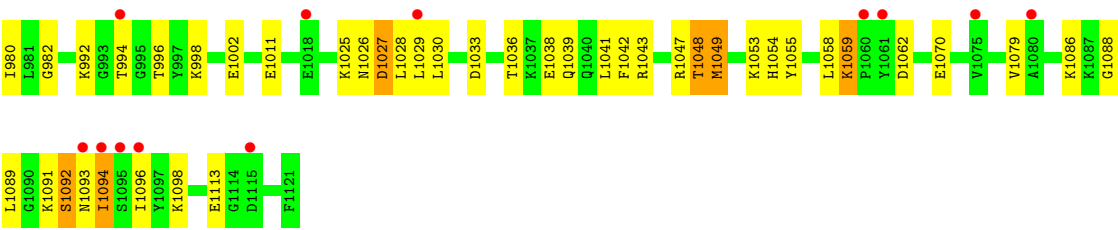
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	22	Total 22	O 22	0	0
7	B	22	Total 22	O 22	0	0
7	C	4	Total 4	O 4	0	0
7	D	3	Total 3	O 3	0	0

3 Residue-property plots

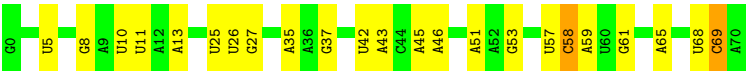
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CRISPR-associated endonuclease Cas9 1

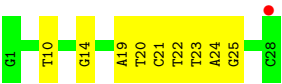




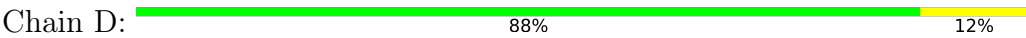
• Molecule 2: RNA (71-MER)



• Molecule 3: DNA (28-MER)



• Molecule 4: DNA (5'-D(*AP*AP*AP*GP*GP*AP*GP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	322.17Å 75.25Å 70.01Å 90.00° 93.28° 90.00°	Depositor
Resolution (Å)	48.90 – 2.56 48.90 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.90-2.56) 99.7 (48.90-2.56)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.226 , 0.256 0.226 , 0.250	Depositor DCC
R_{free} test set	2752 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10523	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.60	3/8373 (0.0%)	0.66	19/11279 (0.2%)
2	B	0.41	0/1679	0.48	0/2615
3	C	0.54	0/625	0.62	0/961
4	D	0.80	0/188	0.96	1/289 (0.3%)
All	All	0.57	3/10865 (0.0%)	0.63	20/15144 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	849	ILE	C-O	-5.79	1.17	1.24
1	A	951	LYS	C-O	-5.14	1.17	1.24
1	A	1059	LYS	C-O	-5.07	1.19	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	DA	C2'-C3'-O3'	-8.45	98.82	111.50
1	A	953	SER	N-CA-C	8.28	122.23	110.23
1	A	1027	ASP	N-CA-C	-8.16	99.76	110.53
1	A	1094	ILE	N-CA-C	8.08	121.29	108.85
1	A	804	PHE	N-CA-C	7.86	119.48	111.07
1	A	521	LYS	N-CA-C	-7.66	102.94	111.82
1	A	517	ASP	N-CA-C	7.01	119.78	111.71
1	A	589	ILE	CB-CA-C	-6.97	103.05	111.97
1	A	590	ASN	N-CA-C	6.66	119.55	111.82
1	A	166	ARG	N-CA-C	6.47	119.63	110.50
1	A	1092	SER	N-CA-C	6.41	118.35	111.36
1	A	514	THR	N-CA-C	-6.29	97.82	108.26
1	A	589	ILE	N-CA-C	6.17	116.34	110.42
1	A	653	SER	N-CA-C	5.92	118.53	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	992	LYS	N-CA-C	-5.50	102.75	110.50
1	A	518	ASP	N-CA-C	-5.37	105.42	111.28
1	A	34	ILE	N-CA-C	5.27	115.49	108.11
1	A	840	ALA	N-CA-C	-5.24	100.87	109.40
1	A	847	GLY	N-CA-C	-5.16	103.27	110.96
1	A	837	LYS	N-CA-C	5.03	119.10	112.92

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	8229	0	8087	205	0
2	B	1500	0	751	12	0
3	C	561	0	321	13	0
4	D	166	0	90	0	0
5	A	6	0	0	0	0
5	B	6	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	2	0	0	0	0
7	A	22	0	0	0	0
7	B	22	0	0	0	0
7	C	4	0	0	0	0
7	D	3	0	0	0	0
All	All	10523	0	9249	217	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 11.

