Full wwPDB X-ray Structure Validation Report (i)

Oct 25, 2022 – 10:56 pm BST

PDB ID	:	7QP8
Title	:	Crystal structure of Vibrio alkaline phosphatase with bound HEPES
Authors	:	Markusson, S.; Hjorleifsson, J.G.; Kursula, P.; Asgeirsson, B.
Deposited on	:	2022-01-03
Resolution	:	1.70 Å(reported)

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

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

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

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

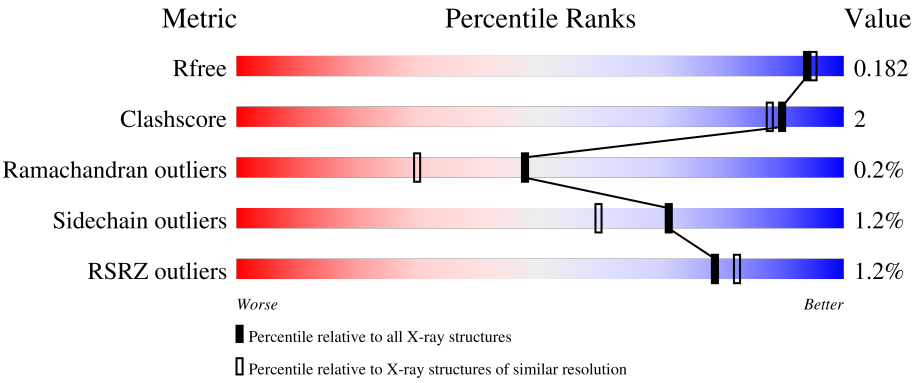
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

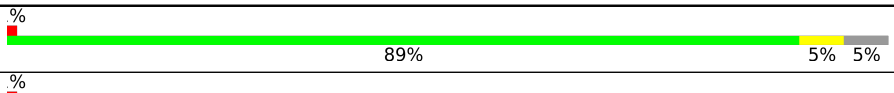
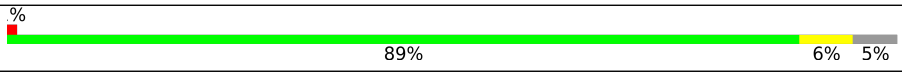
The reported resolution of this entry is 1.70 Å.

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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	531	
1	B	531	

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
6	EPE	A	611	-	X	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 16801 atoms, of which 7890 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 Alkaline phosphatase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	503	Total	C	H	N	O	S	0	14	0
			7854	2493	3880	680	788	13			
1	B	502	Total	C	H	N	O	S	0	16	0
			7883	2501	3897	683	789	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	503	SER	-	expression tag	UNP Q93P54
A	504	ALA	-	expression tag	UNP Q93P54
A	505	TRP	-	expression tag	UNP Q93P54
A	506	SER	-	expression tag	UNP Q93P54
A	507	HIS	-	expression tag	UNP Q93P54
A	508	PRO	-	expression tag	UNP Q93P54
A	509	GLN	-	expression tag	UNP Q93P54
A	510	PHE	-	expression tag	UNP Q93P54
A	511	GLU	-	expression tag	UNP Q93P54
A	512	LYS	-	expression tag	UNP Q93P54
B	503	SER	-	expression tag	UNP Q93P54
B	504	ALA	-	expression tag	UNP Q93P54
B	505	TRP	-	expression tag	UNP Q93P54
B	506	SER	-	expression tag	UNP Q93P54
B	507	HIS	-	expression tag	UNP Q93P54
B	508	PRO	-	expression tag	UNP Q93P54
B	509	GLN	-	expression tag	UNP Q93P54
B	510	PHE	-	expression tag	UNP Q93P54
B	511	GLU	-	expression tag	UNP Q93P54
B	512	LYS	-	expression tag	UNP Q93P54

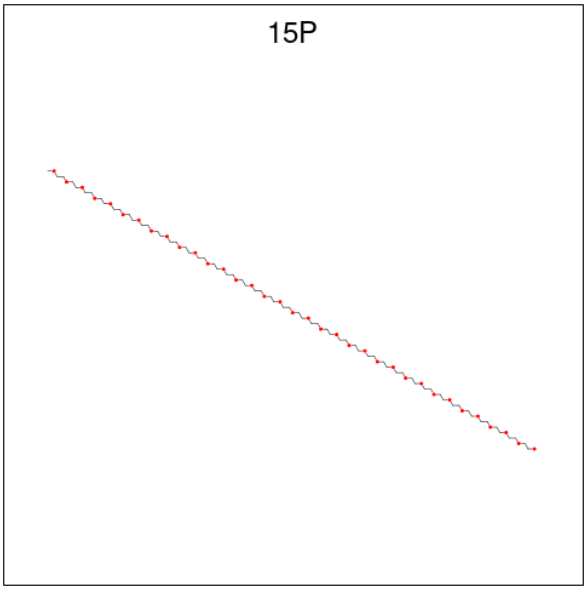
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Mg 3 3	0	0
3	B	3	Total Mg 3 3	0	0

- Molecule 4 is POLYETHYLENE GLYCOL (N=34) (three-letter code: 15P) (formula: $C_{69}H_{140}O_{35}$).

