



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:06 AM UTC

PDB ID : 6LTR / pdb_00006ltr
Title : Crystal structure of Cas12i2 ternary complex with single Mg²⁺ bound in catalytic pocket
Authors : Huang, X.; Sun, W.; Cheng, Z.; Chen, M.; Li, X.; Wang, J.; Sheng, G.; Gong, W.; Wang, Y.
Deposited on : 2020-01-23
Resolution : 2.51 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
Mogul : 2022.3.0, CSD as543be (2022)
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

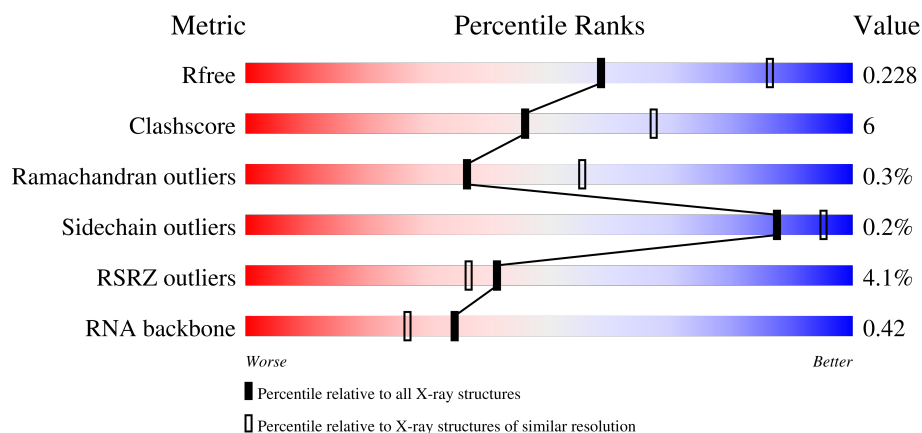
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

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.

Mol	Chain	Length	Quality of chain
1	A	1055	4% 84% 13% ..
2	B	56	4% 54% 21% 12% 12%
3	D	13	8% 46% 38% 15%
4	C	35	3% 60% 29% 11%

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Mol	Chain	Length	Quality of chain
5	E	6	17% 33% 50% 17%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10800 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 Cas12i2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1037	Total	C	N	O	S	0	0	0
			8327	5299	1470	1531	27			

- Molecule 2 is a RNA chain called RNA (56-mer).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	49	Total	C	N	O	P	0	0	0
			1045	469	191	337	48			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	11	Total	C	N	O	P	0	0	0
			217	106	32	69	10			

- Molecule 4 is a DNA chain called DNA (35-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	35	Total	C	N	O	P	0	0	0
			715	341	127	212	35			

- Molecule 5 is a DNA chain called trans ssDNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	5	Total	C	N	O	P	0	0	0
			99	47	19	28	5			

