Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 10:08 PM JST

PDB ID	:	6AFS
Title	:	Proton pyrophosphatase - two phosphates-bound
Authors	:	Tsai, J.-Y.; Li, K.-M.; Sun, Y.-J.
Deposited on	:	2018-08-08
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 (i) symbol.

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

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

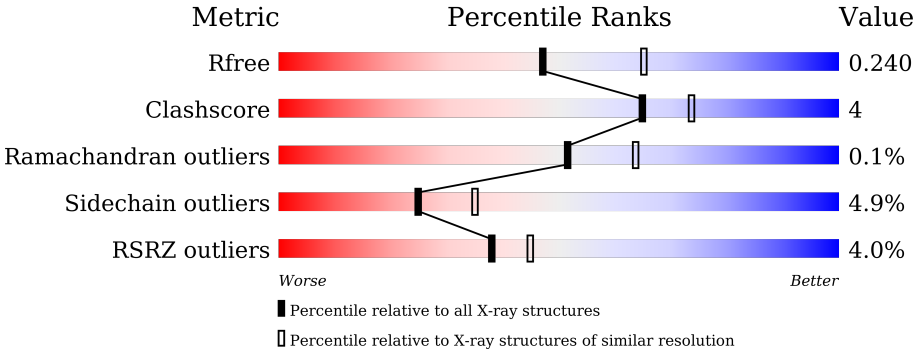
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	766	2% 86% 10% • •
1	B	766	5% 85% 10% • •

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
2	PO4	B	1001	-	-	X	-
2	PO4	B	1002	-	-	X	-
5	1PG	A	1012	-	-	-	X

2 Entry composition (i)

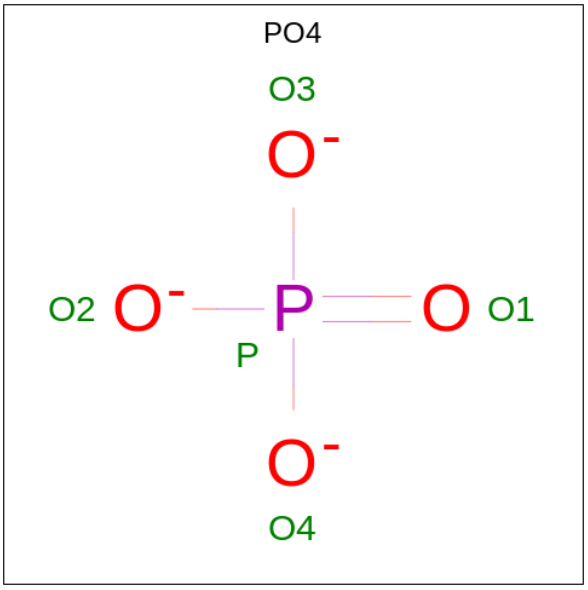
There are 6 unique types of molecules in this entry. The entry contains 11406 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pyrophosphate-energized vacuolar membrane proton pump.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	740	5431	3540	862	1000	29	0	0	0
1	B	739	5424	3535	861	999	29	0	0	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

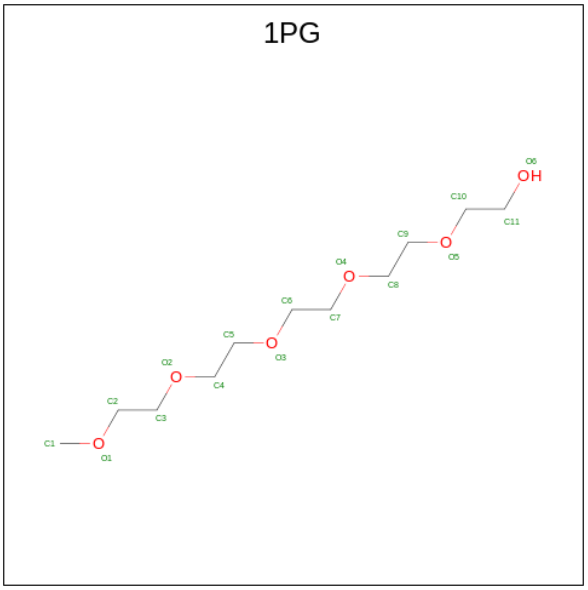
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total Mg 5 5	0	0
3	B	5	Total Mg 5 5	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 5 is 2-(2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHANOL (three-letter code: 1PG) (formula: $C_{11}H_{24}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 17 11 6	0	0
5	A	1	Total C O 17 11 6	0	0
5	A	1	Total C O 17 11 6	0	0
5	A	1	Total C O 17 11 6	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	17	11	6	0	0
			Total	C	O		
5	B	1	17	11	6	0	0
			Total	C	O		
5	B	1	17	11	6	0	0

- Molecule 6 is water.

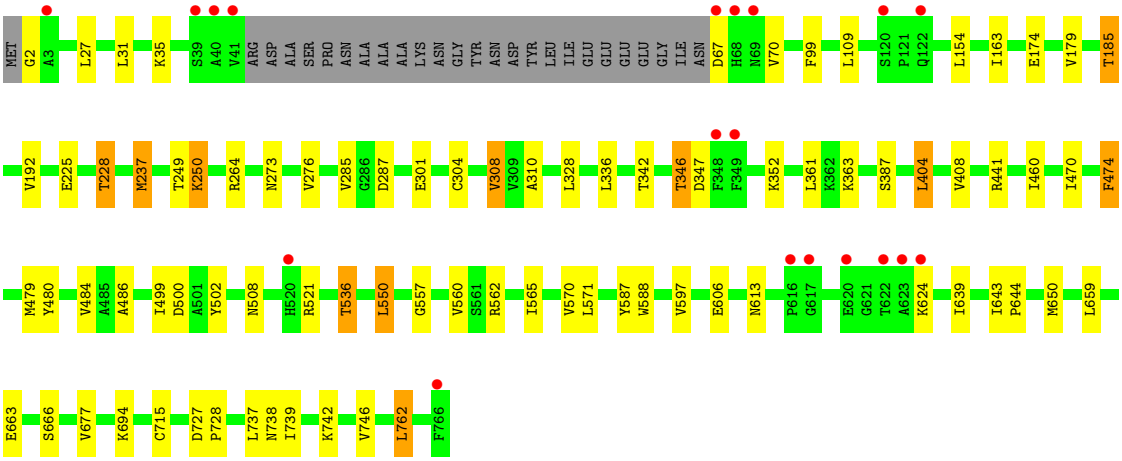
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	223	223	223	0	0
			Total	O		
6	B	177	177	177	0	0

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.

