Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:19 PM GMT

PDB ID	:	4L77
Title	:	P450cin Active Site Water: Implications for Substrate Binding and Solvent Accessibility
Authors	:	Madrona, Y.; Poulos, T.L.
Deposited on	:	2013-06-13
Resolution	:	1.38 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:

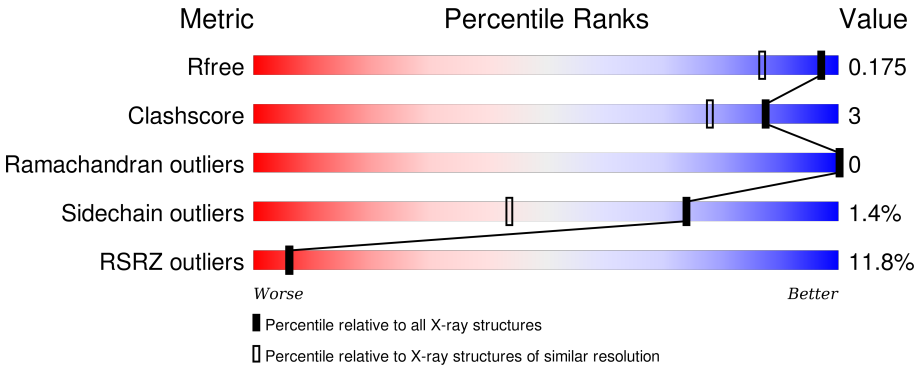
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.38 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	1918 (1.40-1.36)
Clashscore	102246	2042 (1.40-1.36)
Ramachandran outliers	100387	1993 (1.40-1.36)
Sidechain outliers	100360	1992 (1.40-1.36)
RSRZ outliers	91569	1917 (1.40-1.36)

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	398	12% 93% 6% •
1	B	398	12% 94% 6% •

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	CNL	A	502	-	-	-	X
3	CNL	B	502	-	-	-	X
4	PG4	A	503	-	-	-	X
4	PG4	B	503	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7564 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.

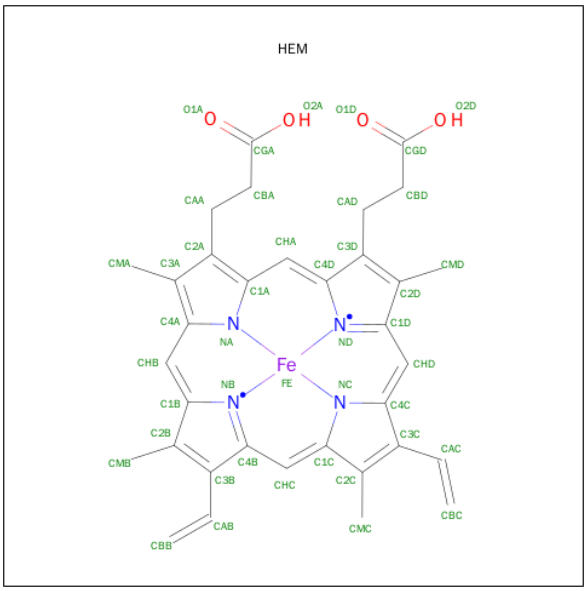
- Molecule 1 is a protein called P450cin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	4	0
			3173	2024	550	588	11			
1	B	397	Total	C	N	O	S	0	3	0
			3162	2018	549	584	11			

There are 4 discrepancies between the modelled and reference sequences:

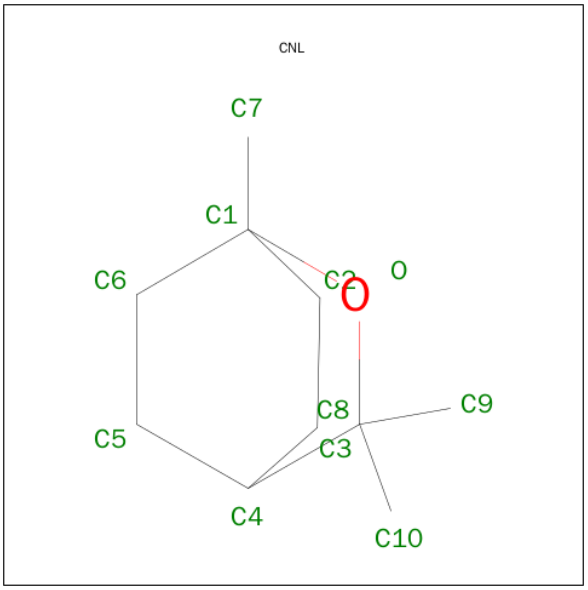
Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	INITIATING METHIONINE	UNP Q8VQF6
A	242	ALA	ASN	ENGINEERED MUTATION	UNP Q8VQF6
B	7	MET	-	INITIATING METHIONINE	UNP Q8VQF6
B	242	ALA	ASN	ENGINEERED MUTATION	UNP Q8VQF6