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		

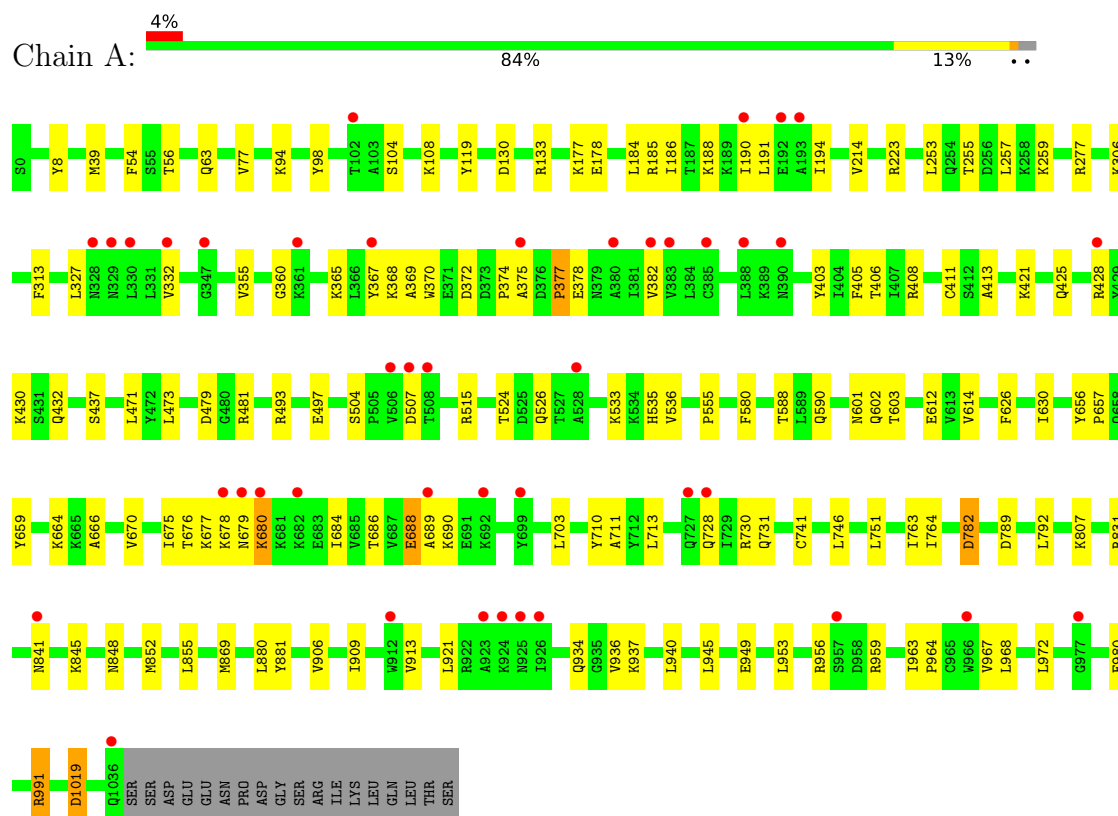
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	259	Total	O	0	0
			259	259		
8	B	65	Total	O	0	0
			65	65		
8	D	20	Total	O	0	0
			20	20		
8	C	47	Total	O	0	0
			47	47		
8	E	1	Total	O	0	0
			1	1		

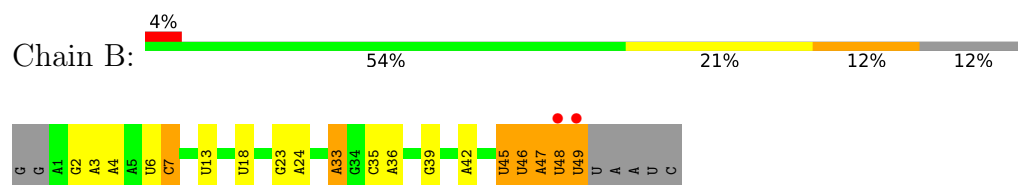
3 Residue-property plots

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: Cas12i2

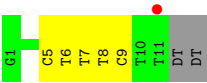


• Molecule 2: RNA (56-mer)



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

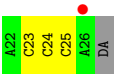




● Molecule 4: DNA (35-MER)



● Molecule 5: trans ssDNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	93.26Å 123.03Å 280.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.74 – 2.51 46.74 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.74-2.51) 98.5 (46.74-2.51)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.61 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874, PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.198 , 0.226 0.199 , 0.228	Depositor DCC
R_{free} test set	2746 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10800	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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, EDO

