wwPDB X-ray Structure Validation Summary Report (i)

Jan 22, 2024 – 03:20 PM EST

PDB ID	:	8VR5
Title	:	crystal structure of the Pcryo_0618 aminotransferase from Psychrobacter cryohalolentis K5 in the presence of PMP and glutamate
Authors	:	Bockhaus, N.J.; Thoden, J.B.; Holden, H.M.
Deposited on	:	2024-01-20
Resolution	:	2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

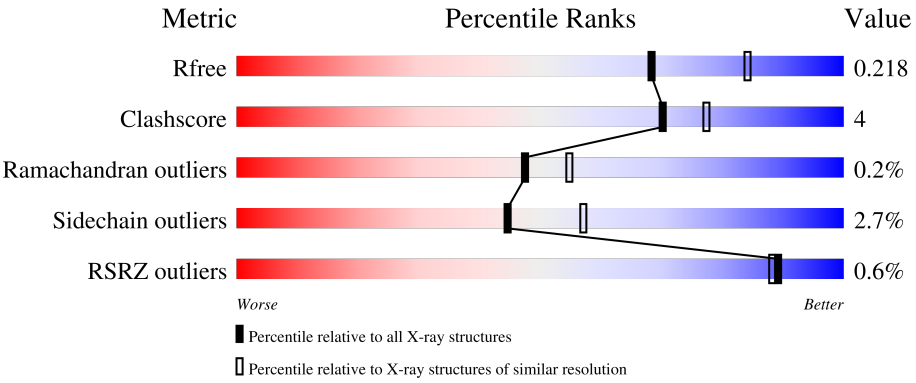
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	380	87% 10% • •
1	B	380	2% 88% 10% • •
1	C	380	91% 7% • •
1	D	380	87% 11% • •

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 12658 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 DegT/DnrJ/EryC1/StrS aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	3	0
			2897	1841	490	550	16			
1	B	376	Total	C	N	O	S	0	3	0
			2930	1861	497	556	16			
1	C	374	Total	C	N	O	S	0	1	0
			2896	1840	489	551	16			
1	D	374	Total	C	N	O	S	0	0	0
			2893	1838	489	550	16			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	373	LEU	-	expression tag	UNP Q1QD52
A	374	GLU	-	expression tag	UNP Q1QD52
A	375	HIS	-	expression tag	UNP Q1QD52
A	376	HIS	-	expression tag	UNP Q1QD52
A	377	HIS	-	expression tag	UNP Q1QD52
A	378	HIS	-	expression tag	UNP Q1QD52
A	379	HIS	-	expression tag	UNP Q1QD52
A	380	HIS	-	expression tag	UNP Q1QD52
B	373	LEU	-	expression tag	UNP Q1QD52
B	374	GLU	-	expression tag	UNP Q1QD52
B	375	HIS	-	expression tag	UNP Q1QD52
B	376	HIS	-	expression tag	UNP Q1QD52
B	377	HIS	-	expression tag	UNP Q1QD52
B	378	HIS	-	expression tag	UNP Q1QD52
B	379	HIS	-	expression tag	UNP Q1QD52
B	380	HIS	-	expression tag	UNP Q1QD52
C	373	LEU	-	expression tag	UNP Q1QD52
C	374	GLU	-	expression tag	UNP Q1QD52
C	375	HIS	-	expression tag	UNP Q1QD52
C	376	HIS	-	expression tag	UNP Q1QD52
C	377	HIS	-	expression tag	UNP Q1QD52

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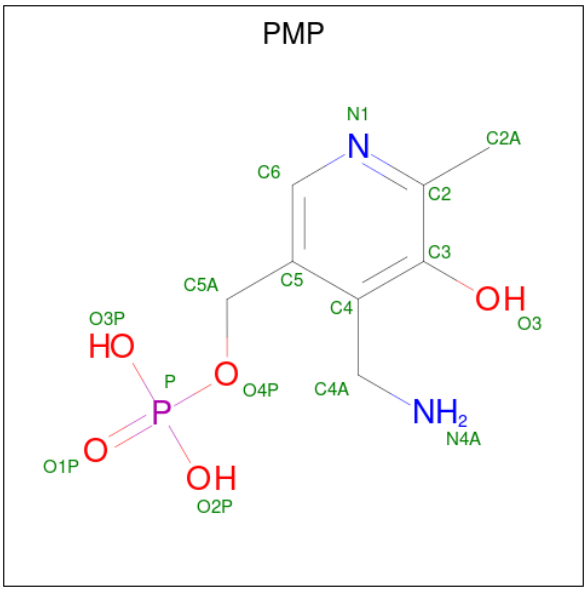
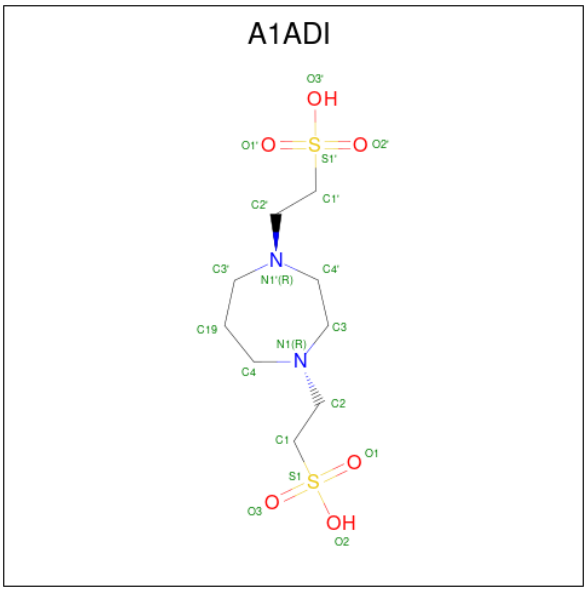
Chain	Residue	Modelled	Actual	Comment	Reference
C	378	HIS	-	expression tag	UNP Q1QD52
C	379	HIS	-	expression tag	UNP Q1QD52
C	380	HIS	-	expression tag	UNP Q1QD52
D	373	LEU	-	expression tag	UNP Q1QD52
D	374	GLU	-	expression tag	UNP Q1QD52
D	375	HIS	-	expression tag	UNP Q1QD52
D	376	HIS	-	expression tag	UNP Q1QD52
D	377	HIS	-	expression tag	UNP Q1QD52
D	378	HIS	-	expression tag	UNP Q1QD52
D	379	HIS	-	expression tag	UNP Q1QD52
D	380	HIS	-	expression tag	UNP Q1QD52

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: $C_8H_{13}N_2O_5P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 3 is 2,2'-(1,4-diazepane-1,4-diyl)di(ethane-1-sulfonic acid) (three-letter code: A1ADI) (formula: $C_9H_{20}N_2O_6S_2$).

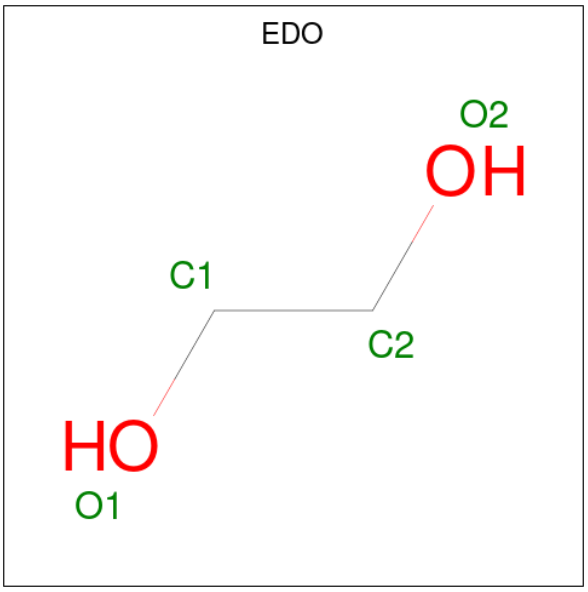


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 19 9 2 6 2	0	0
3	B	1	Total C N O S 19 9 2 6 2	0	0
3	B	1	Total C N O S 19 9 2 6 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

