



Full wwPDB X-ray Structure Validation Report i

Nov 19, 2023 – 07:25 PM JST

PDB ID : 6M0X
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 i symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see references ①) were used in the production of this report:

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

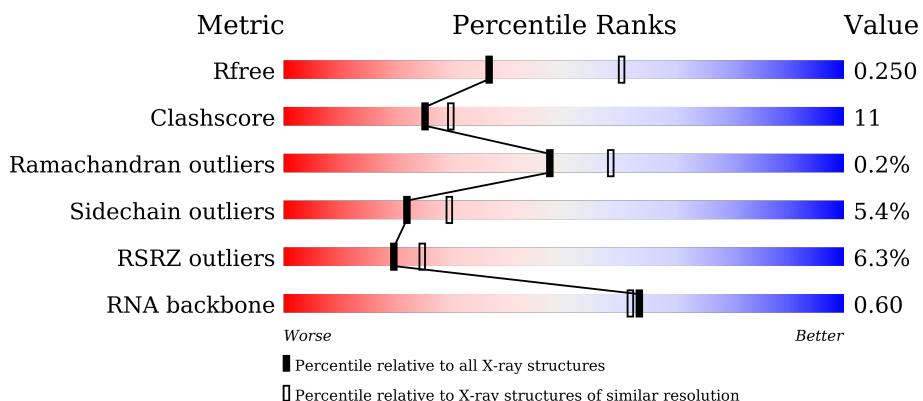
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

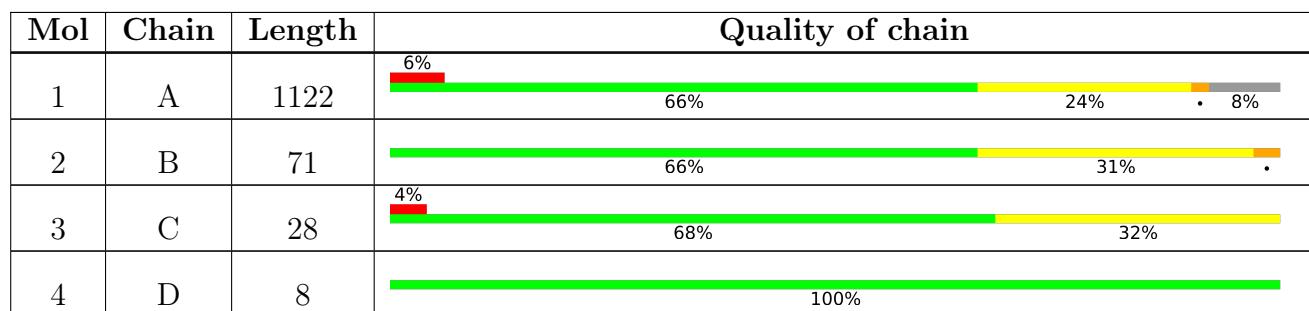
The reported resolution of this entry is 2.56 Å.

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}	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)
RNA backbone	3102	1089 (2.90-2.22)

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.



2 Entry composition [\(i\)](#)

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 8229	N 5213	O 1433	S 1566	17	0	0

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 1500	N 670	O 271	P 488	71	0	0

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

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

- 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 166	N 79	O 38	P 42	7	0	0

- Molecule 5 is BARIUM ION (three-letter code: BA) (formula: Ba).

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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