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	0.42	7/8496 (0.1%)	0.65	3/11469 (0.0%)
2	B	0.42	1/1170 (0.1%)	0.56	1/1822 (0.1%)
3	D	0.33	0/240	0.86	1/368 (0.3%)
4	C	0.39	0/800	1.05	8/1232 (0.6%)
5	E	1.55	3/110 (2.7%)	0.74	0/166
All	All	0.45	11/10816 (0.1%)	0.69	13/15057 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	23	DC	O3'-P	-9.63	1.46	1.61
1	A	676	THR	C-N	7.98	1.43	1.33
5	E	24	DC	O3'-P	-7.54	1.49	1.61
1	A	1019	ASP	C-O	-7.04	1.15	1.24
1	A	675	ILE	C-O	-5.99	1.17	1.24
5	E	24	DC	P-OP2	-5.96	1.36	1.48
1	A	601	ASN	C-O	-5.79	1.16	1.23
1	A	680	LYS	N-CA	5.58	1.53	1.46
1	A	991	ARG	C-O	-5.54	1.16	1.24
2	B	45	U	O3'-P	-5.26	1.53	1.61
1	A	782	ASP	C-O	-5.04	1.18	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	4	DA	C2'-C3'-O3'	-17.94	84.59	111.50
4	C	4	DA	C4'-C3'-O3'	-13.15	90.27	110.00
3	D	9	DC	C2'-C3'-O3'	-7.30	100.55	111.50
4	C	4	DA	C8-N9-C1'	6.75	137.18	127.05
4	C	4	DA	C4-N9-C1'	-6.69	117.02	127.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	LYS	CA-CB-CG	6.38	126.85	114.10
1	A	688	GLU	N-CA-C	6.04	121.70	113.37
4	C	3	DT	C2'-C3'-O3'	-5.86	102.72	111.50
4	C	5	DA	C2'-C3'-O3'	-5.47	103.29	111.50
1	A	677	LYS	CB-CG-CD	-5.42	98.84	111.30
4	C	4	DA	C5'-C4'-O4'	5.21	117.21	109.40
2	B	47	A	C1'-C2'-O2'	-5.17	100.64	108.40
4	C	2	DA	C2'-C3'-O3'	-5.09	103.87	111.50

