Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2017 – 11:24 PM EST

PDB ID	:	5M0O
Title	:	Crystal structure of cytochrome P450 OleT H85Q in complex with arachidonic acid
Authors	:	Tee, K.L.; Munro, A.; Matthews, S.; Leys, D.; Levy, C.
Deposited on	:	2016-10-05
Resolution	:	1.80 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 ①) were used in the production of this report:

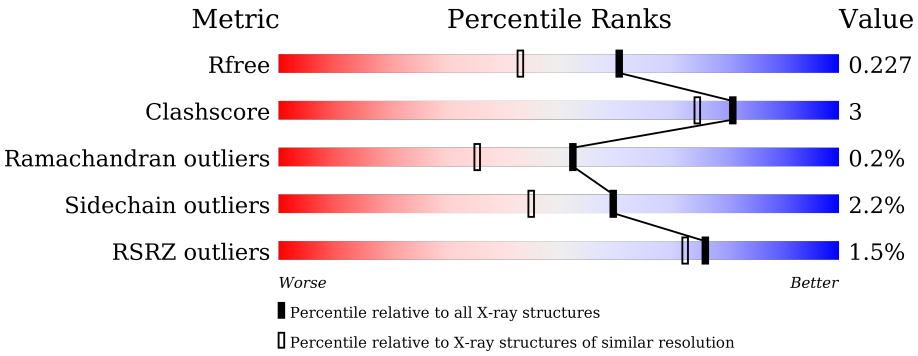
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 <=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	422	2% 90% 8%
2	C	428	3% 89% 8%

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
4	EPA	A	502	-	-	-	X
4	EPA	C	502	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7482 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 Terminal olefin-forming fatty acid decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	4	0
			3407	2164	586	641	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	GLN	HIS	engineered mutation	UNP E9NSU2

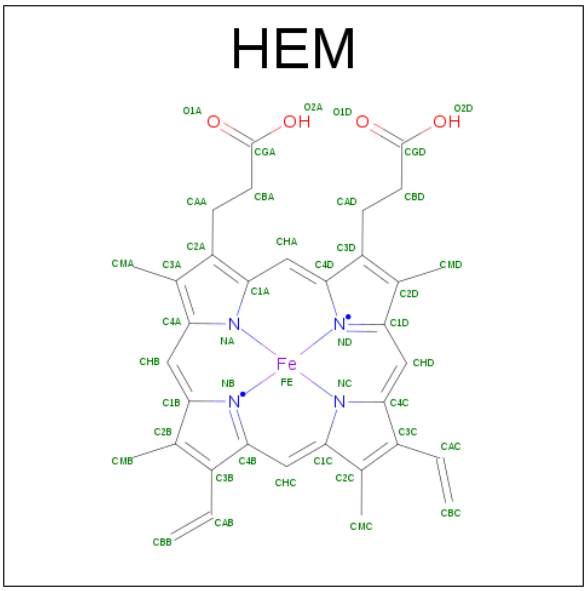
- Molecule 2 is a protein called Terminal olefin-forming fatty acid decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	421	Total	C	N	O	S	0	1	0
			3390	2157	583	634	16			

There are 7 discrepancies between the modelled and reference sequences:

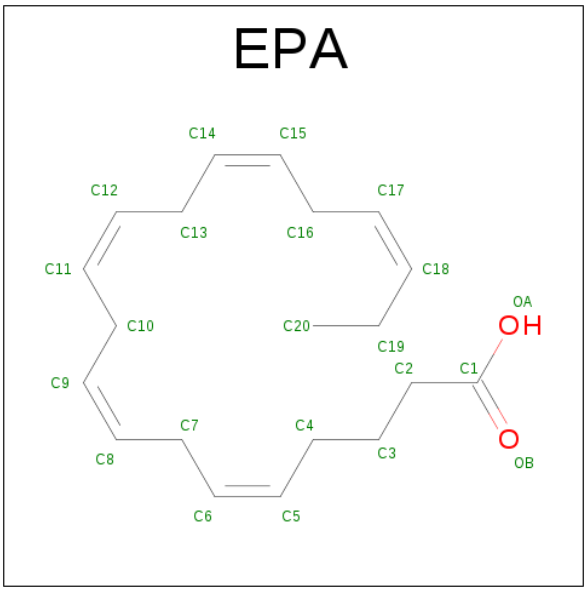
Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	expression tag	UNP E9NSU2
C	-4	HIS	-	expression tag	UNP E9NSU2
C	-3	HIS	-	expression tag	UNP E9NSU2
C	-2	HIS	-	expression tag	UNP E9NSU2
C	-1	HIS	-	expression tag	UNP E9NSU2
C	0	HIS	-	expression tag	UNP E9NSU2
C	85	GLN	HIS	engineered mutation	UNP E9NSU2

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is 5,8,11,14,17-EICOSAPENTAENOIC ACID (three-letter code: EPA) (formula: $C_{20}H_{30}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			22	20	2		

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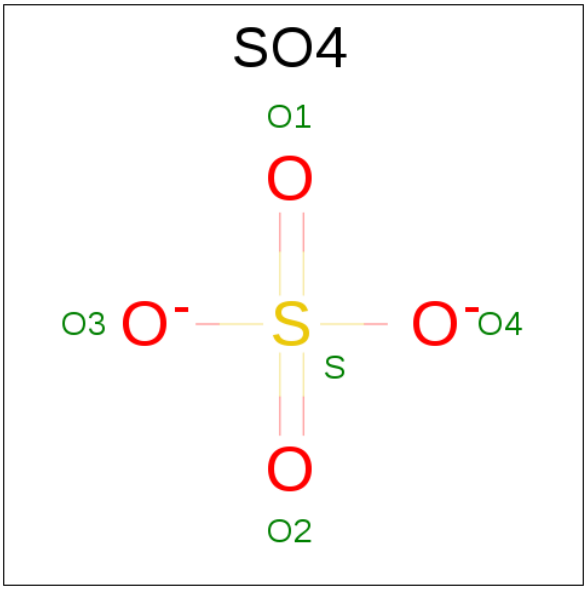
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 22 20 2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

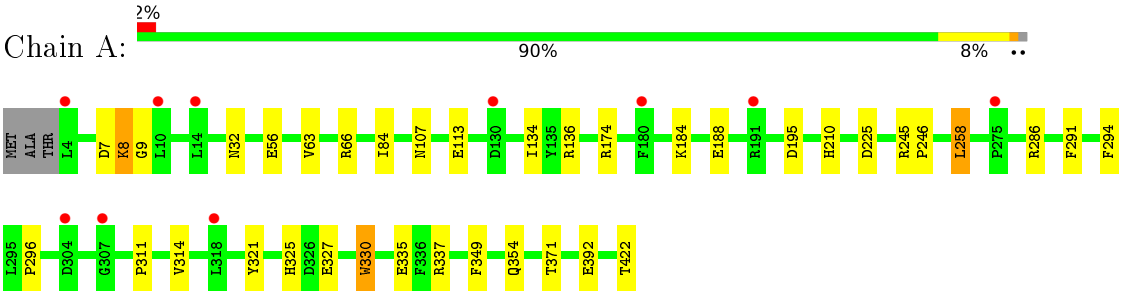
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	248	Total O 248 248	0	0
6	C	302	Total O 302 302	0	0

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 (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.

