Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 07:27 PM GMT

PDB ID	:	4U74
Title	:	Crystal structure of 4-phenylimidazole bound form of human indoleamine 2,3-dioxygenase (G262A mutant)
Authors	:	Sugimoto, H.; Horitani, M.; Kometani, E.; Shiro, Y.
Deposited on	:	2014-07-30
Resolution	:	2.31 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:

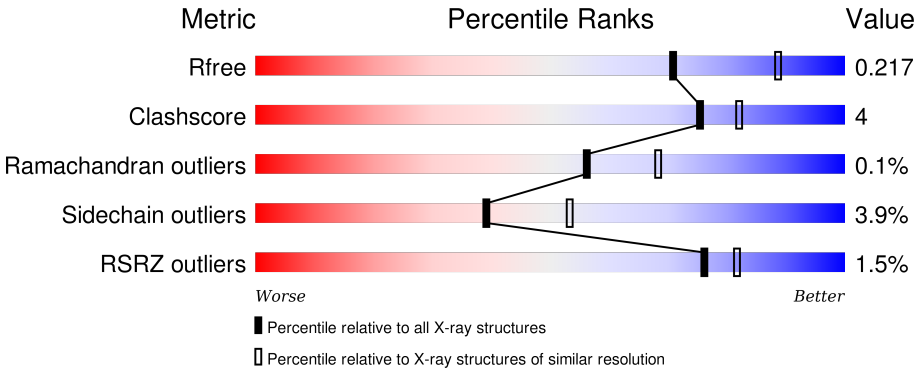
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.31 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	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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	406	% 82% 10% 8%
1	B	406	% 79% 13% • 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6421 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.

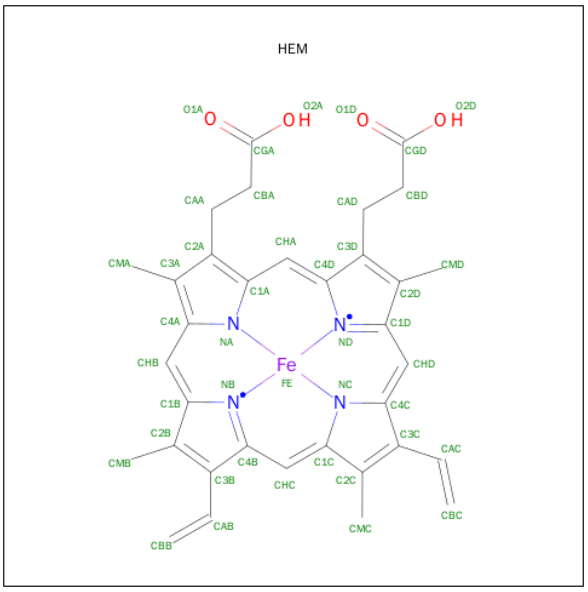
- Molecule 1 is a protein called Indoleamine 2,3-dioxygenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2973	1910	507	539	17			
1	B	374	Total	C	N	O	S	0	4	0
			2981	1918	506	539	18			

There are 8 discrepancies between the modelled and reference sequences:

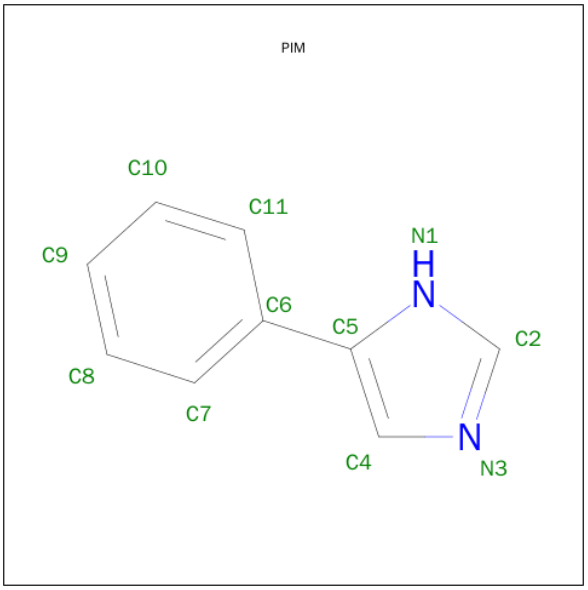
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P14902
A	-1	SER	-	expression tag	UNP P14902
A	0	HIS	-	expression tag	UNP P14902
A	262	ALA	GLY	engineered mutation	UNP P14902
B	-2	GLY	-	expression tag	UNP P14902
B	-1	SER	-	expression tag	UNP P14902
B	0	HIS	-	expression tag	UNP P14902
B	262	ALA	GLY	engineered mutation	UNP P14902

