



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:46 PM UTC

PDB ID : 7OCR / pdb_00007ocr
Title : NADPH and fructose-6-phosphate bound to the dehydrogenase domain of the bifunctional mannitol-1-phosphate dehydrogenase/phosphatase MtlD from *Acinetobacter baumannii*
Authors : Tam, H.K.; Mueller, V.; Pos, K.M.
Deposited on : 2021-04-28
Resolution : 2.60 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

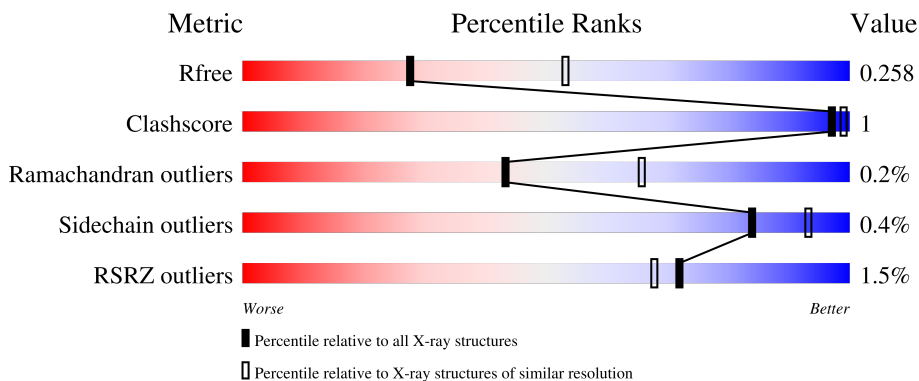
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

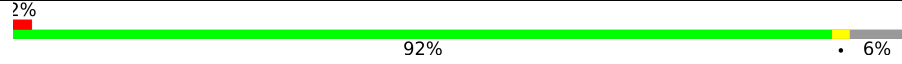
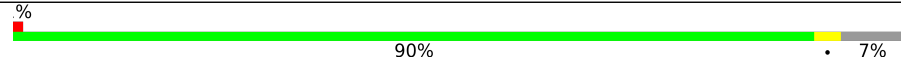
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	 2% 92% 6%
1	B	727	 % 90% 7%

2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 11282 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 HAD hydrolase, family IA, variant 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	687	Total	C	N	O	S	0	0	0
			5540	3518	947	1042	33			
1	B	675	Total	C	N	O	S	0	0	0
			5448	3460	934	1022	32			

There are 26 discrepancies between the modelled and reference sequences:

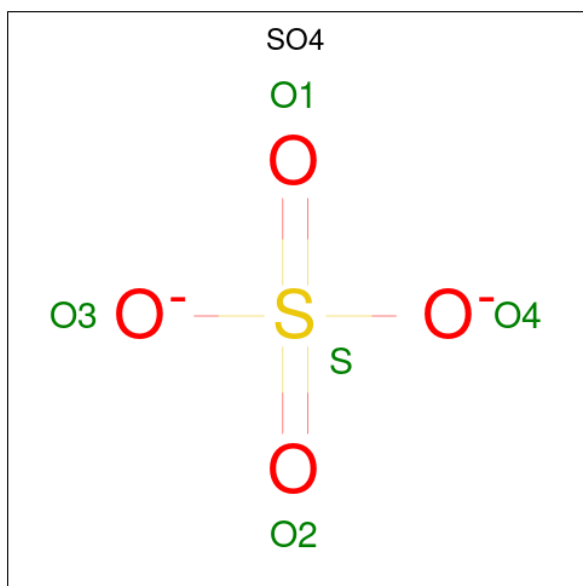
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP D0C7J2
A	2	VAL	-	expression tag	UNP D0C7J2
A	717	ALA	-	expression tag	UNP D0C7J2
A	718	ALA	-	expression tag	UNP D0C7J2
A	719	ALA	-	expression tag	UNP D0C7J2
A	720	LEU	-	expression tag	UNP D0C7J2
A	721	GLU	-	expression 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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	727	HIS	-	expression tag	UNP D0C7J2

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



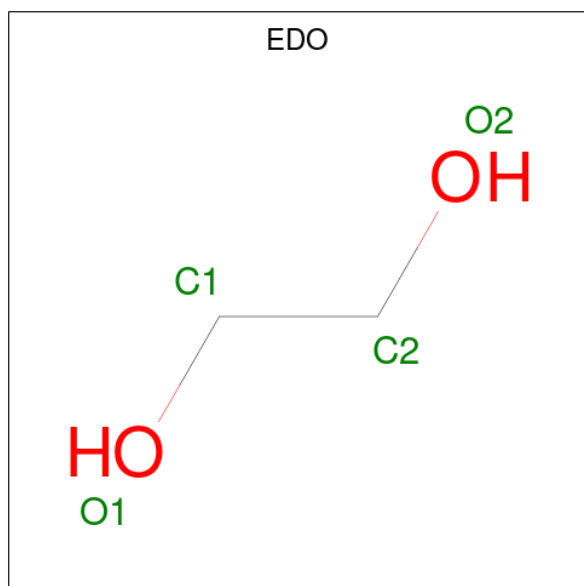
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