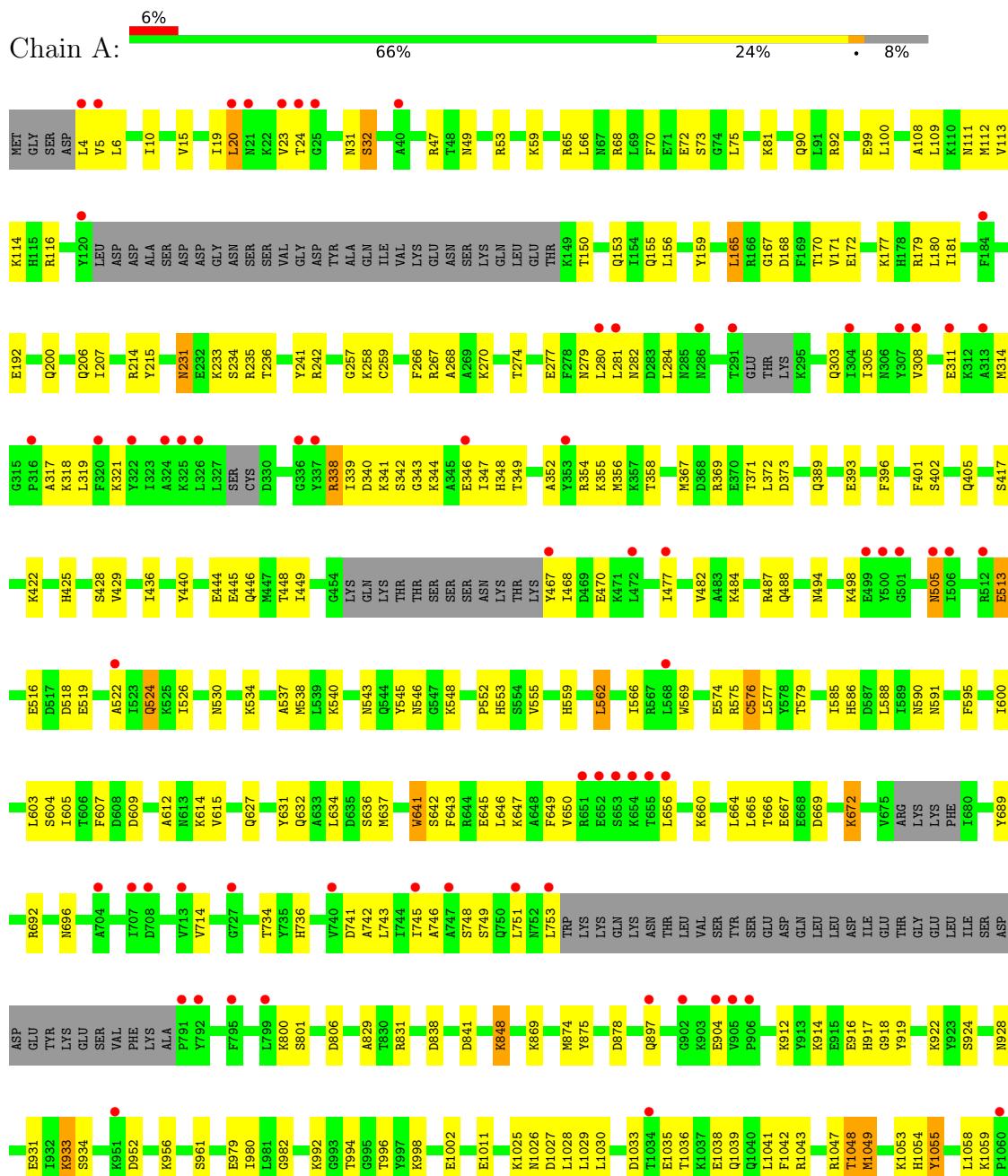
- Molecule 7 is water.

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

Chain B:
66% 31%



- Molecule 3: DNA (28-MER)

Chain C:
4% 68% 32%



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

Chain D:
100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics i

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) 99.8 (48.90-2.56)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.46 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R , R_{free}	0.226 , 0.256 0.225 , 0.250	Depositor DCC
R_{free} test set	2752 reflections (5.09%)	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)	0.30 , 33.5	EDS
L-test for twinning ²	$< L > = 0.49$, $< L^2 > = 0.33$	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 $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [\(i\)](#)

5.1 Standard geometry [\(i\)](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BA, 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	0.51	0/8373	0.58	0/11279
2	B	0.74	0/1679	0.89	0/2615
3	C	1.02	0/625	1.03	0/961
4	D	1.23	0/188	0.95	0/289
All	All	0.61	0/10865	0.69	0/15144

