Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 11:58 AM EDT

PDB ID	:	2I7C
Title	:	The crystal structure of spermidine synthase from p. falciparum in complex with AdoDATO
Authors	:	Qiu, W.; Dong, A.; Ren, H.; Wu, H.; Wasney, G.; Vedadi, M.; Lew, J.; Kozieradski, I.; Edwards, A.M.; Arrowsmith, C.H.; Weigelt, J.; Sundstrom, M.; Plotnikov, A.N.; Bochkarev, A.; Hui, R.; Structural Genomics Consortium (SGC)
Deposited on	:	2006-08-30
Resolution	:	1.71 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

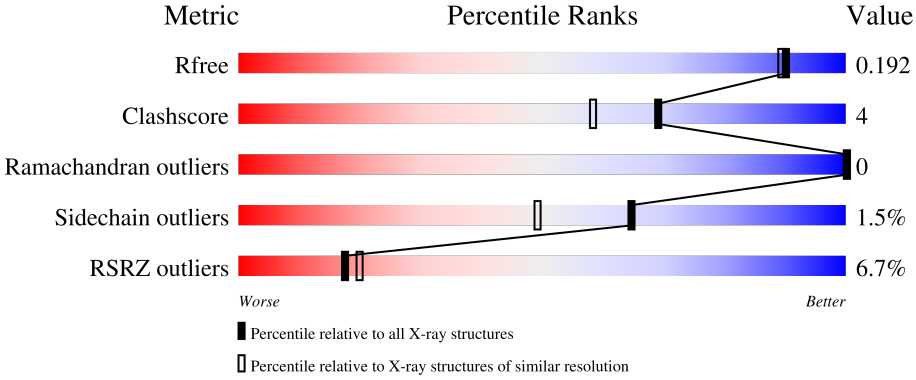
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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 <=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	283	8% 93% 5% ••
1	B	283	7% 88% 9% ••
1	C	283	4% 94% 5% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7559 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.

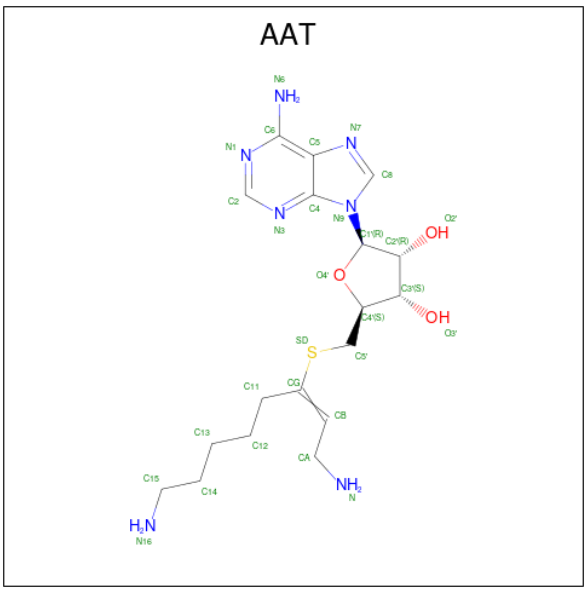
- Molecule 1 is a protein called Spermidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	281	2304	1497	355	437	15	0	9	0
1	B	280	2280	1480	355	430	15	3	7	0
1	C	281	2265	1471	352	427	15	0	3	0

There are 3 discrepancies between the modelled and reference sequences:

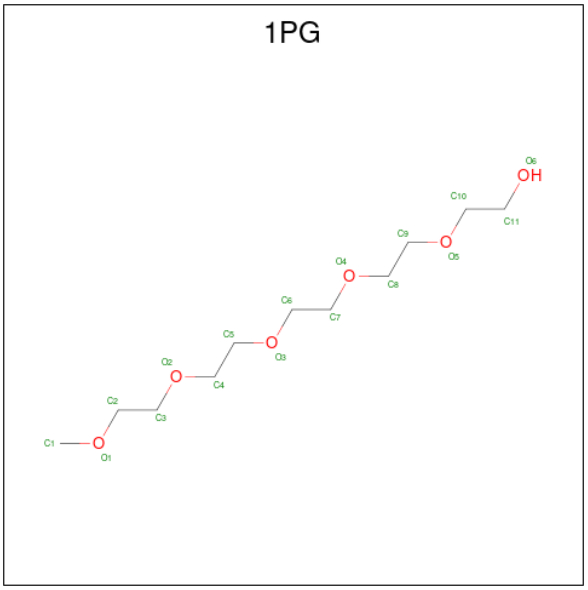
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	cloning artifact	UNP Q8II73
B	0	GLY	-	cloning artifact	UNP Q8II73
C	0	GLY	-	cloning artifact	UNP Q8II73

- Molecule 2 is S-ADENOSYL-1,8-DIAMINO-3-THIOOCTANE (three-letter code: AAT) (formula: $C_{18}H_{29}N_7O_3S$).



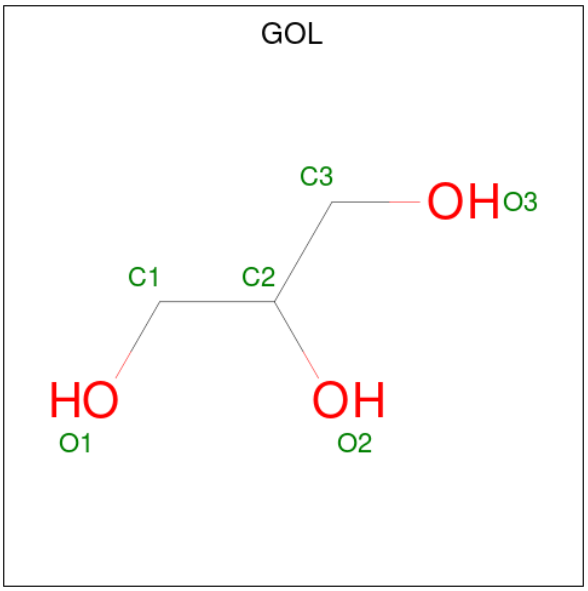
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	29	18	7	3	1	0	0
			Total	C	N	O	S		
2	B	1	29	18	7	3	1	0	0
			Total	C	N	O	S		
2	C	1	29	18	7	3	1	0	0

- Molecule 3 is 2-(2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHANOL (three-letter code: 1PG) (formula: $C_{11}H_{24}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	17	11	6	0	0
			Total	C	O		
3	B	1	17	11	6	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
			Total	C	O		
4	B	1	6	3	3	0	0
			Total	C	O		
4	C	1	6	3	3	0	0

- Molecule 5 is water.