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



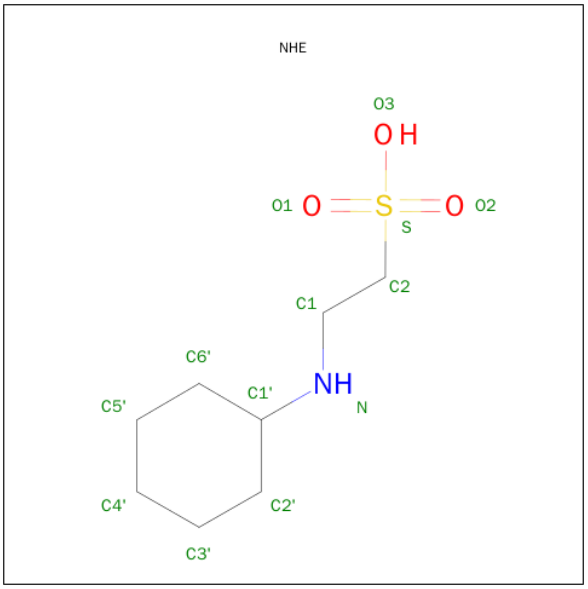
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 4-PHENYL-1H-IMIDAZOLE (three-letter code: PIM) (formula: $C_9H_8N_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N		0	0
			11	9	2			
3	B	1	Total	C	N		0	0
			11	9	2			

- Molecule 4 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: $C_8H_{17}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 5 is water.

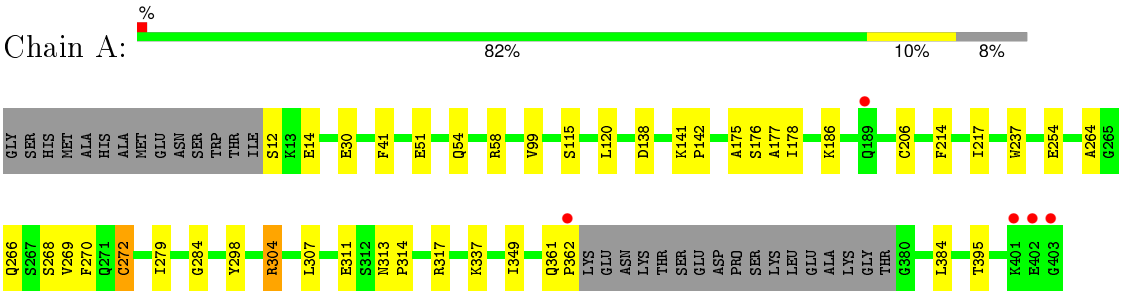
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	155	Total	O	0	0
			155	155		
5	B	152	Total	O	0	0
			152	152		

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.

