



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:49 AM UTC

PDB ID : 7OCS / pdb_00007ocs
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

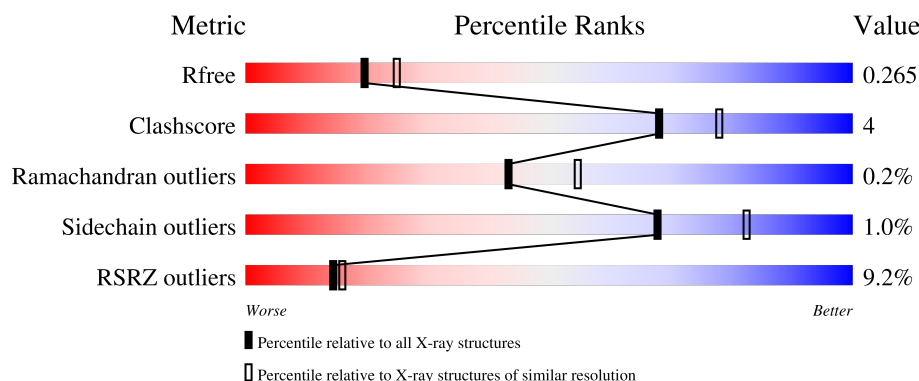
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	727	4% 86% 8% 6%
1	B	727	7% 84% 9% 6%
1	C	727	10% 71% 7% 21%
1	D	727	12% 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	C	804	-	-	X	-

2 Entry composition

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 (CCD ID: GOL) (formula: C₃H₈O₃).



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 (CCD ID: EDO) (formula: $C_2H_6O_2$).



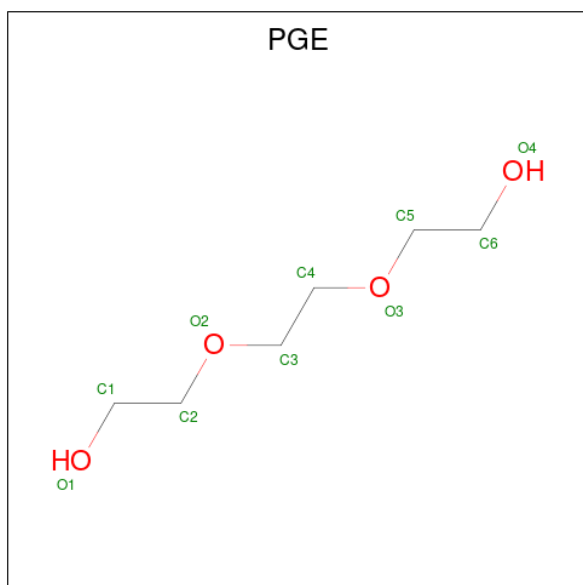
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		

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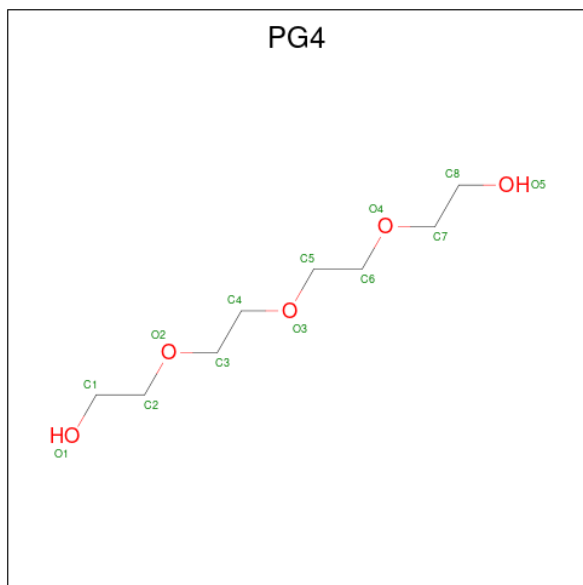
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1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

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



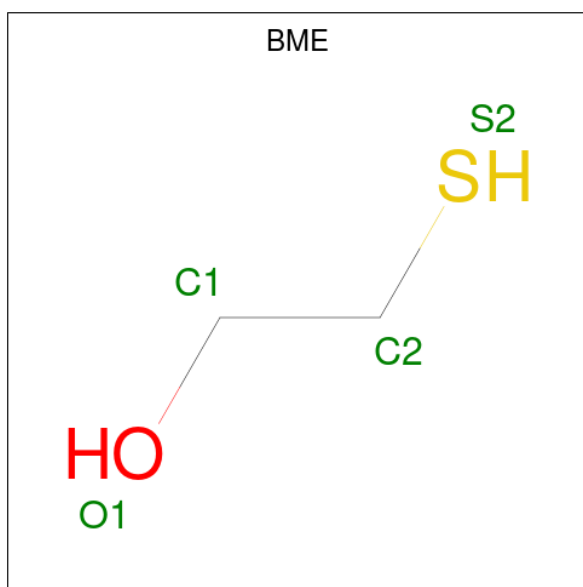
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			24	6	14	4		
4	A	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



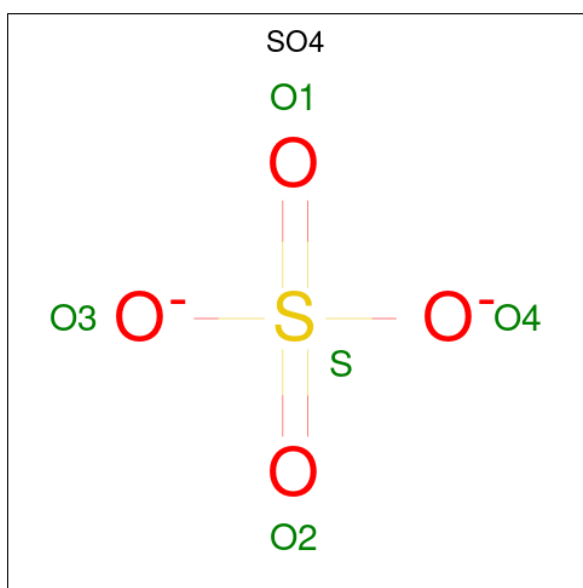
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			31	8	18	5		
5	C	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 6 is BETA-MERCAPTOETHANOL (CCD ID: 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 (CCD ID: SO₄) (formula: O₄S).



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

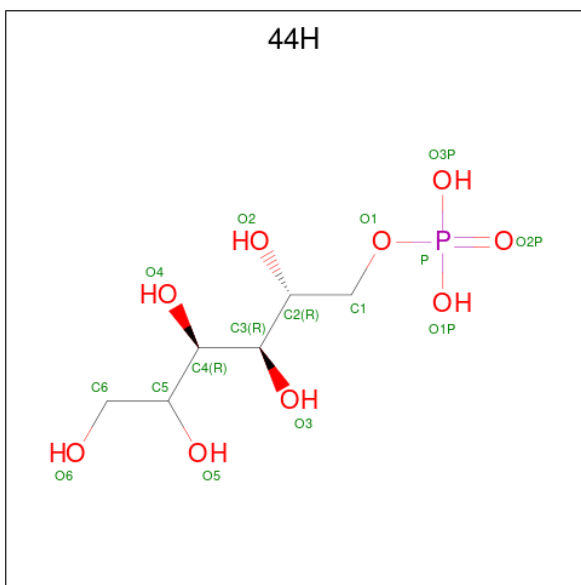
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

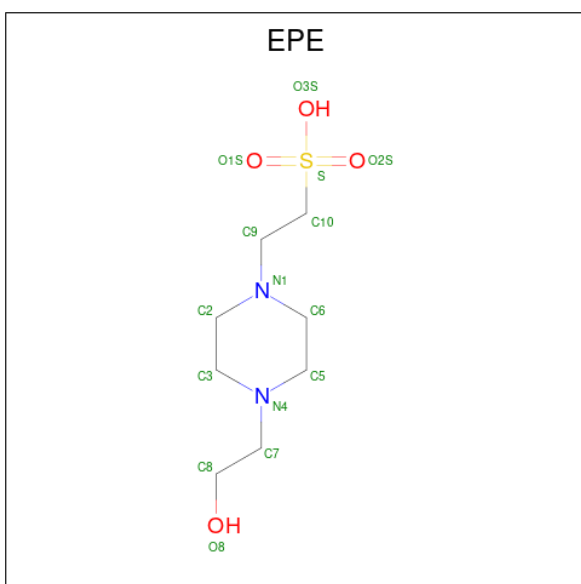
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	3	Total Cl 3 3	0	0
9	B	4	Total Cl 4 4	0	0
9	C	3	Total Cl 3 3	0	0

- Molecule 10 is D-Mannitol-1-phosphate (CCD ID: 44H) (formula: C₆H₁₅O₉P).



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

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

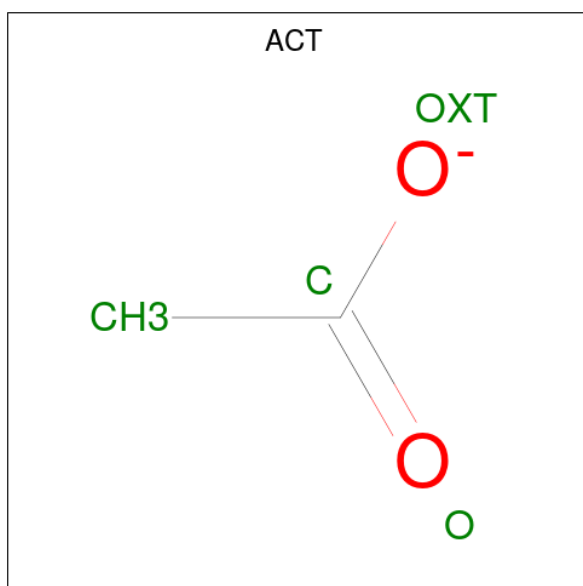


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 12 is SODIUM ION (CCD ID: 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 (CCD ID: ACT) (formula: C₂H₃O₂).



