wwPDB X-ray Structure Validation Summary Report (i)

Apr 20, 2022 – 01:07 am BST

PDB ID	:	7OCS
Title	:	Mannitol-1-phosphate bound to the phosphatase domain of the bifunctional mannitol-1-phosphate dehydrogenase/phosphatase MtlD-D16A from Acinetobacter baumannii
Authors	:	Tam, H.K.; Mueller, V.; Pos, K.M.
Deposited on	:	2021-04-28
Resolution	:	2.30 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 following versions of software and data (see references (i)) were used in the production of this report:

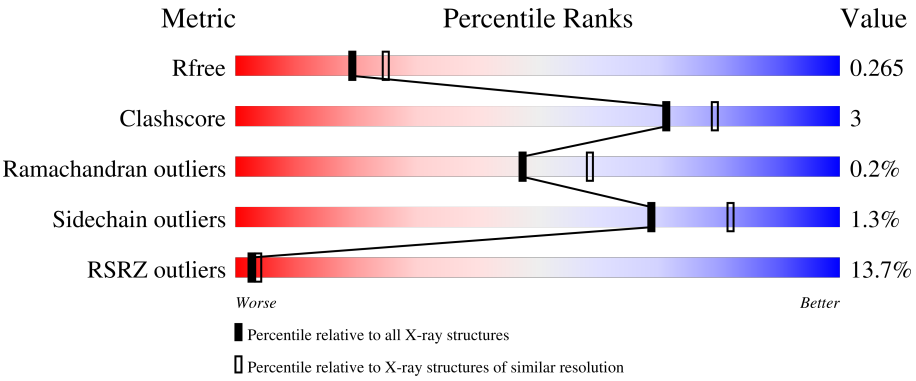
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	727	8% 86% 8% 6%
1	B	727	8% 85% 9% 6%
1	C	727	16% 71% 8% 21%
1	D	727	18% 83% 11% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	EPE	B	805	-	-	X	-
7	SO4	B	808	-	-	-	X
7	SO4	C	804	-	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 22135 atoms, of which 173 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 HAD hydrolase, family IA, variant 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	682	Total	C	N	O	S	0	0	0
			5497	3497	940	1028	32			
1	B	683	Total	C	N	O	S	0	0	0
			5505	3499	942	1031	33			
1	C	572	Total	C	N	O	S	0	0	0
			4601	2921	780	870	30			
1	D	685	Total	C	N	O	S	0	0	0
			5523	3512	944	1035	32			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP D0C7J2
A	2	VAL	-	expression tag	UNP D0C7J2
A	16	ALA	ASP	engineered mutation	UNP D0C7J2
A	717	ALA	-	expression tag	UNP D0C7J2
A	718	ALA	-	expression tag	UNP D0C7J2
A	719	ALA	-	expression tag	UNP D0C7J2
A	720	LEU	-	expression tag	UNP D0C7J2
A	721	GLU	-	expression tag	UNP D0C7J2
A	722	HIS	-	expression tag	UNP D0C7J2
A	723	HIS	-	expression tag	UNP D0C7J2
A	724	HIS	-	expression tag	UNP D0C7J2
A	725	HIS	-	expression tag	UNP D0C7J2
A	726	HIS	-	expression tag	UNP D0C7J2
A	727	HIS	-	expression tag	UNP D0C7J2
B	1	MET	-	initiating methionine	UNP D0C7J2
B	2	VAL	-	expression tag	UNP D0C7J2
B	16	ALA	ASP	engineered mutation	UNP D0C7J2
B	717	ALA	-	expression tag	UNP D0C7J2
B	718	ALA	-	expression tag	UNP D0C7J2
B	719	ALA	-	expression tag	UNP D0C7J2
B	720	LEU	-	expression tag	UNP D0C7J2

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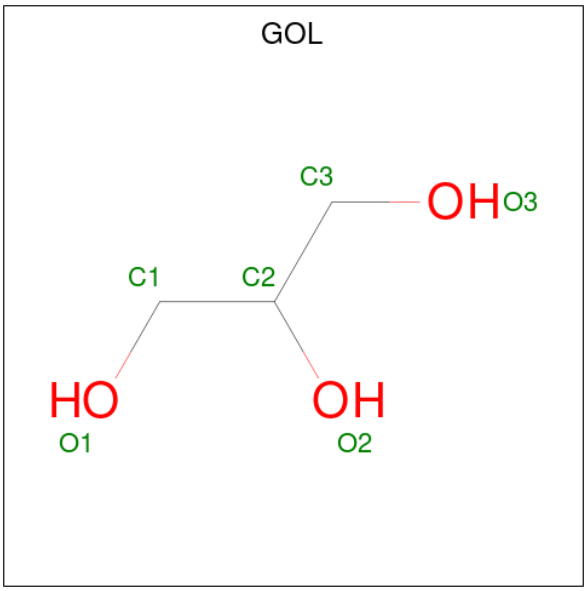
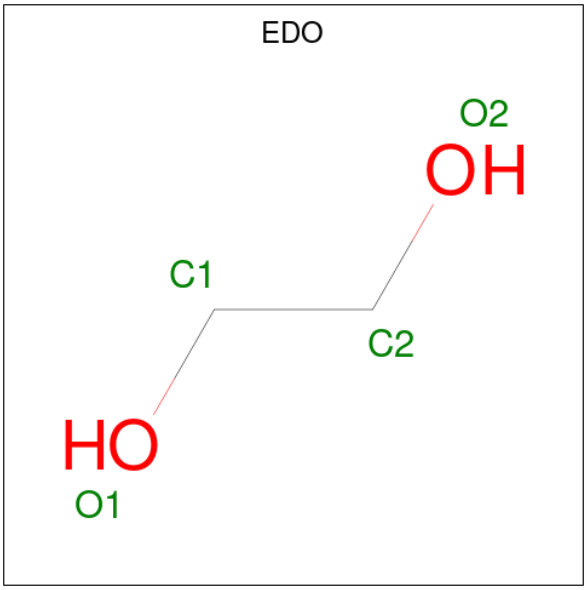
Chain	Residue	Modelled	Actual	Comment	Reference
B	721	GLU	-	expression tag	UNP D0C7J2
B	722	HIS	-	expression tag	UNP D0C7J2
B	723	HIS	-	expression tag	UNP D0C7J2
B	724	HIS	-	expression tag	UNP D0C7J2
B	725	HIS	-	expression tag	UNP D0C7J2
B	726	HIS	-	expression tag	UNP D0C7J2
B	727	HIS	-	expression tag	UNP D0C7J2
C	1	MET	-	initiating methionine	UNP D0C7J2
C	2	VAL	-	expression tag	UNP D0C7J2
C	16	ALA	ASP	engineered mutation	UNP D0C7J2
C	717	ALA	-	expression tag	UNP D0C7J2
C	718	ALA	-	expression tag	UNP D0C7J2
C	719	ALA	-	expression tag	UNP D0C7J2
C	720	LEU	-	expression tag	UNP D0C7J2
C	721	GLU	-	expression tag	UNP D0C7J2
C	722	HIS	-	expression tag	UNP D0C7J2
C	723	HIS	-	expression tag	UNP D0C7J2
C	724	HIS	-	expression tag	UNP D0C7J2
C	725	HIS	-	expression tag	UNP D0C7J2
C	726	HIS	-	expression tag	UNP D0C7J2
C	727	HIS	-	expression tag	UNP D0C7J2
D	1	MET	-	initiating methionine	UNP D0C7J2
D	2	VAL	-	expression tag	UNP D0C7J2
D	16	ALA	ASP	engineered mutation	UNP D0C7J2
D	717	ALA	-	expression tag	UNP D0C7J2
D	718	ALA	-	expression tag	UNP D0C7J2
D	719	ALA	-	expression tag	UNP D0C7J2
D	720	LEU	-	expression tag	UNP D0C7J2
D	721	GLU	-	expression tag	UNP D0C7J2
D	722	HIS	-	expression tag	UNP D0C7J2
D	723	HIS	-	expression tag	UNP D0C7J2
D	724	HIS	-	expression tag	UNP D0C7J2
D	725	HIS	-	expression tag	UNP D0C7J2
D	726	HIS	-	expression tag	UNP D0C7J2
D	727	HIS	-	expression tag	UNP D0C7J2