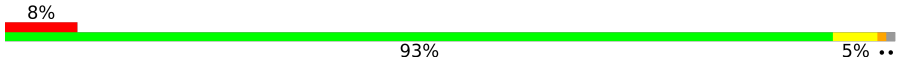
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	152	152	152	0	0
			Total	O		
5	B	154	154	154	0	0
			Total	O		
5	C	265	265	265	0	0

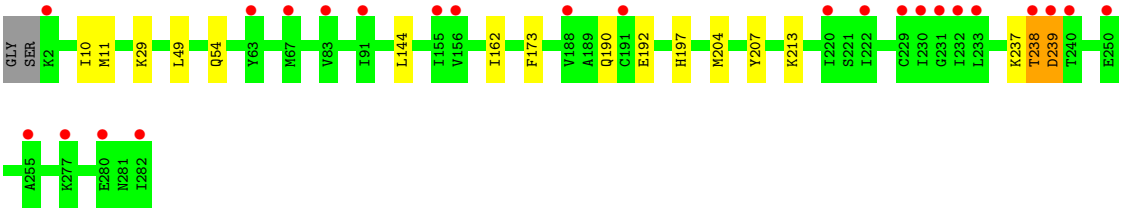
3 Residue-property plots (i)

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: Spermidine synthase

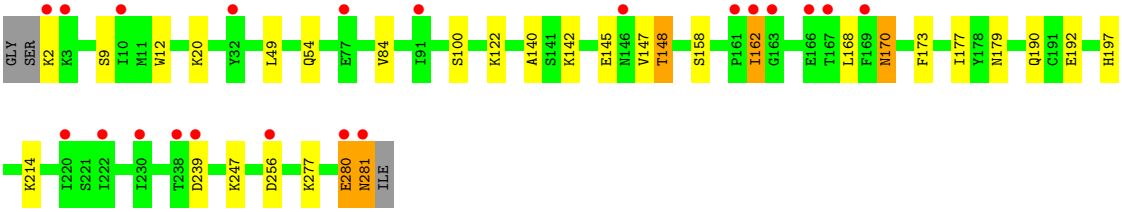
Chain A:





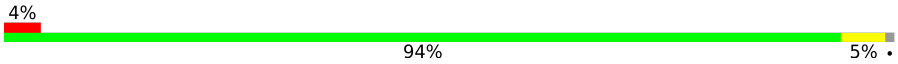
• Molecule 1: Spermidine synthase

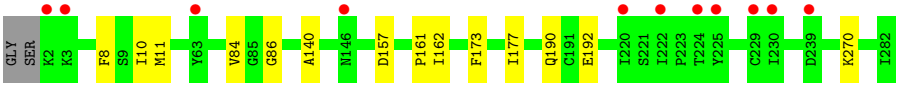
Chain B:



• Molecule 1: Spermidine synthase

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	198.17Å 134.69Å 48.50Å 90.00° 95.44° 90.00°	Depositor
Resolution (Å)	35.92 – 1.71 35.92 – 1.71	Depositor EDS
% Data completeness (in resolution range)	94.0 (35.92-1.71) 94.0 (35.92-1.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.175 , 0.194 0.173 , 0.192	Depositor DCC
R_{free} test set	6456 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7559	wwPDB-VP
Average B, all atoms (Å^2)	25.0	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: AAT, GOL, 1PG

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	0.76	2/2378 (0.1%)	0.58	1/3211 (0.0%)
1	B	0.66	0/2345	0.61	0/3167
1	C	0.72	0/2324	0.61	0/3137
All	All	0.71	2/7047 (0.0%)	0.60	1/9515 (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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	THR	C-N	-19.73	0.88	1.34
1	A	239	ASP	C-N	-15.91	0.97	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	239	ASP	CB-CG-OD2	5.20	122.98	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	280	GLU	Peptide

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	2304	0	2323	20	0
1	B	2280	0	2299	22	0
1	C	2265	0	2284	10	0
2	A	29	0	29	0	0
2	B	29	0	29	1	0
2	C	29	0	29	0	0
3	A	17	0	24	0	0
3	B	17	0	24	1	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
5	A	152	0	0	0	0
5	B	154	0	0	1	0
5	C	265	0	0	1	0
All	All	7559	0	7065	52	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 4.