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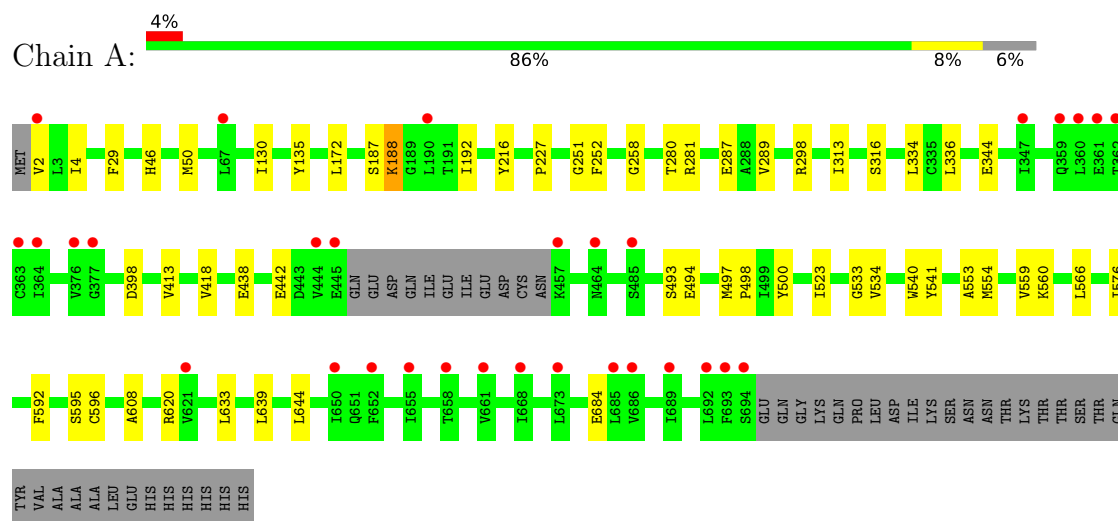
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	D	101	Total 101	O 101	0	0

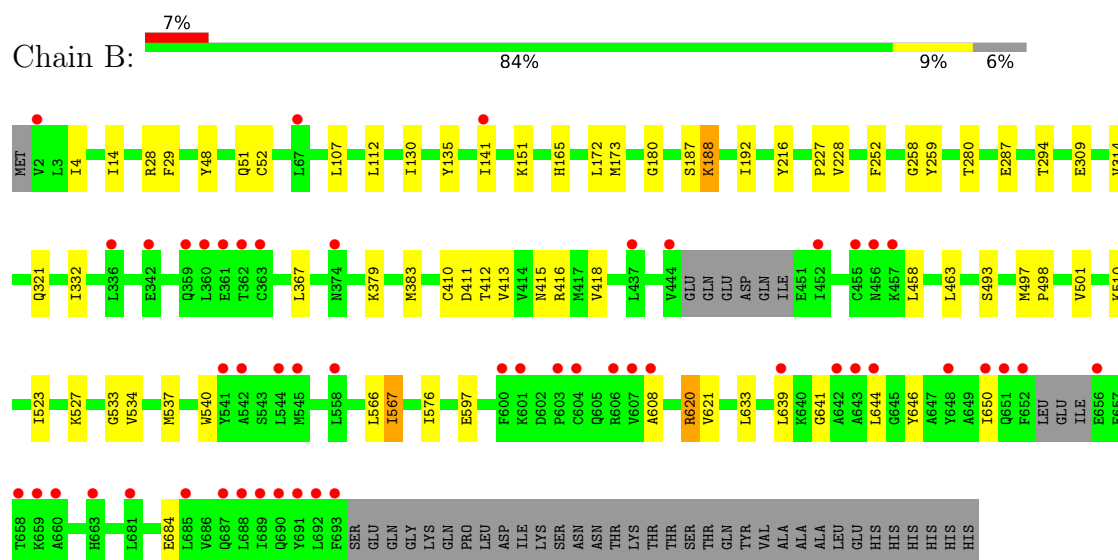
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

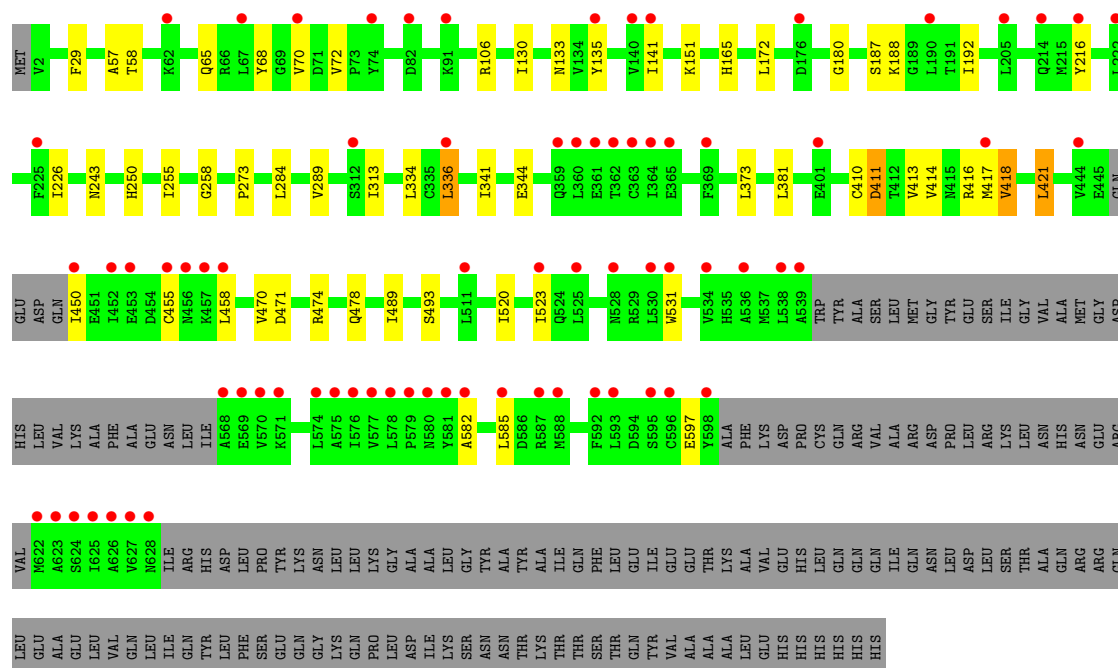


- Molecule 1: HAD hydrolase, family IA, variant 3

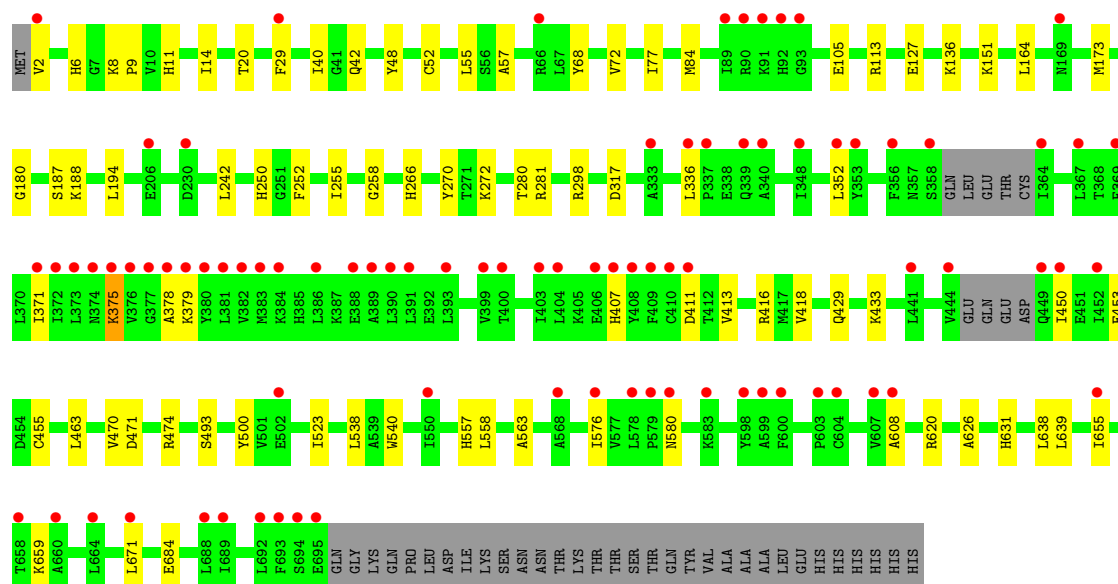
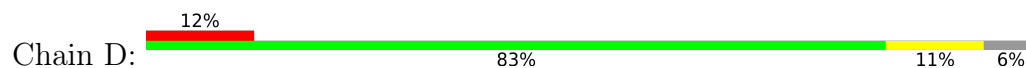