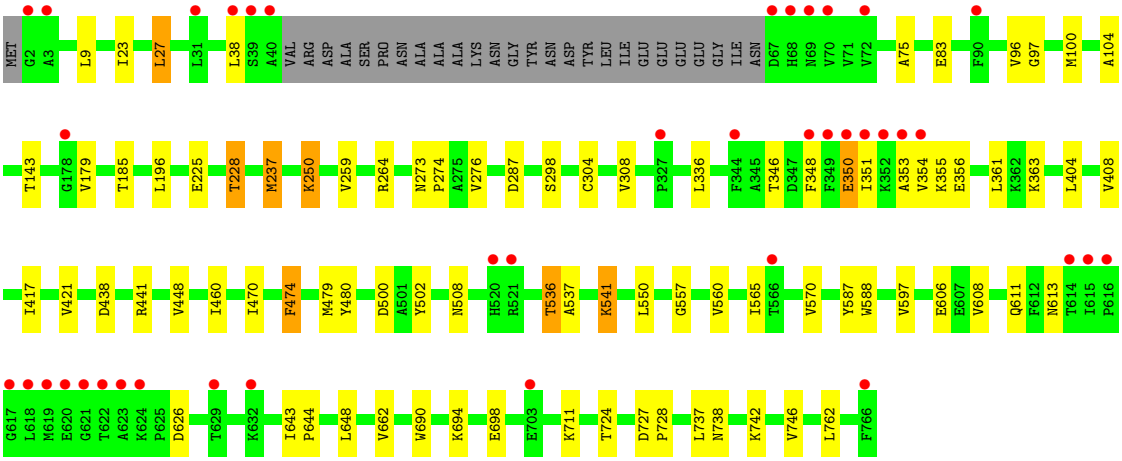
• Molecule 1: Pyrophosphate-energized vacuolar membrane proton pump

Chain A:



• Molecule 1: Pyrophosphate-energized vacuolar membrane proton pump

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	217.64Å 88.43Å 159.05Å 90.00° 125.47° 90.00°	Depositor
Resolution (Å)	24.49 – 2.30 24.49 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.8 (24.49-2.30) 82.6 (24.49-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.208 , 0.240 0.208 , 0.240	Depositor DCC
R_{free} test set	2000 reflections (1.90%)	wwPDB-VP
Wilson B-factor (Å^2)	39.4	Xtriage
Anisotropy	0.756	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11406	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 1PG, MG, PO4, K

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	0.44	0/5537	0.55	0/7524
1	B	0.40	0/5530	0.53	0/7514
All	All	0.42	0/11067	0.54	0/15038