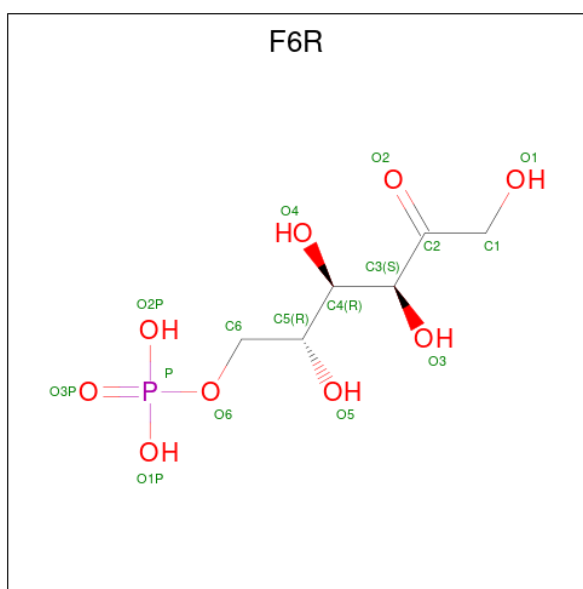
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 8 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 9 is FRUCTOSE -6-PHOSPHATE (CCD ID: F6R) (formula: C₆H₁₃O₉P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	72	Total O 72 72	0	0
10	B	36	Total O 36 36	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	99.89Å 157.56Å 220.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.71 – 2.60 48.71 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.71-2.60) 100.0 (48.71-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.230 , 0.258 0.230 , 0.258	Depositor DCC
R_{free} test set	2617 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	64.3	Xtrriage
Anisotropy	0.613	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11282	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: NDP, MG, EDO, EPE, K, CL, F6R, SO4

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	1.00	0/5644	1.53	0/7620
1	B	1.00	0/5549	1.54	0/7485
All	All	1.00	0/11193	1.54	0/15105

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	5540	0	5516	8	0
1	B	5448	0	5422	11	0
2	A	10	0	0	0	0
3	A	48	0	26	0	0
3	B	48	0	26	0	0
4	A	30	0	36	0	0
5	A	16	0	24	0	0
5	B	8	0	12	0	0
6	A	4	0	0	0	0
6	B	3	0	0	0	0
7	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	1	0	0	0	0
8	A	1	0	0	0	0
9	B	16	0	11	0	0
10	A	72	0	0	0	0
10	B	36	0	0	0	0
All	All	11282	0	11073	19	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 1.

All (19) 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:252:PHE:HB2	1:B:278:ALA:HB1	1.87	0.56
1:A:255:ILE:HD11	1:A:414:VAL:HG11	1.91	0.52
1:A:252:PHE:HB2	1:A:278:ALA:HB1	1.90	0.52
1:B:537:MET:HE1	1:B:638:LEU:HD23	1.95	0.49
1:A:175:GLU:HG2	1:A:180:GLY:C	2.37	0.48
1:B:538:LEU:HD12	1:B:538:LEU:C	2.40	0.47
1:A:259:TYR:CE2	1:A:414:VAL:HG13	2.50	0.47
1:A:187:SER:O	1:A:188:LYS:HB2	2.16	0.44
1:B:250:HIS:CD2	1:B:336:LEU:HD11	2.54	0.43
1:B:336:LEU:HD13	1:B:344:GLU:HG3	2.01	0.43
1:B:286:ARG:HA	1:B:313:ILE:HG21	2.01	0.42
1:A:175:GLU:HG2	1:A:181:LEU:N	2.34	0.42
1:B:259:TYR:CE2	1:B:414:VAL:HG13	2.55	0.42
1:B:537:MET:HE2	1:B:641:GLY:HA3	2.02	0.42
1:B:610:ASP:N	1:B:611:PRO:HD3	2.35	0.41
1:A:508:LEU:HD23	1:A:511:LEU:HD12	2.02	0.41
1:B:508:LEU:HD23	1:B:511:LEU:HD12	2.02	0.41
1:B:96:ILE:HG23	1:B:100:LEU:HD23	2.01	0.41
1:A:34:GLN:HB3	1:A:84:MET:HE1	2.02	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	683/727 (94%)	650 (95%)	31 (4%)	2 (0%)	36	58
1	B	667/727 (92%)	635 (95%)	31 (5%)	1 (0%)	48	70
All	All	1350/1454 (93%)	1285 (95%)	62 (5%)	3 (0%)	43	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	LYS
1	A	455	CYS
1	B	656	GLU

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	606/642 (94%)	604 (100%)	2 (0%)	86	94
1	B	595/642 (93%)	592 (100%)	3 (0%)	81	92
All	All	1201/1284 (94%)	1196 (100%)	5 (0%)	84	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	ARG
1	A	141	ILE
1	B	29	PHE