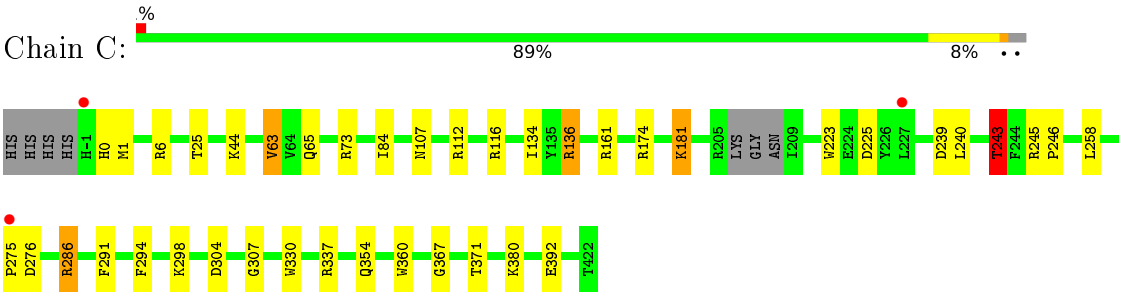
- Molecule 1: Terminal olefin-forming fatty acid decarboxylase

Chain A:



- Molecule 2: Terminal olefin-forming fatty acid decarboxylase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	48.93Å 115.49Å 163.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.50 – 1.80 25.51 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (25.50-1.80) 99.4 (25.51-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.181 , 0.220 0.190 , 0.227	Depositor DCC
R_{free} test set	4230 reflections (5.16%)	DCC
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 45.7	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	0.96	EDS
Total number of atoms	7482	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: HEM, SO4, EPA

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	0.90	1/3486 (0.0%)	0.92	10/4721 (0.2%)
2	C	0.98	3/3469 (0.1%)	1.01	19/4700 (0.4%)
All	All	0.94	4/6955 (0.1%)	0.97	29/9421 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	1	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	360	TRP	CB-CG	6.25	1.61	1.50
2	C	223	TRP	CB-CG	-5.95	1.39	1.50
1	A	392	GLU	CD-OE1	5.24	1.31	1.25
2	C	330	TRP	CE3-CZ3	-5.04	1.29	1.38

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	136	ARG	NE-CZ-NH1	11.75	126.18	120.30
2	C	136	ARG	NE-CZ-NH2	-9.82	115.39	120.30
2	C	136	ARG	CB-CG-CD	8.97	134.92	111.60
1	A	136	ARG	NE-CZ-NH1	8.54	124.57	120.30
2	C	286	ARG	NE-CZ-NH2	8.16	124.38	120.30
2	C	112	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	174	ARG	NE-CZ-NH1	6.98	123.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	243	THR	OG1-CB-CG2	6.89	125.85	110.00
2	C	286	ARG	NE-CZ-NH1	-6.59	117.00	120.30
1	A	225	ASP	CB-CG-OD1	6.45	124.11	118.30
2	C	73	ARG	NE-CZ-NH1	6.16	123.38	120.30
2	C	239	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	66	ARG	NE-CZ-NH2	-6.11	117.24	120.30
2	C	63	VAL	CG1-CB-CG2	6.06	120.60	110.90
2	C	174	ARG	NE-CZ-NH1	5.92	123.26	120.30
2	C	116	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	A	195	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	136	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	330	TRP	N-CA-C	-5.69	95.65	111.00
2	C	161	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	C	225	ASP	CB-CG-OD2	-5.61	113.25	118.30
2	C	245	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	225	ASP	CB-CG-OD2	-5.37	113.47	118.30
2	C	63	VAL	N-CA-CB	-5.28	99.88	111.50
1	A	337	ARG	NE-CZ-NH1	5.27	122.93	120.30
2	C	243	THR	N-CA-CB	-5.24	100.34	110.30
2	C	161	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	A	195	ASP	CB-CG-OD2	-5.05	113.75	118.30
2	C	225	ASP	CB-CG-OD1	5.00	122.80	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	243	THR	CB

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	3407	0	3321	16	1
2	C	3390	0	3312	25	0
3	A	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	43	0	30	5	0
4	A	22	0	27	1	0
4	C	22	0	27	0	0
5	A	5	0	0	0	0
6	A	248	0	0	3	2
6	C	302	0	0	14	3
All	All	7482	0	6747	45	3