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	5431	0	5576	48	0
1	B	5424	0	5567	46	0
2	A	10	0	0	1	0
2	B	10	0	0	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	68	0	96	1	0
5	B	51	0	72	3	0
6	A	223	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	177	0	0	1	0
All	All	11406	0	11311	91	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 (91) 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:174:GLU:HG3	1:A:185:THR:HG21	1.60	0.83
1:B:250:LYS:HG3	1:B:727:ASP:HB3	1.63	0.78
1:B:264:ARG:NH2	1:B:613:ASN:OD1	2.18	0.77
1:A:273:ASN:HB3	1:A:276:VAL:HG23	1.73	0.71
1:A:606:GLU:OE1	1:B:441:ARG:NH2	2.27	0.68
1:B:648:LEU:HA	5:B:1009:1PG:H82	1.75	0.68
1:B:537:ALA:O	1:B:541:LYS:HD3	1.97	0.64
1:A:250:LYS:HG3	1:A:727:ASP:HB3	1.80	0.64
1:A:521:ARG:NH2	6:A:1104:HOH:O	2.31	0.63
1:A:264:ARG:NH2	1:A:613:ASN:OD1	2.34	0.59
1:A:35:LYS:NZ	6:A:1106:HOH:O	2.33	0.58
1:B:404:LEU:HD11	1:B:480:TYR:HE2	1.72	0.54
1:B:460:ILE:HG21	5:B:1011:1PG:H22	1.90	0.54
1:A:570:VAL:HG22	1:B:570:VAL:HG22	1.90	0.53
1:B:351:ILE:HG13	1:B:356:GLU:HB3	1.89	0.53
1:A:249:THR:HG23	1:A:250:LYS:HD2	1.91	0.53
1:B:96:VAL:HG12	1:B:237:MET:HG3	1.91	0.53
1:B:250:LYS:N	1:B:250:LYS:HD2	2.25	0.52
1:A:571:LEU:HD11	1:B:560:VAL:HG21	1.91	0.52
1:A:250:LYS:HD2	1:A:250:LYS:N	2.25	0.52
1:A:346:THR:HG23	1:A:347:ASP:OD1	2.11	0.51
1:B:179:VAL:HG11	1:B:354:VAL:HG12	1.93	0.51
1:B:273:ASN:HB3	1:B:276:VAL:HG23	1.93	0.51
1:A:304:CYS:O	1:A:308:VAL:HG22	2.11	0.51
1:A:663:GLU:O	1:A:666:SER:HB2	2.11	0.50
2:A:1001:PO4:P	2:A:1002:PO4:O1	2.71	0.49
1:A:163:ILE:HG12	1:A:192:VAL:HB	1.94	0.49
1:B:470:ILE:O	1:B:474:PHE:HB2	2.13	0.49
2:B:1001:PO4:O3	2:B:1002:PO4:O1	2.30	0.49
1:A:500:ASP:HA	1:A:536:THR:HG23	1.94	0.49
1:B:250:LYS:NZ	6:B:1112:HOH:O	2.44	0.49
1:B:304:CYS:O	1:B:308:VAL:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ALA:HB2	1:A:550:LEU:HB3	1.96	0.48
1:B:225:GLU:O	1:B:228:THR:HG23	2.14	0.47
1:A:363:LYS:HD3	1:A:363:LYS:HA	1.61	0.47
1:B:724:THR:HA	1:B:727:ASP:OD2	2.14	0.47
1:A:441:ARG:NH2	1:B:606:GLU:OE1	2.48	0.47
1:B:611:GLN:HE22	1:B:626:ASP:HB3	1.80	0.47
1:A:237:MET:HB3	6:A:1270:HOH:O	2.15	0.47
1:A:273:ASN:HB3	1:A:276:VAL:CG2	2.43	0.47
1:B:448:VAL:HA	1:B:690:TRP:CZ2	2.49	0.46
1:A:715:CYS:SG	6:A:1256:HOH:O	2.61	0.46
1:A:560:VAL:HG13	1:A:565:ILE:HB	1.97	0.46
1:A:404:LEU:HD11	1:A:480:TYR:HE2	1.80	0.46
1:B:23:ILE:HG22	1:B:27:LEU:HD22	1.97	0.46
1:A:570:VAL:CG2	1:B:570:VAL:HG22	2.47	0.45
5:A:1011:1PG:H22	5:A:1011:1PG:H42	1.51	0.45
1:A:404:LEU:HD23	1:A:404:LEU:HA	1.73	0.45
1:A:587:TYR:OH	1:B:587:TYR:OH	2.20	0.45
1:A:250:LYS:NZ	6:A:1121:HOH:O	2.50	0.45
1:A:301:GLU:OE2	1:A:742:LYS:HG3	2.16	0.45
1:A:67:ASP:O	1:A:70:VAL:HG12	2.17	0.44
1:A:225:GLU:O	1:A:228:THR:HG23	2.18	0.44
1:B:500:ASP:HA	1:B:536:THR:HG23	1.99	0.44
1:A:154:LEU:HD23	6:A:1270:HOH:O	2.17	0.44
1:A:588:TRP:CD1	1:B:460:ILE:HD11	2.53	0.43
1:B:259:VAL:HG21	1:B:608:VAL:HB	1.99	0.43
1:A:597:VAL:HG11	1:A:728:PRO:HB3	2.00	0.43
1:B:104:ALA:HB1	1:B:143:THR:HG23	2.00	0.43
1:B:479:MET:SD	1:B:557:GLY:HA3	2.59	0.43
1:A:470:ILE:O	1:A:474:PHE:HB2	2.19	0.43
1:B:438:ASP:OD2	1:B:441:ARG:NH1	2.51	0.43
2:B:1001:PO4:P	2:B:1002:PO4:O1	2.77	0.43
1:B:298:SER:OG	1:B:742:LYS:NZ	2.47	0.43
1:B:350:GLU:OE1	1:B:351:ILE:N	2.51	0.43
1:A:99:PHE:CE2	1:A:650:MET:HE2	2.54	0.43
1:B:565:ILE:HD11	1:B:662:VAL:HB	2.00	0.42
1:B:38:LEU:HD12	1:B:75:ALA:HB2	2.01	0.42
1:B:597:VAL:HG11	1:B:728:PRO:HB3	2.01	0.42
5:B:1010:1PG:H21	5:B:1010:1PG:H42	1.80	0.42
1:A:643:ILE:HB	1:A:644:PRO:HD3	2.02	0.42
1:A:659:LEU:HB3	1:A:762:LEU:HD22	2.02	0.42
1:A:694:LYS:HE2	1:A:694:LYS:HB3	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:VAL:HG13	1:B:565:ILE:HB	2.01	0.42
1:A:2:GLY:HA3	6:A:1289:HOH:O	2.20	0.41
1:A:460:ILE:HD11	1:B:588:TRP:CD1	2.56	0.41
1:B:274:PRO:HD2	1:B:608:VAL:HG13	2.02	0.41
1:A:739:ILE:HA	1:A:742:LYS:HE2	2.01	0.41
1:B:417:ILE:O	1:B:421:VAL:HG23	2.21	0.41
1:A:562:ARG:HA	1:A:562:ARG:HD2	1.93	0.41
1:A:639:ILE:HD13	1:A:639:ILE:HA	1.92	0.41
1:B:353:ALA:O	1:B:356:GLU:HB2	2.20	0.41
1:B:694:LYS:HB3	1:B:694:LYS:HE2	1.66	0.41
1:A:499:ILE:O	1:A:536:THR:HG21	2.21	0.41
1:B:643:ILE:HB	1:B:644:PRO:HD3	2.02	0.41
1:A:310:ALA:HB2	1:A:480:TYR:CE1	2.56	0.41
1:B:97:GLY:O	1:B:100:MET:HB3	2.21	0.41
1:B:196:LEU:HD23	1:B:196:LEU:HA	1.88	0.41
1:B:698:GLU:HB3	1:B:711:LYS:HE2	2.03	0.41
1:A:342:THR:O	1:A:346:THR:HB	2.21	0.40
1:A:479:MET:SD	1:A:557:GLY:HA3	2.62	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	736/766 (96%)	726 (99%)	10 (1%)	0	100	100
1	B	735/766 (96%)	718 (98%)	16 (2%)	1 (0%)	51	64
All	All	1471/1532 (96%)	1444 (98%)	26 (2%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	348	PHE

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	568/588 (97%)	537 (94%)	31 (6%)	21	30
1	B	567/588 (96%)	542 (96%)	25 (4%)	28	39
All	All	1135/1176 (96%)	1079 (95%)	56 (5%)	25	35

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	31	LEU
1	A	109	LEU
1	A	179	VAL
1	A	185	THR
1	A	228	THR
1	A	237	MET
1	A	250	LYS
1	A	285	VAL
1	A	287	ASP
1	A	308	VAL
1	A	328	LEU
1	A	336	LEU
1	A	346	THR
1	A	352	LYS
1	A	361	LEU
1	A	387	SER
1	A	404	LEU
1	A	408	VAL
1	A	474	PHE
1	A	484	VAL
1	A	502	TYR
1	A	508	ASN