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8229	0	8087	198	0
2	B	1500	0	751	13	0
3	C	561	0	321	12	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	210	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 (210) 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
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:605:ILE:HG12	1:A:672:LYS:HG3	1.56	0.87
1:A:231:ASN:HD22	1:A:231:ASN:C	1.80	0.83
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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:LYS:NZ	1:A:574:GLU:OE2	2.25	0.61
1:A:367:MET:HE3	1:A:371:THR:HG22	1.83	0.61
1:A:874:MET:HG3	1:A:878:ASP:HB3	1.82	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: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:643:PHE:O	1:A:647:LYS:HG3	2.02	0.58
1:A:467:TYR:CE2	1:A:498:LYS:NZ	2.63	0.58
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:O	1:A:20:LEU:HG	2.03	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: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:H6	3:C:23:DT:H5"	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:634:LEU:HA	1:A:637:MET:HE3	1.91	0.53
1:A:168:ASP:N	1:A:168:ASP:OD1	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
1:A:341:LYS:NZ	2:B:7:A:N3	2.54	0.53
3:C:19:DA:H2'	3:C:20:DT:C6	2.44	0.52
1:A:231:ASN:C	1:A:231:ASN:ND2	2.57	0.52
1:A:281:LEU:CD1	1:A:305:ILE:HD11	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1049:MET:CE	1:A:1086:LYS:HD3	2.40	0.52
1:A:445:GLU:O	1:A:449:ILE:HG13	2.10	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
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:745:ILE:O	1:A:748:SER:OG	2.25	0.50
1:A:49:ASN:O	1:A:53:ARG:HG3	2.12	0.50
3:C:24:DA:H5"	3:C:24:DA:H8	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: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:H5"	3:C:14:DG:H8	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:HD3	1:A:498:LYS:HA	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:HE2	1:A:647:LYS:HB3	1.47	0.48
1:A:317:ALA:O	1:A:321:LYS:N	2.34	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:800:LYS:O	1:A:801:SER:C	2.50	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:H	1:A:672:LYS:CD	2.27	0.47
1:A:743:LEU:HD23	1:A:743:LEU:HA	1.76	0.47
1:A:355:LYS:O	1:A:358:THR:OG1	2.22	0.46
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:207:ILE:HG22	1:A:207:ILE:O	2.15	0.46
1:A:519:GLU:O	1:A:522:ALA:N	2.49	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: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: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: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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:367:MET:HE2	1:A:372:LEU:HD13	2.01	0.42
1:A:534:LYS:NZ	2:B:8:G:OP1	2.49	0.42
1:A:585:ILE:HG22	1:A:586:HIS:CD2	2.54	0.42
1:A:1055:TYR:HA	1:A:1088:GLY:HA2	2.02	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:1049:MET:HE3	1:A:1086:LYS:HD3	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:HD12	1:A:468:ILE:H	1.86	0.41
1:A:590:ASN:C	1:A:591:ASN:OD1	2.59	0.41
1:A:339:ILE:HD11	1:A:343:GLY:C	2.41	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:311:GLU:HG2	1:A:318:LYS:HZ2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H6	2:B:68:U:H5"	1.85	0.40
1:A:165:LEU:H	1:A:165:LEU:HG	1.80	0.40
1:A:1033:ASP:CG	1:A:1036:THR:HG22	2.42	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%)	47 58

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%)	822 (95%)	47 (5%)	22 29

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	32	SER
1	A	65	ARG
1	A	112	MET
1	A	113	VAL
1	A	116	ARG
1	A	159	TYR
1	A	165	LEU
1	A	179	ARG
1	A	231	ASN
1	A	236	THR
1	A	303	GLN
1	A	338	ARG
1	A	342	SER
1	A	505	ASN
1	A	513	GLU
1	A	516	GLU
1	A	518	ASP
1	A	524	GLN
1	A	562	LEU
1	A	576	CYS
1	A	636	SER
1	A	641	TRP
1	A	666	THR
1	A	672	LYS
1	A	689	TYR
1	A	692	ARG
1	A	749	SER
1	A	751	LEU
1	A	753	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	806	ASP
1	A	838	ASP
1	A	841	ASP
1	A	848	LYS
1	A	904	GLU
1	A	933	LYS
1	A	952	ASP
1	A	961	SER
1	A	992	LYS
1	A	994	THR
1	A	1027	ASP
1	A	1035	GLU
1	A	1048	THR
1	A	1055	TYR
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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	153	GLN
1	A	200	GLN
1	A	231	ASN
1	A	282	ASN
1	A	310	ASN
1	A	505	ASN
1	A	586	HIS
1	A	590	ASN
1	A	593	ASN
1	A	627	GLN
1	A	696	ASN
1	A	855	GLN
1	A	1054	HIS