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Mol	Chain	Res	Type
1	B	39	LEU
1	B	421	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	37	GLN
1	A	46	HIS
1	A	133	ASN
1	A	310	ASN
1	A	476	ASN
1	A	557	HIS
1	A	572	GLN
1	B	11	HIS
1	B	133	ASN
1	B	149	GLN
1	B	282	ASN
1	B	301	GLN
1	B	321	GLN
1	B	402	HIS
1	B	423	ASN
1	B	439	GLN
1	B	456	ASN
1	B	476	ASN
1	B	572	GLN
1	B	590	GLN
1	B	617	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 23 ligands modelled in this entry, 10 are monoatomic - leaving 13 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	SO4	A	802	-	4,4,4	0.35	0	6,6,6	0.08	0
3	NDP	B	806	-	51,52,52	2.50	9 (17%)	71,80,80	1.48	15 (21%)
5	EDO	A	806	-	3,3,3	0.07	0	2,2,2	0.13	0
4	EPE	A	813	-	15,15,15	1.33	3 (20%)	19,20,20	1.92	5 (26%)
3	NDP	A	803	-	51,52,52	2.66	9 (17%)	71,80,80	1.41	14 (19%)
5	EDO	A	805	-	3,3,3	0.06	0	2,2,2	0.10	0
5	EDO	B	805	-	3,3,3	0.06	0	2,2,2	0.11	0
5	EDO	A	808	-	3,3,3	0.06	0	2,2,2	0.09	0
5	EDO	A	807	-	3,3,3	0.07	0	2,2,2	0.10	0
5	EDO	B	804	-	3,3,3	0.07	0	2,2,2	0.10	0
4	EPE	A	804	-	15,15,15	1.35	3 (20%)	19,20,20	1.88	4 (21%)
9	F6R	B	807	-	15,15,15	0.40	0	16,21,21	0.53	0
2	SO4	A	801	-	4,4,4	0.34	0	6,6,6	0.07	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
3	NDP	B	806	-	-	11/34/77/77	0/5/5/5
5	EDO	A	806	-	-	1/1/1/1	-
4	EPE	A	813	-	-	4/9/19/19	0/1/1/1
3	NDP	A	803	-	-	7/34/77/77	0/5/5/5
5	EDO	A	805	-	-	1/1/1/1	-
5	EDO	B	805	-	-	1/1/1/1	-
5	EDO	A	808	-	-	0/1/1/1	-
5	EDO	A	807	-	-	1/1/1/1	-
5	EDO	B	804	-	-	1/1/1/1	-
4	EPE	A	804	-	-	4/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	F6R	B	807	-	-	6/20/20/20	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	803	NDP	P2B-O2B	14.50	1.84	1.59
3	B	806	NDP	P2B-O2B	13.68	1.83	1.59
3	A	803	NDP	PA-O3	6.47	1.66	1.59
3	B	806	NDP	PA-O3	5.13	1.65	1.59
3	A	803	NDP	PN-O5D	4.79	1.78	1.59
3	B	806	NDP	PN-O5D	4.42	1.76	1.59
4	A	813	EPE	C10-S	3.62	1.82	1.77
4	A	804	EPE	C10-S	3.56	1.82	1.77
3	A	803	NDP	C5A-C4A	3.12	1.44	1.39
3	B	806	NDP	O2B-C2B	-3.10	1.33	1.44
3	B	806	NDP	C5A-C4A	3.00	1.44	1.39
3	B	806	NDP	C2A-N1A	2.92	1.39	1.33
3	A	803	NDP	O2B-C2B	-2.88	1.34	1.44
3	A	803	NDP	C2A-N1A	2.83	1.39	1.33
3	A	803	NDP	C4A-N3A	2.66	1.39	1.34
3	B	806	NDP	C4A-N3A	2.52	1.39	1.34
4	A	804	EPE	O2S-S	2.46	1.52	1.45
3	A	803	NDP	C8A-N9A	2.37	1.41	1.37
4	A	813	EPE	O1S-S	2.30	1.51	1.45
4	A	813	EPE	O2S-S	2.22	1.51	1.45
4	A	804	EPE	O1S-S	2.19	1.51	1.45
3	B	806	NDP	C8A-N9A	2.14	1.41	1.37
3	B	806	NDP	C7N-N7N	2.07	1.39	1.33
3	A	803	NDP	C2B-C1B	2.06	1.58	1.53

