



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:09 PM UTC

PDB ID : 9MGR / pdb_00009mgr
Title : Crystal structure of PRMT5:MEP50 in complex with MTA and compound 51
Authors : Whittington, D.A.
Deposited on : 2024-12-11
Resolution : 2.07 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

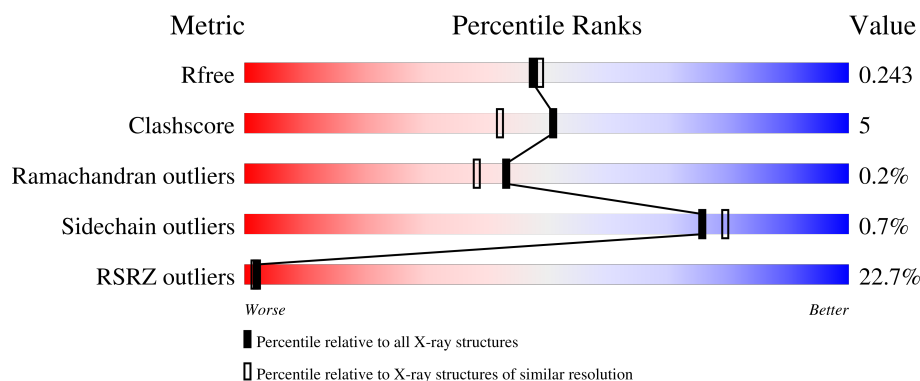
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	645	14% 87% 9% ..
2	B	350	34% 74% 11% 15%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7720 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 Protein arginine N-methyltransferase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	624	Total	C	N	O	S	0	10	0
			5146	3286	892	943	25			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP O14744
A	-6	ASP	-	expression tag	UNP O14744
A	-5	TYR	-	expression tag	UNP O14744
A	-4	LYS	-	expression tag	UNP O14744
A	-3	ASP	-	expression tag	UNP O14744
A	-2	ASP	-	expression tag	UNP O14744
A	-1	ASP	-	expression tag	UNP O14744
A	0	ASP	-	expression tag	UNP O14744
A	1	LYS	-	expression tag	UNP O14744

- Molecule 2 is a protein called Methylosome protein 50.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	298	Total	C	N	O	S	0	8	0
			2317	1450	396	457	14			

There are 9 discrepancies between the modelled and reference sequences:

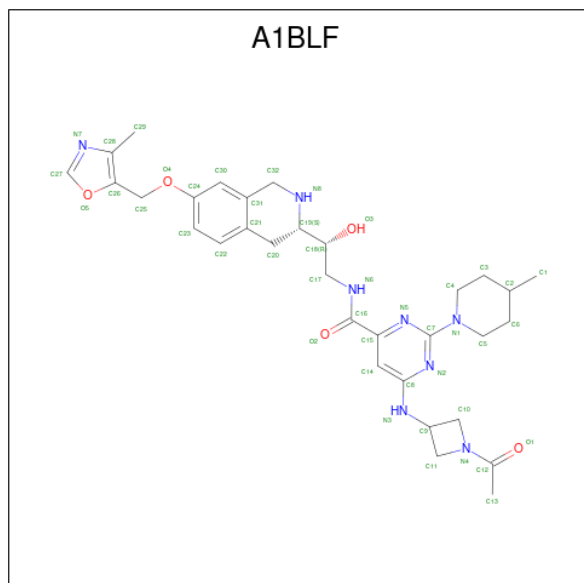
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	initiating methionine	UNP Q9BQA1
B	-6	HIS	-	expression tag	UNP Q9BQA1
B	-5	HIS	-	expression tag	UNP Q9BQA1
B	-4	HIS	-	expression tag	UNP Q9BQA1
B	-3	HIS	-	expression tag	UNP Q9BQA1
B	-2	HIS	-	expression tag	UNP Q9BQA1
B	-1	HIS	-	expression tag	UNP Q9BQA1

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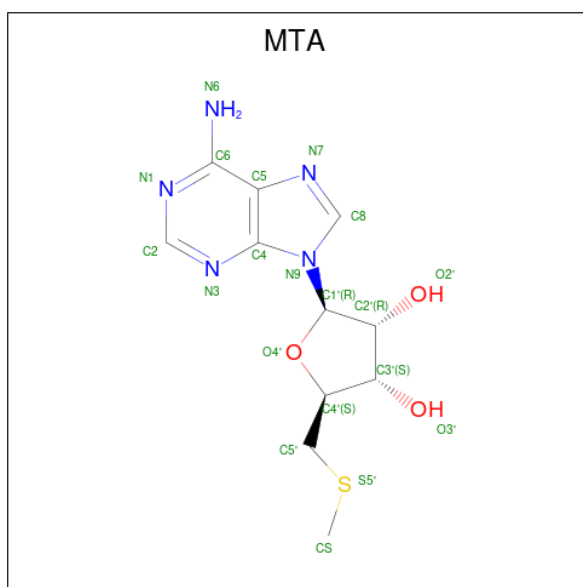
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	expression tag	UNP Q9BQA1
B	1	HIS	-	expression tag	UNP Q9BQA1

- Molecule 3 is 6-[(1-acetylazetidin-3-yl)amino]-N-[(2R)-2-hydroxy-2-[(3S)-7-[(4-methyl-1,3-oxazol-5-yl)methoxy]-1,2,3,4-tetrahydroisoquinolin-3-yl}ethyl]-2-(4-methylpiperidin-1-yl)pyrimidine-4-carboxamide (CCD ID: A1BLF) (formula: C₃₂H₄₂N₈O₅) (labeled as "Ligand of Interest" by depositor).