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	8327	0	8308	97	0
2	B	1045	0	529	10	0
3	D	217	0	128	4	0
4	C	715	0	396	12	0
5	E	99	0	56	1	0
6	A	4	0	6	0	0
7	A	1	0	0	0	0
8	A	259	0	0	6	0
8	B	65	0	0	0	0
8	C	47	0	0	0	0
8	D	20	0	0	0	0
8	E	1	0	0	0	0
All	All	10800	0	9423	114	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 (114) 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)
2:B:46:U:H5''	2:B:46:U:H6	1.18	1.07
2:B:46:U:H5''	2:B:46:U:C6	2.02	0.93
1:A:184:LEU:HG	1:A:188:LYS:HE2	1.54	0.88
1:A:374:PRO:HB3	1:A:408:ARG:HH12	1.42	0.84
4:C:5:DA:H2''	4:C:6:DT:H5'	1.63	0.80
1:A:688:GLU:O	1:A:690:LYS:N	2.19	0.76
1:A:602:GLN:HB2	1:A:751:LEU:HD22	1.74	0.70
1:A:906:VAL:HA	1:A:909:ILE:HD12	1.75	0.68
1:A:533:LYS:O	1:A:536:VAL:HG13	1.94	0.67
1:A:580:PHE:HZ	1:A:869:MET:HG2	1.59	0.67
1:A:524:THR:HG23	1:A:526:GLN:H	1.59	0.66
1:A:945:LEU:HD11	1:A:972:LEU:HD21	1.76	0.66
1:A:178:GLU:HB3	3:D:8:DT:H5''	1.81	0.63
1:A:428:ARG:NH2	8:A:1204:HOH:O	2.31	0.62
1:A:963:ILE:CG1	1:A:967:VAL:HG21	2.29	0.62
1:A:374:PRO:HB3	1:A:408:ARG:NH1	2.14	0.62
1:A:612:GLU:HB2	1:A:630:ILE:HD11	1.81	0.61
1:A:711:ALA:HA	1:A:763:ILE:HD11	1.84	0.59
1:A:688:GLU:C	1:A:690:LYS:H	2.10	0.59
1:A:313:PHE:HE1	1:A:432:GLN:HG2	1.67	0.59
4:C:5:DA:H2'	4:C:6:DT:C6	2.39	0.57
1:A:421:LYS:HE2	1:A:425:GLN:NE2	2.20	0.56
1:A:277:ARG:NH2	8:A:1203:HOH:O	2.30	0.56
1:A:306:LYS:HG3	1:A:437:SER:HA	1.86	0.56
1:A:130:ASP:HA	1:A:133:ARG:HD2	1.87	0.55
1:A:368:LYS:O	1:A:372:ASP:N	2.39	0.55
1:A:688:GLU:O	1:A:688:GLU:HG3	2.07	0.55
2:B:46:U:C6	2:B:46:U:C5'	2.83	0.54
1:A:703:LEU:HD21	1:A:741:CYS:HB3	1.90	0.52
1:A:580:PHE:CZ	1:A:869:MET:HG2	2.43	0.52
1:A:964:PRO:O	1:A:967:VAL:HG22	2.10	0.51
1:A:365:LYS:HG2	1:A:368:LYS:HZ2	1.76	0.51
1:A:185:ARG:HH11	1:A:185:ARG:HG2	1.76	0.51
4:C:32:DC:H2'	4:C:33:DG:C8	2.45	0.51
1:A:365:LYS:O	1:A:368:LYS:HG2	2.11	0.51
1:A:967:VAL:HG23	1:A:968:LEU:N	2.25	0.51
3:D:7:DT:H2'	3:D:8:DT:C6	2.45	0.51
1:A:255:THR:HG22	1:A:259:LYS:HE3	1.93	0.50
1:A:54:PHE:CZ	8:A:1341:HOH:O	2.55	0.50
1:A:54:PHE:CE1	8:A:1341:HOH:O	2.64	0.50
1:A:471:LEU:HB3	1:A:473:LEU:HD21	1.93	0.50
1:A:782:ASP:HB2	4:C:16:DC:OP1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:TYR:OH	1:A:497:GLU:OE1	2.29	0.49
1:A:991:ARG:NH1	1:A:1019:ASP:OD2	2.46	0.49
1:A:186:ILE:O	1:A:190:ILE:HG23	2.12	0.49
1:A:327:LEU:HD21	1:A:421:LYS:HD3	1.94	0.49
1:A:479:ASP:OD2	1:A:481:ARG:HD2	2.13	0.49
1:A:679:ASN:HD21	4:C:5:DA:P	2.36	0.49
1:A:77:VAL:O	1:A:119:TYR:HA	2.12	0.48
1:A:588:THR:O	1:A:590:GLN:NE2	2.46	0.48
1:A:764:ILE:HG23	1:A:792:LEU:HG	1.95	0.48
1:A:845:LYS:HE3	2:B:35:C:OP2	2.14	0.48
