



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2021 – 10:09 AM EDT

PDB ID : 7KWE
Title : Crystal structure of the catalytic domain of human PDE3A bound to DNMDP
Authors : Horner, S.W.; Garvie, C.
Deposited on : 2020-11-30
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.20
buster-report : 1.1.7 (2018)
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) : 2.20

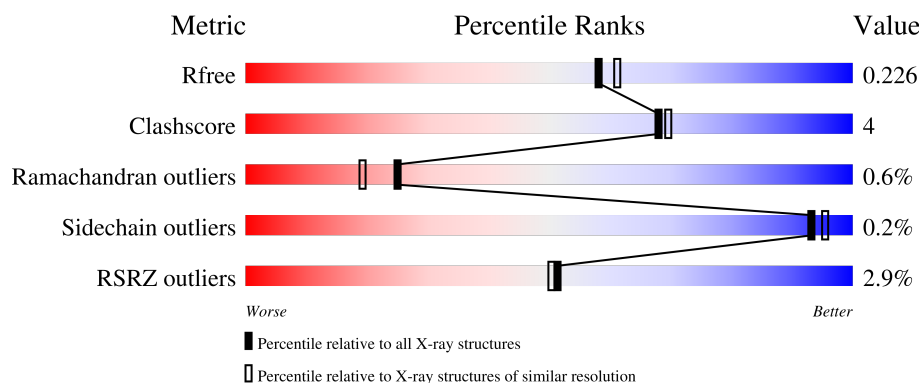
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	380	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div></div> </div> <div>..</div> </div>
1	B	380	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div></div> </div> <div>.</div> </div>
1	C	380	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div></div> </div> <div>.</div> </div>
1	D	380	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div></div> </div> <div>..</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12297 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 cGMP-inhibited 3',5'-cyclic phosphodiesterase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	1	0
			2940	1896	492	533	19			
1	D	371	Total	C	N	O	S	0	1	0
			2990	1924	503	544	19			
1	C	365	Total	C	N	O	S	0	1	0
			2942	1896	493	534	19			
1	B	365	Total	C	N	O	S	0	1	0
			2954	1904	497	534	19			

There are 52 discrepancies between the modelled and reference sequences:

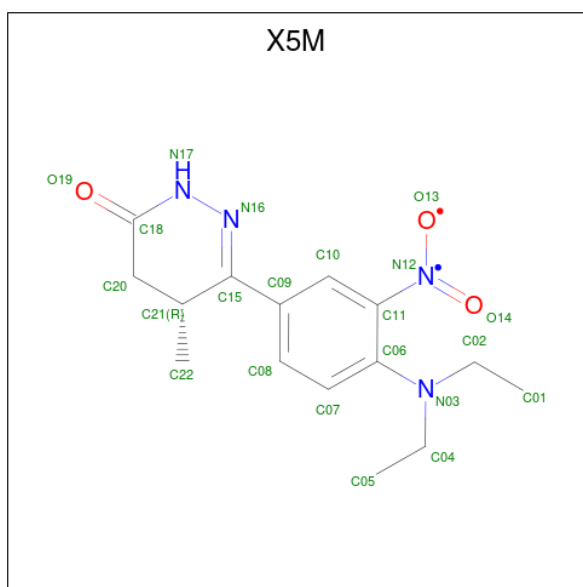
Chain	Residue	Modelled	Actual	Comment	Reference
A	668	GLY	-	expression tag	UNP Q14432
A	795	GLY	-	linker	UNP Q14432
A	796	GLY	-	linker	UNP Q14432
A	797	SER	-	linker	UNP Q14432
A	798	GLY	-	linker	UNP Q14432
A	799	GLY	-	linker	UNP Q14432
A	800	SER	-	linker	UNP Q14432
A	1062	GLY	-	linker	UNP Q14432
A	1063	GLY	-	linker	UNP Q14432
A	1064	SER	-	linker	UNP Q14432
A	1065	GLY	-	linker	UNP Q14432
A	1066	GLY	-	linker	UNP Q14432
A	1067	SER	-	linker	UNP Q14432
D	668	GLY	-	expression tag	UNP Q14432
D	780	GLY	-	linker	UNP Q14432
D	781	GLY	-	linker	UNP Q14432
D	782	SER	-	linker	UNP Q14432
D	783	GLY	-	linker	UNP Q14432
D	784	GLY	-	linker	UNP Q14432
D	785	SER	-	linker	UNP Q14432
D	1062	GLY	-	linker	UNP Q14432

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1063	GLY	-	linker	UNP Q14432
D	1064	SER	-	linker	UNP Q14432
D	1065	GLY	-	linker	UNP Q14432
D	1066	GLY	-	linker	UNP Q14432
D	1067	SER	-	linker	UNP Q14432
C	668	GLY	-	expression tag	UNP Q14432
C	780	GLY	-	linker	UNP Q14432
C	796	GLY	-	linker	UNP Q14432
C	797	SER	-	linker	UNP Q14432
C	798	GLY	-	linker	UNP Q14432
C	799	GLY	-	linker	UNP Q14432
C	800	SER	-	linker	UNP Q14432
C	1029	GLY	-	linker	UNP Q14432
C	1063	GLY	-	linker	UNP Q14432
C	1064	SER	-	linker	UNP Q14432
C	1065	GLY	-	linker	UNP Q14432
C	1066	GLY	-	linker	UNP Q14432
C	1067	SER	-	linker	UNP Q14432
B	668	GLY	-	expression tag	UNP Q14432
B	780	GLY	-	linker	UNP Q14432
B	796	GLY	-	linker	UNP Q14432
B	797	SER	-	linker	UNP Q14432
B	798	GLY	-	linker	UNP Q14432
B	799	GLY	-	linker	UNP Q14432
B	800	SER	-	linker	UNP Q14432
B	1062	GLY	-	linker	UNP Q14432
B	1063	GLY	-	linker	UNP Q14432
B	1064	SER	-	linker	UNP Q14432
B	1065	GLY	-	linker	UNP Q14432
B	1066	GLY	-	linker	UNP Q14432
B	1067	SER	-	linker	UNP Q14432

- Molecule 2 is (4 {R})-3-[4-(diethylamino)-3-[oxidanyl(oxidanylidene)-\$l^{\wedge}\{4\}\$-azanyl]phenyl]-4-methyl-4,5-dihydro-1 {H}-pyridazin-6-one (three-letter code: X5M) (formula: C₁₅H₂₁N₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			22	15	4	3		
2	D	1	Total	C	N	O	0	0
			22	15	4	3		
2	C	1	Total	C	N	O	0	0
			22	15	4	3		
2	B	1	Total	C	N	O	0	0
			22	15	4	3		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