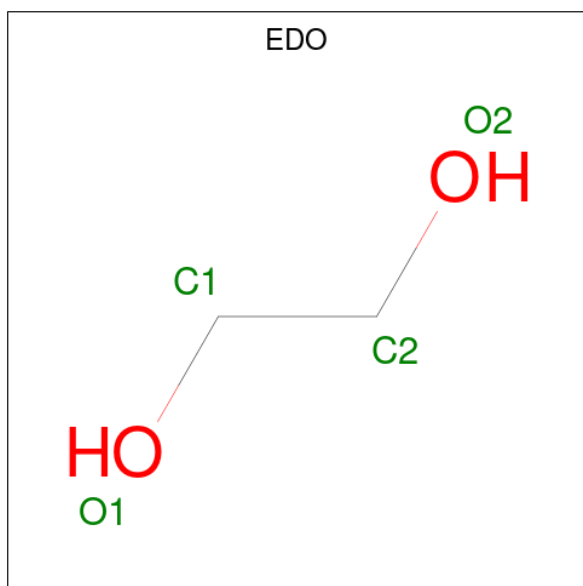
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			45	32	8	5		

- Molecule 4 is 5'-DEOXY-5'-METHYLTHIOADENOSINE (CCD ID: MTA) (formula: C₁₁H₁₅N₅O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

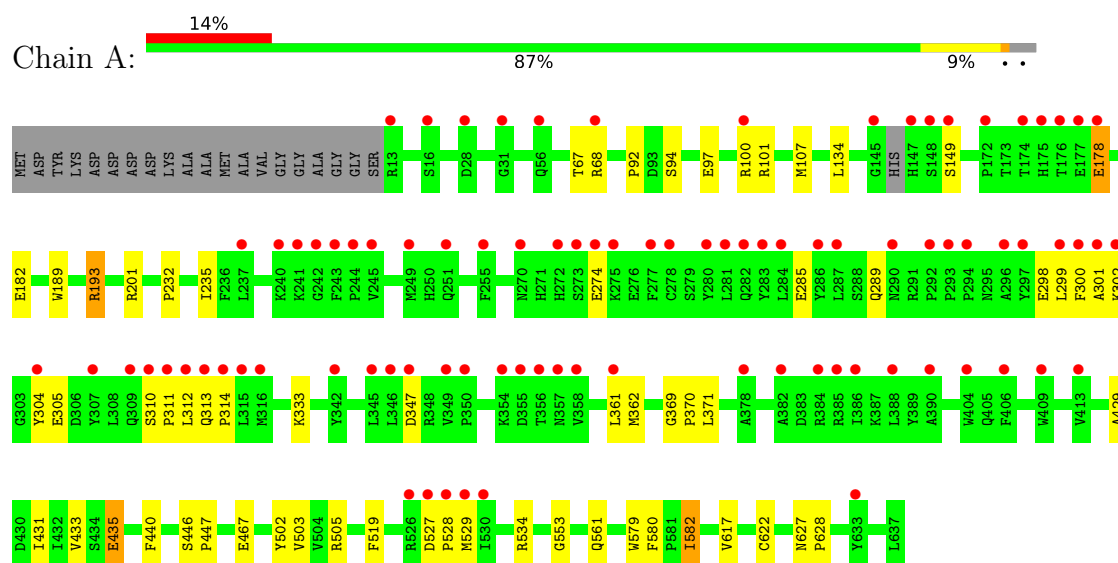
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	115	Total O 115 115	0	0
6	B	17	Total O 17 17	0	0

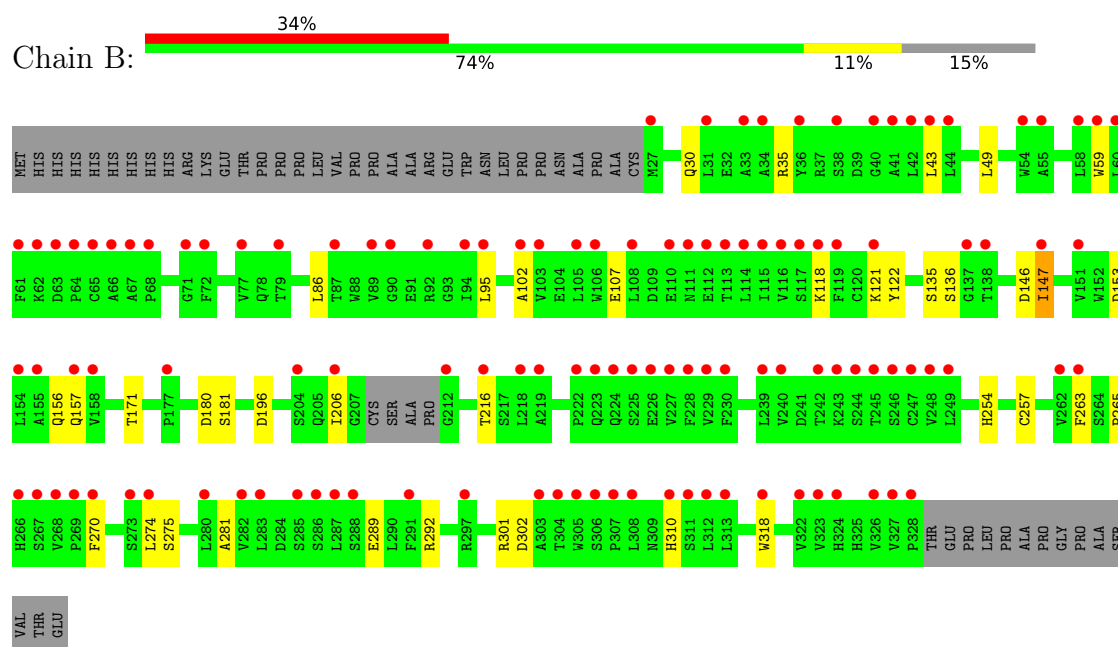
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Protein arginine N-methyltransferase 5