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



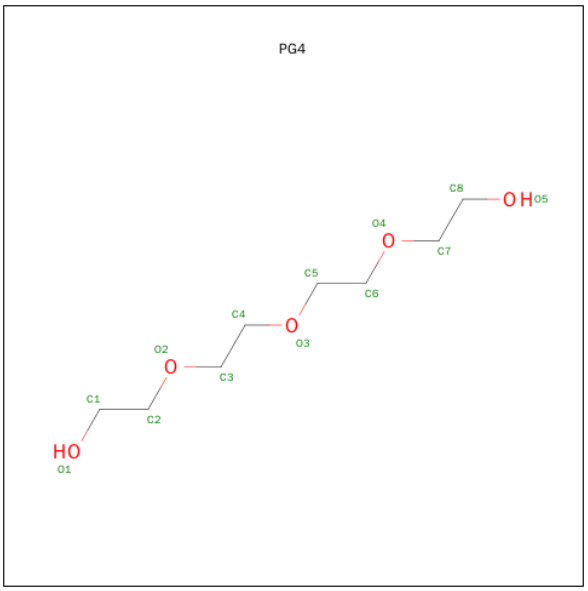
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 1,3,3-TRIMETHYL-2-OXABICYCLO[2.2.2]OCTANE (three-letter code: CNL) (formula: $C_{10}H_{18}O$).



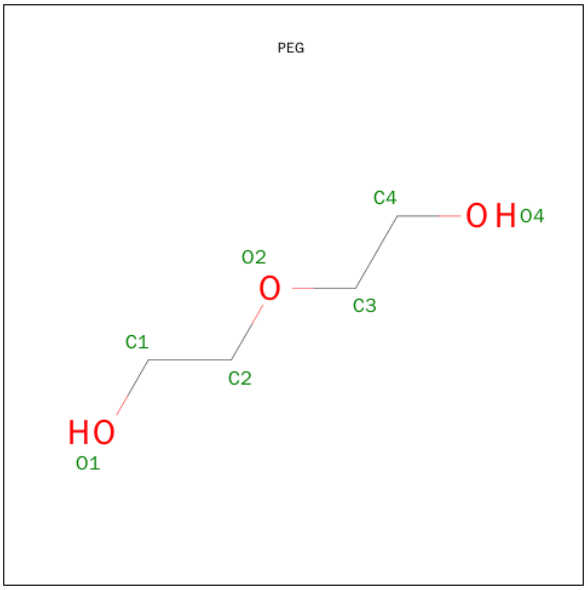
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	10	1		
3	B	1	Total	C	O	0	0
			11	10	1		

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



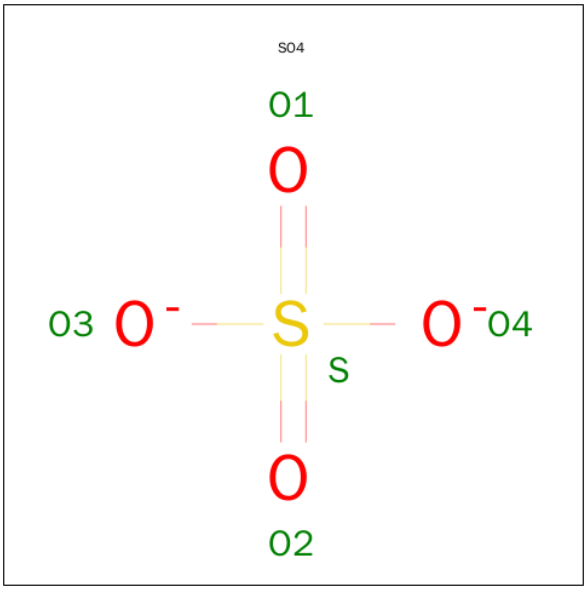
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		

- 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	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 7 is water.

