

Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 08:44 PM EST

PDB ID : 4KVJ

Title : Crystal structure of Oryza sativa fatty acid alpha-dioxygenase with hydrogen

peroxide

Authors: Zhu, G.; Koszelak-Rosenblum, M.; Malkowski, M.G.

Deposited on : 2013-05-22

Resolution : 2.12 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 (1)) 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)

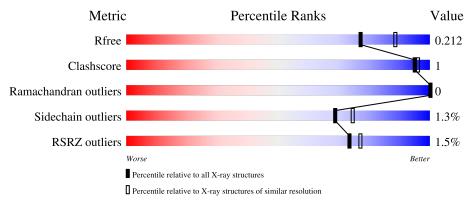
Validation Pipeline (wwPDB-VP) : 2.36

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 2.12 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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
			<u>%</u>
1	A	621	95%



2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 5440 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.

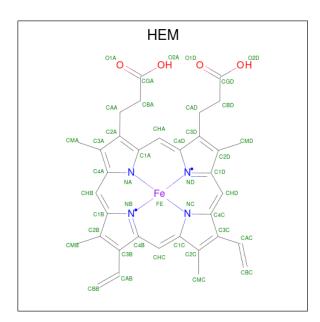
Mo	ol	Chain	Residues		\mathbf{At}	oms			ZeroOcc	AltConf	Trace
1		A	611	Total 4916	C 3137	N 848	O 911	S 20	0	1	0

There are 12 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

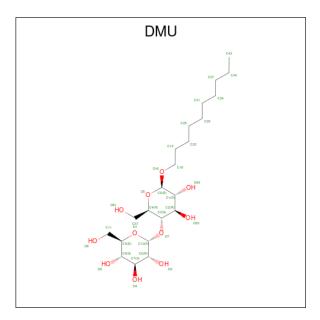
• Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).





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

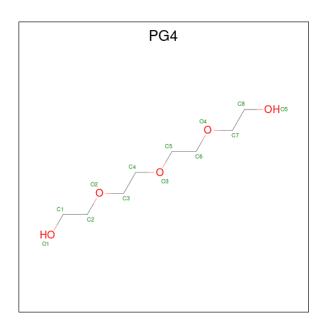
 \bullet Molecule 3 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}).$



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 33	C 22	O 11	0	0

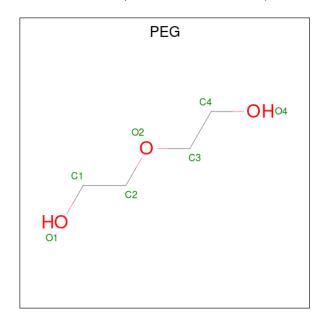
 \bullet Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $\mathrm{C_8H_{18}O_5}).$





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

 $\bullet \ \ Molecule \ 5 \ is \ DI(HYDROXYETHYL)ETHER \ (three-letter \ code: \ PEG) \ (formula: \ C_4H_{10}O_3). \\$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0

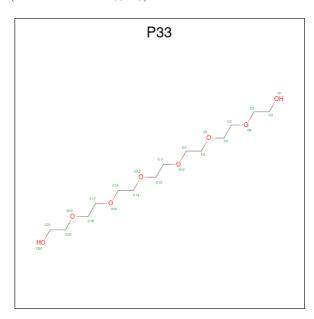
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0

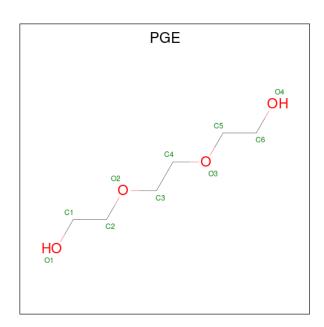
• Molecule 6 is 3,6,9,12,15,18-HEXAOXAICOSANE-1,20-DIOL (three-letter code: P33) (formula: $C_{14}H_{30}O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 22 14 8	0	0

 \bullet Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $\mathrm{C_6H_{14}O_4}).$





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

• Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

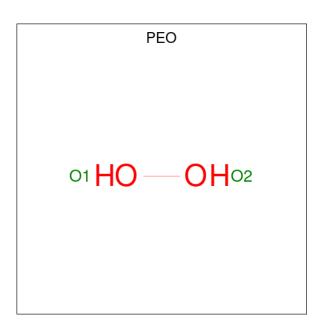
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Ca 1 1	0	0

• Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

• Molecule 10 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H_2O_2).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total O 2 2	0	0

• Molecule 11 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	2	Total Na 2 2	0	0

• Molecule 12 is water.