• Molecule 2: Methylosome protein 50



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	102.95Å 137.89Å 178.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.15 – 2.07 109.15 – 2.07	Depositor EDS
% Data completeness (in resolution range)	47.6 (109.15-2.07) 47.6 (109.15-2.07)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.222 , 0.273 (Not available) , 0.243	Depositor DCC
R_{free} test set	1825 reflections (2.36%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7720	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: MTA, A1BLF, 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	0.46	0/5286	0.87	3/7182 (0.0%)
2	B	0.48	0/2369	0.82	0/3231
All	All	0.46	0/7655	0.86	3/10413 (0.0%)

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
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	435	GLU	N-CA-CB	-5.88	103.42	111.65
1	A	440	PHE	N-CA-CB	-5.80	102.33	111.39
1	A	440	PHE	CB-CA-C	5.51	119.98	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	193[A]	ARG	Sidechain

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	5146	0	5044	47	0
2	B	2317	0	2223	29	0
3	A	45	0	0	2	0
4	A	20	0	15	2	0
5	A	56	0	84	5	0
5	B	4	0	6	0	0
6	A	115	0	0	2	0
6	B	17	0	0	0	0
All	All	7720	0	7372	78	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 5.

All (78) 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:135[B]:SER:HB2	2:B:180[B]:ASP:OD1	1.56	1.06
1:A:299:LEU:HA	1:A:302:LYS:HE3	1.61	0.80
1:A:189:TRP:CE2	1:A:193[A]:ARG:HD3	2.20	0.75
1:A:94:SER:O	1:A:100[A]:ARG:HD3	1.93	0.68
2:B:157[B]:GLN:O	2:B:157[B]:GLN:HG3	1.97	0.65
1:A:314:PRO:HD2	6:A:881:HOH:O	1.99	0.63
2:B:102:ALA:HB2	2:B:122:TYR:CD1	2.33	0.62
1:A:301:ALA:HB1	1:A:505:ARG:HG2	1.83	0.61
1:A:299:LEU:HD23	1:A:302:LYS:CE	2.31	0.61
1:A:285:GLU:O	1:A:289:GLN:OE1	2.21	0.58
2:B:135[B]:SER:CB	2:B:180[B]:ASP:OD1	2.44	0.58
1:A:100[B]:ARG:HH12	5:A:708:EDO:C1	2.17	0.58
1:A:371:LEU:HD11	1:A:435:GLU:HB2	1.87	0.56
1:A:347:ASP:OD2	1:A:561[A]:GLN:NE2	2.38	0.56
2:B:157[B]:GLN:O	2:B:157[B]:GLN:CG	2.53	0.56
1:A:333:LYS:HE3	1:A:579:TRP:CH2	2.41	0.55
1:A:301:ALA:HB2	1:A:580:PHE:CZ	2.41	0.55
1:A:100[B]:ARG:HH12	5:A:708:EDO:H12	1.71	0.54
2:B:156:GLN:O	2:B:157[B]:GLN:HG2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:PRO:HG3	1:A:503:VAL:HG23	1.90	0.54
2:B:180[A]:ASP:O	2:B:180[A]:ASP:CG	2.52	0.53
1:A:299:LEU:HD23	1:A:302:LYS:HE2	1.91	0.53
2:B:171:THR:HG21	2:B:216:THR:HA	1.90	0.53
1:A:301:ALA:HA	1:A:304:TYR:HD2	1.74	0.53
1:A:300:PHE:O	1:A:301:ALA:HB3	2.09	0.52
1:A:301:ALA:HB2	1:A:580:PHE:CE1	2.44	0.52
1:A:67:THR:OG1	1:A:68:ARG:N	2.39	0.51
1:A:371:LEU:HD13	1:A:433:VAL:HG12	1.92	0.51
2:B:30:GLN:HG2	2:B:49:LEU:HD12	1.92	0.51
2:B:102:ALA:HB2	2:B:122:TYR:CE1	2.45	0.51
2:B:107:GLU:HB2	2:B:118:LYS:HE2	1.93	0.51
1:A:299:LEU:HA	1:A:302:LYS:CE	2.37	0.50
3:A:701:A1BLF:C25	4:A:702:MTA:HCS1	2.41	0.50
2:B:147[A]:ILE:HG22	2:B:147[A]:ILE:O	2.12	0.50
1:A:310:SER:H	5:A:707:EDO:H12	1.77	0.49
1:A:189:TRP:CZ2	1:A:193[A]:ARG:HD3	2.47	0.49
1:A:369:GLY:N	1:A:370:PRO:CD	2.74	0.49
2:B:86:LEU:HA	2:B:95:LEU:O	2.12	0.49
1:A:553:GLY:HA3	1:A:582:ILE:HG22	1.94	0.48
2:B:146:ASP:O	2:B:147[B]:ILE:HB	2.13	0.47
2:B:301:ARG:HD2	2:B:318:TRP:NE1	2.30	0.47
1:A:298:GLU:C	1:A:300:PHE:H	2.22	0.47
1:A:302:LYS:HB2	5:A:716:EDO:H11	1.96	0.47
1:A:149:SER:OG	1:A:201[A]:ARG:NH2	2.43	0.47
1:A:529:MET:HA	1:A:529:MET:HE2	1.97	0.47
2:B:281:ALA:HB2	2:B:292:ARG:HE	1.79	0.47
1:A:519:PHE:CE1	1:A:534:ARG:HB3	2.50	0.47
2:B:136:SER:N	2:B:180[B]:ASP:OD1	2.48	0.46
1:A:527:ASP:OD1	1:A:528:PRO:HD2	2.14	0.46
1:A:313:GLN:HB3	6:A:801:HOH:O	2.14	0.45
1:A:446:SER:N	1:A:447:PRO:CD	2.79	0.45
3:A:701:A1BLF:C29	4:A:702:MTA:CS	2.95	0.44
2:B:274:LEU:HD21	2:B:302:ASP:C	2.42	0.44
1:A:100[B]:ARG:HH12	5:A:708:EDO:H21	1.82	0.44
2:B:121:LYS:HE3	2:B:157[B]:GLN:HG3	1.99	0.43
2:B:254:HIS:CG	2:B:275:SER:HB2	2.53	0.43
2:B:153:ASP:OD2	2:B:156:GLN:HB2	2.18	0.43
1:A:100[B]:ARG:NH1	1:A:100[B]:ARG:HG2	2.32	0.43
1:A:178:GLU:O	1:A:182:GLU:HG3	2.19	0.43
1:A:100[B]:ARG:CG	1:A:100[B]:ARG:HH11	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ALA:O	1:A:305:GLU:HG3	2.20	0.42
1:A:362:MET:SD	1:A:429:ALA:HB2	2.60	0.42
2:B:263:PHE:HA	2:B:270:PHE:O	2.19	0.42
2:B:265:PRO:HB2	2:B:310:HIS:CE1	2.55	0.42
1:A:627:ASN:N	1:A:628:PRO:CD	2.83	0.42
2:B:181:SER:O	2:B:196:ASP:HA	2.20	0.42
1:A:107:MET:SD	1:A:134:LEU:HD12	2.60	0.42
2:B:43:LEU:HD12	2:B:59:TRP:O	2.20	0.41
2:B:147[B]:ILE:HG22	2:B:147[B]:ILE:O	2.19	0.41
1:A:361:LEU:HD11	1:A:431:ILE:HD12	2.01	0.41
1:A:92:PRO:O	1:A:100[A]:ARG:HG3	2.20	0.41
2:B:35:ARG:NH1	2:B:86:LEU:O	2.54	0.41
2:B:289:GLU:OE2	2:B:292:ARG:HB2	2.21	0.41
1:A:232:PRO:O	1:A:235:ILE:HG12	2.21	0.41
1:A:97:GLU:OE2	1:A:101:ARG:NH1	2.49	0.40
1:A:311:PRO:HD3	1:A:502:TYR:HA	2.03	0.40
1:A:617:VAL:O	1:A:622:CYS:HA	2.21	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	630/645 (98%)	606 (96%)	24 (4%)	0	100	100
2	B	302/350 (86%)	290 (96%)	8 (3%)	4 (1%)	9	3
All	All	932/995 (94%)	896 (96%)	32 (3%)	4 (0%)	43	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147[A]	ILE