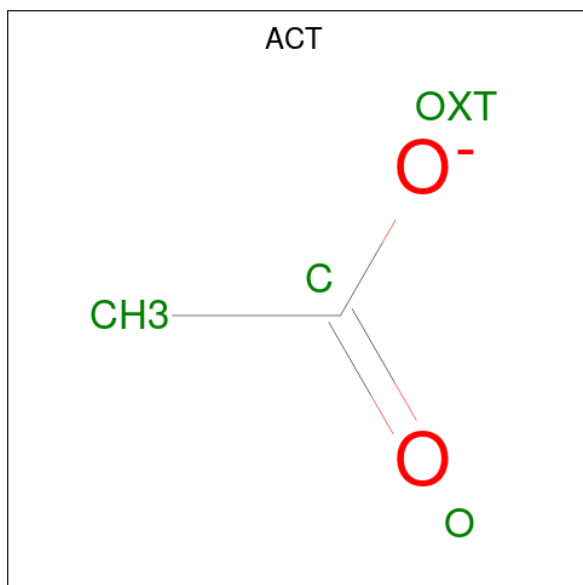
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	75	Total	O	0	0
			75	75		
6	D	104	Total	O	0	0
			104	104		

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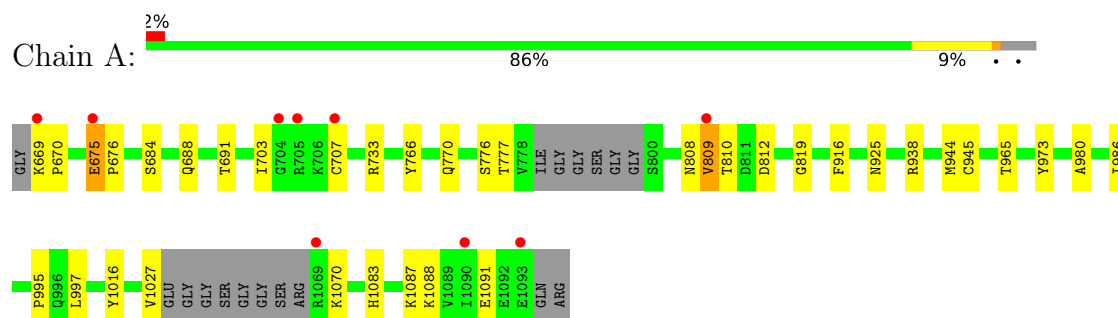
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	110	Total 110	O 110	0	0
6	B	70	Total 70	O 70	0	0

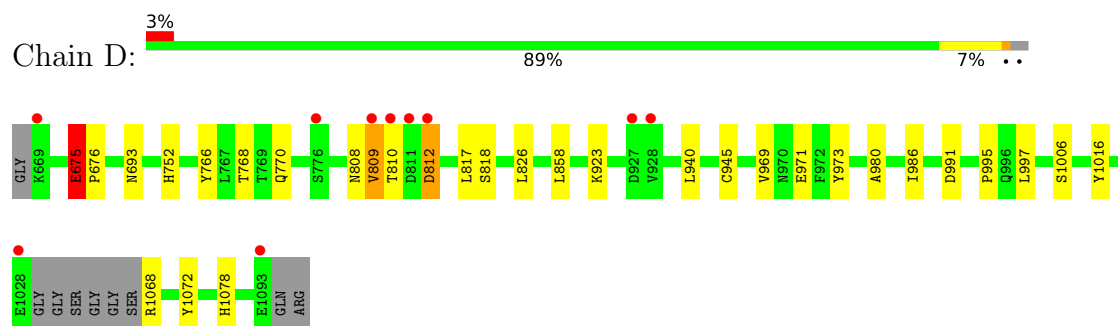
3 Residue-property plots [i](#)

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.

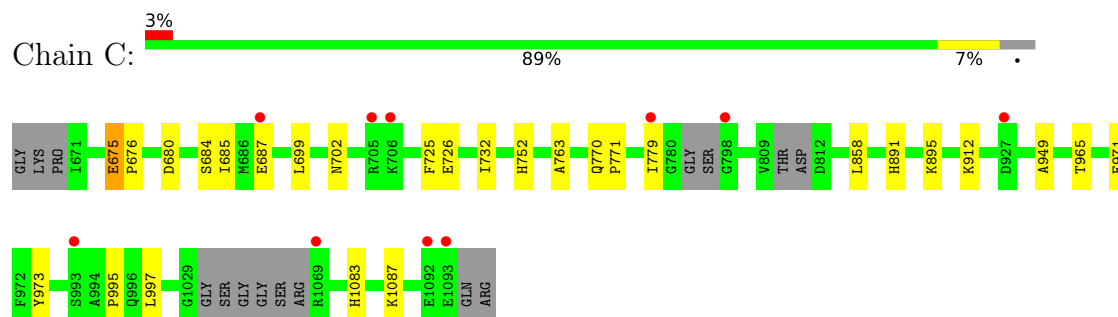
- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase A



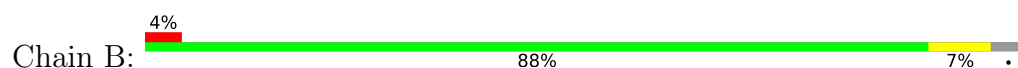
- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase A

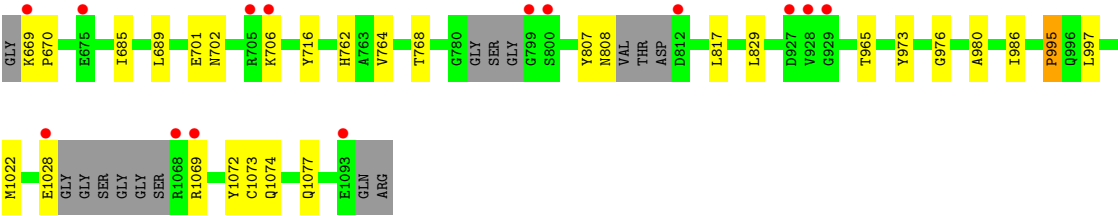


- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase A



- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase A





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.21Å 58.52Å 157.54Å 90.00° 90.66° 90.00°	Depositor
Resolution (Å)	47.70 – 2.00 47.67 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.70-2.00) 99.2 (47.67-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.185 , 0.219 0.195 , 0.226	Depositor DCC
R_{free} test set	5030 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12297	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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, ACT, MN, X5M

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	0.79	0/3022	0.84	2/4104 (0.0%)
1	B	0.78	1/3035 (0.0%)	0.85	0/4117
1	C	0.83	0/3022	0.86	0/4100
1	D	0.82	1/3073 (0.0%)	0.89	1/4172 (0.0%)
All	All	0.80	2/12152 (0.0%)	0.86	3/16493 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	701	GLU	CD-OE2	-6.01	1.19	1.25
1	D	1006	SER	CB-OG	-5.60	1.34	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	675	GLU	CB-CA-C	6.26	122.91	110.40
1	A	938	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	733	ARG	CG-CD-NE	5.07	122.44	111.80

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	2940	0	2866	23	2
1	B	2954	0	2881	19	0
1	C	2942	0	2863	24	0
1	D	2990	0	2914	21	1
2	A	22	0	0	0	0
2	B	22	0	0	2	0
2	C	22	0	0	2	0
2	D	22	0	0	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
5	C	4	0	3	0	0
5	D	4	0	3	0	0
6	A	75	0	0	1	0
6	B	70	0	0	1	0
6	C	110	0	0	6	1
6	D	104	0	0	0	0
All	All	12297	0	11536	89	2

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 4.

