



Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2026 – 02:10 PM EDT

PDB ID : 9ZL4 / pdb_00009zl4
Title : Crystal structure of PRMT5:MEP50 in complex with MTA and TNG456
Authors : Whittington, D.A.
Deposited on : 2025-12-08
Resolution : 1.95 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

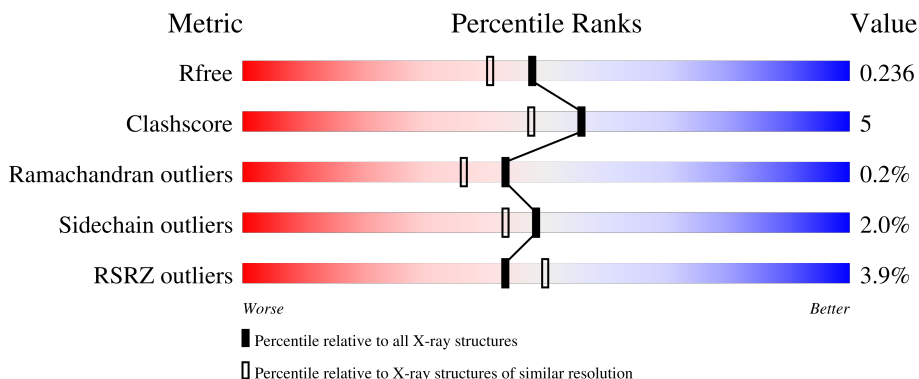
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

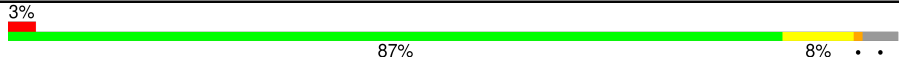
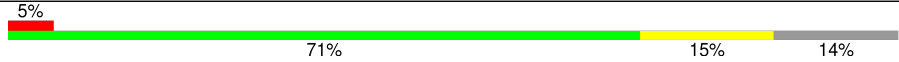
The reported resolution of this entry is 1.95 Å.

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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	
2	B	350	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	EDO	A	717	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8388 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
			Total	C	N	O	S			
1	A	622	5141	3288	882	945	26	0	16	0

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
			Total	C	N	O	S			
2	B	300	2294	1439	391	451	13	0	4	0

There are 9 discrepancies between the modelled and reference sequences:

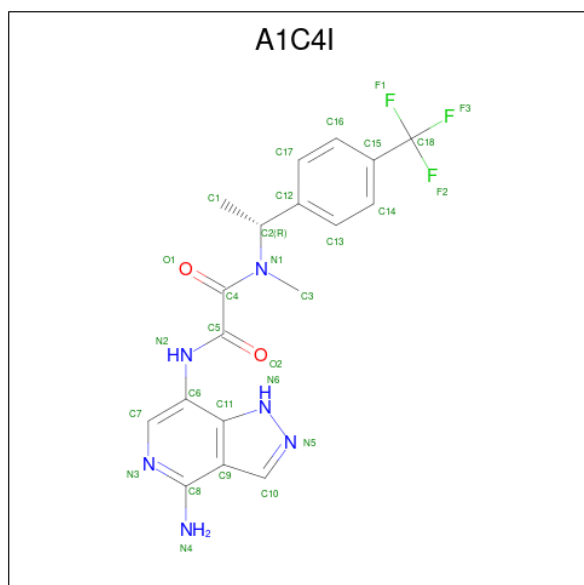
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	initiating methionine	UNP Q9BQA1
B	-6	HIS	-	expression tag	UNP Q9BQA1
B	-5	HIS	-	expression tag	UNP Q9BQA1
B	-4	HIS	-	expression tag	UNP Q9BQA1
B	-3	HIS	-	expression tag	UNP Q9BQA1
B	-2	HIS	-	expression tag	UNP Q9BQA1
B	-1	HIS	-	expression tag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

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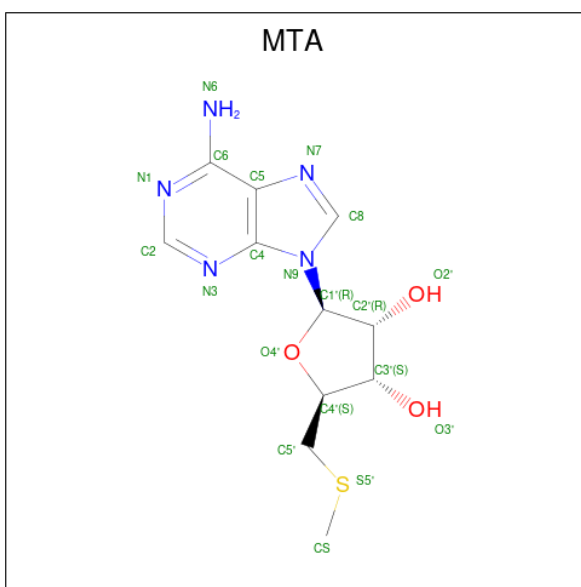
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	expression tag	UNP Q9BQA1
B	1	HIS	-	expression tag	UNP Q9BQA1

- Molecule 3 is N 2 -(4-amino-1H-pyrazolo[4,3-c]pyridin-7-yl)-N 1 -methyl-N 1 -{(1R)-1-[4-(trifluoromethyl)phenyl]ethyl}ethanediamide (CCD ID: A1C4I) (formula: C₁₈H₁₇F₃N₆O₂) (labeled as "Ligand of Interest" by depositor).



