



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 11:47 am GMT

PDB ID : 4C9M
Title : Structure of substrate free, glycerol bound wild type CYP101D1
Authors : Batabyal, D.; L Poulos, T.
Deposited on : 2013-10-02
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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

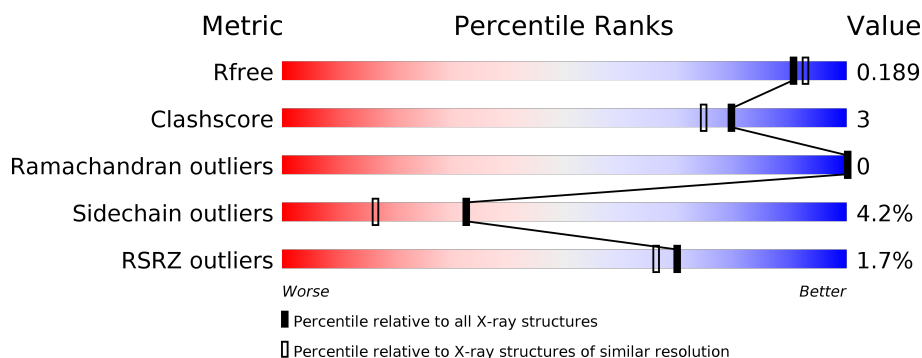
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	111664	5253 (1.80-1.80)
Clashscore	122126	6077 (1.80-1.80)
Ramachandran outliers	120053	6011 (1.80-1.80)
Sidechain outliers	120020	6010 (1.80-1.80)
RSRZ outliers	108989	5157 (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 $\leq 5\%$. 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	421	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 1%; height: 10px; background-color: red;"></div> <div style="width: 89%; height: 10px; background-color: green;"></div> <div style="width: 7%; height: 10px; background-color: yellow;"></div> <div style="width: 3%; height: 10px; background-color: orange;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> </div> </div>
1	B	421	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 90%; height: 10px; background-color: green;"></div> <div style="width: 5%; height: 10px; background-color: yellow;"></div> <div style="width: 3%; height: 10px; background-color: orange;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14014 atoms, of which 6510 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 CYTOCHROME P450.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	408	Total	C	H	N	O	S	0	1	0
			6480	2063	3236	577	591	13			
1	B	407	Total	C	H	N	O	S	0	1	0
			6463	2058	3228	575	589	13			

- 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	H	N	O	0	0
			73	34	1	30	4	4		
2	B	1	Total	C	Fe	N	O		0	0
			43	34	1	4	4			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		

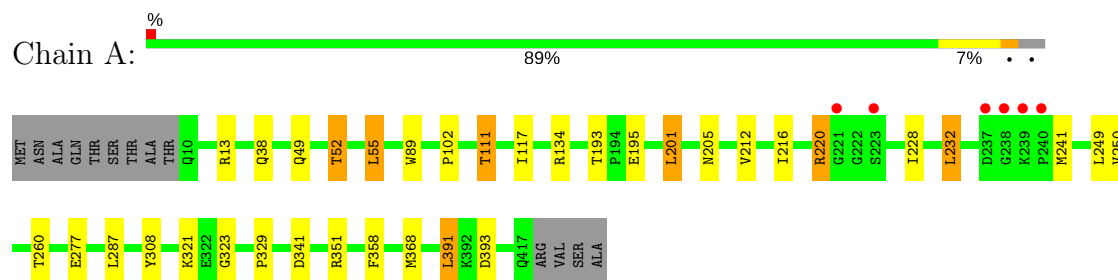
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	514	Total	O	0	0
			514	514		
4	B	413	Total	O	0	0
			413	413		

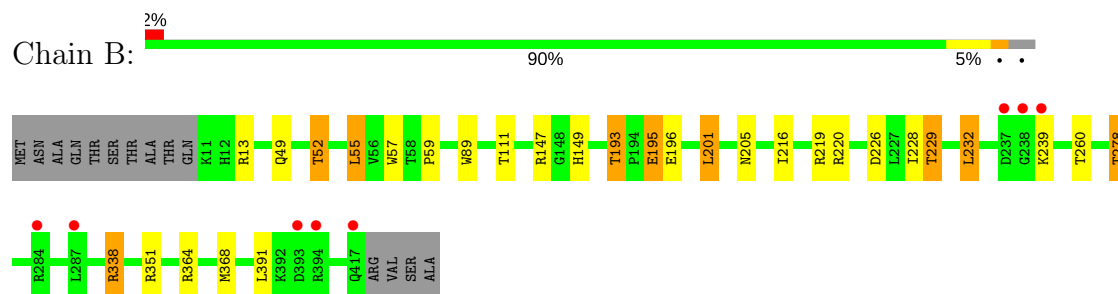
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: CYTOCHROME P450