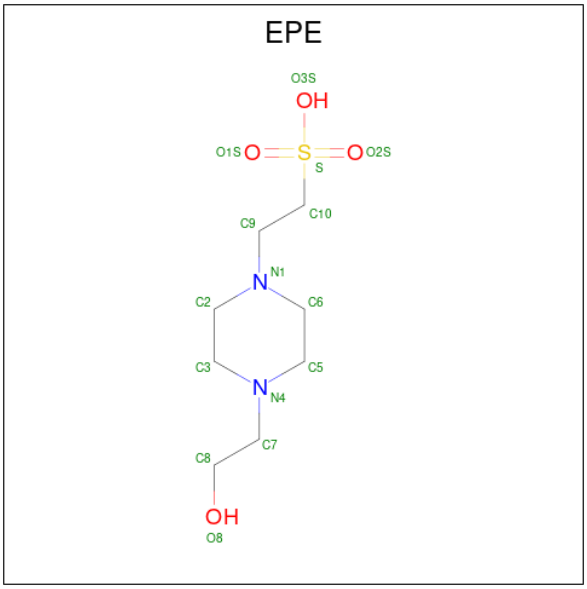


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 50 14 28 8	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

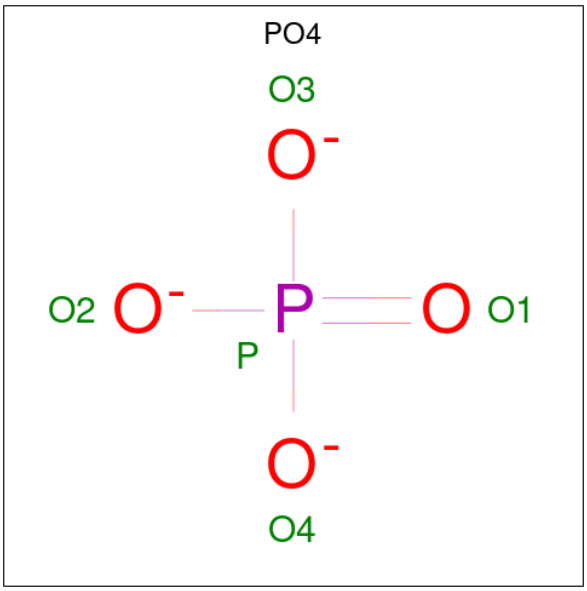
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Cl 2 2	0	0
5	B	1	Total Cl 1 1	0	0

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
6	A	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
6	A	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
6	B	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
6	B	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

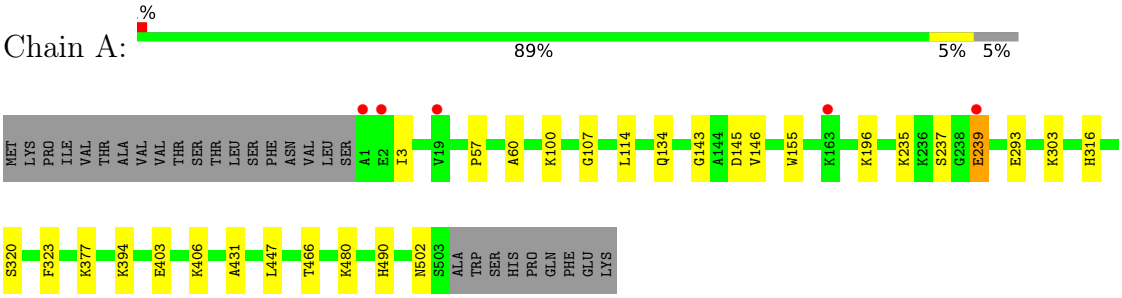
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	421	Total O 421 421	0	0
8	B	410	Total O 410 410	0	0

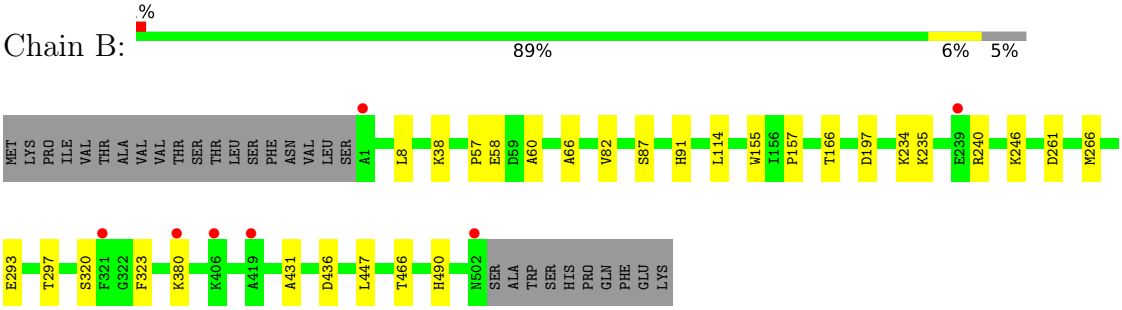
3 Residue-property plots (i)

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

• Molecule 1: Alkaline phosphatase



• Molecule 1: Alkaline phosphatase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.81Å 85.05Å 85.50Å 90.00° 113.90° 90.00°	Depositor
Resolution (Å)	44.10 – 1.70 44.10 – 1.70	Depositor EDS
% Data completeness (in resolution range)	79.7 (44.10-1.70) 74.7 (44.10-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.64 (at 1.70Å)	Xtriage
Refinement program	PHENIX dev_3958	Depositor
R, R_{free}	0.150 , 0.181 0.150 , 0.182	Depositor DCC
R_{free} test set	2015 reflections (2.29%)	wwPDB-VP
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.588	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	0.014 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	16801	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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: ZN, PO4, 15P, EPE, MG, CL

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	0.29	0/4098	0.48	0/5537
1	B	0.29	0/4108	0.48	0/5551
All	All	0.29	0/8206	0.48	0/11088

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	502	ASN	Mainchain

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	3974	3880	3823	14	0
1	B	3986	3897	3853	16	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	22	28	29	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
6	A	45	51	51	0	0
6	B	30	34	34	0	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
8	A	421	0	0	4	0
8	B	410	0	0	4	0
All	All	8911	7890	7790	28	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 2.