All (52) 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:213:LYS:CE	1:A:239:ASP:HB2	1.55	1.37
1:A:213:LYS:HE2	1:A:239:ASP:CB	1.77	1.13
1:A:213:LYS:HE2	1:A:239:ASP:HB2	1.05	1.02
1:B:280:GLU:HB3	1:B:281:ASN:HB2	1.48	0.93
1:B:148:THR:HG22	1:B:179[B]:ASN:HD21	1.39	0.85
1:B:277:LYS:O	1:B:281:ASN:HB3	1.76	0.85
1:B:280:GLU:HB3	1:B:281:ASN:CB	2.08	0.84
1:A:213:LYS:HE2	1:A:239:ASP:CA	2.10	0.80
1:B:281:ASN:C	1:B:281:ASN:HD22	1.90	0.76
1:C:190:GLN:HE21	1:C:192:GLU:H	1.38	0.72
1:A:29:LYS:O	1:B:122:LYS:NZ	2.28	0.66
1:C:11[B]:MET:SD	1:C:161:PRO:HD2	2.36	0.66
1:A:213:LYS:HE3	1:A:239:ASP:HB2	1.69	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LYS:HE2	1:A:239:ASP:N	2.13	0.63
1:A:213:LYS:NZ	1:A:239:ASP:HB2	2.12	0.62
1:B:142:LYS:O	1:B:145:GLU:HG2	1.99	0.62
1:A:213:LYS:CE	1:A:239:ASP:CB	2.48	0.60
1:C:10:ILE:HD11	1:C:162:ILE:HD13	1.83	0.60
1:A:204:MET:HE1	1:A:207:TYR:HE2	1.68	0.57
1:C:190:GLN:NE2	1:C:192:GLU:H	2.01	0.57
1:B:280:GLU:CB	1:B:281:ASN:HB2	2.31	0.57
1:B:192:GLU:HB3	1:B:197:HIS:ND1	2.21	0.55
1:B:162:ILE:O	1:B:162:ILE:HG13	2.07	0.55
1:B:170:ASN:ND2	1:B:173:PHE:H	2.06	0.53
1:B:49:LEU:HG	1:B:54:GLN:HG3	1.91	0.52
1:B:158[B]:SER:OG	1:B:168:LEU:HD12	2.09	0.52
1:B:281:ASN:C	1:B:281:ASN:ND2	2.59	0.52
1:C:270:LYS:HE3	5:C:883:HOH:O	2.09	0.51
1:A:204:MET:CE	1:A:207:TYR:HE2	2.25	0.49
1:B:280:GLU:HB3	1:B:281:ASN:HB3	1.91	0.48
1:B:84:VAL:HG13	1:B:140:ALA:CB	2.43	0.48
1:A:204:MET:CE	1:A:207:TYR:CE2	2.97	0.48
1:A:192:GLU:HB3	1:A:197:HIS:ND1	2.29	0.47
1:A:10:ILE:HD11	1:A:162:ILE:HD13	1.96	0.47
1:B:277:LYS:O	1:B:281:ASN:CB	2.56	0.47
1:C:86:GLY:HA2	1:C:157:ASP:OD2	2.16	0.45
1:C:11[A]:MET:HG2	1:C:162:ILE:HD12	1.99	0.45
1:A:144:LEU:HD12	1:A:173:PHE:CE1	2.51	0.45
1:C:173:PHE:CE2	1:C:177:ILE:HD11	2.52	0.45
1:A:213:LYS:HD3	1:A:238:THR:HA	1.97	0.45
1:B:256:ASP:HB2	5:B:954:HOH:O	2.17	0.44
1:A:49:LEU:HD12	1:A:54:GLN:HG3	2.00	0.44
1:B:173:PHE:CE2	1:B:177[A]:ILE:HD11	2.52	0.44
1:A:11[A]:MET:CG	1:A:162:ILE:HD12	2.48	0.42
1:C:84:VAL:HG13	1:C:140:ALA:CB	2.49	0.42
1:B:9:SER:HB3	1:B:12:TRP:CE2	2.54	0.42
1:A:239:ASP:O	1:A:239:ASP:OD1	2.37	0.42
1:A:213:LYS:HD3	1:A:237:LYS:O	2.19	0.41
1:B:2:LYS:CD	1:B:20:LYS:HE2	2.51	0.41
1:B:2:LYS:HD2	1:B:20:LYS:HE2	2.01	0.41
2:B:802:AAT:H5'2	2:B:802:AAT:HCB	1.91	0.41
3:B:702:1PG:H61	1:C:8:PHE:HZ	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	288/283 (102%)	279 (97%)	9 (3%)	0	100	100
1	B	285/283 (101%)	277 (97%)	8 (3%)	0	100	100
1	C	282/283 (100%)	274 (97%)	8 (3%)	0	100	100
All	All	855/849 (101%)	830 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	262/254 (103%)	261 (100%)	1 (0%)	91	86
1	B	259/254 (102%)	249 (96%)	10 (4%)	32	12
1	C	256/254 (101%)	256 (100%)	0	100	100
All	All	777/762 (102%)	766 (99%)	11 (1%)	65	52

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
1	B	100	SER
1	B	147	VAL
1	B	148	THR
1	B	162	ILE

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Mol	Chain	Res	Type
1	B	170	ASN
1	B	190	GLN
1	B	214	LYS
1	B	239	ASP
1	B	247	LYS
1	B	281	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	103	ASN
1	A	171	GLN
1	A	179	ASN
1	B	103	ASN
1	B	170	ASN
1	B	172	ASN
1	B	246	ASN
1	B	281	ASN
1	C	171	GLN
1	C	172	ASN
1	C	190	GLN
1	C	246	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
4	GOL	B	601	-	5,5,5	0.31	0	5,5,5	0.42	0
2	AAT	B	802	-	26,31,31	0.91	1 (3%)	24,42,42	1.91	4 (16%)
4	GOL	A	603	-	5,5,5	0.35	0	5,5,5	0.31	0
2	AAT	A	801	-	26,31,31	1.26	2 (7%)	24,42,42	1.84	5 (20%)
3	1PG	B	702	-	16,16,16	0.44	0	15,15,15	0.35	0
2	AAT	C	803	-	26,31,31	1.07	2 (7%)	24,42,42	1.86	5 (20%)
3	1PG	A	701	-	16,16,16	0.55	0	15,15,15	0.18	0
4	GOL	C	602	-	5,5,5	0.35	0	5,5,5	0.37	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
4	GOL	B	601	-	-	0/4/4/4	-
2	AAT	B	802	-	-	1/12/34/34	0/3/3/3
4	GOL	A	603	-	-	0/4/4/4	-
2	AAT	A	801	-	-	2/12/34/34	0/3/3/3
3	1PG	B	702	-	-	8/14/14/14	-
2	AAT	C	803	-	-	3/12/34/34	0/3/3/3
3	1PG	A	701	-	-	8/14/14/14	-
4	GOL	C	602	-	-	0/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	AAT	O4'-C1'	3.99	1.46	1.41
2	A	801	AAT	CA-CB	-2.92	1.39	1.49
2	C	803	AAT	O4'-C1'	2.87	1.45	1.41
2	B	802	AAT	CA-CB	-2.83	1.39	1.49
2	C	803	AAT	CA-CB	-2.68	1.40	1.49

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	802	AAT	O4'-C1'-C2'	-4.95	99.69	106.93
2	B	802	AAT	N3-C2-N1	-4.79	121.20	128.68
2	C	803	AAT	N3-C2-N1	-4.75	121.25	128.68
2	C	803	AAT	C12-C11-CG	-4.65	104.64	114.33
2	A	801	AAT	O4'-C1'-C2'	-4.46	100.41	106.93
2	A	801	AAT	N3-C2-N1	-4.20	122.12	128.68
2	A	801	AAT	O4'-C4'-C5'	4.13	119.46	108.83
2	C	803	AAT	O4'-C1'-C2'	-3.99	101.09	106.93
2	B	802	AAT	C12-C11-CG	-3.79	106.43	114.33
2	B	802	AAT	O4'-C4'-C5'	3.40	117.59	108.83
2	A	801	AAT	C12-C11-CG	-3.32	107.42	114.33
2	C	803	AAT	O4'-C4'-C5'	2.60	115.53	108.83
2	A	801	AAT	C4-C5-N7	-2.22	107.08	109.40
2	C	803	AAT	C2-N1-C6	2.05	122.25	118.75

