Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:34 AM GMT

PDB ID	:	3B99
Title	:	Crystal structure of zebrafish prostacyclin synthase (cytochrome P450 8A1) in complex with substrate analog U51605
Authors	:	Li, Y.-C.; Chiang, C.-W.; Yeh, H.-C.; Hsu, P.-Y.; Whitby, F.G.; Wang, L.-H.; Chan, N.-L.
Deposited on	:	2007-11-03
Resolution	:	2.50 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

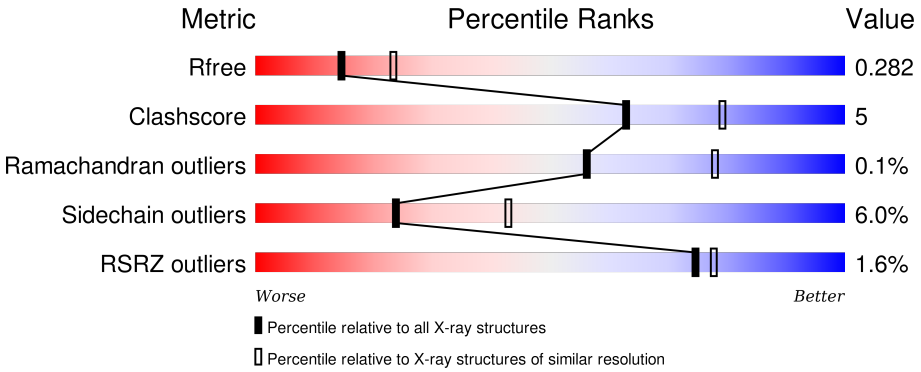
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	475	80% 12% • 6%
1	B	475	3% 74% 12% • 13%

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	U51	A	701	-	-	-	X
3	U51	B	701	-	-	-	X
3	U51	B	702	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7444 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.

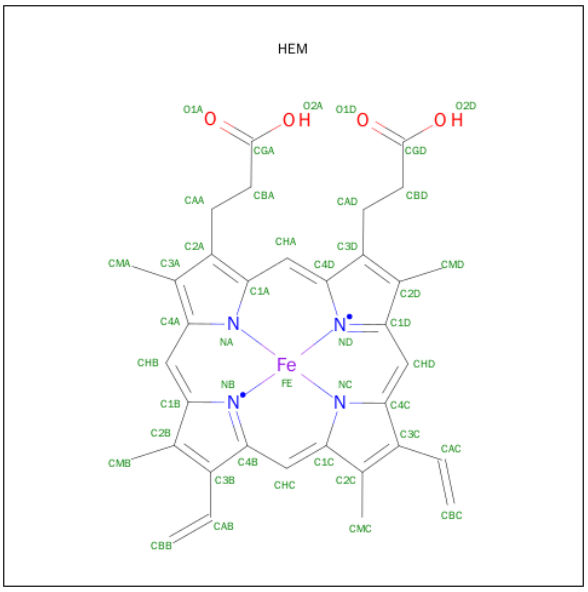
- Molecule 1 is a protein called Prostaglandin I2 synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3605	2296	640	650	19			
1	B	415	Total	C	N	O	S	0	0	0
			3386	2166	599	602	19			

There are 22 discrepancies between the modelled and reference sequences:

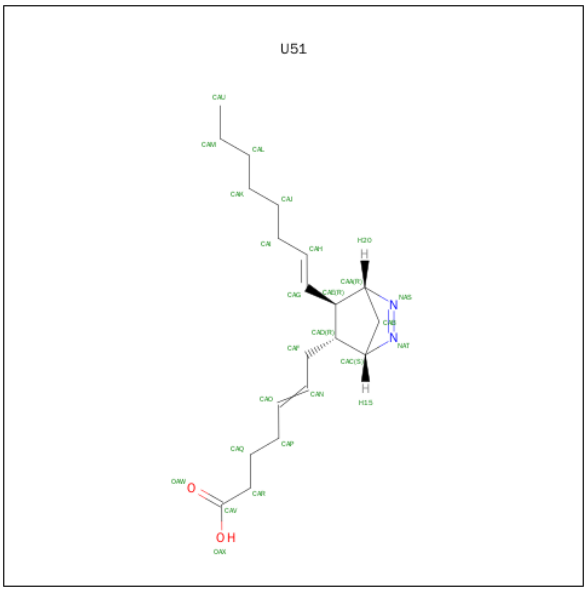
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	MET	-	INITIATING METHIONINE	UNP A9LLA5
A	11	ALA	-	EXPRESSION TAG	UNP A9LLA5
A	12	LYS	-	EXPRESSION TAG	UNP A9LLA5
A	13	LYS	-	EXPRESSION TAG	UNP A9LLA5
A	14	THR	-	EXPRESSION TAG	UNP A9LLA5
A	15	SER	-	EXPRESSION TAG	UNP A9LLA5
A	16	SER	-	EXPRESSION TAG	UNP A9LLA5
A	481	HIS	-	EXPRESSION TAG	UNP A9LLA5
A	482	HIS	-	EXPRESSION TAG	UNP A9LLA5
A	483	HIS	-	EXPRESSION TAG	UNP A9LLA5
A	484	HIS	-	EXPRESSION TAG	UNP A9LLA5
B	10	MET	-	INITIATING METHIONINE	UNP A9LLA5
B	11	ALA	-	EXPRESSION TAG	UNP A9LLA5
B	12	LYS	-	EXPRESSION TAG	UNP A9LLA5
B	13	LYS	-	EXPRESSION TAG	UNP A9LLA5
B	14	THR	-	EXPRESSION TAG	UNP A9LLA5
B	15	SER	-	EXPRESSION TAG	UNP A9LLA5
B	16	SER	-	EXPRESSION TAG	UNP A9LLA5
B	481	HIS	-	EXPRESSION TAG	UNP A9LLA5
B	482	HIS	-	EXPRESSION TAG	UNP A9LLA5
B	483	HIS	-	EXPRESSION TAG	UNP A9LLA5
B	484	HIS	-	EXPRESSION TAG	UNP A9LLA5

- 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 (5Z)-7-{(1R,4S,5R,6R)-6-[(1E)-OCT-1-EN-1-YL]-2,3-DIAZABICYCLO[2.2.1]HEPT-2-EN-5-YL}HEPT-5-ENOIC ACID (three-letter code: U51) (formula: $C_{20}H_{32}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	20	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	20	2	2		
3	A	1	Total	C	N	O	0	0
			24	20	2	2		
3	B	1	Total	C	N	O	0	0
			24	20	2	2		
3	B	1	Total	C	N	O	0	0
			24	20	2	2		
3	B	1	Total	C	N	O	0	0
			24	20	2	2		

- Molecule 4 is water.

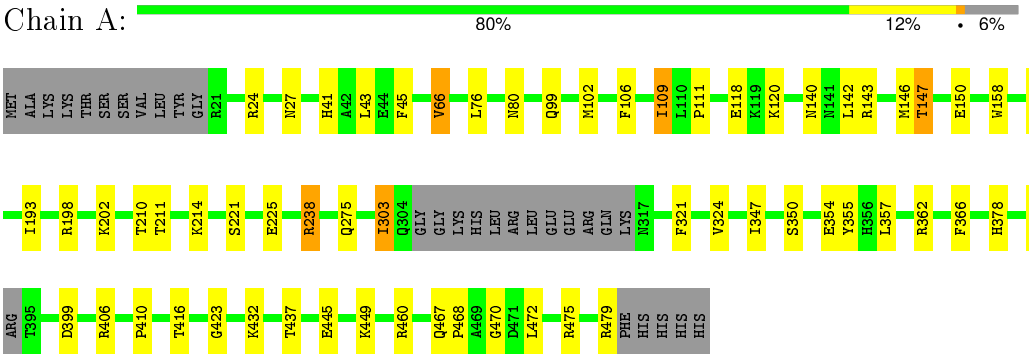
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	154	Total	O	0	0
			154	154		
4	B	69	Total	O	0	0
			69	69		

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.

