



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:11 PM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

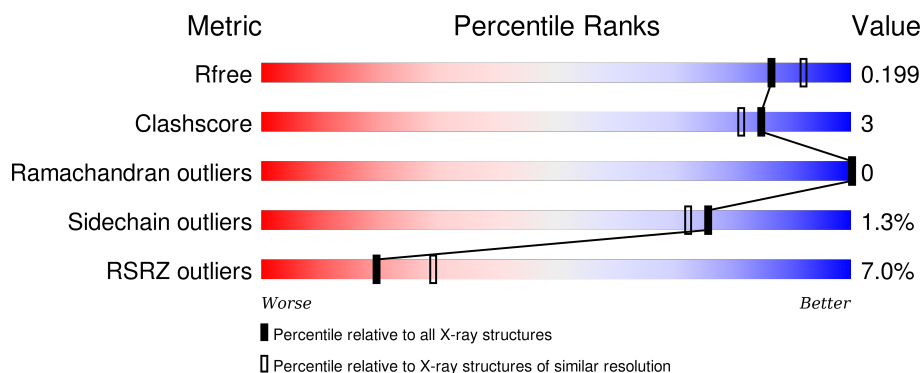
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

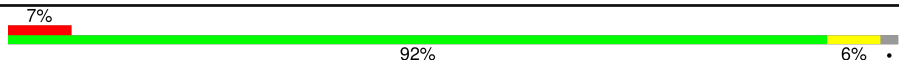
The reported resolution of this entry is 1.96 Å.

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}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	621	

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
3	PLM	A	704	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	BOG	A	710	-	-	-	X
8	PGE	A	712	-	-	-	X
8	PGE	A	713	-	-	-	X
8	PGE	A	714	-	-	-	X

2 Entry composition

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:

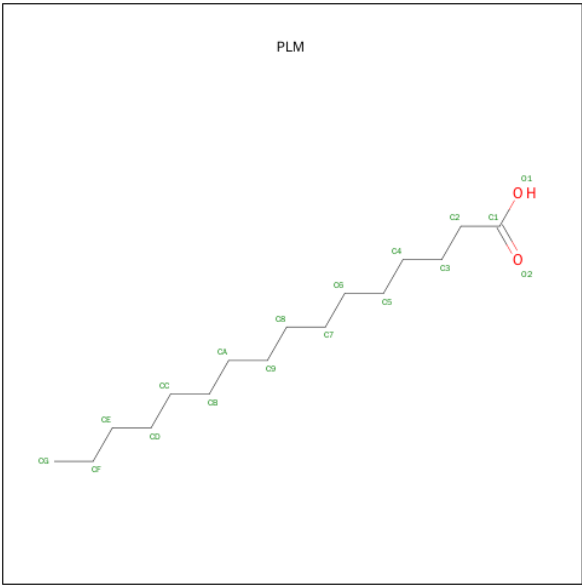
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP Q9M5J1
A	-1	ARG	-	EXPRESSION TAG	UNP Q9M5J1
A	0	GLY	-	EXPRESSION TAG	UNP Q9M5J1
A	1	SER	-	EXPRESSION TAG	UNP Q9M5J1
A	2	HIS	-	EXPRESSION TAG	UNP Q9M5J1
A	3	HIS	-	EXPRESSION TAG	UNP Q9M5J1
A	4	HIS	-	EXPRESSION TAG	UNP Q9M5J1
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: C₁₆H₃₂O₂).