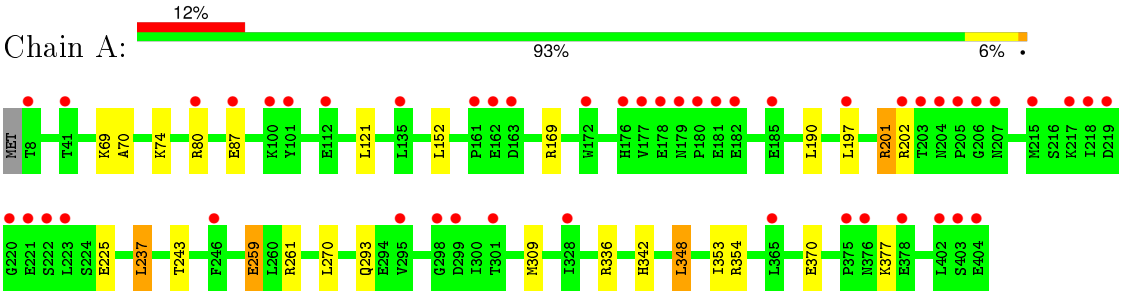
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	504	Total O 516 516	0	12
7	B	546	Total O 566 566	0	19

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.

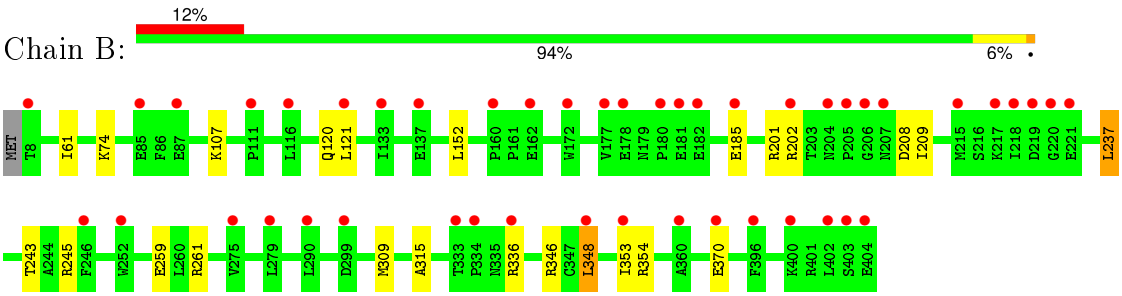
- Molecule 1: P450cin

Chain A:



- Molecule 1: P450cin

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.40Å 68.10Å 103.66Å 90.00° 96.12° 90.00°	Depositor
Resolution (Å)	43.79 – 1.38 43.79 – 1.38	Depositor EDS
% Data completeness (in resolution range)	99.2 (43.79-1.38) 99.2 (43.79-1.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 1.38Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.142 , 0.178 0.142 , 0.175	Depositor DCC
R_{free} test set	9126 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	13.5	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 181964 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7564	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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, 0.375 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: CNL, HEM, PG4, PEG, SO4

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	0.68	1/3259 (0.0%)	0.86	11/4432 (0.2%)
1	B	0.68	0/3251	0.77	7/4420 (0.2%)
All	All	0.68	1/6510 (0.0%)	0.82	18/8852 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	259	GLU	CD-OE2	-5.27	1.19	1.25

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	336	ARG	NE-CZ-NH1	18.52	129.56	120.30
1	A	336	ARG	NE-CZ-NH2	-13.83	113.39	120.30
1	B	309	MET	CG-SD-CE	9.22	114.94	100.20
1	A	261	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	A	309	MET	CG-SD-CE	8.09	113.14	100.20
1	A	261	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	B	261	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	B	201	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	169	ARG	NE-CZ-NH1	-6.11	117.25	120.30
1	B	237	LEU	CB-CG-CD2	5.95	121.11	111.00
1	A	80	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	B	237	LEU	CA-CB-CG	5.47	127.89	115.30
1	B	348	LEU	CB-CG-CD2	5.21	119.86	111.00
1	A	348	LEU	CB-CG-CD2	5.16	119.77	111.00
1	A	354	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	237	LEU	CA-CB-CG	5.06	126.94	115.30
1	A	201	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	261	ARG	NE-CZ-NH1	5.05	122.83	120.30