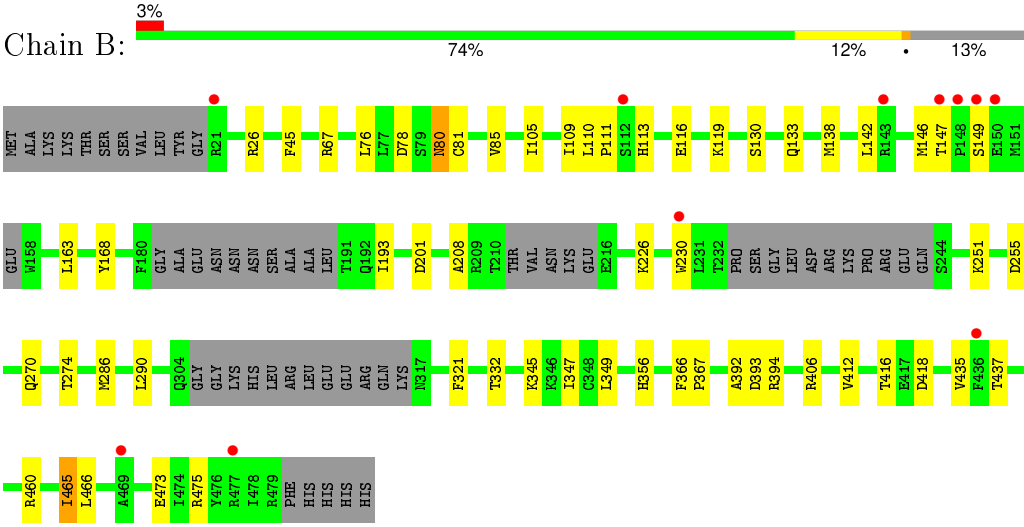
- Molecule 1: Prostaglandin I2 synthase

Chain A:



- Molecule 1: Prostaglandin I2 synthase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.47Å 88.04Å 190.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.75 – 2.50 27.75 – 2.48	Depositor EDS
% Data completeness (in resolution range)	91.6 (27.75-2.50) 91.7 (27.75-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 2.47Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.214 , 0.292 0.207 , 0.282	Depositor DCC
R_{free} test set	1621 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 39.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 32600 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7444	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 4.69% 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: HEM, U51

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	0/3686	0.60	0/4979
1	B	0.44	0/3462	0.55	0/4672
All	All	0.47	0/7148	0.58	0/9651

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	3605	0	3609	42	0
1	B	3386	0	3389	29	0
2	A	43	0	30	2	0
2	B	43	0	30	4	0
3	A	72	0	93	8	0
3	B	72	0	93	3	0
4	A	154	0	0	3	0
4	B	69	0	0	1	0
All	All	7444	0	7244	77	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 5.