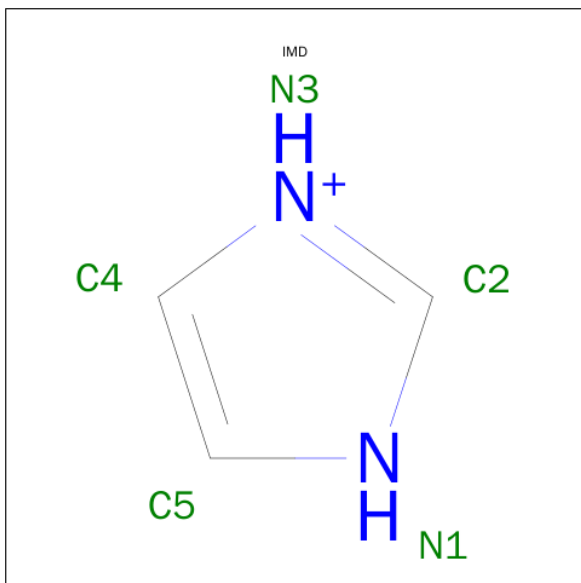


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			18	16	2		
3	A	1	Total	C	O	0	0
			18	16	2		

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

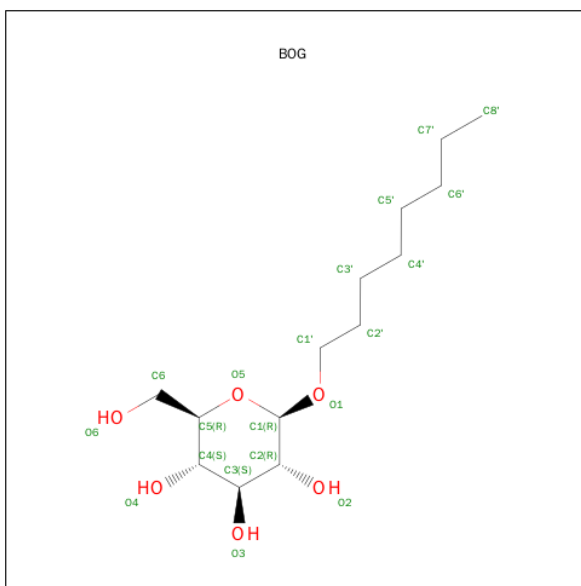
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

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



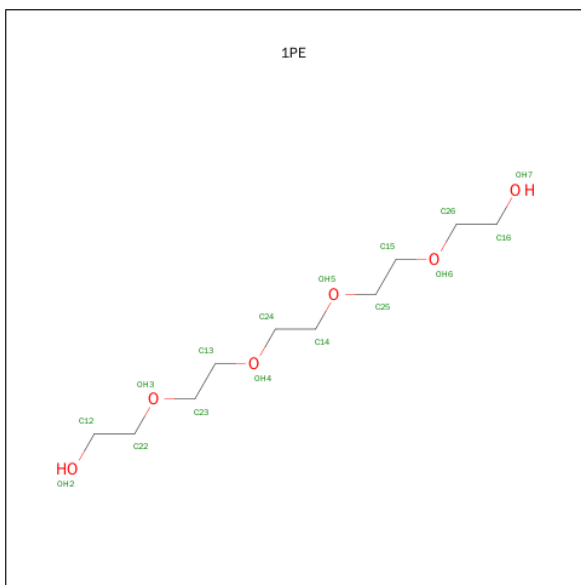
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			5	3	2		

- Molecule 6 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



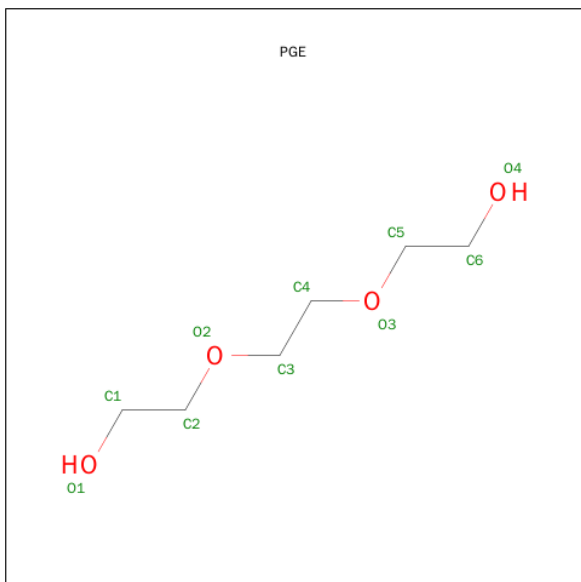
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			20	14	6		
6	A	1	Total	C	O	0	0
			20	14	6		

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $\text{C}_{10}\text{H}_{22}\text{O}_6$).