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Mol	Chain	Res	Type
2	B	147[B]	ILE
2	B	257[A]	CYS
2	B	257[B]	CYS

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	567/570 (100%)	562 (99%)	5 (1%)	70	74
2	B	262/298 (88%)	261 (100%)	1 (0%)	84	87
All	All	829/868 (96%)	823 (99%)	6 (1%)	76	79

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	GLU
1	A	274	GLU
1	A	312	LEU
1	A	467	GLU
1	A	582	ILE
2	B	206	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	147	HIS
1	A	251	GLN
1	A	263	GLN
1	A	282	GLN
1	A	290	ASN
1	A	309	GLN
1	A	336	GLN
1	A	627	ASN

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Mol	Chain	Res	Type
2	B	169	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 ⓘ

17 ligands are modelled in this entry.

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	$\# Z > 2$
5	EDO	A	704	-	3,3,3	0.12	0	2,2,2	0.32	0
5	EDO	A	716	-	3,3,3	0.07	0	2,2,2	0.20	0
5	EDO	A	713	-	3,3,3	0.10	0	2,2,2	0.19	0
5	EDO	B	401	-	3,3,3	0.07	0	2,2,2	0.17	0
5	EDO	A	703	-	3,3,3	0.07	0	2,2,2	0.26	0
5	EDO	A	706	-	3,3,3	0.17	0	2,2,2	0.52	0
5	EDO	A	709	-	3,3,3	0.07	0	2,2,2	0.17	0
5	EDO	A	708	-	3,3,3	0.12	0	2,2,2	0.11	0
5	EDO	A	705	-	3,3,3	0.06	0	2,2,2	0.08	0
4	MTA	A	702	-	22,22,22	0.21	0	32,32,32	0.31	0
5	EDO	A	712	-	3,3,3	0.08	0	2,2,2	0.26	0
5	EDO	A	710	-	3,3,3	0.10	0	2,2,2	0.20	0
5	EDO	A	714	-	3,3,3	0.10	0	2,2,2	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	707	-	3,3,3	0.06	0	2,2,2	0.19	0
5	EDO	A	715	-	3,3,3	0.08	0	2,2,2	0.17	0
5	EDO	A	711	-	3,3,3	0.08	0	2,2,2	0.16	0
3	A1BLF	A	701	-	47,50,50	0.94	4 (8%)	56,71,71	1.86	12 (21%)