All (217) 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)
1:A:513:GLU:HG3	3:C:22:DT:H5"	1.26	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ARG:HH21	1:A:346:GLU:HG3	1.25	0.97
1:A:642:SER:OG	1:A:645:GLU:HG3	1.70	0.91
1:A:231:ASN:C	1:A:231:ASN:HD22	1.80	0.87
1:A:605:ILE:HG12	1:A:672:LYS:HG3	1.56	0.87
1:A:519:GLU:O	1:A:522:ALA:HB3	1.80	0.82
1:A:575:ARG:HE	1:A:649:PHE:HE2	1.25	0.80
1:A:1049:MET:HE3	1:A:1086:LYS:HD3	1.66	0.77
1:A:75:LEU:HD11	1:A:206:GLN:HB3	1.67	0.76
1:A:1048:THR:HG21	1:A:1086:LYS:HE2	1.65	0.76
1:A:634:LEU:HA	1:A:637:MET:HE3	1.66	0.75
1:A:92:ARG:NH1	1:A:111:ASN:OD1	2.21	0.74
1:A:99:GLU:HA	1:A:200:GLN:HE22	1.54	0.72
1:A:231:ASN:ND2	1:A:234:SER:H	1.89	0.71
1:A:150:THR:H	1:A:153:GLN:HE21	1.39	0.69
1:A:68:ARG:NH1	2:B:58:C:O2'	2.26	0.69
1:A:277:GLU:OE1	1:A:369:ARG:NH1	2.27	0.67
1:A:609:ASP:OD1	1:A:614:LYS:NZ	2.26	0.67
1:A:467:TYR:CZ	1:A:498:LYS:NZ	2.63	0.67
1:A:100:LEU:H	1:A:200:GLN:NE2	1.93	0.67
1:A:444:GLU:HG2	1:A:448:THR:HG21	1.78	0.66
1:A:1028:LEU:HD23	1:A:1043:ARG:HB3	1.78	0.64
1:A:1098:LYS:NZ	1:A:1113:GLU:OE1	2.20	0.64
1:A:268:ALA:HB2	1:A:429:VAL:HG23	1.79	0.64
1:A:848:LYS:HD2	1:A:934:SER:HB3	1.79	0.64
1:A:569:TRP:CZ2	1:A:574:GLU:HG2	2.32	0.63
1:A:916:GLU:HG2	1:A:917:HIS:CE1	2.33	0.63
1:A:274:THR:HG21	1:A:429:VAL:HG13	1.80	0.63
1:A:996:THR:HG22	1:A:998:LYS:HG2	1.81	0.63
1:A:341:LYS:NZ	3:C:23:DT:O2	2.30	0.62
1:A:31:ASN:OD1	1:A:32:SER:N	2.32	0.62
1:A:874:MET:HG3	1:A:878:ASP:HB3	1.82	0.60
1:A:467:TYR:CE2	1:A:498:LYS:NZ	2.63	0.60
1:A:47:ARG:NH2	2:B:13:A:OP2	2.34	0.60
1:A:59:LYS:NZ	1:A:114:LYS:O	2.32	0.60
1:A:612:ALA:HA	1:A:660:LYS:HE3	1.84	0.60
1:A:540:LYS:NZ	1:A:574:GLU:OE2	2.25	0.59
1:A:150:THR:HB	1:A:192:GLU:HB2	1.83	0.59
1:A:1025:LYS:O	1:A:1026:ASN:HB2	2.01	0.59
1:A:874:MET:HE1	1:A:886:ILE:HD12	1.85	0.59
1:A:643:PHE:O	1:A:647:LYS:HG3	2.02	0.58
1:A:308:VAL:HG12	1:A:314:MET:HE3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:SER:HB2	1:A:627:GLN:HE21	1.67	0.58
1:A:979:GLU:HA	1:A:1054:HIS:CD2	2.39	0.58