All (89) 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:D:1101:X5M:O13	2:D:1101:X5M:C02	2.25	0.84
1:D:969:VAL:HG11	1:D:997:LEU:HD13	1.62	0.82
1:C:726:GLU:OE2	6:C:1201:HOH:O	1.97	0.82
1:B:764:VAL:HG21	1:B:829:LEU:HG	1.67	0.77
1:C:675:GLU:HB2	1:C:676:PRO:HD3	1.68	0.76
1:A:965:THR:CG2	1:A:997:LEU:HD21	2.22	0.70
2:D:1101:X5M:O13	2:D:1101:X5M:C01	2.40	0.69
1:A:965:THR:HG21	1:A:997:LEU:HD21	1.76	0.68
1:C:687:GLU:OE2	1:C:687:GLU:O	2.12	0.67
1:A:777:THR:HG23	1:A:819:GLY:HA3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:965:THR:HG21	1:C:997:LEU:HD21	1.76	0.67
1:D:969:VAL:HG11	1:D:997:LEU:CD1	2.25	0.66
1:B:980:ALA:HB2	1:B:986:ILE:HD11	1.82	0.62
1:C:912:LYS:HD2	6:C:1238:HOH:O	2.00	0.61
1:A:980:ALA:HB2	1:A:986:ILE:HD11	1.83	0.61
1:D:980:ALA:HB2	1:D:986:ILE:HD11	1.82	0.60
1:A:776:SER:OG	6:A:1201:HOH:O	2.15	0.60
1:B:807:TYR:O	1:B:808:ASN:OD1	2.21	0.59
2:B:1101:X5M:C01	2:B:1101:X5M:O13	2.52	0.57
1:C:965:THR:CG2	1:C:997:LEU:HD21	2.35	0.57
1:B:965:THR:CG2	1:B:997:LEU:HD21	2.35	0.57
1:A:688:GLN:O	1:A:691:THR:HG22	2.05	0.57
1:C:684:SER:HB2	1:B:1074:GLN:HG3	1.87	0.57
1:C:680:ASP:OD2	1:B:1028:GLU:HB3	2.06	0.56
1:A:916:PHE:HB3	1:A:944:MET:CE	2.34	0.56
1:D:923:LYS:HD2	1:D:940:LEU:HD23	1.87	0.56
1:B:1072:TYR:OH	1:B:1077:GLN:HG2	2.06	0.56
1:A:1027:VAL:HG23	1:A:1027:VAL:O	2.07	0.54
1:B:689:LEU:O	1:B:762:HIS:HE1	1.90	0.54
1:D:809:VAL:HG23	1:D:809:VAL:O	2.08	0.53
1:C:685:ILE:HD13	1:C:699:LEU:HA	1.90	0.53
1:A:916:PHE:HB3	1:A:944:MET:HE1	1.90	0.52
1:B:965:THR:HG21	1:B:997:LEU:HD21	1.90	0.52
1:B:762:HIS:HD2	6:B:1206:HOH:O	1.92	0.52
2:C:1101:X5M:C02	2:C:1101:X5M:O13	2.57	0.52
1:D:675:GLU:HB3	1:D:676:PRO:CD	2.39	0.52
1:D:945[B]:CYS:HG	1:D:1016:TYR:HH	1.58	0.51
1:A:1088:LYS:HA	1:A:1091:GLU:OE2	2.11	0.51
1:D:693:ASN:HD21	1:D:1078:HIS:CE1	2.29	0.50
1:C:1083:HIS:NE2	1:C:1087:LYS:HE3	2.27	0.49
1:B:973:TYR:OH	1:B:995:PRO:HB3	2.12	0.49
1:C:912:LYS:HE2	6:C:1238:HOH:O	2.12	0.49
1:D:675:GLU:HB3	1:D:676:PRO:HD3	1.94	0.49
1:A:945[B]:CYS:HG	1:A:1016:TYR:HH	1.58	0.48
1:C:702:ASN:OD1	1:B:1077:GLN:NE2	2.46	0.48
1:C:725:PHE:CE1	1:C:732:ILE:HD13	2.48	0.48
1:C:726:GLU:OE2	6:C:1202:HOH:O	2.20	0.48
2:C:1101:X5M:O13	2:C:1101:X5M:C01	2.63	0.47
1:D:812:ASP:N	1:D:812:ASP:OD1	2.47	0.47
1:D:752:HIS:ND1	1:D:971:GLU:OE2	2.32	0.47
1:D:858:LEU:HD11	1:C:858:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1101:X5M:O13	2:B:1101:X5M:C02	2.63	0.46
1:B:1022:MET:HG3	1:B:1073:CYS:SG	2.56	0.46
1:C:891:HIS:CE1	1:C:895:LYS:HE2	2.50	0.46
1:B:716:TYR:CD1	1:B:716:TYR:C	2.89	0.46
1:A:669:LYS:N	1:A:670:PRO:CD	2.79	0.45
1:A:1083:HIS:NE2	1:A:1087:LYS:HE3	2.32	0.45
1:D:858:LEU:HD21	1:C:858:LEU:HD11	1.99	0.45
1:C:912:LYS:CE	6:C:1238:HOH:O	2.64	0.44
1:A:1027:VAL:HG21	1:A:1070:LYS:HG2	1.98	0.44
1:A:973:TYR:OH	1:A:995:PRO:HB3	2.18	0.44
1:C:752:HIS:ND1	1:C:971:GLU:OE2	2.36	0.44
1:B:669:LYS:N	1:B:670:PRO:CD	2.81	0.44
1:D:973:TYR:OH	1:D:995:PRO:HB3	2.18	0.43
2:D:1101:X5M:O13	2:D:1101:X5M:N03	2.50	0.43
1:C:891:HIS:O	1:C:895:LYS:HG2	2.19	0.43
1:C:912:LYS:CD	6:C:1238:HOH:O	2.64	0.43
1:B:997:LEU:HD23	1:B:997:LEU:O	2.19	0.42
1:C:770:GLN:HA	1:C:771:PRO:HD3	1.91	0.42
1:D:808:ASN:O	1:D:809:VAL:C	2.57	0.42
1:D:986:ILE:HG21	1:D:991:ASP:HB2	2.00	0.42
1:A:669:LYS:N	1:A:670:PRO:HD2	2.34	0.42
1:D:818:SER:HA	1:D:826:LEU:HD11	2.02	0.42
1:A:808:ASN:O	1:A:809:VAL:C	2.59	0.41
1:D:766:TYR:CE2	1:D:770:GLN:HG3	2.54	0.41
1:A:675:GLU:HB2	1:A:676:PRO:HD3	2.02	0.41
1:B:976:GLY:O	1:B:986:ILE:CD1	2.68	0.41
1:A:916:PHE:HB3	1:A:944:MET:HE3	2.01	0.41
1:A:703:ILE:HG22	1:A:707:CYS:HB3	2.02	0.41
1:D:1068:ARG:HD2	1:D:1068:ARG:HA	1.81	0.41
1:A:808:ASN:O	1:A:810:THR:HG23	2.21	0.41
1:B:768:THR:HA	1:B:817:LEU:HB2	2.02	0.41
1:C:973:TYR:OH	1:C:995:PRO:HB3	2.20	0.41
1:D:808:ASN:O	1:D:810:THR:HG23	2.20	0.41
1:A:766:TYR:CE2	1:A:770:GLN:HG3	2.56	0.41
1:A:1027:VAL:O	1:A:1027:VAL:CG2	2.68	0.41
1:B:706:LYS:O	1:B:706:LYS:HG2	2.20	0.40
1:D:768:THR:HA	1:D:817:LEU:HB2	2.04	0.40
1:C:763:ALA:HB3	1:C:949:ALA:HB1	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:SER:OG	1:D:1072:TYR:OH[1_556]	2.14	0.06
1:A:925:ASN:O	6:C:1201:HOH:O[2_555]	2.15	0.05