• Molecule 1: CYTOCHROME P450



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	151.52Å 151.52Å 195.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.08 – 1.80 48.08 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.08-1.80) 98.4 (48.08-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.77 (at 1.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.154 , 0.188 0.156 , 0.189	Depositor DCC
R_{free} test set	2000 reflections (1.64%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14014	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: GOL, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	0/3329	0.70	5/4524 (0.1%)
1	B	0.45	0/3320	0.68	3/4512 (0.1%)
All	All	0.47	0/6649	0.69	8/9036 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	A	55	LEU	CA-CB-CG	6.28	129.74	115.30
1	B	201	LEU	CA-CB-CG	5.46	127.87	115.30
1	A	220	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	201	LEU	CA-CB-CG	5.43	127.80	115.30
1	B	55	LEU	CA-CB-CG	5.37	127.66	115.30
1	A	391	LEU	CA-CB-CG	5.18	127.22	115.30
1	B	338	ARG	NE-CZ-NH2	-5.15	117.72	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	3244	3236	3222	15	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3235	3228	3214	18	1
2	A	43	30	30	3	0
2	B	43	0	30	4	0
3	A	6	8	8	0	0
3	B	6	8	8	0	0
4	A	514	0	0	2	0
4	B	413	0	0	3	0
All	All	7504	6510	6512	39	1

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 (39) 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:B:1418:HEM:HMB1	2:B:1418:HEM:HBB2	1.74	0.68
1:A:212:VAL:HG11	1:A:250:VAL:HB	1.77	0.66
1:A:49:GLN:HB2	1:A:52:THR:HG22	1.78	0.66
1:B:278:THR:HG21	4:B:2310:HOH:O	2.01	0.60
1:B:111:THR:HG22	4:B:2172:HOH:O	2.02	0.59
1:B:13:ARG:HG3	1:B:59:PRO:HB2	1.86	0.57
1:A:111:THR:HG21	4:A:2226:HOH:O	2.03	0.57
1:B:226:ASP:OD1	1:B:229:THR:HG23	2.06	0.55
1:B:49:GLN:HB2	1:B:52:THR:HG22	1.87	0.54
2:B:1418:HEM:HHD	2:B:1418:HEM:HBC2	1.89	0.53
2:B:1418:HEM:CMB	2:B:1418:HEM:HBB2	2.40	0.52
1:B:364:ARG:HG2	1:B:368:MET:CE	2.41	0.51
1:A:220:ARG:NH2	1:A:241:MET:O	2.37	0.51
1:B:219:ARG:HD3	1:B:229:THR:HG22	1.92	0.50
1:B:193:THR:HG22	1:B:196:GLU:H	1.76	0.50
1:B:57:TRP:CH2	1:B:59:PRO:HA	2.48	0.49
1:A:212:VAL:HG12	1:A:216:ILE:CD1	2.44	0.48
1:B:229:THR:HG21	4:B:2287:HOH:O	2.14	0.48
1:A:102:PRO:HD3	1:A:117:ILE:HD11	1.96	0.47
1:A:341:ASP:OD2	1:B:338:ARG:NH2	2.48	0.47
1:A:193:THR:HG22	1:A:195:GLU:H	1.78	0.47
2:A:1418:HEM:HBB2	2:A:1418:HEM:HMB1	1.96	0.46
2:B:1418:HEM:HHD	2:B:1418:HEM:CBC	2.46	0.45
1:A:49:GLN:HB2	1:A:52:THR:CG2	2.46	0.45
1:A:216:ILE:O	1:A:220:ARG:HG3	2.17	0.45
1:B:147:ARG:HG2	1:B:149:HIS:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:PHE:CE2	1:A:368:MET:HG3	2.52	0.44
1:A:228:ILE:O	1:A:232:LEU:HB2	2.17	0.44
1:B:49:GLN:H	1:B:52:THR:CG2	2.31	0.44
1:B:226:ASP:OD1	1:B:229:THR:CG2	2.66	0.44
2:A:1418:HEM:HHD	2:A:1418:HEM:HBC2	1.99	0.43
1:B:216:ILE:O	1:B:220:ARG:HG3	2.19	0.43
4:A:2450:HOH:O	1:B:338:ARG:HD3	2.19	0.42
1:B:228:ILE:O	1:B:232:LEU:HB2	2.19	0.42
1:A:117:ILE:HD11	1:A:249:LEU:CD2	2.49	0.42
1:A:49:GLN:H	1:A:52:THR:CG2	2.33	0.41
1:B:193:THR:HG22	1:B:195:GLU:N	2.36	0.41
1:A:308:TYR:CZ	1:A:323:GLY:HA2	2.56	0.41
2:A:1418:HEM:CBC	2:A:1418:HEM:HHD	2.51	0.40

All (1) 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)
1:A:13:ARG:O	1:B:351:ARG:HH22[8_555]	1.53	0.07