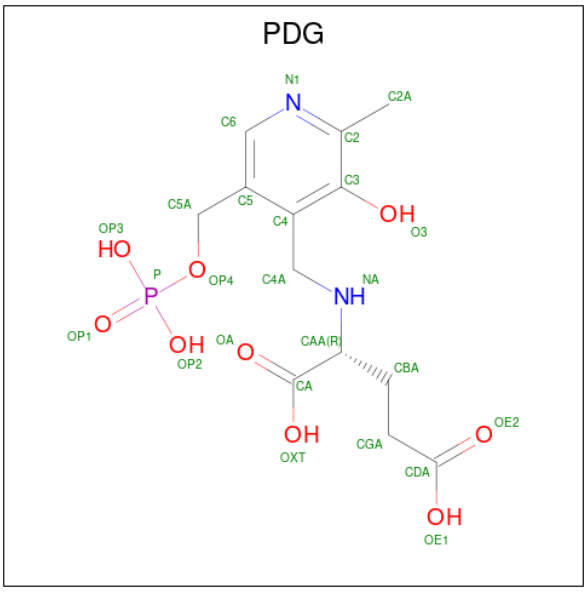


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0
6	B	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0

- Molecule 7 is N-({3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PYRIDIN-4-YL}METHYL)-D-GLUTAMIC ACID (three-letter code: PDG) (formula: $C_{13}H_{19}N_2O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O P 25 13 2 9 1	0	0
7	C	1	Total C N O P 25 13 2 9 1	0	0
7	D	1	Total C N O P 25 13 2 9 1	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Na 1 1	0	0
8	C	1	Total Na 1 1	0	0
8	D	1	Total Na 1 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	246	Total O 246 246	0	0
9	B	257	Total O 257 257	0	0
9	C	195	Total O 195 195	0	0

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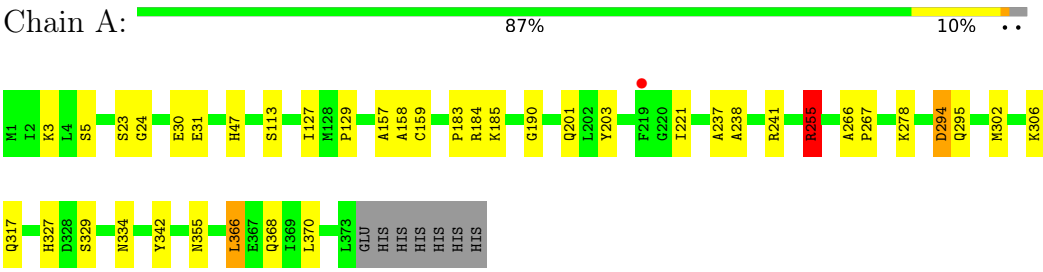
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	159	Total 159	O 159	0	0

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.

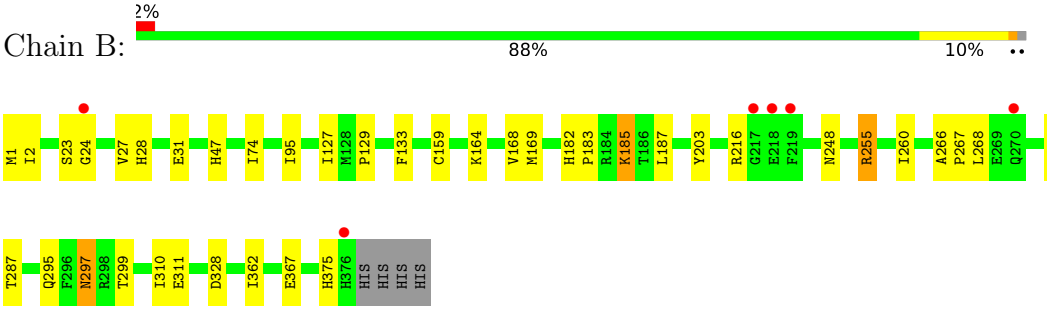
• Molecule 1: DegT/DnrJ/EryC1/StrS aminotransferase

Chain A:



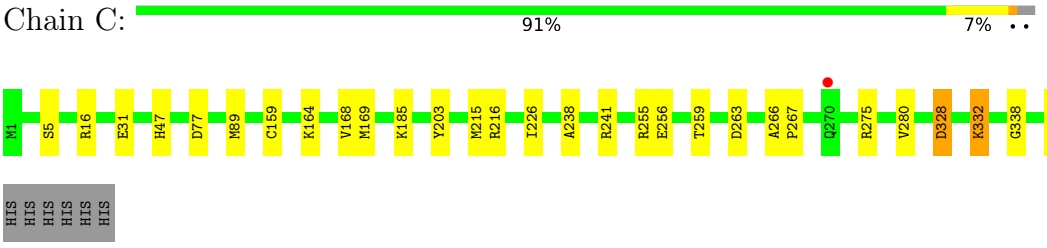
• Molecule 1: DegT/DnrJ/EryC1/StrS aminotransferase

Chain B:



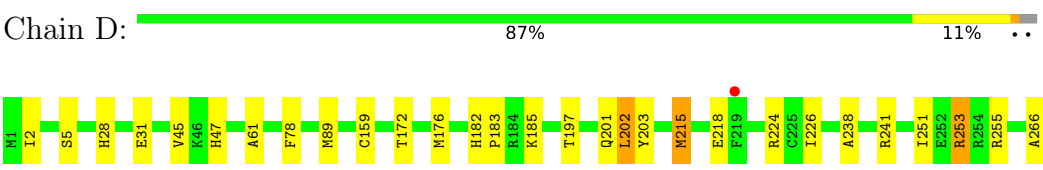
• Molecule 1: DegT/DnrJ/EryC1/StrS aminotransferase

Chain C:



• Molecule 1: DegT/DnrJ/EryC1/StrS aminotransferase

Chain D:




I279
V280
Y288
A316
H327
D328
S329
K332
L350
I362
L366
E367
Q368
I369
L370
E374
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	131.49Å 159.82Å 115.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.89 – 2.20 32.89 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (32.89-2.20) 99.7 (32.89-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.178 , 0.213 0.185 , 0.218	Depositor DCC
R_{free} test set	6297 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	19.2	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12658	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2739e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1ADI, NA, CL, PDG, EDO, MG, PMP

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	0.48	0/2953	0.79	0/3991
1	B	0.48	0/2988	0.80	1/4038 (0.0%)
1	C	0.45	0/2946	0.75	0/3981
1	D	0.43	0/2940	0.74	0/3973
All	All	0.46	0/11827	0.77	1/15983 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	295	GLN	CB-CA-C	-5.15	100.10	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	255	ARG	Sidechain
1	B	255	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	16	ARG	Sidechain
1	C	275	ARG	Sidechain

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	2897	0	2946	19	0
1	B	2930	0	2969	21	0
1	C	2896	0	2940	15	0
1	D	2893	0	2935	26	0
2	A	16	0	11	1	0
3	A	19	0	0	0	0
3	B	38	0	0	0	0
4	A	1	0	0	1	0
4	B	1	0	0	0	0
4	C	1	0	0	1	0
5	A	16	0	24	0	0
5	B	12	0	18	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	B	25	0	15	1	0
7	C	25	0	15	2	0
7	D	25	0	15	2	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	246	0	0	2	1
9	B	257	0	0	2	0
9	C	195	0	0	1	0
9	D	159	0	0	3	0
All	All	12658	0	11888	84	1

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.

The worst 5 of 84 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:159:CYS:SG	1:A:185:LYS:NZ	2.35	0.99
1:B:159:CYS:SG	1:B:185:LYS:NZ	2.36	0.98
1:D:253:ARG:HH11	1:D:253:ARG:HG2	1.37	0.86
1:D:159:CYS:SG	1:D:185:LYS:NZ	2.53	0.81
7:D:401:PDG:H4A1	7:D:401:PDG:HGA1	1.66	0.78

All (1) 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)
9:A:724:HOH:O	9:A:724:HOH:O[2_555]	1.25	0.95

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	374/380 (98%)	361 (96%)	12 (3%)	1 (0%)	41	46
1	B	377/380 (99%)	365 (97%)	11 (3%)	1 (0%)	41	46
1	C	373/380 (98%)	362 (97%)	11 (3%)	0	100	100
1	D	372/380 (98%)	360 (97%)	11 (3%)	1 (0%)	41	46
All	All	1496/1520 (98%)	1448 (97%)	45 (3%)	3 (0%)	47	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	ASP
1	B	375	HIS
1	D	28	HIS

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	314/318 (99%)	302 (96%)	12 (4%)	33	42
1	B	317/318 (100%)	311 (98%)	6 (2%)	57	71
1	C	313/318 (98%)	306 (98%)	7 (2%)	52	65
1	D	312/318 (98%)	303 (97%)	9 (3%)	42	54
All	All	1256/1272 (99%)	1222 (97%)	34 (3%)	44	57

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	218	GLU
1	D	253	ARG
1	D	366	LEU
1	B	31	GLU
1	A	368	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	297	ASN
1	D	116	GLN
1	D	353	HIS
1	D	182	HIS
1	B	201	GLN

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)