5.3.3 RNA (i)

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
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 monosaccharides 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

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1032/1122 (91%)	0.48	71 (6%) 16 22	29, 61, 105, 166	0
2	B	71/71 (100%)	-0.28	0 100 100	29, 41, 72, 93	0
3	C	28/28 (100%)	0.22	1 (3%) 42 51	31, 44, 89, 93	0
4	D	8/8 (100%)	-0.09	0 100 100	33, 35, 39, 43	0
All	All	1139/1229 (92%)	0.42	72 (6%) 20 25	29, 60, 102, 166	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	654	LYS	6.6
1	A	308	VAL	5.6
1	A	905	VAL	5.5
1	A	500	TYR	5.3
1	A	23	VAL	5.2
1	A	747	ALA	4.9
1	A	707	ILE	4.9
1	A	656	LEU	4.8
1	A	652	GLU	4.8
1	A	325	LYS	4.7
1	A	499	GLU	4.6
1	A	708	ASP	4.4
1	A	505	ASN	4.1
1	A	897	GLN	4.1
1	A	792	TYR	4.0
3	C	28	DC	4.0
1	A	322	TYR	3.9
1	A	337	TYR	3.8
1	A	20	LEU	3.7
1	A	5	VAL	3.7
1	A	25	GLY	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	704	ALA	3.5
1	A	727	GLY	3.5
1	A	651	ARG	3.4
1	A	21	ASN	3.4
1	A	467	TYR	3.4
1	A	326	LEU	3.4
1	A	795	PHE	3.2
1	A	316	PRO	3.1
1	A	40	ALA	3.1
1	A	477	ILE	3.0
1	A	4	LEU	3.0
1	A	753	LEU	2.9
1	A	353	TYR	2.9
1	A	311	GLU	2.8
1	A	902	GLY	2.8
1	A	291	THR	2.7
1	A	336	GLY	2.7
1	A	740	VAL	2.7
1	A	313	ALA	2.7
1	A	281	LEU	2.6
1	A	522	ALA	2.6
1	A	1034	THR	2.6
1	A	799	LEU	2.6
1	A	24	THR	2.5
1	A	304	ILE	2.5
1	A	307	TYR	2.5
1	A	745	ILE	2.5
1	A	280	LEU	2.4
1	A	568	LEU	2.3
1	A	751	LEU	2.3
1	A	791	PRO	2.3
1	A	346	GLU	2.3
1	A	512	ARG	2.3
1	A	653	SER	2.3
1	A	906	PRO	2.2
1	A	501	GLY	2.2
1	A	324	ALA	2.2
1	A	506	ILE	2.2
1	A	320	PHE	2.2
1	A	951	LYS	2.2
1	A	1108	HIS	2.1
1	A	655	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1060	PRO	2.1
1	A	472	LEU	2.1
1	A	1092	SER	2.1
1	A	286	ASN	2.1
1	A	904	GLU	2.1
1	A	120	TYR	2.0
1	A	713	VAL	2.0
1	A	1093	ASN	2.0
1	A	184	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BA	B	105	1/1	0.71	0.09	182,182,182,182	0
6	MG	A	1208	1/1	0.82	0.11	45,45,45,45	0
5	BA	B	106	1/1	0.83	0.06	162,162,162,162	0
5	BA	A	1206	1/1	0.84	0.15	152,152,152,152	0
6	MG	A	1207	1/1	0.87	0.15	48,48,48,48	0
5	BA	A	1205	1/1	0.88	0.10	156,156,156,156	0
5	BA	A	1203	1/1	0.88	0.10	141,141,141,141	0
5	BA	C	101	1/1	0.90	0.08	115,115,115,115	0
5	BA	A	1201	1/1	0.96	0.04	94,94,94,94	0
5	BA	B	104	1/1	0.97	0.04	105,105,105,105	0
5	BA	A	1202	1/1	0.97	0.03	106,106,106,106	0
5	BA	B	102	1/1	0.98	0.03	83,83,83,83	0
5	BA	D	101	1/1	0.99	0.07	55,55,55,55	0
5	BA	A	1204	1/1	0.99	0.06	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BA	B	103	1/1	0.99	0.03	125,125,125,125	0
5	BA	B	101	1/1	1.00	0.17	40,40,40,40	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.