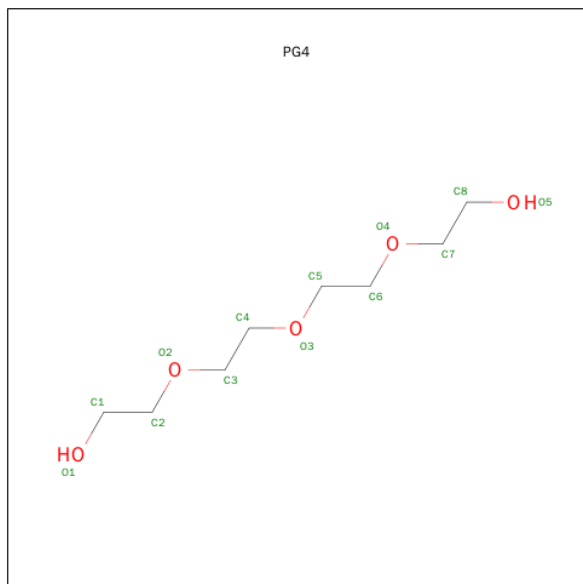
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $\text{C}_6\text{H}_{14}\text{O}_4$).



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

- 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	0	0
			13	8	5		

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

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

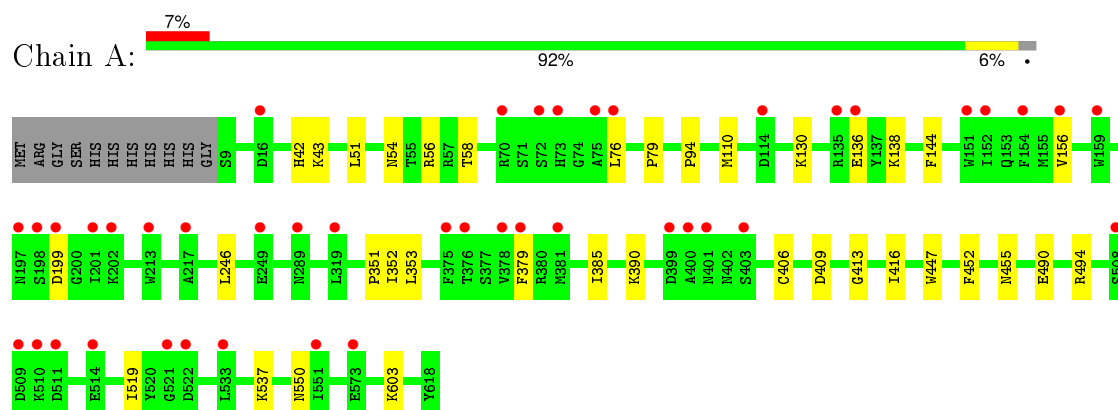
- Molecule 11 is water.

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

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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

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
$\langle I/\sigma(I) \rangle$ 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	3248 reflections (5.33%)	DCC
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 , 45.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 64389 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PGE, IMD, CL, CA, 1PE, PG4, HEM, PLM, BOG

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:C1	8:A:714:PGE:H42	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:C1	8:A:714:PGE:C4	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:416[A]:ILE:HD11	1:A:452:PHE:CE1	2.52	0.45
1:A:385:ILE:HG21	1:A:452:PHE:HZ	1.82	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:H4	8:A:708:PGE:H6	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%)	76	72