1:A:90:GLN:HA	1:A:156:LEU:HD22	1.87	0.57
1:A:10:ILE:HA	1:A:15:VAL:HG22	1.86	0.57
1:A:349:THR:OG1	1:A:354:ARG:NH2	2.37	0.57
1:A:99:GLU:HA	1:A:200:GLN:NE2	2.20	0.57
1:A:235:ARG:CZ	1:A:241:TYR:HB3	2.34	0.57
1:A:20:LEU:HG	1:A:20:LEU:O	2.03	0.56
1:A:367:MET:HE2	1:A:372:LEU:HD13	1.88	0.56
1:A:349:THR:O	1:A:354:ARG:NH2	2.36	0.56
1:A:150:THR:H	1:A:153:GLN:NE2	2.04	0.55
1:A:168:ASP:HB3	1:A:181:ILE:HD12	1.88	0.55
1:A:340:ASP:HB3	1:A:343:GLY:H	1.71	0.55
1:A:586:HIS:O	1:A:590:ASN:HB2	2.06	0.55
1:A:745:ILE:O	1:A:748:SER:OG	2.25	0.55
1:A:279:ASN:HB3	1:A:348:HIS:CD2	2.40	0.55
1:A:534:LYS:O	1:A:538:MET:HG2	2.06	0.55
1:A:543:ASN:ND2	1:A:548:LYS:O	2.37	0.55
1:A:734:THR:HG22	1:A:736:HIS:H	1.72	0.55
3:C:23:DT:H5''	3:C:23:DT:H6	1.73	0.54
1:A:470:GLU:HG3	1:A:487:ARG:HG2	1.90	0.53
1:A:314:MET:SD	1:A:319:LEU:HB2	2.48	0.53
1:A:933:LYS:HD3	2:B:43:A:H5''	1.90	0.53
1:A:168:ASP:OD1	1:A:168:ASP:N	2.42	0.53
1:A:282:ASN:ND2	1:A:446:GLN:H	2.07	0.53
1:A:311:GLU:HG2	1:A:318:LYS:NZ	2.24	0.53
1:A:1011:GLU:HA	1:A:1053:LYS:HE3	1.91	0.53
1:A:73:SER:HB3	1:A:75:LEU:HD13	1.90	0.53
3:C:19:DA:H2'	3:C:20:DT:C6	2.44	0.52
1:A:281:LEU:CD1	1:A:305:ILE:HD11	2.39	0.52
1:A:627:GLN:NE2	3:C:10:DT:H5''	2.25	0.52
1:A:308:VAL:HG11	1:A:319:LEU:HD12	1.91	0.52
1:A:1036:THR:HG23	1:A:1038:GLU:HG3	1.91	0.52
1:A:800:LYS:O	1:A:801:SER:C	2.50	0.51
1:A:445:GLU:O	1:A:449:ILE:HG13	2.10	0.51
1:A:355:LYS:O	1:A:358:THR:OG1	2.22	0.51
1:A:577:LEU:O	1:A:646:LEU:HD13	2.10	0.51
1:A:305:ILE:HD12	1:A:440:TYR:OH	2.10	0.51
1:A:1002:GLU:OE1	1:A:1002:GLU:N	2.36	0.51
2:B:68:U:H5'	2:B:69:C:OP2	2.11	0.51
1:A:231:ASN:ND2	1:A:234:SER:N	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:NH2	1:A:155:GLN:OE1	2.44	0.51
1:A:402:SER:OG	1:A:405:GLN:HG3	2.10	0.51
1:A:257:GLY:O	1:A:267:ARG:HG3	2.11	0.51
1:A:590:ASN:O	1:A:591:ASN:OD1	2.29	0.50
1:A:734:THR:HG21	1:A:736:HIS:CD2	2.45	0.50
1:A:109:LEU:HB3	1:A:215:TYR:CE1	2.47	0.50
1:A:338:ARG:HA	3:C:25:DG:O4'	2.12	0.50
1:A:444:GLU:HB3	1:A:448:THR:HB	1.94	0.50
1:A:49:ASN:O	1:A:53:ARG:HG3	2.12	0.50