All (77) 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:142:LEU:HG	1:A:146:MET:HE2	1.40	0.98
1:A:146:MET:HE3	1:A:437:THR:HG21	1.53	0.90
1:A:142:LEU:HG	1:A:146:MET:CE	2.04	0.88
1:A:106:PHE:HE2	3:A:701:U51:H28	1.41	0.83
1:A:146:MET:CE	1:A:437:THR:HG21	2.11	0.81
1:A:158:TRP:CE3	1:A:475:ARG:HG3	2.18	0.78
1:A:80:ASN:HD21	1:A:350:SER:HB3	1.53	0.73
1:A:321:PHE:CE2	1:A:432:LYS:HG2	2.23	0.73
1:A:140:ASN:OD1	1:A:143:ARG:NH2	2.28	0.66
1:B:85:VAL:HG22	1:B:347:ILE:HD12	1.78	0.66
1:A:189:ALA:O	1:A:193:ILE:HG13	1.97	0.64
1:A:80:ASN:ND2	1:A:350:SER:HB3	2.13	0.64
1:A:303:ILE:O	1:A:303:ILE:HG22	1.99	0.63
1:A:221:SER:O	1:A:225:GLU:HG3	1.99	0.62
1:A:303:ILE:O	1:A:303:ILE:CG2	2.48	0.61
1:A:211:THR:HG22	1:A:211:THR:O	1.99	0.61
1:B:116:GLU:HA	1:B:119:LYS:HE3	1.82	0.61
1:A:175:GLY:HA3	1:A:275:GLN:OE1	2.01	0.61
3:B:702:U51:H24	3:B:702:U51:H17	1.84	0.60
1:A:347:ILE:HD12	1:A:357:LEU:HD11	1.83	0.60
1:B:345:LYS:HE3	1:B:347:ILE:HD11	1.84	0.60
1:B:290:LEU:HB3	1:B:446:LEU:HD21	1.83	0.59
1:B:201:ASP:O	1:B:460:ARG:NH2	2.36	0.59
1:B:105:ILE:HD11	1:B:208:ALA:HB2	1.84	0.59
1:B:146:MET:HE3	1:B:437:THR:HG21	1.84	0.59
1:A:146:MET:HE3	4:A:844:HOH:O	2.01	0.58
1:A:378:HIS:HE1	1:A:410:PRO:O	1.87	0.58
2:A:600:HEM:HMB1	2:A:600:HEM:HBB2	1.85	0.56
1:A:106:PHE:CE2	3:A:701:U51:H28	2.31	0.56
1:A:109:ILE:HG22	1:A:111:PRO:HD3	1.87	0.55
1:A:147:THR:HG22	1:A:150:GLU:H	1.71	0.55
1:B:367:PRO:HB3	1:B:412:VAL:HB	1.88	0.54
1:B:332:THR:HA	1:B:466:LEU:HD12	1.88	0.54
1:B:270:GLN:OE1	1:B:270:GLN:HA	2.07	0.54
1:B:146:MET:CE	1:B:437:THR:HG21	2.38	0.54
1:A:324:VAL:HG22	1:A:386:PHE:HB2	1.90	0.53
1:A:109:ILE:CG2	1:A:111:PRO:HD3	2.39	0.53
1:A:41:HIS:CD2	1:A:66:VAL:HG22	2.43	0.52
1:A:468:PRO:HB2	1:A:470:GLY:O	2.10	0.52
1:A:385:GLN:NE2	4:A:816:HOH:O	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:GLU:CD	1:B:264:ARG:HH21	2.13	0.52
1:B:274:THR:HG22	2:B:600:HEM:HAC	1.91	0.52
1:B:460:ARG:HD2	4:B:710:HOH:O	2.10	0.50
1:B:465:ILE:CD1	2:B:600:HEM:HMB2	2.41	0.50
1:A:146:MET:CE	4:A:844:HOH:O	2.59	0.50
1:A:41:HIS:HD2	1:A:66:VAL:HG22	1.77	0.50
2:B:600:HEM:C1D	3:B:700:U51:H20	2.47	0.50
2:B:600:HEM:ND	3:B:700:U51:H20	2.27	0.49
1:A:99:GLN:NE2	3:A:701:U51:H5	2.27	0.49
1:B:416:THR:HG22	1:B:418:ASP:H	1.79	0.48
1:B:109:ILE:HG23	1:B:111:PRO:HD3	1.96	0.48
1:A:102:MET:HE3	3:A:701:U51:H23	1.95	0.48
1:B:110:LEU:HD13	1:B:113:HIS:ND1	2.29	0.47
3:A:700:U51:H5	3:A:700:U51:H10	1.67	0.47
1:A:211:THR:CG2	1:A:211:THR:O	2.62	0.47
1:A:445:GLU:OE1	1:A:475:ARG:HD3	2.16	0.46
1:B:251:LYS:O	1:B:255:ASP:HB2	2.16	0.46
1:B:78:ASP:OD1	1:B:80:ASN:ND2	2.49	0.45
1:A:238:ARG:HA	1:A:238:ARG:HD2	1.52	0.45
1:A:423:GLY:HA3	2:A:600:HEM:C3C	2.52	0.44
1:B:81:CYS:SG	1:B:349:LEU:HA	2.58	0.44
1:A:99:GLN:HE21	3:A:701:U51:H5	1.82	0.44
3:A:702:U51:H12	3:A:702:U51:H6	1.85	0.43
1:A:27:ASN:O	1:A:355:TYR:HA	2.19	0.43
1:A:102:MET:CE	3:A:701:U51:H21	2.49	0.42
1:A:347:ILE:HD12	1:A:357:LEU:CD1	2.48	0.42
1:B:109:ILE:O	1:B:262:MET:HG2	2.19	0.42
1:B:163:LEU:HD21	1:B:286:MET:HB3	2.01	0.42
1:B:392:ALA:C	1:B:394:ARG:H	2.22	0.42
1:B:142:LEU:HG	1:B:146:MET:HE2	2.01	0.42
1:B:142:LEU:HG	1:B:146:MET:CE	2.50	0.42
1:A:460:ARG:HG3	1:A:467:GLN:HB2	2.02	0.41
1:B:110:LEU:HB3	1:B:113:HIS:HB2	2.02	0.41
1:B:147:THR:HG22	1:B:149:SER:H	1.86	0.41
1:B:321:PHE:CE1	1:B:435:VAL:HG11	2.56	0.40
1:A:321:PHE:HE2	1:A:432:LYS:HG2	1.79	0.40
1:A:347:ILE:CD1	1:A:357:LEU:HD11	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	439/475 (92%)	424 (97%)	14 (3%)	1 (0%)	52 75
1	B	403/475 (85%)	390 (97%)	13 (3%)	0	100 100
All	All	842/950 (89%)	814 (97%)	27 (3%)	1 (0%)	56 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	303	ILE

