Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 09:12 PM EST

PDB ID	:	4KVL
Title	:	Crystal structure of Oryza sativa fatty acid alpha-dioxygenase Y379F with palmitic acid
Authors	:	Zhu, G.; Koszelak-Rosenblum, M.; Malkowski, M.G.
Deposited on	:	2013-05-22
Resolution	:	1.96 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:

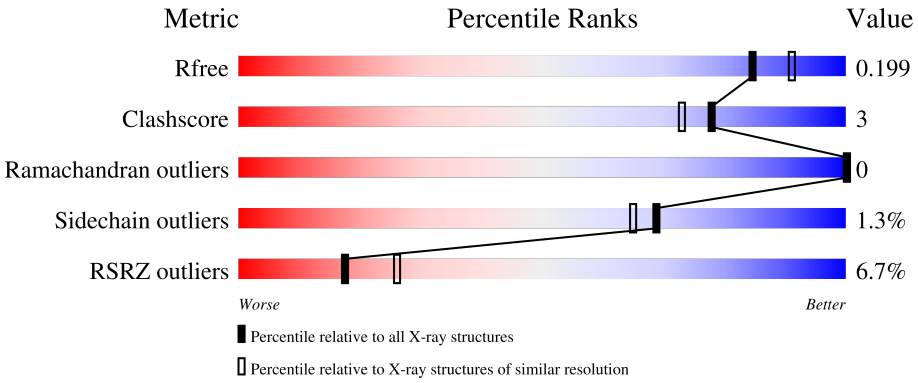
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	621	7% 92% 6% ·

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 5694 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.

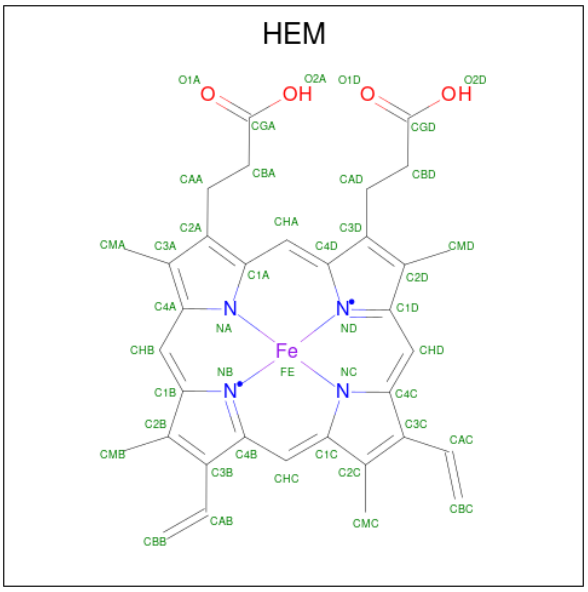
- Molecule 1 is a protein called Fatty acid alpha-oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	610	Total	C	N	O	S	0	12	0
			4973	3180	858	914	21			

There are 13 discrepancies between the modelled and reference sequences:

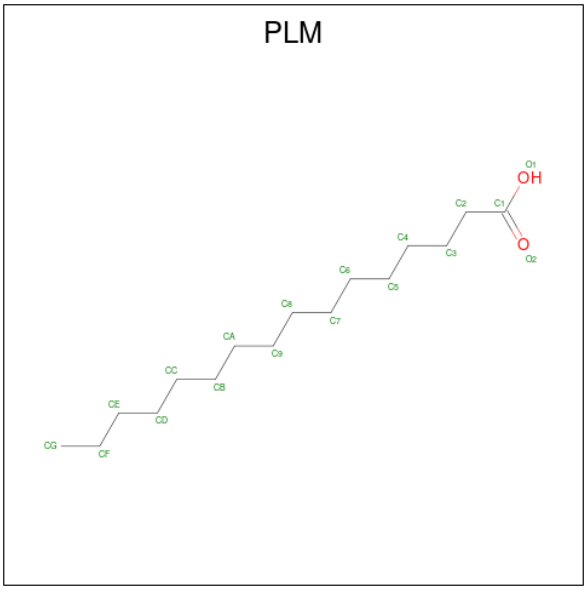
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP Q9M5J1
A	-1	ARG	-	expression tag	UNP Q9M5J1
A	0	GLY	-	expression tag	UNP Q9M5J1
A	1	SER	-	expression tag	UNP Q9M5J1
A	2	HIS	-	expression tag	UNP Q9M5J1
A	3	HIS	-	expression tag	UNP Q9M5J1
A	4	HIS	-	expression tag	UNP Q9M5J1
A	5	HIS	-	expression tag	UNP Q9M5J1
A	6	HIS	-	expression tag	UNP Q9M5J1
A	7	HIS	-	expression tag	UNP Q9M5J1
A	8	GLY	-	expression tag	UNP Q9M5J1
A	9	SER	-	expression tag	UNP Q9M5J1
A	379	PHE	TYR	engineered mutation	UNP Q9M5J1

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).

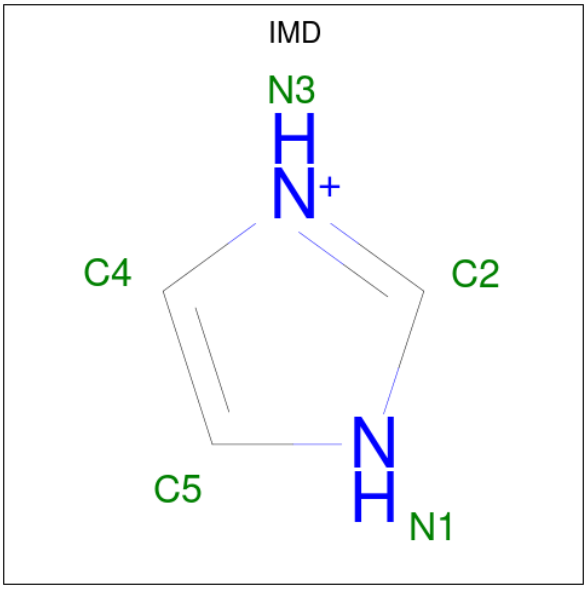


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			18	16	2		
3	A	1	Total	C	O	0	0
			18	16	2		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

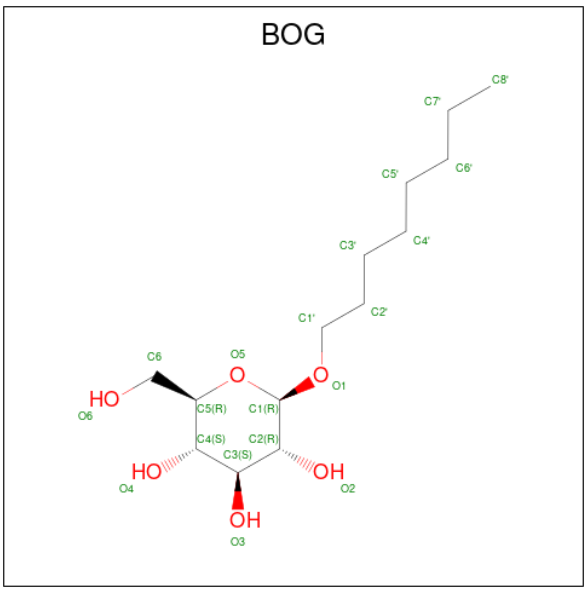
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