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	407/421 (97%)	397 (98%)	10 (2%)	0	100	100
1	B	406/421 (96%)	394 (97%)	12 (3%)	0	100	100
All	All	813/842 (97%)	791 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	347/356 (98%)	330 (95%)	17 (5%)	27	12
1	B	346/356 (97%)	332 (96%)	14 (4%)	34	18
All	All	693/712 (97%)	662 (96%)	31 (4%)	32	14

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	52	THR
1	A	55	LEU
1	A	89	TRP
1	A	111	THR
1	A	201	LEU
1	A	205	ASN
1	A	232	LEU
1	A	260[A]	THR
1	A	260[B]	THR
1	A	277	GLU
1	A	287	LEU
1	A	321	LYS
1	A	329	PRO
1	A	351	ARG
1	A	391	LEU
1	A	393	ASP
1	B	52	THR
1	B	55	LEU
1	B	89	TRP
1	B	193	THR
1	B	195	GLU
1	B	201	LEU
1	B	205	ASN
1	B	229	THR
1	B	232	LEU
1	B	239	LYS

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Mol	Chain	Res	Type
1	B	260[A]	THR
1	B	260[B]	THR
1	B	278	THR
1	B	391	LEU

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

Mol	Chain	Res	Type
1	B	149	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	1418	1	27,50,50	1.88	5 (18%)	17,82,82	1.37	3 (17%)
3	GOL	A	1419	-	5,5,5	0.64	0	5,5,5	0.65	0
2	HEM	B	1418	1	27,50,50	2.02	7 (25%)	17,82,82	1.87	5 (29%)
3	GOL	B	1419	-	5,5,5	0.39	0	5,5,5	0.23	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	1418	1	-	0/6/54/54	0/0/8/8
3	GOL	A	1419	-	-	0/4/4/4	0/0/0/0
2	HEM	B	1418	1	-	0/6/54/54	0/0/8/8
3	GOL	B	1419	-	-	0/4/4/4	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1418	HEM	C3C-C2C	-4.84	1.33	1.40
2	B	1418	HEM	C3C-C2C	-4.69	1.33	1.40
2	B	1418	HEM	C3B-C2B	-4.22	1.34	1.40
2	A	1418	HEM	C3B-C2B	-4.04	1.34	1.40
2	B	1418	HEM	C1D-ND	2.40	1.41	1.36
2	B	1418	HEM	CMA-C3A	2.53	1.56	1.51
2	B	1418	HEM	C3B-CAB	2.85	1.53	1.47
2	A	1418	HEM	C3C-CAC	2.88	1.53	1.47
2	B	1418	HEM	C3C-CAC	3.20	1.54	1.47
2	A	1418	HEM	C3B-CAB	3.77	1.55	1.47
2	A	1418	HEM	C3D-C2D	4.10	1.49	1.37
2	B	1418	HEM	C3D-C2D	4.39	1.50	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1418	HEM	CMA-C3A-C4A	-3.55	123.00	128.46
2	B	1418	HEM	C3C-C4C-NC	-2.96	105.36	110.94
2	B	1418	HEM	CAD-CBD-CGD	-2.49	108.40	112.66
2	A	1418	HEM	CMA-C3A-C4A	-2.11	125.23	128.46
2	A	1418	HEM	C1D-C2D-C3D	-2.07	105.56	107.00
2	B	1418	HEM	CMA-C3A-C2A	2.01	128.74	124.94
2	A	1418	HEM	CMB-C2B-C3B	2.98	130.31	124.88
2	B	1418	HEM	C4C-C3C-C2C	3.39	109.27	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1418	HEM	3	0
2	B	1418	HEM	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 [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, 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	408/421 (96%)	-0.53	6 (1%) 73 70	11, 18, 34, 52	0
1	B	407/421 (96%)	-0.41	8 (1%) 65 61	11, 21, 39, 62	0
All	All	815/842 (96%)	-0.47	14 (1%) 70 66	11, 20, 37, 62	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	417	GLN	4.3
1	B	237	ASP	3.9
1	B	239	LYS	3.8
1	B	238	GLY	3.3
1	A	237	ASP	3.1
1	A	239	LYS	3.0
1	A	223	SER	2.4
1	A	238	GLY	2.3
1	B	394	ARG	2.3
1	A	240	PRO	2.2
1	B	393	ASP	2.1
1	B	284	ARG	2.1
1	B	287	LEU	2.1
1	A	221	GLY	2.1

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. 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	B-factors(\AA^2)	Q<0.9
3	GOL	A	1419	6/6	0.85	0.20	14,48,57,65	0
3	GOL	B	1419	6/6	0.90	0.15	27,50,63,72	0
2	HEM	B	1418	43/43	0.98	0.12	8,12,15,22	0
2	HEM	A	1418	43/43	0.99	0.08	9,13,22,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.