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	3173	0	3127	11	0
1	B	3162	0	3121	14	0
2	A	43	0	30	1	0
2	B	43	0	30	3	0
3	A	11	0	18	2	0
3	B	11	0	18	1	0
4	A	10	0	13	0	0
4	B	10	0	13	2	0
5	A	7	0	10	0	0
5	B	7	0	10	1	0
6	A	5	0	0	0	0
7	A	516	0	0	5	0
7	B	566	0	0	10	0
All	All	7564	0	6390	34	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 (34) 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:B:354:ARG:NH1	7:B:1101:HOH:O	2.20	0.69
1:A:259:GLU:OE2	7:A:657:HOH:O	2.09	0.69
1:B:185:GLU:HG3	7:B:1132:HOH:O	1.94	0.67
1:A:225:GLU:OE1	7:A:1084:HOH:O	2.12	0.67
1:B:208:ASP:OD2	7:B:1126:HOH:O	2.13	0.67
2:B:501:HEM:HBB2	2:B:501:HEM:HMB1	1.76	0.66
1:B:336:ARG:HA	7:B:954:HOH:O	2.00	0.61
3:A:502:CNL:H73	7:A:1104[A]:HOH:O	1.99	0.61
1:A:121:LEU:HD21	1:A:152:LEU:HD22	1.82	0.61
4:B:503:PG4:O1	5:B:504:PEG:O1	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LYS:NZ	7:B:1133:HOH:O	2.34	0.60
1:A:377:LYS:NZ	7:A:915:HOH:O	2.35	0.59
3:B:502:CNL:H73	7:B:838[A]:HOH:O	2.00	0.59
1:A:74:LYS:NZ	1:A:87:GLU:OE2	2.18	0.59
2:A:501:HEM:HMB1	2:A:501:HEM:HBB2	1.85	0.58
1:B:243:THR:HG22	1:B:353:ILE:HD13	1.87	0.56
1:B:121:LEU:HD21	1:B:152:LEU:HD22	1.88	0.55
1:A:70:ALA:HA	1:A:293:GLN:HG2	1.90	0.54
1:B:346:ARG:HH22	1:B:354:ARG:HH12	1.56	0.53
1:B:209[B]:ILE:HG13	7:B:866:HOH:O	2.08	0.53
1:B:259:GLU:OE2	7:B:672:HOH:O	2.20	0.49
2:B:501:HEM:HBB2	2:B:501:HEM:CMB	2.44	0.48
1:B:61:ILE:HD12	1:B:315:ALA:HB2	1.95	0.48
4:B:503:PG4:H62	7:B:1114:HOH:O	2.16	0.45
1:A:190:LEU:C	1:A:190:LEU:HD23	2.37	0.44
1:A:342:HIS:ND1	7:A:1066:HOH:O	2.36	0.44
1:B:120[A]:GLN:NE2	7:B:1070:HOH:O	2.51	0.44
1:A:243:THR:HG22	1:A:353:ILE:HD13	1.99	0.44
1:A:69:LYS:HE3	1:A:69:LYS:HB2	1.59	0.43
2:B:501:HEM:HBC2	2:B:501:HEM:HMC1	2.00	0.42
1:B:74:LYS:HA	1:B:74:LYS:HD3	1.90	0.42
1:B:245:ARG:HA	1:B:245:ARG:NE	2.36	0.41
1:A:197[B]:LEU:HD11	1:A:201:ARG:NH2	2.36	0.41
3:A:502:CNL:H31	3:A:502:CNL:H92	1.86	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	399/398 (100%)	392 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	398/398 (100%)	392 (98%)	6 (2%)	0	100 100
All	All	797/796 (100%)	784 (98%)	13 (2%)	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	336/333 (101%)	331 (98%)	5 (2%)	72 40
1	B	335/333 (101%)	331 (99%)	4 (1%)	78 51
All	All	671/666 (101%)	662 (99%)	9 (1%)	74 46

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	ARG
1	A	237	LEU
1	A	270	LEU
1	A	348	LEU
1	A	370	GLU
1	B	202	ARG
1	B	237	LEU
1	B	348	LEU
1	B	370	GLU