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 (45) 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)
2:C:275:PRO:HA	6:C:750:HOH:O	1.60	1.00
1:A:113[A]:GLU:OE2	6:A:601:HOH:O	1.84	0.93
2:C:25:THR:HG21	6:C:886:HOH:O	1.74	0.87
2:C:25:THR:HG23	6:C:626:HOH:O	1.76	0.86
2:C:25:THR:CG2	6:C:886:HOH:O	2.25	0.84
2:C:276:ASP:HB3	6:C:864:HOH:O	1.81	0.81
3:A:501:HEM:HMC2	3:A:501:HEM:HBC2	1.68	0.76
2:C:337:ARG:HD2	6:C:636:HOH:O	1.88	0.73
2:C:25:THR:HG22	6:C:749:HOH:O	1.92	0.68
3:A:501:HEM:CMC	3:A:501:HEM:HBC2	2.30	0.61
2:C:286:ARG:HH21	2:C:354:GLN:NE2	2.01	0.59
3:C:501:HEM:HBC2	3:C:501:HEM:HMC2	1.85	0.59
1:A:246:PRO:HB2	3:A:501:HEM:C1C	2.39	0.57
2:C:246:PRO:HB2	3:C:501:HEM:C1C	2.40	0.55
2:C:44:LYS:HD2	6:C:810:HOH:O	2.07	0.55
1:A:184:LYS:HE2	1:A:188:GLU:OE1	2.07	0.54
2:C:380:LYS:HD3	6:C:891:HOH:O	2.09	0.53
2:C:181:LYS:HD3	6:C:792:HOH:O	2.09	0.52
1:A:286:ARG:HH21	1:A:354:GLN:NE2	2.08	0.52
2:C:134:ILE:HG13	2:C:258:LEU:HD12	1.93	0.51
3:C:501:HEM:HBC2	3:C:501:HEM:CMC	2.40	0.51
1:A:354:GLN:HE22	1:A:371:THR:HG21	1.75	0.51
2:C:6:ARG:NH1	6:C:604:HOH:O	2.44	0.50
1:A:134:ILE:HG13	1:A:258:LEU:HD12	1.93	0.50
1:A:296:PRO:HB3	4:A:502:EPA:H151	1.94	0.48
2:C:240:LEU:O	2:C:243:THR:HG22	2.15	0.47
1:A:311:PRO:O	1:A:314:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:354:GLN:HE22	2:C:371:THR:HG21	1.80	0.47
2:C:298:LYS:HE2	6:C:602:HOH:O	2.14	0.46
2:C:65:GLN:OE1	2:C:298:LYS:HE2	2.16	0.45
1:A:321:TYR:CE2	1:A:325:HIS:CE1	3.05	0.45
1:A:327:GLU:O	1:A:330:TRP:O	2.34	0.45
2:C:275:PRO:O	2:C:276:ASP:HB2	2.16	0.45
2:C:298:LYS:HE3	6:C:724:HOH:O	2.17	0.43
2:C:367:GLY:HA3	3:C:501:HEM:C3C	2.53	0.43
2:C:1:MET:HE3	2:C:307:GLY:HA2	2.01	0.42
1:A:7:ASP:OD1	1:A:8:LYS:HG2	2.20	0.41
1:A:210:HIS:CE1	6:A:656:HOH:O	2.72	0.41
2:C:0:HIS:HE1	2:C:304:ASP:OD2	2.03	0.41
2:C:246:PRO:HB2	3:C:501:HEM:C2C	2.55	0.41
1:A:56:GLU:HG2	1:A:349:PHE:CZ	2.57	0.40
1:A:245:ARG:HB3	1:A:246:PRO:HD3	2.04	0.40
1:A:335:GLU:HB3	6:A:617:HOH:O	2.22	0.40
1:A:184:LYS:O	1:A:188:GLU:HG3	2.21	0.40
2:C:337:ARG:CD	6:C:636:HOH:O	2.59	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:602:HOH:O	6:C:703:HOH:O[3_644]	1.09	1.11
6:A:772:HOH:O	6:C:703:HOH:O[3_644]	1.95	0.25
1:A:422:THR:C	6:C:703:HOH:O[3_644]	2.17	0.03