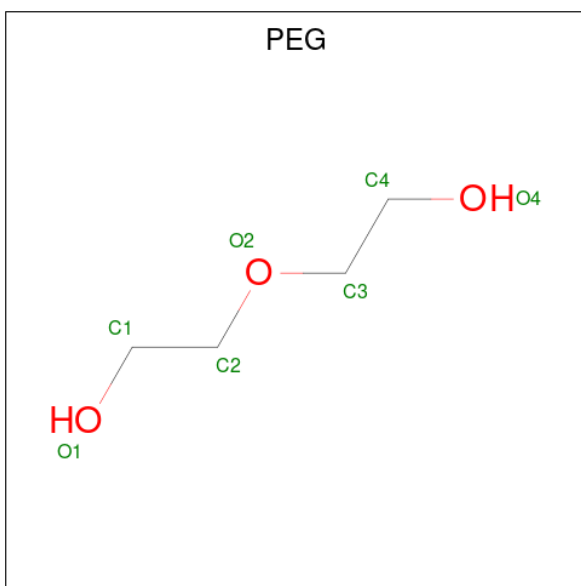
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			29	18	3	6	2		
3	B	1	Total	C	F	N	O	0	0
			29	18	3	6	2		

- 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 DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).

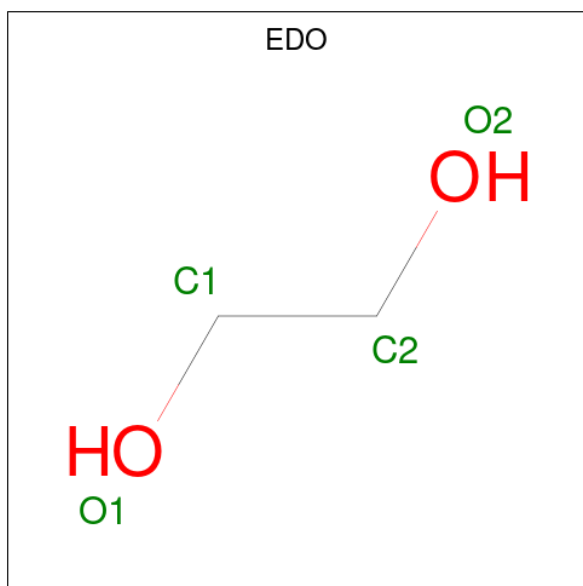


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	4	Total Cl 4 4	0	0

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

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

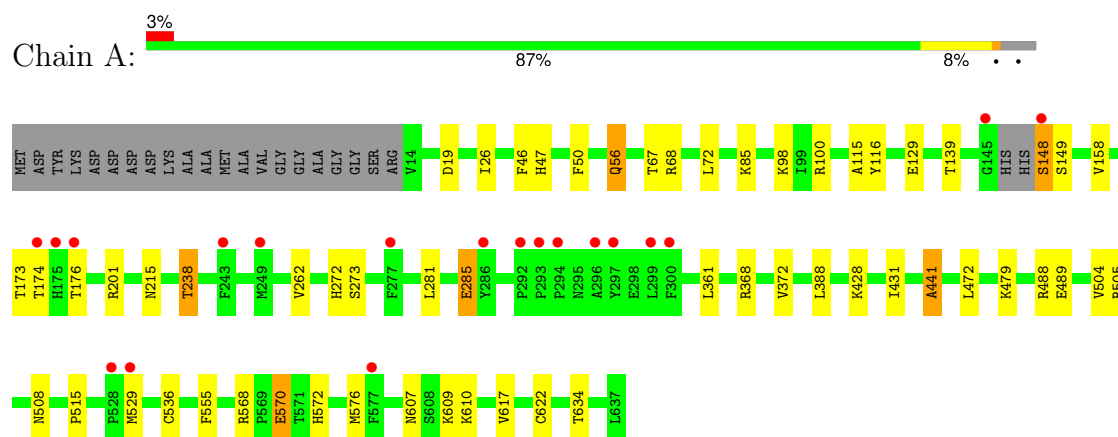
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	538	Total 541	O 541	0	4
8	B	167	Total 167	O 167	0	0

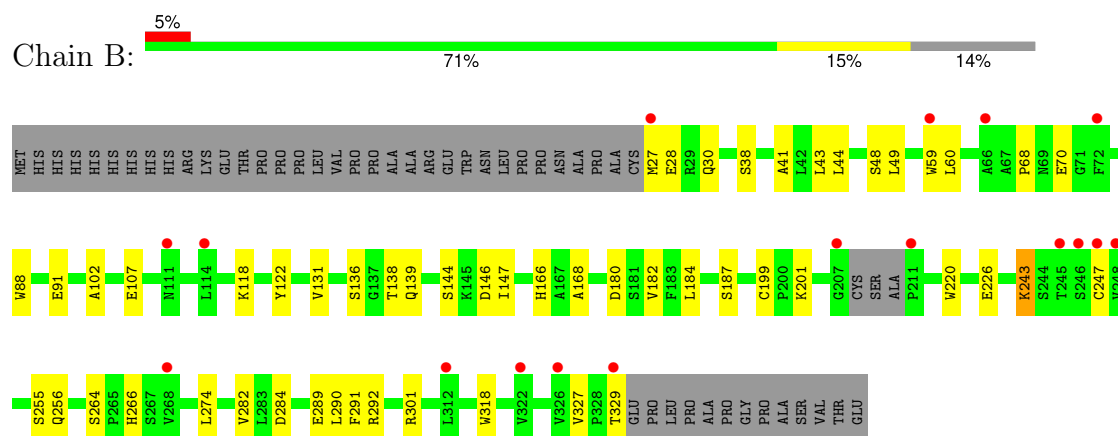
3 Residue-property plots

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: 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	100.51Å 138.26Å 178.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.66 – 1.95 45.66 – 1.95	Depositor EDS
% Data completeness (in resolution range)	72.6 (45.66-1.95) 72.6 (45.66-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0267, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.176 , 0.236 0.181 , 0.236	Depositor DCC
R_{free} test set	3257 reflections (3.61%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.2	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	0.96	EDS
Total number of atoms	8388	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MTA, PEG, A1C4I, EDO, CL

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	0.30	0/5307	0.48	0/7209
2	B	0.27	0/2353	0.48	0/3211
All	All	0.29	0/7660	0.48	0/10420