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

Mol	Chain	Res	Type
1	A	293	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

9 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	$\#\|Z\| > 2$
2	HEM	A	501	1,7	30,50,50	2.12	7 (23%)	24,82,82	2.28	6 (25%)
3	CNL	A	502	-	12,12,12	2.17	3 (25%)	18,20,20	1.20	3 (16%)
4	PG4	A	503	-	9,9,12	0.89	0	8,8,11	0.74	0
5	PEG	A	504	-	6,6,6	0.94	0	5,5,5	0.53	0
6	SO4	A	505	-	4,4,4	0.56	0	6,6,6	0.70	0
2	HEM	B	501	1,7	30,50,50	2.43	9 (30%)	24,82,82	2.30	9 (37%)
3	CNL	B	502	-	12,12,12	2.09	3 (25%)	18,20,20	1.04	0
4	PG4	B	503	-	9,9,12	0.94	0	8,8,11	0.81	0
5	PEG	B	504	-	6,6,6	0.87	0	5,5,5	0.62	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	501	1,7	-	0/10/54/54	0/0/8/8
3	CNL	A	502	-	-	0/0/24/24	0/0/2/2
4	PG4	A	503	-	-	0/7/7/10	0/0/0/0
5	PEG	A	504	-	-	0/4/4/4	0/0/0/0
6	SO4	A	505	-	-	0/0/0/0	0/0/0/0
2	HEM	B	501	1,7	-	0/10/54/54	0/0/8/8
3	CNL	B	502	-	-	0/0/24/24	0/0/2/2
4	PG4	B	503	-	-	0/7/7/10	0/0/0/0
5	PEG	B	504	-	-	0/4/4/4	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3B-C4B	-7.60	1.45	1.51
2	B	501	HEM	C3B-C4B	-6.60	1.46	1.51
2	B	501	HEM	C3D-C4D	-6.39	1.43	1.51
2	A	501	HEM	C3D-C4D	-4.61	1.45	1.51
2	B	501	HEM	C2C-C1C	-3.98	1.45	1.52
3	B	502	CNL	C5-C4	-3.19	1.44	1.53
3	A	502	CNL	C5-C4	-2.95	1.45	1.53
3	B	502	CNL	C2-C3	-2.66	1.47	1.53
2	A	501	HEM	C2C-C1C	-2.63	1.47	1.52
3	A	502	CNL	C2-C3	-2.52	1.47	1.53
2	A	501	HEM	C2D-C1D	-2.25	1.44	1.51
2	B	501	HEM	C2D-C3D	-2.18	1.48	1.54
2	B	501	HEM	C2B-C1B	-2.17	1.44	1.51
2	B	501	HEM	C2D-C1D	-2.17	1.44	1.51
2	A	501	HEM	C2D-C3D	-2.03	1.48	1.54
2	B	501	HEM	C3C-CAC	2.04	1.55	1.51
2	A	501	HEM	C4C-NC	2.16	1.38	1.36
2	B	501	HEM	C4C-NC	2.61	1.39	1.36
2	A	501	HEM	C1C-NC	4.34	1.41	1.36
3	B	502	CNL	O-C8	4.82	1.55	1.46
3	A	502	CNL	O-C8	5.31	1.56	1.46
2	B	501	HEM	C1C-NC	6.17	1.43	1.36