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Mol	Chain	Res	Type
1	A	536	THR
1	A	550	LEU
1	A	624	LYS
1	A	677	VAL
1	A	737	LEU
1	A	738	ASN
1	A	746	VAL
1	A	762	LEU
1	B	9	LEU
1	B	27	LEU
1	B	83	GLU
1	B	185	THR
1	B	228	THR
1	B	237	MET
1	B	250	LYS
1	B	287	ASP
1	B	336	LEU
1	B	346	THR
1	B	350	GLU
1	B	355	LYS
1	B	361	LEU
1	B	363	LYS
1	B	408	VAL
1	B	474	PHE
1	B	502	TYR
1	B	508	ASN
1	B	536	THR
1	B	541	LYS
1	B	550	LEU
1	B	737	LEU
1	B	738	ASN
1	B	746	VAL
1	B	762	LEU

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 23 ligands modelled in this entry, 12 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	1PG	B	1009	-	16,16,16	0.82	0	15,15,15	0.61	0
2	PO4	B	1002	3	4,4,4	0.68	0	6,6,6	0.94	0
2	PO4	B	1001	3,4	4,4,4	1.22	1 (25%)	6,6,6	0.55	0
2	PO4	A	1001	3,4	4,4,4	1.24	1 (25%)	6,6,6	0.78	0
5	1PG	A	1011	-	16,16,16	0.80	0	15,15,15	0.35	0
5	1PG	B	1011	-	16,16,16	0.81	0	15,15,15	0.32	0
2	PO4	A	1002	3	4,4,4	0.76	0	6,6,6	1.20	1 (16%)
5	1PG	A	1012	-	16,16,16	0.78	0	15,15,15	0.27	0
5	1PG	A	1009	-	16,16,16	0.79	0	15,15,15	0.40	0
5	1PG	B	1010	-	16,16,16	0.77	0	15,15,15	0.33	0
5	1PG	A	1010	-	16,16,16	0.83	0	15,15,15	0.36	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
5	1PG	B	1009	-	-	9/14/14/14	-
5	1PG	A	1011	-	-	13/14/14/14	-
5	1PG	B	1011	-	-	10/14/14/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1PG	A	1012	-	-	6/14/14/14	-
5	1PG	A	1009	-	-	7/14/14/14	-
5	1PG	B	1010	-	-	10/14/14/14	-
5	1PG	A	1010	-	-	8/14/14/14	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	PO4	P-O1	2.24	1.56	1.50
2	B	1001	PO4	P-O1	2.06	1.55	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1002	PO4	O3-P-O1	-2.37	102.21	110.89

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1009	1PG	C7-C6-O3-C5
5	A	1011	1PG	C2-C3-O2-C4
5	A	1010	1PG	O2-C4-C5-O3
5	B	1010	1PG	O4-C8-C9-O5
5	B	1010	1PG	O2-C4-C5-O3
5	A	1009	1PG	O2-C4-C5-O3
5	A	1009	1PG	O1-C2-C3-O2
5	B	1010	1PG	C2-C3-O2-C4
5	A	1011	1PG	O4-C8-C9-O5
5	B	1009	1PG	O3-C6-C7-O4
5	B	1010	1PG	O3-C6-C7-O4
5	B	1011	1PG	O3-C6-C7-O4
5	A	1009	1PG	O5-C10-C11-O6
5	B	1010	1PG	O5-C10-C11-O6
5	A	1010	1PG	O1-C2-C3-O2
5	A	1011	1PG	O3-C6-C7-O4
5	A	1012	1PG	C9-C8-O4-C7
5	B	1010	1PG	C3-C2-O1-C1
5	A	1011	1PG	O5-C10-C11-O6
5	B	1009	1PG	O1-C2-C3-O2

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Mol	Chain	Res	Type	Atoms
5	B	1011	1PG	O1-C2-C3-O2
5	A	1009	1PG	O3-C6-C7-O4
5	B	1009	1PG	O5-C10-C11-O6
5	A	1011	1PG	C3-C2-O1-C1
5	A	1011	1PG	C6-C7-O4-C8
5	B	1009	1PG	C3-C2-O1-C1
5	B	1011	1PG	C3-C2-O1-C1
5	B	1010	1PG	O1-C2-C3-O2
5	A	1011	1PG	C9-C8-O4-C7
5	A	1012	1PG	C7-C6-O3-C5
5	A	1011	1PG	C4-C5-O3-C6
5	A	1011	1PG	O2-C4-C5-O3
5	A	1009	1PG	C7-C6-O3-C5
5	A	1010	1PG	C6-C7-O4-C8
5	B	1009	1PG	C6-C7-O4-C8
5	A	1011	1PG	C11-C10-O5-C9
5	B	1010	1PG	C7-C6-O3-C5
5	B	1010	1PG	C5-C4-O2-C3
5	B	1009	1PG	C11-C10-O5-C9
5	B	1011	1PG	C4-C5-O3-C6
5	A	1012	1PG	C6-C7-O4-C8
5	B	1011	1PG	O5-C10-C11-O6
5	B	1010	1PG	C6-C7-O4-C8
5	A	1012	1PG	O4-C8-C9-O5
5	B	1011	1PG	C11-C10-O5-C9
5	A	1011	1PG	C8-C9-O5-C10
5	B	1011	1PG	C6-C7-O4-C8
5	A	1009	1PG	C4-C5-O3-C6
5	A	1010	1PG	C11-C10-O5-C9
5	A	1011	1PG	C7-C6-O3-C5
5	A	1009	1PG	C2-C3-O2-C4
5	A	1011	1PG	C5-C4-O2-C3
5	A	1010	1PG	O5-C10-C11-O6
5	A	1012	1PG	O2-C4-C5-O3
5	B	1009	1PG	O2-C4-C5-O3
5	A	1012	1PG	O1-C2-C3-O2
5	B	1011	1PG	O2-C4-C5-O3
5	A	1010	1PG	O3-C6-C7-O4
5	B	1011	1PG	C7-C6-O3-C5
5	A	1010	1PG	C7-C6-O3-C5
5	B	1011	1PG	O4-C8-C9-O5
5	A	1010	1PG	O4-C8-C9-O5

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Mol	Chain	Res	Type	Atoms
5	B	1009	1PG	O4-C8-C9-O5