Of 23 ligands modelled in this entry, 9 are monoatomic - leaving 14 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	EDO	B	407	-	3,3,3	0.17	0	2,2,2	0.35	0
5	EDO	B	406	-	3,3,3	0.40	0	2,2,2	0.46	0
2	PMP	A	401	-	16,16,16	0.55	0	21,23,23	0.80	0
3	A1ADI	B	402	-	19,19,19	2.16	2 (10%)	19,27,27	2.98	9 (47%)
7	PDG	C	401	-	25,25,25	0.80	1 (4%)	31,35,35	1.16	3 (9%)
5	EDO	A	405	-	3,3,3	0.37	0	2,2,2	0.82	0
5	EDO	A	404	-	3,3,3	0.14	0	2,2,2	0.32	0
5	EDO	A	407	-	3,3,3	0.43	0	2,2,2	0.54	0
7	PDG	D	401	-	25,25,25	0.96	0	31,35,35	1.51	4 (12%)
3	A1ADI	B	403	-	19,19,19	2.10	5 (26%)	19,27,27	2.84	5 (26%)
5	EDO	A	406	-	3,3,3	0.19	0	2,2,2	0.36	0
7	PDG	B	401	-	25,25,25	0.84	0	31,35,35	1.02	1 (3%)
5	EDO	B	405	-	3,3,3	0.39	0	2,2,2	0.52	0
3	A1ADI	A	402	-	19,19,19	2.12	2 (10%)	19,27,27	2.60	4 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	407	-	-	1/1/1/1	-
5	EDO	B	406	-	-	0/1/1/1	-
2	PMP	A	401	-	-	2/8/8/8	0/1/1/1
3	A1ADI	B	402	-	-	6/12/23/23	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PDG	C	401	-	-	10/20/20/20	0/1/1/1
5	EDO	A	405	-	-	0/1/1/1	-
5	EDO	A	404	-	-	0/1/1/1	-
5	EDO	A	407	-	-	0/1/1/1	-
7	PDG	D	401	-	-	5/20/20/20	0/1/1/1
3	A1ADI	B	403	-	-	10/12/23/23	0/1/1/1
5	EDO	A	406	-	-	0/1/1/1	-
7	PDG	B	401	-	-	9/20/20/20	0/1/1/1
5	EDO	B	405	-	-	0/1/1/1	-
3	A1ADI	A	402	-	-	4/12/23/23	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	A1ADI	C1'-S1'	-5.99	1.69	1.77
3	B	402	A1ADI	C1-S1	-5.87	1.69	1.77
3	A	402	A1ADI	C1'-S1'	-5.48	1.69	1.77
3	A	402	A1ADI	C1-S1	-5.39	1.69	1.77
3	B	403	A1ADI	C1'-S1'	-5.08	1.70	1.77

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	403	A1ADI	O3-S1-C1	9.49	118.34	106.92
3	B	402	A1ADI	O2'-S1'-C1'	7.94	116.47	106.92
3	A	402	A1ADI	O2'-S1'-C1'	7.34	115.75	106.92
3	B	402	A1ADI	O1-S1-C1	5.77	113.86	106.92
3	B	402	A1ADI	O1'-S1'-C1'	-5.14	100.72	106.92

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	A1ADI	C1-C2-N1-C4
3	A	402	A1ADI	S1-C1-C2-N1
3	B	402	A1ADI	C1'-C2'-N1'-C3'
3	B	403	A1ADI	C2'-C1'-S1'-O1'
3	B	403	A1ADI	S1'-C1'-C2'-N1'

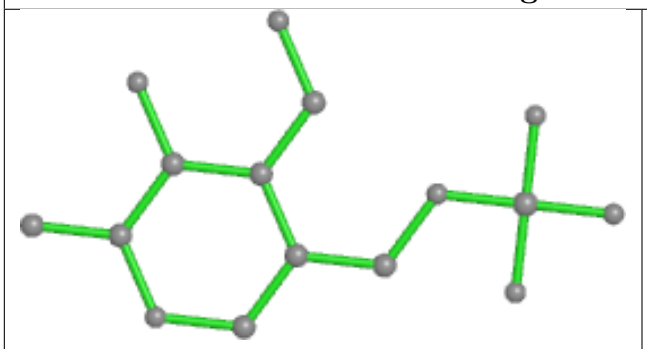
There are no ring outliers.

4 monomers are involved in 6 short contacts:

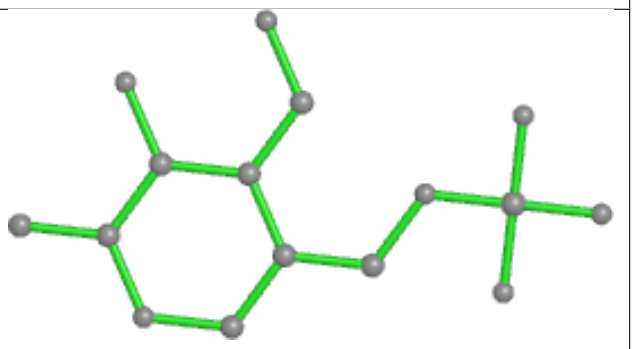
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	PMP	1	0
7	C	401	PDG	2	0
7	D	401	PDG	2	0
7	B	401	PDG	1	0

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.