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	388/414 (94%)	364 (94%)	24 (6%)	23 41
1	B	364/414 (88%)	343 (94%)	21 (6%)	25 45
All	All	752/828 (91%)	707 (94%)	45 (6%)	24 43

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	43	LEU
1	A	45	PHE
1	A	66	VAL
1	A	76	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	109	ILE
1	A	118	GLU
1	A	120	LYS
1	A	147	THR
1	A	168	TYR
1	A	198	ARG
1	A	202	LYS
1	A	210	THR
1	A	214	LYS
1	A	238	ARG
1	A	354	GLU
1	A	362	ARG
1	A	366	PHE
1	A	399	ASP
1	A	406	ARG
1	A	416	THR
1	A	449	LYS
1	A	472	LEU
1	A	479	ARG
1	B	26	ARG
1	B	45	PHE
1	B	67	ARG
1	B	76	LEU
1	B	80	ASN
1	B	130	SER
1	B	133	GLN
1	B	138	MET
1	B	168	TYR
1	B	193	ILE
1	B	226	LYS
1	B	230	TRP
1	B	264	ARG
1	B	356	HIS
1	B	366	PHE
1	B	393	ASP
1	B	406	ARG
1	B	448	ASP
1	B	465	ILE
1	B	473	GLU
1	B	475	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	125	HIS
1	A	185	ASN
1	A	378	HIS
1	A	385	GLN
1	A	391	ASN
1	A	467	GLN
1	B	80	ASN
1	B	94	GLN
1	B	376	GLN
1	B	378	HIS
1	B	380	GLN
1	B	385	GLN
1	B	391	ASN
1	B	403	ASN
1	B	419	ASN
1	B	467	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

8 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	600	1,3	30,50,50	2.17	5 (16%)	24,82,82	2.23	7 (29%)
3	U51	A	700	2	18,25,25	0.64	0	19,31,31	2.19	4 (21%)
3	U51	A	701	-	18,25,25	0.47	0	19,31,31	2.20	4 (21%)
3	U51	A	702	-	18,25,25	0.52	0	19,31,31	2.73	3 (15%)
2	HEM	B	600	1,3	30,50,50	2.20	8 (26%)	24,82,82	2.31	8 (33%)
3	U51	B	700	2	18,25,25	0.53	0	19,31,31	2.32	7 (36%)
3	U51	B	701	-	18,25,25	0.44	0	19,31,31	2.38	3 (15%)
3	U51	B	702	-	18,25,25	0.52	0	19,31,31	2.49	2 (10%)

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	600	1,3	-	0/10/54/54	0/0/8/8
3	U51	A	700	2	-	0/15/38/38	0/0/2/2
3	U51	A	701	-	-	0/15/38/38	0/0/2/2
3	U51	A	702	-	-	0/15/38/38	0/0/2/2
2	HEM	B	600	1,3	-	0/10/54/54	0/0/8/8
3	U51	B	700	2	-	0/15/38/38	0/0/2/2
3	U51	B	701	-	-	0/15/38/38	0/0/2/2
3	U51	B	702	-	-	0/15/38/38	0/0/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	HEM	C3B-C4B	-7.28	1.45	1.51
2	B	600	HEM	C3B-C4B	-7.02	1.45	1.51
2	B	600	HEM	C3D-C4D	-5.37	1.44	1.51
2	A	600	HEM	C3D-C4D	-4.76	1.45	1.51
2	B	600	HEM	C2C-C1C	-4.07	1.44	1.52
2	A	600	HEM	C2C-C1C	-3.85	1.45	1.52
2	B	600	HEM	C2B-C1B	-2.11	1.45	1.51
2	B	600	HEM	C2D-C1D	-2.07	1.45	1.51
2	B	600	HEM	C3B-CAB	2.02	1.55	1.51
2	B	600	HEM	C4C-NC	2.04	1.38	1.36
2	A	600	HEM	C3B-CAB	2.83	1.56	1.51
2	A	600	HEM	FE-NC	2.98	2.07	1.95
2	B	600	HEM	FE-NC	3.14	2.08	1.95