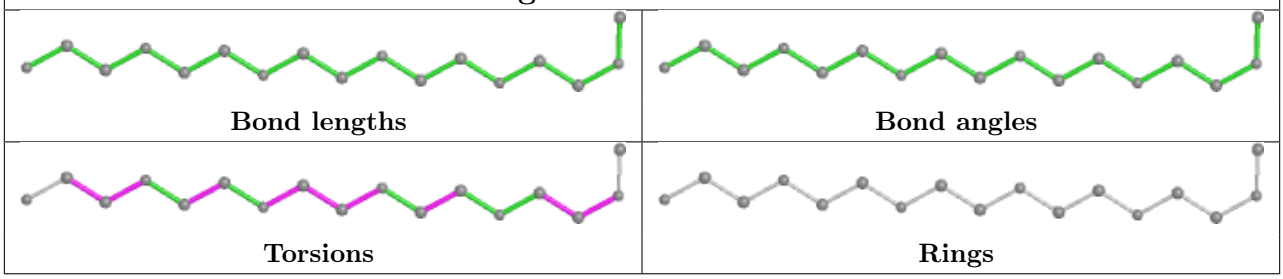
There are no ring outliers.

8 monomers are involved in 7 short contacts:

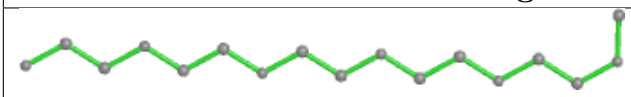
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1009	1PG	1	0
2	B	1002	PO4	2	0
2	B	1001	PO4	2	0
2	A	1001	PO4	1	0
5	A	1011	1PG	1	0
5	B	1011	1PG	1	0
2	A	1002	PO4	1	0
5	B	1010	1PG	1	0

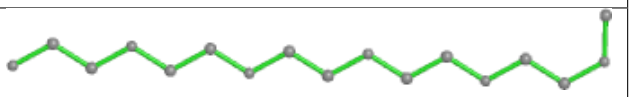
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

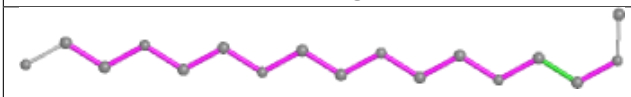
Ligand 1PG B 1009

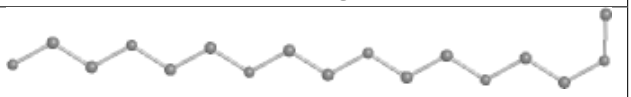


Ligand 1PG A 1011

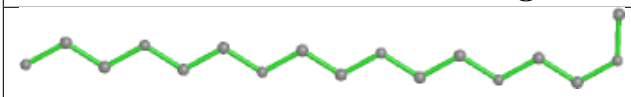

Bond lengths

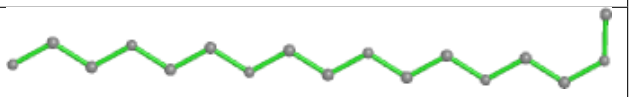

Bond angles

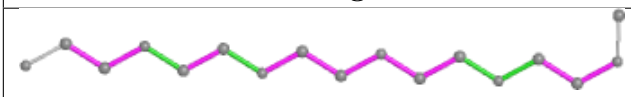

Torsions


Rings

Ligand 1PG B 1011


Bond lengths


Bond angles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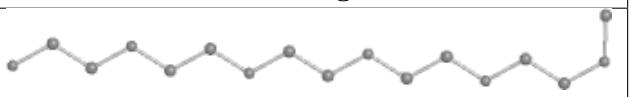
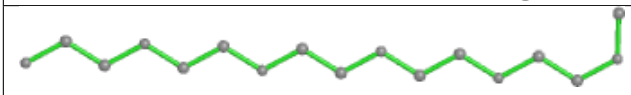
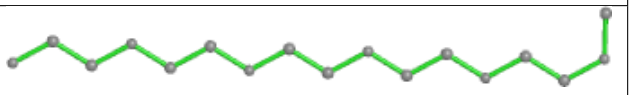
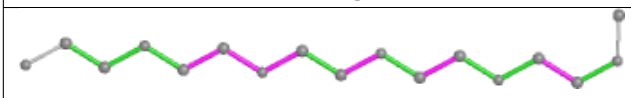
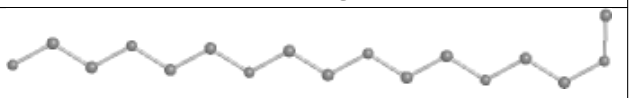

Rings

Ligand 1PG A 1012

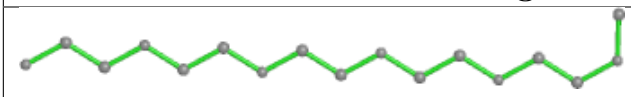

Bond lengths

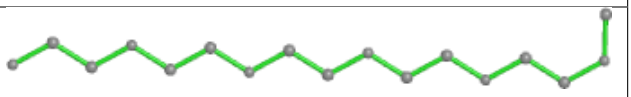

Bond angles

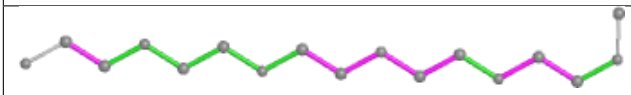

Torsions

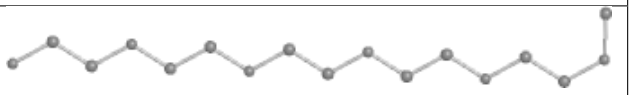

Rings

Ligand 1PG A 1009

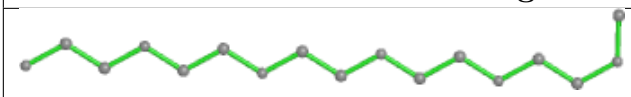

Bond lengths


Bond angles


Torsions

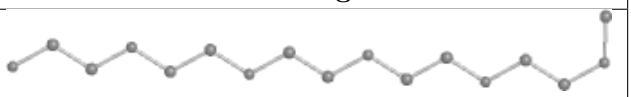

Rings

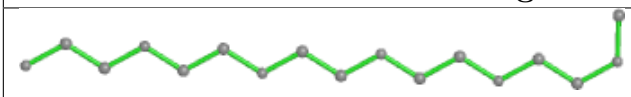
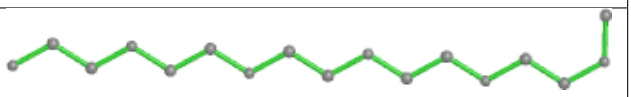
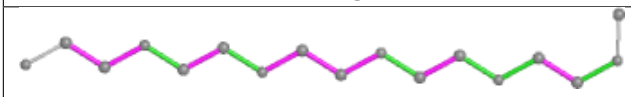
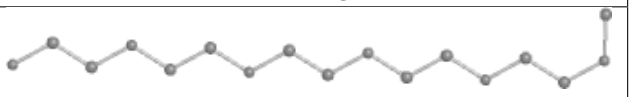
Ligand 1PG B 1010