3:C:24:DA:H8	3:C:24:DA:H5''	1.76	0.50
1:A:742:ALA:HA	1:A:745:ILE:HD12	1.92	0.49
1:A:5:VAL:HG22	1:A:505:ASN:HB3	1.94	0.49
1:A:1049:MET:HE3	1:A:1086:LYS:CD	2.39	0.49
1:A:924:SER:OG	1:A:928:ASN:N	2.40	0.49
1:A:519:GLU:O	1:A:522:ALA:CB	2.55	0.49
1:A:1029:LEU:O	1:A:1041:LEU:HD12	2.13	0.49
3:C:14:DG:H8	3:C:14:DG:H5''	1.78	0.49
1:A:279:ASN:HB3	1:A:348:HIS:CG	2.48	0.48
1:A:588:LEU:HA	1:A:595:PHE:CE2	2.48	0.48
1:A:1089:LEU:HB3	1:A:1096:ILE:HD11	1.95	0.48
1:A:389:GLN:O	1:A:393:GLU:HG3	2.13	0.48
1:A:75:LEU:CD1	1:A:206:GLN:HB3	2.42	0.48
1:A:498:LYS:HA	1:A:498:LYS:HD3	1.54	0.48
1:A:339:ILE:CG2	3:C:24:DA:H2''	2.44	0.48
1:A:72:GLU:OE1	1:A:214:ARG:NH2	2.41	0.48
1:A:647:LYS:HB3	1:A:647:LYS:HE2	1.47	0.48
1:A:317:ALA:O	1:A:321:LYS:N	2.34	0.48
1:A:1049:MET:CE	1:A:1086:LYS:HD3	2.40	0.48
1:A:231:ASN:HD22	1:A:234:SER:H	1.58	0.47
1:A:545:TYR:HB2	1:A:585:ILE:HG21	1.96	0.47
1:A:267:ARG:HD3	1:A:425:HIS:O	2.13	0.47
1:A:352:ALA:O	1:A:356:MET:HG3	2.15	0.47
1:A:537:ALA:HB1	1:A:566:ILE:HG22	1.97	0.47
1:A:92:ARG:HG2	1:A:108:ALA:HB1	1.95	0.47
1:A:696:ASN:N	1:A:696:ASN:HD22	2.13	0.47
1:A:559:HIS:CE1	1:A:562:LEU:HG	2.49	0.47
1:A:714:VAL:HG21	1:A:748:SER:OG	2.14	0.47
1:A:741:ASP:O	1:A:745:ILE:HG13	2.15	0.47
1:A:546:ASN:ND2	1:A:552:PRO:HD3	2.30	0.47
1:A:672:LYS:CD	1:A:672:LYS:H	2.27	0.47
1:A:743:LEU:HD23	1:A:743:LEU:HA	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1062:ASP:OD1	1:A:1062:ASP:N	2.49	0.46
1:A:631:TYR:CE1	1:A:667:GLU:HG2	2.49	0.46
1:A:6:LEU:HD12	1:A:19:ILE:HG12	1.97	0.46
1:A:274:THR:OG1	1:A:373:ASP:OD2	2.27	0.46
1:A:367:MET:HE3	1:A:371:THR:HG22	1.98	0.46
1:A:207:ILE:O	1:A:207:ILE:HG22	2.15	0.46
1:A:519:GLU:O	1:A:522:ALA:N	2.49	0.46
1:A:590:ASN:C	1:A:591:ASN:OD1	2.59	0.46
1:A:650:VAL:HG13	1:A:656:LEU:HD13	1.98	0.46
1:A:919:TYR:HB2	1:A:931:GLU:HG2	1.98	0.46
1:A:311:GLU:HG2	1:A:318:LYS:HZ2	1.81	0.46
1:A:168:ASP:HA	1:A:180:LEU:O	2.16	0.46
1:A:519:GLU:HA	1:A:522:ALA:HB3	1.97	0.46
1:A:534:LYS:NZ	2:B:8:G:OP1	2.49	0.46
1:A:1043:ARG:HG3	1:A:1059:LYS:HB2	1.97	0.46