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		

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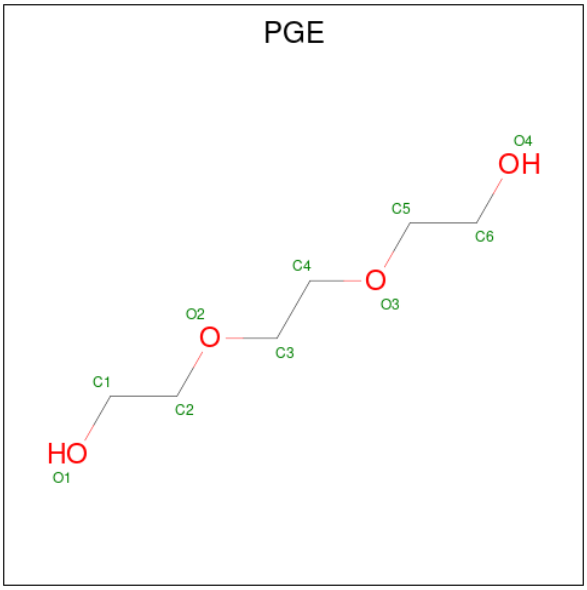
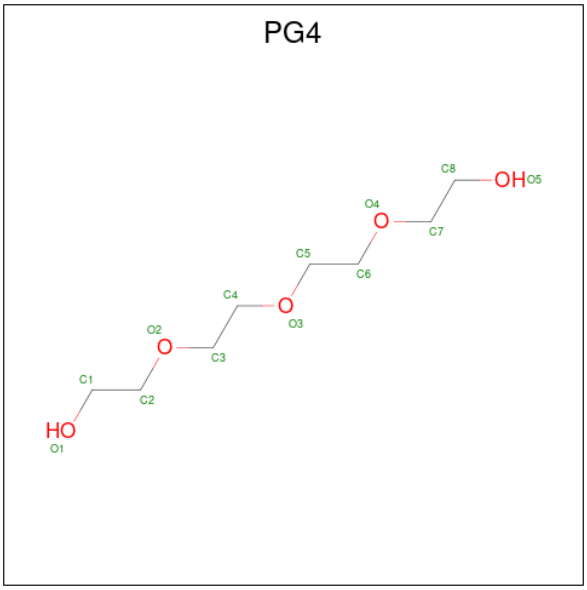
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	D	1	Total C H O 10 2 6 2	0	0
3	D	1	Total C H O 10 2 6 2	0	0
3	D	1	Total C H O 10 2 6 2	0	0
3	D	1	Total C H O 10 2 6 2	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



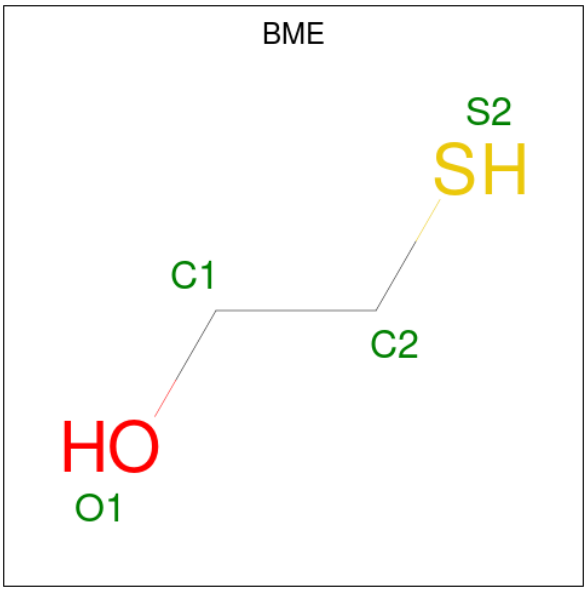
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 24 6 14 4	0	0
4	A	1	Total C H O 24 6 14 4	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



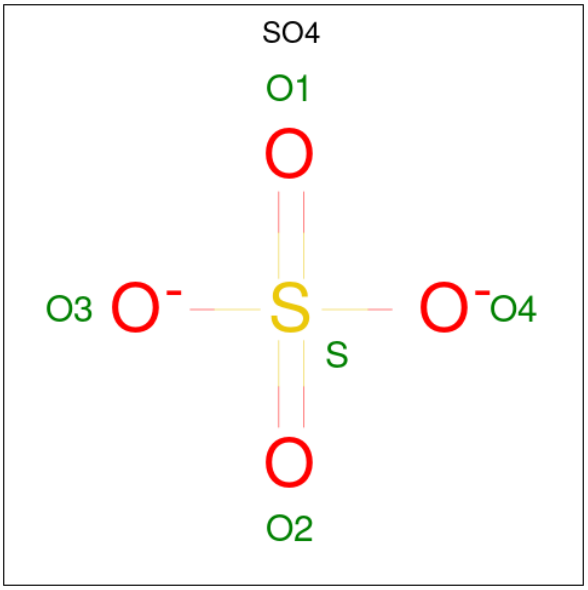
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 31 8 18 5	0	0
5	C	1	Total C H O 31 8 18 5	0	0

- Molecule 6 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	D	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

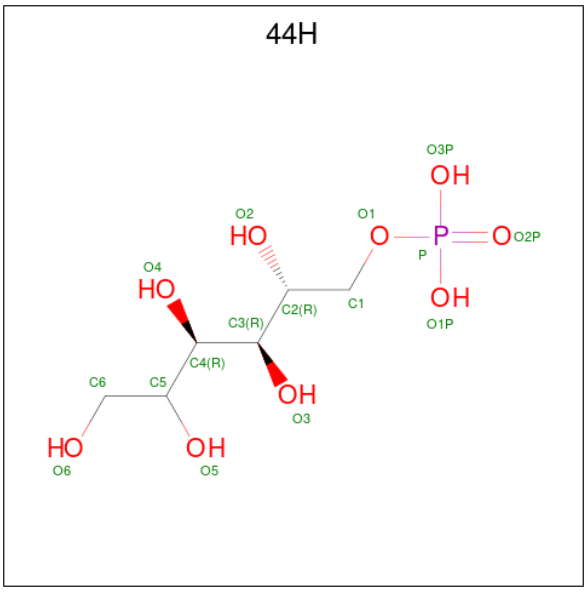
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

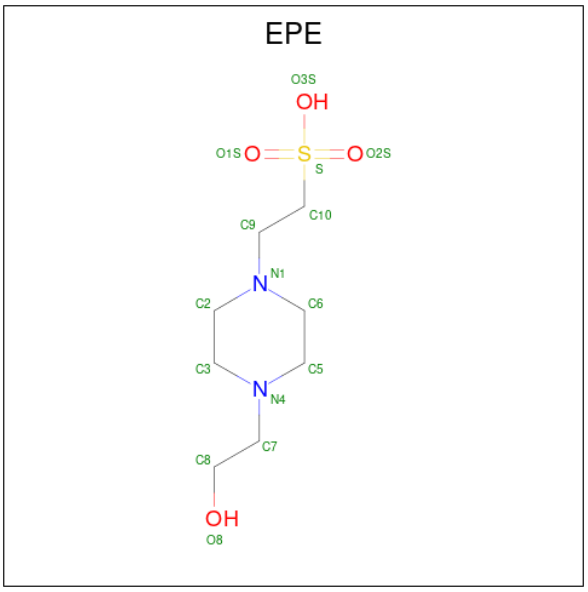
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	3	Total Cl 3 3	0	0
9	B	4	Total Cl 4 4	0	0
9	C	3	Total Cl 3 3	0	0

- Molecule 10 is D-Mannitol-1-phosphate (three-letter code: 44H) (formula: $C_6H_{15}O_9P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O P 16 6 9 1	0	0
10	B	1	Total C O P 16 6 9 1	0	0
10	C	1	Total C O P 16 6 9 1	0	0
10	D	1	Total C O P 16 6 9 1	0	0

- Molecule 11 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).