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	358/380 (94%)	349 (98%)	6 (2%)	3 (1%)	19	13
1	B	358/380 (94%)	348 (97%)	9 (2%)	1 (0%)	41	37
1	C	358/380 (94%)	346 (97%)	10 (3%)	2 (1%)	25	19
1	D	368/380 (97%)	359 (98%)	6 (2%)	3 (1%)	19	13
All	All	1442/1520 (95%)	1402 (97%)	31 (2%)	9 (1%)	25	19

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	675	GLU
1	A	809	VAL
1	D	675	GLU
1	D	809	VAL
1	C	675	GLU
1	C	779	ILE
1	D	812	ASP
1	A	812	ASP
1	B	1069	ARG

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	320/327 (98%)	320 (100%)	0	100	100
1	B	320/327 (98%)	317 (99%)	3 (1%)	78	83
1	C	318/327 (97%)	318 (100%)	0	100	100
1	D	324/327 (99%)	324 (100%)	0	100	100
All	All	1282/1308 (98%)	1279 (100%)	3 (0%)	93	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	685	ILE
1	B	702	ASN
1	B	995	PRO

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	702	ASN
1	A	820	ASN
1	A	860	ASN
1	A	1074	GLN
1	A	1081	GLN
1	D	996	GLN
1	D	1074	GLN
1	D	1078	HIS
1	D	1081	GLN
1	C	855	GLN
1	C	891	HIS
1	B	762	HIS
1	B	808	ASN
1	B	860	ASN

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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
5	ACT	C	1104	-	1,3,3	4.69	1 (100%)	0,3,3	0.00	-
2	X5M	A	1101	-	22,23,23	3.82	7 (31%)	26,32,32	2.04	10 (38%)
2	X5M	C	1101	-	22,23,23	3.66	7 (31%)	26,32,32	1.88	7 (26%)
5	ACT	D	1104	-	1,3,3	4.98	1 (100%)	0,3,3	0.00	-
2	X5M	D	1101	-	22,23,23	3.27	5 (22%)	26,32,32	2.01	9 (34%)
2	X5M	B	1101	-	22,23,23	3.71	8 (36%)	26,32,32	1.86	5 (19%)
5	ACT	A	1104	-	1,3,3	4.37	1 (100%)	0,3,3	0.00	-
5	ACT	B	1104	-	1,3,3	3.08	1 (100%)	0,3,3	0.00	-

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
2	X5M	C	1101	-	-	6/14/29/29	0/2/2/2
2	X5M	A	1101	-	-	4/14/29/29	0/2/2/2
2	X5M	B	1101	-	-	4/14/29/29	0/2/2/2
2	X5M	D	1101	-	-	2/14/29/29	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	X5M	C15-N16	14.36	1.43	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	X5M	C15-N16	13.93	1.43	1.29
2	C	1101	X5M	C15-N16	13.76	1.43	1.29
2	D	1101	X5M	C15-N16	12.17	1.41	1.29
2	A	1101	X5M	C18-N17	8.02	1.49	1.34
2	C	1101	X5M	C18-N17	7.73	1.48	1.34
2	B	1101	X5M	C18-N17	7.29	1.47	1.34
2	D	1101	X5M	C18-N17	6.48	1.46	1.34
5	D	1104	ACT	CH3-C	4.98	1.55	1.48
5	C	1104	ACT	CH3-C	4.69	1.54	1.48
5	A	1104	ACT	CH3-C	4.37	1.54	1.48
2	C	1101	X5M	C21-C15	-3.88	1.46	1.51
2	B	1101	X5M	N17-N16	3.52	1.47	1.38
2	A	1101	X5M	N17-N16	3.18	1.46	1.38
2	B	1101	X5M	C21-C15	-3.17	1.47	1.51
2	D	1101	X5M	O14-N12	-3.16	1.17	1.22
5	B	1104	ACT	CH3-C	3.08	1.52	1.48
2	A	1101	X5M	O19-C18	-3.03	1.17	1.23
2	B	1101	X5M	C06-N03	2.81	1.47	1.41
2	A	1101	X5M	C09-C15	2.78	1.52	1.48
2	B	1101	X5M	O14-N12	-2.77	1.18	1.22
2	C	1101	X5M	C06-N03	2.61	1.47	1.41
2	B	1101	X5M	O19-C18	-2.53	1.18	1.23
2	C	1101	X5M	O19-C18	-2.44	1.18	1.23
2	C	1101	X5M	O14-N12	-2.37	1.18	1.22
2	A	1101	X5M	C21-C15	-2.34	1.48	1.51
2	D	1101	X5M	C06-N03	2.34	1.46	1.41
2	D	1101	X5M	C21-C15	-2.33	1.48	1.51
2	A	1101	X5M	O14-N12	-2.13	1.19	1.22
2	C	1101	X5M	N17-N16	2.07	1.43	1.38
2	B	1101	X5M	C09-C15	2.02	1.51	1.48