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	CNL	O-C1-C2	-2.43	100.59	108.51
2	B	501	HEM	C3B-CAB-CBB	-2.29	120.95	124.46
2	A	501	HEM	CBD-CAD-C3D	-2.20	107.14	113.55
3	A	502	CNL	C3-C4-C8	-2.17	104.62	109.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	HEM	CAA-C2A-C1A	-2.10	124.73	127.01
2	A	501	HEM	CMD-C2D-C3D	2.14	123.81	114.35
3	A	502	CNL	O-C1-C7	2.14	112.69	105.12
2	B	501	HEM	C3B-C4B-CHC	2.17	126.22	123.16
2	B	501	HEM	C2D-C3D-C4D	3.12	106.79	101.50
2	B	501	HEM	CMD-C2D-C3D	3.17	128.39	114.35
2	A	501	HEM	CAD-C3D-C2D	4.01	124.74	113.22
2	B	501	HEM	CAD-C3D-C4D	4.27	127.53	112.47
2	B	501	HEM	CAD-C3D-C2D	4.33	125.67	113.22
2	B	501	HEM	CMC-C2C-C3C	4.43	127.59	116.53
2	B	501	HEM	CMB-C2B-C3B	4.84	128.60	116.53
2	A	501	HEM	CMC-C2C-C3C	5.02	129.05	116.53
2	A	501	HEM	CAD-C3D-C4D	5.15	130.64	112.47
2	A	501	HEM	CMB-C2B-C3B	5.74	130.86	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	1	0
3	A	502	CNL	2	0
2	B	501	HEM	3	0
3	B	502	CNL	1	0
4	B	503	PG4	2	0
5	B	504	PEG	1	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, 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	397/398 (99%)	1.20	48 (12%)	6	6	8, 16, 35, 57	0
1	B	397/398 (99%)	1.13	46 (11%)	6	6	7, 14, 32, 60	0
All	All	794/796 (99%)	1.16	94 (11%)	6	6	7, 15, 33, 60	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	THR	12.1
1	B	404	GLU	9.0
1	B	8	THR	8.4
1	A	219	ASP	7.9
1	A	218	ILE	7.3
1	A	207	ASN	6.8
1	B	207	ASN	6.5
1	A	404	GLU	6.2
1	A	220	GLY	6.1
1	B	402	LEU	5.9
1	B	219	ASP	5.7
1	A	177	VAL	5.3
1	A	221	GLU	5.2
1	B	220	GLY	4.6
1	B	403	SER	4.5
1	A	180	PRO	4.4
1	B	177	VAL	4.2
1	B	181	GLU	4.1
1	B	334	PRO	4.0
1	A	403	SER	4.0
1	A	172	TRP	3.9
1	A	402	LEU	3.9
1	B	180	PRO	3.9
1	A	204	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	178	GLU	3.1
1	A	181	GLU	3.1
1	A	135	LEU	3.1
1	A	162[A]	GLU	3.1
1	B	172	TRP	3.1
1	B	221	GLU	3.1
1	A	215	MET	3.0
1	A	205	PRO	3.0
1	B	205	PRO	3.0
1	B	178	GLU	3.0
1	B	299	ASP	2.9
1	B	215	MET	2.9
1	B	333	THR	2.9
1	B	206	GLY	2.9
1	B	160	PRO	2.9
1	A	217	LYS	2.8
1	B	400	LYS	2.8
1	A	197[A]	LEU	2.8
1	B	336	ARG	2.8
1	A	112	GLU	2.8
1	A	206	GLY	2.7
1	B	218	ILE	2.7
1	A	365	LEU	2.6
1	B	137	GLU	2.6
1	A	179	ASN	2.6
1	A	376	ASN	2.6
1	B	348	LEU	2.6
1	A	378	GLU	2.6
1	A	299	ASP	2.6
1	B	162	GLU	2.6
1	B	121	LEU	2.5
1	A	203	THR	2.5
1	B	185	GLU	2.5
1	A	295	VAL	2.5
1	A	163	ASP	2.5
1	A	41	THR	2.5
1	B	217	LYS	2.5
1	B	111	PRO	2.4
1	A	176	HIS	2.4
1	B	116	LEU	2.4
1	A	80	ARG	2.4
1	A	101	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	87	GLU	2.3
1	A	375	PRO	2.3
1	A	182	GLU	2.3
1	B	275	VAL	2.3
1	A	246	PHE	2.2
1	A	301	THR	2.2
1	B	202	ARG	2.2
1	B	396	PHE	2.2
1	B	133	ILE	2.2
1	B	87	GLU	2.2
1	B	370	GLU	2.2
1	A	298	GLY	2.1
1	B	360	ALA	2.1
1	B	353	ILE	2.1
1	B	252	TRP	2.1
1	B	279	LEU	2.1
1	A	100	LYS	2.1
1	B	246	PHE	2.1
1	A	222	SER	2.1
1	A	185	GLU	2.1
1	A	161	PRO	2.1
1	B	204	ASN	2.1
1	B	85	GLU	2.1
1	A	223	LEU	2.1
1	B	182	GLU	2.0
1	B	290	LEU	2.0
1	A	328	ILE	2.0
1	A	202	ARG	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, 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
3	CNL	A	502	11/11	0.74	0.17	6.16	20,23,26,26	0
3	CNL	B	502	11/11	0.81	0.15	3.65	17,20,22,24	0
4	PG4	B	503	10/13	0.82	0.16	2.86	30,32,37,39	0
4	PG4	A	503	10/13	0.77	0.20	2.35	32,34,38,41	0
6	SO4	A	505	5/5	0.88	0.14	1.67	25,26,28,30	4
2	HEM	A	501	43/43	0.96	0.12	0.42	7,11,15,26	0
2	HEM	B	501	43/43	0.97	0.12	0.25	6,8,13,25	0
5	PEG	A	504	7/7	0.84	0.23	-	38,39,40,41	0
5	PEG	B	504	7/7	0.63	0.31	-	40,40,41,42	0

6.5 Other polymers (i)

There are no such residues in this entry.