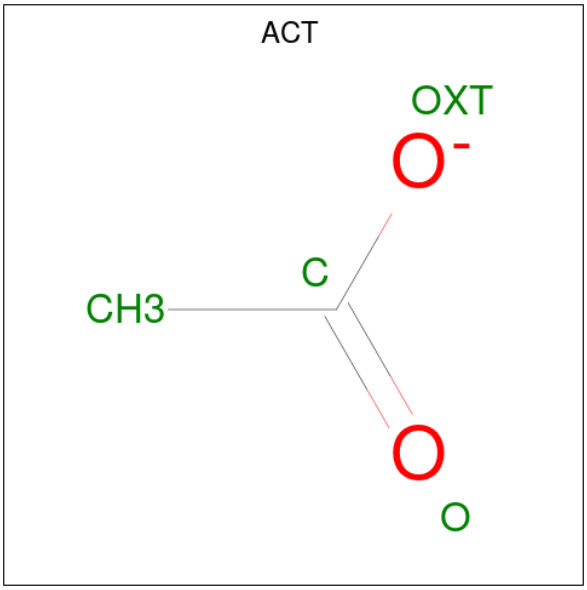


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 12 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 13 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	196	Total	O	0	0
			196	196		
14	B	200	Total	O	0	0
			200	200		
14	C	75	Total	O	0	0
			75	75		

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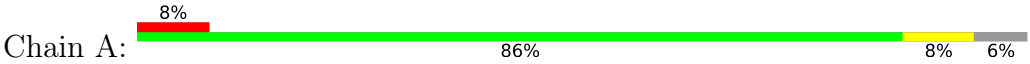
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	D	101	Total	O	0	0
			101	101		

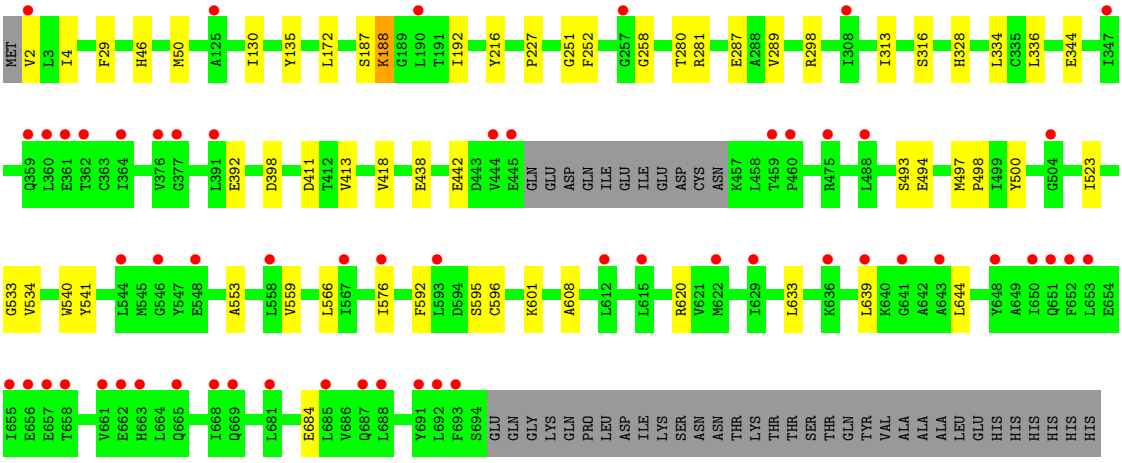
3 Residue-property plots (i)

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: HAD hydrolase, family IA, variant 3

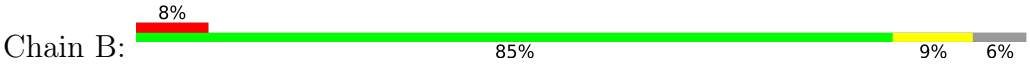
Chain A:

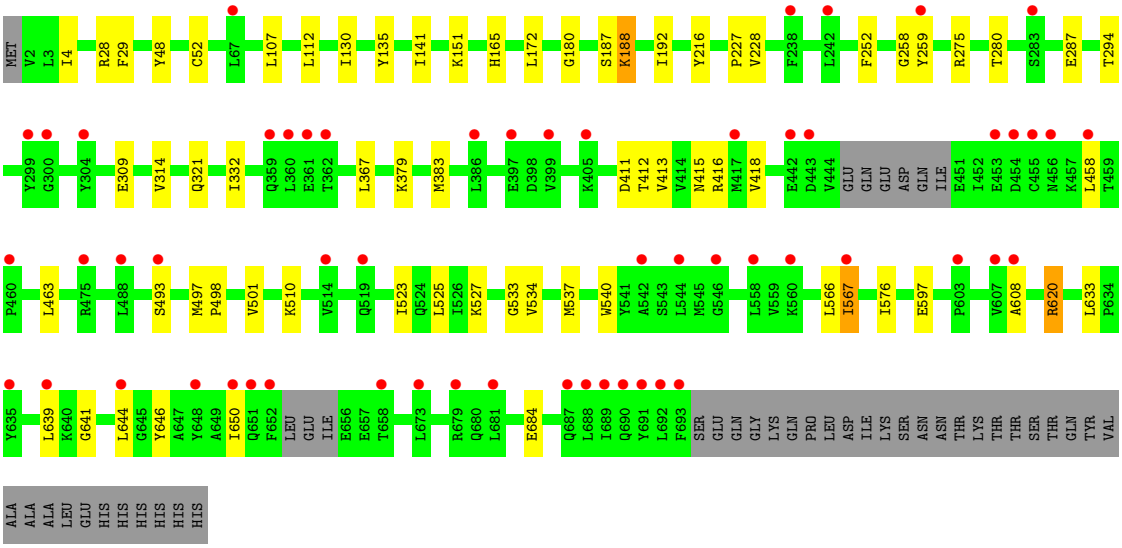




• Molecule 1: HAD hydrolase, family IA, variant 3

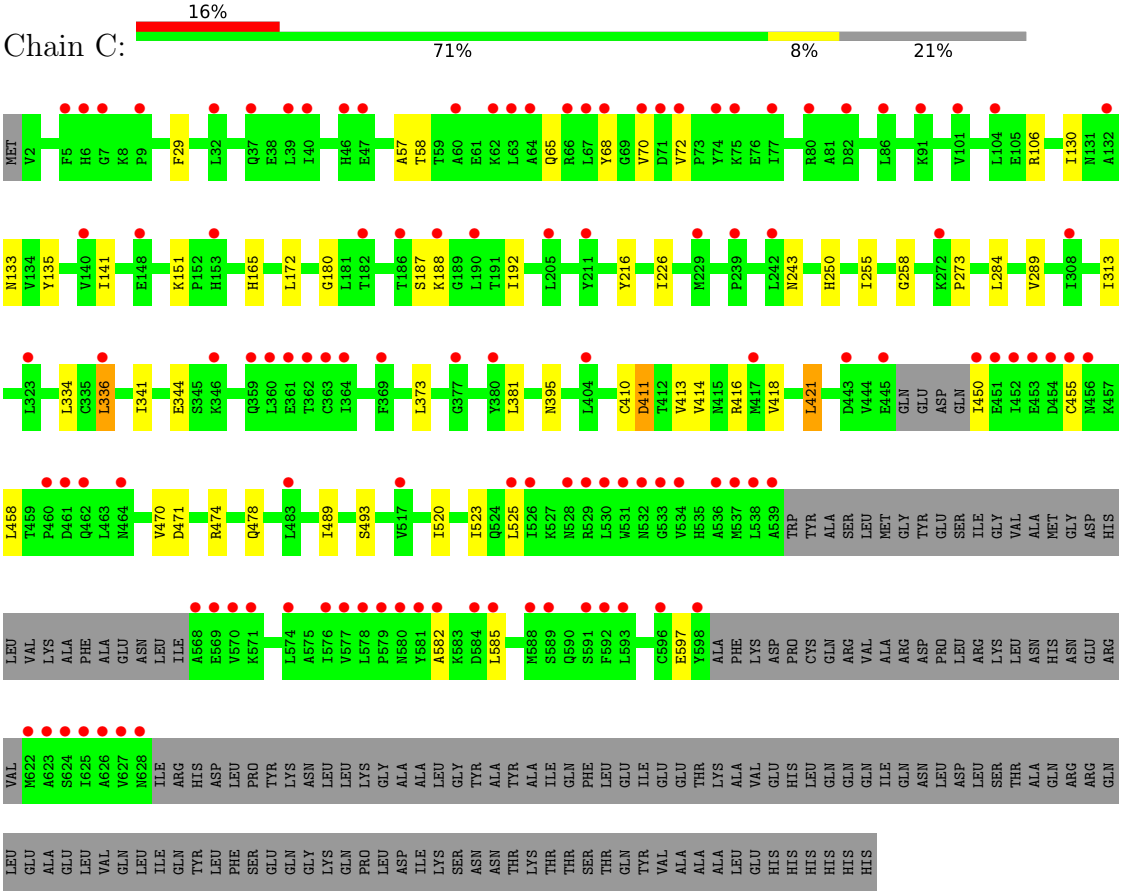
Chain B:





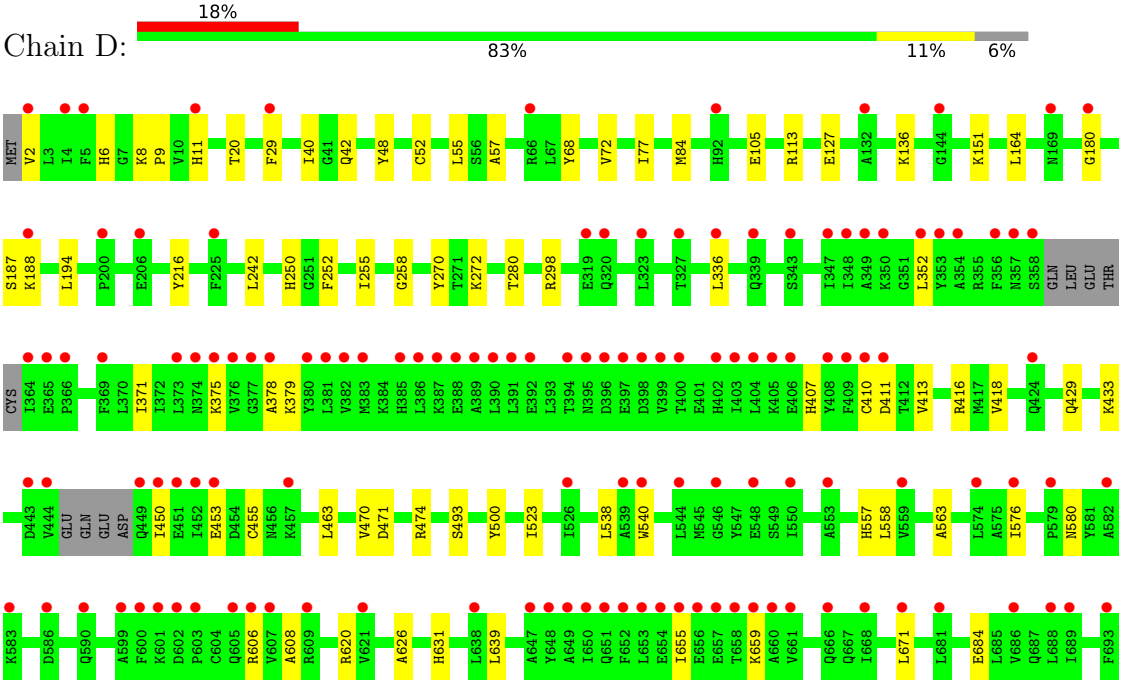
• Molecule 1: HAD hydrolase, family IA, variant 3

Chain C:



• Molecule 1: HAD hydrolase, family IA, variant 3

Chain D:




S694
E695
GLN
GLY
LYS
GLN
PRO
LEU
ASP
ILE
LYS
SER
ASN
ASN
THR
LYS
THR
THR
SER
THR
GLN
TYR
VAL
ALA
ALA
ALA
LEU
GLU
HIS
HIS
HIS
HIS
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HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.89Å 212.63Å 98.82Å 90.00° 112.81° 90.00°	Depositor
Resolution (Å)	48.61 – 2.30 48.61 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.61-2.30) 99.8 (48.61-2.30)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.29Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.215 , 0.247 0.229 , 0.265	Depositor DCC
R_{free} test set	7389 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	1.159	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	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	0.93	EDS
Total number of atoms	22135	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MG, NA, EPE, BME, PGE, 44H, GOL, PG4, ACT, CL, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.40	0/5602	0.37	0/7563
1	B	0.39	0/5609	0.36	0/7571
1	C	0.35	0/4685	0.33	0/6320
1	D	0.36	0/5627	0.34	0/7595
All	All	0.38	0/21523	0.35	0/29049

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5497	0	5485	33	0
1	B	5505	0	5483	38	0
1	C	4601	0	4575	36	0
1	D	5523	0	5504	48	0
2	A	6	8	8	0	0
2	C	6	8	8	0	0
3	A	20	30	30	0	0
3	B	16	24	24	0	0
3	D	16	24	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	20	28	28	1	0
5	A	13	18	18	4	0
5	C	13	18	18	4	0
6	A	4	6	6	3	0
6	D	4	6	6	1	0
7	A	20	0	0	0	0
7	B	15	0	0	0	0
7	C	5	0	0	2	0
7	D	10	0	0	1	0
8	A	1	0	0	0	0
9	A	3	0	0	0	0
9	B	4	0	0	0	0
9	C	3	0	0	0	0
10	A	16	0	0	0	0
10	B	16	0	0	1	0
10	C	16	0	0	0	0
10	D	16	0	0	0	0
11	B	15	0	18	7	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
13	C	4	3	3	0	0
14	A	196	0	0	0	0
14	B	200	0	0	0	0
14	C	75	0	0	1	0
14	D	101	0	0	0	0
All	All	21962	173	21238	148	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 3.

The worst 5 of 148 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:B:130:ILE:HA	11:B:805:EPE:O1S	1.57	1.04
1:D:250:HIS:CD2	1:D:336:LEU:HD11	2.13	0.82
1:A:135:TYR:HB3	5:A:809:PG4:H11	1.62	0.81
1:A:2:VAL:HA	4:A:807:PGE:H62	1.63	0.80
1:A:130:ILE:HA	5:A:809:PG4:H22	1.66	0.76

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	678/727 (93%)	662 (98%)	15 (2%)	1 (0%)	51	64
1	B	677/727 (93%)	659 (97%)	16 (2%)	2 (0%)	41	50
1	C	564/727 (78%)	545 (97%)	19 (3%)	0	100	100
1	D	679/727 (93%)	653 (96%)	25 (4%)	1 (0%)	51	64
All	All	2598/2908 (89%)	2519 (97%)	75 (3%)	4 (0%)	47	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	LYS
1	B	620	ARG
1	B	188	LYS
1	D	620	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	600/641 (94%)	593 (99%)	7 (1%)	71	84
1	B	601/641 (94%)	594 (99%)	7 (1%)	71	84
1	C	508/641 (79%)	500 (98%)	8 (2%)	62	78
1	D	603/641 (94%)	596 (99%)	7 (1%)	71	84
All	All	2312/2564 (90%)	2283 (99%)	29 (1%)	69	82

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	29	PHE
1	D	580	ASN
1	C	395	ASN
1	D	127	GLU
1	C	336	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	133	ASN
1	C	535	HIS