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	X5M	C18-N17-N16	-5.67	119.76	126.33
2	A	1101	X5M	C20-C21-C15	5.17	115.03	108.13
2	C	1101	X5M	C18-N17-N16	-4.76	120.81	126.33
2	D	1101	X5M	C10-C11-C06	4.60	123.85	118.69
2	D	1101	X5M	C07-C06-N03	-4.47	115.17	122.30
2	C	1101	X5M	C20-C21-C15	4.35	113.93	108.13
2	C	1101	X5M	C07-C06-N03	-4.18	115.64	122.30
2	A	1101	X5M	C21-C15-N16	-4.09	117.65	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	X5M	C21-C20-C18	4.00	116.35	111.22
2	D	1101	X5M	C20-C21-C15	3.55	112.86	108.13
2	A	1101	X5M	C09-C15-N16	-3.35	114.24	117.14
2	B	1101	X5M	C10-C11-C06	3.32	122.42	118.69
2	A	1101	X5M	C18-N17-N16	-3.11	122.72	126.33
2	D	1101	X5M	C08-C09-C15	-3.06	117.12	120.75
2	A	1101	X5M	C07-C06-N03	-2.95	117.59	122.30
2	D	1101	X5M	C09-C10-C11	-2.79	115.43	118.88
2	B	1101	X5M	C04-N03-C02	2.71	121.54	116.34
2	D	1101	X5M	C18-N17-N16	-2.57	123.35	126.33
2	B	1101	X5M	C20-C21-C15	2.53	111.51	108.13
2	A	1101	X5M	C08-C09-C15	2.53	123.75	120.75
2	D	1101	X5M	C21-C20-C18	2.51	114.44	111.22
2	C	1101	X5M	C21-C20-C18	2.51	114.44	111.22
2	C	1101	X5M	C22-C21-C15	-2.50	105.73	109.70
2	C	1101	X5M	C21-C15-N16	-2.47	119.70	122.84
2	A	1101	X5M	C04-N03-C02	2.46	121.06	116.34
2	A	1101	X5M	C10-C11-C06	2.38	121.36	118.69
2	D	1101	X5M	C08-C09-C10	2.34	122.00	119.24
2	A	1101	X5M	C21-C20-C18	2.29	114.16	111.22
2	A	1101	X5M	C22-C21-C15	-2.28	106.08	109.70
2	C	1101	X5M	C10-C11-C06	2.20	121.16	118.69
2	D	1101	X5M	C21-C15-N16	-2.02	120.28	122.84

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1101	X5M	C01-C02-N03-C06
2	C	1101	X5M	C01-C02-N03-C06
2	A	1101	X5M	C11-C06-N03-C04
2	B	1101	X5M	C01-C02-N03-C06
2	C	1101	X5M	C01-C02-N03-C04
2	D	1101	X5M	C01-C02-N03-C04
2	B	1101	X5M	C01-C02-N03-C04
2	C	1101	X5M	C11-C06-N03-C04
2	C	1101	X5M	C05-C04-N03-C06
2	C	1101	X5M	C05-C04-N03-C02
2	A	1101	X5M	C07-C06-N03-C04
2	A	1101	X5M	C05-C04-N03-C02
2	B	1101	X5M	C11-C06-N03-C04
2	B	1101	X5M	C07-C06-N03-C04

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Mol	Chain	Res	Type	Atoms
2	A	1101	X5M	C05-C04-N03-C06
2	C	1101	X5M	C07-C06-N03-C04

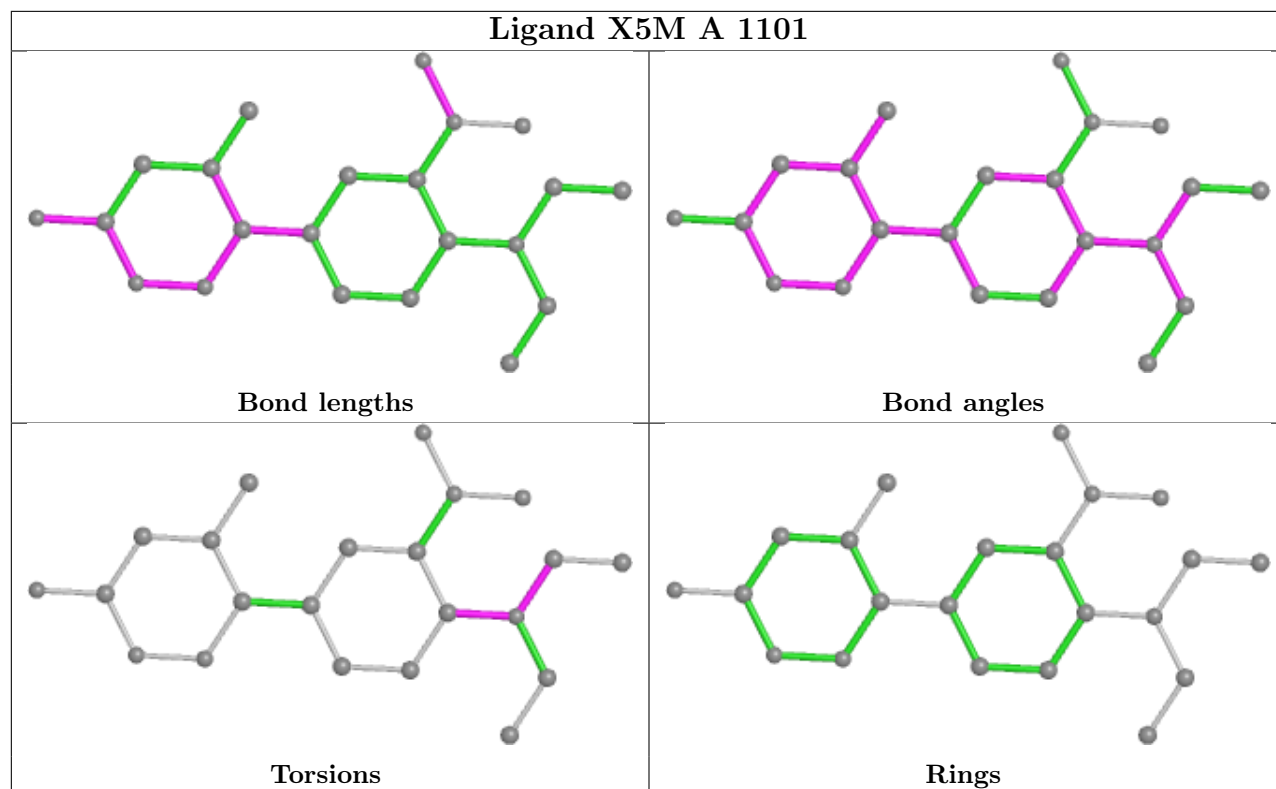
There are no ring outliers.