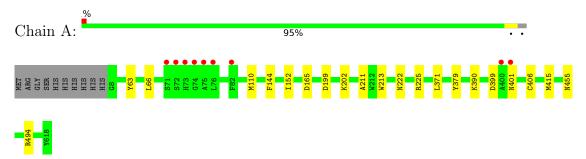
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	332	Total O 332 332	0	0



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: Fatty acid alpha-oxidase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	72.28Å 129.65Å 187.71Å	Donositon
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.86 - 2.12	Depositor
Resolution (A)	93.86 - 2.12	EDS
% Data completeness	99.3 (93.86-2.12)	Depositor
(in resolution range)	99.3 (93.86-2.12)	EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.56 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
P. P.	0.170 , 0.208	Depositor
R, R_{free}	0.176 , 0.212	DCC
R_{free} test set	2564 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36, 46.8	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5440	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: PGE, CL, PEG, PEO, PG4, DMU, CA, P33, HEM, NA

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).

Mal	Chain	Bond lengths		Bond angles	
MIOI		RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.37	0/5038	0.57	0/6812

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	4916	0	4850	9	0
2	A	43	0	30	2	0
3	A	33	0	42	0	0
4	A	26	0	36	0	0
5	A	49	0	70	0	0
6	A	22	0	30	1	0
7	A	10	0	14	1	0
8	A	1	0	0	0	0
9	A	4	0	0	0	0
10	A	2	0	0	0	0
11	A	2	0	0	0	0
12	A	332	0	0	1	0
All	All	5440	0	5072	12	0



The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (12) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:399:ASP:O	1:A:401:ASN:O	2.16	0.62
2:A:701:HEM:HBB2	2:A:701:HEM:HMB1	1.82	0.62
2:A:701:HEM:HHD	2:A:701:HEM:HBC2	1.86	0.57
1:A:390:LYS:HD3	1:A:406[A]:CYS:SG	2.46	0.55
1:A:494:ARG:HA	7:A:706:PGE:H42	1.94	0.48
6:A:705:P33:H111	6:A:705:P33:H142	1.52	0.47
1:A:211:ALA:HB1	1:A:371:LEU:HG	1.98	0.46
1:A:199:ASP:O	1:A:202:LYS:NZ	2.51	0.43
1:A:152:ILE:HD11	1:A:379:TYR:CE1	2.53	0.43
1:A:63:TYR:OH	12:A:1024:HOH:O	2.21	0.42
1:A:222:ASN:OD1	1:A:225:ARG:HG2	2.20	0.40
1:A:390:LYS:HG3	1:A:406[B]:CYS:SG	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	610/621 (98%)	589 (97%)	21 (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	527/535 (98%)	520 (99%)	7 (1%)	69 74

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

Mol	Chain	Res	Type
1	A	66	LEU
1	A	110	MET
1	A	144	PHE
1	A	165	ASP
1	A	213	TRP
1	A	415	MET
1	A	455	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	455	ASN

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, 7 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	Trino	Chain	Res	Link	Во	ond leng	$_{ m ths}$	Е	ond ang	gles			
MIOI	Type	Cham	Chain	Chain	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	HEM	A	701	10,1	41,50,50	1.32	5 (12%)	45,82,82	1.82	10 (22%)			
5	PEG	A	708	-	6,6,6	0.56	0	5,5,5	0.22	0			
7	PGE	A	706	-	9,9,9	0.50	0	8,8,8	0.47	0			
10	PEO	A	719	2	1,1,1	0.46	0	-					
4	PG4	A	707	11	12,12,12	0.42	0	11,11,11	0.34	0			
3	DMU	A	702	-	34,34,34	0.58	0	45,45,45	0.99	1 (2%)			
4	PG4	A	703	-	12,12,12	0.53	0	11,11,11	0.30	0			
5	PEG	A	711	-	6,6,6	0.45	0	5,5,5	0.34	0			
5	PEG	A	713	-	6,6,6	0.56	0	5,5,5	0.21	0			
5	PEG	A	704	-	6,6,6	0.43	0	5,5,5	0.34	0			
5	PEG	A	709	-	6,6,6	0.40	0	5,5,5	0.36	0			
5	PEG	A	712	-	6,6,6	0.42	0	5,5,5	0.30	0			
6	P33	A	705	11	21,21,21	0.64	0	20,20,20	0.67	0			
5	PEG	A	710	-	6,6,6	0.44	0	5,5,5	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
2	HEM	A	701	10,1	-	2/12/54/54	-
5	PEG	A	708	-	-	2/4/4/4	-
7	PGE	A	706	-	-	3/7/7/7	-
4	PG4	A	707	11	-	2/10/10/10	-
3	DMU	A	702	-	-	3/19/59/59	0/2/2/2
4	PG4	A	703	-	-	4/10/10/10	-
5	PEG	A	711	-	-	2/4/4/4	-
5	PEG	A	713	-	-	1/4/4/4	-
5	PEG	A	704	-	-	2/4/4/4	-
5	PEG	A	709	-	-	2/4/4/4	-
5	PEG	A	712	-	-	1/4/4/4	-
6	P33	A	705	11	-	9/19/19/19	_
5	PEG	A	710	-	-	3/4/4/4	_