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	804	EPE	O2S-S-C10	5.20	114.59	106.73
4	A	813	EPE	O3S-S-O1S	-4.38	100.44	111.40
4	A	813	EPE	O1S-S-C10	4.33	113.27	106.73
3	B	806	NDP	P2B-O2B-C2B	-4.20	112.23	123.43
4	A	804	EPE	O2S-S-O1S	-4.05	100.64	113.82
3	B	806	NDP	O3-PA-O1A	-3.70	99.58	110.70
3	B	806	NDP	O2B-P2B-O1X	-3.66	96.28	109.33
3	A	803	NDP	O3-PA-O1A	-3.56	100.00	110.70
3	A	803	NDP	O2B-P2B-O1X	-3.42	97.15	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	NDP	P2B-O2B-C2B	-3.41	114.33	123.43
4	A	813	EPE	O3S-S-C10	2.96	111.79	106.00
3	B	806	NDP	PA-O5B-C5B	-2.85	105.05	121.35
3	A	803	NDP	PA-O5B-C5B	-2.79	105.36	121.35
4	A	804	EPE	O1S-S-C10	2.72	110.83	106.73
3	B	806	NDP	O3X-P2B-O2X	2.54	117.32	107.80
4	A	813	EPE	C6-N1-C2	2.51	114.25	108.84
4	A	813	EPE	C9-N1-C2	2.48	117.84	111.24
3	A	803	NDP	O3X-P2B-O2X	2.48	117.09	107.80
3	A	803	NDP	N3A-C4A-N9A	2.43	131.29	127.17
3	B	806	NDP	C3N-C2N-N1N	-2.37	119.73	123.20
3	A	803	NDP	C2A-N1A-C6A	-2.36	114.85	118.73
3	B	806	NDP	N3A-C4A-N9A	2.36	131.18	127.17
3	B	806	NDP	C2A-N1A-C6A	-2.33	114.91	118.73
3	B	806	NDP	O7N-C7N-N7N	-2.32	117.68	122.89
4	A	804	EPE	C9-N1-C6	2.32	117.42	111.24
3	A	803	NDP	O2N-PN-O1N	2.30	123.15	112.44
3	B	806	NDP	PN-O5D-C5D	-2.30	108.18	121.35
3	B	806	NDP	C5B-C4B-C3B	-2.23	107.17	115.21
3	A	803	NDP	C5A-C4A-N3A	-2.23	123.65	126.72
3	B	806	NDP	O2N-PN-O1N	2.19	122.62	112.44
3	A	803	NDP	O4B-C4B-C3B	2.18	109.47	105.15
3	A	803	NDP	O2N-PN-O3	2.16	113.10	107.27
3	B	806	NDP	O4B-C4B-C3B	2.15	109.42	105.15
3	A	803	NDP	PN-O5D-C5D	-2.15	109.03	121.35
3	A	803	NDP	O7N-C7N-N7N	-2.07	118.25	122.89
3	B	806	NDP	C5A-C4A-N3A	-2.07	123.87	126.72
3	A	803	NDP	C3N-C2N-N1N	-2.04	120.22	123.20
3	B	806	NDP	O3X-P2B-O2B	-2.02	97.97	105.85

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	NDP	C2N-C3N-C7N-N7N
3	B	806	NDP	C5B-O5B-PA-O1A
3	B	806	NDP	C5B-O5B-PA-O3
3	B	806	NDP	O4B-C4B-C5B-O5B
3	B	806	NDP	O4D-C4D-C5D-O5D
3	B	806	NDP	C2N-C3N-C7N-N7N
4	A	804	EPE	C10-C9-N1-C6
4	A	804	EPE	N4-C7-C8-O8