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

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	5141	0	5062	41	0
2	B	2294	0	2216	29	0
3	A	29	0	0	0	0
3	B	29	0	0	0	0
4	A	20	0	15	0	0
5	A	7	0	10	0	0
6	A	4	0	0	0	0
7	A	116	0	174	16	0
7	B	40	0	60	4	0
8	A	541	0	0	6	0
8	B	167	0	0	2	0
All	All	8388	0	7537	72	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 (72) 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:149[A]:SER:OG	7:A:736:EDO:O2	2.10	0.69
1:A:26:ILE:HD11	1:A:68:ARG:HD3	1.77	0.65
1:A:479:LYS:NZ	7:A:717:EDO:H22	2.11	0.65
1:A:428:LYS:HE2	7:A:722:EDO:H12	1.81	0.63
2:B:27:MET:HE3	2:B:68:PRO:HB2	1.81	0.62
2:B:136:SER:OG	2:B:138:THR:HG22	2.04	0.58
1:A:508:ASN:HD22	7:A:717:EDO:H11	1.68	0.58
2:B:28:GLU:HG2	2:B:48[A]:SER:HB2	1.86	0.58
1:A:508:ASN:ND2	7:A:717:EDO:H11	2.19	0.57
2:B:41:ALA:HB1	2:B:60:LEU:HD11	1.86	0.57
1:A:610[A]:LYS:HD2	1:A:634:THR:HG21	1.88	0.56
1:A:56:GLN:HG2	8:B:530:HOH:O	2.04	0.56
1:A:158:VAL:O	7:A:710:EDO:H11	2.06	0.55
1:A:479:LYS:HZ1	7:A:717:EDO:H22	1.72	0.54
1:A:129:GLU:O	7:A:711:EDO:H22	2.09	0.52
2:B:182:VAL:HG11	7:B:406:EDO:H12	1.91	0.52
1:A:19:ASP:OD1	1:A:85:LYS:NZ	2.43	0.51
7:A:735:EDO:H12	8:A:1262:HOH:O	2.10	0.51
2:B:30:GLN:HG2	2:B:49:LEU:HD12	1.92	0.51
2:B:70:GLU:H	2:B:70:GLU:CD	2.19	0.51
1:A:173:THR:HB	7:A:714:EDO:H11	1.93	0.50
2:B:102:ALA:HB2	2:B:122:TYR:CE1	2.47	0.50
2:B:199:CYS:HB3	7:B:403:EDO:H21	1.93	0.49
2:B:301:ARG:HD2	2:B:318:TRP:NE1	2.28	0.49
1:A:116:TYR:HB2	7:A:716:EDO:H12	1.94	0.49
1:A:47:HIS:HB3	1:A:50:PHE:HB2	1.95	0.48
2:B:144:SER:HB3	2:B:146:ASP:OD1	2.14	0.48
2:B:264:SER:HB2	2:B:266:HIS:HD2	1.78	0.48
1:A:68:ARG:HG3	1:A:72:LEU:HD12	1.95	0.48
2:B:284:ASP:HB3	2:B:290:LEU:HD11	1.96	0.48
1:A:115:ALA:HB2	7:A:736:EDO:H11	1.97	0.47
2:B:327:VAL:O	2:B:329:THR:HG23	2.14	0.47
1:A:98:LYS:HD2	8:B:625:HOH:O	2.14	0.46
1:A:238:THR:HG23	1:A:272:HIS:CD2	2.50	0.46
1:A:100[A]:ARG:NH2	8:A:823[A]:HOH:O	2.44	0.46
1:A:174:THR:HG22	1:A:176:THR:H	1.81	0.46
2:B:243:LYS:HA	2:B:243:LYS:HD2	1.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488[A]:ARG:HG3	1:A:489:GLU:N	2.31	0.46
7:A:713:EDO:H21	8:A:814:HOH:O	2.15	0.46
1:A:139:THR:HG23	8:A:1121:HOH:O	2.15	0.45
1:A:576:MET:HE3	1:A:576:MET:HB3	1.88	0.45
1:A:368:ARG:HH12	7:A:709:EDO:H21	1.81	0.45
2:B:255:SER:C	2:B:256:GLN:HG2	2.42	0.45
1:A:570:GLU:H	1:A:570:GLU:CD	2.25	0.45
2:B:282:VAL:HB	2:B:291:PHE:HB3	1.99	0.45
2:B:166:HIS:ND1	2:B:187:SER:HB3	2.32	0.44
1:A:609[B]:LYS:NZ	8:A:808:HOH:O	2.35	0.44
1:A:536[B]:CYS:HA	7:A:732:EDO:H12	2.00	0.44
1:A:361:LEU:HD11	1:A:431:ILE:HD12	1.99	0.44
2:B:168:ALA:HB1	7:B:408:EDO:H21	1.98	0.44
1:A:281:LEU:O	1:A:285:GLU:HG2	2.17	0.44
2:B:38:SER:OG	2:B:91:GLU:OE2	2.28	0.44
2:B:107:GLU:HB2	2:B:118:LYS:HE3	1.99	0.44
1:A:607:ASN:HD21	1:A:610[A]:LYS:HE3	1.83	0.44
1:A:26:ILE:HD11	1:A:68:ARG:CD	2.44	0.44
1:A:441:ALA:HB2	1:A:555:PHE:HB2	1.99	0.43
1:A:568:ARG:NH2	8:A:833:HOH:O	2.50	0.43
2:B:289:GLU:OE2	2:B:292:ARG:HB2	2.19	0.43
1:A:148:SER:HB2	1:A:201[B]:ARG:NH1	2.34	0.42
2:B:44:LEU:HB2	2:B:59:TRP:HB2	2.01	0.42
1:A:372:VAL:HG13	1:A:388:LEU:HD13	2.01	0.42
2:B:201:LYS:O	7:B:403:EDO:H12	2.20	0.42
1:A:617:VAL:O	1:A:622:CYS:HA	2.20	0.42
1:A:46:PHE:CD2	1:A:67:THR:HB	2.55	0.41
2:B:138:THR:HG23	2:B:139:GLN:HG3	2.01	0.41
2:B:118:LYS:HA	2:B:118:LYS:HD3	1.86	0.41
2:B:107:GLU:CD	2:B:118:LYS:HG3	2.46	0.41
2:B:43:LEU:HB2	2:B:88:TRP:CZ2	2.56	0.41
1:A:572:HIS:HE1	1:A:576:MET:O	2.04	0.40
1:A:505:ARG:HG3	7:A:725:EDO:H11	2.04	0.40
2:B:184:LEU:HG	2:B:220:TRP:CZ2	2.56	0.40
1:A:472:LEU:O	1:A:515:PRO:HA	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	634/645 (98%)	615 (97%)	18 (3%)	1 (0%)	43	36
2	B	300/350 (86%)	292 (97%)	7 (2%)	1 (0%)	36	28
All	All	934/995 (94%)	907 (97%)	25 (3%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147	ILE
1	A	441	ALA