- Molecule 1: HAD hydrolase, family IA, variant 3





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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	7404 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)	0.34 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.74	0/5602	0.86	0/7563
1	B	0.73	0/5609	0.85	0/7571
1	C	0.69	0/4685	0.81	0/6320
1	D	0.70	0/5627	0.84	0/7595
All	All	0.72	0/21523	0.84	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 [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	5497	0	5485	34	0
1	B	5505	0	5483	41	0
1	C	4601	0	4575	37	0
1	D	5523	0	5504	50	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	1	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	155	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 (155) 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
1:D:57:ALA:HB3	7:D:807:SO4:O1	1.86	0.74
11:B:805:EPE:H71	1:C:421:LEU:HD11	1.71	0.71
1:D:371:ILE:HB	1:D:411:ASP:HA	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:GLY:HA2	1:B:620:ARG:HB3	1.73	0.71
11:B:805:EPE:H62	1:C:489:ILE:HB	1.72	0.70
1:C:450:ILE:HD12	1:C:471:ASP:HA	1.79	0.65
1:A:258:GLY:HA3	1:A:418:VAL:HG11	1.80	0.64
1:A:540:TRP:CD1	1:A:608:ALA:HB1	2.34	0.63
1:C:130:ILE:HA	5:C:801:PG4:H72	1.81	0.63
1:D:576:ILE:HG21	1:D:631:HIS:CE1	2.34	0.63
1:D:639:LEU:HD21	1:D:684:GLU:HB3	1.81	0.62
1:B:534:VAL:HG13	1:B:566:LEU:HD23	1.82	0.62
1:B:130:ILE:CA	11:B:805:EPE:O1S	2.39	0.62
1:A:418:VAL:HG13	1:A:493:SER:HB3	1.81	0.62
1:D:576:ILE:HG21	1:D:631:HIS:ND1	2.14	0.62
1:C:57:ALA:HB3	7:C:804:SO4:O3	1.99	0.62
1:D:258:GLY:HA3	1:D:418:VAL:HG11	1.82	0.61
1:D:538:LEU:HD21	1:D:563:ALA:HB2	1.83	0.61
1:A:172:LEU:HD22	1:A:192:ILE:HD11	1.85	0.59
1:C:58:THR:HG23	7:C:804:SO4:O3	2.03	0.59
1:C:336:LEU:HD22	1:C:344:GLU:HG3	1.84	0.59
1:D:450:ILE:HD11	1:D:474:ARG:HD3	1.85	0.57
1:D:2:VAL:HG12	1:D:11:HIS:NE2	2.20	0.57
1:A:494:GLU:HG3	1:A:595:SER:HB2	1.87	0.56
11:B:805:EPE:H32	14:C:926:HOH:O	2.05	0.56
1:D:455:CYS:HB2	1:D:463:LEU:HD21	1.86	0.56
1:A:413:VAL:HG21	1:A:523:ILE:HG23	1.86	0.56
1:B:187:SER:O	1:B:188:LYS:HB2	2.05	0.56
1:B:639:LEU:HD21	1:B:684:GLU:HB3	1.88	0.56
11:B:805:EPE:H62	1:C:489:ILE:CB	2.37	0.55
1:B:416:ARG:HD3	1:B:493:SER:OG	2.07	0.55
1:A:287:GLU:HB3	1:D:470:VAL:HG11	1.88	0.54
1:B:646:TYR:O	1:B:650:ILE:HG12	2.08	0.54
1:B:151:LYS:HD3	1:B:180:GLY:HA2	1.91	0.53
1:B:258:GLY:HA3	1:B:418:VAL:HG11	1.90	0.53
1:A:227:PRO:HB3	1:B:4:ILE:HD12	1.90	0.53
1:D:375:LYS:HB3	1:D:378:ALA:HB2	1.90	0.53
1:C:68:TYR:HB2	1:C:72:VAL:HG11	1.91	0.53
1:A:334:LEU:HD11	1:A:336:LEU:HD22	1.91	0.53
1:B:534:VAL:HG21	1:B:567:ILE:HD12	1.90	0.52
1:D:418:VAL:HG13	1:D:493:SER:HB2	1.91	0.52
1:B:130:ILE:HG23	11:B:805:EPE:H91	1.92	0.52
1:D:655:ILE:HG23	1:D:659:LYS:HE3	1.91	0.52
1:B:172:LEU:HD22	1:B:192:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:GLU:HB3	1:C:470:VAL:HG11	1.93	0.51
1:D:540:TRP:CD1	1:D:608:ALA:HB1	2.46	0.51
1:A:438:GLU:O	1:A:442:GLU:HG2	2.11	0.50
1:C:258:GLY:HA3	1:C:418:VAL:HG11	1.93	0.50
1:B:413:VAL:HG21	1:B:523:ILE:HG23	1.93	0.50
1:D:52:CYS:HA	1:D:55:LEU:HD12	1.93	0.50
1:A:187:SER:O	1:A:188:LYS:HB2	2.12	0.50
1:D:68:TYR:CB	1:D:72:VAL:HG11	2.41	0.50
1:D:20:THR:HG23	1:D:194:LEU:HD12	1.93	0.50
5:A:809:PG4:H12	1:D:298:ARG:HH22	1.77	0.50
1:A:4:ILE:HD12	1:B:227:PRO:HB3	1.94	0.49
1:C:135:TYR:HE1	1:C:141:ILE:HG13	1.78	0.49
1:C:250:HIS:HB3	1:C:334:LEU:HD12	1.95	0.49
1:C:135:TYR:HB3	5:C:801:PG4:H71	1.95	0.48
1:A:554:MET:HE3	1:A:560:LYS:HD3	1.93	0.48
1:B:540:TRP:CD1	1:B:608:ALA:HB1	2.48	0.48
1:B:314:VAL:HB	1:B:321:GLN:HB3	1.94	0.48
1:C:417:MET:HE2	1:C:531:TRP:HE1	1.79	0.48
1:D:151:LYS:HD3	1:D:180:GLY:HA2	1.96	0.48
1:C:416:ARG:HD3	1:C:493:SER:OG	2.13	0.48
1:D:557:HIS:CE1	1:D:558:LEU:HG	2.48	0.48
1:D:450:ILE:HD12	1:D:471:ASP:HA	1.94	0.48
1:B:228:VAL:HG22	1:B:510:LYS:HD3	1.96	0.48
1:A:336:LEU:HD11	6:A:810:BME:S2	2.54	0.47
1:D:252:PHE:HB3	1:D:280:THR:HB	1.96	0.47
1:C:133:ASN:HA	5:C:801:PG4:H81	1.96	0.47
1:A:576:ILE:HD12	1:A:633:LEU:HD11	1.96	0.47
1:D:626:ALA:HB2	1:D:671:LEU:HD22	1.96	0.47
1:D:68:TYR:HB3	1:D:72:VAL:HG11	1.97	0.47
1:D:2:VAL:CG1	1:D:11:HIS:NE2	2.79	0.46
1:D:113:ARG:HB3	1:D:164:LEU:HD22	1.96	0.46
1:D:453:GLU:HA	1:D:463:LEU:HD13	1.96	0.46
1:A:336:LEU:HD21	1:A:344:GLU:HG3	1.98	0.46
1:A:336:LEU:CD1	6:A:810:BME:S2	3.04	0.46
1:B:135:TYR:HE1	1:B:141:ILE:HG13	1.80	0.46
1:C:187:SER:O	1:C:188:LYS:HB2	2.16	0.46
1:D:84:MET:HG2	6:D:805:BME:H11	1.98	0.46
1:C:474:ARG:O	1:C:478:GLN:HB2	2.16	0.46
1:A:252:PHE:HB3	1:A:280:THR:HB	1.98	0.45
1:A:553:ALA:HB1	1:A:559:VAL:HG11	1.99	0.45
1:D:413:VAL:HG21	1:D:523:ILE:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ILE:HA	5:C:801:PG4:C7	2.46	0.45
1:C:172:LEU:HD22	1:C:192:ILE:HD11	1.98	0.45
1:A:289:VAL:HB	1:A:313:ILE:HG13	1.98	0.45
1:D:416:ARG:HD3	1:D:493:SER:OG	2.17	0.44
1:B:252:PHE:HB3	1:B:280:THR:HB	1.99	0.44
1:B:597:GLU:O	1:C:165:HIS:HE1	2.00	0.44
1:C:289:VAL:HB	1:C:313:ILE:HG13	1.99	0.44
1:A:251:GLY:HA2	6:A:810:BME:H22	1.99	0.44
1:D:429:GLN:O	1:D:433:LYS:HG2	2.16	0.44
1:C:341:ILE:HD12	1:C:381:LEU:HD23	2.00	0.44
1:D:2:VAL:HG12	1:D:11:HIS:CE1	2.52	0.44
1:A:639:LEU:HD21	1:A:684:GLU:HB3	2.00	0.44
1:C:455:CYS:HB2	1:C:458:LEU:HD12	2.00	0.44
1:D:14:ILE:HD12	1:D:173:MET:HE2	1.98	0.44
1:C:411:ASP:HB3	1:C:520:ILE:HG12	2.00	0.44
1:D:281:ARG:HE	1:D:317:ASP:CG	2.26	0.44
1:D:379:LYS:HB2	1:D:411:ASP:HB3	1.99	0.44
1:A:46:HIS:O	1:A:50:MET:HG2	2.18	0.43
1:D:576:ILE:CG2	1:D:631:HIS:CE1	2.99	0.43
1:A:413:VAL:HB	1:A:500:TYR:HB2	2.00	0.43
1:C:151:LYS:HD3	1:C:180:GLY:HA2	2.01	0.43
1:B:14:ILE:HD12	1:B:173:MET:HE2	2.01	0.43
1:C:582:ALA:HA	1:C:585:LEU:HD12	2.01	0.43
1:B:48:TYR:CZ	1:B:52:CYS:SG	3.12	0.43
1:B:107:LEU:HB3	1:B:112:LEU:HD12	2.00	0.43
1:B:259:TYR:CD1	1:B:416:ARG:HD2	2.54	0.43
1:A:541:TYR:HB2	1:A:644:LEU:HD13	1.99	0.43
1:D:187:SER:O	1:D:188:LYS:HB2	2.19	0.42
1:A:592:PHE:CZ	1:A:596:CYS:SG	3.12	0.42
1:C:106:ARG:HG2	1:C:226:ILE:HG21	2.01	0.42
5:A:809:PG4:H12	1:D:298:ARG:NH2	2.34	0.42
1:B:51:GLN:CD	9:B:810:CL:CL	3.00	0.42
1:A:497:MET:HB2	1:A:498:PRO:HD3	2.02	0.42
1:C:255:ILE:HD11	1:C:414:VAL:HG11	2.02	0.42
1:D:6:HIS:HA	3:D:801:EDO:H21	2.02	0.42
1:A:281:ARG:HG3	1:A:316:SER:HB2	2.02	0.42
1:C:413:VAL:HG21	1:C:523:ILE:HG23	2.01	0.42
1:D:48:TYR:CZ	1:D:52:CYS:SG	3.13	0.42
1:B:332:ILE:HG13	1:B:367:LEU:HD11	2.01	0.42
1:C:418:VAL:HG13	1:C:493:SER:HB2	2.02	0.42
1:D:242:LEU:HD23	1:D:272:LYS:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:LEU:HD22	1:D:407:HIS:CD2	2.54	0.42
1:D:500:TYR:CG	1:D:523:ILE:HG12	2.55	0.42
1:B:458:LEU:HD11	1:C:284:LEU:HD22	2.01	0.41
1:B:537:MET:HB2	1:B:566:LEU:HD21	2.02	0.41
1:C:243:ASN:OD1	1:C:273:PRO:HA	2.20	0.41
1:B:165:HIS:HD2	1:C:597:GLU:OE2	2.04	0.41
1:A:534:VAL:HG22	1:A:566:LEU:HG	2.02	0.41
1:B:28:ARG:HD2	10:B:814:44H:O4	2.20	0.41
1:B:379:LYS:O	1:B:383:MET:HG2	2.20	0.41
1:A:298:ARG:CZ	1:D:136:LYS:HB3	2.51	0.41
1:B:294:THR:HG22	1:B:309:GLU:HA	2.03	0.41
1:B:576:ILE:HD12	1:B:633:LEU:HD11	2.02	0.41
1:B:641:GLY:HA2	1:B:644:LEU:HD12	2.03	0.41
1:C:65:GLN:HG2	1:C:70:VAL:HA	2.03	0.41
1:C:341:ILE:HD11	1:C:373:LEU:HD22	2.03	0.41
1:D:40:ILE:HG23	1:D:77:ILE:HD11	2.03	0.41
1:B:497:MET:HB2	1:B:498:PRO:HD3	2.02	0.41
1:D:255:ILE:HD12	1:D:255:ILE:HA	1.98	0.40
1:A:533:GLY:CA	1:A:620:ARG:HB2	2.51	0.40
1:B:412:THR:HG22	1:B:501:VAL:HG22	2.03	0.40
1:B:415:ASN:OD1	1:B:527:LYS:HD3	2.22	0.40
1:B:537:MET:HE2	1:B:621:VAL:HG22	2.02	0.40
1:D:8:LYS:HA	1:D:9:PRO:HD3	1.96	0.40
1:D:105:GLU:HG2	1:D:270:TYR:O	2.21	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	678/727 (93%)	662 (98%)	15 (2%)	1 (0%)	48 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	677/727 (93%)	659 (97%)	16 (2%)	2 (0%)	36	46
1	C	564/727 (78%)	545 (97%)	19 (3%)	0	100	100
1	D	679/727 (93%)	653 (96%)	25 (4%)	1 (0%)	48	60
All	All	2598/2908 (89%)	2519 (97%)	75 (3%)	4 (0%)	43	55