All (28) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:GLN:OE1	8:A:701:HOH:O	1.97	0.81
1:A:145:ASP:OD2	8:A:702:HOH:O	2.09	0.69
1:A:303:LYS:NZ	8:A:703:HOH:O	2.23	0.68
1:B:261:ASP:OD2	8:B:701:HOH:O	2.10	0.68
1:B:197[B]:ASP:OD2	8:B:702:HOH:O	2.14	0.65
1:A:100[A]:LYS:NZ	1:A:143:GLY:O	2.30	0.52
1:A:323:PHE:O	1:B:466:THR:HA	2.10	0.52
1:A:403:GLU:OE2	1:A:406:LYS:NZ	2.40	0.52
1:B:157:PRO:HG2	1:B:166:THR:HG21	1.93	0.50
1:B:436:ASP:OD2	8:B:703:HOH:O	2.19	0.50
1:B:114:LEU:HD23	1:B:155:TRP:CZ2	2.47	0.50
1:B:431:ALA:O	1:B:447:LEU:HD21	2.14	0.48
1:A:466:THR:HA	1:B:323:PHE:O	2.13	0.47
1:A:114:LEU:HD23	1:A:155:TRP:CZ2	2.49	0.47
1:B:235:LYS:NZ	1:B:293:GLU:OE2	2.48	0.47
1:B:66:ALA:HB1	1:B:82:VAL:O	2.15	0.46
1:B:8:LEU:O	1:B:266:MET:HA	2.16	0.46
1:B:58:GLU:OE1	1:B:87:SER:OG	2.21	0.45
1:B:234:LYS:HB3	1:B:240:ARG:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:LYS:NZ	8:A:722:HOH:O	2.51	0.44
1:A:235:LYS:NZ	1:A:293:GLU:OE2	2.50	0.44
1:A:107:GLY:HA2	1:A:146:VAL:O	2.19	0.43
1:A:431:ALA:O	1:A:447:LEU:HD21	2.20	0.42
1:B:246:LYS:HG3	1:B:297:THR:OG1	2.20	0.41
1:B:38:LYS:HE3	8:B:721:HOH:O	2.20	0.41
1:A:57:PRO:HG2	1:A:60:ALA:HB3	2.02	0.41
1:B:57:PRO:HG2	1:B:60:ALA:HB3	2.01	0.41
1:A:3:ILE:HD11	1:A:480:LYS:HD2	2.02	0.41

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	515/531 (97%)	503 (98%)	10 (2%)	2 (0%)	34 18
1	B	516/531 (97%)	505 (98%)	11 (2%)	0	100 100
All	All	1031/1062 (97%)	1008 (98%)	21 (2%)	2 (0%)	47 30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	GLU
1	A	316	HIS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/443 (97%)	424 (99%)	6 (1%)	67	53
1	B	431/443 (97%)	427 (99%)	4 (1%)	78	70
All	All	861/886 (97%)	851 (99%)	10 (1%)	71	59

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	LYS
1	A	237	SER
1	A	239	GLU
1	A	320	SER
1	A	394	LYS
1	A	490	HIS
1	B	91	HIS
1	B	320	SER
1	B	380	LYS
1	B	490	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 21 ligands modelled in this entry, 13 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
6	EPE	A	611	-	15,15,15	3.79	7 (46%)	18,20,20	3.10	10 (55%)
7	PO4	B	609	2	4,4,4	0.87	0	6,6,6	0.46	0
6	EPE	A	610	-	15,15,15	3.80	7 (46%)	18,20,20	3.07	9 (50%)
6	EPE	B	608	-	15,15,15	3.77	7 (46%)	18,20,20	2.85	8 (44%)
6	EPE	B	607	-	15,15,15	3.73	8 (53%)	18,20,20	2.91	10 (55%)
4	15P	A	604	-	21,21,103	0.51	0	20,20,102	0.41	0
6	EPE	A	609	-	15,15,15	3.65	7 (46%)	18,20,20	2.81	11 (61%)
7	PO4	A	612	2	4,4,4	0.81	0	6,6,6	0.31	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
6	EPE	A	611	-	-	5/9/19/19	0/1/1/1
6	EPE	A	610	-	-	3/9/19/19	0/1/1/1
6	EPE	B	608	-	-	3/9/19/19	0/1/1/1
6	EPE	B	607	-	-	2/9/19/19	0/1/1/1
4	15P	A	604	-	-	9/19/19/101	-
6	EPE	A	609	-	-	2/9/19/19	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	611	EPE	C2-N1	-6.31	1.29	1.46
6	B	607	EPE	C5-N4	-6.26	1.29	1.46
6	B	608	EPE	C2-N1	-6.24	1.29	1.46
6	A	609	EPE	C5-N4	-6.20	1.29	1.46
6	A	611	EPE	C5-N4	-6.18	1.29	1.46
6	B	607	EPE	C2-N1	-6.18	1.29	1.46
6	A	610	EPE	C2-N1	-6.18	1.29	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	609	EPE	C2-N1	-6.15	1.30	1.46
6	A	610	EPE	C5-N4	-6.10	1.30	1.46
6	B	608	EPE	C5-N4	-6.02	1.30	1.46
6	A	611	EPE	C3-N4	-5.88	1.30	1.46
6	A	610	EPE	C3-N4	-5.81	1.30	1.46
6	A	610	EPE	C6-N1	-5.71	1.31	1.46
6	B	608	EPE	C6-N1	-5.66	1.31	1.46
6	B	607	EPE	C6-N1	-5.65	1.31	1.46
6	A	609	EPE	C3-N4	-5.62	1.31	1.46
6	B	608	EPE	C3-N4	-5.60	1.31	1.46
6	B	607	EPE	C3-N4	-5.59	1.31	1.46
6	A	611	EPE	C6-N1	-5.51	1.31	1.46
6	B	608	EPE	C7-N4	-5.45	1.34	1.47
6	A	609	EPE	C6-N1	-5.45	1.31	1.46
6	A	610	EPE	C7-N4	-5.44	1.34	1.47
6	B	608	EPE	C9-N1	-5.44	1.34	1.47
6	A	610	EPE	C9-N1	-5.42	1.35	1.47
6	A	611	EPE	C9-N1	-5.36	1.35	1.47
6	A	611	EPE	C7-N4	-5.26	1.35	1.47
6	B	607	EPE	C9-N1	-5.14	1.35	1.47
6	A	609	EPE	C7-N4	-5.06	1.35	1.47
6	A	609	EPE	C9-N1	-5.03	1.35	1.47
6	B	607	EPE	C7-N4	-4.86	1.36	1.47
6	B	607	EPE	C10-S	3.12	1.81	1.77
6	B	608	EPE	C10-S	3.05	1.81	1.77
6	A	610	EPE	C10-S	2.94	1.81	1.77
6	A	611	EPE	C10-S	2.91	1.81	1.77
6	B	607	EPE	C6-C5	2.14	1.59	1.51
6	A	609	EPE	C10-S	2.06	1.80	1.77