1:A:56:THR:HG21	1:A:63:GLN:HB2	1.95	0.48
1:A:253:LEU:O	1:A:257:LEU:HG	2.14	0.48
1:A:375:ALA:O	1:A:377:PRO:HD3	2.14	0.47
1:A:603:THR:HG23	5:E:25:DC:H5''	1.96	0.47
1:A:504:SER:OG	1:A:507:ASP:HB2	2.13	0.47
1:A:332:VAL:HG12	1:A:411:CYS:SG	2.55	0.47
2:B:48:U:H2'	2:B:49:U:C6	2.49	0.47
1:A:104:SER:O	1:A:108:LYS:HG2	2.14	0.47
1:A:921:LEU:HD13	1:A:936:VAL:CG1	2.45	0.46
1:A:507:ASP:HB3	1:A:555:PRO:HG3	1.97	0.46
1:A:968:LEU:HD23	1:A:972:LEU:HD11	1.97	0.46
1:A:403:TYR:O	1:A:406:THR:HB	2.16	0.46
1:A:678:LYS:NZ	1:A:684:ILE:HD11	2.30	0.46
1:A:940:LEU:CD1	1:A:949:GLU:HG3	2.46	0.46
1:A:845:LYS:HB2	1:A:845:LYS:HE2	1.68	0.45
1:A:378:GLU:O	1:A:382:VAL:HG13	2.16	0.45
4:C:1:DA:N6	4:C:2:DA:N6	2.65	0.45
1:A:614:VAL:O	1:A:626:PHE:HB2	2.16	0.45
1:A:177:LYS:NZ	3:D:7:DT:OP1	2.48	0.45
1:A:191:LEU:HA	1:A:194:ILE:HG22	1.98	0.45
1:A:367:TYR:CD1	1:A:413:ALA:HB2	2.52	0.45
3:D:5:DC:H2'	3:D:6:DT:C6	2.52	0.44
1:A:656:TYR:HB3	1:A:657:PRO:HD3	1.98	0.44
1:A:190:ILE:HG22	1:A:214:VAL:HG11	1.98	0.44
1:A:841:ASN:N	2:B:33:A:OP1	2.50	0.44
1:A:223:ARG:HH21	4:C:31:DG:H5'	1.82	0.44
1:A:524:THR:HG23	1:A:526:GLN:N	2.30	0.44
1:A:953:LEU:O	1:A:956:ARG:NH1	2.45	0.44
1:A:493:ARG:NH1	8:A:1211:HOH:O	2.46	0.44
1:A:728:GLN:HA	1:A:731:GLN:OE1	2.18	0.44
1:A:848:ASN:O	1:A:852:MET:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:CYS:HA	1:A:746:LEU:HD12	1.99	0.44
2:B:45:U:H2'	2:B:46:U:C6	2.53	0.43
1:A:369:ALA:HA	1:A:372:ASP:HB3	2.01	0.43
1:A:880:LEU:HG	1:A:881:TYR:CD2	2.54	0.43
1:A:909:ILE:HG23	1:A:913:VAL:HG11	2.00	0.43
1:A:831:ARG:NH2	8:A:1207:HOH:O	2.40	0.43
1:A:956:ARG:HB2	1:A:959:ARG:HG3	2.00	0.43
2:B:35:C:H2'	2:B:36:A:C8	2.53	0.43
1:A:664:LYS:HB2	1:A:664:LYS:HE2	1.73	0.43
1:A:670:VAL:HG21	1:A:713:LEU:HD21	2.00	0.43
1:A:355:VAL:HG12	1:A:360:GLY:HA2	2.00	0.43
4:C:18:DT:H2''	4:C:19:DG:H8	1.83	0.42
1:A:666:ALA:HB1	1:A:710:TYR:CE1	2.53	0.42
1:A:656:TYR:HA	1:A:659:TYR:CE1	2.54	0.42
4:C:13:DC:H2'	4:C:14:DT:C6	2.54	0.42
1:A:730:ARG:NH1	1:A:789:ASP:OD2	2.50	0.42
4:C:13:DC:H2''	4:C:14:DT:H5'	2.01	0.42
1:A:906:VAL:HA	1:A:909:ILE:CD1	2.47	0.42
4:C:1:DA:N6	4:C:2:DA:C6	2.87	0.42
1:A:493:ARG:HB2	2:B:7:C:C4	2.55	0.42
1:A:533:LYS:C	1:A:535:HIS:H	2.28	0.42
1:A:807:LYS:HB3	1:A:855:LEU:HD11	2.02	0.41
1:A:934:GLN:O	1:A:937:LYS:HB2	2.20	0.41
4:C:3:DT:H2''	4:C:4:DA:C5'	2.50	0.41
1:A:313:PHE:CE1	1:A:432:GLN:HG2	2.50	0.41
1:A:370:TRP:CZ3	1:A:405:PHE:HA	2.56	0.41
1:A:678:LYS:HZ2	1:A:684:ILE:HD11	1.85	0.41
1:A:670:VAL:HG13	1:A:690:LYS:HD3	2.03	0.40
1:A:39:MET:HE2	1:A:39:MET:HB3	1.92	0.40
1:A:94:LYS:HG3	1:A:98:TYR:CE2	2.57	0.40
1:A:515:ARG:HD3	2:B:23:G:OP1	2.22	0.40