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 ⓘ

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%)	597 (100%)	3 (0%)	81	90
1	B	601/641 (94%)	595 (99%)	6 (1%)	68	82
1	C	508/641 (79%)	501 (99%)	7 (1%)	59	76
1	D	603/641 (94%)	596 (99%)	7 (1%)	63	79
All	All	2312/2564 (90%)	2289 (99%)	23 (1%)	68	82

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	PHE
1	A	216	TYR
1	A	398	ASP
1	B	29	PHE
1	B	216	TYR
1	B	410	CYS
1	B	411	ASP

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Mol	Chain	Res	Type
1	B	463	LEU
1	B	567	ILE
1	C	29	PHE
1	C	216	TYR
1	C	336	LEU
1	C	410	CYS
1	C	411	ASP
1	C	418	VAL
1	C	421	LEU
1	D	29	PHE
1	D	42	GLN
1	D	127	GLU
1	D	266	HIS
1	D	375	LYS
1	D	580	ASN
1	D	638	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	37	GLN
1	A	88	HIS
1	A	92	HIS
1	A	131	ASN
1	A	149	GLN
1	A	169	ASN
1	A	519	GLN
1	A	528	ASN
1	B	133	ASN
1	B	402	HIS
1	B	476	ASN
1	B	528	ASN
1	B	680	GLN
1	C	34	GLN
1	C	301	GLN
1	C	478	GLN
1	D	30	GLN
1	D	37	GLN
1	D	149	GLN
1	D	235	GLN
1	D	320	GLN

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Mol	Chain	Res	Type
1	D	472	ASN
1	D	557	HIS
1	D	666	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 oligosaccharides 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	$\# Z > 2$
10	44H	C	809	-	15,15,15	1.12	1 (6%)	20,21,21	0.55	0
3	EDO	A	803	-	3,3,3	0.48	0	2,2,2	0.39	0
3	EDO	B	802	-	3,3,3	0.51	0	2,2,2	0.32	0
7	SO4	B	808	-	4,4,4	0.23	0	6,6,6	0.09	0
10	44H	B	814	-	15,15,15	1.07	2 (13%)	20,21,21	0.75	0
11	EPE	B	805	-	15,15,15	1.57	3 (20%)	19,20,20	2.01	7 (36%)
2	GOL	C	802	-	5,5,5	0.06	0	5,5,5	0.12	0
7	SO4	B	806	-	4,4,4	0.55	0	6,6,6	0.20	0
3	EDO	D	801	-	3,3,3	0.55	0	2,2,2	0.34	0
7	SO4	C	804	-	4,4,4	0.21	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PG4	A	809	-	12,12,12	0.25	0	11,11,11	0.18	0
13	ACT	C	803	-	3,3,3	1.14	0	3,3,3	0.86	0
6	BME	D	805	-	3,3,3	0.16	0	2,2,2	1.16	0
4	PGE	A	807	-	9,9,9	0.13	0	8,8,8	0.09	0
3	EDO	B	804	-	3,3,3	0.62	0	2,2,2	0.29	0
7	SO4	A	813	-	4,4,4	0.30	0	6,6,6	0.09	0
7	SO4	A	812	-	4,4,4	0.36	0	6,6,6	0.15	0
7	SO4	B	807	-	4,4,4	0.26	0	6,6,6	0.12	0
3	EDO	A	802	-	3,3,3	0.50	0	2,2,2	0.38	0
7	SO4	A	811	-	4,4,4	0.19	0	6,6,6	0.11	0
7	SO4	D	806	-	4,4,4	0.33	0	6,6,6	0.11	0
3	EDO	D	802	-	3,3,3	0.55	0	2,2,2	0.37	0
5	PG4	C	801	-	12,12,12	0.23	0	11,11,11	0.11	0
6	BME	A	810	-	3,3,3	0.30	0	2,2,2	1.26	0
3	EDO	D	803	-	3,3,3	0.51	0	2,2,2	0.37	0
3	EDO	A	806	-	3,3,3	0.49	0	2,2,2	0.39	0
2	GOL	A	801	-	5,5,5	0.08	0	5,5,5	0.17	0
4	PGE	A	808	-	9,9,9	0.24	0	8,8,8	0.09	0
7	SO4	D	807	-	4,4,4	0.22	0	6,6,6	0.12	0
3	EDO	B	803	-	3,3,3	0.55	0	2,2,2	0.36	0
3	EDO	B	801	-	3,3,3	0.48	0	2,2,2	0.37	0
10	44H	A	819	-	15,15,15	1.05	1 (6%)	20,21,21	0.60	0
7	SO4	A	814	-	4,4,4	0.33	0	6,6,6	0.20	0
3	EDO	A	805	-	3,3,3	0.57	0	2,2,2	0.33	0
10	44H	D	808	-	15,15,15	0.75	0	20,21,21	0.66	0
3	EDO	A	804	-	3,3,3	0.52	0	2,2,2	0.35	0
3	EDO	D	804	-	3,3,3	0.49	0	2,2,2	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
10	44H	C	809	-	-	0/20/20/20	-
3	EDO	A	803	-	-	0/1/1/1	-
3	EDO	B	802	-	-	0/1/1/1	-
10	44H	B	814	-	-	0/20/20/20	-
11	EPE	B	805	-	-	4/9/19/19	0/1/1/1
2	GOL	C	802	-	-	0/4/4/4	-
3	EDO	D	801	-	-	0/1/1/1	-
5	PG4	A	809	-	-	4/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BME	D	805	-	-	0/1/1/1	-
4	PGE	A	807	-	-	3/7/7/7	-
3	EDO	B	804	-	-	0/1/1/1	-
3	EDO	A	802	-	-	0/1/1/1	-
3	EDO	D	802	-	-	0/1/1/1	-
5	PG4	C	801	-	-	3/10/10/10	-
6	BME	A	810	-	-	0/1/1/1	-
3	EDO	D	803	-	-	0/1/1/1	-
3	EDO	A	806	-	-	0/1/1/1	-
2	GOL	A	801	-	-	0/4/4/4	-
4	PGE	A	808	-	-	3/7/7/7	-
3	EDO	B	803	-	-	0/1/1/1	-
3	EDO	B	801	-	-	0/1/1/1	-
10	44H	A	819	-	-	0/20/20/20	-
3	EDO	A	805	-	-	0/1/1/1	-
10	44H	D	808	-	-	1/20/20/20	-
3	EDO	A	804	-	-	0/1/1/1	-
3	EDO	D	804	-	-	0/1/1/1	-