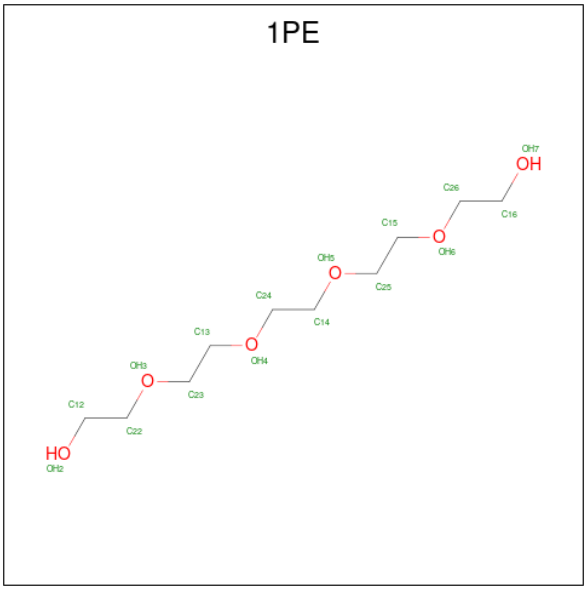
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 5 3 2	0	0

- Molecule 6 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



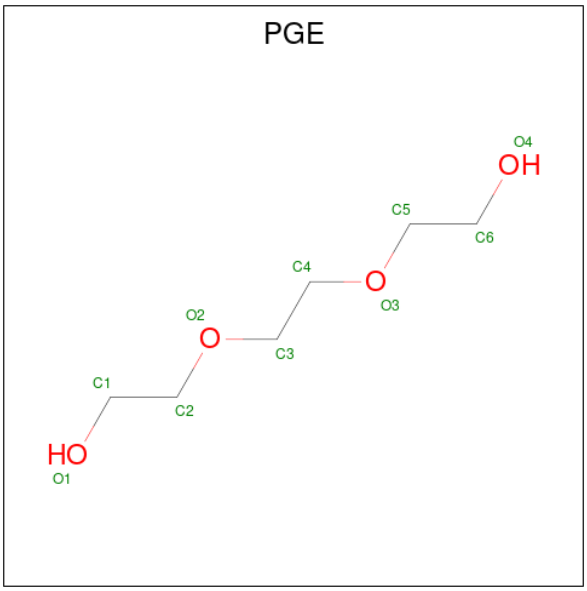
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 20 14 6	0	0
6	A	1	Total C O 20 14 6	0	0

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



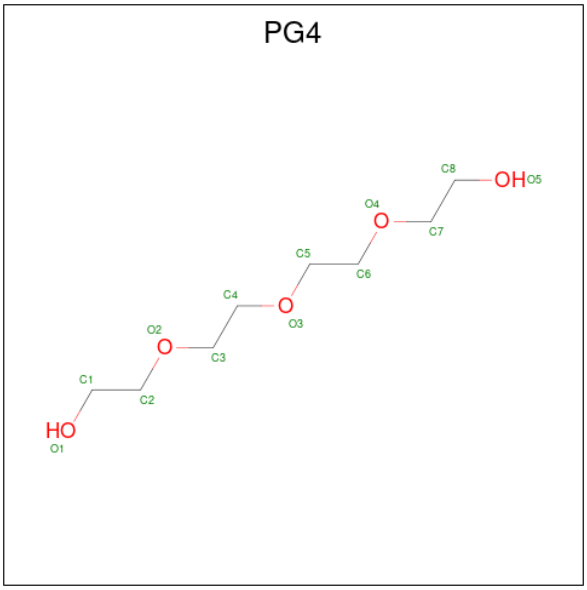
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 16 10 6	0	0

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 10 6 4	0	0
8	A	1	Total C O 10 6 4	0	0
8	A	1	Total C O 10 6 4	0	0
8	A	1	Total C O 10 6 4	0	0
8	A	1	Total C O 10 6 4	0	0
8	A	1	Total C O 10 6 4	0	0

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 13 8 5	0	0

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	2	Total Cl 2 2	0	0

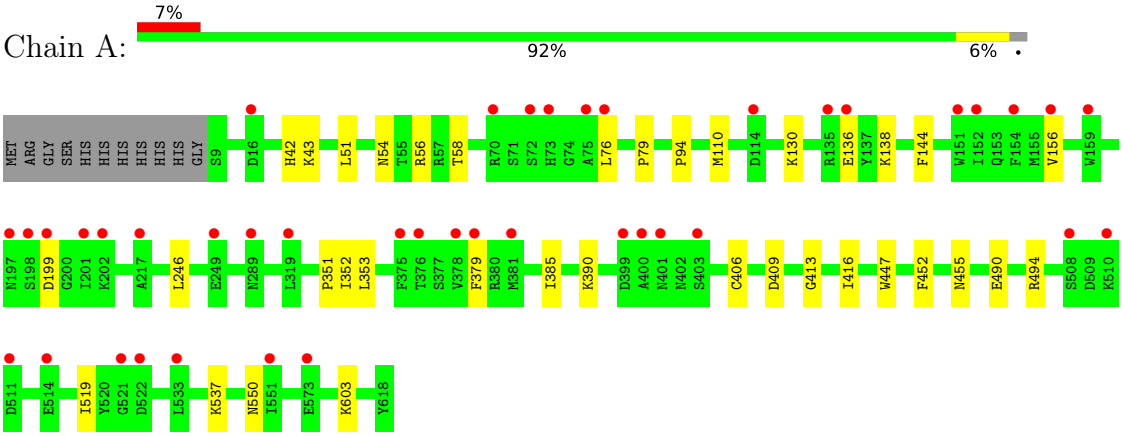
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	505	Total	O	0	0
			505	505		

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: Fatty acid alpha-oxidase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	72.89Å 130.20Å 188.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.07 – 1.96 37.29 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.3 (107.07-1.96) 99.3 (37.29-1.96)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.20 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.157 , 0.186 0.170 , 0.199	Depositor DCC
R_{free} test set	3256 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5694	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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: PLM, CA, CL, BOG, IMD, 1PE, PGE, PG4, HEM

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	0.58	0/5128	0.59	0/6931

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4973	0	4952	23	0
2	A	43	0	30	1	0
3	A	36	0	62	1	0
4	A	1	0	0	0	0
5	A	5	0	4	0	0
6	A	40	0	56	5	0
7	A	16	0	22	1	0
8	A	60	0	84	6	0
9	A	13	0	18	2	0
10	A	2	0	0	0	0
11	A	505	0	0	4	0
All	All	5694	0	5228	30	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 3.