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	421/422 (100%)	409 (97%)	10 (2%)	2 (0%)	34 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	C	418/428 (98%)	409 (98%)	9 (2%)	0	100 100
All	All	839/850 (99%)	818 (98%)	19 (2%)	2 (0%)	52 35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	9	GLY

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	364/365 (100%)	357 (98%)	7 (2%)	65 52
2	C	361/371 (97%)	352 (98%)	9 (2%)	55 39
All	All	725/736 (98%)	709 (98%)	16 (2%)	60 45

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	63	VAL
1	A	84	ILE
1	A	107	ASN
1	A	258	LEU
1	A	291	PHE
1	A	294	PHE
2	C	63	VAL
2	C	84	ILE
2	C	107	ASN
2	C	136	ARG
2	C	181	LYS
2	C	243	THR
2	C	291	PHE

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Mol	Chain	Res	Type
2	C	294	PHE
2	C	392	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	61	ASN
1	A	107	ASN
1	A	124	GLN
1	A	334	ASN
1	A	354	GLN
2	C	0	HIS
2	C	32	ASN
2	C	61	ASN
2	C	107	ASN
2	C	122	ASN
2	C	334	ASN
2	C	354	GLN

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

5 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
3	HEM	A	501	1,6	24,50,50	1.45	2 (8%)	16,82,82	1.43	3 (18%)
4	EPA	A	502	-	18,21,21	2.11	7 (38%)	18,21,21	4.14	10 (55%)
5	SO4	A	503	-	4,4,4	2.23	2 (50%)	6,6,6	0.59	0
3	HEM	C	501	2,6	24,50,50	1.84	5 (20%)	16,82,82	1.59	4 (25%)
4	EPA	C	502	-	18,21,21	2.07	7 (38%)	18,21,21	4.24	10 (55%)

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
3	HEM	A	501	1,6	-	0/6/54/54	0/0/8/8
4	EPA	A	502	-	-	0/17/19/19	0/0/0/0
5	SO4	A	503	-	-	0/0/0/0	0/0/0/0
3	HEM	C	501	2,6	-	0/6/54/54	0/0/8/8
4	EPA	C	502	-	-	0/17/19/19	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	HEM	C3B-C2B	-5.23	1.33	1.40
3	C	501	HEM	C3B-C2B	-4.88	1.34	1.40
3	C	501	HEM	C1B-NB	-4.59	1.30	1.36
4	C	502	EPA	C16-C17	-3.09	1.33	1.50
4	A	502	EPA	C20-C19	-3.07	1.29	1.48
4	A	502	EPA	C16-C17	-2.86	1.34	1.50
4	C	502	EPA	C20-C19	-2.83	1.31	1.48
3	C	501	HEM	C3C-C2C	-2.82	1.36	1.40
3	C	501	HEM	C3D-C2D	-2.45	1.30	1.37
5	A	503	SO4	O2-S	2.09	1.54	1.47
3	C	501	HEM	CAA-C2A	2.45	1.56	1.52
3	A	501	HEM	CAA-C2A	2.51	1.56	1.52
4	C	502	EPA	C9-C8	3.19	1.50	1.31
4	C	502	EPA	C12-C11	3.34	1.51	1.31
4	A	502	EPA	C18-C17	3.36	1.51	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	503	SO4	O3-S	3.37	1.59	1.47
4	A	502	EPA	C6-C5	3.45	1.52	1.31
4	C	502	EPA	C15-C14	3.48	1.52	1.31
4	A	502	EPA	C15-C14	3.49	1.52	1.31
4	C	502	EPA	C18-C17	3.51	1.52	1.31
4	A	502	EPA	C9-C8	3.52	1.52	1.31
4	C	502	EPA	C6-C5	3.61	1.53	1.31
4	A	502	EPA	C12-C11	3.65	1.53	1.31