There are no symmetry-related clashes.

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	
1	A	1035/1055 (98%)	1001 (97%)	31 (3%)	3 (0%)	36	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	689	ALA
1	A	377	PRO
1	A	680	LYS

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	
1	A	888/930 (96%)	886 (100%)	2 (0%)	87	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	686	THR
1	A	980	GLU

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

Mol	Chain	Res	Type
1	A	20	GLN
1	A	109	GLN
1	A	165	ASN
1	A	254	GLN
1	A	459	ASN
1	A	496	GLN
1	A	519	HIS
1	A	679	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	48/56 (85%)	15 (31%)	1 (2%)

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	G
2	B	3	A
2	B	4	A
2	B	6	U
2	B	7	C
2	B	13	U
2	B	18	U
2	B	24	A
2	B	33	A
2	B	39	G
2	B	42	A
2	B	46	U
2	B	47	A
2	B	48	U
2	B	49	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	46	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	EDO	A	1101	-	3,3,3	0.40	0	2,2,2	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	1101	-	-	0/1/1/1	-

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	1037/1055 (98%)	0.28	42 (4%) 41 37	15, 38, 73, 109	0
2	B	49/56 (87%)	-0.42	2 (4%) 41 37	19, 35, 77, 132	0
3	D	11/13 (84%)	-0.15	1 (9%) 15 13	26, 30, 64, 89	0
4	C	35/35 (100%)	-0.14	1 (2%) 53 49	24, 35, 117, 120	0
5	E	5/6 (83%)	0.24	1 (20%) 3 2	35, 35, 42, 76	0
All	All	1137/1165 (97%)	0.24	47 (4%) 41 37	15, 37, 76, 132	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	925	ASN	4.3
1	A	923	ALA	3.7
1	A	508	THR	3.6
3	D	11	DT	3.5
1	A	329	ASN	3.4
1	A	193	ALA	3.4
1	A	1036	GLN	3.2
1	A	328	ASN	3.2
1	A	375	ALA	3.1
1	A	977	GLY	3.0
1	A	957	SER	2.8
1	A	380	ALA	2.8
1	A	689	ALA	2.8
1	A	699	TYR	2.7
1	A	682	LYS	2.7
1	A	528	ALA	2.7
1	A	728	GLN	2.6
1	A	102	THR	2.6
1	A	361	LYS	2.6
1	A	385	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	507	ASP	2.5
1	A	383	VAL	2.5
1	A	390	ASN	2.5
1	A	367	TYR	2.4
2	B	49	U	2.4
1	A	347	GLY	2.4
1	A	506	VAL	2.4
1	A	388	LEU	2.3
1	A	330	LEU	2.3
5	E	26	DA	2.3
4	C	2	DA	2.3
1	A	679	ASN	2.2
1	A	727	GLN	2.2
1	A	192	GLU	2.2
1	A	382	VAL	2.2
1	A	190	ILE	2.1
1	A	428	ARG	2.1
1	A	680	LYS	2.1
1	A	332	VAL	2.1
1	A	966	TRP	2.1
1	A	841	ASN	2.1
1	A	926	ILE	2.1
1	A	692	LYS	2.1
2	B	48	U	2.1
1	A	678	LYS	2.1
1	A	912	TRP	2.0
1	A	924	LYS	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.