1:A:235:ARG:HD2	1:A:242:ARG:O	2.16	0.45
1:A:339:ILE:HD11	1:A:343:GLY:C	2.41	0.45
1:A:170:THR:HG22	1:A:171:VAL:N	2.32	0.45
1:A:513:GLU:CG	3:C:22:DT:H5''	2.19	0.45
2:B:26:U:H2'	2:B:27:G:H8	1.81	0.45
1:A:258:LYS:HE2	1:A:266:PHE:CZ	2.52	0.45
1:A:1033:ASP:CG	1:A:1036:THR:HG22	2.42	0.45
1:A:1042:PHE:CG	1:A:1058:LEU:HD13	2.52	0.45
1:A:897:GLN:OE1	1:A:912:LYS:HE3	2.16	0.45
1:A:631:TYR:CD2	1:A:667:GLU:HA	2.52	0.45
1:A:600:ILE:HD11	1:A:615:VAL:HG13	1.98	0.44
1:A:338:ARG:HE	1:A:338:ARG:HB2	1.27	0.44
1:A:552:PRO:O	1:A:555:VAL:HG22	2.17	0.44
1:A:649:PHE:CD1	1:A:649:PHE:C	2.95	0.44
3:C:14:DG:H5''	3:C:14:DG:C8	2.52	0.44
1:A:603:LEU:HG	1:A:607:PHE:HA	1.98	0.44
1:A:922:LYS:HD3	2:B:42:U:H1'	1.98	0.44
1:A:524:GLN:H	1:A:524:GLN:HG2	1.65	0.44
1:A:259:CYS:HB2	1:A:428:SER:HB3	2.00	0.44
3:C:20:DT:H2'	3:C:21:DC:C6	2.53	0.44
1:A:494:ASN:O	1:A:498:LYS:HE2	2.17	0.44
1:A:829:ALA:HB1	1:A:831:ARG:HH22	1.83	0.44
1:A:914:LYS:HA	1:A:918:GLY:O	2.18	0.44
1:A:340:ASP:HB3	1:A:344:LYS:H	1.83	0.43
2:B:26:U:H2'	2:B:27:G:C8	2.53	0.43
1:A:576:CYS:SG	1:A:579:THR:HG23	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:LEU:O	1:A:665:LEU:HD23	2.17	0.43
1:A:280:LEU:HD13	1:A:348:HIS:O	2.18	0.43
1:A:23:VAL:HG23	1:A:24:THR:N	2.33	0.43
1:A:980:ILE:H	1:A:1054:HIS:HD2	1.67	0.43
1:A:869:LYS:HE3	1:A:875:TYR:CE2	2.54	0.43
1:A:855:GLN:HE21	1:A:907:CYS:C	2.27	0.43
1:A:5:VAL:HG12	1:A:746:ALA:HB1	2.01	0.42
1:A:66:LEU:HD11	1:A:70:PHE:HE1	1.84	0.42
1:A:632:GLN:HE21	1:A:669:ASP:HA	1.84	0.42
1:A:276:GLN:CD	1:A:352:ALA:HB3	2.44	0.42
1:A:339:ILE:HD11	1:A:343:GLY:O	2.20	0.42
1:A:270:LYS:HE2	1:A:422:LYS:O	2.18	0.42
1:A:347:ILE:HG12	1:A:348:HIS:H	1.83	0.42
1:A:1028:LEU:HA	1:A:1043:ARG:HA	2.00	0.42
1:A:585:ILE:HG22	1:A:586:HIS:CD2	2.54	0.42
1:A:627:GLN:CD	3:C:10:DT:H5''	2.45	0.42
1:A:1055:TYR:HA	1:A:1088:GLY:HA2	2.02	0.42
1:A:112:MET:HE2	1:A:112:MET:HB2	1.75	0.42
1:A:280:LEU:O	1:A:284:LEU:HG	2.19	0.42
1:A:281:LEU:HD22	1:A:436:ILE:HG23	2.02	0.42
1:A:172:GLU:HA	1:A:177:LYS:HE2	2.01	0.42