All (30) 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:494:ARG:HA	8:A:708:PGE:H42	1.65	0.78
8:A:714:PGE:C4	8:A:714:PGE:H1	2.19	0.72
8:A:714:PGE:H42	8:A:714:PGE:C1	2.17	0.72
1:A:351:PRO:HG2	6:A:710:BOG:H62	1.74	0.70
8:A:714:PGE:H1	8:A:714:PGE:H42	1.77	0.67
9:A:711:PG4:H82	11:A:1028:HOH:O	1.96	0.66
1:A:352:ILE:CD1	6:A:710:BOG:H1'1	2.29	0.63
1:A:351:PRO:HG2	6:A:710:BOG:C6	2.31	0.61
1:A:54:ASN:O	1:A:58[B]:THR:HG23	2.03	0.58
1:A:156:VAL:HG21	2:A:701:HEM:HBC2	1.86	0.56
8:A:714:PGE:C4	8:A:714:PGE:C1	2.82	0.56
1:A:390:LYS:HD3	1:A:406:CYS:SG	2.47	0.55
1:A:51:LEU:HD21	6:A:706:BOG:H4'2	1.89	0.54
1:A:56:ARG:HD3	1:A:550:ASN:OD1	2.10	0.52
1:A:413:GLY:HA2	1:A:416[A]:ILE:HD12	1.94	0.50
1:A:537:LYS:HE3	7:A:707:1PE:H162	1.95	0.48
1:A:79:PRO:HG3	1:A:94:PRO:HG3	1.94	0.48
9:A:711:PG4:H81	9:A:711:PG4:H62	1.73	0.47
1:A:76:LEU:HA	11:A:1045:HOH:O	2.15	0.47
1:A:447:TRP:HD1	11:A:871:HOH:O	1.98	0.45
1:A:352:ILE:HD11	6:A:710:BOG:H1'1	1.97	0.45
1:A:385:ILE:HG21	1:A:452:PHE:HZ	1.82	0.45
1:A:416[A]:ILE:HD11	1:A:452:PHE:CE1	2.52	0.45
1:A:136:GLU:O	1:A:138:LYS:HD3	2.17	0.45
1:A:490:GLU:O	1:A:494:ARG:HG2	2.18	0.44
1:A:42:HIS:CE1	1:A:43:LYS:HE3	2.55	0.42
8:A:708:PGE:H6	8:A:708:PGE:H4	1.85	0.42
1:A:353:LEU:HD21	3:A:704:PLM:H71	2.03	0.40
1:A:130:LYS:HB2	1:A:519:ILE:HD11	2.03	0.40
1:A:455[B]:ASN:ND2	11:A:1050:HOH:O	2.53	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	620/621 (100%)	600 (97%)	20 (3%)	0	100 100

There are no Ramachandran outliers to report.

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	538/535 (101%)	531 (99%)	7 (1%)	69 65

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	MET
1	A	144	PHE
1	A	199	ASP
1	A	246	LEU
1	A	379	PHE
1	A	409	ASP
1	A	603	LYS

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
8	PGE	A	713	-	9,9,9	0.52	0	8,8,8	0.25	0
6	BOG	A	706	-	20,20,20	0.67	0	25,25,25	0.96	1 (4%)
7	1PE	A	707	-	15,15,15	0.44	0	14,14,14	0.37	0
3	PLM	A	704	-	17,17,17	0.51	0	17,17,17	0.96	1 (5%)
2	HEM	A	701	1,5	41,50,50	2.05	10 (24%)	45,82,82	2.17	12 (26%)
8	PGE	A	715	-	9,9,9	0.51	0	8,8,8	0.33	0
5	IMD	A	705	2	3,5,5	0.33	0	4,5,5	0.52	0
6	BOG	A	710	-	20,20,20	0.50	0	25,25,25	1.79	7 (28%)
8	PGE	A	709	-	9,9,9	0.40	0	8,8,8	0.44	0
8	PGE	A	712	-	9,9,9	0.43	0	8,8,8	0.38	0
3	PLM	A	702	-	17,17,17	0.57	0	17,17,17	0.89	0
8	PGE	A	708	-	9,9,9	0.46	0	8,8,8	0.38	0
8	PGE	A	714	-	9,9,9	0.62	0	8,8,8	1.03	1 (12%)
9	PG4	A	711	-	12,12,12	0.53	0	11,11,11	0.41	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
8	PGE	A	713	-	-	3/7/7/7	-
6	BOG	A	706	-	-	8/11/31/31	0/1/1/1
3	PLM	A	702	-	-	4/15/15/15	-
7	1PE	A	707	-	-	5/13/13/13	-
3	PLM	A	704	-	-	10/15/15/15	-
2	HEM	A	701	1,5	-	2/12/54/54	-
8	PGE	A	715	-	-	4/7/7/7	-
5	IMD	A	705	2	-	-	0/1/1/1
8	PGE	A	709	-	-	3/7/7/7	-
8	PGE	A	712	-	-	2/7/7/7	-
6	BOG	A	710	-	-	6/11/31/31	0/1/1/1
8	PGE	A	708	-	-	4/7/7/7	-
8	PGE	A	714	-	-	6/7/7/7	-
9	PG4	A	711	-	-	4/10/10/10	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	HEM	C3D-C2D	7.64	1.53	1.36
2	A	701	HEM	C3C-C2C	-3.98	1.34	1.40
2	A	701	HEM	C3C-CAC	3.43	1.54	1.47
2	A	701	HEM	FE-ND	3.21	2.12	1.96
2	A	701	HEM	CMB-C2B	2.95	1.57	1.50
2	A	701	HEM	FE-NB	2.83	2.10	1.96
2	A	701	HEM	CAA-C2A	2.58	1.55	1.52
2	A	701	HEM	CAB-C3B	2.58	1.54	1.47
2	A	701	HEM	CMD-C2D	2.45	1.56	1.50
2	A	701	HEM	CMC-C2C	2.16	1.56	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	HEM	C4D-ND-C1D	7.86	113.19	105.07
2	A	701	HEM	C4C-CHD-C1D	5.05	129.23	122.56
2	A	701	HEM	C1B-NB-C4B	4.70	109.92	105.07
6	A	710	BOG	O2-C2-C3	-3.62	101.98	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	HEM	C4B-CHC-C1C	3.38	127.02	122.56
6	A	710	BOG	O5-C5-C4	-3.14	103.98	109.69
2	A	701	HEM	CMD-C2D-C1D	2.98	129.58	125.04
6	A	710	BOG	O5-C5-C6	2.95	113.78	106.44
2	A	701	HEM	CHA-C4D-ND	2.92	127.99	124.38
6	A	710	BOG	O4-C4-C3	-2.83	103.80	110.35
2	A	701	HEM	CAD-CBD-CGD	-2.73	107.72	113.60
2	A	701	HEM	CAA-CBA-CGA	-2.55	106.60	113.76
2	A	701	HEM	C3D-C4D-ND	-2.47	107.41	110.17
6	A	710	BOG	C4-C3-C2	2.47	115.14	110.82
6	A	710	BOG	C6-C5-C4	2.39	118.61	113.00
2	A	701	HEM	C4B-C3B-C2B	2.30	108.94	107.11
6	A	706	BOG	O5-C1-C2	-2.29	105.50	110.35
8	A	714	PGE	C3-O2-C2	2.15	122.59	113.29
2	A	701	HEM	CMA-C3A-C4A	-2.13	125.19	128.46
2	A	701	HEM	C2C-C3C-C4C	2.12	108.38	106.90
6	A	710	BOG	C3-C4-C5	-2.11	106.48	110.24
3	A	704	PLM	O1-C1-C2	2.04	120.60	114.03