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	AAT	CB-CG-SD-C5'
2	A	801	AAT	C11-CG-SD-C5'
2	B	802	AAT	CB-CG-SD-C5'
2	C	803	AAT	CA-CB-CG-C11
2	C	803	AAT	CB-CG-SD-C5'
2	C	803	AAT	C11-CG-SD-C5'
3	A	701	1PG	O2-C4-C5-O3
3	B	702	1PG	O5-C10-C11-O6
3	B	702	1PG	O2-C4-C5-O3
3	B	702	1PG	O4-C8-C9-O5
3	A	701	1PG	C3-C2-O1-C1
3	B	702	1PG	C3-C2-O1-C1
3	A	701	1PG	O3-C6-C7-O4
3	A	701	1PG	C8-C9-O5-C10
3	A	701	1PG	O4-C8-C9-O5
3	B	702	1PG	C9-C8-O4-C7
3	A	701	1PG	C5-C4-O2-C3
3	B	702	1PG	C6-C7-O4-C8
3	B	702	1PG	C4-C5-O3-C6
3	A	701	1PG	C4-C5-O3-C6
3	B	702	1PG	O3-C6-C7-O4
3	A	701	1PG	O1-C2-C3-O2

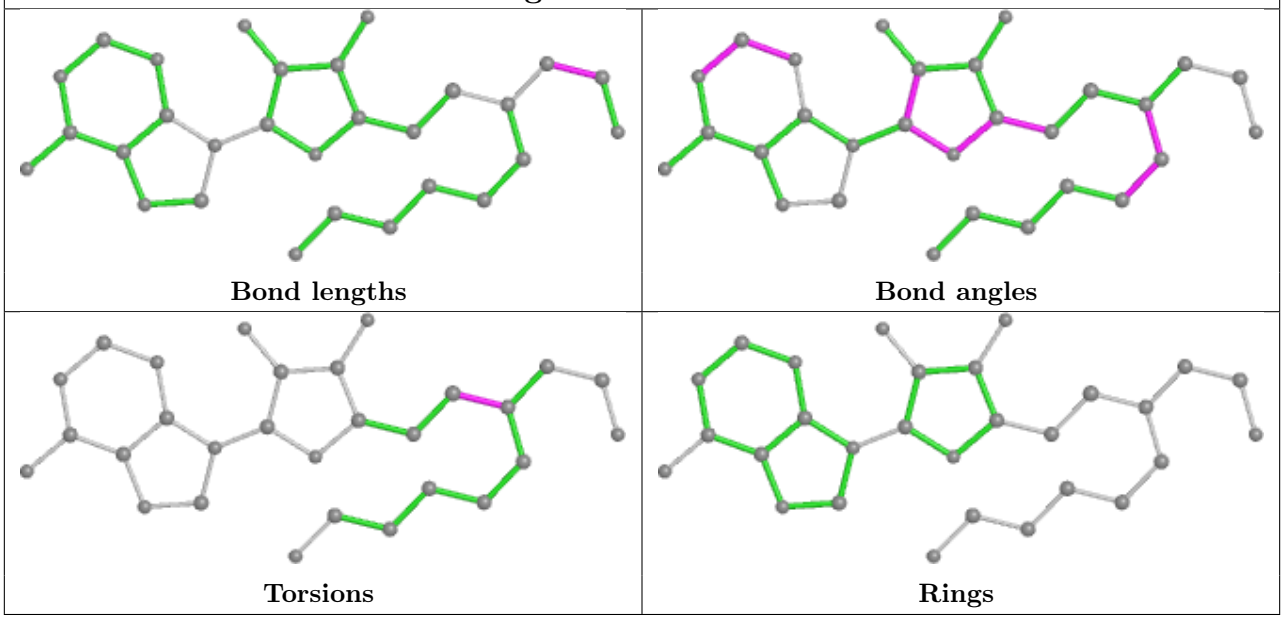
There are no ring outliers.

2 monomers are involved in 2 short contacts:

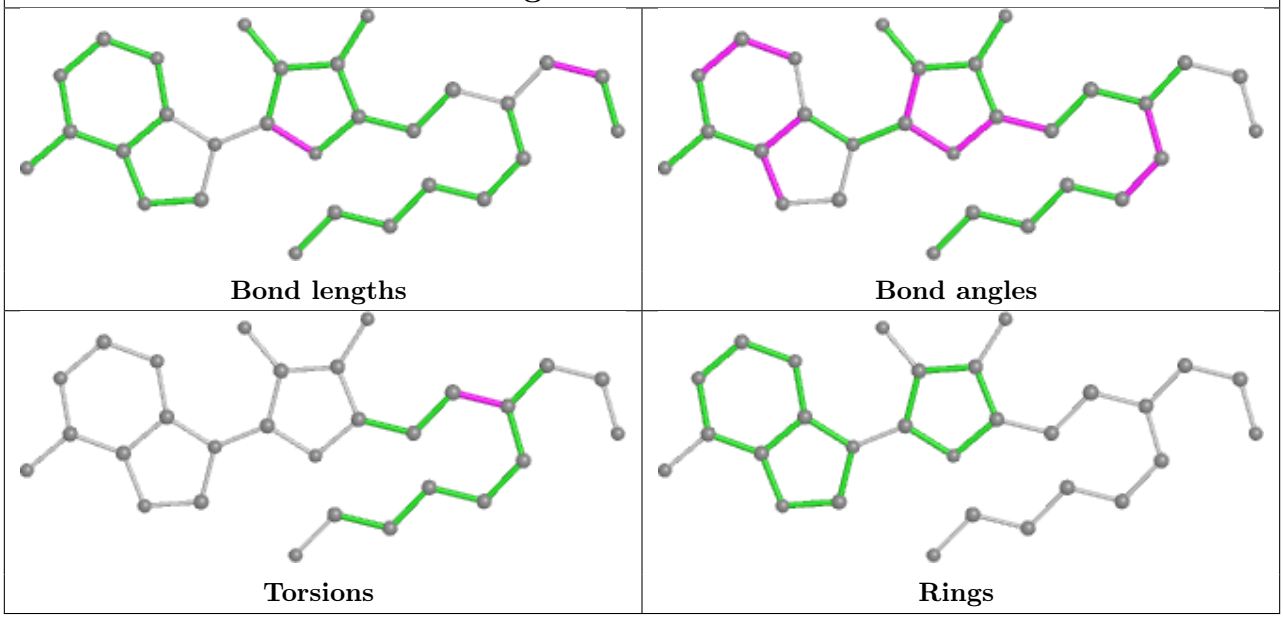
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	802	AAT	1	0
3	B	702	1PG	1	0

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 then 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.