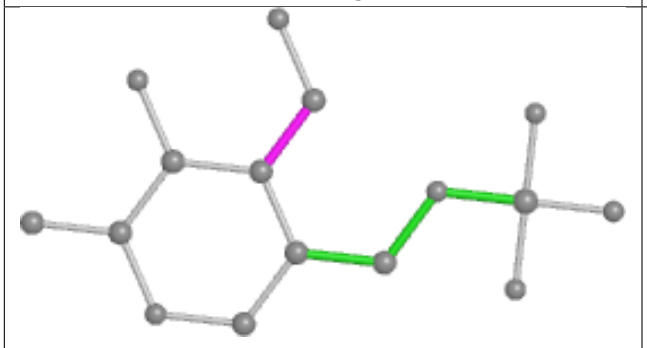
Ligand PMP A 401



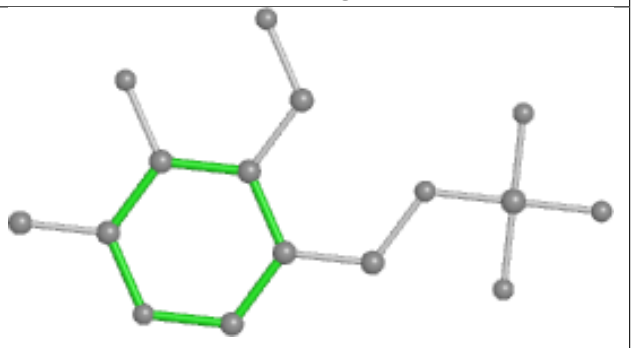
Bond lengths



Bond angles

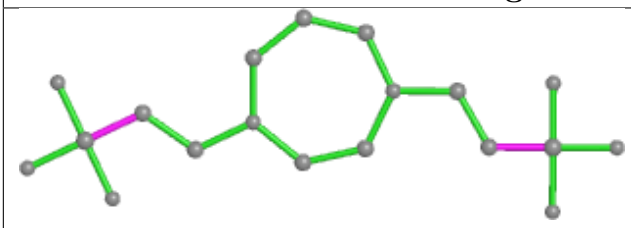


Torsions

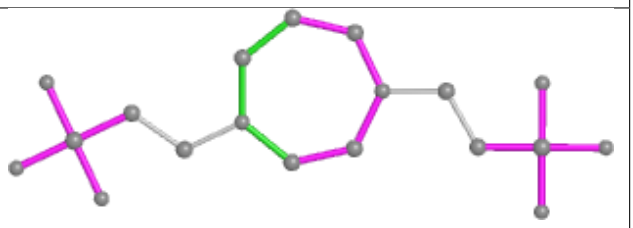


Rings

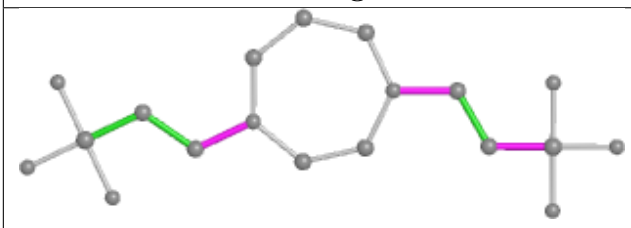
Ligand A1ADI B 402



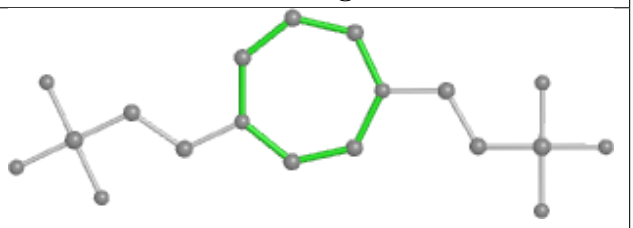
Bond lengths



Bond angles

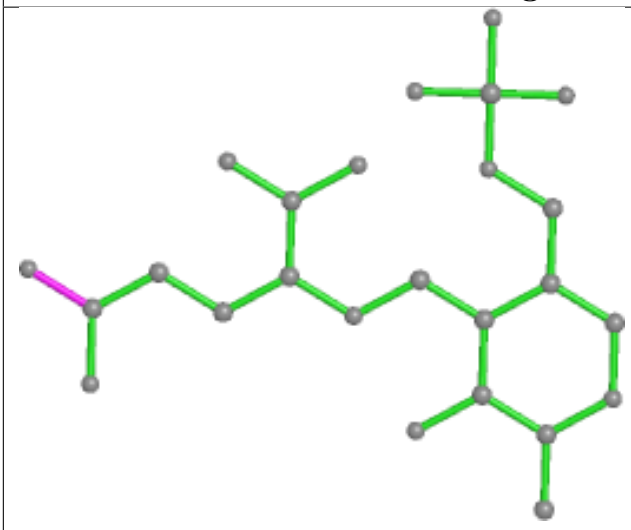


Torsions

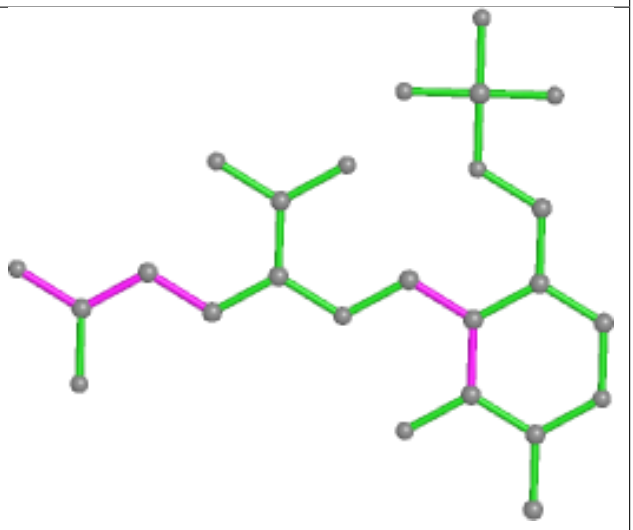


Rings

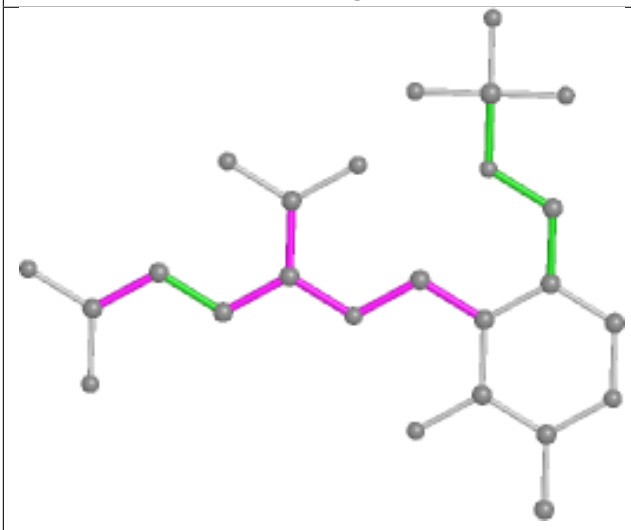
Ligand PDG C 401



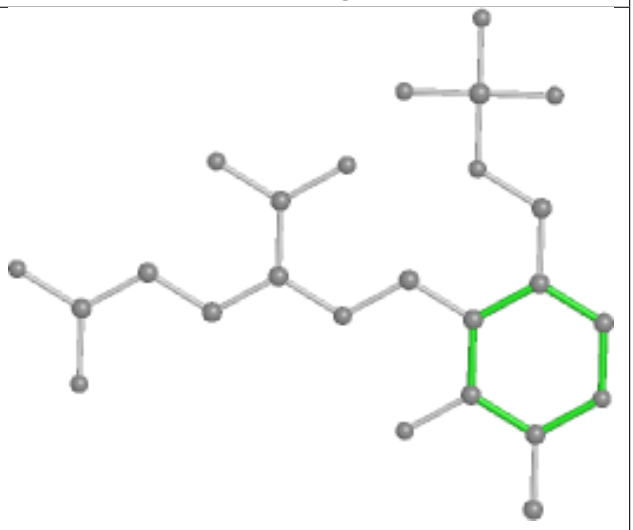
Bond lengths



Bond angles

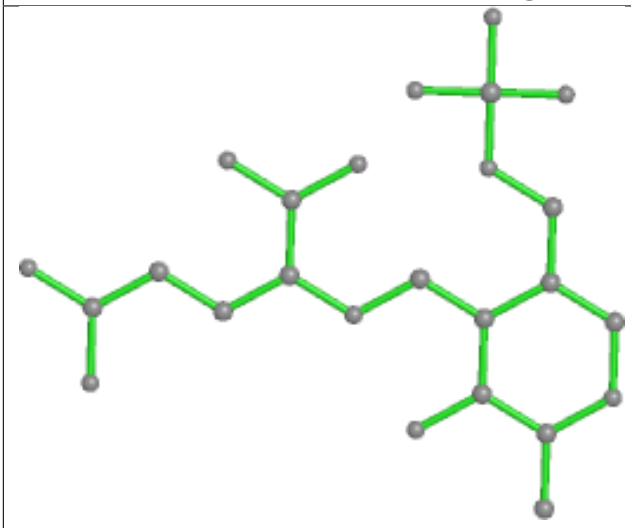


Torsions

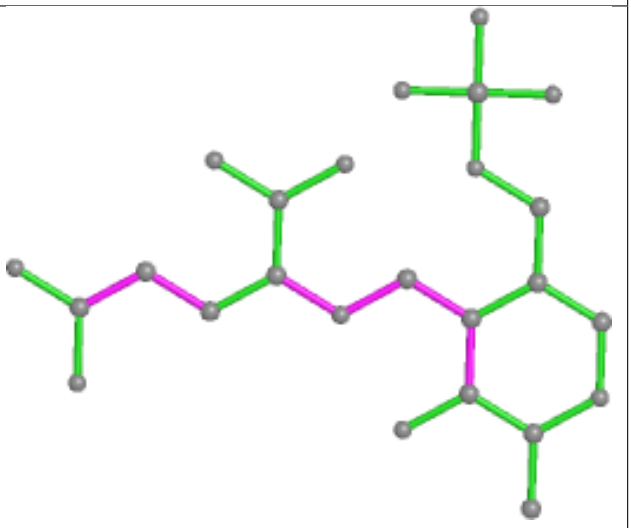


Rings

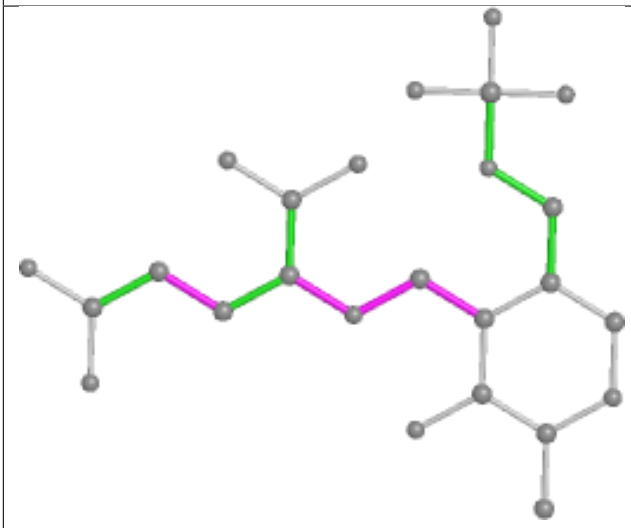
Ligand PDG D 401



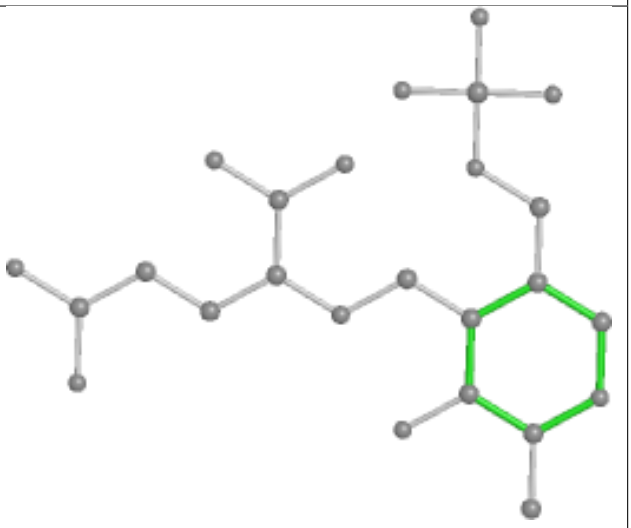
Bond lengths



Bond angles

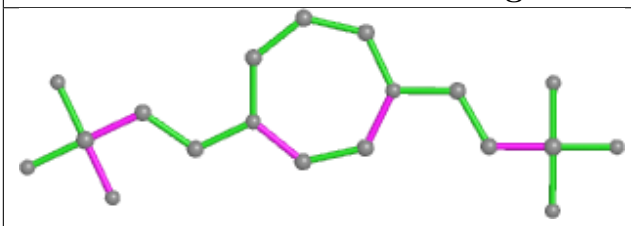


Torsions

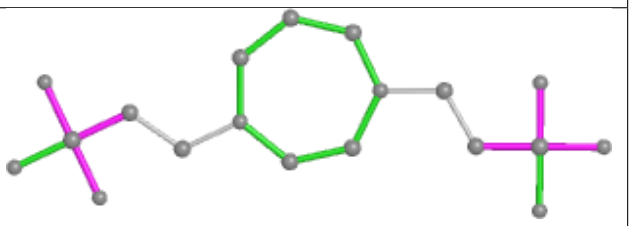


Rings

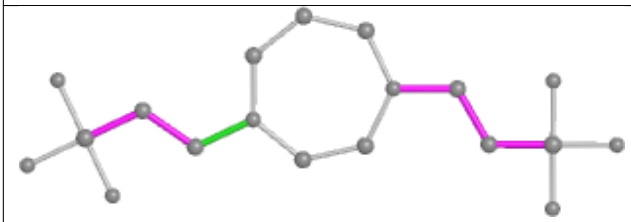
Ligand A1ADI B 403



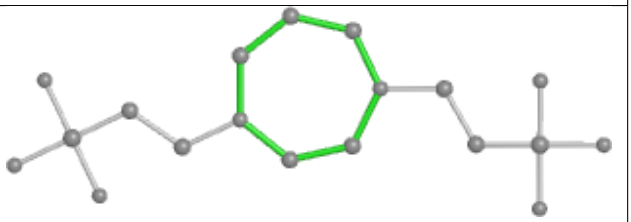