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	714	PGE	C1-C2-O2-C3
8	A	714	PGE	C4-C3-O2-C2
9	A	711	PG4	C8-C7-O4-C6
8	A	713	PGE	O1-C1-C2-O2
8	A	714	PGE	O2-C3-C4-O3
8	A	708	PGE	O2-C3-C4-O3
8	A	714	PGE	O1-C1-C2-O2
8	A	715	PGE	O1-C1-C2-O2
3	A	704	PLM	C8-C9-CA-CB
3	A	704	PLM	C4-C5-C6-C7
3	A	704	PLM	C9-CA-CB-CC
3	A	704	PLM	C7-C8-C9-CA
6	A	706	BOG	C4'-C5'-C6'-C7'
6	A	710	BOG	O1-C1'-C2'-C3'
7	A	707	1PE	OH7-C16-C26-OH6
6	A	710	BOG	C2'-C3'-C4'-C5'
6	A	710	BOG	C3'-C4'-C5'-C6'
6	A	706	BOG	C1'-C2'-C3'-C4'
3	A	704	PLM	C6-C7-C8-C9

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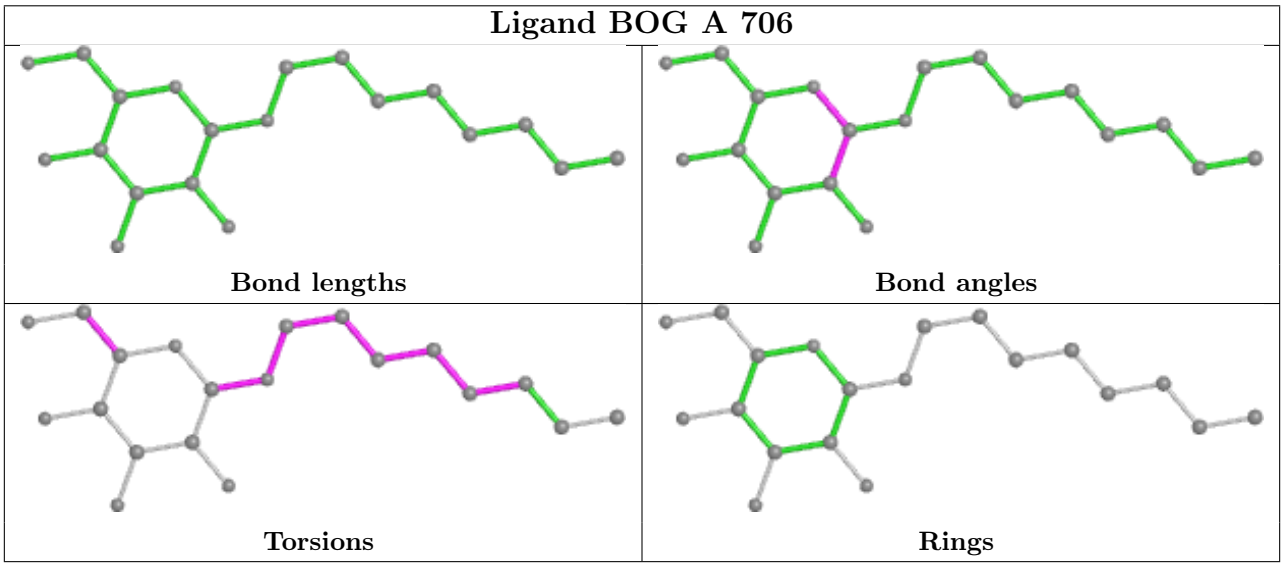
Mol	Chain	Res	Type	Atoms
6	A	710	BOG	C1'-C2'-C3'-C4'
3	A	704	PLM	CB-CC-CD-CE
3	A	702	PLM	C1-C2-C3-C4
8	A	709	PGE	O1-C1-C2-O2
6	A	706	BOG	O1-C1'-C2'-C3'
6	A	706	BOG	C3'-C4'-C5'-C6'
8	A	713	PGE	O3-C5-C6-O4
7	A	707	1PE	OH6-C15-C25-OH5
3	A	702	PLM	CD-CE-CF-CG
8	A	714	PGE	O3-C5-C6-O4
8	A	708	PGE	C6-C5-O3-C4
6	A	706	BOG	C2'-C1'-O1-C1
3	A	702	PLM	C2-C3-C4-C5
6	A	706	BOG	O5-C5-C6-O6
3	A	704	PLM	CC-CD-CE-CF
6	A	706	BOG	O5-C1-O1-C1'
6	A	706	BOG	C2'-C3'-C4'-C5'
3	A	704	PLM	C3-C4-C5-C6
8	A	714	PGE	C3-C4-O3-C5
7	A	707	1PE	C14-C24-OH4-C13
6	A	710	BOG	C4'-C5'-C6'-C7'
8	A	712	PGE	C1-C2-O2-C3
8	A	709	PGE	O3-C5-C6-O4
9	A	711	PG4	O3-C5-C6-O4
8	A	715	PGE	C4-C3-O2-C2
8	A	713	PGE	C3-C4-O3-C5
3	A	702	PLM	CA-CB-CC-CD
3	A	704	PLM	O1-C1-C2-C3
7	A	707	1PE	C12-C22-OH3-C23
3	A	704	PLM	O2-C1-C2-C3
8	A	708	PGE	C4-C3-O2-C2
2	A	701	HEM	CAA-CBA-CGA-O2A
7	A	707	1PE	C24-C14-OH5-C25
6	A	710	BOG	C4-C5-C6-O6
8	A	715	PGE	C6-C5-O3-C4
2	A	701	HEM	CAA-CBA-CGA-O1A
8	A	708	PGE	O1-C1-C2-O2
8	A	709	PGE	O2-C3-C4-O3
9	A	711	PG4	O2-C3-C4-O3
8	A	712	PGE	C6-C5-O3-C4
8	A	715	PGE	O3-C5-C6-O4
9	A	711	PG4	C5-C6-O4-C7

There are no ring outliers.