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
5	EDO	A	704	-	-	1/1/1/1	-
5	EDO	A	716	-	-	0/1/1/1	-
5	EDO	A	713	-	-	0/1/1/1	-
5	EDO	B	401	-	-	1/1/1/1	-
5	EDO	A	703	-	-	1/1/1/1	-
5	EDO	A	706	-	-	1/1/1/1	-
5	EDO	A	709	-	-	1/1/1/1	-
5	EDO	A	708	-	-	0/1/1/1	-
5	EDO	A	705	-	-	0/1/1/1	-
4	MTA	A	702	-	-	1/7/23/23	0/3/3/3
5	EDO	A	712	-	-	1/1/1/1	-
5	EDO	A	710	-	-	1/1/1/1	-
5	EDO	A	714	-	-	0/1/1/1	-
5	EDO	A	707	-	-	0/1/1/1	-
5	EDO	A	715	-	-	0/1/1/1	-
5	EDO	A	711	-	-	0/1/1/1	-
3	A1BLF	A	701	-	-	7/30/57/57	0/6/6/6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	A1BLF	C28-N7	-3.36	1.33	1.38
3	A	701	A1BLF	O5-C26	-2.38	1.34	1.37
3	A	701	A1BLF	C25-C26	2.17	1.51	1.48
3	A	701	A1BLF	C7-N1	2.03	1.40	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	A1BLF	C15-N5-C7	7.53	121.51	115.85
3	A	701	A1BLF	O5-C27-N7	-4.15	109.14	115.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	A1BLF	O5-C26-C25	3.93	121.22	117.15
3	A	701	A1BLF	N5-C7-N2	-3.48	120.09	126.27
3	A	701	A1BLF	C25-O4-C24	3.41	123.75	117.63
3	A	701	A1BLF	C5-N1-C7	-2.74	116.26	121.67
3	A	701	A1BLF	N5-C7-N1	2.70	120.96	117.12
3	A	701	A1BLF	C18-C19-N8	-2.38	106.76	110.85
3	A	701	A1BLF	C11-N4-C10	-2.36	93.04	94.69
3	A	701	A1BLF	C14-C15-N5	-2.21	119.57	123.41
3	A	701	A1BLF	C14-C8-N2	-2.18	118.83	123.35
3	A	701	A1BLF	C4-N1-C7	-2.15	117.42	121.67

There are no chirality outliers.

All (15) torsion outliers are listed below:

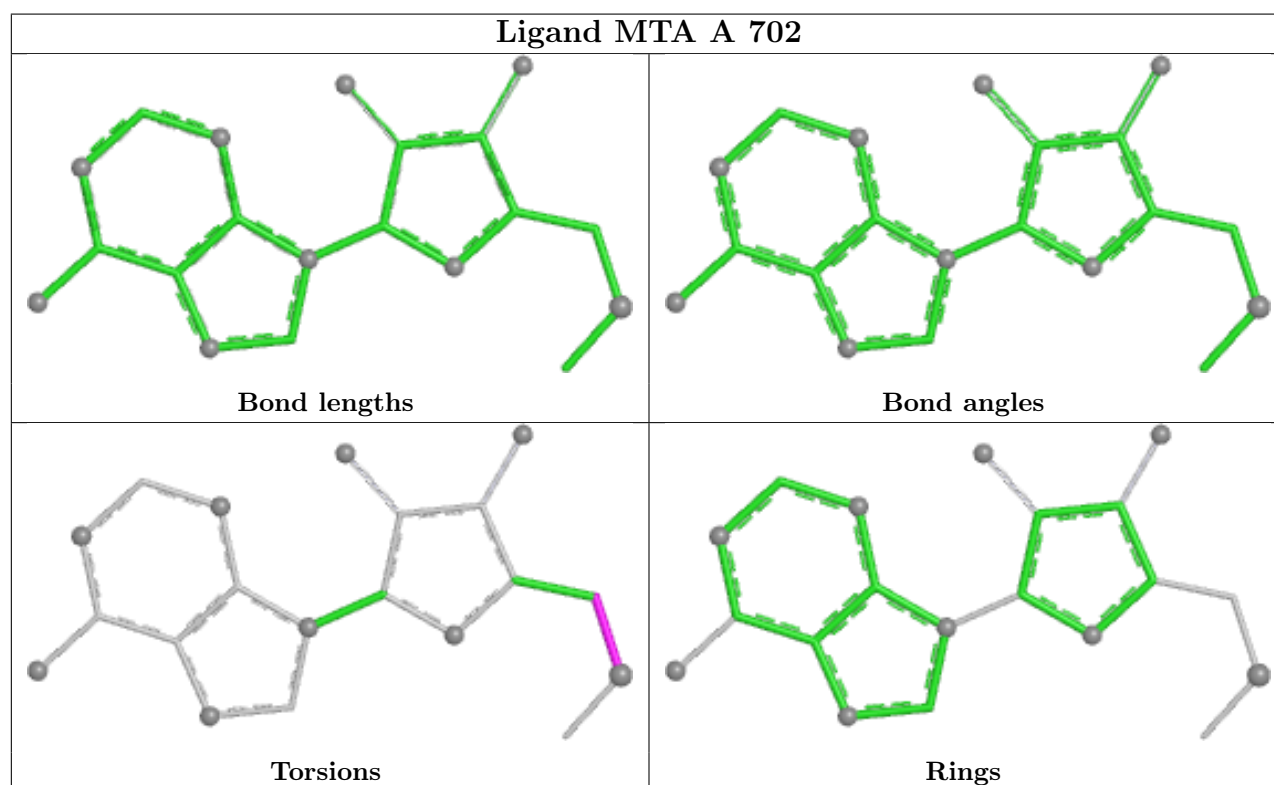
Mol	Chain	Res	Type	Atoms
4	A	702	MTA	C4'-C5'-S5'-CS
3	A	701	A1BLF	C14-C15-C16-N6
3	A	701	A1BLF	C14-C15-C16-O2
3	A	701	A1BLF	N5-C15-C16-O2
3	A	701	A1BLF	N5-C15-C16-N6
3	A	701	A1BLF	N6-C17-C18-C19
5	A	712	EDO	O1-C1-C2-O2
5	A	704	EDO	O1-C1-C2-O2
5	A	703	EDO	O1-C1-C2-O2
5	A	709	EDO	O1-C1-C2-O2
5	A	710	EDO	O1-C1-C2-O2
5	A	706	EDO	O1-C1-C2-O2
5	B	401	EDO	O1-C1-C2-O2
3	A	701	A1BLF	N5-C7-N1-C4
3	A	701	A1BLF	N2-C7-N1-C4