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	608	EPE	O1S-S-C10	6.49	114.73	106.92
6	A	611	EPE	O1S-S-C10	6.24	114.43	106.92
6	A	609	EPE	O2S-S-C10	6.15	114.33	106.92
6	A	610	EPE	O2S-S-C10	6.03	114.18	106.92
6	B	607	EPE	O1S-S-C10	5.99	114.13	106.92
6	B	607	EPE	O2S-S-C10	5.89	114.00	106.92
6	A	611	EPE	O2S-S-C10	5.85	113.95	106.92
6	A	610	EPE	O1S-S-C10	5.76	113.85	106.92
6	B	608	EPE	O2S-S-C10	5.52	113.56	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	607	EPE	O3S-S-C10	5.17	114.14	105.77
6	B	608	EPE	O3S-S-C10	5.14	114.09	105.77
6	A	611	EPE	O3S-S-C10	5.14	114.08	105.77
6	A	609	EPE	O1S-S-C10	5.04	112.99	106.92
6	A	610	EPE	O3S-S-C10	4.80	113.53	105.77
6	A	609	EPE	O3S-S-C10	4.65	113.30	105.77
6	A	610	EPE	C3-C2-N1	4.41	119.69	110.64
6	A	610	EPE	C6-N1-C2	4.33	118.56	108.83
6	A	611	EPE	C6-N1-C2	4.15	118.18	108.83
6	A	611	EPE	C3-C2-N1	3.56	117.94	110.64
6	B	608	EPE	C3-C2-N1	3.13	117.06	110.64
6	B	607	EPE	O3S-S-O1S	-3.03	103.87	111.27
6	A	609	EPE	C3-C2-N1	2.87	116.52	110.64
6	B	607	EPE	O3S-S-O2S	-2.84	104.32	111.27
6	B	608	EPE	O3S-S-O2S	-2.84	104.34	111.27
6	A	611	EPE	O3S-S-O1S	-2.83	104.36	111.27
6	B	608	EPE	O3S-S-O1S	-2.80	104.44	111.27
6	A	611	EPE	O3S-S-O2S	-2.79	104.46	111.27
6	A	609	EPE	C6-N1-C2	2.78	115.08	108.83
6	A	610	EPE	O3S-S-O1S	-2.77	104.50	111.27
6	A	611	EPE	O2S-S-O1S	-2.76	104.40	113.95
6	A	609	EPE	O3S-S-O2S	-2.76	104.54	111.27
6	B	608	EPE	C7-N4-C5	2.73	118.21	111.23
6	B	608	EPE	O2S-S-O1S	-2.72	104.55	113.95
6	B	607	EPE	C3-C2-N1	2.69	116.16	110.64
6	A	611	EPE	C7-N4-C5	2.64	118.00	111.23
6	A	610	EPE	O3S-S-O2S	-2.64	104.82	111.27
6	A	610	EPE	O2S-S-O1S	-2.60	104.94	113.95
6	A	609	EPE	O3S-S-O1S	-2.55	105.04	111.27
6	A	609	EPE	C7-N4-C5	2.53	117.69	111.23
6	B	607	EPE	O2S-S-O1S	-2.51	105.26	113.95
6	B	607	EPE	C7-N4-C5	2.43	117.44	111.23
6	A	611	EPE	C5-C6-N1	2.42	115.60	110.64
6	A	609	EPE	C5-C6-N1	2.41	115.58	110.64
6	A	609	EPE	O2S-S-O1S	-2.36	105.77	113.95
6	B	607	EPE	C5-C6-N1	2.19	115.13	110.64
6	A	610	EPE	C2-C3-N4	2.12	115.00	110.64
6	A	609	EPE	C2-C3-N4	2.05	114.86	110.64
6	B	607	EPE	C6-N1-C2	2.02	113.37	108.83

There are no chirality outliers.

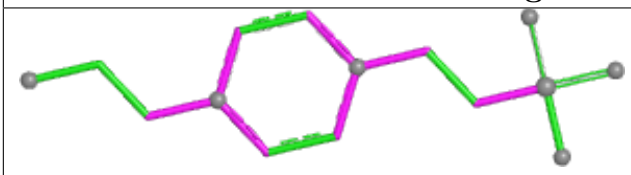
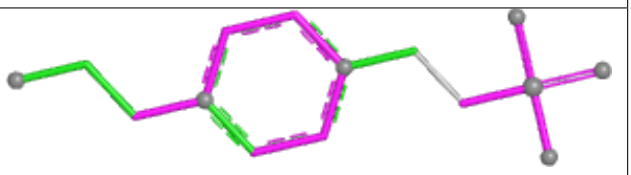
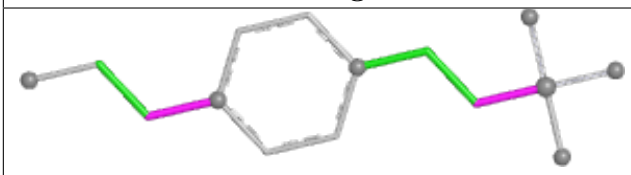
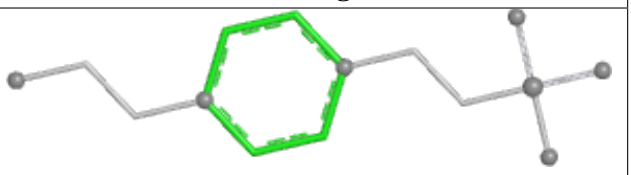
All (24) torsion outliers are listed below:

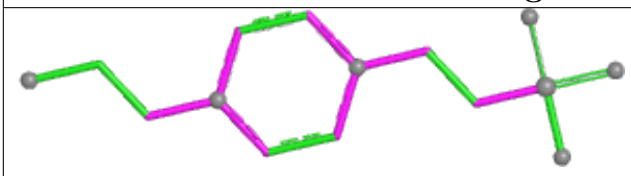
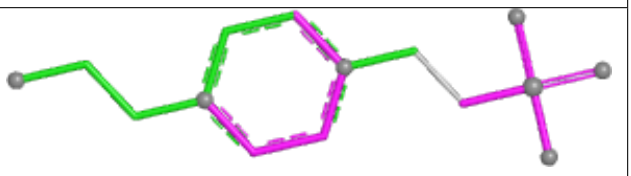
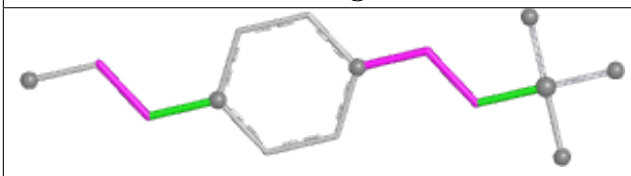
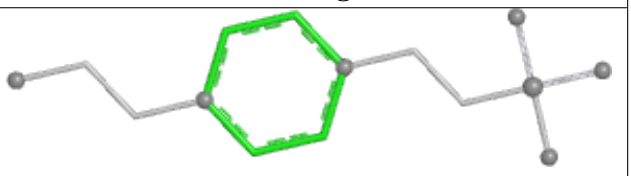
Mol	Chain	Res	Type	Atoms
6	A	609	EPE	C8-C7-N4-C5
6	A	610	EPE	N4-C7-C8-O8
6	A	611	EPE	C8-C7-N4-C5
6	A	611	EPE	C9-C10-S-O1S
6	B	607	EPE	C8-C7-N4-C5
6	B	608	EPE	C8-C7-N4-C5
6	B	608	EPE	S-C10-C9-N1
4	A	604	15P	O1-C3-C4-O2
4	A	604	15P	O2-C5-C6-O3
4	A	604	15P	O5-C10-C9-O4
6	A	611	EPE	C9-C10-S-O3S
4	A	604	15P	C3-C4-O2-C5
6	B	608	EPE	C8-C7-N4-C3
4	A	604	15P	O3-C7-C8-O4
6	A	610	EPE	S-C10-C9-N1
6	A	610	EPE	C10-C9-N1-C6
4	A	604	15P	C5-C6-O3-C7
6	A	611	EPE	C8-C7-N4-C3
4	A	604	15P	C4-C3-O1-C2
6	A	609	EPE	C8-C7-N4-C3
4	A	604	15P	C10-C9-O4-C8
6	A	611	EPE	C9-C10-S-O2S
4	A	604	15P	C8-C7-O3-C6
6	B	607	EPE	C8-C7-N4-C3

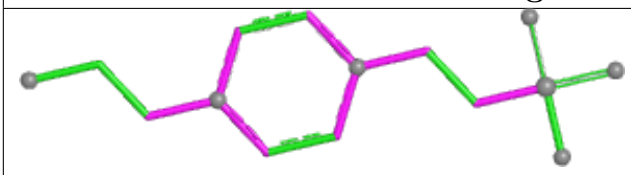
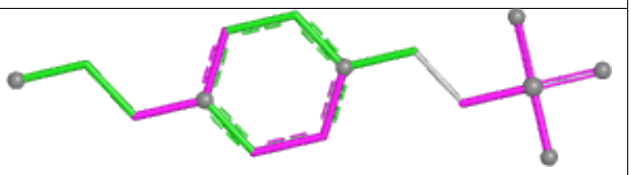
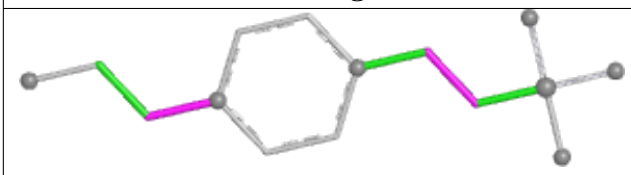
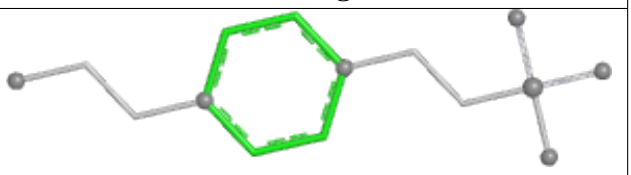
There are no ring outliers.

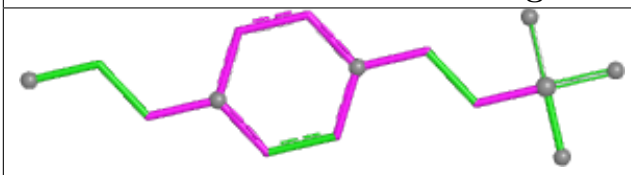
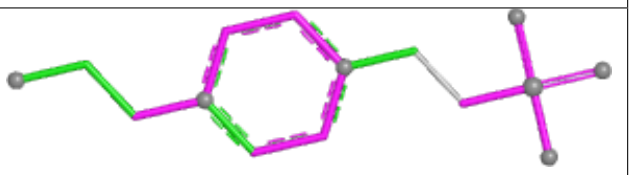
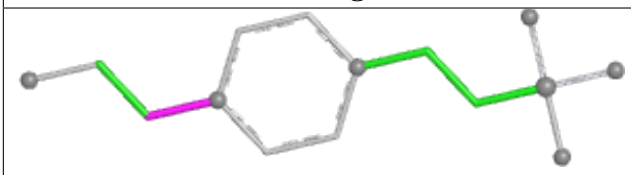
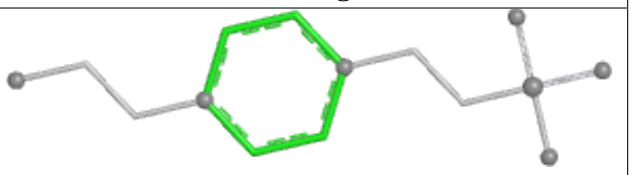
No monomer is involved in short contacts.