Bond lengths

Bond angles

Torsions


Rings

Ligand 1PG A 1010	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	740/766 (96%)	-0.16	19 (2%)	56	63	26, 37, 53, 77	0
1	B	739/766 (96%)	0.16	40 (5%)	25	32	26, 45, 69, 87	0
All	All	1479/1532 (96%)	-0.00	59 (3%)	38	45	26, 40, 64, 87	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	68	HIS	7.0
1	A	68	HIS	6.7
1	B	40	ALA	6.1
1	B	39	SER	5.8
1	B	349	PHE	5.7
1	A	41	VAL	5.6
1	B	2	GLY	5.5
1	A	67	ASP	5.2
1	B	614	THR	5.2
1	B	622	THR	5.0
1	B	352	LYS	4.9
1	A	622	THR	4.9
1	A	623	ALA	4.9
1	B	69	ASN	4.9
1	B	520	HIS	4.6
1	B	67	ASP	4.4
1	A	616	PRO	4.3
1	A	40	ALA	4.3
1	B	38	LEU	4.3
1	B	623	ALA	4.2
1	A	766	PHE	4.2
1	B	766	PHE	4.2
1	B	353	ALA	4.1
1	B	351	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	348	PHE	4.0
1	A	624	LYS	4.0
1	B	615	ILE	3.9
1	B	616	PRO	3.8
1	B	348	PHE	3.7
1	B	620	GLU	3.5
1	B	72	VAL	3.4
1	A	349	PHE	3.3
1	B	632	LYS	3.2
1	B	90	PHE	3.1
1	B	350	GLU	3.1
1	B	617	GLY	3.0
1	A	520	HIS	3.0
1	A	39	SER	2.9
1	A	617	GLY	2.9
1	B	619	MET	2.8
1	A	3	ALA	2.7
1	A	69	ASN	2.6
1	B	354	VAL	2.6
1	B	621	GLY	2.6
1	B	624	LYS	2.5
1	B	31	LEU	2.5
1	B	629	THR	2.5
1	A	122	GLN	2.4
1	B	70	VAL	2.4
1	A	120	SER	2.3
1	B	566	THR	2.3
1	B	327	PRO	2.2
1	A	620	GLU	2.2
1	B	521	ARG	2.2
1	B	618	LEU	2.1
1	B	3	ALA	2.0
1	B	344	PHE	2.0
1	B	703	GLU	2.0
1	B	178	GLY	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 monosaccharides in this entry.

6.4 Ligands (i)

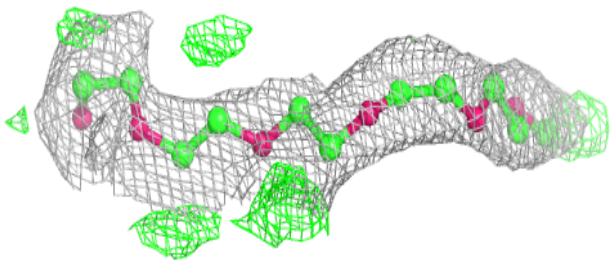
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

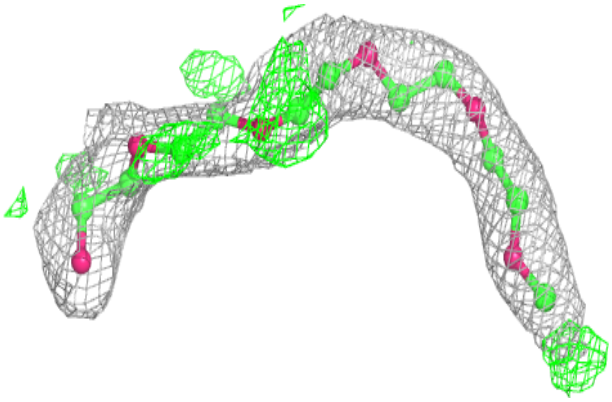
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	1PG	A	1010	17/17	0.76	0.23	49,59,74,77	0
5	1PG	A	1012	17/17	0.76	0.52	52,68,83,85	0
5	1PG	A	1011	17/17	0.77	0.30	52,60,70,71	0
5	1PG	B	1011	17/17	0.78	0.34	46,54,61,63	0
3	MG	B	1007	1/1	0.79	0.09	44,44,44,44	0
5	1PG	A	1009	17/17	0.79	0.23	37,51,64,65	0
3	MG	B	1005	1/1	0.83	0.18	38,38,38,38	0
5	1PG	B	1010	17/17	0.84	0.29	43,52,58,60	0
4	K	B	1008	1/1	0.84	0.21	57,57,57,57	0
3	MG	B	1004	1/1	0.88	0.07	44,44,44,44	0
3	MG	A	1004	1/1	0.89	0.12	39,39,39,39	0
5	1PG	B	1009	17/17	0.90	0.25	41,47,58,59	0
2	PO4	B	1001	5/5	0.91	0.13	32,41,45,52	0
3	MG	A	1007	1/1	0.92	0.09	37,37,37,37	0
3	MG	A	1003	1/1	0.92	0.13	32,32,32,32	0
3	MG	A	1006	1/1	0.93	0.10	37,37,37,37	0
3	MG	B	1003	1/1	0.95	0.09	45,45,45,45	0
2	PO4	A	1001	5/5	0.95	0.11	29,32,36,50	0
2	PO4	B	1002	5/5	0.96	0.10	35,39,41,41	0
3	MG	B	1006	1/1	0.97	0.13	44,44,44,44	0
4	K	A	1008	1/1	0.98	0.08	41,41,41,41	0
3	MG	A	1005	1/1	0.98	0.17	32,32,32,32	0
2	PO4	A	1002	5/5	0.98	0.11	27,30,34,38	0