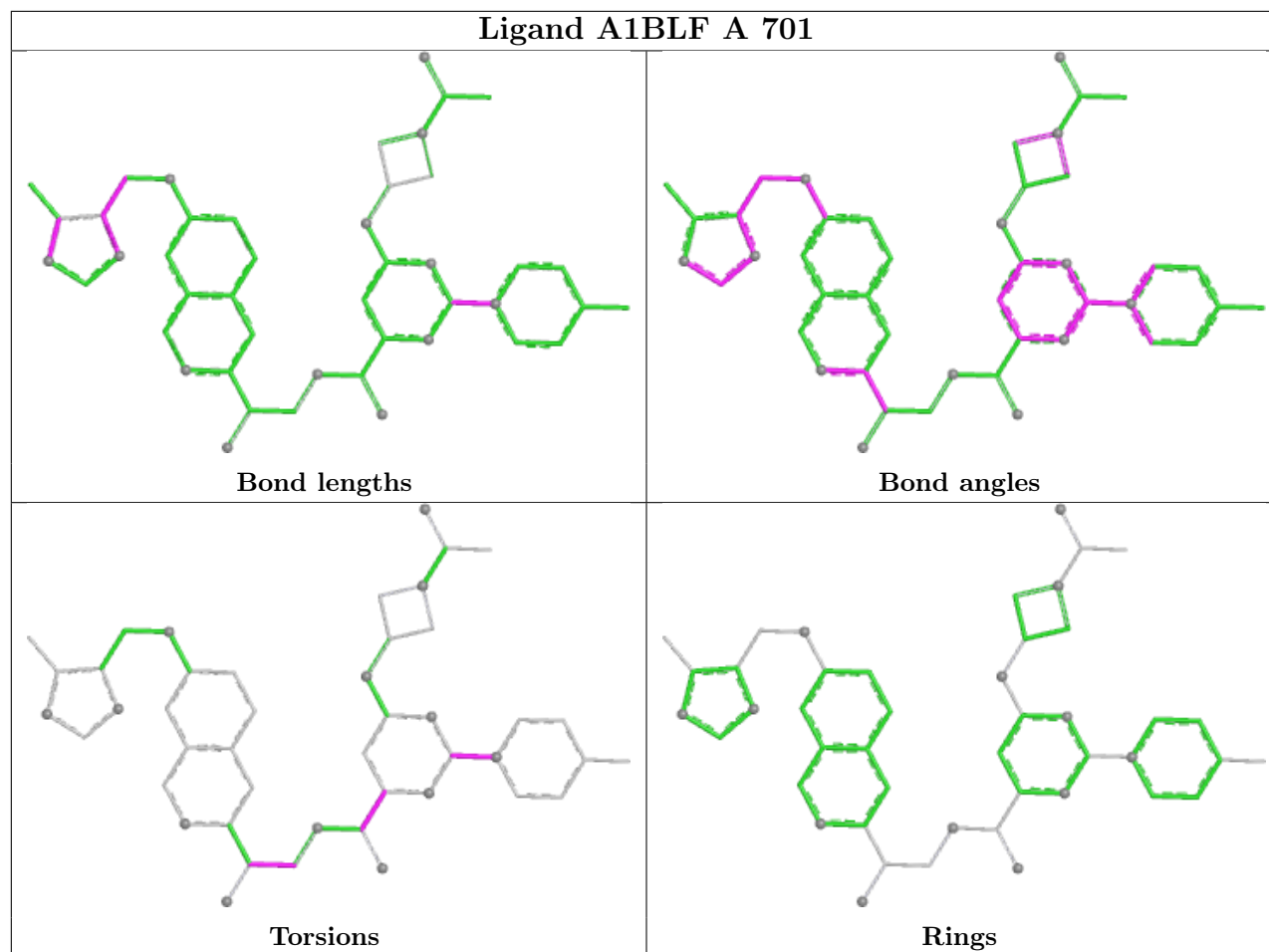
There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	716	EDO	1	0
5	A	708	EDO	3	0
4	A	702	MTA	2	0
5	A	707	EDO	1	0
3	A	701	A1BLF	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	624/645 (96%)	0.81	90 (14%) 6 6	11, 34, 76, 111	10 (1%)
2	B	298/350 (85%)	1.83	119 (39%) 1 0	18, 53, 77, 111	8 (2%)
All	All	922/995 (92%)	1.14	209 (22%) 2 2	11, 41, 77, 111	18 (1%)