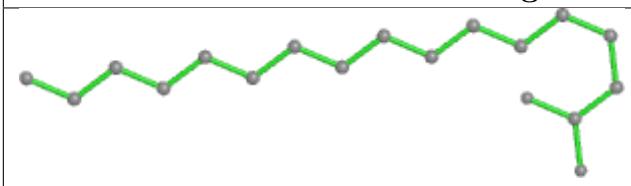
8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	706	BOG	1	0
7	A	707	1PE	1	0
3	A	704	PLM	1	0
2	A	701	HEM	1	0
6	A	710	BOG	4	0
8	A	708	PGE	2	0
8	A	714	PGE	4	0
9	A	711	PG4	2	0

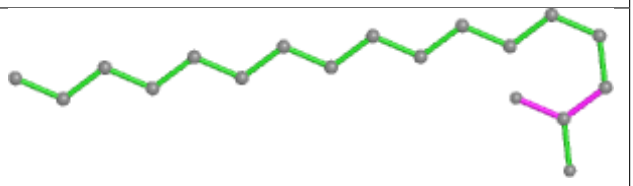
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



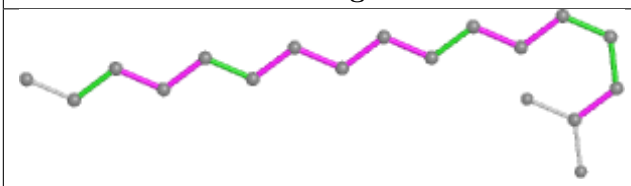
Ligand PLM A 704



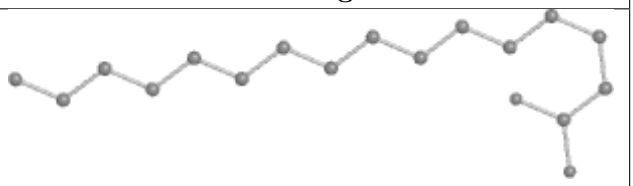
Bond lengths



Bond angles

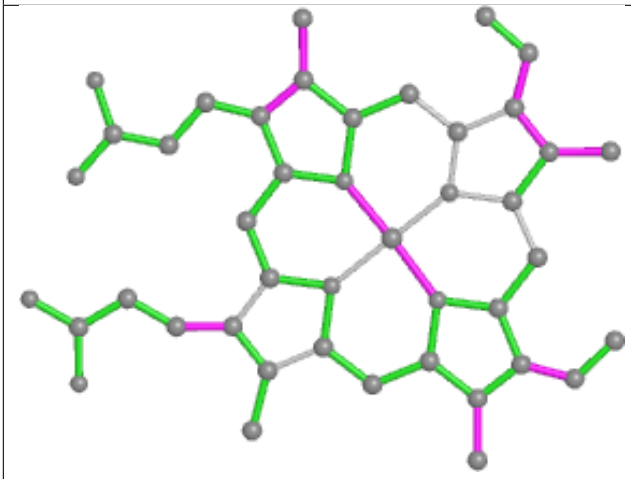


Torsions

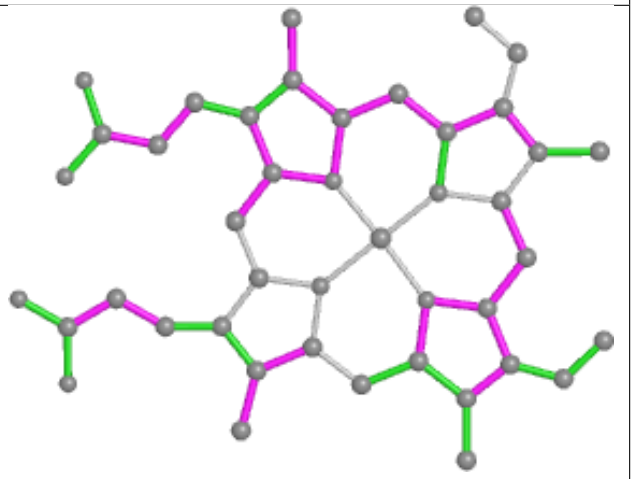


Rings

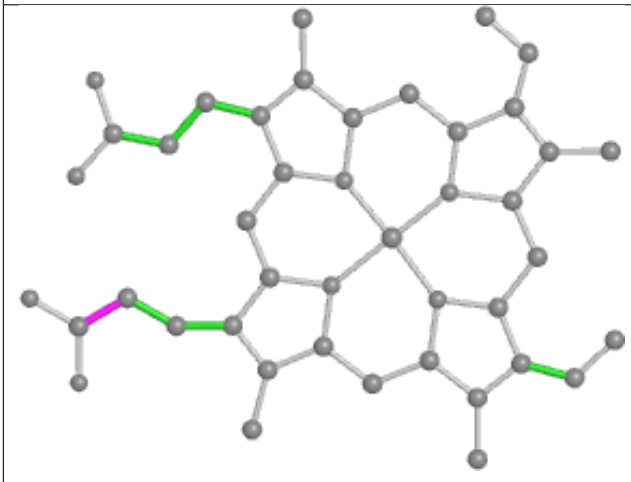
Ligand HEM A 701



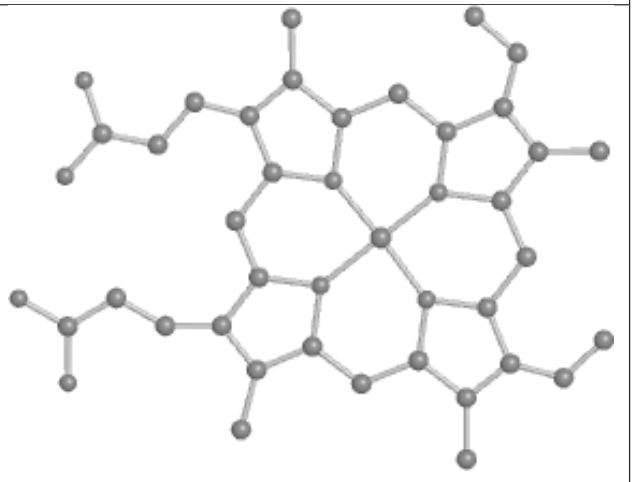
Bond lengths



Bond angles

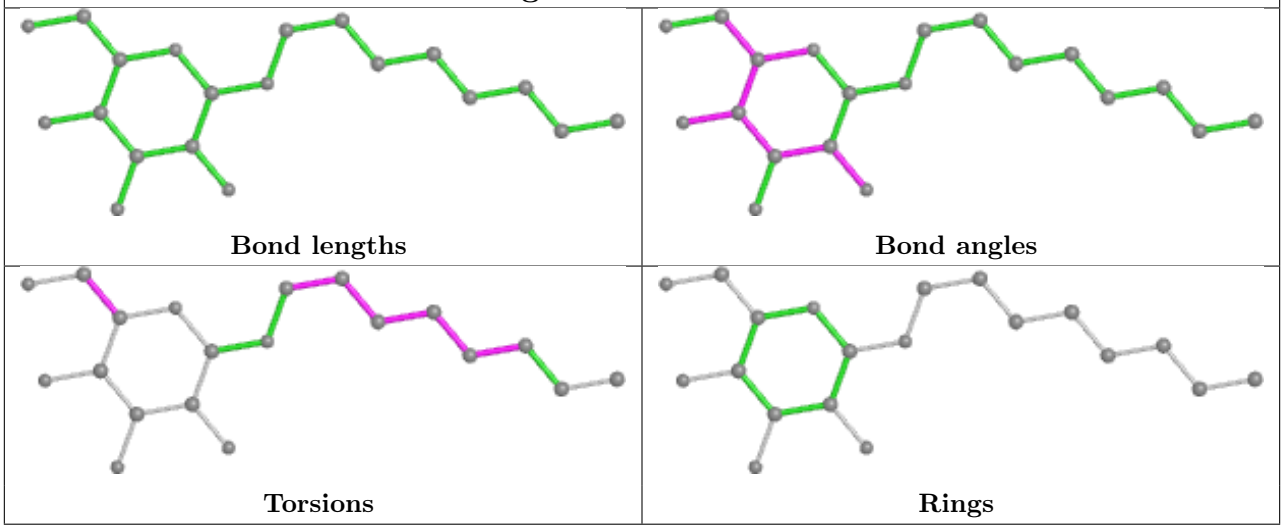


Torsions

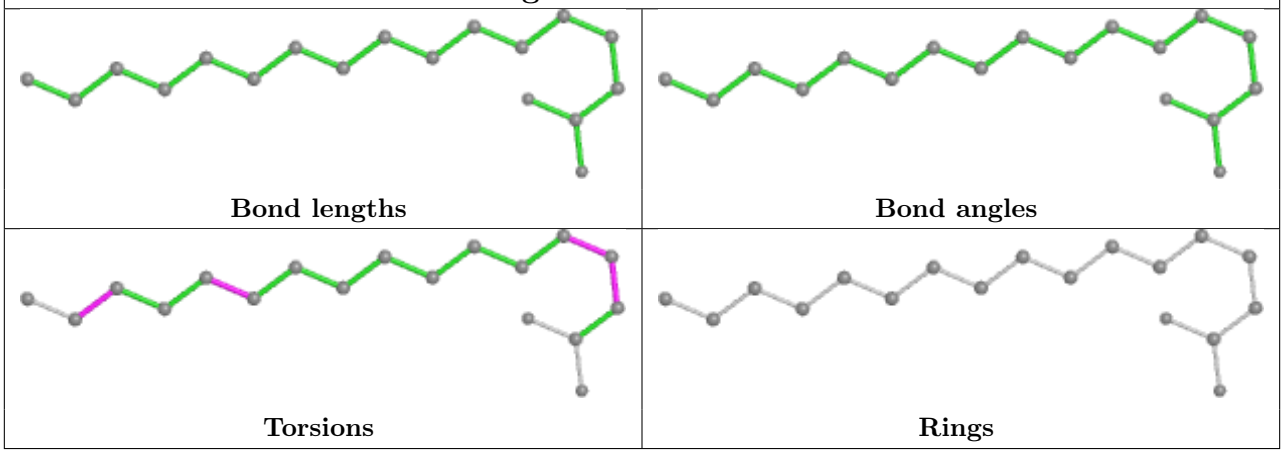


Rings

Ligand BOG A 710



Ligand PLM A 702



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	610/621 (98%)	0.16	41 (6%)	17	26	17, 30, 51, 75	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	400	ALA	9.8
1	A	76	LEU	6.6
1	A	401	ASN	6.5
1	A	73	HIS	6.1
1	A	156	VAL	5.0
1	A	72	SER	4.6