All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
2	A	701	HEM	C1B-NB	-4.32	1.32	1.40
2	A	701	HEM	FE-NB	2.64	2.09	1.96
2	A	701	HEM	CHB-C1B	2.40	1.41	1.35
2	A	701	HEM	C4B-NB	-2.36	1.33	1.38
2	A	701	HEM	C4D-ND	-2.34	1.36	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
2	A	701	HEM	C1B-NB-C4B	5.14	110.39	105.07
2	A	701	HEM	CHC-C4B-NB	4.73	129.57	124.43
2	A	701	HEM	CHD-C1D-ND	3.64	128.38	124.43
2	A	701	HEM	CHA-C4D-ND	3.51	128.71	124.38
3	A	702	DMU	C10-O7-C3	-3.22	110.00	117.96
2	A	701	HEM	CHA-C4D-C3D	-3.06	119.58	125.33
2	A	701	HEM	CHD-C1D-C2D	-2.96	120.35	124.98
2	A	701	HEM	C4B-C3B-C2B	-2.29	105.30	107.11
2	A	701	HEM	C3C-C4C-NC	-2.28	106.63	110.94
2	A	701	HEM	CBD-CAD-C3D	-2.18	106.58	112.63
2	A	701	HEM	C2C-C3C-C4C	2.07	108.34	106.90

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	705	P33	C11-C12-O13-C14
6	A	705	P33	O16-C17-C18-O19
4	A	703	PG4	O3-C5-C6-O4
6	A	705	P33	O10-C11-C12-O13
4	A	707	PG4	O4-C7-C8-O5
5	A	710	PEG	O2-C3-C4-O4
7	A	706	PGE	O3-C5-C6-O4
5	A	712	PEG	O2-C3-C4-O4
6	A	705	P33	O4-C5-C6-O7
5	A	711	PEG	O2-C3-C4-O4
5	A	708	PEG	O2-C3-C4-O4
5	A	709	PEG	O1-C1-C2-O2
6	A	705	P33	O7-C8-C9-O10
3	A	702	DMU	C31-C34-C37-C40
3	A	702	DMU	O16-C18-C19-C22
7	A	706	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
5	A	704	PEG	O1-C1-C2-O2
4	A	703	PG4	O2-C3-C4-O3
5	A	708	PEG	C1-C2-O2-C3
6	A	705	P33	C9-C8-O7-C6
4	A	703	PG4	C3-C4-O3-C5
6	A	705	P33	C21-C20-O19-C18
6	A	705	P33	C15-C14-O13-C12
3	A	702	DMU	C34-C37-C40-C43
5	A	709	PEG	C4-C3-O2-C2
4	A	707	PG4	C1-C2-O2-C3
5	A	710	PEG	C1-C2-O2-C3
5	A	704	PEG	O2-C3-C4-O4
5	A	710	PEG	O1-C1-C2-O2
5	A	711	PEG	C4-C3-O2-C2
6	A	705	P33	O1-C2-C3-O4
2	A	701	HEM	CAA-CBA-CGA-O2A
2	A	701	HEM	CAA-CBA-CGA-O1A
7	A	706	PGE	C6-C5-O3-C4
5	A	713	PEG	O1-C1-C2-O2
4	A	703	PG4	C4-C3-O2-C2