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	312	LEU	7.7
1	A	299	LEU	6.7
2	B	248	VAL	6.7
2	B	249	LEU	6.1
1	A	311	PRO	6.0
1	A	314	PRO	6.0
2	B	287	LEU	5.8
1	A	301	ALA	5.7
1	A	300	PHE	5.6
1	A	243	PHE	5.4
1	A	297	TYR	5.2
2	B	245	THR	5.2
1	A	277	PHE	5.0
2	B	246	SER	4.8
2	B	116	VAL	4.7
1	A	292	PRO	4.5
1	A	293	PRO	4.5
2	B	41	ALA	4.5
2	B	114	LEU	4.5
2	B	312	LEU	4.3
2	B	303	ALA	4.1
2	B	268	VAL	4.1
1	A	302	LYS	4.1
2	B	157[A]	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	243	LYS	4.1
1	A	147	HIS	4.1
1	A	294	PRO	4.1
1	A	296	ALA	4.1
2	B	313	LEU	4.0
2	B	308	LEU	4.0
1	A	406	PHE	4.0
2	B	72	PHE	3.9
2	B	61	PHE	3.9
1	A	354	LYS	3.8
1	A	242	GLY	3.7
2	B	282	VAL	3.7
1	A	175	HIS	3.7
1	A	240	LYS	3.7
2	B	108	LEU	3.6
1	A	529	MET	3.6
2	B	64	PRO	3.6
2	B	34	ALA	3.6
1	A	286	TYR	3.5
2	B	247	CYS	3.5
1	A	356	THR	3.5
2	B	326	VAL	3.5
2	B	27	MET	3.4
1	A	275	LYS	3.4
2	B	270	PHE	3.4
2	B	43	LEU	3.4
2	B	266	HIS	3.4
2	B	285	SER	3.4
1	A	307	TYR	3.3
2	B	322	VAL	3.3
2	B	206	ILE	3.3
2	B	90	GLY	3.3
2	B	59	TRP	3.2
1	A	148	SER	3.2
2	B	158	VAL	3.2
1	A	346	LEU	3.2
1	A	174	THR	3.2
2	B	40	GLY	3.2
1	A	283	TYR	3.2
2	B	115	ILE	3.2
2	B	63	ASP	3.2
2	B	244	SER	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	328	PRO	3.2
1	A	290	ASN	3.2
2	B	327	VAL	3.1
1	A	284	LEU	3.1
1	A	633	TYR	3.1
2	B	283	LEU	3.1
2	B	103	VAL	3.1
1	A	404	TRP	3.1
2	B	62	LYS	3.1
1	A	386	ILE	3.1
2	B	106	TRP	3.0
1	A	316	MET	3.0
2	B	87	THR	3.0
1	A	244	PRO	3.0
1	A	527	ASP	3.0
1	A	528	PRO	3.0
2	B	66	ALA	2.9
2	B	218	LEU	2.9
2	B	242	THR	2.9
1	A	56	GLN	2.9
1	A	241	LYS	2.9
1	A	287	LEU	2.9
1	A	315	LEU	2.9
2	B	323	VAL	2.9
2	B	110	GLU	2.9
2	B	286	SER	2.9
2	B	155	ALA	2.9
2	B	225	SER	2.8
2	B	306	SER	2.8
1	A	361	LEU	2.8
1	A	273	SER	2.8
1	A	272	HIS	2.8
2	B	112	GLU	2.8
2	B	102	ALA	2.8
1	A	281	LEU	2.8
2	B	68	PRO	2.8
2	B	229	VAL	2.8
2	B	60	LEU	2.7
2	B	280	LEU	2.7
2	B	269	PRO	2.7
2	B	263	PHE	2.7
2	B	291	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	36	TYR	2.7
2	B	77	VAL	2.7
2	B	226	GLU	2.7
2	B	117	SER	2.7
2	B	288	SER	2.7
2	B	239	LEU	2.7
2	B	307	PRO	2.7
1	A	382	ALA	2.6
1	A	249	MET	2.6
2	B	119	PHE	2.6
2	B	262	VAL	2.6
2	B	65	CYS	2.6
1	A	13	ARG	2.6
2	B	105	LEU	2.6
1	A	304	TYR	2.6
2	B	92	ARG	2.6
1	A	145	GLY	2.6
1	A	357	ASN	2.6
2	B	154	LEU	2.6
1	A	345	LEU	2.6
1	A	342	TYR	2.5
1	A	237	LEU	2.5
2	B	230	PHE	2.5
2	B	137	GLY	2.5
2	B	240	VAL	2.5
2	B	311	SER	2.5
2	B	177	PRO	2.5
2	B	42	LEU	2.5
1	A	526	ARG	2.5
2	B	310	HIS	2.5
2	B	89	VAL	2.4
2	B	138	THR	2.4
2	B	55	ALA	2.4
1	A	388	LEU	2.4
1	A	177	GLU	2.4
1	A	245	VAL	2.4
1	A	409	TRP	2.4
2	B	273	SER	2.4
2	B	118	LYS	2.4
2	B	224	GLN	2.4
1	A	68	ARG	2.4
1	A	413	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	227	VAL	2.4
2	B	212	GLY	2.3
1	A	255	PHE	2.3
1	A	349	VAL	2.3
2	B	151	VAL	2.3
2	B	113	THR	2.3
2	B	219	ALA	2.3
2	B	58	LEU	2.3
1	A	310	SER	2.3
2	B	31	LEU	2.3
1	A	274	GLU	2.3
2	B	222	PRO	2.3
1	A	31	GLY	2.3
2	B	95	LEU	2.3
2	B	94	ILE	2.2
1	A	358	VAL	2.2
1	A	355	ASP	2.2
2	B	267	SER	2.2
1	A	530	ILE	2.2
2	B	147[A]	ILE	2.2
2	B	71	GLY	2.2
2	B	33	ALA	2.2
1	A	278	CYS	2.2
2	B	274	LEU	2.2
1	A	280	TYR	2.2
1	A	309	GLN	2.2
1	A	149	SER	2.2
1	A	176	THR	2.2
1	A	251	GLN	2.1
1	A	313	GLN	2.1
2	B	38	SER	2.1
1	A	270	ASN	2.1
1	A	350	PRO	2.1
2	B	54	TRP	2.1
2	B	318	TRP	2.1
1	A	282	GLN	2.1
2	B	223	GLN	2.1
1	A	378	ALA	2.1
2	B	121	LYS	2.1
2	B	324	HIS	2.1
1	A	385	ARG	2.1
2	B	297	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	228	PHE	2.1
2	B	305	TRP	2.1
1	A	390	ALA	2.1
2	B	67	ALA	2.1
1	A	16	SER	2.1
2	B	79	THR	2.1
2	B	204	SER	2.1
2	B	44	LEU	2.0
2	B	111	ASN	2.0
2	B	304	THR	2.0
1	A	178	GLU	2.0
1	A	28	ASP	2.0
1	A	347	ASP	2.0
1	A	100[A]	ARG	2.0
1	A	384	ARG	2.0
1	A	172	PRO	2.0
2	B	216	THR	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	EDO	A	716	4/4	0.62	0.20	44,44,46,46	0
5	EDO	A	706	4/4	0.63	0.29	44,45,45,47	0
5	EDO	A	714	4/4	0.70	0.17	36,36,37,37	0
5	EDO	A	711	4/4	0.78	0.20	42,42,43,43	0
5	EDO	A	708	4/4	0.80	0.18	47,48,48,49	0
5	EDO	A	707	4/4	0.81	0.19	44,44,44,44	0