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	571/570 (100%)	561 (98%)	10 (2%)	51	47
2	B	260/298 (87%)	254 (98%)	6 (2%)	44	38
All	All	831/868 (96%)	815 (98%)	16 (2%)	48	45

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	148	SER
1	A	215	ASN
1	A	238	THR

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Mol	Chain	Res	Type
1	A	262	VAL
1	A	273	SER
1	A	285	GLU
1	A	504	VAL
1	A	529	MET
1	A	570	GLU
2	B	131	VAL
2	B	180	ASP
2	B	226	GLU
2	B	243	LYS
2	B	247	CYS
2	B	274	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 47 ligands modelled in this entry, 4 are monoatomic - leaving 43 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
7	EDO	A	732	-	3,3,3	0.52	0	2,2,2	0.25	0
7	EDO	A	717	-	3,3,3	0.47	0	2,2,2	0.20	0
7	EDO	A	725	-	3,3,3	0.46	0	2,2,2	0.18	0
7	EDO	A	714	-	3,3,3	0.54	0	2,2,2	0.35	0
7	EDO	A	729	-	3,3,3	0.42	0	2,2,2	0.64	0
7	EDO	A	716	-	3,3,3	0.41	0	2,2,2	0.57	0
7	EDO	A	733	-	3,3,3	0.48	0	2,2,2	0.30	0
7	EDO	A	708	-	3,3,3	0.43	0	2,2,2	0.66	0
7	EDO	B	405	-	3,3,3	0.47	0	2,2,2	0.18	0
7	EDO	A	730	-	3,3,3	0.55	0	2,2,2	0.28	0
7	EDO	B	407	-	3,3,3	0.47	0	2,2,2	0.32	0
3	A1C4I	B	401	-	31,31,31	2.38	11 (35%)	41,46,46	2.89	11 (26%)
7	EDO	A	719	-	3,3,3	0.59	0	2,2,2	0.12	0
7	EDO	A	722	-	3,3,3	0.52	0	2,2,2	0.28	0
7	EDO	A	735	-	3,3,3	0.56	0	2,2,2	0.25	0
7	EDO	B	403	-	3,3,3	0.48	0	2,2,2	0.20	0
5	PEG	A	703	-	6,6,6	0.21	0	5,5,5	0.11	0
7	EDO	A	720	-	3,3,3	0.41	0	2,2,2	0.53	0
7	EDO	B	402	-	3,3,3	0.41	0	2,2,2	0.44	0
3	A1C4I	A	701	-	31,31,31	2.41	9 (29%)	41,46,46	2.85	17 (41%)
7	EDO	A	727	-	3,3,3	0.43	0	2,2,2	0.44	0
7	EDO	A	724	-	3,3,3	0.57	0	2,2,2	0.18	0
7	EDO	A	713	-	3,3,3	0.52	0	2,2,2	0.34	0
7	EDO	B	410	-	3,3,3	0.45	0	2,2,2	0.56	0
7	EDO	B	409	-	3,3,3	0.44	0	2,2,2	0.33	0
7	EDO	B	411	-	3,3,3	0.59	0	2,2,2	0.24	0
7	EDO	A	712	-	3,3,3	0.38	0	2,2,2	0.63	0
7	EDO	A	710	-	3,3,3	0.57	0	2,2,2	0.40	0
4	MTA	A	702	-	22,22,22	0.56	0	32,32,32	0.58	0
7	EDO	A	726	-	3,3,3	0.57	0	2,2,2	0.30	0
7	EDO	A	709	-	3,3,3	0.39	0	2,2,2	0.21	0
7	EDO	A	734	-	3,3,3	0.35	0	2,2,2	0.71	0
7	EDO	A	711	-	3,3,3	0.47	0	2,2,2	0.39	0
7	EDO	A	715	-	3,3,3	0.48	0	2,2,2	0.34	0
7	EDO	A	718	-	3,3,3	0.49	0	2,2,2	0.16	0
7	EDO	A	721	-	3,3,3	0.63	0	2,2,2	0.16	0
7	EDO	A	731	-	3,3,3	0.52	0	2,2,2	0.29	0
7	EDO	A	736	-	3,3,3	0.73	0	2,2,2	0.21	0
7	EDO	A	728	-	3,3,3	0.49	0	2,2,2	0.43	0
7	EDO	A	723	-	3,3,3	0.51	0	2,2,2	0.14	0
7	EDO	B	404	-	3,3,3	0.42	0	2,2,2	0.30	0
7	EDO	B	406	-	3,3,3	0.42	0	2,2,2	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	B	408	-	3,3,3	0.50	0	2,2,2	0.23	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
7	EDO	A	732	-	-	0/1/1/1	-
7	EDO	A	717	-	-	0/1/1/1	-
7	EDO	A	725	-	-	0/1/1/1	-
7	EDO	A	714	-	-	0/1/1/1	-
7	EDO	A	729	-	-	0/1/1/1	-
7	EDO	A	716	-	-	1/1/1/1	-
7	EDO	A	733	-	-	0/1/1/1	-
7	EDO	A	708	-	-	0/1/1/1	-
7	EDO	B	405	-	-	0/1/1/1	-
7	EDO	A	730	-	-	0/1/1/1	-
7	EDO	B	407	-	-	0/1/1/1	-
3	A1C4I	B	401	-	-	1/26/26/26	0/3/3/3
7	EDO	A	719	-	-	0/1/1/1	-
7	EDO	A	722	-	-	1/1/1/1	-