1:A:231:ASN:ND2	1:A:233:LYS:H	2.17	0.42
1:A:445:GLU:H	1:A:445:GLU:HG3	1.69	0.42
1:A:522:ALA:O	1:A:526:ILE:HG13	2.18	0.42
1:A:633:ALA:HB1	1:A:637:MET:HE2	2.02	0.42
2:B:45:A:H2'	2:B:46:A:C8	2.55	0.42
1:A:484:LYS:O	1:A:488:GLN:HG2	2.19	0.41
1:A:1030:LEU:HD21	1:A:1039:GLN:OE1	2.20	0.41
1:A:338:ARG:NH1	2:B:5:U:O2'	2.54	0.41
1:A:417:SER:OG	1:A:553:HIS:NE2	2.53	0.41
1:A:4:LEU:HD22	1:A:19:ILE:HG22	2.03	0.41
1:A:396:PHE:CG	1:A:401:PHE:HE2	2.38	0.41
1:A:468:ILE:H	1:A:468:ILE:HD12	1.86	0.41
1:A:569:TRP:CH2	1:A:574:GLU:HG2	2.56	0.41
1:A:660:LYS:HE3	1:A:660:LYS:HB2	1.89	0.41
1:A:1033:ASP:OD2	1:A:1036:THR:HG22	2.20	0.41
1:A:477:ILE:HD11	1:A:482:VAL:HG12	2.03	0.41
1:A:604:SER:CB	1:A:627:GLN:HE21	2.33	0.41
1:A:982:GLY:HA3	1:A:1047:ARG:HG2	2.01	0.40
1:A:167:GLY:O	1:A:181:ILE:HA	2.21	0.40
1:A:530:ASN:O	1:A:534:LYS:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:SER:OG	1:A:645:GLU:CG	2.55	0.40
2:B:25:U:H2'	2:B:26:U:C6	2.56	0.40
1:A:641:TRP:HH2	1:A:649:PHE:CD2	2.39	0.40
1:A:848:LYS:CD	1:A:934:SER:HB3	2.49	0.40
1:A:81:LYS:H	1:A:81:LYS:HG2	1.66	0.40
1:A:347:ILE:HG12	1:A:348:HIS:N	2.36	0.40
1:A:912:LYS:HD3	1:A:912:LYS:HA	1.92	0.40
1:A:956:LYS:HB3	1:A:956:LYS:HE3	1.84	0.40
1:A:1070:GLU:O	1:A:1079:VAL:HG12	2.22	0.40
2:B:68:U:H5''	2:B:68:U:H6	1.85	0.40
1:A:165:LEU:H	1:A:165:LEU:HG	1.80	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	1018/1122 (91%)	981 (96%)	35 (3%)	2 (0%)	43 54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1093	ASN
1	A	1049	MET

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	869/1000 (87%)	833 (96%)	36 (4%)	27	39

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	32	SER
1	A	112	MET
1	A	113	VAL
1	A	165	LEU
1	A	206	GLN
1	A	231	ASN
1	A	236	THR
1	A	338	ARG
1	A	342	SER
1	A	347	ILE
1	A	349	THR
1	A	513	GLU
1	A	516	GLU
1	A	518	ASP
1	A	524	GLN
1	A	636	SER
1	A	666	THR
1	A	672	LYS
1	A	749	SER
1	A	751	LEU
1	A	753	LEU
1	A	798	THR
1	A	799	LEU
1	A	806	ASP
1	A	838	ASP
1	A	848	LYS
1	A	904	GLU
1	A	933	LYS
1	A	961	SER
1	A	994	THR