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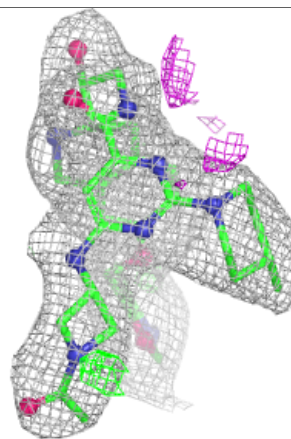
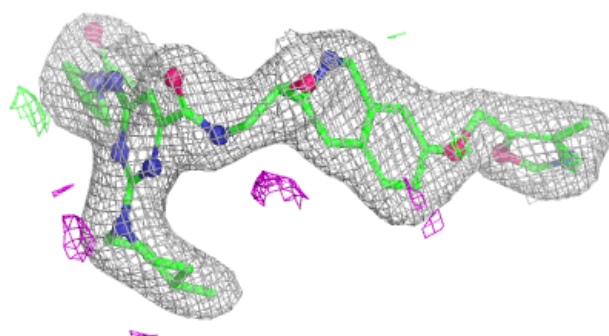
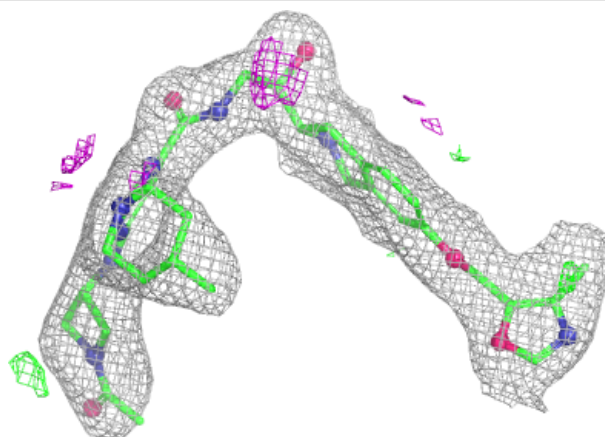
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	A	713	4/4	0.82	0.17	38,39,40,41	0
5	EDO	A	709	4/4	0.83	0.16	42,43,43,43	0
5	EDO	B	401	4/4	0.83	0.19	59,59,60,61	0
5	EDO	A	710	4/4	0.84	0.12	36,36,36,37	0
5	EDO	A	703	4/4	0.84	0.20	40,40,40,40	0
5	EDO	A	704	4/4	0.84	0.22	38,38,39,39	0
5	EDO	A	712	4/4	0.89	0.20	34,34,34,35	0
5	EDO	A	715	4/4	0.90	0.14	53,53,54,54	0
5	EDO	A	705	4/4	0.92	0.08	27,28,28,28	0
3	A1BLF	A	701	45/45	0.94	0.08	25,27,40,45	0
4	MTA	A	702	20/20	0.96	0.08	25,26,28,29	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.

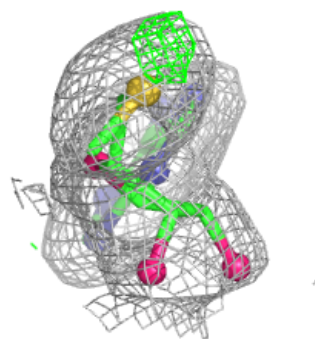
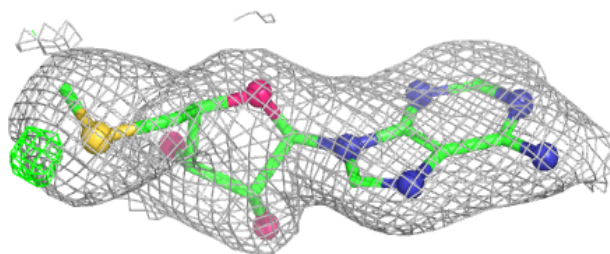
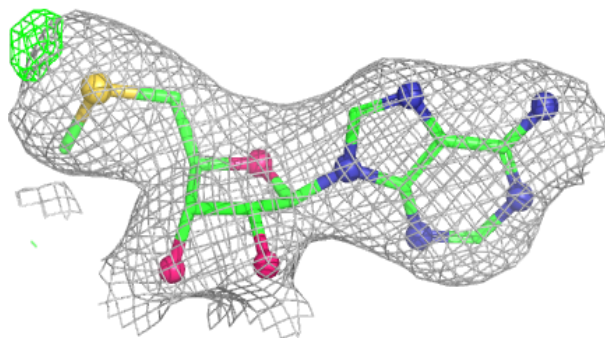
Electron density around A1BLF A 701:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MTA A 702:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.