1	A	199	ASP	4.0
1	A	510	LYS	3.4
1	A	152	ILE	3.3
1	A	136	GLU	3.2
1	A	70	ARG	3.1
1	A	249	GLU	3.1
1	A	159	TRP	3.0
1	A	403	SER	2.9
1	A	511	ASP	2.9
1	A	197	ASN	2.9
1	A	375	PHE	2.9
1	A	16	ASP	2.9
1	A	399	ASP	2.9
1	A	378	VAL	2.6
1	A	514	GLU	2.5
1	A	522	ASP	2.5
1	A	75	ALA	2.5
1	A	154	PHE	2.4
1	A	379	PHE	2.4
1	A	202	LYS	2.3
1	A	289	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	217	ALA	2.2
1	A	201	ILE	2.2
1	A	508	SER	2.2
1	A	376	THR	2.2
1	A	198	SER	2.1
1	A	573	GLU	2.1
1	A	114	ASP	2.1
1	A	381	MET	2.1
1	A	151	TRP	2.1
1	A	521	GLY	2.1
1	A	135	ARG	2.0
1	A	319	LEU	2.0
1	A	551	ILE	2.0
1	A	533	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 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
8	PGE	A	715	10/10	0.77	0.19	73,78,81,81	0
8	PGE	A	714	10/10	0.78	0.15	56,70,72,74	0
6	BOG	A	710	20/20	0.81	0.19	57,73,81,82	0
8	PGE	A	713	10/10	0.81	0.16	55,62,66,67	0
9	PG4	A	711	13/13	0.81	0.24	35,60,69,69	0
8	PGE	A	708	10/10	0.89	0.17	40,49,56,60	0
8	PGE	A	712	10/10	0.89	0.17	50,54,62,66	0
8	PGE	A	709	10/10	0.91	0.16	47,53,58,62	0
3	PLM	A	704	18/18	0.92	0.15	32,43,48,48	0