Bond lengths



Bond angles

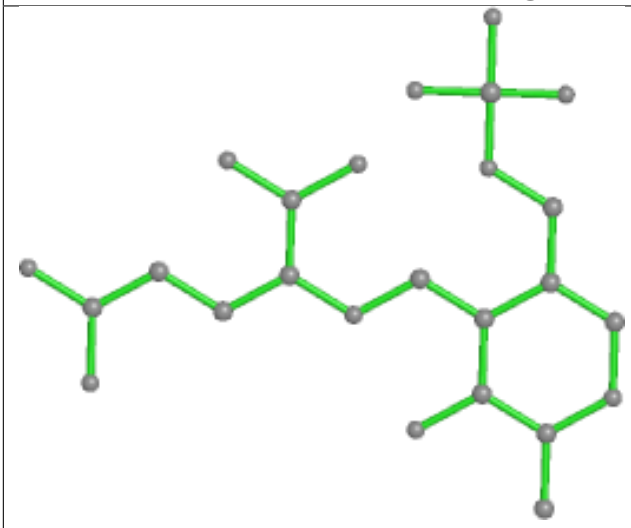


Torsions

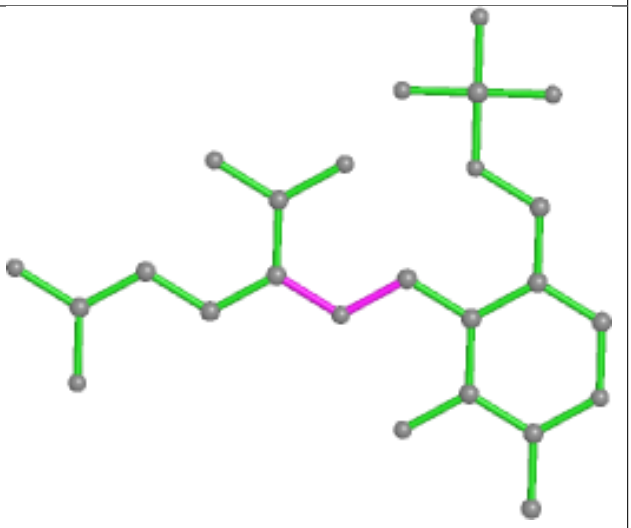


Rings

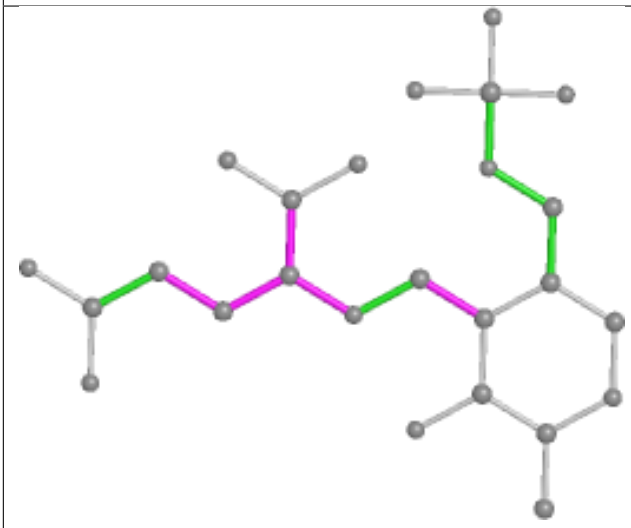
Ligand PDG B 401



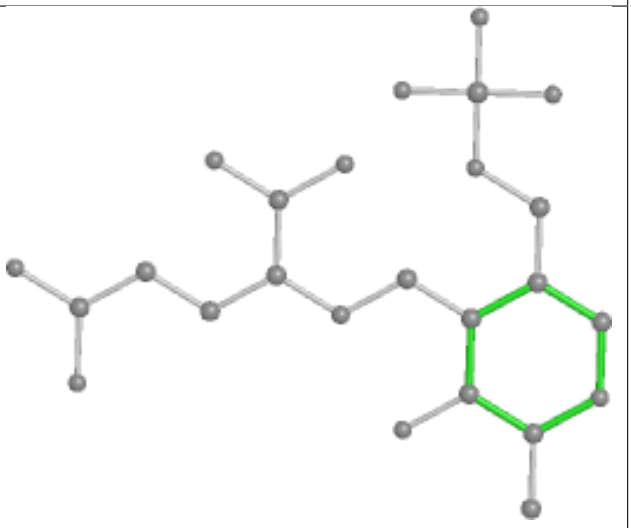
Bond lengths



Bond angles

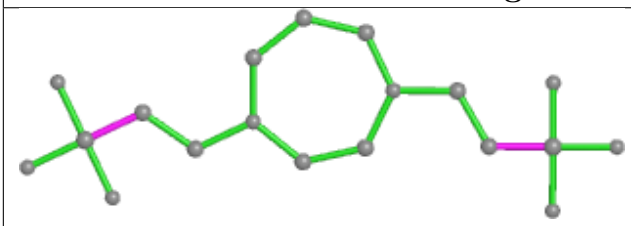


Torsions

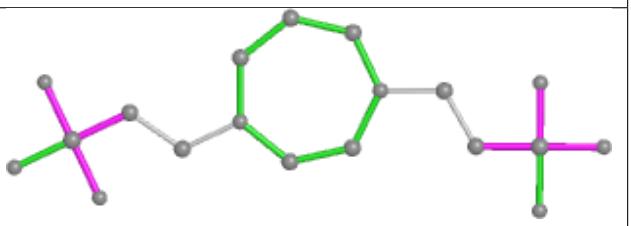


Rings

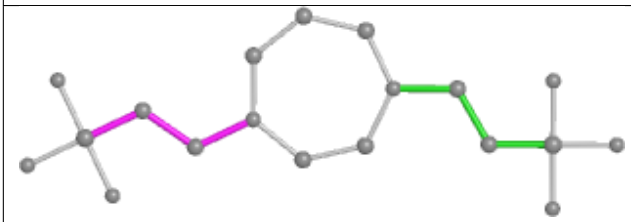
Ligand A1ADI A 402



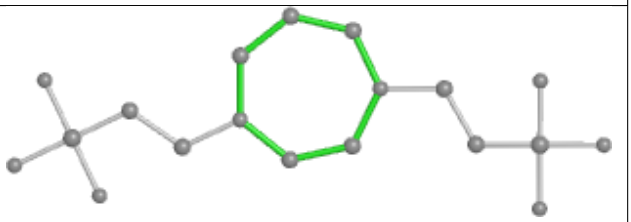
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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, 95^{th} 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	373/380 (98%)	-0.75	1 (0%)	94	93	6, 17, 41, 80	0
1	B	376/380 (98%)	-0.70	6 (1%)	72	70	9, 18, 40, 95	0
1	C	374/380 (98%)	-0.57	1 (0%)	94	93	11, 22, 48, 70	0
1	D	374/380 (98%)	-0.54	1 (0%)	94	93	13, 24, 52, 86	0
All	All	1497/1520 (98%)	-0.64	9 (0%)	89	88	6, 21, 47, 95	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	219	PHE	3.9
1	B	376	HIS	3.7
1	A	219	PHE	3.1
1	B	270	GLN	2.8
1	C	270	GLN	2.7