All (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
10	C	809	44H	P-O2P	3.23	1.60	1.50
10	B	814	44H	P-O2P	3.18	1.60	1.50
10	A	819	44H	P-O2P	2.95	1.59	1.50
11	B	805	EPE	O2S-S	2.58	1.52	1.45
11	B	805	EPE	O1S-S	2.36	1.51	1.45
10	B	814	44H	P-O3P	-2.02	1.47	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	805	EPE	C6-N1-C2	4.12	117.72	108.84
11	B	805	EPE	O3S-S-O2S	-3.75	102.03	111.40
11	B	805	EPE	O2S-S-C10	3.09	111.40	106.73
11	B	805	EPE	C5-C6-N1	2.76	116.21	110.65
11	B	805	EPE	O3S-S-C10	2.67	111.23	106.00
11	B	805	EPE	O1S-S-C10	2.57	110.61	106.73
11	B	805	EPE	C9-N1-C6	2.09	116.81	111.24

There are no chirality outliers.

All (18) 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
4	A	808	PGE	O3-C5-C6-O4
11	B	805	EPE	C8-C7-N4-C3
4	A	808	PGE	O2-C3-C4-O3
5	A	809	PG4	C5-C6-O4-C7
5	C	801	PG4	C4-C3-O2-C2
5	C	801	PG4	C5-C6-O4-C7
4	A	807	PGE	C6-C5-O3-C4
5	A	809	PG4	C3-C4-O3-C5
4	A	808	PGE	O1-C1-C2-O2
5	A	809	PG4	C4-C3-O2-C2
4	A	807	PGE	C4-C3-O2-C2
10	D	808	44H	O5-C5-C6-O6
4	A	807	PGE	O2-C3-C4-O3

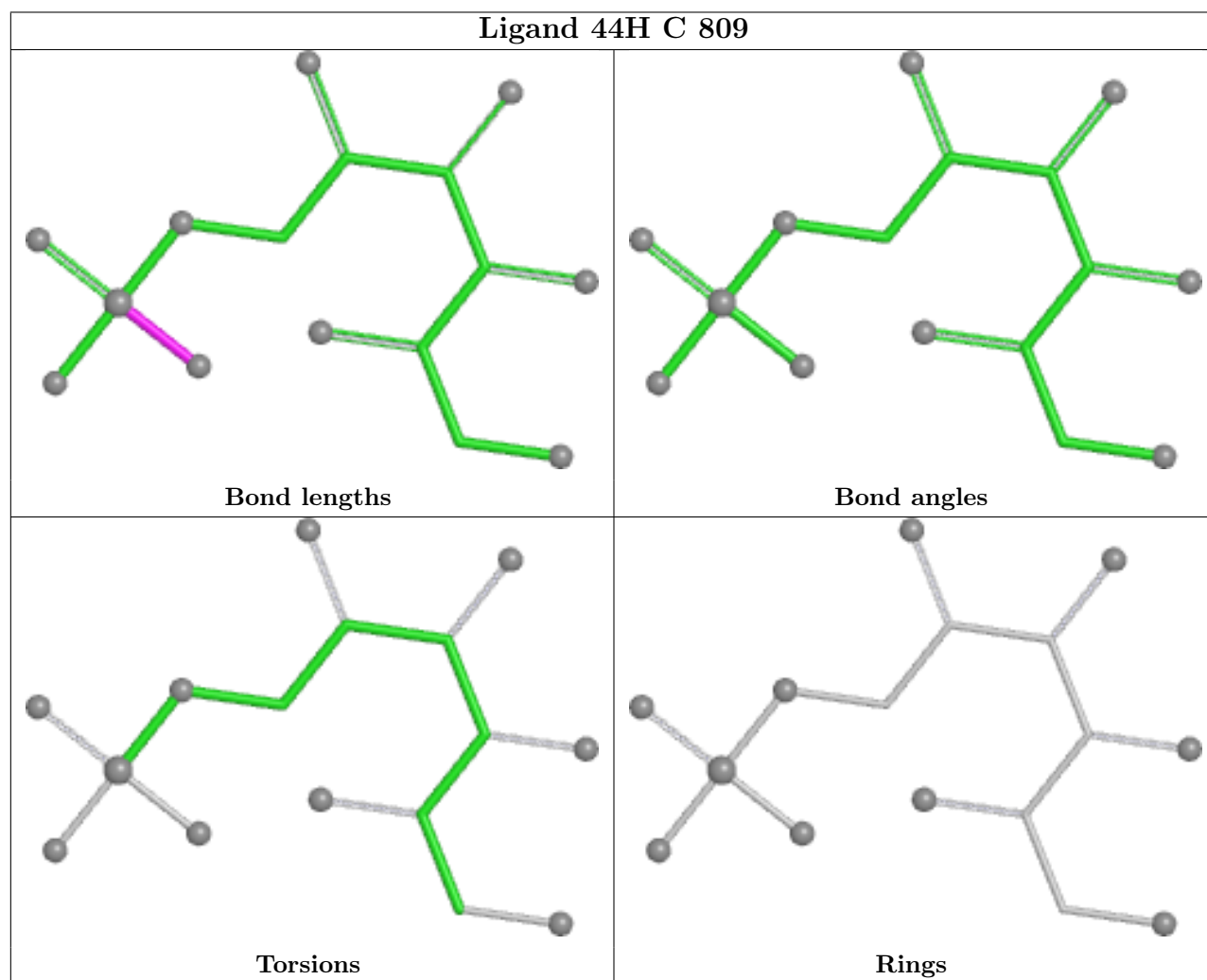
There are no ring outliers.

10 monomers are involved in 25 short contacts:

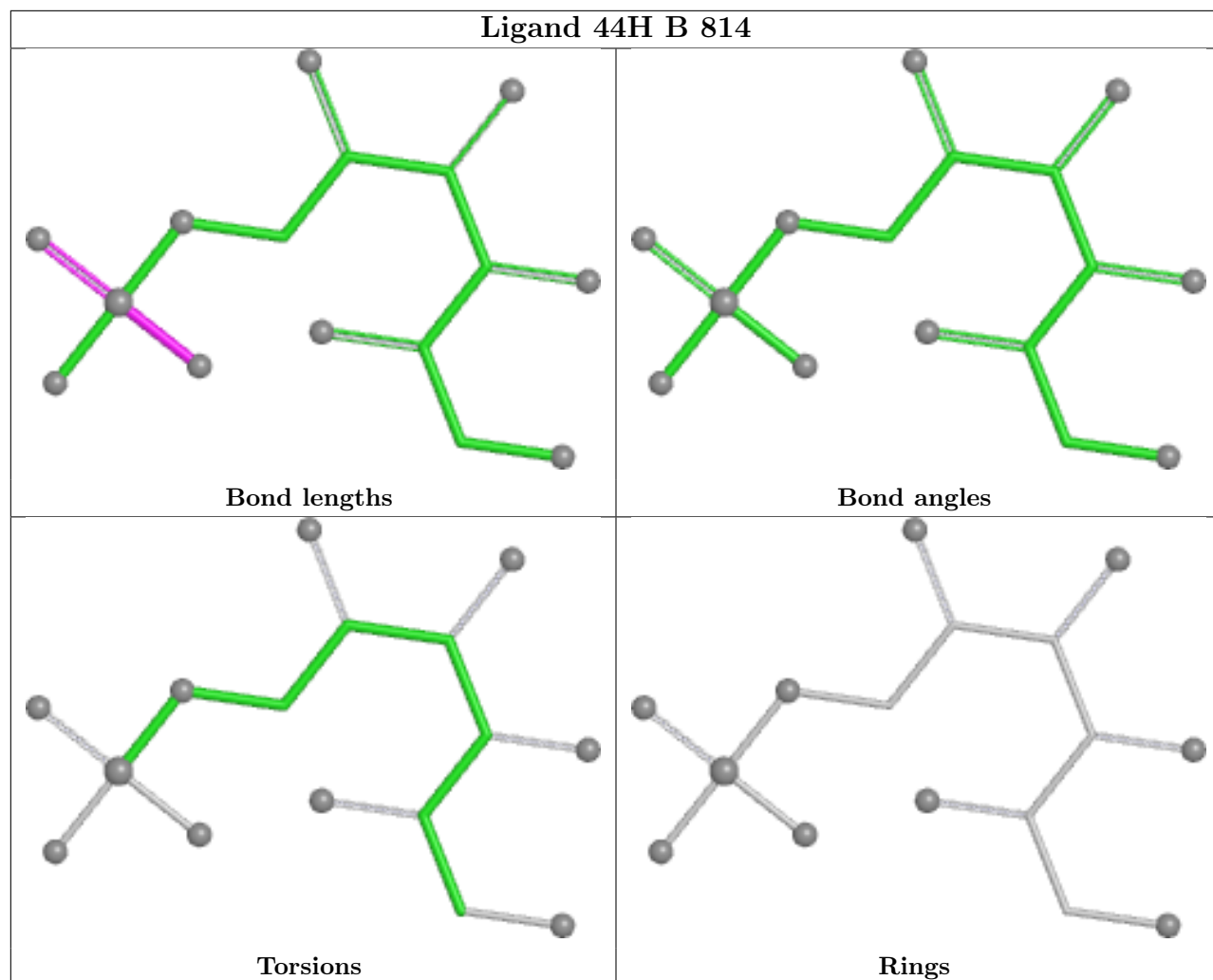
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	814	44H	1	0
11	B	805	EPE	7	0
3	D	801	EDO	1	0
7	C	804	SO4	2	0
5	A	809	PG4	4	0
6	D	805	BME	1	0
4	A	807	PGE	1	0
5	C	801	PG4	4	0
6	A	810	BME	3	0
7	D	807	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