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

Some 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 carbohydrates 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	$\# Z > 2$
2	HEM	A	701	1,5	30,50,50	2.30	8 (26%)	24,82,82	2.47	13 (54%)
3	PLM	A	702	-	14,17,17	0.31	0	14,17,17	0.72	0
3	PLM	A	704	-	14,17,17	0.17	0	14,17,17	0.67	0
5	IMD	A	705	2	3,5,5	0.49	0	4,5,5	0.52	0
6	BOG	A	706	-	20,20,20	0.66	0	25,25,25	0.95	1 (4%)
7	1PE	A	707	-	15,15,15	0.45	0	14,14,14	0.38	0
8	PGE	A	708	-	9,9,9	0.46	0	8,8,8	0.37	0
8	PGE	A	709	-	9,9,9	0.41	0	8,8,8	0.46	0
6	BOG	A	710	-	20,20,20	0.48	0	25,25,25	1.79	8 (32%)
9	PG4	A	711	-	12,12,12	0.54	0	11,11,11	0.42	0
8	PGE	A	712	-	9,9,9	0.44	0	8,8,8	0.37	0
8	PGE	A	713	-	9,9,9	0.52	0	8,8,8	0.28	0
8	PGE	A	714	-	9,9,9	0.62	0	8,8,8	1.00	1 (12%)
8	PGE	A	715	-	9,9,9	0.51	0	8,8,8	0.33	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	1,5	-	0/10/54/54	0/0/8/8
3	PLM	A	702	-	-	0/13/15/15	0/0/0/0
3	PLM	A	704	-	-	0/13/15/15	0/0/0/0
5	IMD	A	705	2	-	0/0/0/0	0/1/1/1
6	BOG	A	706	-	-	0/11/31/31	0/1/1/1
7	1PE	A	707	-	-	0/13/13/13	0/0/0/0
8	PGE	A	708	-	-	0/7/7/7	0/0/0/0
8	PGE	A	709	-	-	0/7/7/7	0/0/0/0
6	BOG	A	710	-	-	0/11/31/31	0/1/1/1
9	PG4	A	711	-	-	0/10/10/10	0/0/0/0
8	PGE	A	712	-	-	0/7/7/7	0/0/0/0
8	PGE	A	713	-	-	0/7/7/7	0/0/0/0
8	PGE	A	714	-	-	0/7/7/7	0/0/0/0
8	PGE	A	715	-	-	0/7/7/7	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	HEM	C3B-C4B	-6.78	1.45	1.51
2	A	701	HEM	C3D-C4D	-5.39	1.44	1.51
2	A	701	HEM	C2C-C1C	-2.97	1.46	1.52
2	A	701	HEM	CAA-C2A	2.23	1.55	1.52
2	A	701	HEM	FE-NB	2.53	2.10	1.97
2	A	701	HEM	FE-ND	2.89	2.12	1.97
2	A	701	HEM	FE-NC	3.43	2.09	1.95
2	A	701	HEM	C4C-NC	3.57	1.40	1.36