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 50 ligands modelled in this entry, 13 are monoatomic - leaving 37 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	$\#\|Z\| > 2$
2	GOL	A	801	-	5,5,5	0.08	0	5,5,5	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	SO4	A	812	-	4,4,4	0.36	0	6,6,6	0.11	0
5	PG4	C	801	-	12,12,12	0.23	0	11,11,11	0.11	0
7	SO4	B	806	-	4,4,4	0.66	0	6,6,6	0.23	0
4	PGE	A	808	-	9,9,9	0.24	0	8,8,8	0.09	0
3	EDO	B	802	-	3,3,3	0.57	0	2,2,2	0.27	0
3	EDO	A	803	-	3,3,3	0.53	0	2,2,2	0.34	0
10	44H	D	808	-	15,15,15	0.73	0	21,21,21	0.63	0
3	EDO	D	802	-	3,3,3	0.62	0	2,2,2	0.33	0
7	SO4	D	807	-	4,4,4	0.18	0	6,6,6	0.14	0
3	EDO	A	805	-	3,3,3	0.64	0	2,2,2	0.29	0
7	SO4	C	804	-	4,4,4	0.14	0	6,6,6	0.12	0
6	BME	A	810	-	3,3,3	0.29	0	1,2,2	1.45	0
3	EDO	D	801	-	3,3,3	0.62	0	2,2,2	0.30	0
13	ACT	C	803	-	1,3,3	3.34	1 (100%)	0,3,3	-	-
3	EDO	A	804	-	3,3,3	0.58	0	2,2,2	0.31	0
5	PG4	A	809	-	12,12,12	0.25	0	11,11,11	0.18	0
7	SO4	B	807	-	4,4,4	0.15	0	6,6,6	0.08	0
7	SO4	D	806	-	4,4,4	0.26	0	6,6,6	0.08	0
10	44H	A	819	-	15,15,15	1.02	1 (6%)	21,21,21	0.59	0
3	EDO	B	801	-	3,3,3	0.54	0	2,2,2	0.33	0
3	EDO	B	803	-	3,3,3	0.61	0	2,2,2	0.31	0
11	EPE	B	805	-	15,15,15	1.54	3 (20%)	18,20,20	2.18	7 (38%)
7	SO4	A	813	-	4,4,4	0.20	0	6,6,6	0.06	0
4	PGE	A	807	-	9,9,9	0.13	0	8,8,8	0.09	0
2	GOL	C	802	-	5,5,5	0.05	0	5,5,5	0.12	0
7	SO4	A	811	-	4,4,4	0.15	0	6,6,6	0.10	0
10	44H	B	814	-	15,15,15	1.03	1 (6%)	21,21,21	0.76	0
7	SO4	A	814	-	4,4,4	0.34	0	6,6,6	0.19	0
6	BME	D	805	-	3,3,3	0.15	0	1,2,2	1.41	0
3	EDO	D	804	-	3,3,3	0.54	0	2,2,2	0.33	0
3	EDO	B	804	-	3,3,3	0.69	0	2,2,2	0.24	0
3	EDO	A	806	-	3,3,3	0.55	0	2,2,2	0.35	0
3	EDO	D	803	-	3,3,3	0.57	0	2,2,2	0.32	0
3	EDO	A	802	-	3,3,3	0.56	0	2,2,2	0.33	0
7	SO4	B	808	-	4,4,4	0.12	0	6,6,6	0.07	0
10	44H	C	809	-	15,15,15	1.08	1 (6%)	21,21,21	0.55	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
2	GOL	A	801	-	-	0/4/4/4	-
5	PG4	C	801	-	-	3/10/10/10	-
4	PGE	A	808	-	-	3/7/7/7	-
3	EDO	B	802	-	-	0/1/1/1	-
3	EDO	A	803	-	-	0/1/1/1	-
10	44H	D	808	-	-	0/20/20/20	-
3	EDO	D	802	-	-	0/1/1/1	-
3	EDO	A	805	-	-	0/1/1/1	-
6	BME	A	810	-	-	0/1/1/1	-
3	EDO	D	801	-	-	0/1/1/1	-
3	EDO	A	804	-	-	0/1/1/1	-
5	PG4	A	809	-	-	4/10/10/10	-
10	44H	A	819	-	-	0/20/20/20	-
3	EDO	B	801	-	-	0/1/1/1	-
3	EDO	B	803	-	-	0/1/1/1	-
11	EPE	B	805	-	-	4/9/19/19	0/1/1/1
4	PGE	A	807	-	-	3/7/7/7	-
2	GOL	C	802	-	-	0/4/4/4	-
10	44H	B	814	-	-	0/20/20/20	-
6	BME	D	805	-	-	0/1/1/1	-
3	EDO	D	804	-	-	0/1/1/1	-
3	EDO	B	804	-	-	0/1/1/1	-
3	EDO	A	806	-	-	0/1/1/1	-
3	EDO	D	803	-	-	0/1/1/1	-
3	EDO	A	802	-	-	0/1/1/1	-
10	44H	C	809	-	-	0/20/20/20	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	805	EPE	C10-S	4.25	1.83	1.77
13	C	803	ACT	CH3-C	3.34	1.53	1.48
10	C	809	44H	P-O2P	3.09	1.60	1.50
10	B	814	44H	P-O2P	3.04	1.60	1.50
10	A	819	44H	P-O2P	2.82	1.59	1.50

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	805	EPE	C6-N1-C2	3.95	117.72	108.83
11	B	805	EPE	O3S-S-O2S	-3.78	102.03	111.27
11	B	805	EPE	O2S-S-C10	3.73	111.40	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	805	EPE	O3S-S-C10	3.37	111.23	105.77
11	B	805	EPE	O1S-S-C10	3.07	110.61	106.92

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	B	805	EPE	C10-C9-N1-C2
11	B	805	EPE	C10-C9-N1-C6
5	A	809	PG4	O3-C5-C6-O4
5	C	801	PG4	O2-C3-C4-O3
11	B	805	EPE	C8-C7-N4-C5

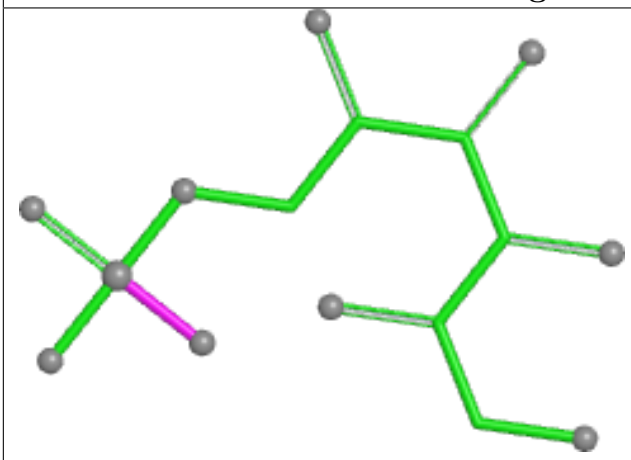
There are no ring outliers.

10 monomers are involved in 25 short contacts:

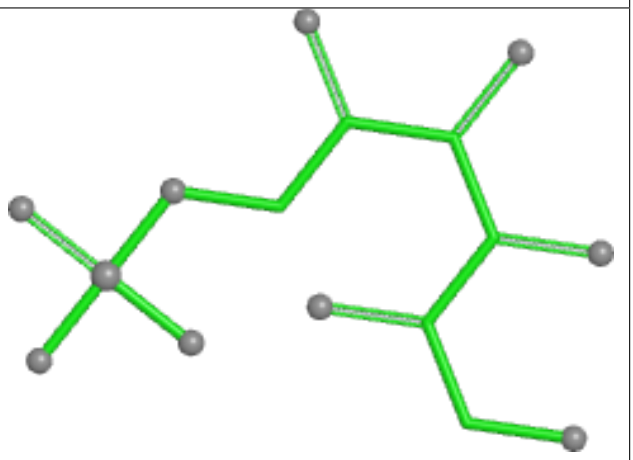
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	801	PG4	4	0
7	D	807	SO4	1	0
7	C	804	SO4	2	0
6	A	810	BME	3	0
3	D	801	EDO	1	0
5	A	809	PG4	4	0
11	B	805	EPE	7	0
4	A	807	PGE	1	0
10	B	814	44H	1	0
6	D	805	BME	1	0

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.