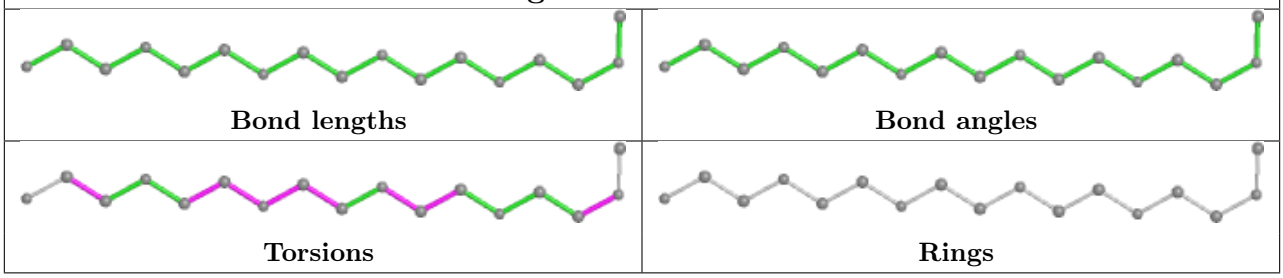
Ligand AAT B 802



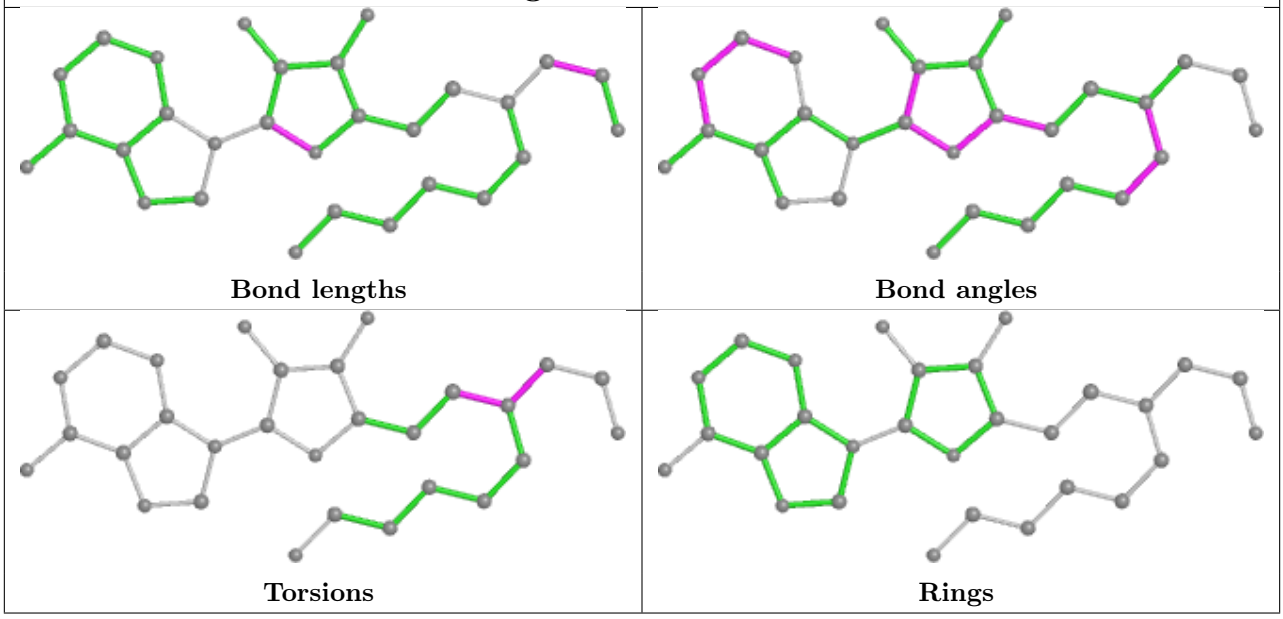
Ligand AAT A 801

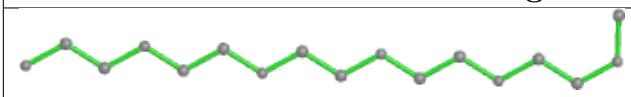
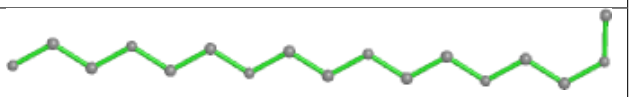
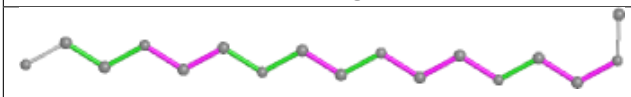
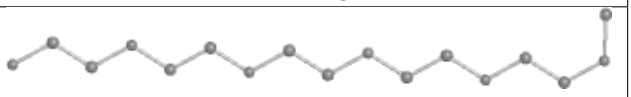


Ligand 1PG B 702



Ligand AAT C 803



Ligand 1PG A 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	239:ASP	C	240:THR	N	0.97
1	A	238:THR	C	239:ASP	N	0.88