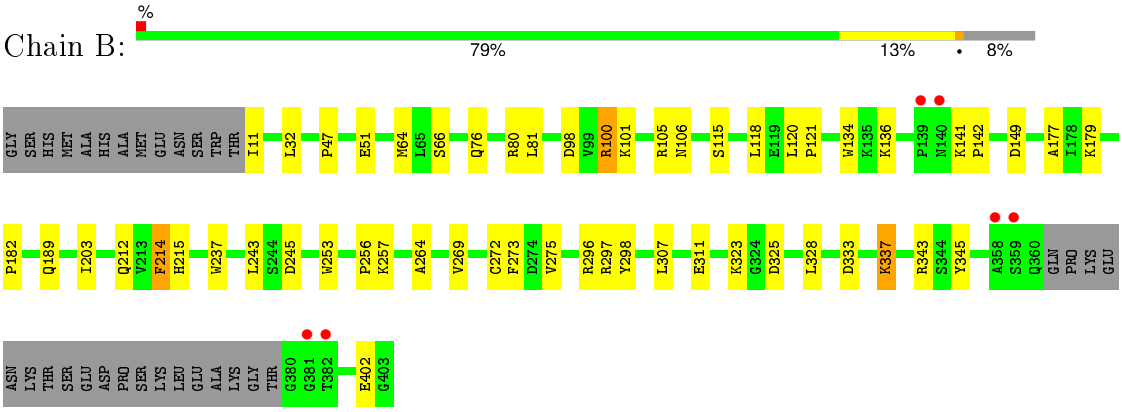
- Molecule 1: Indoleamine 2,3-dioxygenase 1

Chain A:



- Molecule 1: Indoleamine 2,3-dioxygenase 1

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	85.88Å 99.54Å 132.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 2.31 39.77 – 2.31	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.89-2.31) 97.1 (39.77-2.31)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.44 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.171 , 0.220 0.170 , 0.217	Depositor DCC
R_{free} test set	2387 reflections (5.12%)	DCC
Wilson B-factor (Å^2)	31.5	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 39.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 49175 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6421	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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: NHE, HEM, PIM

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	0.93	0/3042	0.96	3/4113 (0.1%)
1	B	0.95	1/3061 (0.0%)	0.97	7/4139 (0.2%)
All	All	0.94	1/6103 (0.0%)	0.97	10/8252 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	134	TRP	CE3-CZ3	6.79	1.50	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	304	ARG	NE-CZ-NH2	7.53	124.06	120.30
1	A	304	ARG	NE-CZ-NH1	-7.50	116.55	120.30
1	B	325	ASP	CB-CG-OD1	6.43	124.08	118.30
1	A	317	ARG	NE-CZ-NH1	-6.31	117.15	120.30
1	B	81	LEU	CB-CG-CD2	-6.08	100.67	111.00
1	B	100	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	B	80	ARG	NE-CZ-NH1	-5.41	117.59	120.30
1	B	98	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	297	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	343	ARG	NE-CZ-NH2	-5.29	117.66	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	2973	0	2984	22	0
1	B	2981	0	3007	22	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
3	A	11	0	8	2	0
3	B	11	0	8	2	0
4	A	26	0	33	0	0
4	B	26	0	34	0	0
5	A	155	0	0	1	0
5	B	152	0	0	1	0
All	All	6421	0	6134	48	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 4.