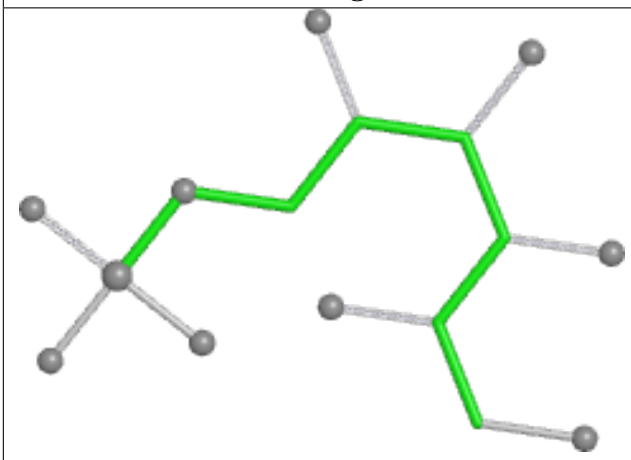
Ligand 44H A 819



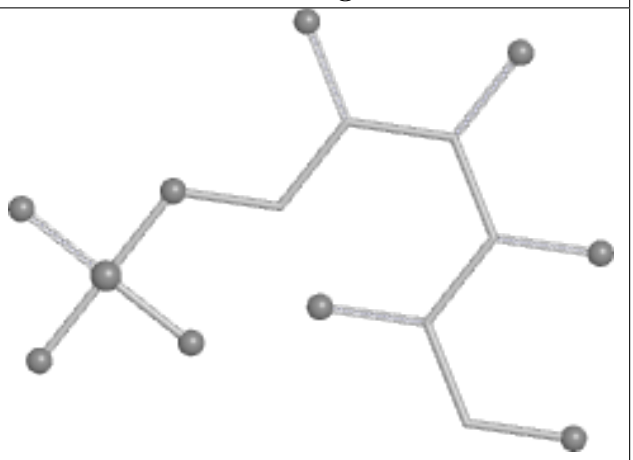
Bond lengths



Bond angles

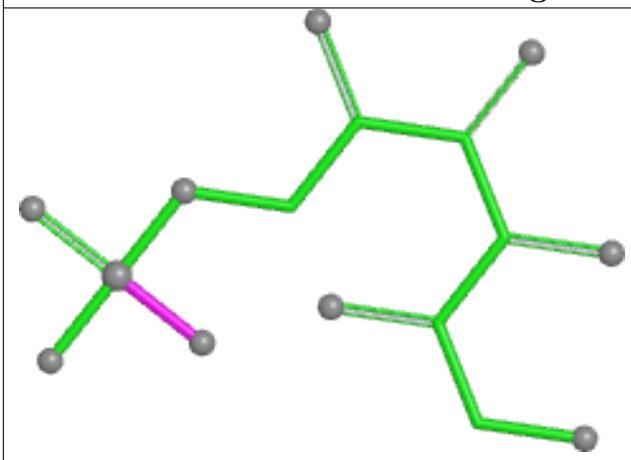


Torsions

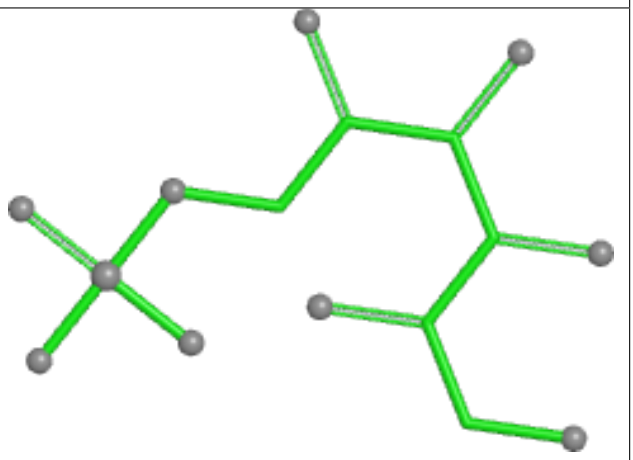


Rings

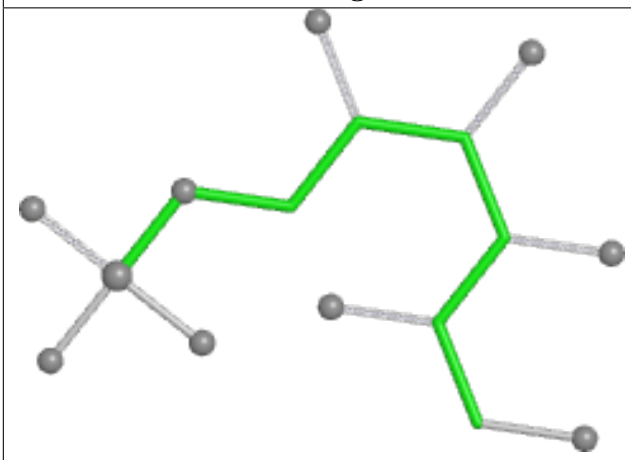
Ligand 44H B 814



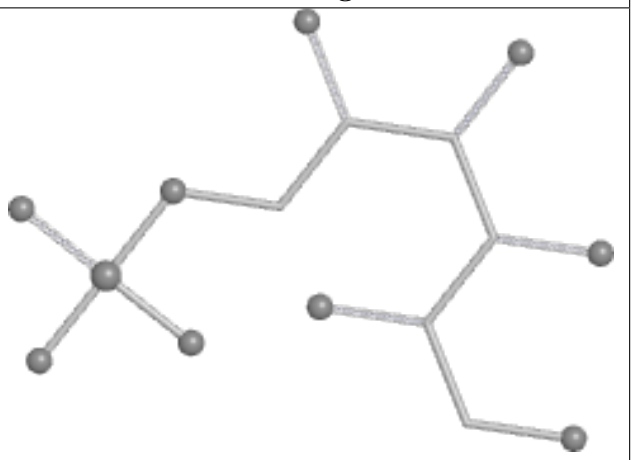
Bond lengths



Bond angles

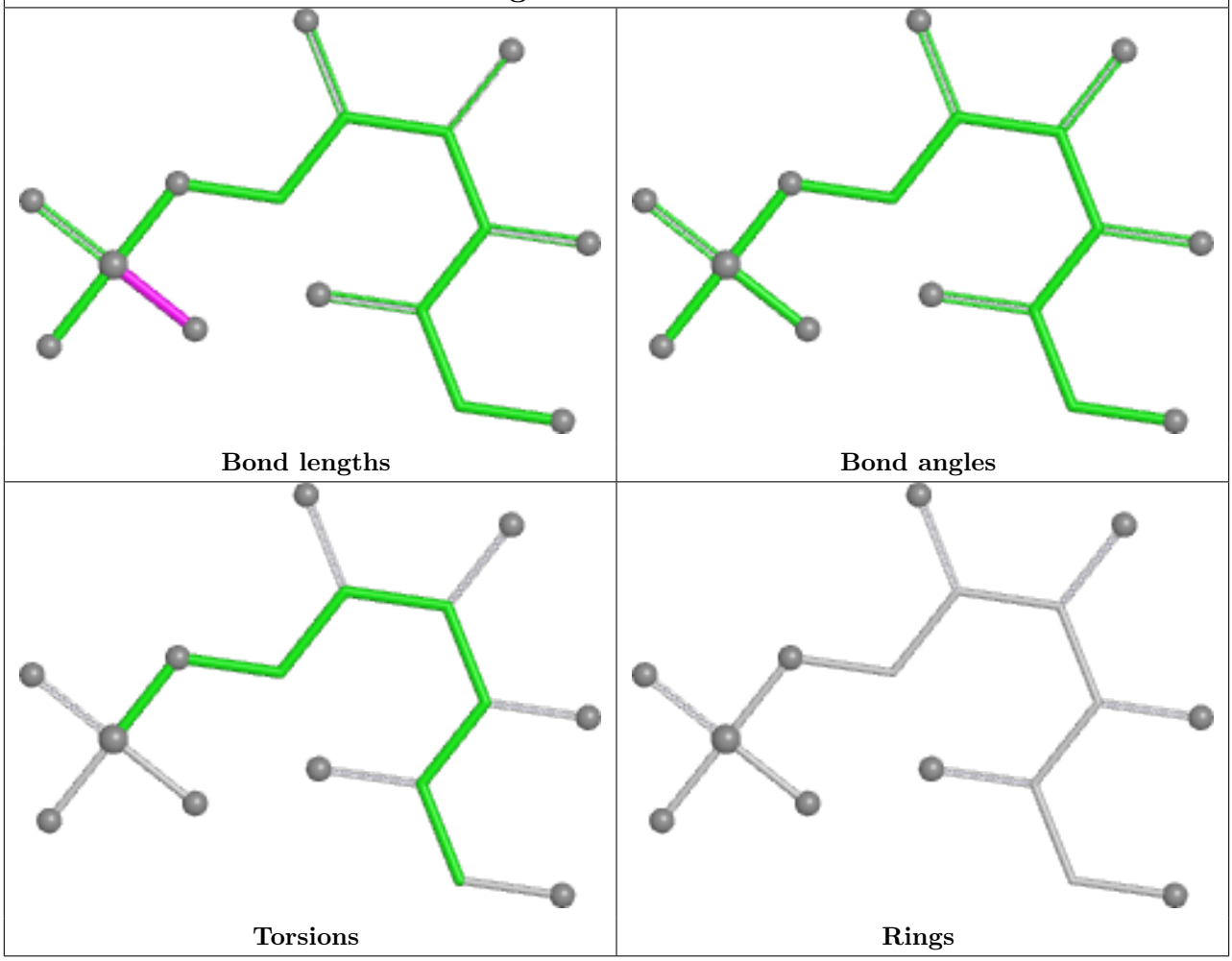


Torsions



Rings

Ligand 44H C 809



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	682/727 (93%)	0.87	58 (8%)	10	14	26, 44, 74, 97	0
1	B	683/727 (93%)	0.91	57 (8%)	11	15	29, 45, 72, 102	0
1	C	572/727 (78%)	1.29	114 (19%)	1	1	33, 56, 92, 114	0
1	D	685/727 (94%)	1.16	129 (18%)	1	1	34, 56, 90, 116	0
All	All	2622/2908 (90%)	1.05	358 (13%)	3	4	26, 50, 86, 116	0

The worst 5 of 358 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	692	LEU	13.9
1	D	381	LEU	9.9
1	C	538	LEU	9.8
1	D	376	VAL	8.6
1	A	661	VAL	8.5

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
3	EDO	A	805	4/4	0.64	0.29	60,72,72,72	0
3	EDO	B	804	4/4	0.64	0.26	66,79,79,79	0
2	GOL	C	802	6/6	0.66	0.23	73,88,88,89	0
3	EDO	D	802	4/4	0.66	0.19	71,86,86,86	0
7	SO4	B	808	5/5	0.68	0.40	125,125,125,125	0
4	PGE	A	808	10/10	0.69	0.31	46,56,60,60	0
3	EDO	A	803	4/4	0.72	0.18	84,101,101,101	0
12	NA	C	808	1/1	0.72	0.30	60,60,60,60	0
5	PG4	C	801	13/13	0.74	0.31	47,56,65,66	0
11	EPE	B	805	15/15	0.75	0.35	73,73,73,74	0
7	SO4	C	804	5/5	0.77	0.28	98,98,98,98	0
7	SO4	A	813	5/5	0.77	0.27	135,135,135,135	0
3	EDO	A	804	4/4	0.77	0.16	69,83,83,83	0
13	ACT	C	803	4/4	0.78	0.17	46,47,55,55	0
3	EDO	A	802	4/4	0.81	0.17	77,92,93,93	0