1	A	1027	ASP
1	A	1048	THR
1	A	1091	LYS
1	A	1092	SER
1	A	1094	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	39	GLN
1	A	49	ASN
1	A	102	ASN
1	A	153	GLN
1	A	200	GLN
1	A	204	ASN
1	A	231	ASN
1	A	310	ASN
1	A	389	GLN
1	A	505	ASN
1	A	586	HIS
1	A	593	ASN
1	A	627	GLN
1	A	696	ASN
1	A	699	GLN
1	A	855	GLN
1	A	880	GLN
1	A	1054	HIS
1	A	1106	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	69/71 (97%)	12 (17%)	0

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	10	U
2	B	11	U
2	B	35	A
2	B	37	G
2	B	51	A
2	B	53	G
2	B	57	U
2	B	58	C
2	B	59	A
2	B	61	G
2	B	65	A

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Mol	Chain	Res	Type
2	B	69	C

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 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, 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	1032/1122 (91%)	0.87	117 (11%) 10 9	29, 61, 105, 166	0
2	B	71/71 (100%)	-0.39	0 100 100	29, 41, 72, 93	0
3	C	28/28 (100%)	-0.07	1 (3%) 46 47	31, 44, 89, 93	0
4	D	8/8 (100%)	-0.50	0 100 100	33, 35, 39, 43	0
All	All	1139/1229 (92%)	0.76	118 (10%) 11 12	29, 60, 102, 166	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	477	ILE	5.8
1	A	38	ALA	5.1
1	A	747	ALA	4.8
1	A	467	TYR	4.8
1	A	40	ALA	4.6
1	A	729	GLU	4.4
1	A	291	THR	4.4
1	A	336	GLY	4.4
1	A	656	LEU	4.3
1	A	327	LEU	4.3
1	A	675	VAL	4.2
1	A	262	TYR	4.1
1	A	740	VAL	3.7
1	A	931	GLU	3.7
1	A	333	ASP	3.6
1	A	793	GLN	3.6
1	A	500	TYR	3.5
1	A	928	ASN	3.4
1	A	708	ASP	3.4
1	A	727	GLY	3.3
1	A	337	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	120	TYR	3.3
1	A	308	VAL	3.2
1	A	603	LEU	3.2
1	A	330	ASP	3.1
1	A	323	ILE	3.1
1	A	232	GLU	3.1
1	A	592	SER	3.1
1	A	726	TRP	3.1
1	A	725	HIS	3.0
1	A	282	ASN	3.0
1	A	364	ILE	3.0
1	A	326	LEU	3.0
1	A	806	ASP	3.0
1	A	454	GLY	3.0
1	A	338	ARG	2.9
1	A	837	LYS	2.9
1	A	290	PRO	2.9
1	A	655	THR	2.8
1	A	178	HIS	2.8
1	A	1061	TYR	2.8
1	A	343	GLY	2.8
1	A	505	ASN	2.7
1	A	342	SER	2.7
1	A	654	LYS	2.7
1	A	204	ASN	2.7
1	A	653	SER	2.7
1	A	165	LEU	2.7
1	A	499	GLU	2.7
1	A	840	ALA	2.7