3 monomers are involved in 7 short contacts:

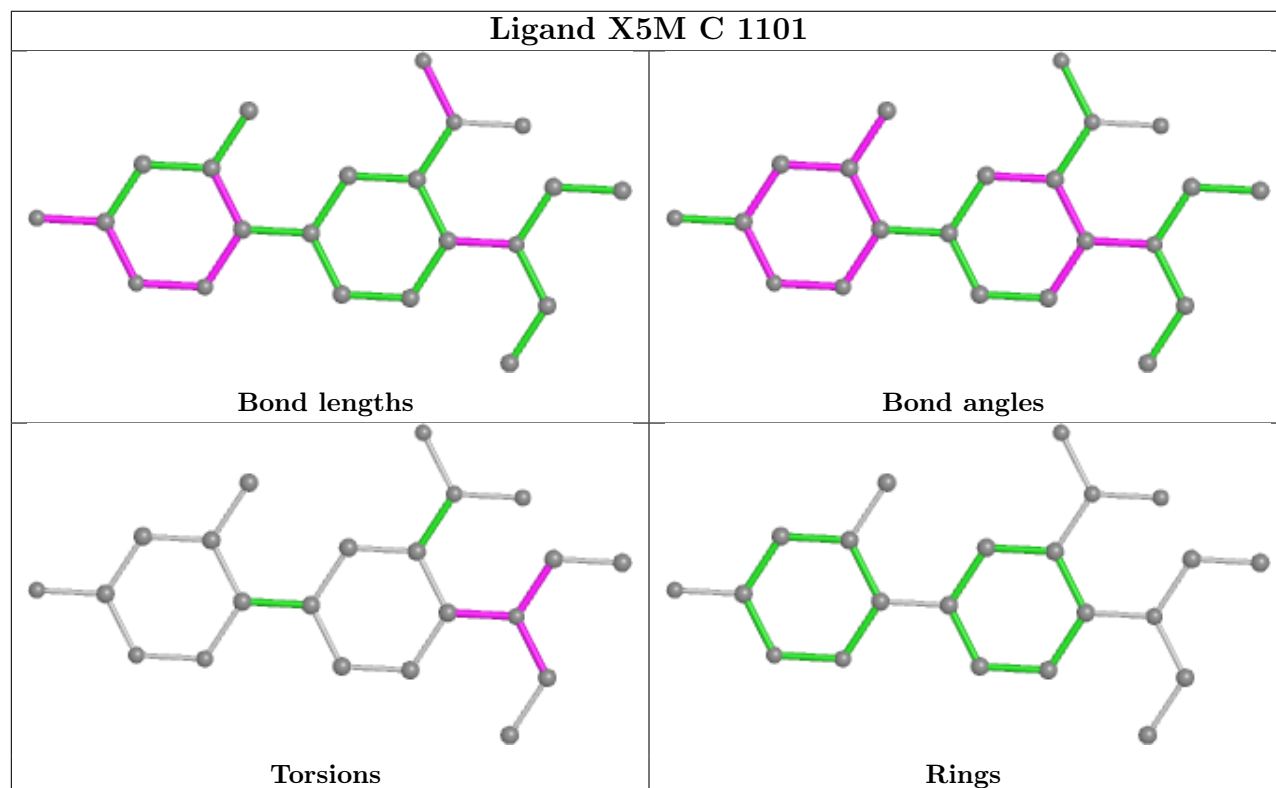
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1101	X5M	2	0
2	D	1101	X5M	3	0
2	B	1101	X5M	2	0

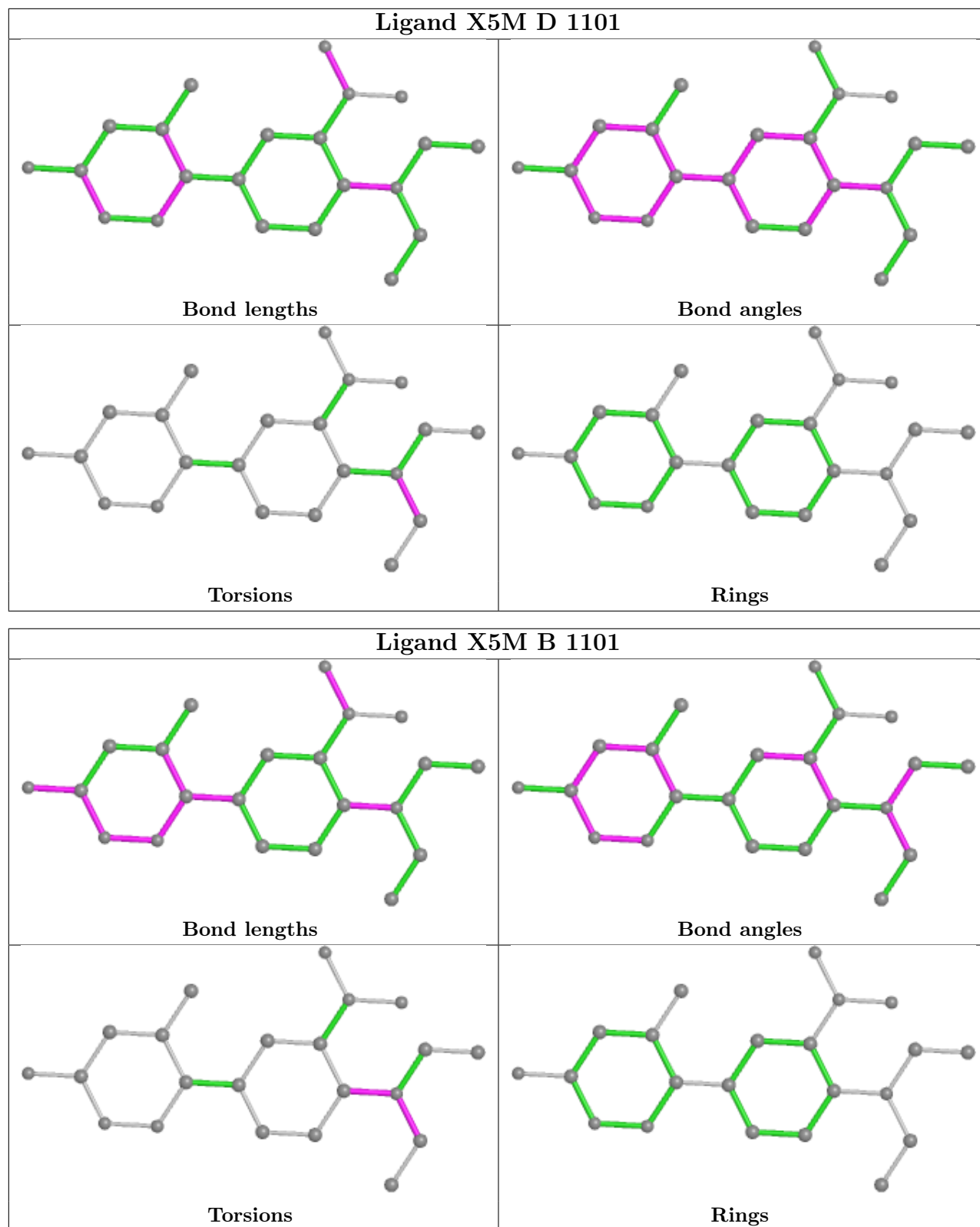
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand X5M A 1101