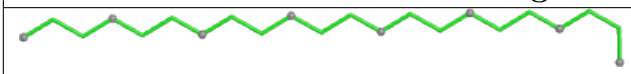
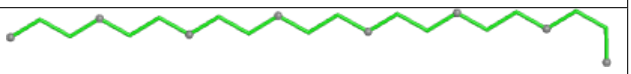
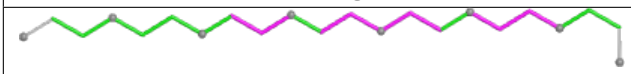
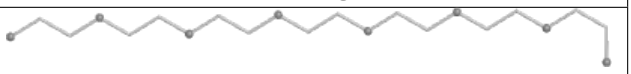
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

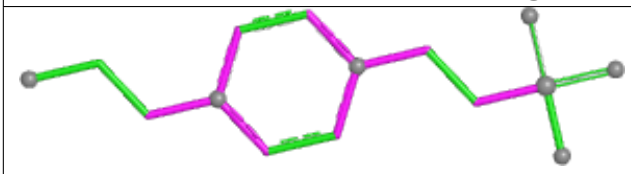
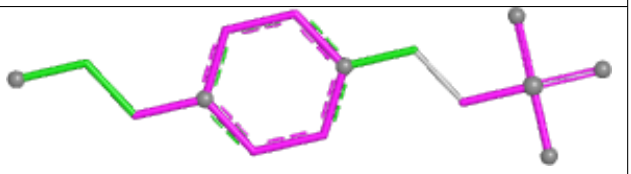
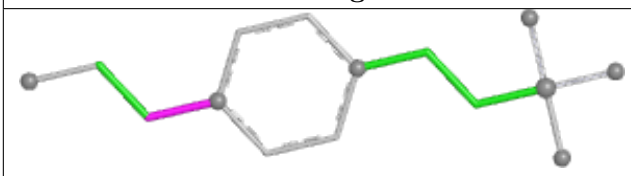
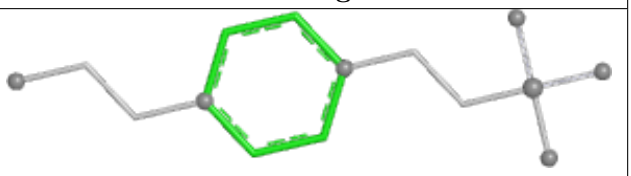
Ligand EPE A 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand EPE A 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand EPE B 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand EPE B 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 15P A 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand EPE A 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	503/531 (94%)	-0.12	5 (0%)	82 85	22, 30, 45, 58	0
1	B	502/531 (94%)	-0.15	7 (1%)	75 79	23, 31, 44, 61	0
All	All	1005/1062 (94%)	-0.13	12 (1%)	79 82	22, 30, 45, 61	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	239	GLU	4.5
1	A	1	ALA	4.3
1	A	239	GLU	3.4
1	B	502	ASN	2.8
1	B	1	ALA	2.8
1	B	406	LYS	2.5
1	A	163	LYS	2.2
1	B	321	PHE	2.2
1	A	19	VAL	2.2
1	A	2	GLU	2.1
1	B	380	LYS	2.1
1	B	419	ALA	2.0

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 (i)

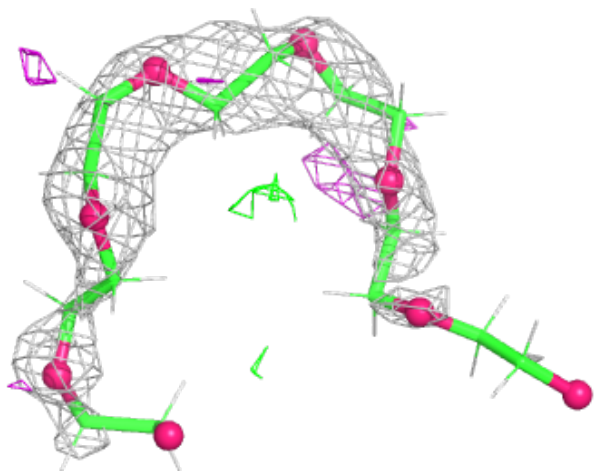
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

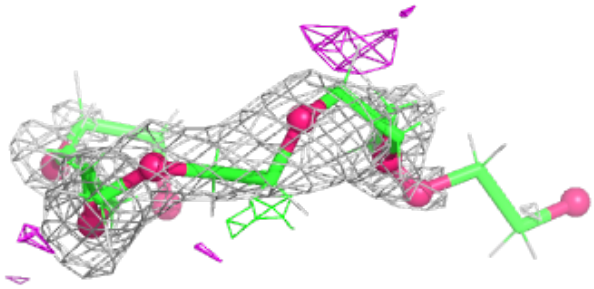
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	15P	A	604	22/104	0.69	0.33	83,100,113,114	0
6	EPE	A	611	15/15	0.71	0.25	80,96,104,106	0
3	MG	A	606	1/1	0.88	0.09	69,69,69,69	0
6	EPE	B	608	15/15	0.92	0.13	58,72,77,77	0
6	EPE	A	610	15/15	0.94	0.12	60,73,75,75	0
6	EPE	B	607	15/15	0.95	0.10	39,49,53,53	0
6	EPE	A	609	15/15	0.95	0.09	34,43,47,48	0
3	MG	A	605	1/1	0.97	0.07	31,31,31,31	0
3	MG	B	605	1/1	0.97	0.07	30,30,30,30	0
5	CL	A	608	1/1	0.98	0.08	59,59,59,59	0
7	PO4	B	609	5/5	0.98	0.13	28,28,29,29	0
3	MG	B	604	1/1	0.99	0.05	32,32,32,32	0
5	CL	A	607	1/1	0.99	0.03	32,32,32,32	0
7	PO4	A	612	5/5	0.99	0.09	24,25,25,25	0
3	MG	A	603	1/1	0.99	0.09	22,22,22,22	0
2	ZN	A	601	1/1	1.00	0.10	24,24,24,24	0
2	ZN	A	602	1/1	1.00	0.09	25,25,25,25	0
2	ZN	B	601	1/1	1.00	0.10	28,28,28,28	0
3	MG	B	603	1/1	1.00	0.06	24,24,24,24	0
5	CL	B	606	1/1	1.00	0.04	34,34,34,34	0
2	ZN	B	602	1/1	1.00	0.10	26,26,26,26	0