All (48) 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:175:ALA:HA	1:A:178:ILE:HD12	1.62	0.80
2:B:501:HEM:HBB2	2:B:501:HEM:HMB2	1.68	0.75
2:A:501:HEM:HMB2	2:A:501:HEM:HBB2	1.71	0.73
1:A:217:ILE:HG21	1:A:349:ILE:HD13	1.77	0.66
1:A:217:ILE:HG21	1:A:349:ILE:CD1	2.29	0.62
1:B:214:PHE:HD1	1:B:214:PHE:O	1.82	0.61
1:B:141:LYS:HB3	1:B:142:PRO:HD2	1.83	0.58
2:B:501:HEM:C1A	3:B:502:PIM:H2	2.38	0.58
1:B:264:ALA:H	3:B:502:PIM:HN1	1.52	0.56
1:A:268:SER:O	1:A:272:CYS:HB3	2.05	0.56
1:A:384:LEU:HD11	2:A:501:HEM:HMA3	1.88	0.56
1:A:279:ILE:HD13	1:A:395:THR:HG23	1.88	0.55
1:A:54:GLN:O	1:A:58:ARG:HG2	2.08	0.53
1:A:141:LYS:HB3	1:A:142:PRO:HD2	1.91	0.52
1:A:313:ASN:HB3	1:A:314:PRO:HD2	1.91	0.52
1:B:64:MET:HB2	1:B:106:ASN:OD1	2.09	0.52
1:B:296:ARG:CZ	1:B:307[B]:LEU:HD21	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ALA:HB1	1:B:203:ILE:HG12	1.93	0.50
1:A:264:ALA:H	3:A:502:PIM:HN1	1.59	0.50
1:B:136:LYS:HE2	1:B:141:LYS:O	2.12	0.50
1:A:138:ASP:OD2	1:A:141:LYS:HD2	2.12	0.49
1:A:176:SER:HB2	1:A:206:CYS:SG	2.54	0.48
1:B:253:TRP:CE3	1:B:257:LYS:HG3	2.49	0.48
1:A:361:GLN:HA	1:A:362:PRO:HD3	1.70	0.47
1:A:115:SER:HB3	1:A:120:LEU:O	2.14	0.47
2:A:501:HEM:C1A	3:A:502:PIM:H2	2.51	0.46
1:A:141:LYS:HB3	1:A:142:PRO:CD	2.45	0.46
1:B:11:ILE:HG13	1:B:182:PRO:HG3	1.98	0.46
1:B:76:GLN:HB3	1:B:118:LEU:HD11	1.99	0.45
1:B:115:SER:HB3	1:B:120:LEU:O	2.16	0.45
1:A:307:LEU:O	1:A:311:GLU:HG2	2.18	0.43
1:A:384:LEU:CD1	2:A:501:HEM:HMA3	2.47	0.43
1:A:41:PHE:CE2	1:A:58:ARG:NH2	2.87	0.43
1:B:121:PRO:HG2	1:B:298:TYR:CD2	2.54	0.42
1:B:328:LEU:HA	1:B:328:LEU:HD23	1.92	0.42
1:B:215:HIS:HD2	1:B:345:TYR:CZ	2.37	0.42
1:B:47:PRO:HD2	5:B:608:HOH:O	2.20	0.42
1:A:284:GLY:HA3	5:A:715:HOH:O	2.19	0.41
1:A:177:ALA:HB2	1:A:206:CYS:HB2	2.03	0.41
1:B:333:ASP:O	1:B:337:LYS:HB2	2.20	0.41
1:B:177:ALA:HB3	1:B:273:PHE:CZ	2.55	0.41
1:B:245:ASP:O	1:B:256:PRO:HB2	2.21	0.41
1:B:101:LYS:HG2	1:B:243:LEU:CD2	2.51	0.41
1:B:323:LYS:HD3	1:B:323:LYS:HA	1.90	0.41
1:A:269:VAL:HG12	1:A:270:PHE:N	2.36	0.41
1:B:32:LEU:HD23	1:B:32:LEU:HA	1.86	0.41
1:B:275:VAL:HG11	1:B:311:GLU:HG3	2.02	0.40
1:A:266:GLN:HG2	1:A:298:TYR:HB2	2.02	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	371/406 (91%)	363 (98%)	8 (2%)	0	100 100
1	B	374/406 (92%)	362 (97%)	11 (3%)	1 (0%)	46 56
All	All	745/812 (92%)	725 (97%)	19 (3%)	1 (0%)	56 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	402	GLU

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	324/350 (93%)	312 (96%)	12 (4%)	41 55
1	B	327/350 (93%)	313 (96%)	14 (4%)	35 48
All	All	651/700 (93%)	625 (96%)	26 (4%)	39 52

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	14	GLU
1	A	30	GLU
1	A	51	GLU
1	A	99	VAL
1	A	186	LYS
1	A	214	PHE
1	A	237	TRP
1	A	254	GLU
1	A	272	CYS
1	A	304	ARG
1	A	337	LYS

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Mol	Chain	Res	Type
1	B	51	GLU
1	B	66	SER
1	B	100	ARG
1	B	105	ARG
1	B	149	ASP
1	B	179	LYS
1	B	189	GLN
1	B	212	GLN
1	B	214	PHE
1	B	237	TRP
1	B	269	VAL
1	B	272[A]	CYS
1	B	272[B]	CYS
1	B	337	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	189	GLN
1	B	215	HIS
1	B	313	ASN