7	EDO	A	735	-	-	1/1/1/1	-
7	EDO	B	403	-	-	1/1/1/1	-
5	PEG	A	703	-	-	2/4/4/4	-
7	EDO	A	720	-	-	0/1/1/1	-
7	EDO	B	402	-	-	0/1/1/1	-
3	A1C4I	A	701	-	-	1/26/26/26	0/3/3/3
7	EDO	A	727	-	-	1/1/1/1	-
7	EDO	A	724	-	-	1/1/1/1	-
7	EDO	A	713	-	-	1/1/1/1	-
7	EDO	B	410	-	-	0/1/1/1	-
7	EDO	B	409	-	-	0/1/1/1	-
7	EDO	B	411	-	-	1/1/1/1	-
7	EDO	A	712	-	-	1/1/1/1	-
7	EDO	A	710	-	-	1/1/1/1	-
4	MTA	A	702	-	-	0/7/23/23	0/3/3/3
7	EDO	A	726	-	-	1/1/1/1	-
7	EDO	A	709	-	-	0/1/1/1	-
7	EDO	A	734	-	-	1/1/1/1	-
7	EDO	A	711	-	-	1/1/1/1	-
7	EDO	A	715	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	718	-	-	1/1/1/1	-
7	EDO	A	721	-	-	0/1/1/1	-
7	EDO	A	731	-	-	0/1/1/1	-
7	EDO	A	736	-	-	1/1/1/1	-
7	EDO	A	728	-	-	0/1/1/1	-
7	EDO	A	723	-	-	1/1/1/1	-
7	EDO	B	404	-	-	0/1/1/1	-
7	EDO	B	406	-	-	0/1/1/1	-
7	EDO	B	408	-	-	0/1/1/1	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	A1C4I	C11-C6	5.85	1.46	1.40
3	B	401	A1C4I	C11-C6	5.54	1.46	1.40
3	B	401	A1C4I	C11-N6	-5.50	1.31	1.36
3	A	701	A1C4I	C4-C5	-5.40	1.47	1.53
3	B	401	A1C4I	N6-N5	5.31	1.41	1.36
3	A	701	A1C4I	C11-N6	-5.13	1.31	1.36
3	B	401	A1C4I	C10-N5	4.07	1.35	1.32
3	A	701	A1C4I	N6-N5	3.92	1.39	1.36
3	B	401	A1C4I	C9-C11	3.84	1.48	1.41
3	B	401	A1C4I	C9-C10	-3.59	1.38	1.42
3	A	701	A1C4I	C10-N5	3.56	1.34	1.32
3	A	701	A1C4I	C9-C8	3.47	1.46	1.42
3	A	701	A1C4I	C9-C10	-3.41	1.38	1.42
3	A	701	A1C4I	C9-C11	3.18	1.47	1.41
3	B	401	A1C4I	C9-C8	3.02	1.45	1.42
3	B	401	A1C4I	C4-C5	-2.98	1.50	1.53
3	B	401	A1C4I	F1-C18	2.37	1.41	1.33
3	B	401	A1C4I	F2-C18	2.18	1.40	1.33
3	B	401	A1C4I	F3-C18	2.05	1.40	1.33
3	A	701	A1C4I	F1-C18	2.04	1.40	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	A1C4I	C9-C10-N5	-9.95	107.18	111.34
3	B	401	A1C4I	C10-N5-N6	8.62	110.52	106.02
3	A	701	A1C4I	C9-C10-N5	-7.71	108.12	111.34
3	A	701	A1C4I	C10-N5-N6	7.48	109.92	106.02
3	B	401	A1C4I	C11-N6-N5	-6.41	108.34	111.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	A1C4I	C11-N6-N5	-6.17	108.45	111.42
3	A	701	A1C4I	C7-N3-C8	5.46	123.92	118.64
3	B	401	A1C4I	C7-N3-C8	4.93	123.40	118.64
3	B	401	A1C4I	C11-C9-C10	4.58	106.83	104.35
3	A	701	A1C4I	C4-C5-N2	4.43	120.07	112.28
3	B	401	A1C4I	C9-C8-N4	-4.41	117.73	122.42
3	A	701	A1C4I	C1-C2-N1	-3.84	105.20	110.64
3	A	701	A1C4I	C9-C11-C6	-3.75	116.80	121.55
3	B	401	A1C4I	C9-C11-C6	-3.54	117.06	121.55
3	A	701	A1C4I	C17-C12-C13	3.17	122.24	118.30
3	A	701	A1C4I	O2-C5-C4	-2.96	116.70	120.45
3	B	401	A1C4I	C4-C5-N2	2.89	117.36	112.28
3	A	701	A1C4I	C3-N1-C2	2.87	123.09	117.05
3	A	701	A1C4I	C16-C15-C14	2.79	122.20	118.03
3	A	701	A1C4I	C11-C9-C10	2.75	105.83	104.35
3	A	701	A1C4I	F3-C18-C15	-2.73	107.04	112.90
3	A	701	A1C4I	F1-C18-C15	-2.34	107.89	112.90
3	A	701	A1C4I	C14-C13-C12	-2.29	118.89	121.18
3	B	401	A1C4I	F2-C18-C15	-2.23	108.11	112.90
3	A	701	A1C4I	C16-C17-C12	-2.23	118.96	121.18
3	B	401	A1C4I	O1-C4-C5	2.15	118.81	116.72
3	B	401	A1C4I	F3-C18-C15	-2.11	108.37	112.90
3	A	701	A1C4I	O1-C4-C5	2.07	118.73	116.72