Ligand X5M C 1101





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 ⓘ

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	363/380 (95%)	0.06	9 (2%) 57 56	27, 52, 89, 129	0
1	B	365/380 (96%)	0.15	14 (3%) 40 39	30, 56, 96, 131	0
1	C	365/380 (96%)	0.04	10 (2%) 54 53	27, 45, 82, 116	0
1	D	371/380 (97%)	0.05	10 (2%) 54 53	26, 45, 79, 115	0
All	All	1464/1520 (96%)	0.08	43 (2%) 51 50	26, 49, 90, 131	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	675	GLU	5.7
1	D	669	LYS	5.3
1	A	705	ARG	5.2
1	C	1069	ARG	5.1
1	B	675	GLU	4.4
1	B	927	ASP	4.4
1	B	928	VAL	4.0
1	C	779	ILE	4.0
1	C	1092	GLU	3.9
1	C	1093	GLU	3.8
1	A	809	VAL	3.7
1	D	810	THR	3.6
1	D	1028	GLU	3.5
1	C	927	ASP	3.5
1	A	707	CYS	3.5
1	B	706	LYS	3.5
1	B	799	GLY	3.2
1	C	706	LYS	3.1
1	D	811	ASP	3.1
1	D	1093	GLU	3.0
1	D	776	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	927	ASP	2.7
1	D	928	VAL	2.7
1	B	1093	GLU	2.7
1	A	1090	ILE	2.6
1	B	929	GLY	2.6
1	B	812	ASP	2.6
1	D	809	VAL	2.5
1	B	1028	GLU	2.5
1	C	993	SER	2.4
1	C	798	GLY	2.4
1	B	705	ARG	2.4
1	B	669	LYS	2.4
1	C	687	GLU	2.4
1	A	704	GLY	2.4
1	D	812	ASP	2.3
1	A	669	LYS	2.2
1	C	705	ARG	2.2
1	B	1068	ARG	2.2
1	B	800	SER	2.1
1	A	1069	ARG	2.1
1	A	1093	GLU	2.0
1	B	1069	ARG	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.

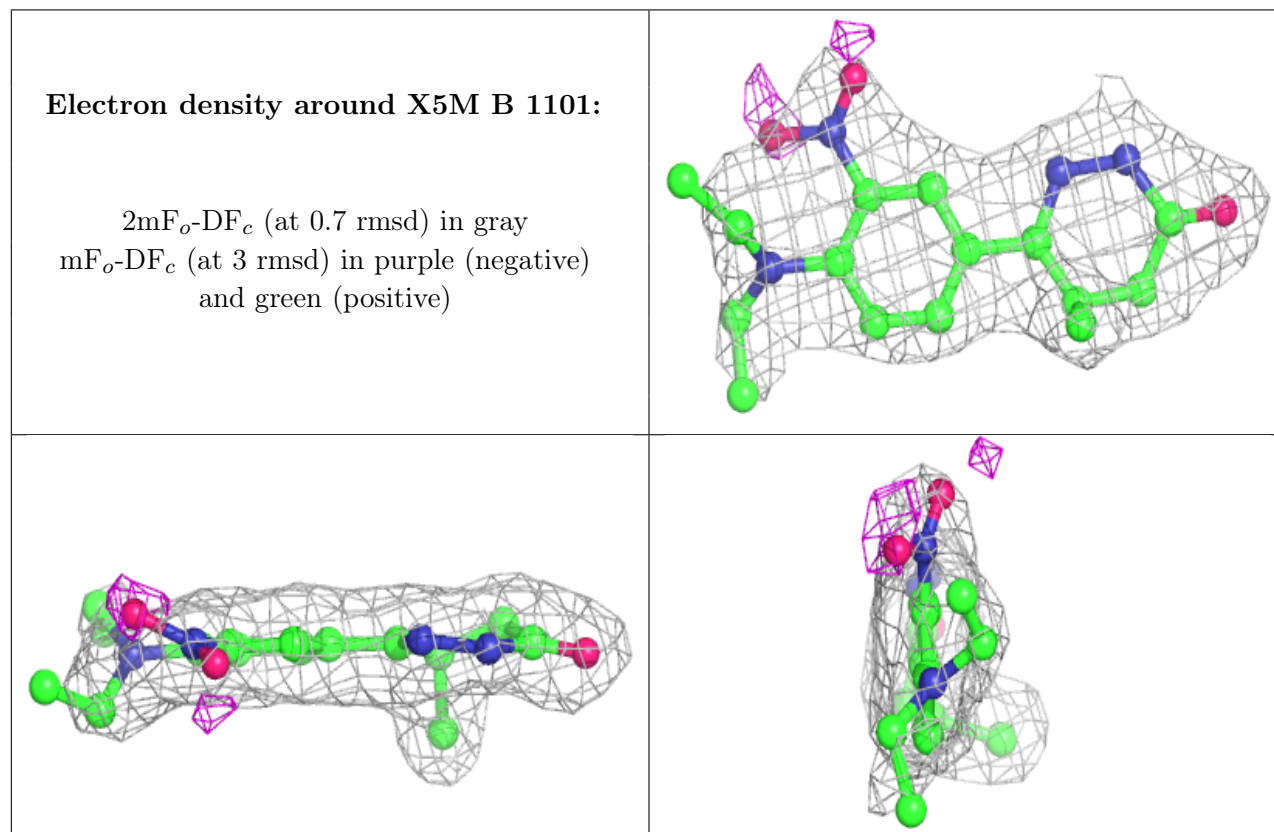
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	ACT	B	1104	4/4	0.91	0.20	54,63,76,79	0