1	A	296	LEU	2.6
1	A	704	ALA	2.6
1	A	792	TYR	2.6
1	A	1115	ASP	2.6
1	A	795	PHE	2.6
1	A	286	ASN	2.6
1	A	905	VAL	2.6
1	A	325	LYS	2.6
1	A	304	ILE	2.6
1	A	611	LEU	2.6
1	A	322	TYR	2.6
1	A	916	GLU	2.5
1	A	331	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	994	THR	2.5
1	A	1095	SER	2.5
1	A	1060	PRO	2.5
1	A	20	LEU	2.5
1	A	898	ILE	2.5
1	A	522	ALA	2.5
1	A	902	GLY	2.5
1	A	37	ALA	2.5
1	A	722	LEU	2.4
1	A	85	ASN	2.4
1	A	289	VAL	2.4
1	A	184	PHE	2.4
1	A	652	GLU	2.4
1	A	524	GLN	2.4
1	A	791	PRO	2.3
1	A	515	ASN	2.3
1	A	332	ALA	2.3
1	A	443	SER	2.3
1	A	750	GLN	2.3
1	A	753	LEU	2.3
1	A	1096	ILE	2.3
1	A	174	ASP	2.3
1	A	951	LYS	2.3
1	A	295	LYS	2.3
3	C	28	DC	2.3
1	A	512	ARG	2.3
1	A	476	GLU	2.2
1	A	21	ASN	2.2
1	A	162	TYR	2.2
1	A	897	GLN	2.2
1	A	4	LEU	2.2
1	A	1094	ILE	2.2
1	A	1080	ALA	2.2
1	A	173	LYS	2.2
1	A	175	GLY	2.2
1	A	453	LEU	2.2
1	A	81	LYS	2.2
1	A	5	VAL	2.1
1	A	899	ASN	2.1
1	A	334	ILE	2.1
1	A	1018	GLU	2.1
1	A	1029	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	181	ILE	2.1
1	A	353	TYR	2.1
1	A	1093	ASN	2.1
1	A	399	GLY	2.1
1	A	41	GLU	2.1
1	A	504	ASP	2.1
1	A	433	MET	2.1
1	A	593	ASN	2.0
1	A	80	THR	2.0
1	A	1075	VAL	2.0
1	A	528	LYS	2.0
1	A	851	ASP	2.0
1	A	297	SER	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	BA	B	105	1/1	0.66	0.16	182,182,182,182	0
6	MG	A	1208	1/1	0.84	0.11	45,45,45,45	0
5	BA	B	106	1/1	0.87	0.12	162,162,162,162	0
5	BA	A	1205	1/1	0.88	0.17	156,156,156,156	0
5	BA	C	101	1/1	0.91	0.18	115,115,115,115	0
5	BA	A	1206	1/1	0.92	0.12	152,152,152,152	0
5	BA	A	1203	1/1	0.94	0.08	141,141,141,141	0
5	BA	A	1202	1/1	0.95	0.16	106,106,106,106	0
5	BA	B	104	1/1	0.95	0.14	105,105,105,105	0
6	MG	A	1207	1/1	0.96	0.05	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BA	B	103	1/1	0.96	0.10	125,125,125,125	0
5	BA	B	102	1/1	0.97	0.09	83,83,83,83	0
5	BA	A	1201	1/1	0.97	0.12	94,94,94,94	0
5	BA	A	1204	1/1	0.99	0.06	68,68,68,68	0
5	BA	B	101	1/1	1.00	0.04	40,40,40,40	0
5	BA	D	101	1/1	1.00	0.05	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.