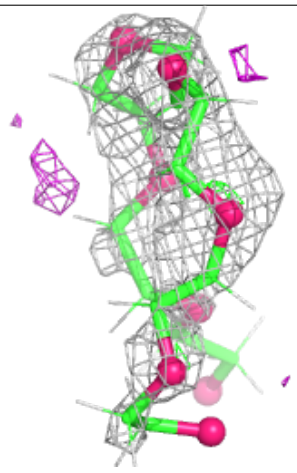
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 15P A 604:

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

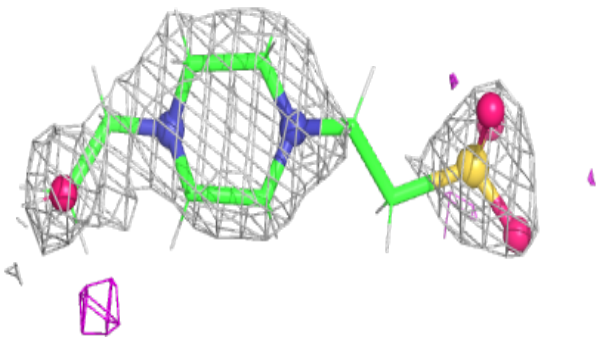


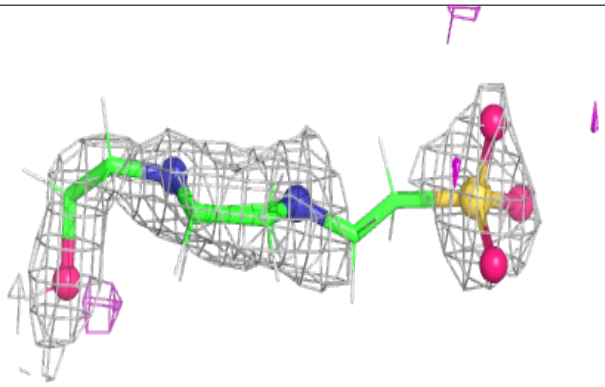


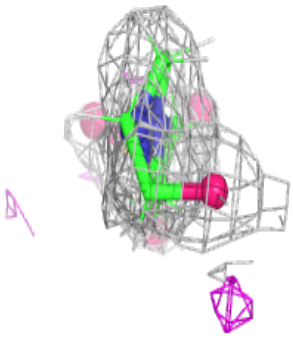


Electron density around EPE A 611:

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

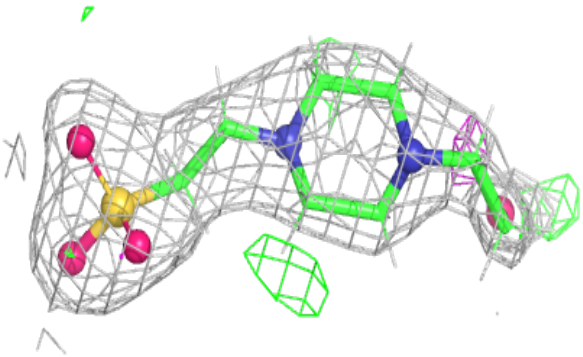


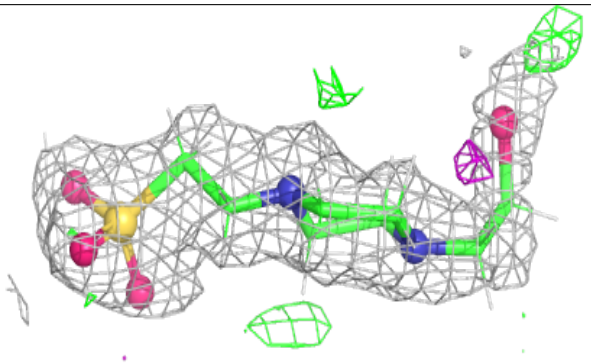


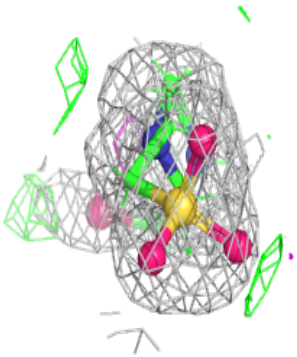


Electron density around EPE B 608:

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

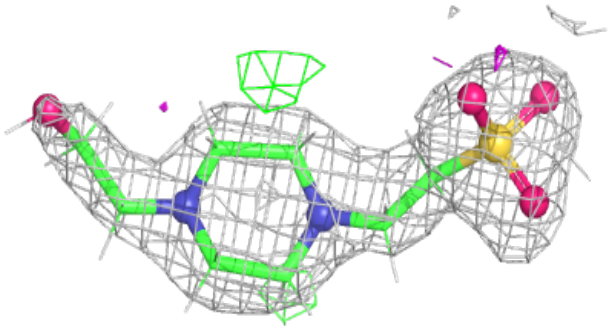


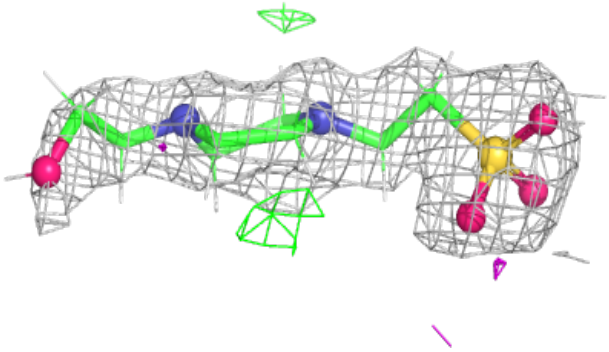


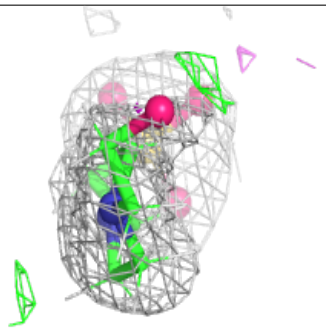


Electron density around EPE A 610:

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

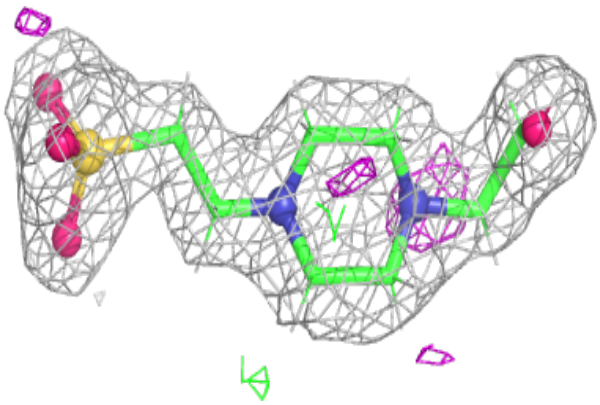


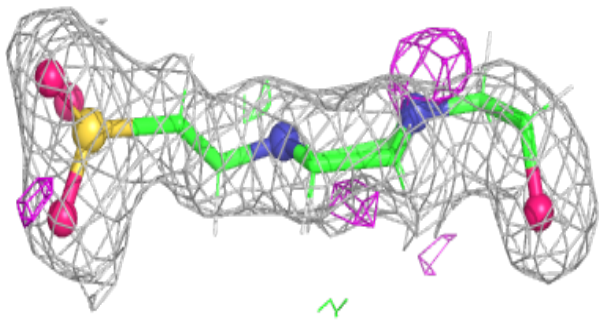


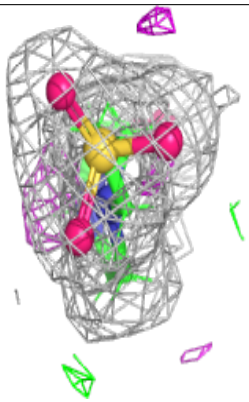


Electron density around EPE B 607:

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

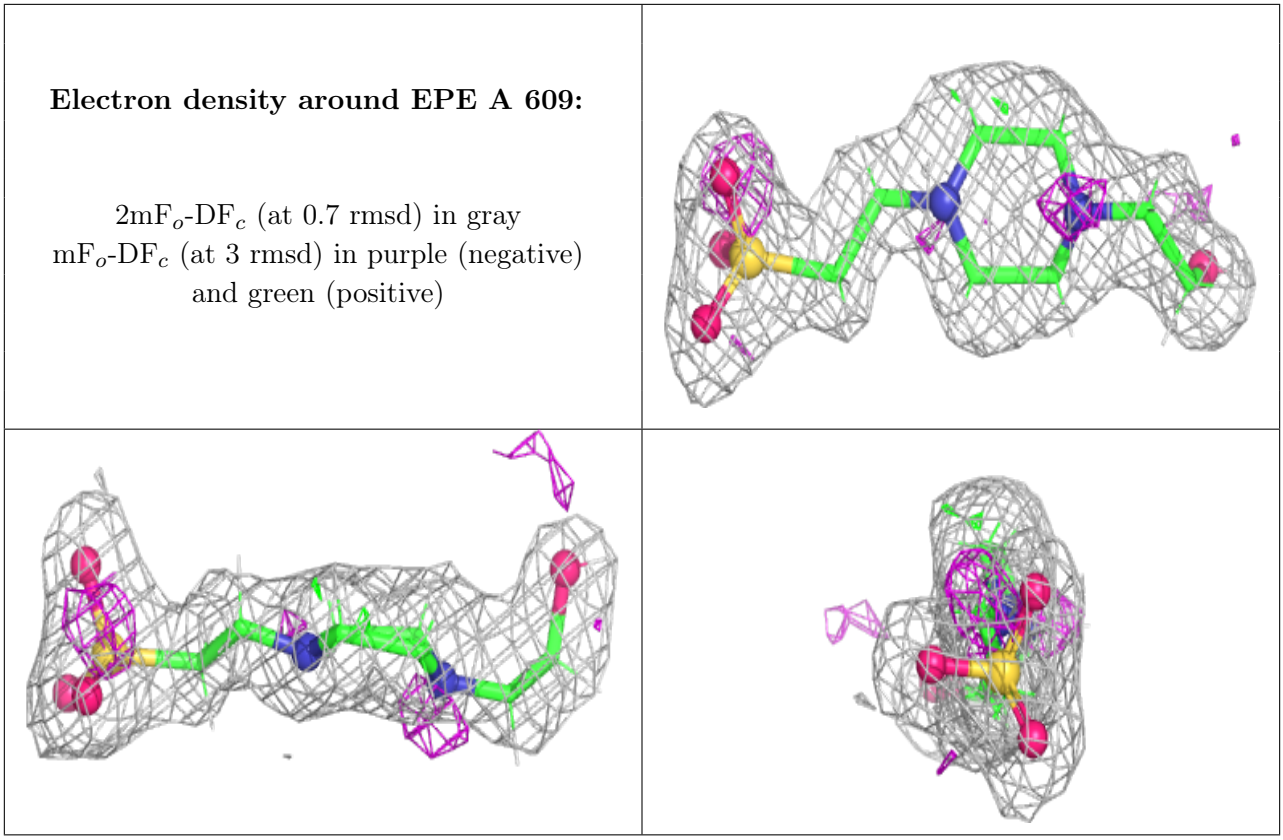






Electron density around EPE A 609:

$2mF_o$-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.