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	710	BOG	O2-C2-C3	-3.71	101.98	110.34
2	A	701	HEM	CAA-CBA-CGA	-3.35	106.60	112.75
6	A	710	BOG	O5-C5-C4	-3.04	103.98	109.68
6	A	710	BOG	O4-C4-C3	-2.90	103.80	110.34
2	A	701	HEM	C3B-C4B-NB	-2.60	106.67	111.63
6	A	706	BOG	O5-C1-C2	-2.33	105.50	110.28
2	A	701	HEM	CBD-CAD-C3D	-2.15	107.30	113.55
2	A	701	HEM	CAA-C2A-C1A	-2.13	124.69	127.01
6	A	710	BOG	C3-C4-C5	-2.13	106.48	110.20
6	A	710	BOG	O5-C1-C2	2.04	114.45	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	HEM	C1D-CHD-C4C	2.04	129.23	125.82
8	A	714	PGE	C3-O2-C2	2.16	122.59	113.31
6	A	710	BOG	C6-C5-C4	2.27	118.61	113.02
6	A	710	BOG	C4-C3-C2	2.33	115.14	110.79
2	A	701	HEM	C2C-C1C-CHC	2.33	127.23	123.68
2	A	701	HEM	CMD-C2D-C3D	2.46	125.23	114.35
2	A	701	HEM	C3B-C4B-CHC	2.72	126.99	123.16
6	A	710	BOG	O5-C5-C6	2.94	113.78	106.36
2	A	701	HEM	C2D-C3D-C4D	2.98	106.56	101.50
2	A	701	HEM	CAD-C3D-C4D	3.90	126.22	112.47
2	A	701	HEM	CMC-C2C-C3C	3.94	126.38	116.53
2	A	701	HEM	CMB-C2B-C3B	4.32	127.31	116.53
2	A	701	HEM	CAD-C3D-C2D	4.87	127.21	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 16 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	610/621 (98%)	0.20	43 (7%) 19 29	17, 30, 51, 75	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	400	ALA	10.0
1	A	76	LEU	6.7
1	A	401	ASN	6.6
1	A	73	HIS	6.2
1	A	156	VAL	5.1
1	A	72	SER	4.7
1	A	199	ASP	4.1
1	A	510	LYS	3.5
1	A	152	ILE	3.4
1	A	136	GLU	3.2
1	A	70	ARG	3.1
1	A	249	GLU	3.1
1	A	159	TRP	3.1
1	A	403	SER	3.0
1	A	511	ASP	3.0
1	A	375	PHE	3.0
1	A	399	ASP	3.0
1	A	16	ASP	3.0
1	A	197	ASN	2.9
1	A	378	VAL	2.7
1	A	522	ASP	2.6
1	A	75	ALA	2.6
1	A	514	GLU	2.6
1	A	154	PHE	2.5
1	A	379	PHE	2.5
1	A	202	LYS	2.4
1	A	289	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	201	ILE	2.3
1	A	217	ALA	2.3
1	A	508	SER	2.3
1	A	376	THR	2.2
1	A	198	SER	2.2
1	A	114	ASP	2.2
1	A	573	GLU	2.1
1	A	151	TRP	2.1
1	A	381	MET	2.1
1	A	551	ILE	2.1
1	A	319	LEU	2.1
1	A	521	GLY	2.1
1	A	533	LEU	2.1
1	A	135	ARG	2.0
1	A	509	ASP	2.0
1	A	213	TRP	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
6	BOG	A	710	20/20	0.81	0.19	4.41	57,73,81,82	0
8	PGE	A	714	10/10	0.78	0.15	4.39	56,70,72,74	0
3	PLM	A	704	18/18	0.92	0.15	3.42	32,43,48,48	0
8	PGE	A	712	10/10	0.89	0.17	2.96	50,54,62,66	0
8	PGE	A	713	10/10	0.81	0.16	2.67	55,62,66,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	PLM	A	702	18/18	0.94	0.24	1.90	18,25,39,41	0
6	BOG	A	706	20/20	0.93	0.12	1.75	26,47,62,64	0
7	1PE	A	707	16/16	0.95	0.12	1.49	37,45,50,52	0
8	PGE	A	709	10/10	0.91	0.16	1.25	47,53,58,62	0
8	PGE	A	708	10/10	0.89	0.17	1.19	40,49,56,60	0
9	PG4	A	711	13/13	0.81	0.24	0.82	35,60,69,69	0
2	HEM	A	701	43/43	0.98	0.16	0.03	22,26,31,39	0
5	IMD	A	705	5/5	0.97	0.10	-1.38	30,36,37,40	0
10	CL	A	716	1/1	0.98	0.05	-1.74	30,30,30,30	0
4	CA	A	703	1/1	0.99	0.08	-1.87	29,29,29,29	0
10	CL	A	717	1/1	0.99	0.05	-	32,32,32,32	0
8	PGE	A	715	10/10	0.77	0.19	-	73,78,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.