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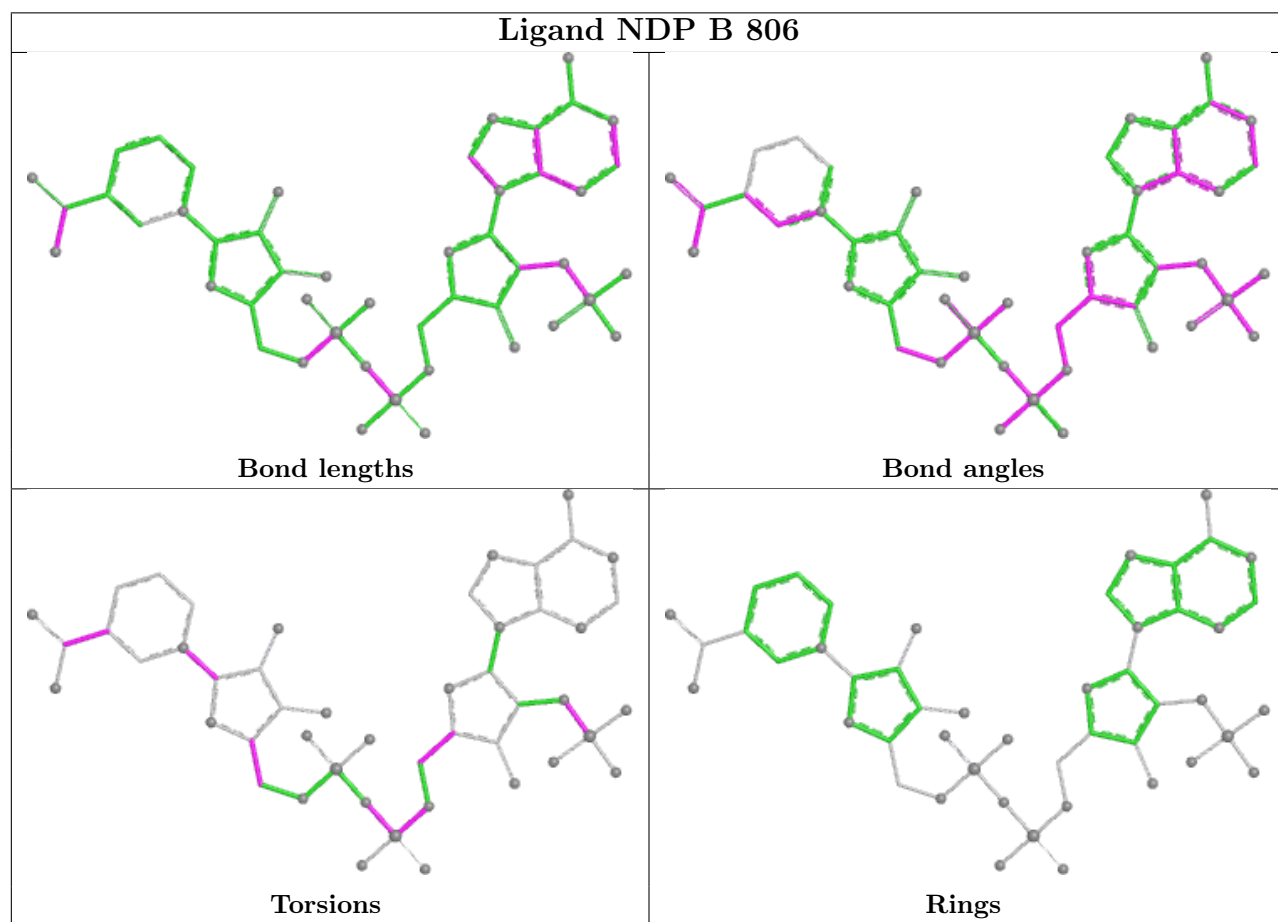
Mol	Chain	Res	Type	Atoms
4	A	804	EPE	S-C10-C9-N1
4	A	813	EPE	C10-C9-N1-C2
4	A	813	EPE	S-C10-C9-N1
9	B	807	F6R	O1-C1-C2-C3
9	B	807	F6R	O1-C1-C2-O2
9	B	807	F6R	C1-C2-C3-C4
9	B	807	F6R	O2-C2-C3-C4
9	B	807	F6R	O2-C2-C3-O3
4	A	813	EPE	N4-C7-C8-O8
3	B	806	NDP	C3B-C4B-C5B-O5B
3	B	806	NDP	C3D-C4D-C5D-O5D
3	A	803	NDP	C3B-C2B-O2B-P2B
3	A	803	NDP	O4B-C4B-C5B-O5B
3	A	803	NDP	C1B-C2B-O2B-P2B
5	B	804	EDO	O1-C1-C2-O2
4	A	804	EPE	C10-C9-N1-C2
4	A	813	EPE	C10-C9-N1-C6
3	A	803	NDP	O4D-C1D-N1N-C6N
3	A	803	NDP	C3B-C4B-C5B-O5B
3	B	806	NDP	PN-O3-PA-O5B
5	A	805	EDO	O1-C1-C2-O2
3	A	803	NDP	C5B-O5B-PA-O1A
3	B	806	NDP	O4D-C1D-N1N-C6N
3	B	806	NDP	C2D-C1D-N1N-C6N
5	A	807	EDO	O1-C1-C2-O2
5	B	805	EDO	O1-C1-C2-O2
9	B	807	F6R	C1-C2-C3-O3
3	B	806	NDP	C2B-O2B-P2B-O3X
5	A	806	EDO	O1-C1-C2-O2

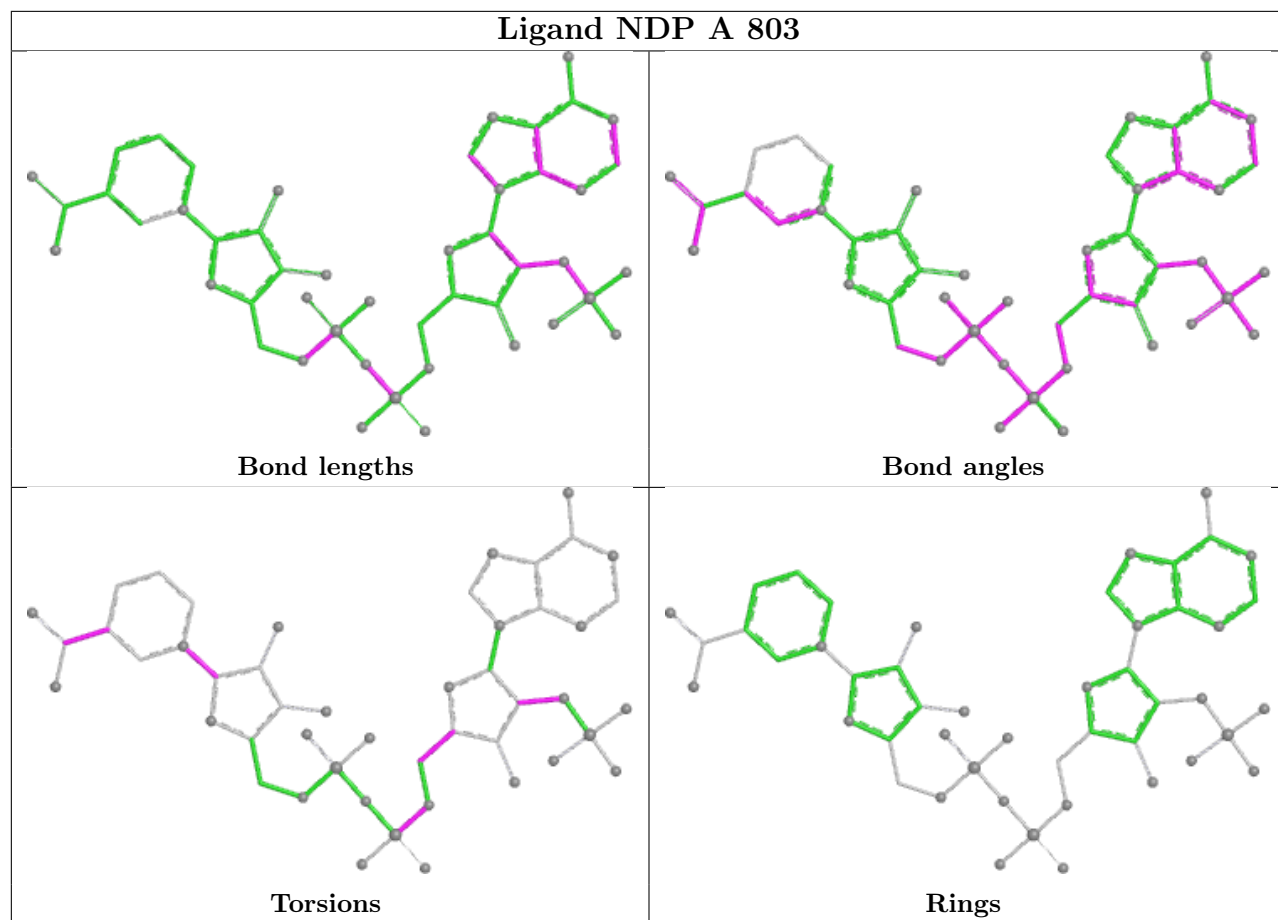
There are no ring outliers.