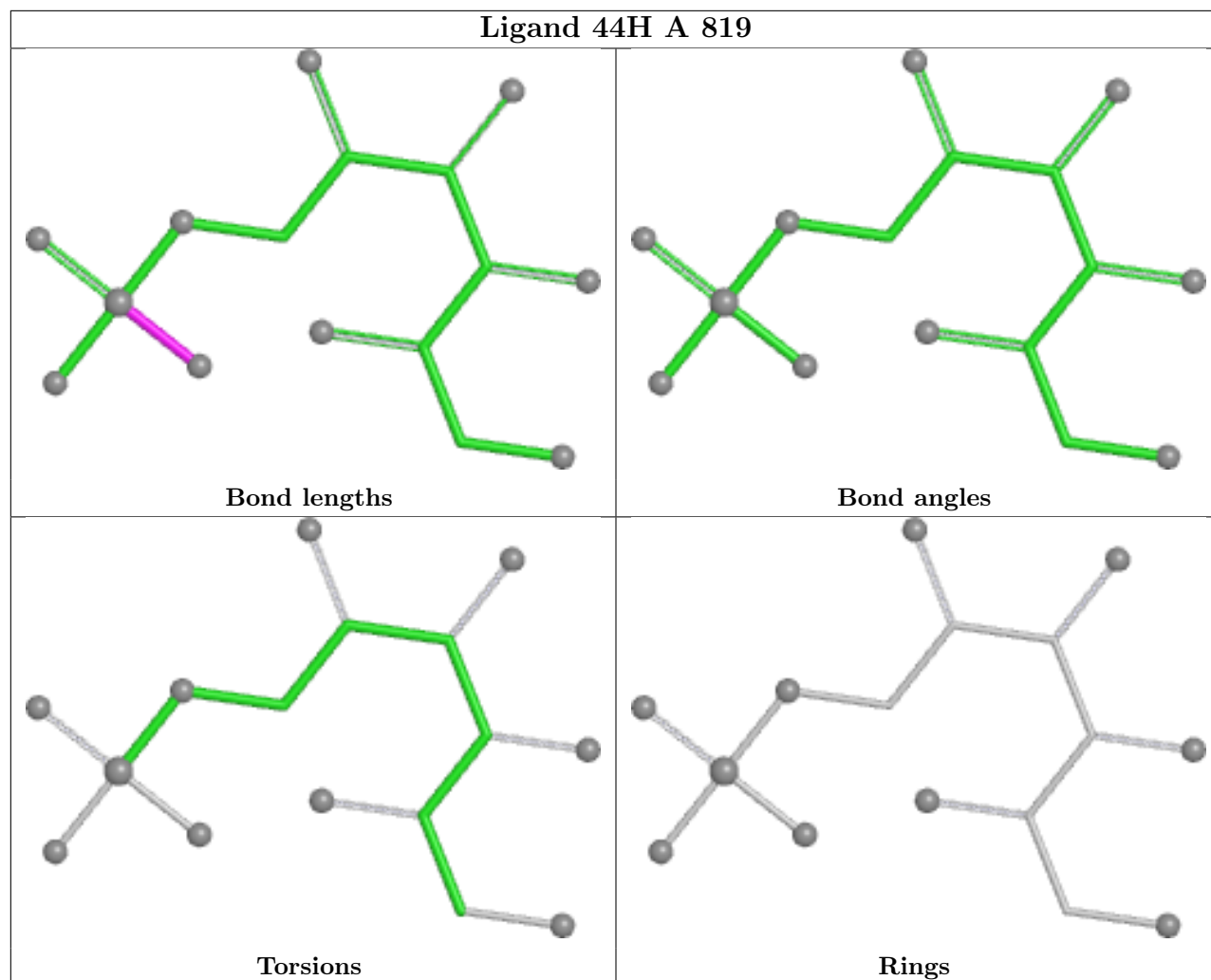
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

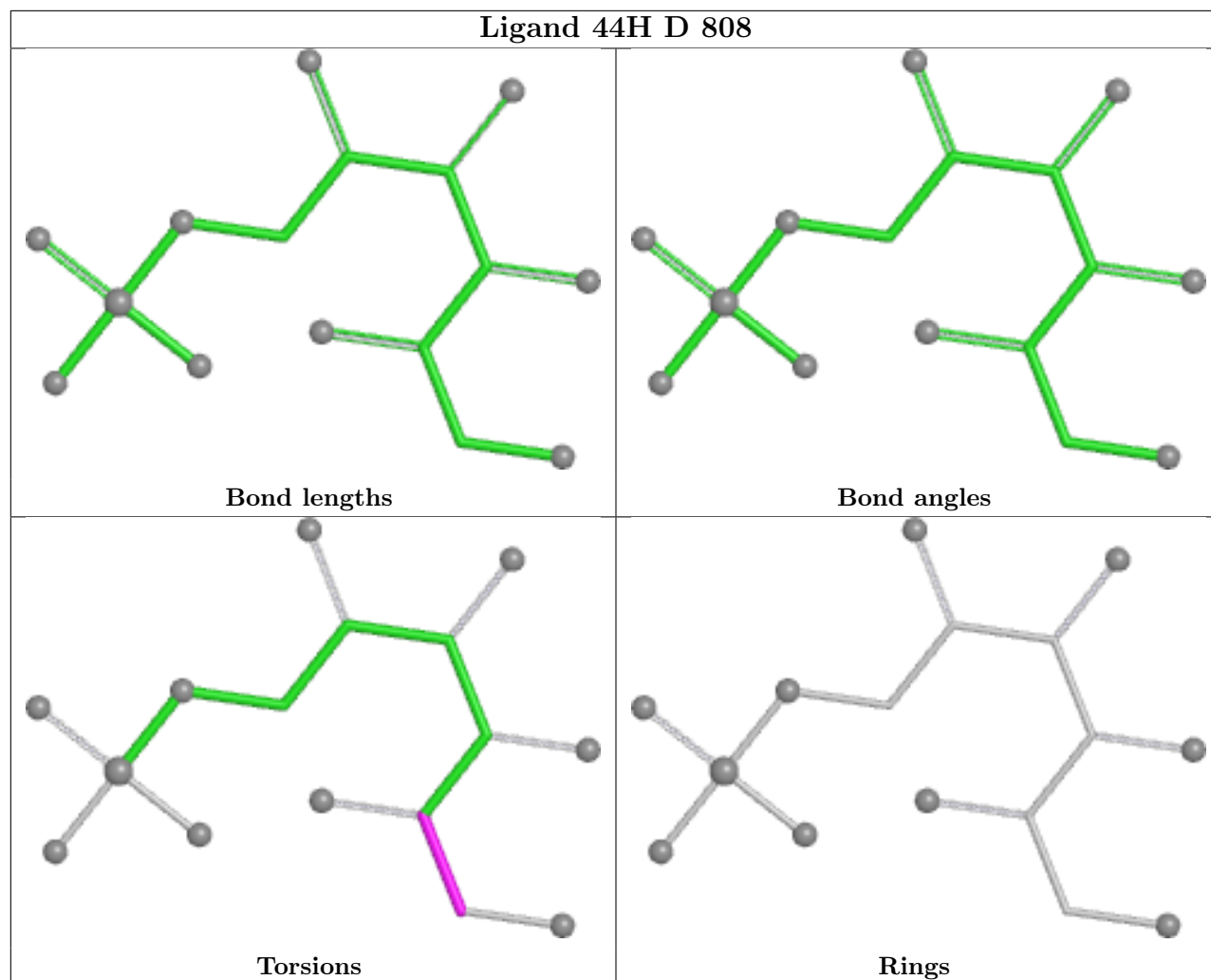


Ligand 44H B 814



Ligand 44H A 819





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	682/727 (93%)	0.58	31 (4%) 38 40	26, 44, 74, 97	0
1	B	683/727 (93%)	0.66	51 (7%) 20 22	29, 45, 72, 102	0
1	C	572/727 (78%)	1.02	74 (12%) 7 8	33, 56, 92, 114	0
1	D	685/727 (94%)	1.02	85 (12%) 8 9	34, 56, 90, 116	0
All	All	2622/2908 (90%)	0.81	241 (9%) 14 16	26, 50, 86, 116	0