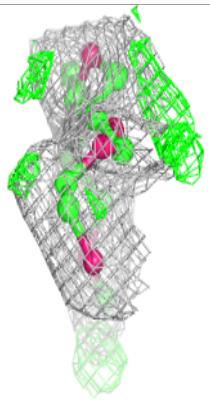
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 1PG A 1010:

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

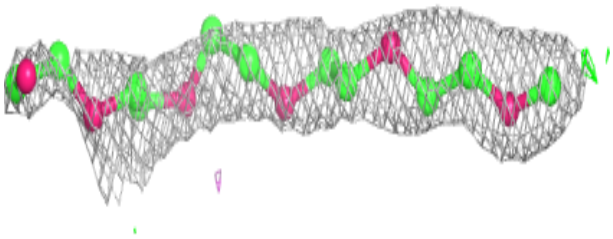


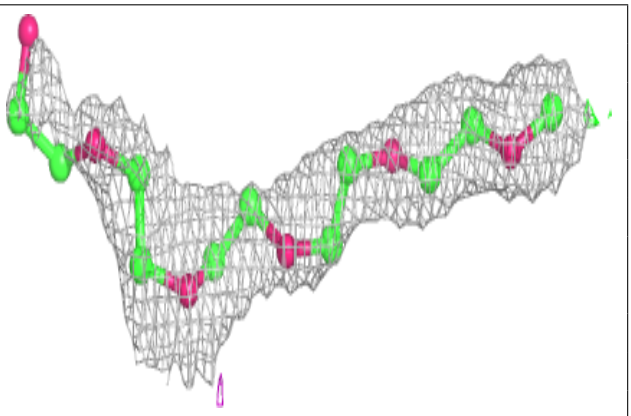


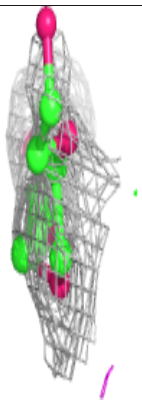


Electron density around 1PG A 1012:

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

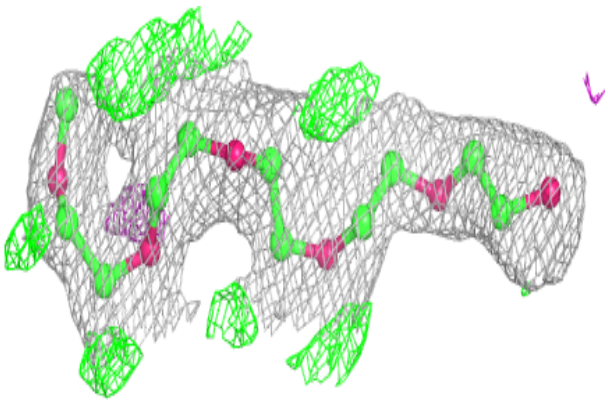


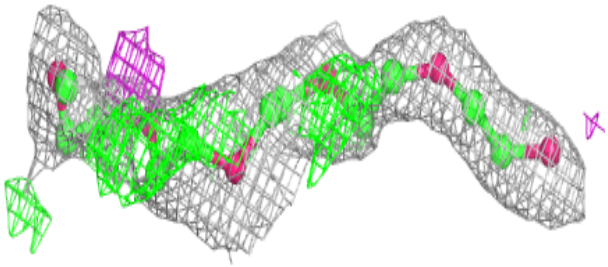


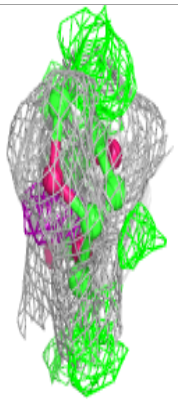


Electron density around 1PG A 1011:

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

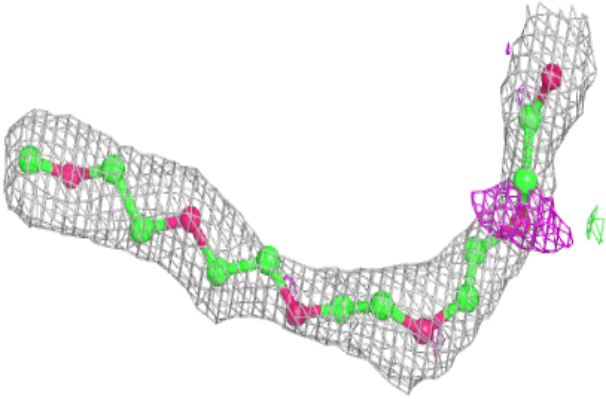


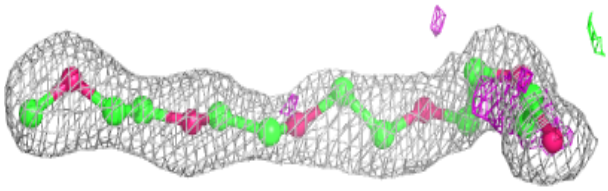


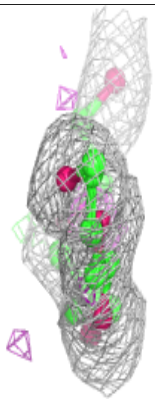


Electron density around 1PG B 1011:

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

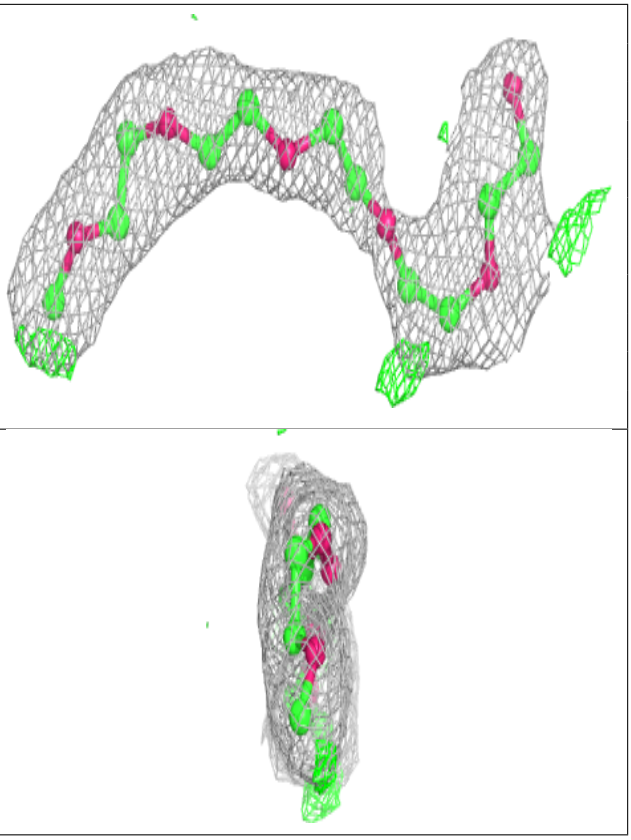


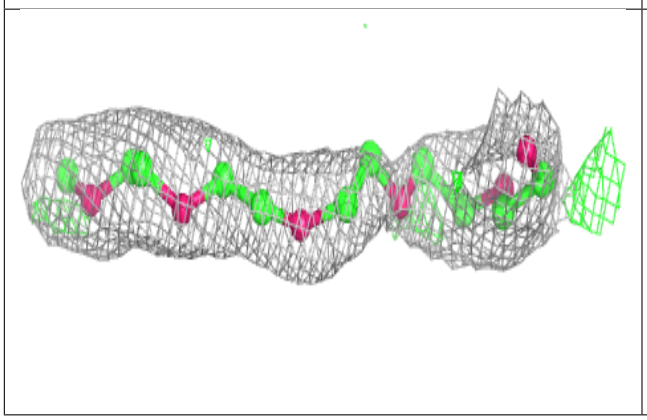




Electron density around 1PG A 1009:

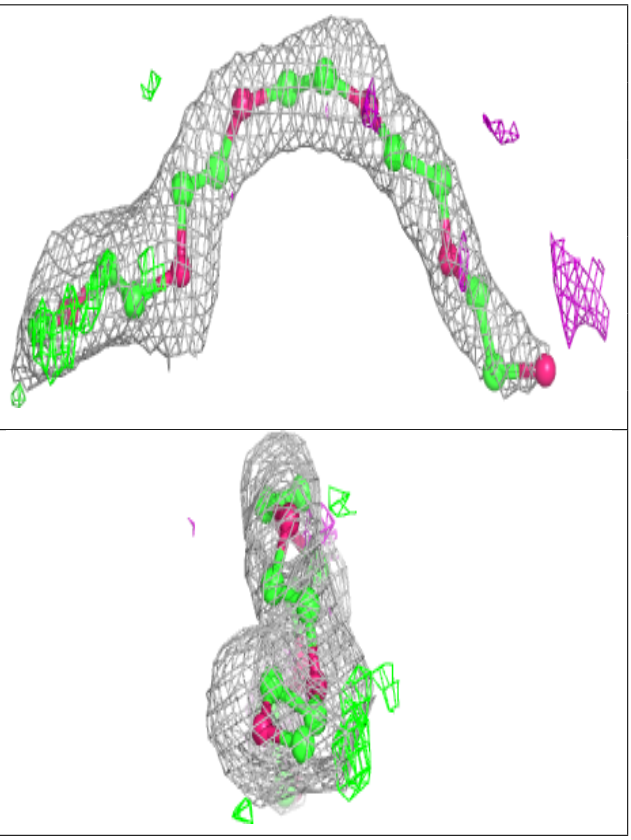
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

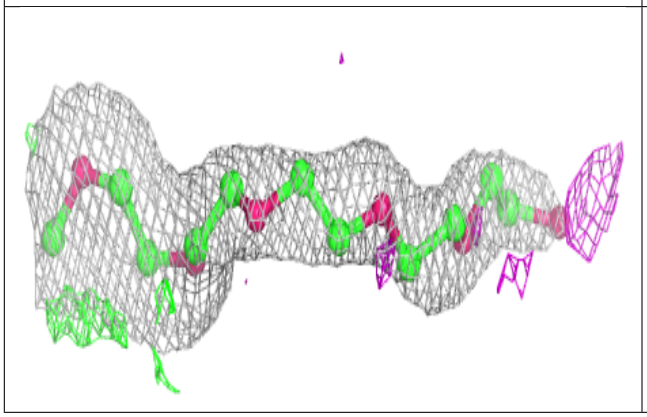




Electron density around 1PG B 1010:

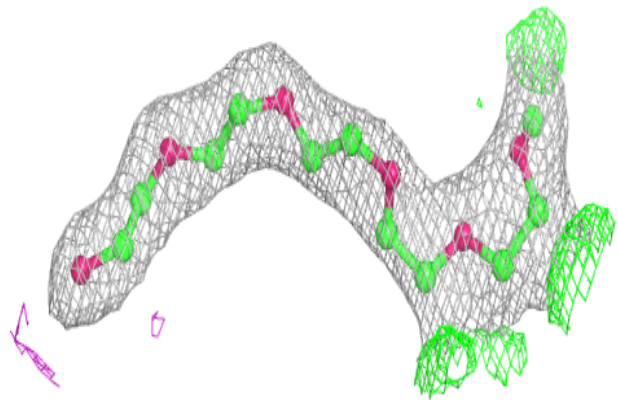
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

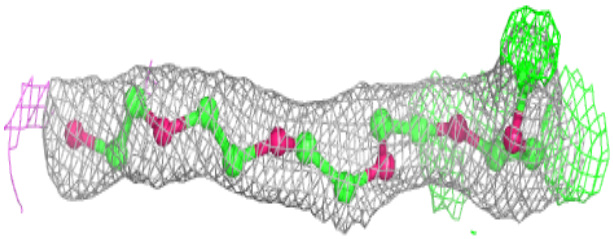


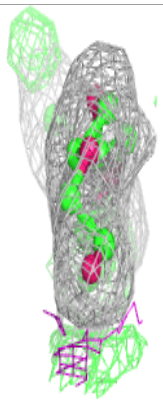


Electron density around 1PG B 1009:

$2mF_o$-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.