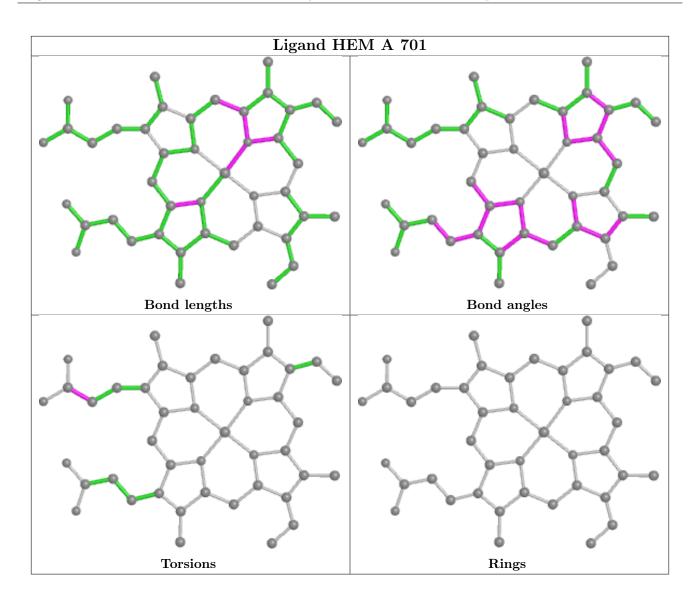
There are no ring outliers.

3 monomers are involved in 4 short contacts:

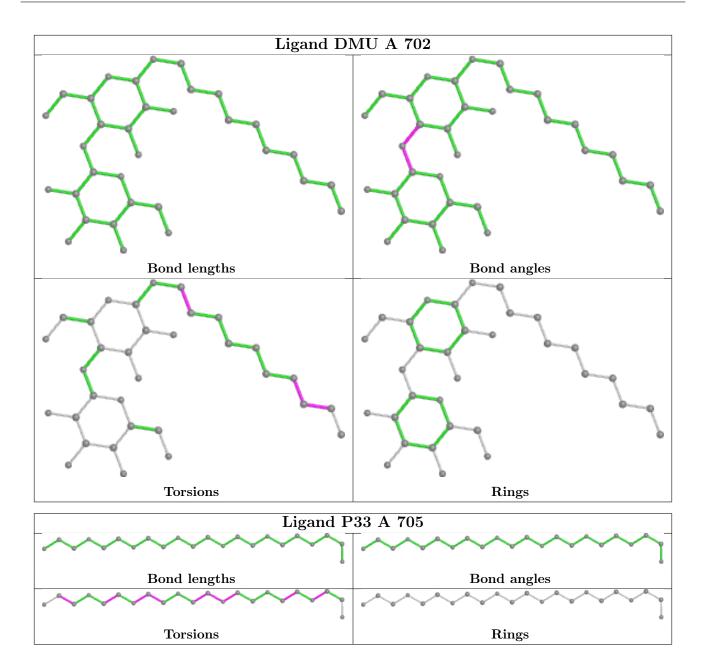
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	HEM	2	0
7	A	706	PGE	1	0
6	A	705	P33	1	0

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.









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, 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>	# RSRZ > 2	$OWAB(Å^2)$	Q < 0.9
1	A	611/621 (98%)	-0.12	9 (1%) 73 77	28, 41, 63, 115	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	400	ALA	6.8
1	A	75	ALA	6.4
1	A	74	GLY	4.8
1	A	73	HIS	4.8
1	A	76	LEU	3.7
1	A	72	SER	3.6
1	A	401	ASN	3.3
1	A	71	SER	3.0
1	A	82	PHE	2.2

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)

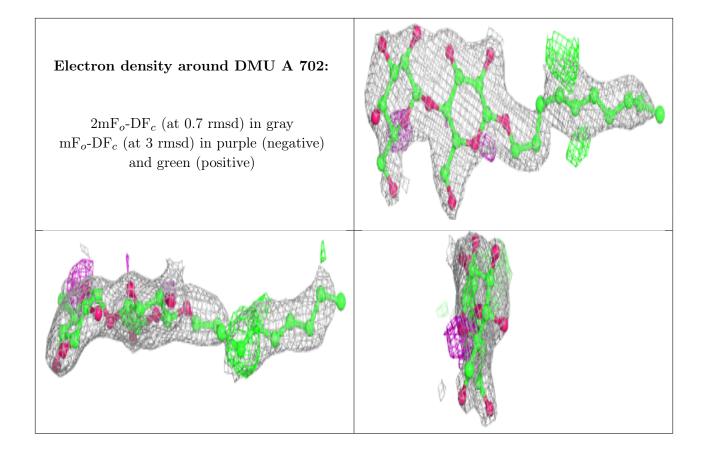
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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