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	A1C4I	O1-C4-C5-N2
3	A	701	A1C4I	O1-C4-C5-N2
7	A	712	EDO	O1-C1-C2-O2
7	A	724	EDO	O1-C1-C2-O2
7	A	734	EDO	O1-C1-C2-O2
7	B	411	EDO	O1-C1-C2-O2
7	A	723	EDO	O1-C1-C2-O2
5	A	703	PEG	O1-C1-C2-O2
7	A	711	EDO	O1-C1-C2-O2
7	A	726	EDO	O1-C1-C2-O2
7	A	727	EDO	O1-C1-C2-O2
7	A	735	EDO	O1-C1-C2-O2
5	A	703	PEG	C1-C2-O2-C3
7	A	713	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	A	710	EDO	O1-C1-C2-O2
7	A	716	EDO	O1-C1-C2-O2
7	A	736	EDO	O1-C1-C2-O2
7	B	403	EDO	O1-C1-C2-O2
7	A	718	EDO	O1-C1-C2-O2
7	A	722	EDO	O1-C1-C2-O2

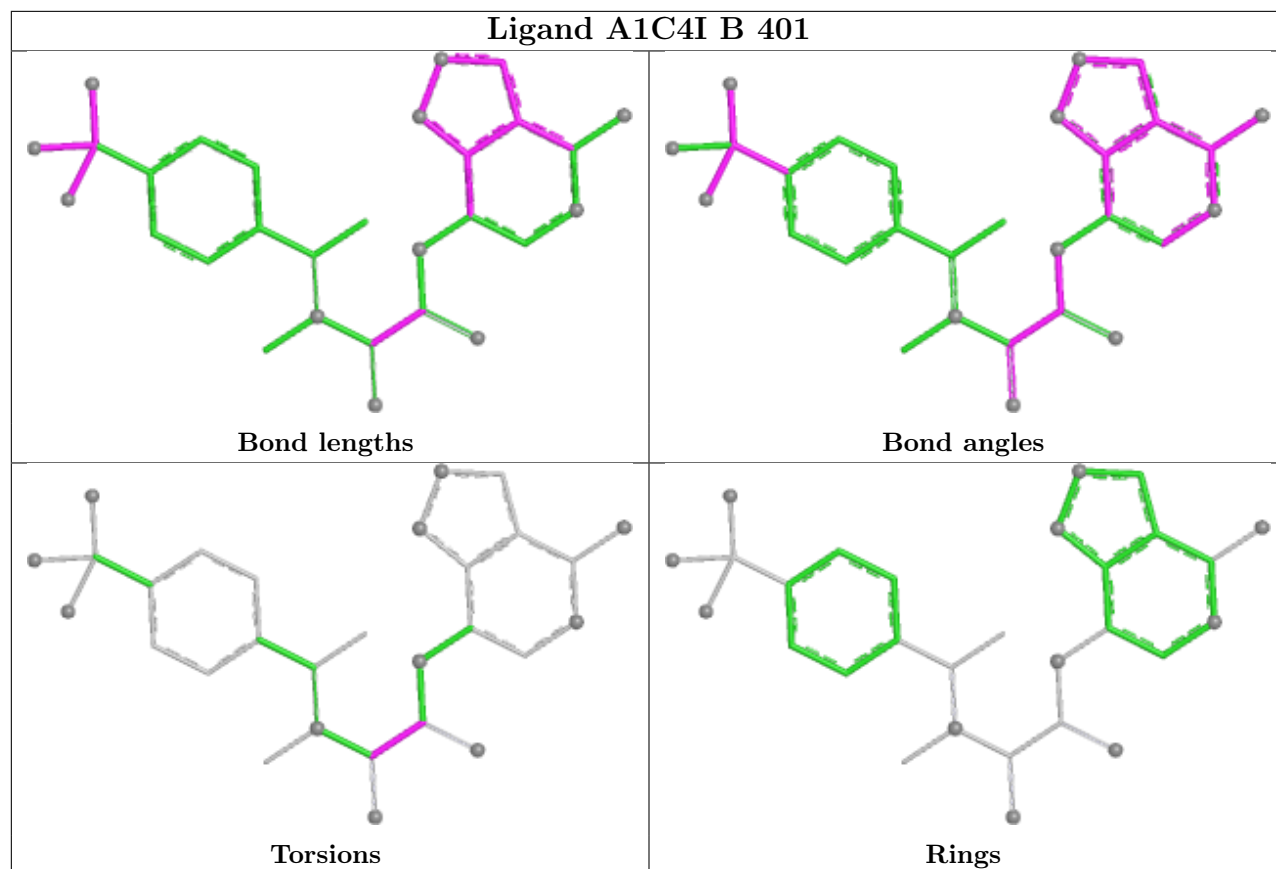
There are no ring outliers.

15 monomers are involved in 20 short contacts:

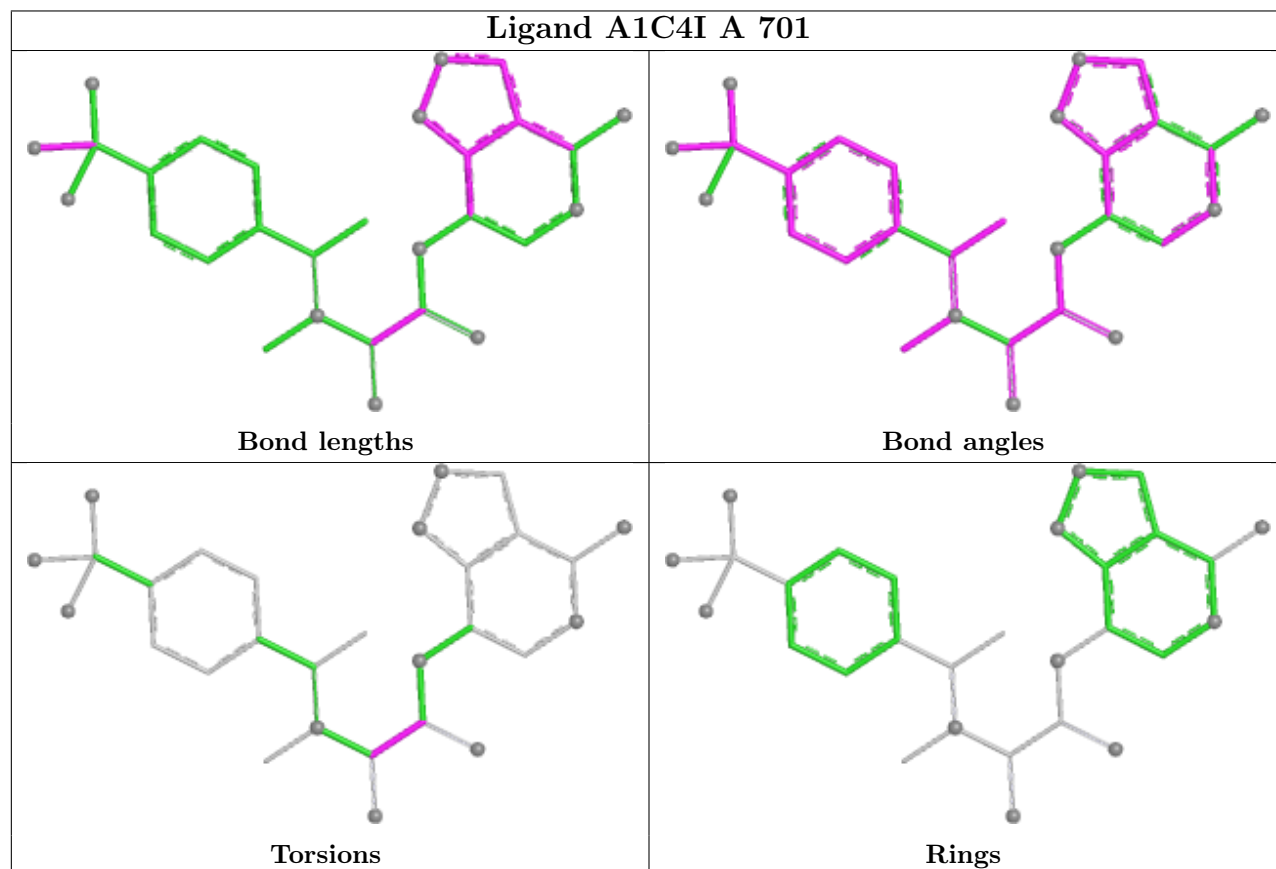
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	732	EDO	1	0
7	A	717	EDO	4	0
7	A	725	EDO	1	0
7	A	714	EDO	1	0
7	A	716	EDO	1	0
7	A	722	EDO	1	0
7	A	735	EDO	1	0
7	B	403	EDO	2	0
7	A	713	EDO	1	0
7	A	710	EDO	1	0
7	A	709	EDO	1	0
7	A	711	EDO	1	0
7	A	736	EDO	2	0
7	B	406	EDO	1	0
7	B	408	EDO	1	0

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.

Ligand A1C4I B 401



Ligand A1C4I A 701



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	622/645 (96%)	-0.17	19 (3%)	51	58	11, 26, 62, 95	16 (2%)
2	B	300/350 (85%)	0.57	17 (5%)	29	34	14, 36, 63, 92	4 (1%)
All	All	922/995 (92%)	0.07	36 (3%)	43	50	11, 30, 62, 95	20 (2%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	TYR	4.2
2	B	207	GLY	4.0
1	A	294	PRO	3.9
1	A	176	THR	3.8
2	B	246	SER	3.8
1	A	292	PRO	3.5
2	B	329	THR	3.5
2	B	211	PRO	3.4
1	A	175	HIS	3.2
1	A	577	PHE	3.2
2	B	245	THR	3.2
1	A	277	PHE	3.1
1	A	299	LEU	3.0
2	B	114	LEU	2.9
1	A	300	PHE	2.8
1	A	145	GLY	2.7
1	A	148	SER	2.7
2	B	312	LEU	2.7
1	A	529	MET	2.6
2	B	72	PHE	2.6
1	A	296	ALA	2.5
1	A	293	PRO	2.5
2	B	111	ASN	2.4
1	A	528	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	248	VAL	2.4
1	A	243	PHE	2.4
1	A	249	MET	2.3
2	B	66	ALA	2.3
1	A	286	TYR	2.3
2	B	247	CYS	2.3
2	B	322	VAL	2.2
2	B	27	MET	2.1
2	B	59	TRP	2.1
1	A	174	THR	2.1
2	B	326	VAL	2.1
2	B	268	VAL	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(\AA^2)	Q<0.9
7	EDO	A	735	4/4	0.73	0.23	43,45,49,53	0
7	EDO	B	407	4/4	0.80	0.15	42,54,58,63	0
7	EDO	B	411	4/4	0.80	0.17	39,42,46,51	0
7	EDO	A	723	4/4	0.81	0.24	51,54,55,58	0
3	A1C4I	B	401	29/29	0.82	0.13	35,52,58,62	0
5	PEG	A	703	7/7	0.82	0.13	44,47,57,58	0
7	EDO	A	734	4/4	0.83	0.17	39,44,47,49	0
7	EDO	A	733	4/4	0.83	0.12	48,53,59,60	0
7	EDO	A	729	4/4	0.84	0.14	34,35,36,53	0
7	EDO	B	410	4/4	0.84	0.15	44,45,46,58	0
7	EDO	B	405	4/4	0.84	0.22	46,50,52,59	0