All (241) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	693	PHE	6.3
1	B	692	LEU	6.2
1	B	652	PHE	6.1
1	C	362	THR	6.0
1	D	381	LEU	5.9
1	B	544	LEU	5.8
1	D	364	ILE	5.5
1	D	376	VAL	5.5
1	C	360	LEU	5.5
1	C	539	ALA	5.4
1	C	626	ALA	5.3
1	D	382	VAL	4.9
1	D	391	LEU	4.9
1	C	576	ILE	4.7
1	C	625	ILE	4.7
1	D	393	LEU	4.6
1	C	363	CYS	4.4
1	B	603	PRO	4.4
1	C	570	VAL	4.4
1	C	577	VAL	4.4
1	C	598	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	356	PHE	4.3
1	A	360	LEU	4.2
1	D	380	TYR	4.1
1	C	575	ALA	4.0
1	A	362	THR	4.0
1	C	627	VAL	4.0
1	D	2	VAL	3.9
1	D	378	ALA	3.9
1	B	688	LEU	3.8
1	A	694	SER	3.8
1	C	364	ILE	3.7
1	C	538	LEU	3.7
1	D	336	LEU	3.7
1	D	452	ILE	3.7
1	B	444	VAL	3.7
1	B	361	GLU	3.7
1	A	376	VAL	3.7
1	D	599	ALA	3.6
1	B	650	ILE	3.6
1	D	411	ASP	3.6
1	B	658	THR	3.6
1	B	607	VAL	3.6
1	D	576	ILE	3.5
1	C	578	LEU	3.5
1	D	386	LEU	3.5
1	B	452	ILE	3.5
1	D	377	GLY	3.5
1	A	444	VAL	3.5
1	B	604	CYS	3.5
1	C	361	GLU	3.5
1	B	542	ALA	3.4
1	C	579	PRO	3.4
1	A	2	VAL	3.4
1	C	67	LEU	3.4
1	C	450	ILE	3.4
1	C	568	ALA	3.4
1	C	623	ALA	3.4
1	D	383	MET	3.3
1	B	558	LEU	3.3
1	D	658	THR	3.3
1	C	574	LEU	3.3
1	D	600	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	452	ILE	3.3
1	D	655	ILE	3.3
1	A	658	THR	3.3
1	B	689	ILE	3.2
1	D	91	LYS	3.2
1	B	639	LEU	3.2
1	D	450	ILE	3.2
1	C	140	VAL	3.2
1	C	444	VAL	3.2
1	D	608	ALA	3.2
1	C	622	MET	3.2
1	B	541	TYR	3.1
1	B	648	TYR	3.1
1	A	377	GLY	3.1
1	A	686	VAL	3.1
1	B	601	LYS	3.1
1	C	581	TYR	3.1
1	C	580	ASN	3.1
1	B	651	GLN	3.0
1	D	410	CYS	3.0
1	D	598	TYR	3.0
1	D	375	LYS	3.0
1	A	693	PHE	3.0
1	D	403	ILE	3.0
1	D	408	TYR	3.0
1	B	360	LEU	2.9
1	A	364	ILE	2.9
1	B	691	TYR	2.9
1	B	545	MET	2.9
1	C	534	VAL	2.9
1	D	399	VAL	2.9
1	C	336	LEU	2.9
1	C	536	ALA	2.9
1	C	585	LEU	2.9
1	A	661	VAL	2.9
1	A	361	GLU	2.9
1	C	624	SER	2.9
1	D	550	ILE	2.9
1	C	458	LEU	2.8
1	D	389	ALA	2.8
1	D	693	PHE	2.8
1	C	628	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	595	SER	2.8
1	B	642	ALA	2.8
1	D	388	GLU	2.8
1	D	66	ARG	2.8
1	B	456	ASN	2.8
1	C	593	LEU	2.8
1	C	525	LEU	2.8
1	B	342	GLU	2.7
1	D	406	GLU	2.7
1	A	457	LYS	2.7
1	A	485	SER	2.7
1	D	358	SER	2.7
1	D	352	LEU	2.7
1	A	652	PHE	2.7
1	D	369	PHE	2.7
1	B	362	THR	2.7
1	D	502	GLU	2.7
1	A	363	CYS	2.7
1	C	530	LEU	2.7
1	D	230	ASP	2.6
1	C	531	TRP	2.6
1	C	401	GLU	2.6
1	D	374	ASN	2.6
1	D	694	SER	2.6
1	B	336	LEU	2.6
1	D	390	LEU	2.6
1	D	404	LEU	2.6
1	D	409	PHE	2.6
1	C	596	CYS	2.6
1	A	347	ILE	2.6
1	D	664	LEU	2.5
1	D	688	LEU	2.5
1	B	455	CYS	2.5
1	B	608	ALA	2.5
1	D	444	VAL	2.5
1	A	650	ILE	2.5
1	D	353	TYR	2.5
1	D	660	ALA	2.5
1	D	400	THR	2.5
1	A	359	GLN	2.5
1	C	453	GLU	2.5
1	C	62	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	580	ASN	2.5
1	C	70	VAL	2.5
1	C	205	LEU	2.5
1	C	582	ALA	2.5
1	C	592	PHE	2.4
1	B	685	LEU	2.4
1	D	93	GLY	2.4
1	D	579	PRO	2.4
1	C	369	PHE	2.4
1	A	692	LEU	2.4
1	C	82	ASP	2.4
1	C	176	ASP	2.4
1	D	604	CYS	2.4
1	C	417	MET	2.4
1	D	367	LEU	2.4
1	D	441	LEU	2.4
1	D	92	HIS	2.4
1	D	339	GLN	2.4
1	C	222	LEU	2.4
1	B	663	HIS	2.4
1	B	690	GLN	2.4
1	D	695	GLU	2.4
1	D	568	ALA	2.3
1	C	588	MET	2.3
1	A	67	LEU	2.3
1	C	528	ASN	2.3
1	A	655	ILE	2.3
1	A	685	LEU	2.3
1	D	583	LYS	2.3
1	C	587	ARG	2.3
1	D	90	ARG	2.3
1	B	656	GLU	2.3
1	C	569	GLU	2.3
1	D	206	GLU	2.3
1	D	449	GLN	2.3
1	D	348	ILE	2.3
1	B	659	LYS	2.3
1	A	689	ILE	2.3
1	C	456	ASN	2.2
1	D	169	ASN	2.2
1	D	379	LYS	2.2
1	D	692	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	643	ALA	2.2
1	C	91	LYS	2.2
1	D	340	ALA	2.2
1	A	668	ILE	2.2
1	C	141	ILE	2.2
1	C	523	ILE	2.2
1	D	371	ILE	2.2
1	A	190	LEU	2.2
1	D	578	LEU	2.2
1	B	359	GLN	2.2
1	C	359	GLN	2.2
1	C	571	LYS	2.2
1	B	606	ARG	2.1
1	C	135	TYR	2.1
1	C	216	TYR	2.1
1	B	67	LEU	2.1
1	B	374	ASN	2.1
1	C	457	LYS	2.1
1	D	333	ALA	2.1
1	B	141	ILE	2.1
1	D	373	LEU	2.1
1	C	365	GLU	2.1
1	A	621	VAL	2.1
1	D	29	PHE	2.1
1	B	660	ALA	2.1
1	B	437	LEU	2.1
1	A	464	ASN	2.1
1	C	74	TYR	2.1
1	D	372	ILE	2.1
1	D	671	LEU	2.1
1	D	689	ILE	2.1
1	C	214	GLN	2.1
1	D	603	PRO	2.1
1	B	363	CYS	2.1
1	B	457	LYS	2.1
1	C	190	LEU	2.1
1	D	337	PRO	2.1
1	B	2	VAL	2.1
1	C	225	PHE	2.1
1	C	455	CYS	2.0
1	D	89	ILE	2.0
1	D	607	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	600	PHE	2.0
1	A	445	GLU	2.0
1	C	312	SER	2.0
1	B	687	GLN	2.0
1	D	407	HIS	2.0
1	A	673	LEU	2.0
1	B	644	LEU	2.0
1	B	681	LEU	2.0
1	C	511	LEU	2.0
1	D	384	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
13	ACT	C	803	4/4	0.59	0.20	46,47,55,55	0
3	EDO	D	802	4/4	0.72	0.15	71,86,86,86	0
11	EPE	B	805	15/15	0.72	0.29	73,73,73,74	0
3	EDO	B	804	4/4	0.72	0.26	66,79,79,79	0
7	SO4	C	804	5/5	0.73	0.16	98,98,98,98	0
4	PGE	A	808	10/10	0.73	0.22	46,56,60,60	0
7	SO4	B	807	5/5	0.73	0.15	99,99,99,99	0
2	GOL	C	802	6/6	0.76	0.13	73,88,88,89	0
3	EDO	A	803	4/4	0.77	0.17	84,101,101,101	0
7	SO4	A	814	5/5	0.77	0.27	71,71,71,71	0
7	SO4	B	808	5/5	0.78	0.16	125,125,125,125	0
7	SO4	A	813	5/5	0.78	0.18	135,135,135,135	0
3	EDO	A	805	4/4	0.78	0.16	60,72,72,72	0