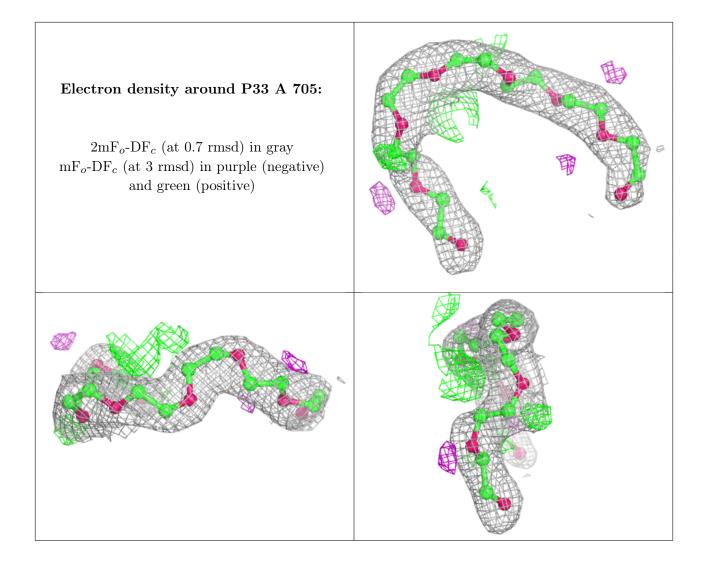
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}({ ext{\AA}}^2)$	Q < 0.9
5	PEG	A	712	7/7	0.70	0.28	78,79,82,82	0
5	PEG	A	713	7/7	0.73	0.19	68,70,74,74	0
5	PEG	A	711	7/7	0.81	0.15	77,77,79,79	0
3	DMU	A	702	33/33	0.82	0.17	58,69,82,82	0
7	PGE	A	706	10/10	0.87	0.19	57,63,66,69	0
5	PEG	A	708	7/7	0.88	0.14	61,62,64,64	0
4	PG4	A	703	13/13	0.89	0.20	57,63,67,68	0
5	PEG	A	704	7/7	0.90	0.25	60,60,62,63	0
11	NA	A	720	1/1	0.90	0.09	64,64,64,64	0
5	PEG	A	710	7/7	0.91	0.17	72,73,74,75	0
6	P33	A	705	22/22	0.92	0.17	50,58,64,66	0
10	PEO	A	719	2/2	0.94	0.12	58,58,58,60	0
5	PEG	A	709	7/7	0.94	0.20	63,64,65,68	0
4	PG4	A	707	13/13	0.95	0.16	54,57,65,69	0
9	CL	A	718	1/1	0.95	0.07	49,49,49,49	0
11	NA	A	721	1/1	0.96	0.14	61,61,61,61	0
2	HEM	A	701	43/43	0.97	0.12	38,41,44,46	0
9	CL	A	717	1/1	0.97	0.08	51,51,51,51	0
8	CA	A	714	1/1	0.98	0.05	57,57,57,57	0
9	CL	A	715	1/1	0.99	0.11	38,38,38,38	0
9	CL	A	716	1/1	1.00	0.10	40,40,40,40	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.

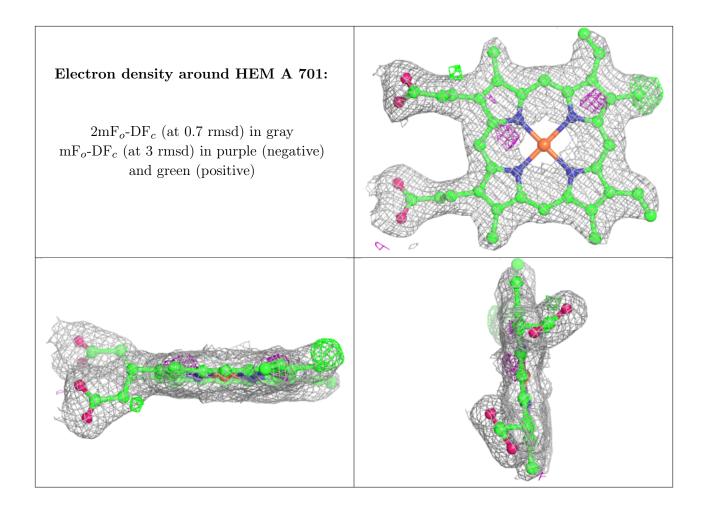












6.5 Other polymers (i)

There are no such residues in this entry.