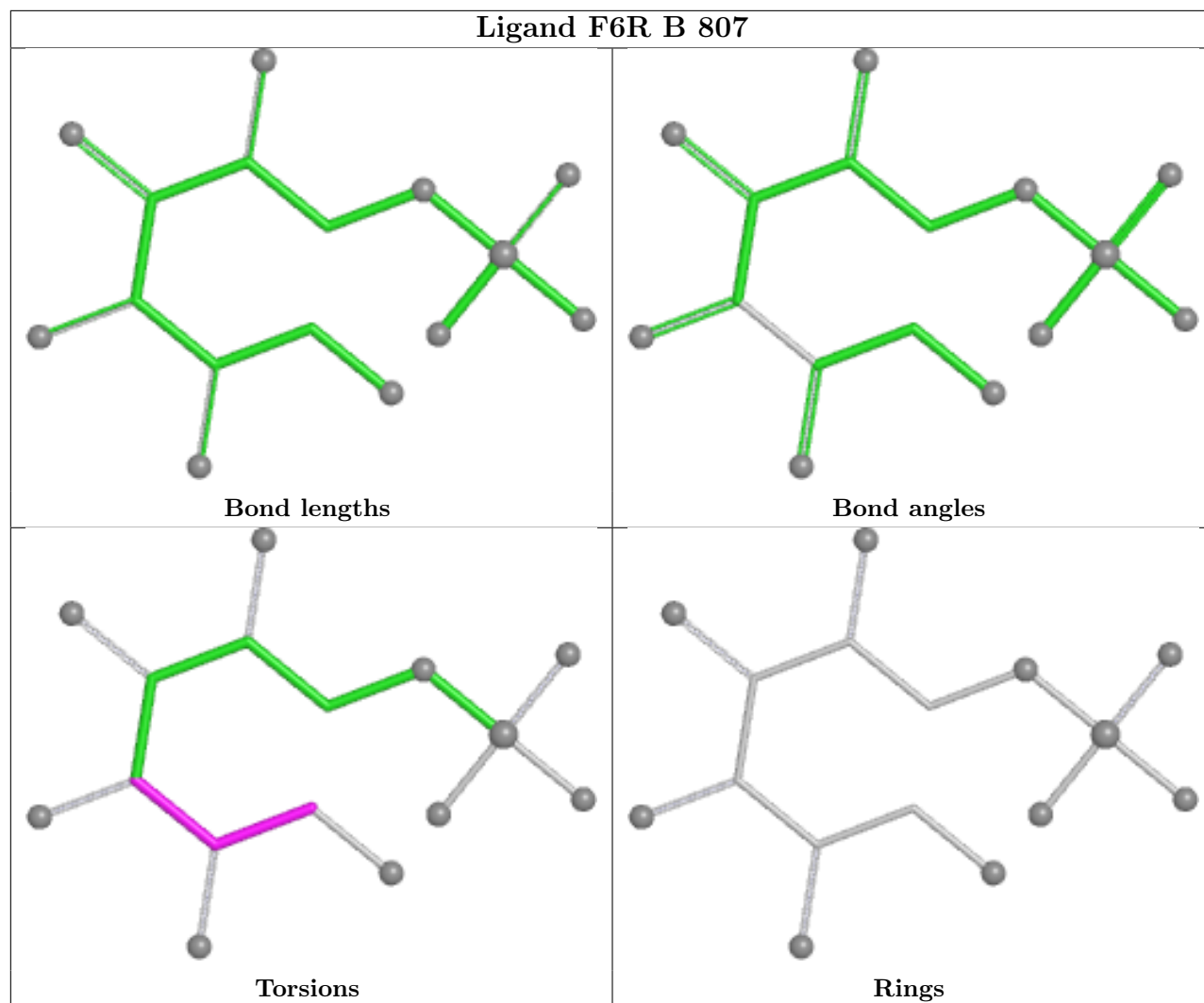
No monomer is involved in short contacts.