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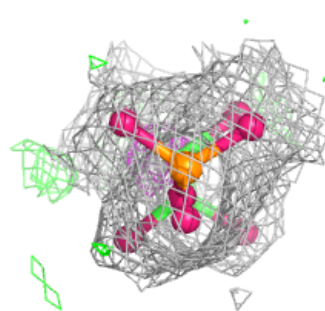
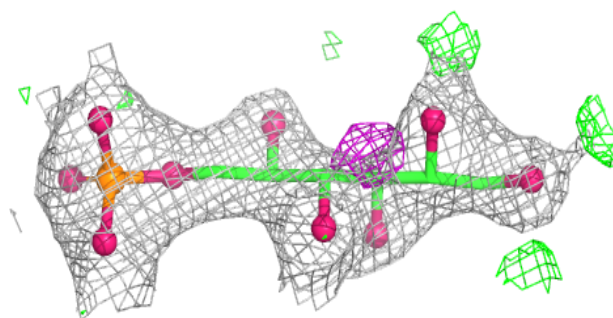
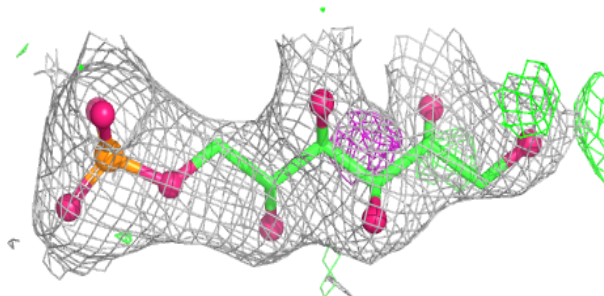
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	804	4/4	0.78	0.16	69,83,83,83	0
4	PGE	A	807	10/10	0.79	0.15	69,84,84,84	0
3	EDO	D	803	4/4	0.81	0.16	70,84,84,84	0
3	EDO	A	802	4/4	0.81	0.15	77,92,93,93	0
5	PG4	C	801	13/13	0.82	0.17	47,56,65,66	0
3	EDO	B	803	4/4	0.82	0.23	52,62,63,63	0
12	NA	C	808	1/1	0.83	0.21	60,60,60,60	0
5	PG4	A	809	13/13	0.84	0.13	42,51,57,57	0
2	GOL	A	801	6/6	0.85	0.16	45,55,55,55	0
3	EDO	A	806	4/4	0.85	0.14	56,67,67,67	0
3	EDO	D	801	4/4	0.86	0.10	74,88,88,88	0
8	MG	A	815	1/1	0.87	0.16	66,66,66,66	0
3	EDO	B	802	4/4	0.88	0.13	40,48,48,49	0
3	EDO	B	801	4/4	0.90	0.12	42,50,51,51	0
3	EDO	D	804	4/4	0.91	0.10	48,58,58,58	0
6	BME	A	810	4/4	0.91	0.13	48,58,58,58	0
10	44H	C	809	16/16	0.91	0.10	47,49,51,51	0
7	SO4	D	807	5/5	0.92	0.12	78,78,78,78	0
9	CL	C	807	1/1	0.92	0.10	64,64,64,64	0
7	SO4	D	806	5/5	0.93	0.13	54,54,55,55	0
6	BME	D	805	4/4	0.93	0.16	19,25,28,31	0
7	SO4	A	811	5/5	0.93	0.14	70,70,70,70	0
7	SO4	B	806	5/5	0.93	0.14	33,34,35,35	0
7	SO4	A	812	5/5	0.94	0.11	35,35,36,36	5
12	NA	B	813	1/1	0.94	0.12	39,39,39,39	0
9	CL	B	812	1/1	0.95	0.09	37,37,37,37	0
10	44H	D	808	16/16	0.95	0.09	41,42,42,42	0
10	44H	A	819	16/16	0.95	0.08	32,33,34,34	0
10	44H	B	814	16/16	0.96	0.07	33,36,37,38	0
9	CL	C	806	1/1	0.97	0.16	58,58,58,58	0
9	CL	A	818	1/1	0.98	0.05	38,38,38,38	0
9	CL	B	809	1/1	0.98	0.05	36,36,36,36	0
9	CL	B	810	1/1	0.98	0.07	51,51,51,51	0
9	CL	B	811	1/1	0.98	0.08	39,39,39,39	0
9	CL	A	816	1/1	0.98	0.05	31,31,31,31	0
9	CL	A	817	1/1	0.99	0.09	34,34,34,34	0
9	CL	C	805	1/1	0.99	0.09	49,49,49,49	0

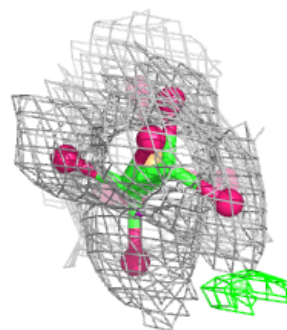
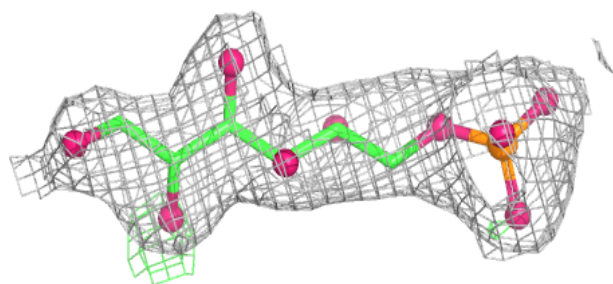
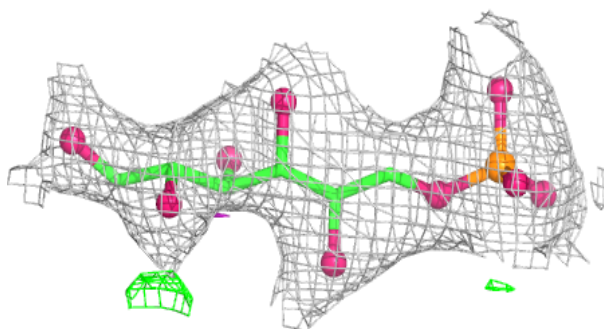
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

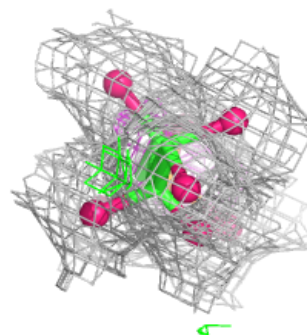
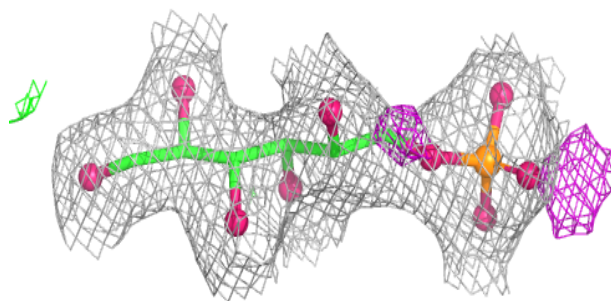
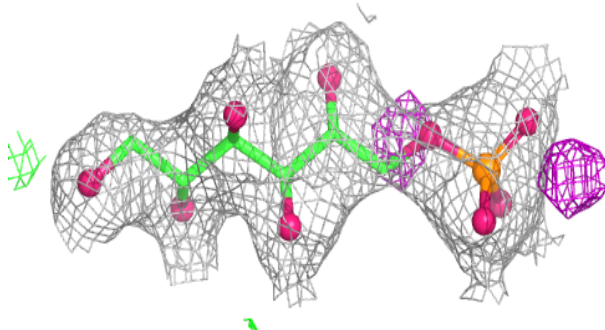
**Electron density around 44H D 808:**

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

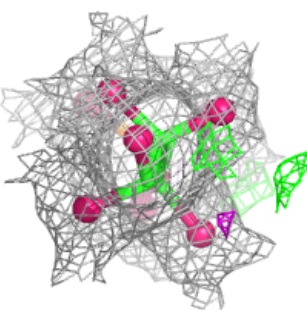
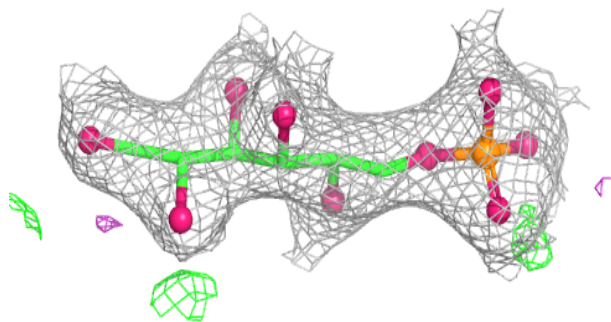
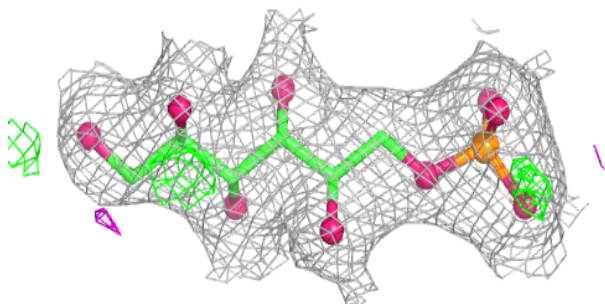


Electron density around 44H A 819:

$2mF_o-DF_c$ (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.