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	281/283 (99%)	0.32	24 (8%)	10	12	22, 27, 35, 42	12 (4%)
1	B	280/283 (98%)	0.20	21 (7%)	14	16	16, 22, 33, 51	9 (3%)
1	C	281/283 (99%)	-0.06	11 (3%)	39	44	14, 19, 28, 37	3 (1%)
All	All	842/849 (99%)	0.15	56 (6%)	17	20	14, 24, 34, 51	24 (2%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	162	ILE	6.0
1	A	239	ASP	5.2
1	A	238	THR	5.2
1	B	281	ASN	5.1
1	B	10	ILE	4.6
1	B	238	THR	4.3
1	A	282	ILE	4.2
1	B	146[A]	ASN	4.0
1	B	280	GLU	3.8
1	A	230	ILE	3.7
1	A	280	GLU	3.6
1	A	156	VAL	3.6
1	A	63	TYR	3.4
1	C	230	ILE	3.3
1	A	250	GLU	3.2
1	B	2	LYS	3.1
1	A	240	THR	3.0
1	B	169	PHE	3.0
1	A	2	LYS	3.0
1	B	220	ILE	2.9
1	C	222	ILE	2.9
1	B	161	PRO	2.9
1	C	146	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	155	ILE	2.9
1	A	91	ILE	2.8
1	A	220	ILE	2.8
1	A	232	ILE	2.7
1	B	239	ASP	2.7
1	B	166	GLU	2.7
1	C	3	LYS	2.7
1	A	83	VAL	2.6
1	A	188	VAL	2.6
1	B	163	GLY	2.6
1	C	220	ILE	2.6
1	B	256	ASP	2.6
1	C	239	ASP	2.6
1	A	67	MET	2.5
1	B	222	ILE	2.5
1	A	229	CYS	2.4
1	B	3	LYS	2.4
1	A	233	LEU	2.3
1	C	63	TYR	2.3
1	B	91	ILE	2.3
1	C	2	LYS	2.3
1	B	32	TYR	2.2
1	B	167	THR	2.2
1	A	222	ILE	2.2
1	C	229	CYS	2.2
1	C	225	TYR	2.1
1	A	277	LYS	2.1
1	A	191	CYS	2.1
1	B	230	ILE	2.0
1	C	224	THR	2.0
1	A	231	GLY	2.0
1	A	255	ALA	2.0
1	B	77	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

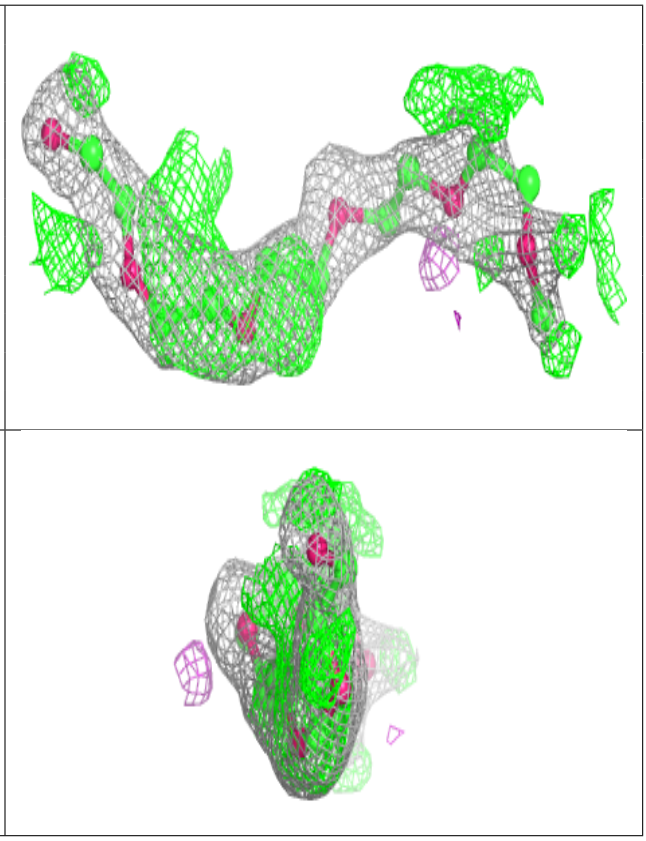
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	1PG	B	702	17/17	0.73	0.19	31,35,41,41	17
3	1PG	A	701	17/17	0.90	0.22	40,42,49,50	17
4	GOL	A	603	6/6	0.90	0.12	47,48,48,49	0
2	AAT	B	802	29/29	0.92	0.09	25,28,30,33	0
4	GOL	B	601	6/6	0.92	0.08	32,34,35,37	0
4	GOL	C	602	6/6	0.94	0.09	31,33,35,35	0
2	AAT	C	803	29/29	0.95	0.09	17,20,22,24	0
2	AAT	A	801	29/29	0.95	0.08	26,28,32,34	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.

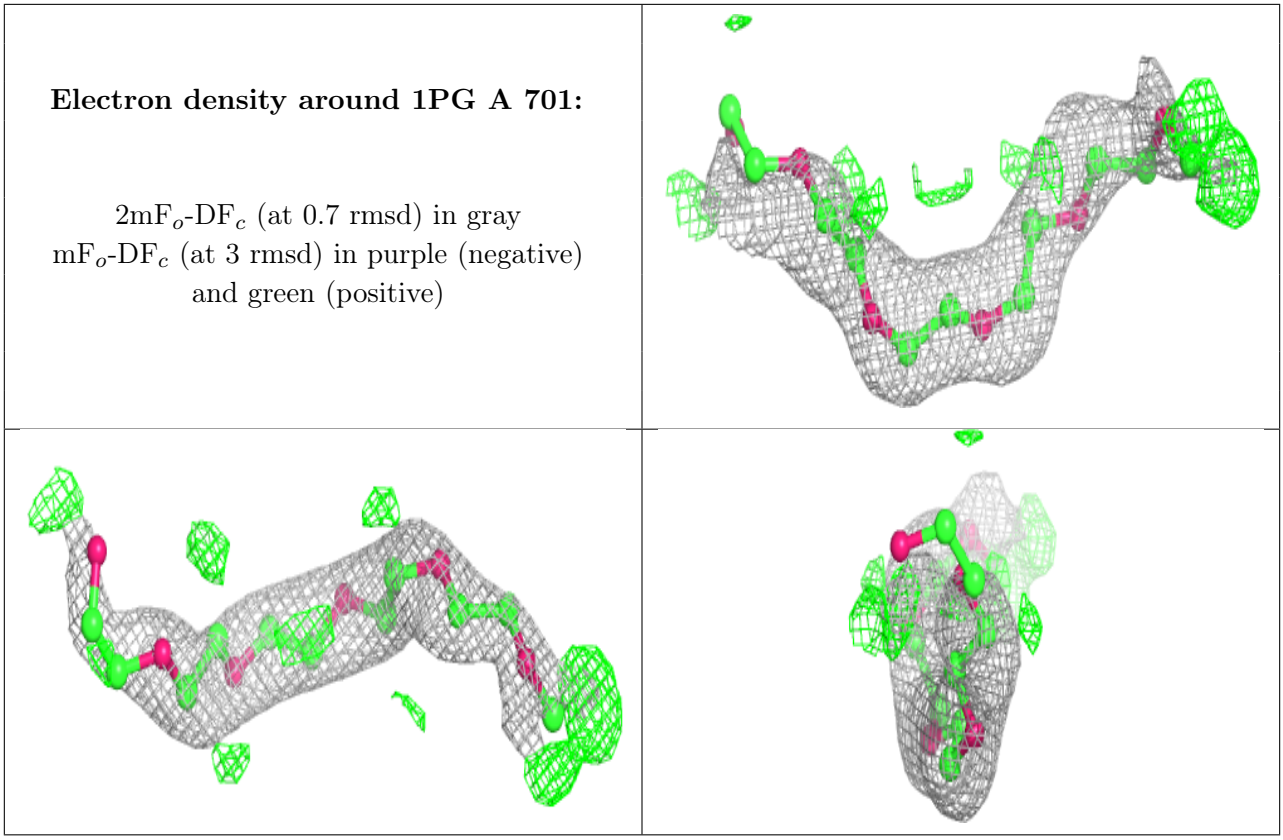
Electron density around 1PG B 702:

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



Electron density around 1PG 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 AAT B 802:

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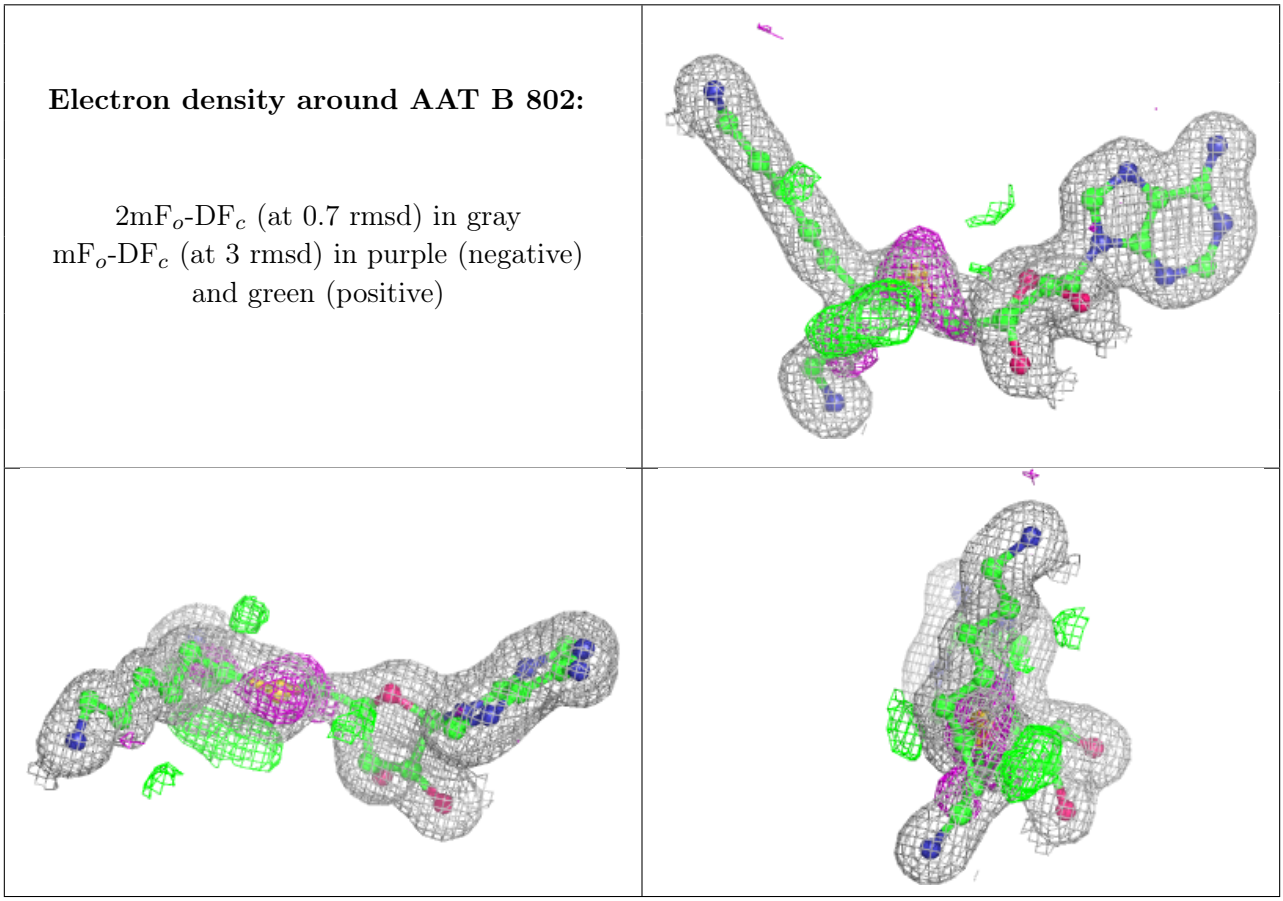
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AAT C 803:

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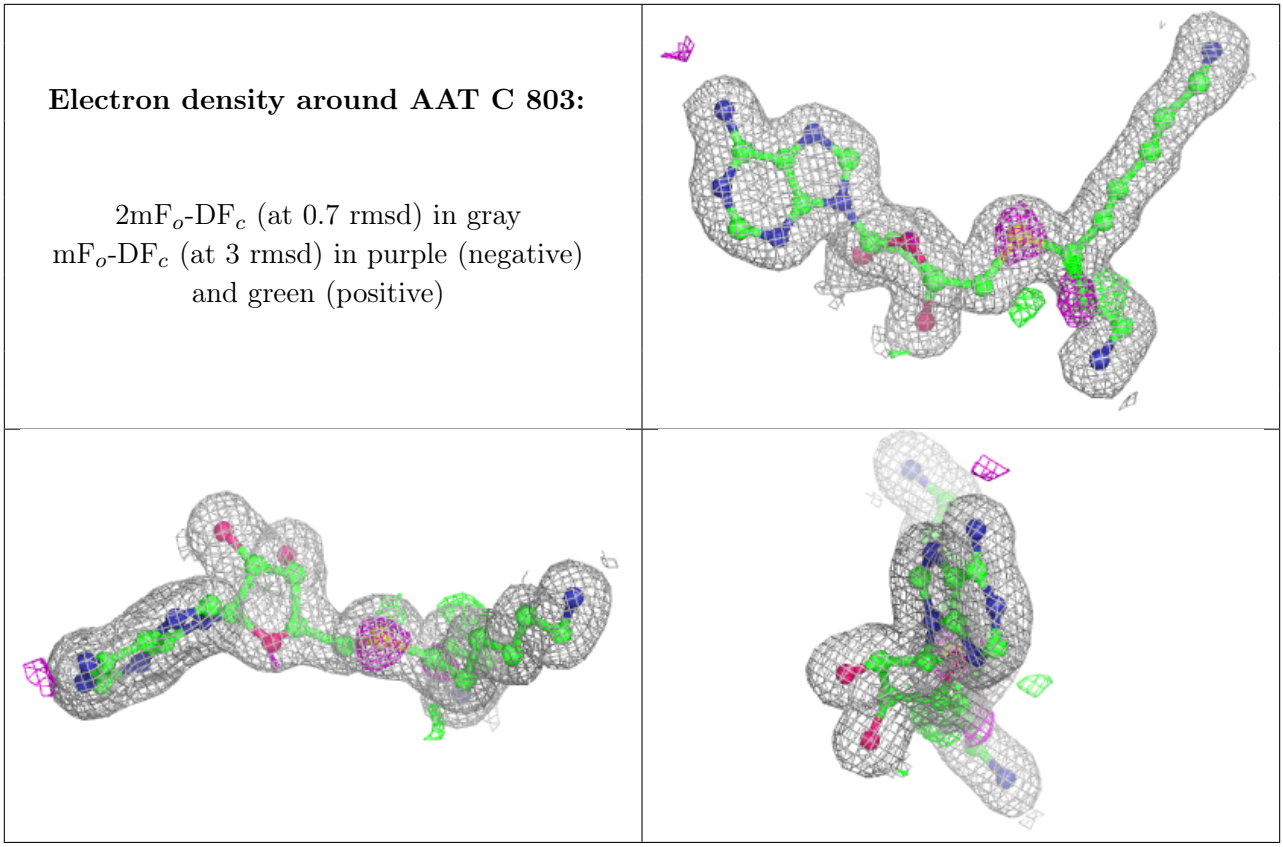
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AAT A 801:

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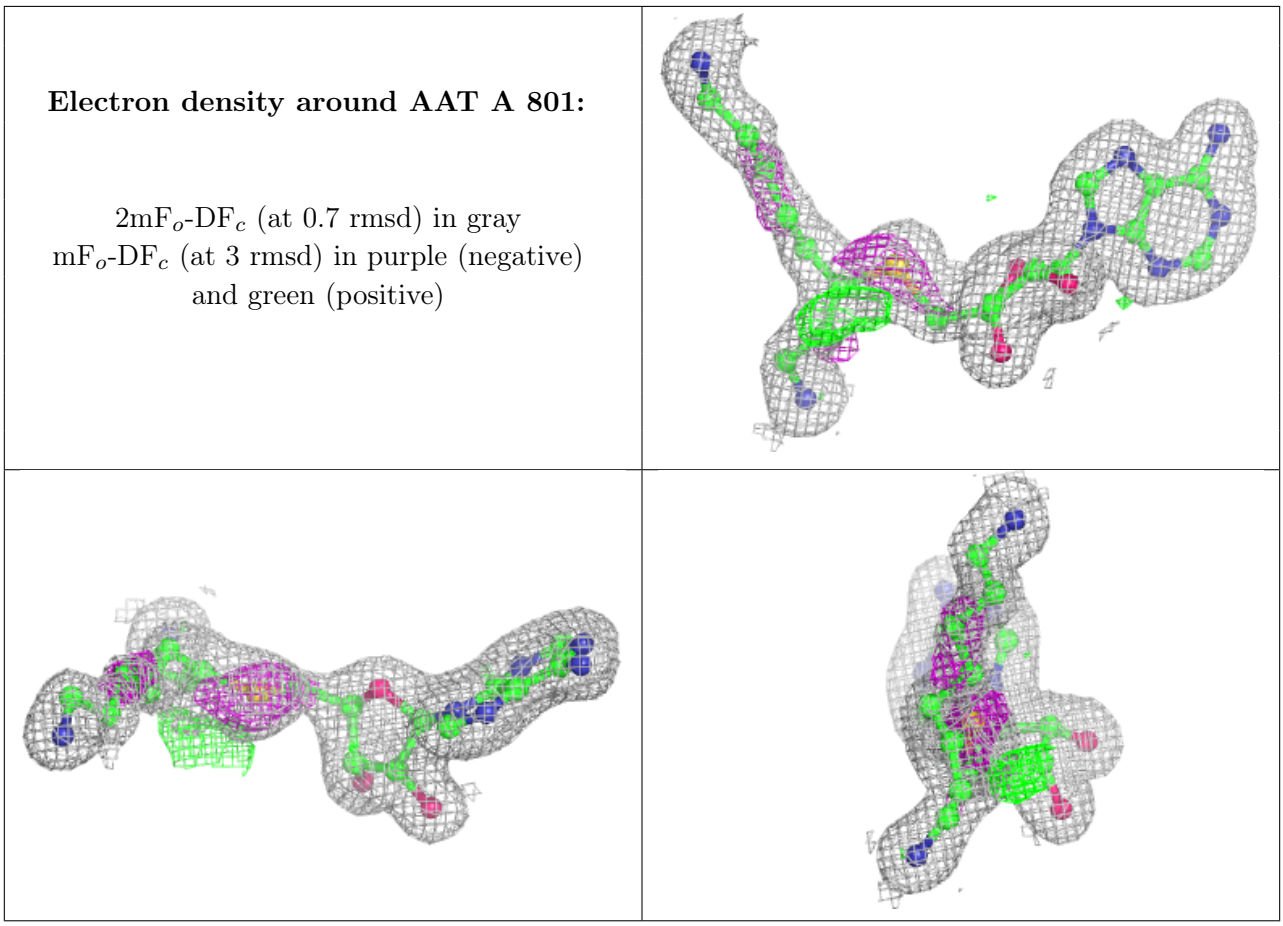
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.