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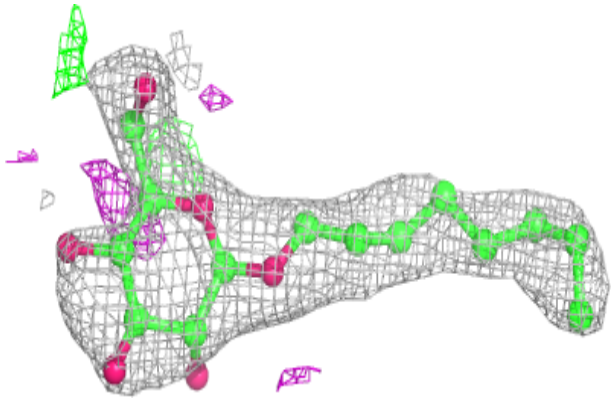
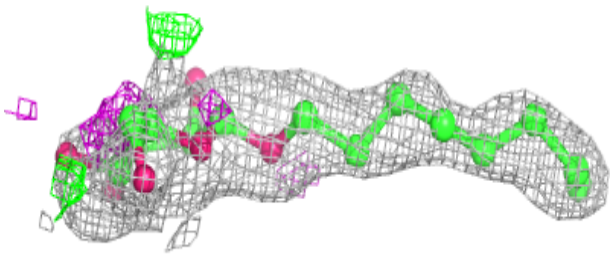
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	BOG	A	706	20/20	0.93	0.12	26,47,62,64	0
3	PLM	A	702	18/18	0.94	0.24	18,25,39,41	0
7	1PE	A	707	16/16	0.95	0.12	37,45,50,52	0
5	IMD	A	705	5/5	0.97	0.10	30,36,37,40	0
2	HEM	A	701	43/43	0.98	0.16	22,26,31,39	0
10	CL	A	716	1/1	0.98	0.05	30,30,30,30	0
4	CA	A	703	1/1	0.99	0.08	29,29,29,29	0
10	CL	A	717	1/1	0.99	0.05	32,32,32,32	0

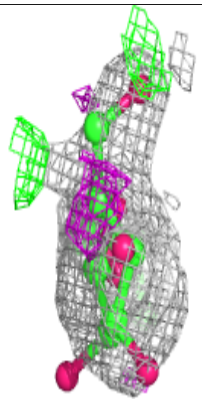
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BOG A 710:

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

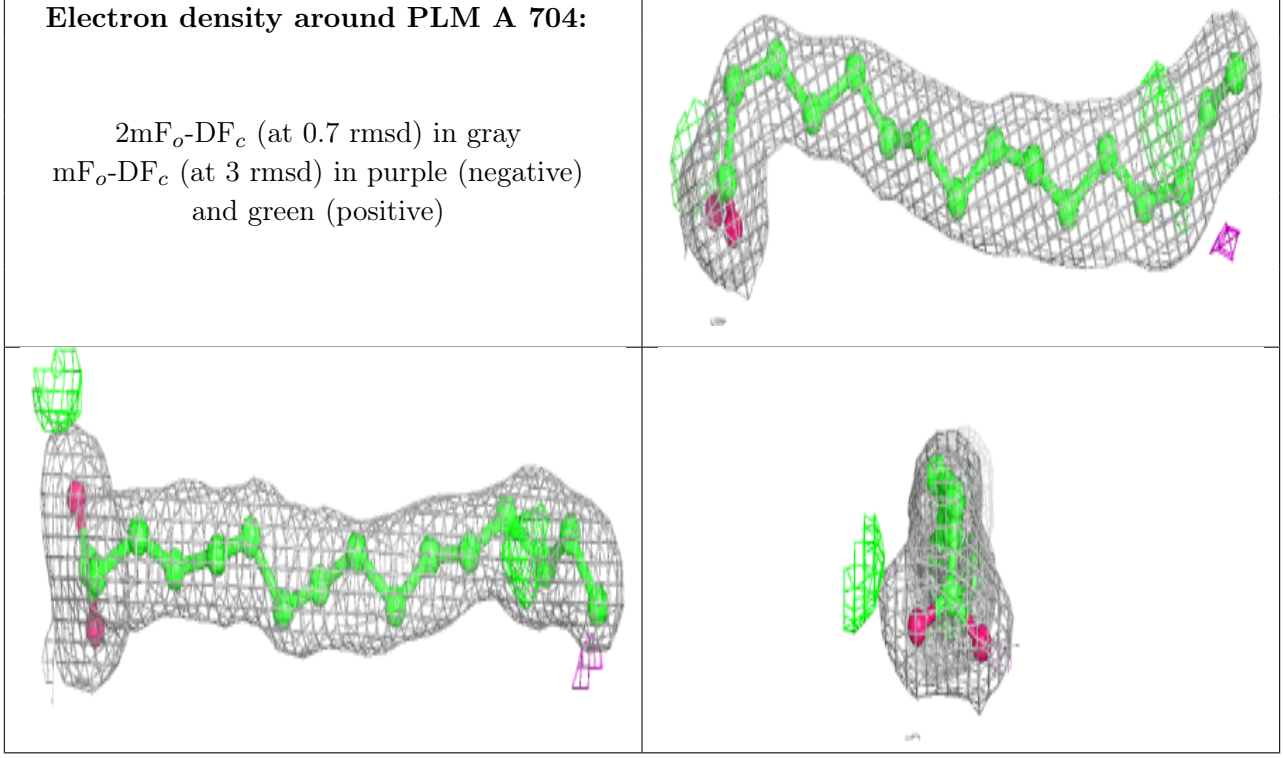






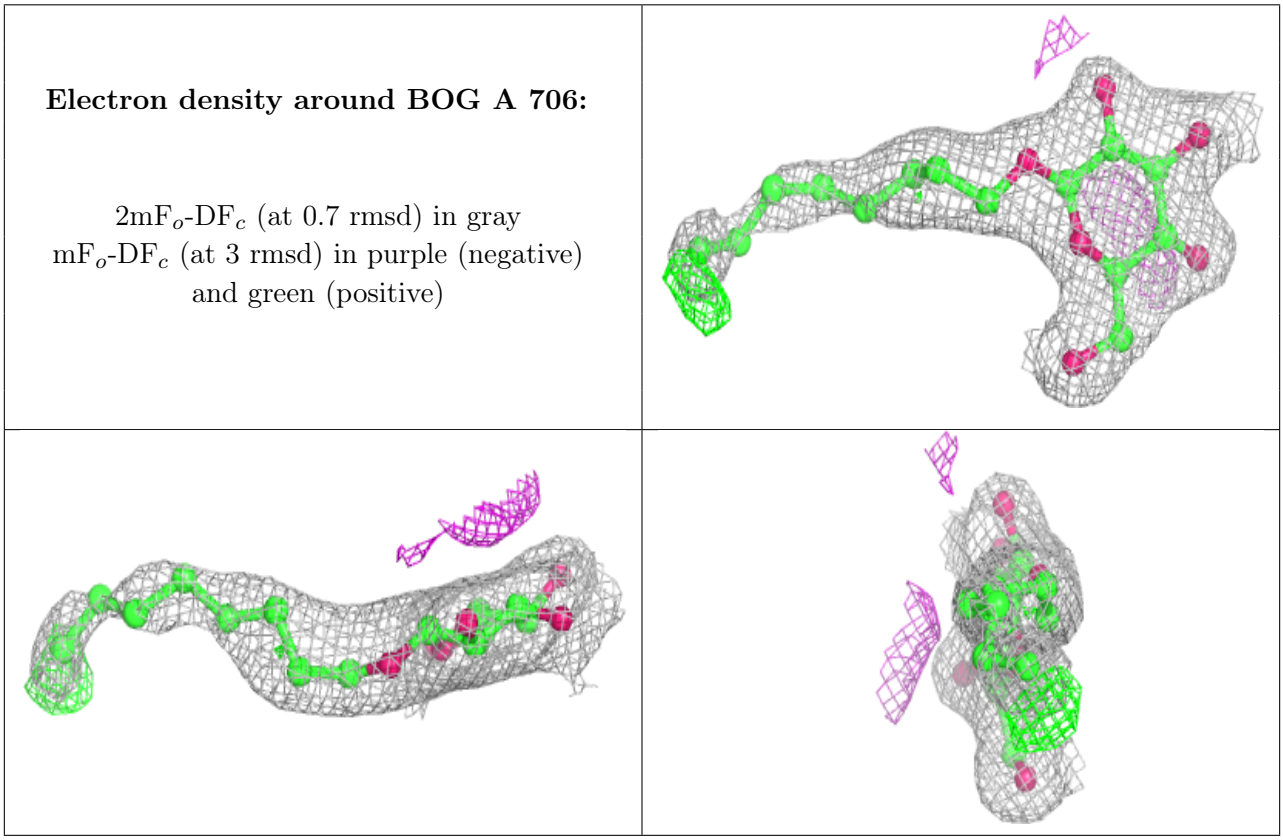
Electron density around PLM A 704:

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



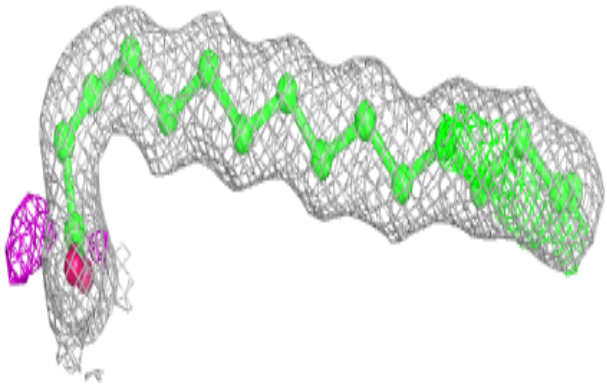
Electron density around BOG A 706:

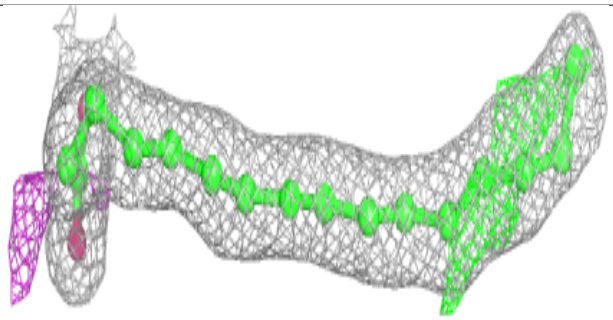
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

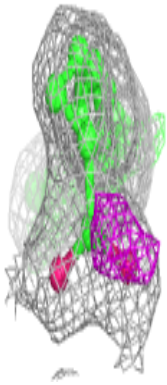


Electron density around PLM A 702:

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

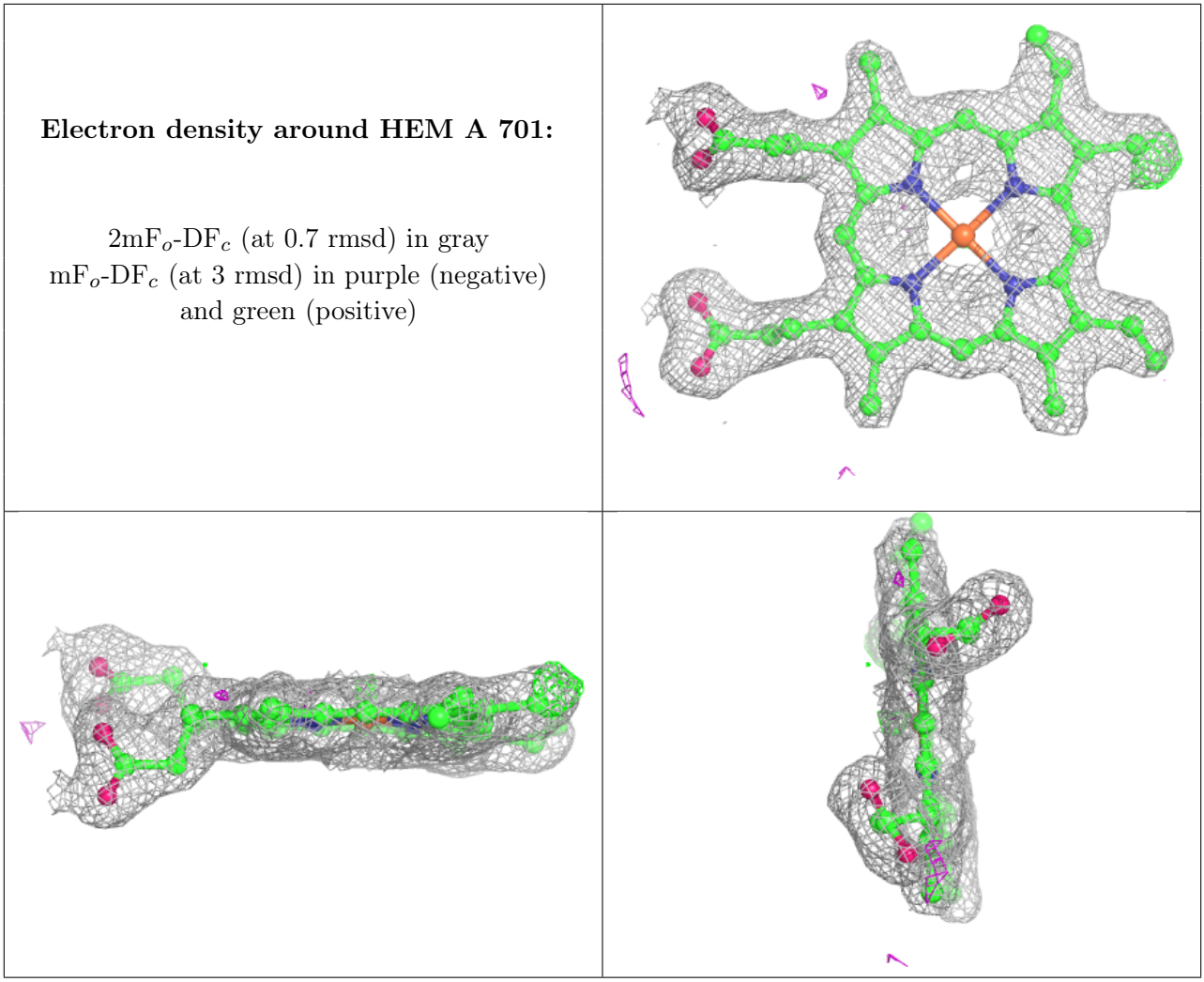






Electron density around HEM A 701:

$2mF_o$-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

There are no such residues in this entry.