3	EDO	D	801	4/4	0.82	0.30	74,88,88,88	0
4	PGE	A	807	10/10	0.82	0.26	69,84,84,84	0
3	EDO	A	806	4/4	0.83	0.16	56,67,67,67	0
5	PG4	A	809	13/13	0.84	0.19	42,51,57,57	0
3	EDO	B	802	4/4	0.86	0.27	40,48,48,49	0
2	GOL	A	801	6/6	0.87	0.24	45,55,55,55	0
3	EDO	B	803	4/4	0.88	0.27	52,62,63,63	0
10	44H	D	808	16/16	0.90	0.19	41,42,42,42	0
7	SO4	B	807	5/5	0.90	0.17	99,99,99,99	0
3	EDO	D	803	4/4	0.90	0.13	70,84,84,84	0
3	EDO	B	801	4/4	0.90	0.21	42,50,51,51	0
9	CL	C	807	1/1	0.91	0.18	64,64,64,64	0
10	44H	C	809	16/16	0.91	0.17	47,49,51,51	0
7	SO4	A	814	5/5	0.91	0.28	71,71,71,71	0
9	CL	B	812	1/1	0.92	0.15	37,37,37,37	0
6	BME	A	810	4/4	0.92	0.14	48,58,58,58	0
10	44H	A	819	16/16	0.92	0.19	32,33,34,34	0
9	CL	B	810	1/1	0.92	0.14	51,51,51,51	0
7	SO4	B	806	5/5	0.93	0.30	33,34,35,35	0
3	EDO	D	804	4/4	0.93	0.17	48,58,58,58	0
8	MG	A	815	1/1	0.93	0.18	66,66,66,66	0
9	CL	B	809	1/1	0.94	0.18	36,36,36,36	0
6	BME	D	805	4/4	0.94	0.27	19,25,28,31	0
10	44H	B	814	16/16	0.94	0.17	33,36,37,38	0
9	CL	A	816	1/1	0.94	0.15	31,31,31,31	0
9	CL	A	818	1/1	0.95	0.09	38,38,38,38	0
7	SO4	A	811	5/5	0.95	0.24	70,70,70,70	0
7	SO4	D	807	5/5	0.95	0.21	78,78,78,78	0

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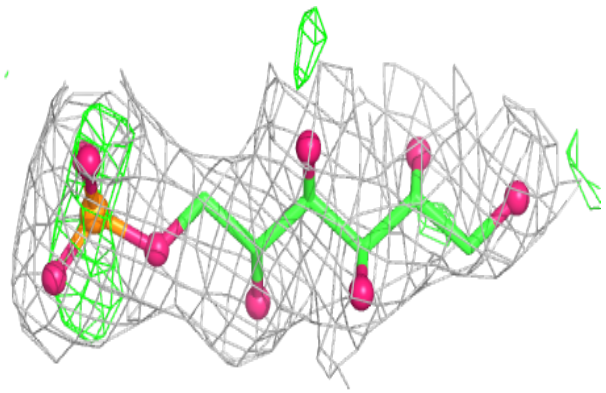
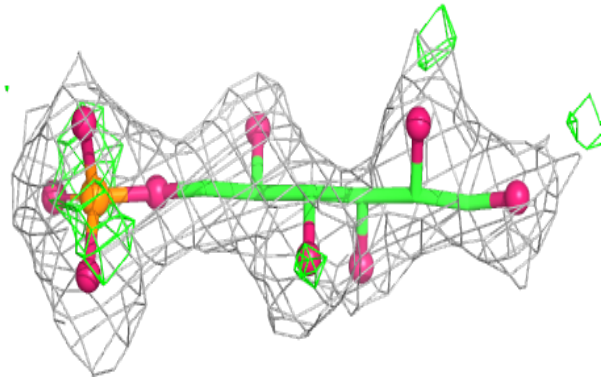
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	SO4	A	812	5/5	0.96	0.22	35,35,36,36	5
9	CL	C	805	1/1	0.96	0.28	49,49,49,49	0
12	NA	B	813	1/1	0.97	0.21	39,39,39,39	0
7	SO4	D	806	5/5	0.97	0.16	54,54,55,55	0
9	CL	C	806	1/1	0.97	0.16	58,58,58,58	0
9	CL	A	817	1/1	0.98	0.17	34,34,34,34	0
9	CL	B	811	1/1	0.99	0.09	39,39,39,39	0