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.







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	687/727 (94%)	0.20	13 (1%) 66 61	47, 80, 134, 157	0
1	B	675/727 (92%)	0.30	7 (1%) 79 76	55, 88, 142, 177	0
All	All	1362/1454 (93%)	0.25	20 (1%) 72 68	47, 84, 138, 177	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	453	GLU	3.6
1	A	691	TYR	3.5
1	A	689	ILE	3.2
1	B	27	LEU	3.1
1	A	362	THR	3.1
1	B	67	LEU	2.7
1	B	29	PHE	2.4
1	A	452	ILE	2.4
1	A	567	ILE	2.4
1	A	360	LEU	2.3
1	B	655	ILE	2.3
1	A	2	VAL	2.3
1	A	646	TYR	2.3
1	A	380	TYR	2.2
1	B	2	VAL	2.2
1	B	441	LEU	2.1
1	A	601	LYS	2.1
1	A	363	CYS	2.1
1	A	482	ILE	2.1
1	A	688	LEU	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](#)

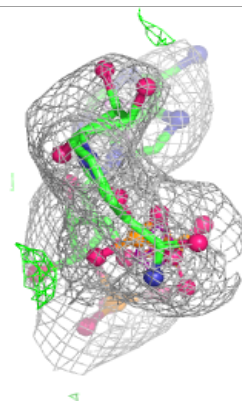
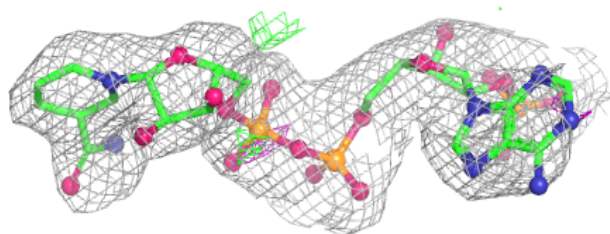
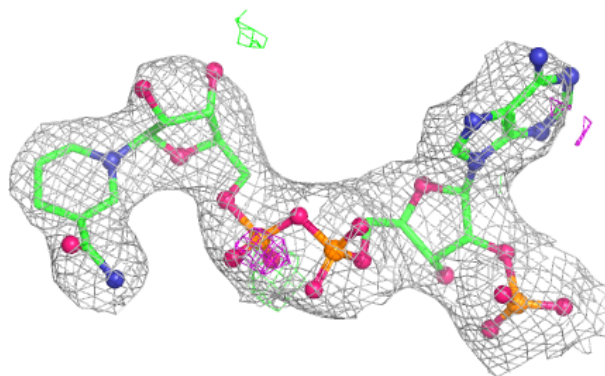
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	B	805	4/4	0.70	0.17	97,99,99,100	0
2	SO4	A	801	5/5	0.75	0.13	108,108,108,108	0
4	EPE	A	804	15/15	0.76	0.25	73,74,76,77	0
5	EDO	A	807	4/4	0.81	0.19	74,75,75,76	0
4	EPE	A	813	15/15	0.81	0.20	99,102,106,106	0
2	SO4	A	802	5/5	0.82	0.07	115,115,115,115	0
8	K	A	815	1/1	0.82	0.13	90,90,90,90	0
5	EDO	B	804	4/4	0.83	0.22	117,118,118,119	0
5	EDO	A	805	4/4	0.88	0.13	77,78,78,79	0
5	EDO	A	806	4/4	0.88	0.10	84,84,84,85	0
5	EDO	A	808	4/4	0.89	0.13	79,80,82,82	0
6	CL	B	803	1/1	0.89	0.09	85,85,85,85	0
3	NDP	A	803	48/48	0.89	0.10	91,96,103,107	0
6	CL	A	812	1/1	0.91	0.09	67,67,67,67	0
7	MG	A	814	1/1	0.93	0.18	60,60,60,60	0
7	MG	B	808	1/1	0.93	0.16	88,88,88,88	0
3	NDP	B	806	48/48	0.93	0.08	62,70,84,86	0
9	F6R	B	807	16/16	0.93	0.09	70,70,71,72	0
6	CL	A	809	1/1	0.94	0.14	75,75,75,75	0
6	CL	B	801	1/1	0.96	0.06	64,64,64,64	0
6	CL	B	802	1/1	0.97	0.11	50,50,50,50	0
6	CL	A	811	1/1	0.98	0.11	75,75,75,75	0
6	CL	A	810	1/1	0.99	0.04	57,57,57,57	0