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	502	EPA	C2-C3-C4	-4.15	105.69	113.41
4	C	502	EPA	C7-C6-C5	-3.55	102.95	124.38
4	A	502	EPA	C7-C6-C5	-3.18	105.19	124.38
4	C	502	EPA	C7-C8-C9	-3.06	105.94	124.38
3	A	501	HEM	C3C-C4C-NC	-2.94	105.40	110.94
4	A	502	EPA	C2-C3-C4	-2.86	108.10	113.41
4	A	502	EPA	C7-C8-C9	-2.70	108.11	124.38
4	A	502	EPA	C10-C9-C8	-2.61	108.62	124.38
3	A	501	HEM	C3B-C4B-NB	-2.50	105.98	109.21
4	A	502	EPA	C19-C18-C17	-2.47	115.65	127.15
3	C	501	HEM	C3B-C4B-NB	-2.38	106.13	109.21
4	C	502	EPA	C16-C15-C14	-2.37	110.11	124.38
4	A	502	EPA	C10-C11-C12	-2.22	110.99	124.38
4	A	502	EPA	C16-C15-C14	-2.19	111.15	124.38
4	C	502	EPA	C10-C11-C12	-2.19	111.16	124.38
4	C	502	EPA	C10-C9-C8	-2.12	111.57	124.38
3	C	501	HEM	CAA-C2A-C3A	-2.10	123.00	129.00
4	C	502	EPA	C13-C12-C11	-2.10	111.72	124.38
4	A	502	EPA	C4-C5-C6	-2.05	108.51	124.66
4	C	502	EPA	C4-C5-C6	-2.05	108.54	124.66
3	A	501	HEM	CMC-C2C-C3C	2.04	129.07	125.09
3	C	501	HEM	CBD-CAD-C3D	3.18	118.04	112.47
4	A	502	EPA	C17-C16-C15	3.24	122.93	112.17
3	C	501	HEM	CBA-CAA-C2A	3.27	118.23	112.49
4	C	502	EPA	C17-C16-C15	4.00	125.47	112.17
4	A	502	EPA	C20-C19-C18	15.37	175.11	112.69
4	C	502	EPA	C20-C19-C18	15.40	175.21	112.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	HEM	3	0
4	A	502	EPA	1	0
3	C	501	HEM	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	419/422 (99%)	0.05	10 (2%) 62 57	15, 27, 52, 66	0
2	C	421/428 (98%)	-0.23	3 (0%) 89 87	14, 22, 40, 56	0
All	All	840/850 (98%)	-0.09	13 (1%) 76 72	14, 24, 47, 66	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	GLY	3.8
1	A	275	PRO	3.1
2	C	275	PRO	3.1
2	C	227	LEU	3.0
1	A	10	LEU	2.9
2	C	-1	HIS	2.5
1	A	14	LEU	2.4
1	A	130	ASP	2.3
1	A	318	LEU	2.3
1	A	191	ARG	2.3
1	A	180	PHE	2.2
1	A	304	ASP	2.1
1	A	4	LEU	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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, 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	LLDF	B-factors(Å^2)	Q<0.9
4	EPA	C	502	22/22	0.89	0.20	5.17	27,34,40,44	0
4	EPA	A	502	22/22	0.89	0.21	2.72	35,42,51,51	0
3	HEM	C	501	43/43	0.97	0.12	0.95	13,16,18,23	0
5	SO4	A	503	5/5	0.97	0.12	0.75	23,24,27,29	0
3	HEM	A	501	43/43	0.98	0.10	-0.42	16,20,25,28	0

6.5 Other polymers

There are no such residues in this entry.