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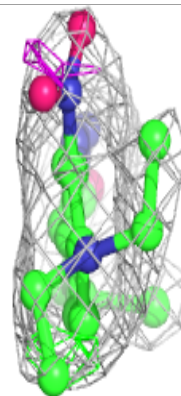
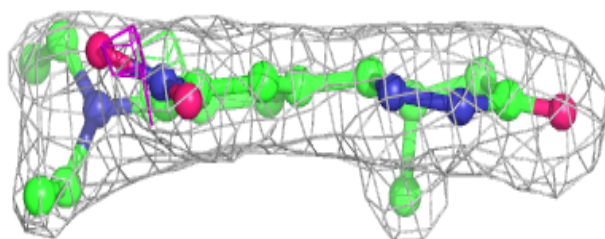
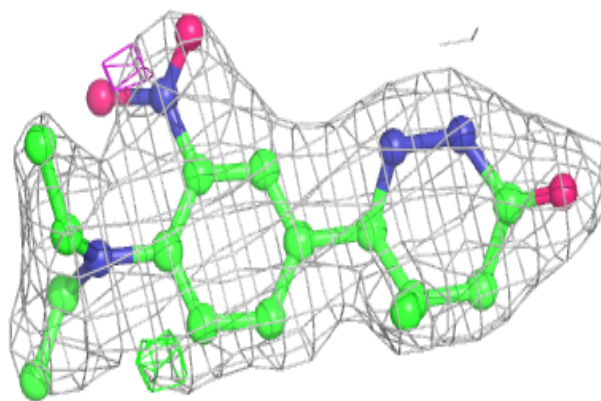
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	X5M	B	1101	22/22	0.92	0.16	33,45,71,77	0
5	ACT	A	1104	4/4	0.92	0.22	58,58,62,63	0
2	X5M	A	1101	22/22	0.92	0.15	38,50,66,82	0
5	ACT	C	1104	4/4	0.93	0.17	47,55,61,62	0
2	X5M	D	1101	22/22	0.95	0.14	27,35,61,68	0
2	X5M	C	1101	22/22	0.95	0.13	32,43,67,77	0
5	ACT	D	1104	4/4	0.96	0.13	45,47,47,53	0
4	MG	A	1103	1/1	0.98	0.07	27,27,27,27	0
4	MG	C	1103	1/1	0.98	0.08	27,27,27,27	0
4	MG	B	1103	1/1	0.99	0.08	29,29,29,29	0
3	MN	B	1102	1/1	0.99	0.10	37,37,37,37	0
3	MN	D	1102	1/1	0.99	0.06	32,32,32,32	0
4	MG	D	1103	1/1	0.99	0.12	25,25,25,25	0
3	MN	C	1102	1/1	0.99	0.09	36,36,36,36	0
3	MN	A	1102	1/1	1.00	0.07	37,37,37,37	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.

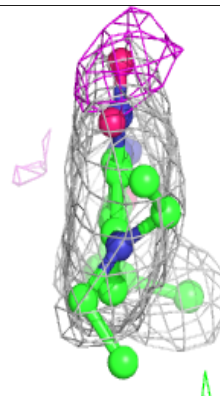
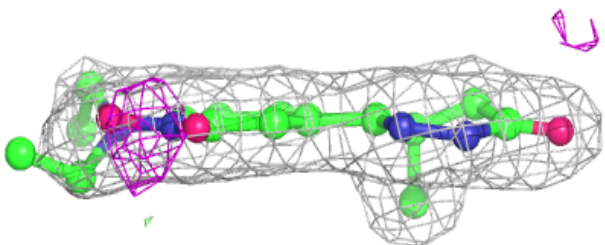
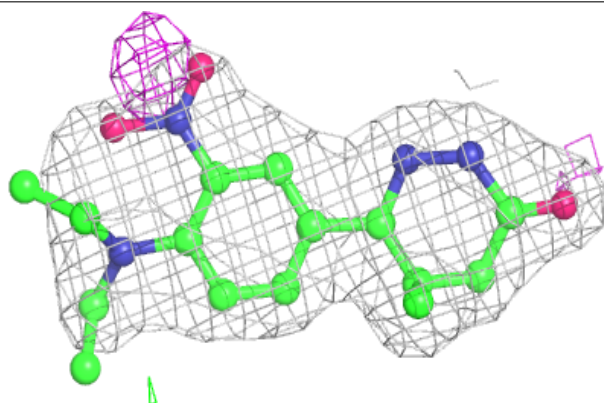


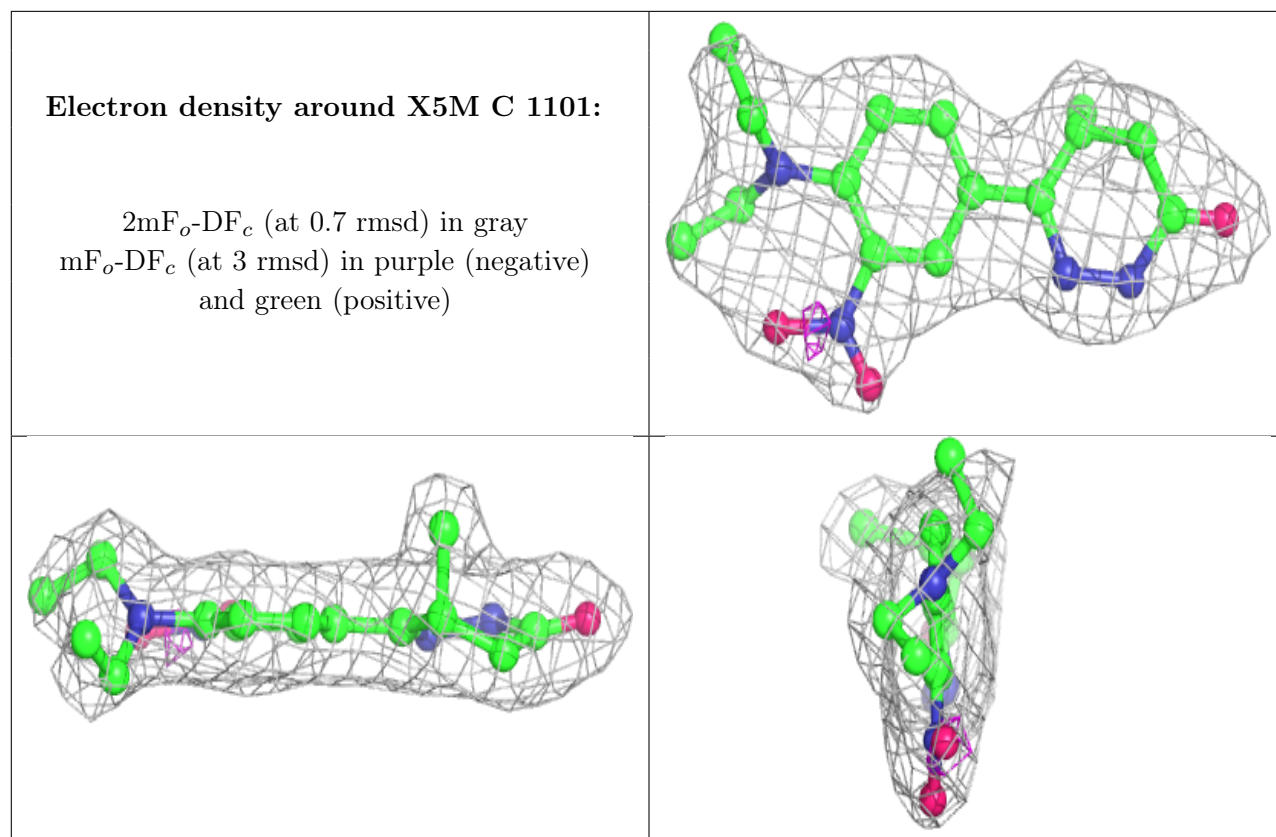
Electron density around X5M A 1101:

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

**Electron density around X5M D 1101:**

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 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.