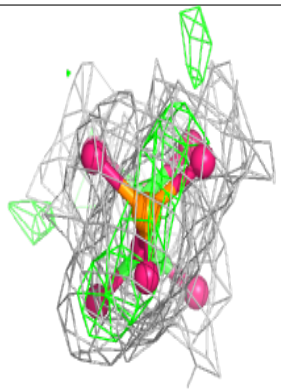
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 44H C 809:

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

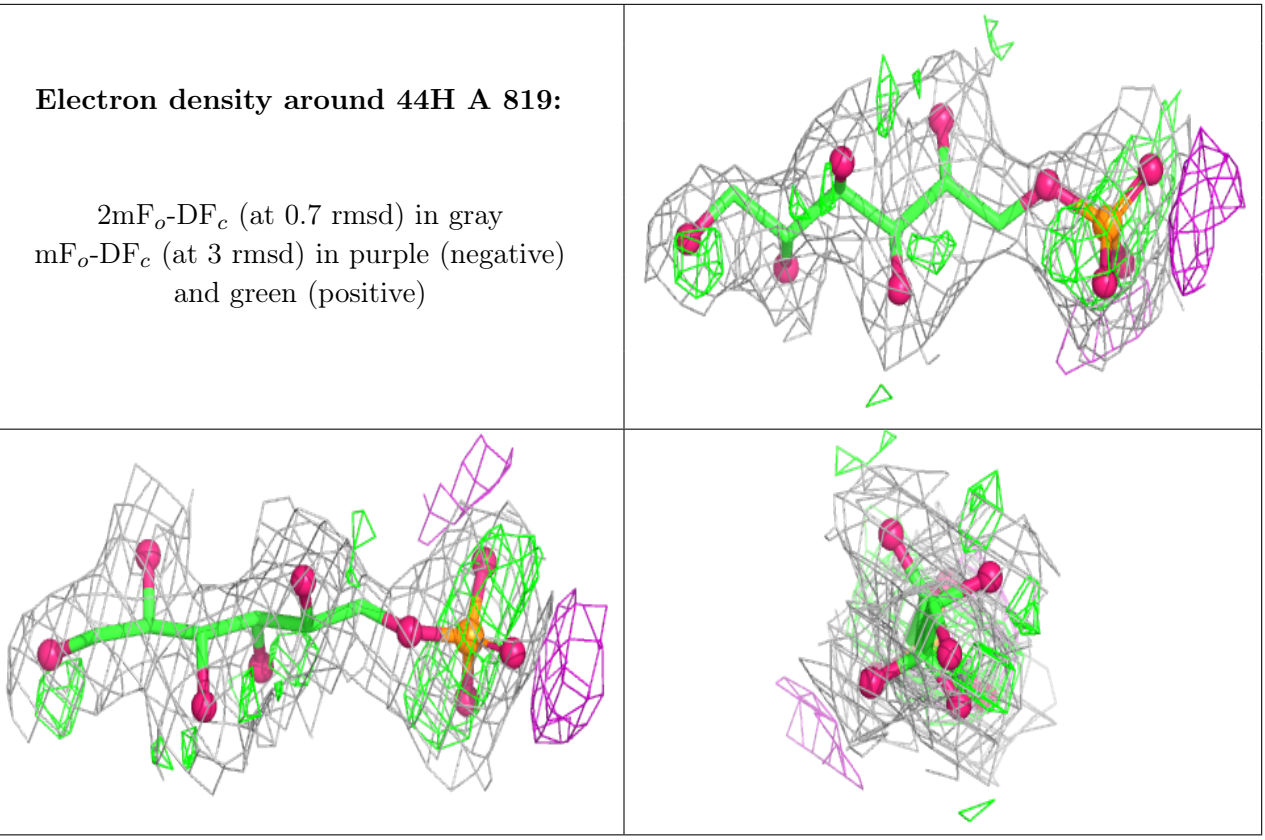






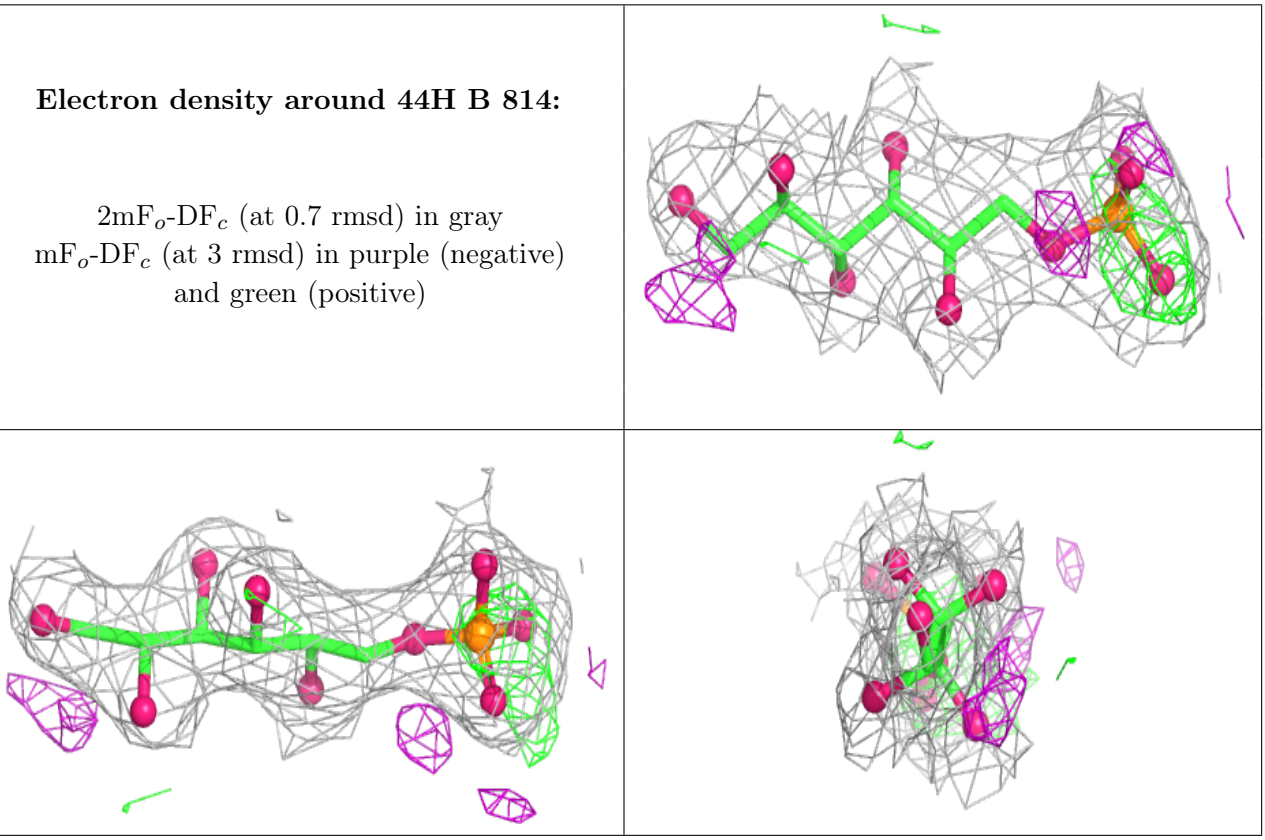
Electron density around 44H A 819:

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



Electron density around 44H B 814:

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



6.5 Other polymers (i)

There are no such residues in this entry.