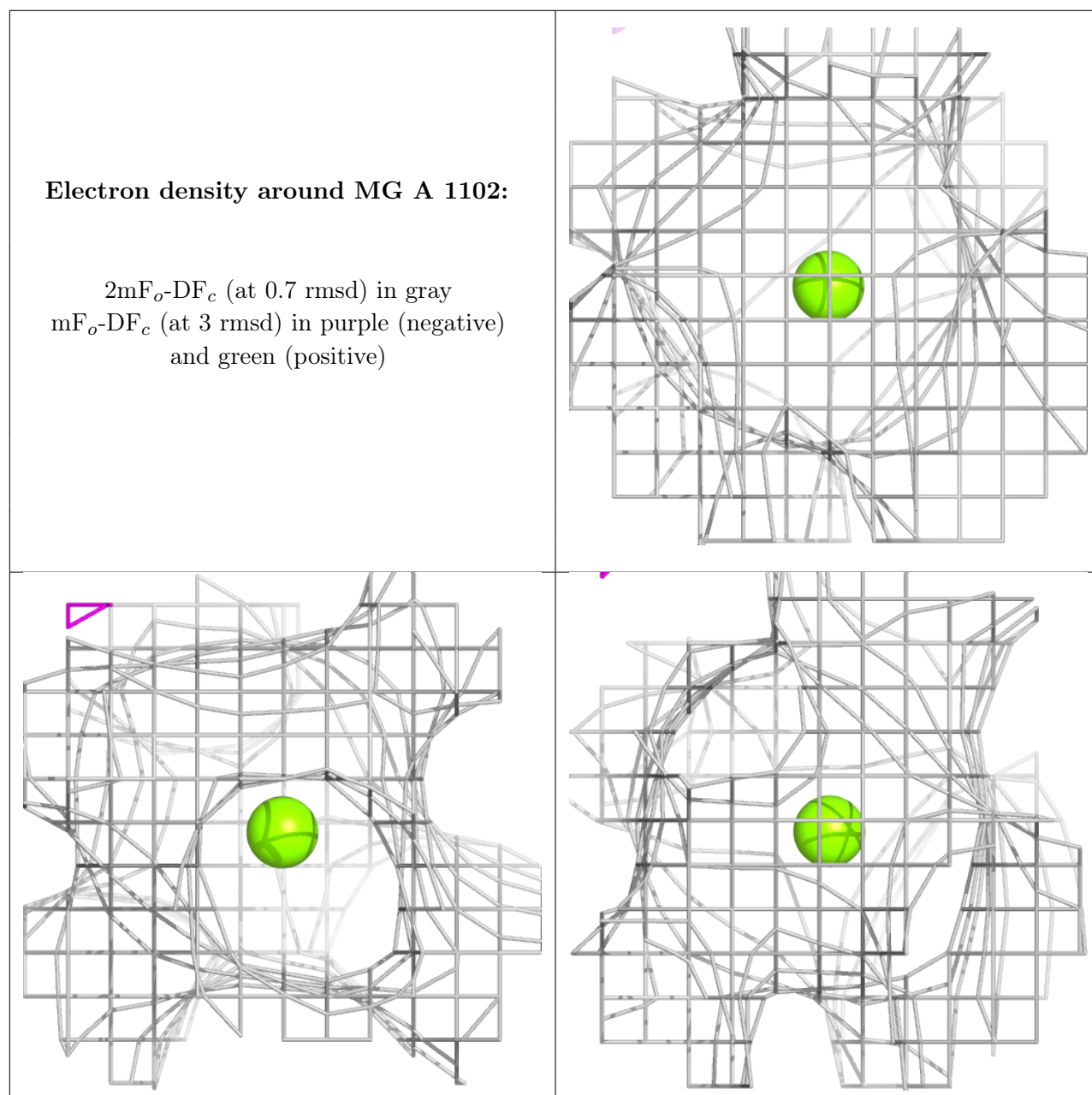
6.4 Ligands [i](#)

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
6	EDO	A	1101	4/4	0.97	0.12	26,26,27,28	0
7	MG	A	1102	1/1	0.99	0.03	15,15,15,15	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.