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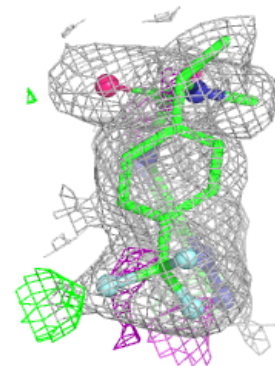
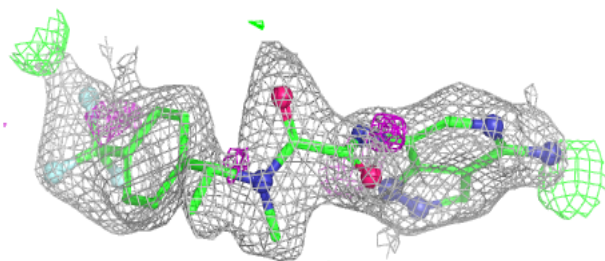
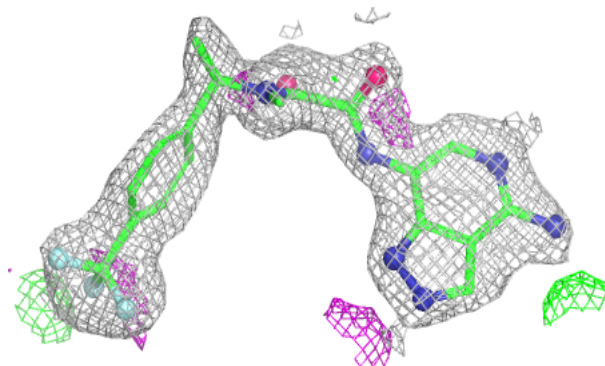
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	EDO	A	718	4/4	0.85	0.12	41,49,51,59	0
7	EDO	A	713	4/4	0.86	0.18	36,39,46,48	0
7	EDO	A	715	4/4	0.86	0.14	41,47,53,60	0
7	EDO	A	719	4/4	0.87	0.16	40,40,42,43	0
7	EDO	A	721	4/4	0.88	0.16	36,39,40,49	0
7	EDO	A	736	4/4	0.88	0.10	22,28,28,32	0
7	EDO	A	730	4/4	0.88	0.21	32,36,41,47	0
7	EDO	B	404	4/4	0.89	0.11	40,41,44,49	0
7	EDO	A	722	4/4	0.89	0.12	47,48,56,56	0
7	EDO	A	710	4/4	0.89	0.13	27,32,33,36	0
7	EDO	A	714	4/4	0.89	0.21	38,40,43,46	0
7	EDO	A	711	4/4	0.89	0.11	32,32,34,42	0
7	EDO	B	406	4/4	0.90	0.13	41,47,50,52	0
7	EDO	A	724	4/4	0.90	0.15	31,38,42,48	0
7	EDO	B	409	4/4	0.90	0.11	37,49,51,55	0
7	EDO	A	717	4/4	0.90	0.10	33,37,41,48	0
6	CL	A	705	1/1	0.90	0.10	57,57,57,57	0
7	EDO	B	408	4/4	0.91	0.14	38,43,44,46	0
7	EDO	A	716	4/4	0.91	0.16	30,30,32,46	0
7	EDO	B	403	4/4	0.92	0.14	36,39,40,55	0
7	EDO	A	712	4/4	0.92	0.14	28,34,37,41	0
7	EDO	A	727	4/4	0.92	0.15	28,37,46,46	0
7	EDO	A	720	4/4	0.93	0.08	39,40,41,43	0
7	EDO	A	726	4/4	0.93	0.16	23,30,36,39	0
7	EDO	A	732	4/4	0.93	0.10	29,29,34,42	0
6	CL	A	707	1/1	0.93	0.10	51,51,51,51	0
7	EDO	A	725	4/4	0.94	0.13	29,29,31,35	0
7	EDO	A	728	4/4	0.94	0.14	25,26,35,45	0
6	CL	A	704	1/1	0.94	0.12	53,53,53,53	0
7	EDO	A	709	4/4	0.95	0.07	29,31,31,32	0
3	A1C4I	A	701	29/29	0.95	0.07	16,24,45,51	0
7	EDO	A	708	4/4	0.96	0.06	16,18,18,19	0
6	CL	A	706	1/1	0.96	0.10	43,43,43,43	0
7	EDO	B	402	4/4	0.96	0.07	31,34,36,37	0
7	EDO	A	731	4/4	0.97	0.07	21,26,26,27	0
4	MTA	A	702	20/20	0.98	0.04	16,18,26,31	0

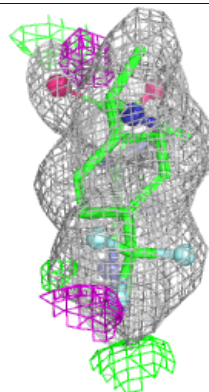
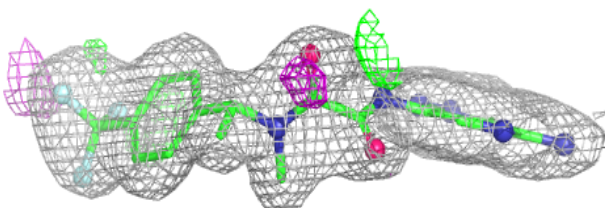
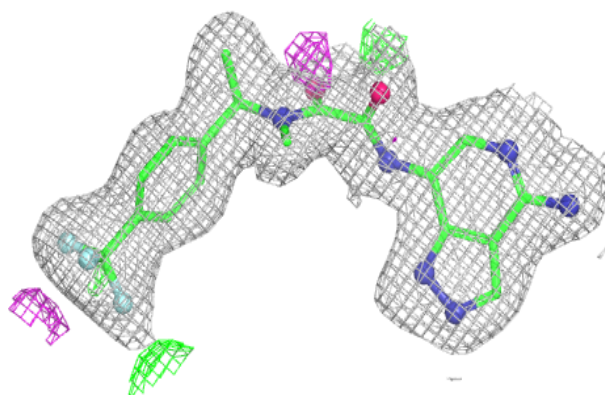
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1C4I B 401:

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

**Electron density around A1C4I 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.