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

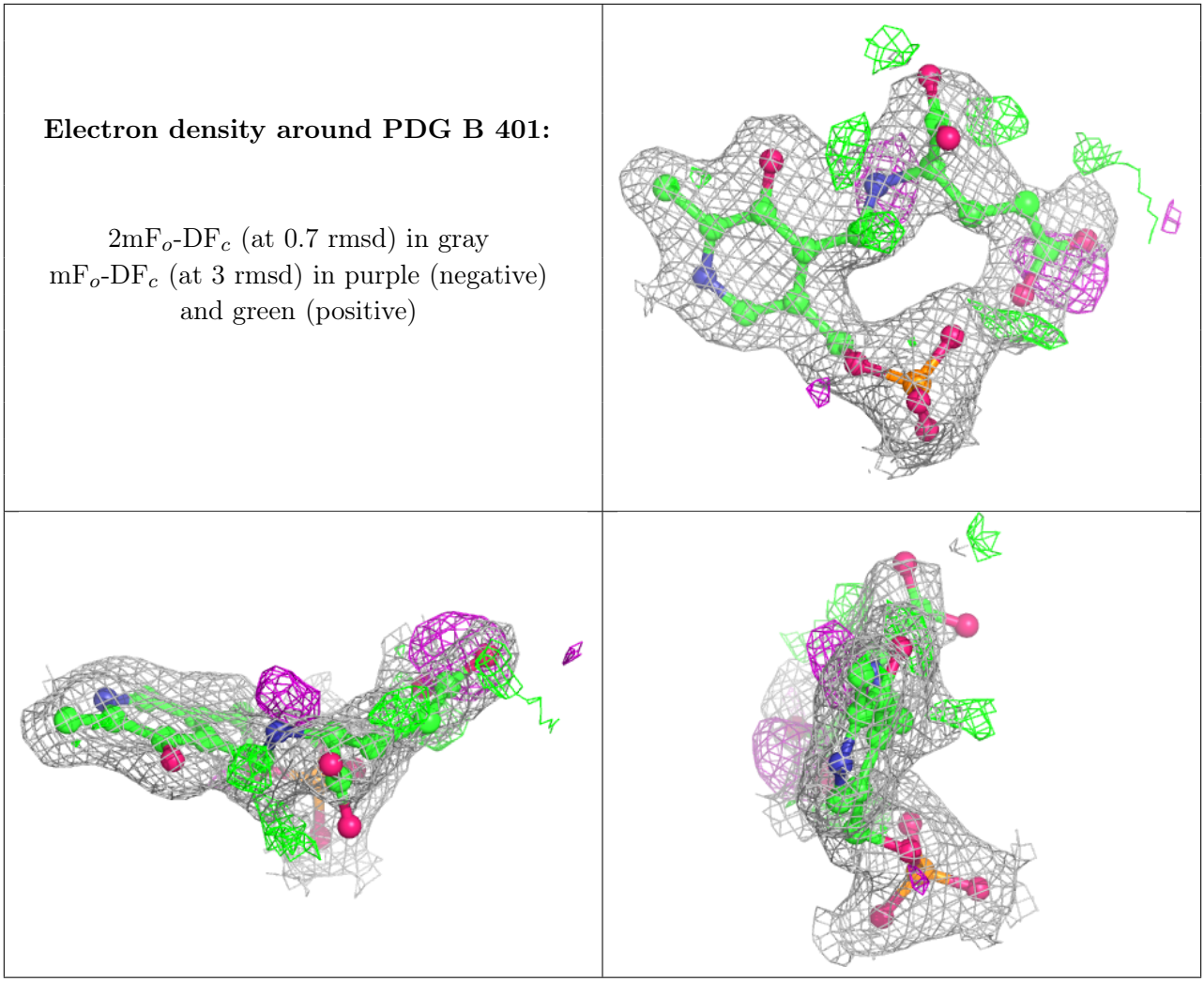
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	EDO	B	406	4/4	0.73	0.20	52,57,60,63	0
6	MG	B	408	1/1	0.85	0.15	43,43,43,43	0
8	NA	B	409	1/1	0.90	0.17	34,34,34,34	0
5	EDO	A	407	4/4	0.91	0.17	32,33,37,37	4
5	EDO	B	405	4/4	0.92	0.11	34,35,35,36	0
5	EDO	A	404	4/4	0.92	0.13	43,44,45,45	0
6	MG	D	402	1/1	0.93	0.14	41,41,41,41	0
5	EDO	A	406	4/4	0.93	0.11	27,31,34,37	0
6	MG	A	408	1/1	0.94	0.11	41,41,41,41	0
7	PDG	B	401	25/25	0.95	0.15	10,14,61,69	0
3	A1ADI	A	402	19/19	0.95	0.19	41,60,93,104	0
3	A1ADI	B	403	19/19	0.96	0.17	32,50,72,74	0
3	A1ADI	B	402	19/19	0.96	0.13	27,40,59,62	0
7	PDG	C	401	25/25	0.96	0.17	11,14,60,65	0
5	EDO	A	405	4/4	0.96	0.10	21,21,22,22	0
7	PDG	D	401	25/25	0.97	0.19	14,20,68,72	0
8	NA	C	403	1/1	0.97	0.08	27,27,27,27	0
8	NA	D	403	1/1	0.97	0.14	33,33,33,33	0
4	CL	B	404	1/1	0.98	0.05	35,35,35,35	0
4	CL	C	402	1/1	0.98	0.04	22,22,22,22	0
5	EDO	B	407	4/4	0.98	0.07	20,21,22,23	0
4	CL	A	403	1/1	0.98	0.05	32,32,32,32	0
2	PMP	A	401	16/16	0.99	0.13	8,11,16,21	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.

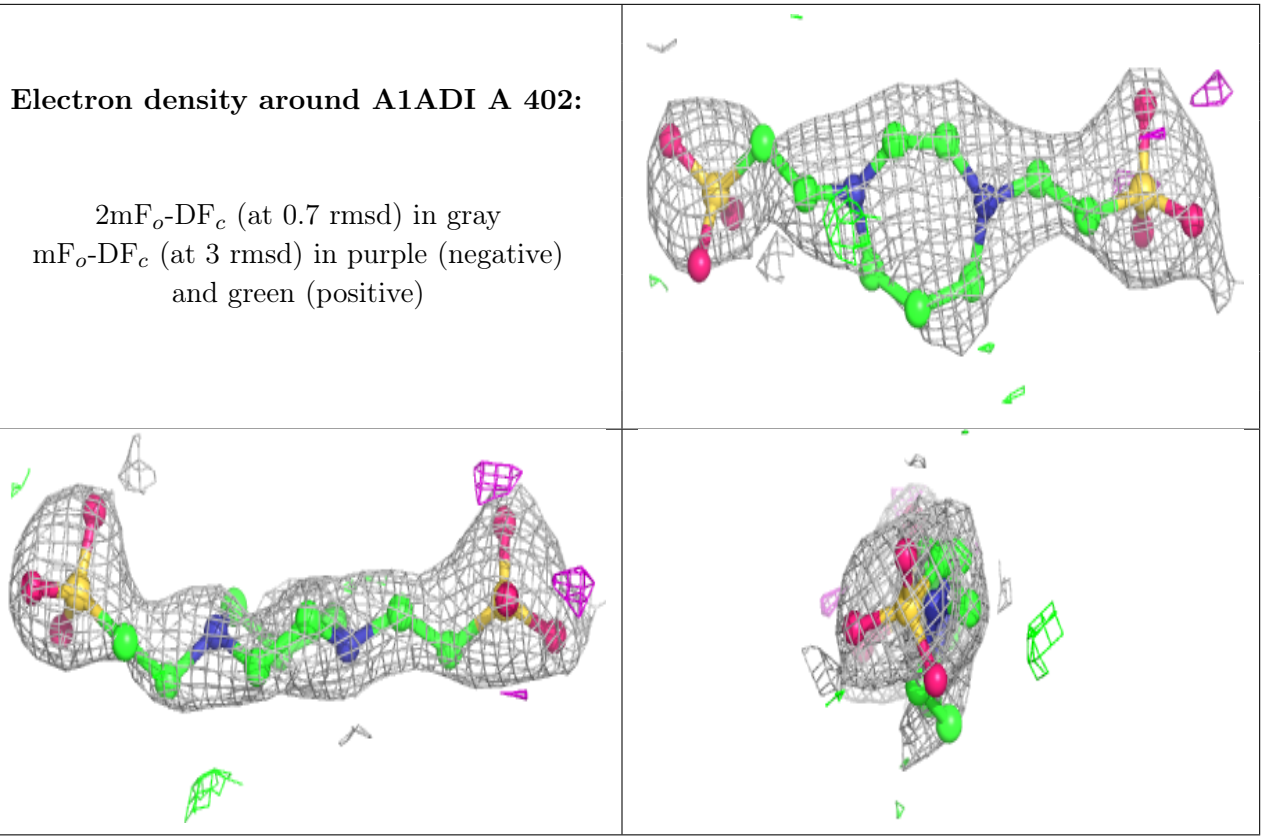
Electron density around PDG B 401:

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



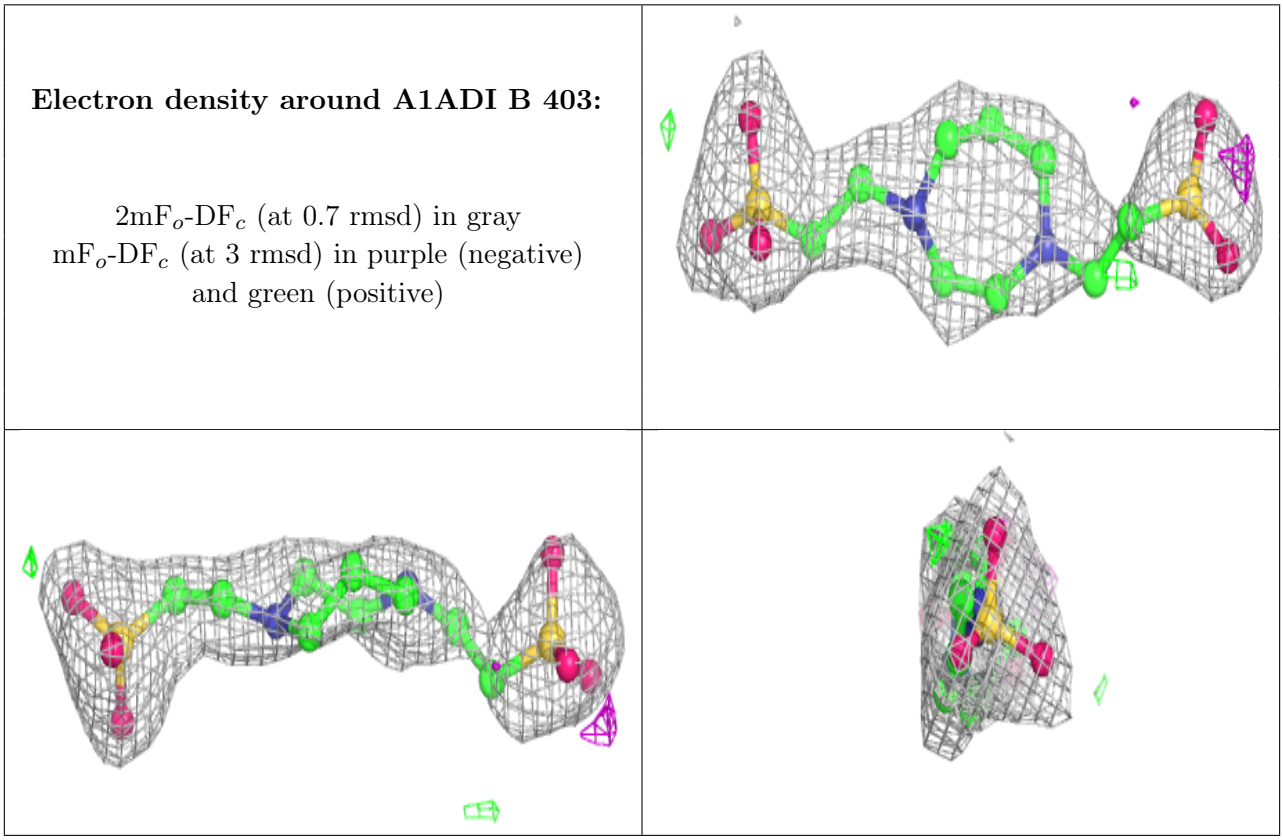
Electron density around A1ADI A 402:

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



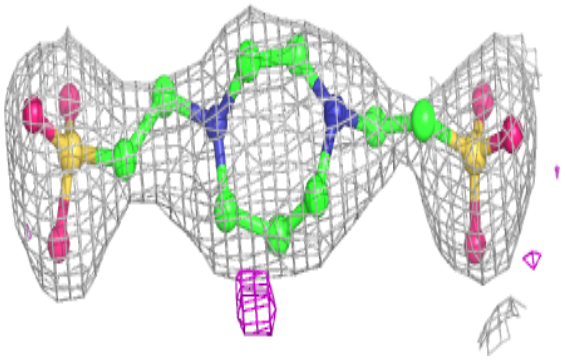
Electron density around A1ADI B 403:

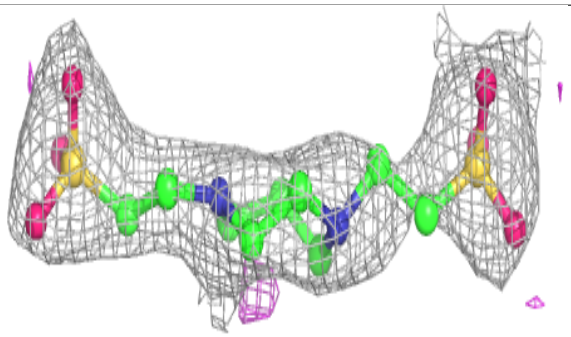
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

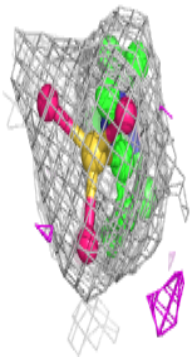


Electron density around A1ADI B 402:

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

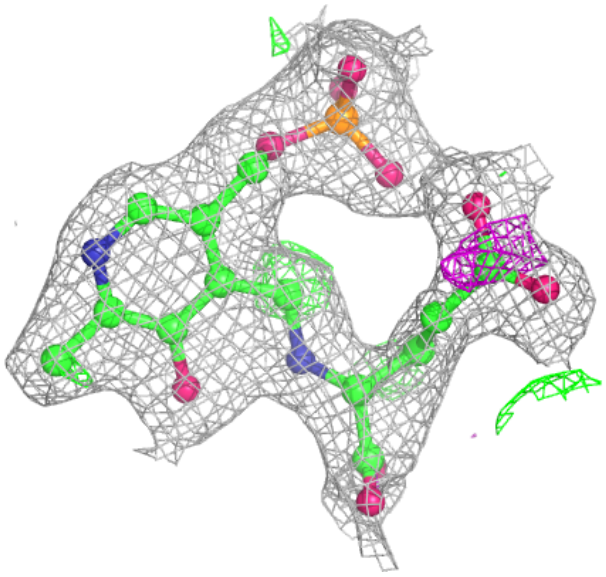


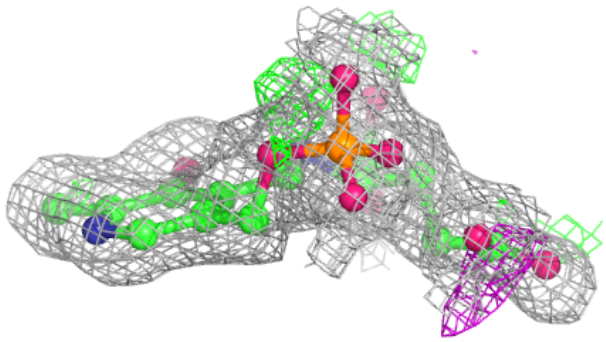


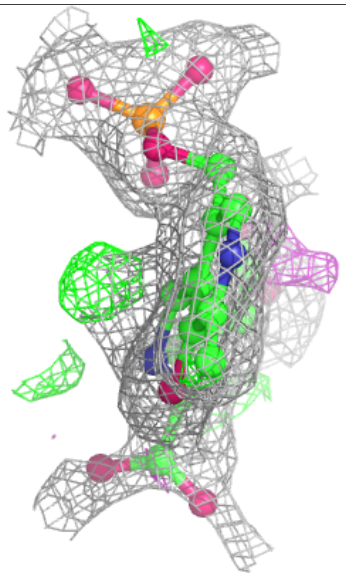


Electron density around PDG C 401:

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

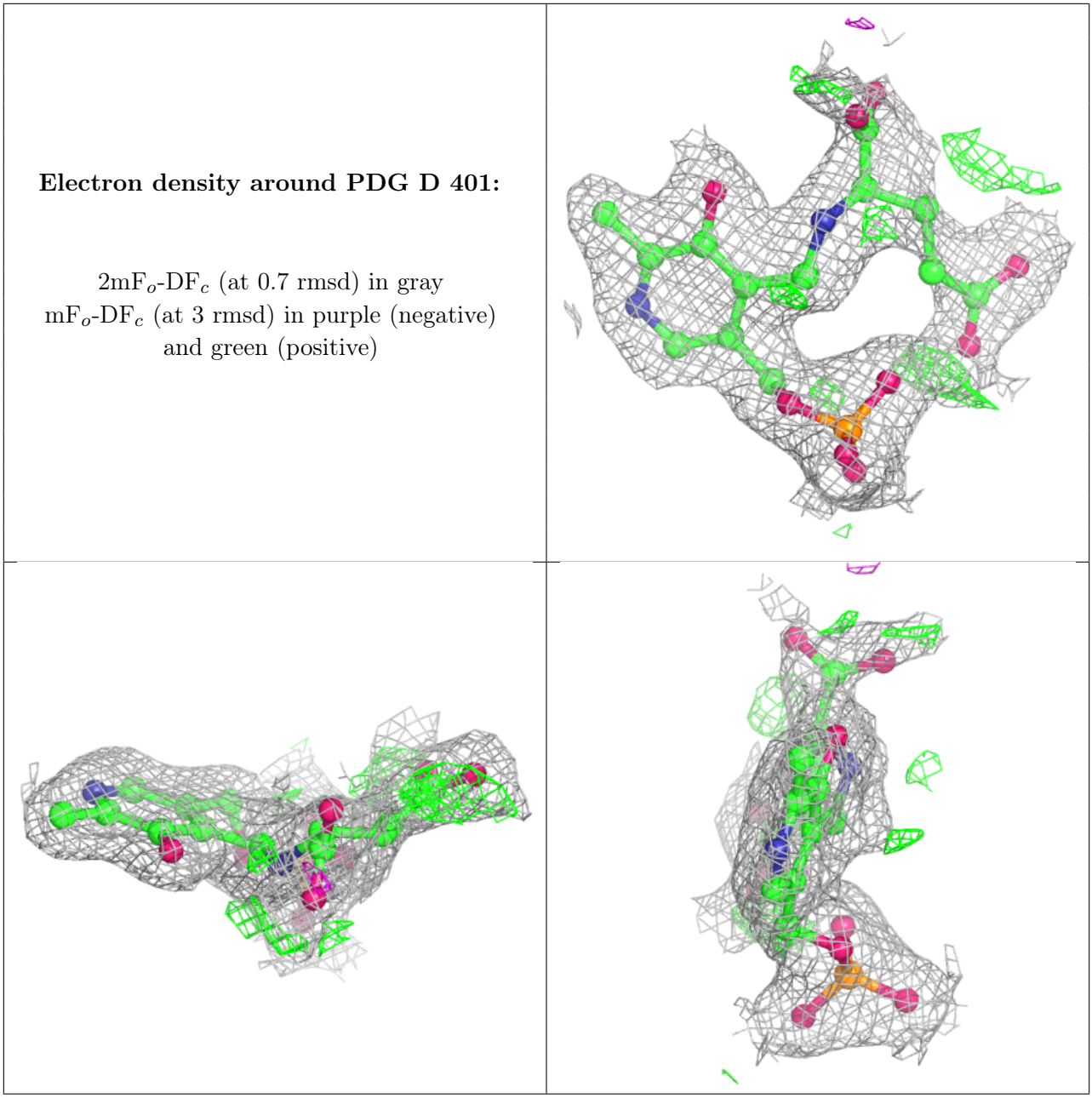






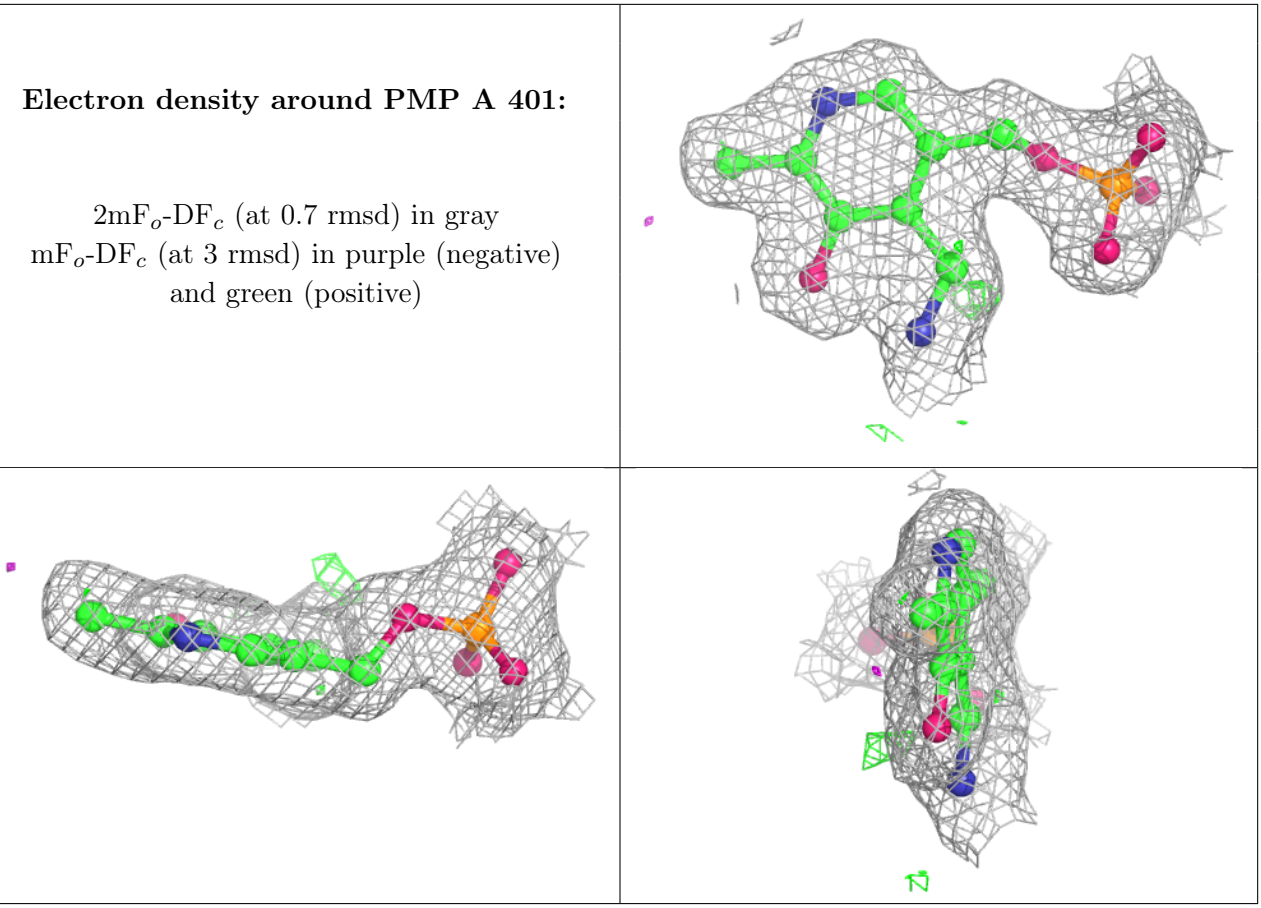
Electron density around PDG D 401:

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



Electron density around PMP A 401:

$2mF_o$-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

There are no such residues in this entry.