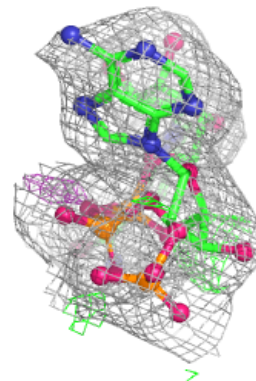
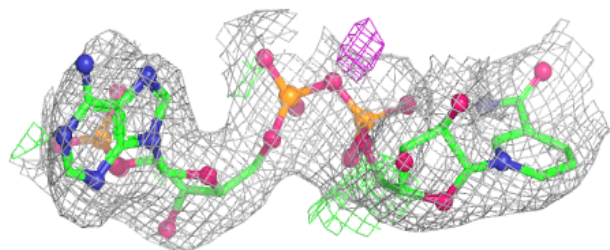
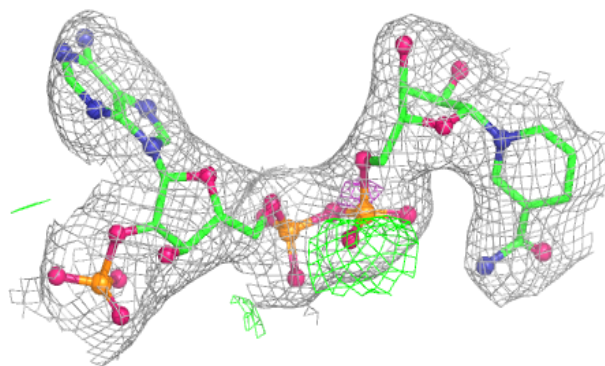
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

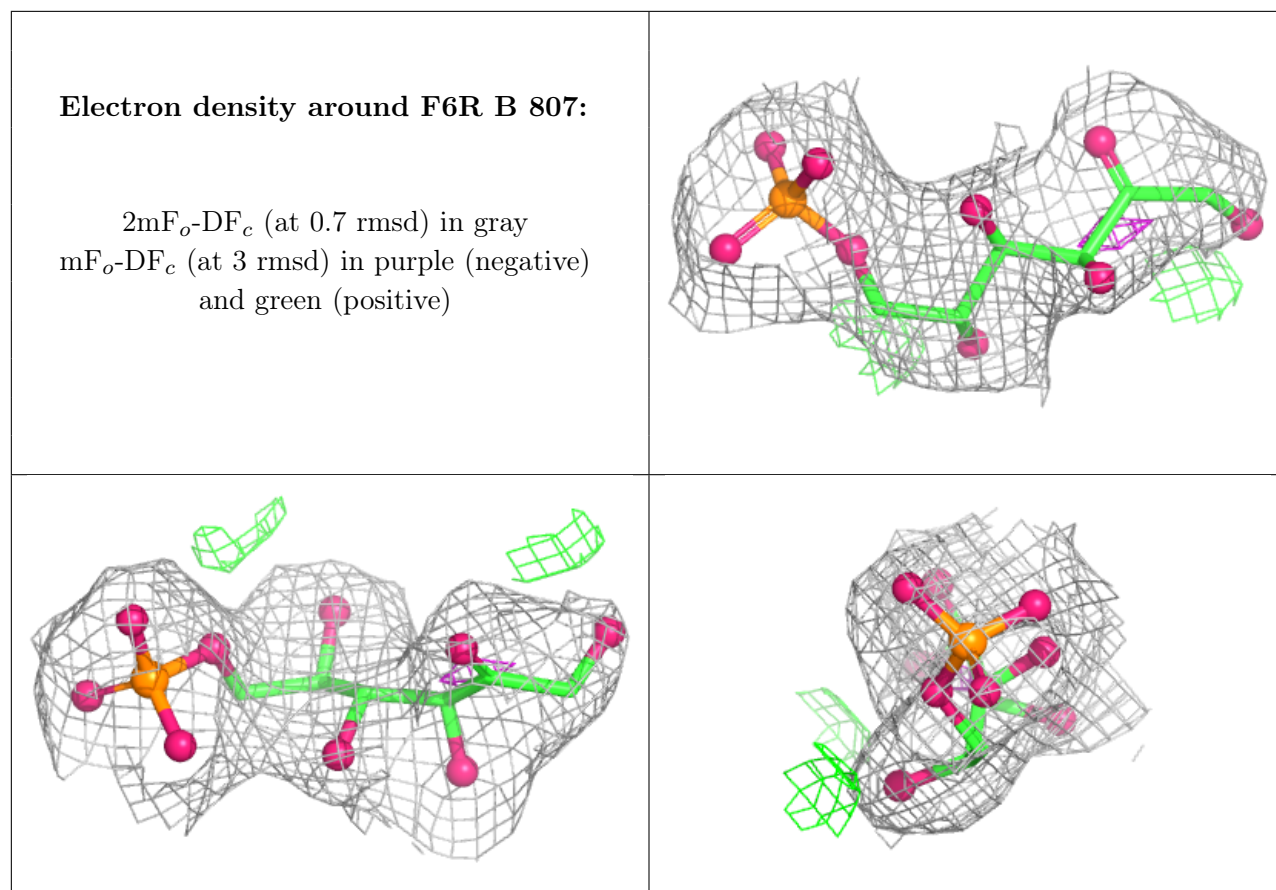
Electron density around NDP A 803:

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

**Electron density around NDP B 806:**

$2mF_o-DF_c$ (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.