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	702	U51	CAB-CAC-NAT	-7.69	94.14	103.62
3	A	702	U51	CAB-CAC-NAT	-7.59	94.27	103.62
3	A	702	U51	CAB-CAA-NAS	-7.49	94.40	103.62
3	B	701	U51	CAB-CAC-NAT	-7.07	94.91	103.62
3	B	702	U51	CAB-CAA-NAS	-6.85	95.18	103.62
3	B	701	U51	CAB-CAA-NAS	-6.58	95.51	103.62
3	B	700	U51	CAB-CAC-NAT	-6.27	95.89	103.62
3	A	700	U51	CAB-CAC-NAT	-6.08	96.13	103.62
3	A	701	U51	CAB-CAC-NAT	-6.03	96.20	103.62
3	A	701	U51	CAB-CAA-NAS	-5.71	96.59	103.62
3	B	700	U51	CAB-CAA-NAS	-5.60	96.72	103.62
3	A	700	U51	CAB-CAA-NAS	-5.28	97.12	103.62
3	A	701	U51	CAI-CAH-CAG	-2.86	116.56	125.14
3	B	700	U51	CAA-CAE-CAG	-2.76	107.45	114.62
3	A	700	U51	CAI-CAH-CAG	-2.70	117.05	125.14
2	B	600	HEM	CAA-C2A-C1A	-2.48	124.31	127.01
3	B	700	U51	CAR-CAQ-CAP	-2.42	108.47	113.25
3	A	700	U51	CAA-CAE-CAG	-2.39	108.41	114.62
3	B	700	U51	CAF-CAD-CAC	-2.35	108.17	114.68
3	A	701	U51	CAA-CAE-CAG	-2.35	108.53	114.62
3	B	700	U51	CAI-CAH-CAG	-2.31	118.22	125.14
3	B	701	U51	CAI-CAH-CAG	-2.24	118.42	125.14
2	B	600	HEM	C3C-CAC-CBC	-2.15	121.16	124.46
3	B	700	U51	CAF-CAN-CAO	-2.01	119.72	126.58
2	A	600	HEM	CAD-CBD-CGD	-2.00	104.85	113.02
2	A	600	HEM	C2D-C3D-C4D	2.20	105.23	101.50
2	B	600	HEM	C3B-C4B-CHC	2.53	126.72	123.16
2	B	600	HEM	CMD-C2D-C3D	2.90	127.18	114.35
2	A	600	HEM	CMD-C2D-C3D	2.91	127.22	114.35
3	A	702	U51	CAE-CAG-CAH	3.49	136.75	125.12
2	B	600	HEM	CAD-C3D-C4D	4.08	126.85	112.47
2	B	600	HEM	CMC-C2C-C3C	4.08	126.71	116.53
2	A	600	HEM	CAD-C3D-C2D	4.42	125.93	113.22
2	A	600	HEM	CMB-C2B-C3B	4.43	127.59	116.53
2	B	600	HEM	CMB-C2B-C3B	4.63	128.09	116.53
2	A	600	HEM	CAD-C3D-C4D	4.63	128.81	112.47
2	A	600	HEM	CMC-C2C-C3C	4.97	128.93	116.53
2	B	600	HEM	CAD-C3D-C2D	5.37	128.64	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	HEM	2	0
3	A	700	U51	1	0
3	A	701	U51	6	0
3	A	702	U51	1	0
2	B	600	HEM	4	0
3	B	700	U51	2	0
3	B	702	U51	1	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	445/475 (93%)	-0.28	1 (0%) 95 96	9, 22, 43, 57	0
1	B	415/475 (87%)	0.15	13 (3%) 52 57	13, 37, 71, 86	0
All	All	860/950 (90%)	-0.07	14 (1%) 74 78	9, 28, 64, 86	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	21	ARG	3.8
1	B	112	SER	3.6
1	B	150	GLU	3.5
1	B	147	THR	3.3
1	B	436	PHE	3.2
1	B	469	ALA	3.1
1	B	148	PRO	3.0
1	B	450	ASN	2.6
1	B	230	TRP	2.6
1	B	477	ARG	2.5
1	B	143	ARG	2.4
1	B	149	SER	2.3
1	A	392	ALA	2.1
1	B	446	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
3	U51	B	702	24/24	0.80	0.24	4.40	44,53,62,62	0
3	U51	B	701	24/24	0.76	0.31	4.18	36,62,75,75	0
3	U51	A	701	24/24	0.88	0.23	2.39	35,39,45,46	0
3	U51	A	702	24/24	0.88	0.18	1.69	18,29,36,37	0
3	U51	A	700	24/24	0.96	0.18	0.90	15,19,28,29	0
3	U51	B	700	24/24	0.97	0.15	0.27	21,25,33,37	0
2	HEM	A	600	43/43	0.98	0.14	-0.17	7,10,21,27	0
2	HEM	B	600	43/43	0.97	0.13	-0.24	13,17,28,34	0

6.5 Other polymers

There are no such residues in this entry.