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	501	1,3	24,50,50	1.32	2 (8%)	16,82,82	2.11	5 (31%)
3	PIM	A	502	2	10,12,12	0.98	0	11,15,15	1.42	2 (18%)
4	NHE	A	503	-	13,13,13	1.88	2 (15%)	16,17,17	5.05	6 (37%)
4	NHE	A	504	-	13,13,13	1.58	1 (7%)	16,17,17	1.70	5 (31%)
2	HEM	B	501	1,3	24,50,50	1.01	1 (4%)	16,82,82	1.94	5 (31%)
3	PIM	B	502	2	10,12,12	0.78	0	11,15,15	1.96	2 (18%)
4	NHE	B	503	-	13,13,13	1.74	2 (15%)	16,17,17	2.61	6 (37%)
4	NHE	B	504	-	13,13,13	2.16	2 (15%)	16,17,17	3.37	6 (37%)

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	1,3	-	0/6/54/54	0/0/8/8
3	PIM	A	502	2	-	0/4/4/4	0/2/2/2
4	NHE	A	503	-	-	0/7/15/15	0/1/1/1
4	NHE	A	504	-	-	0/7/15/15	0/1/1/1
2	HEM	B	501	1,3	-	0/6/54/54	0/0/8/8
3	PIM	B	502	2	-	0/4/4/4	0/2/2/2
4	NHE	B	503	-	-	0/7/15/15	0/1/1/1
4	NHE	B	504	-	-	0/7/15/15	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	504	NHE	C2-S	-6.62	1.67	1.77
4	A	503	NHE	C2-S	-5.51	1.69	1.77
4	A	504	NHE	C2-S	-4.98	1.70	1.77
4	B	503	NHE	C2-S	-4.96	1.70	1.77
2	A	501	HEM	C1B-NB	-3.78	1.31	1.36
2	B	501	HEM	C1B-NB	-2.75	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	NHE	C1-N	-2.52	1.41	1.46
4	B	504	NHE	C1'-N	-2.49	1.43	1.48
4	A	503	NHE	O2-S	2.76	1.53	1.45
2	A	501	HEM	CAD-C3D	2.88	1.56	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	503	NHE	O1-S-C2	-7.58	101.51	106.87
4	A	503	NHE	C4'-C3'-C2'	-6.22	98.57	111.44
4	B	503	NHE	O2-S-O1	-6.06	96.84	113.96
2	A	501	HEM	C3B-CAB-CBB	-5.37	115.60	126.40
4	A	503	NHE	O3-S-O1	-4.40	101.52	111.26
4	B	504	NHE	O2-S-O1	-3.77	103.32	113.96
2	B	501	HEM	CAA-CBA-CGA	-3.53	105.90	112.78
3	B	502	PIM	C5-C4-N3	-3.36	102.08	109.08
2	B	501	HEM	C3B-CAB-CBB	-3.19	119.99	126.40
2	A	501	HEM	CMA-C3A-C4A	-3.07	123.10	128.31
4	B	504	NHE	C5'-C6'-C1'	-2.97	106.61	111.15
4	B	503	NHE	C5'-C6'-C1'	-2.67	107.06	111.15
2	B	501	HEM	C3C-CAC-CBC	-2.61	121.16	126.40
3	A	502	PIM	C11-C6-C5	-2.44	117.27	121.30
4	A	503	NHE	C1-C2-S	-2.27	106.89	113.66
4	B	504	NHE	C4'-C3'-C2'	-2.25	106.78	111.44
4	A	504	NHE	O2-S-O1	-2.21	107.73	113.96
2	A	501	HEM	C3C-C4C-NC	-2.17	106.86	110.94
3	A	502	PIM	C5-C4-N3	-2.07	104.77	109.08
4	A	503	NHE	C5'-C4'-C3'	-2.06	104.87	111.24
4	A	504	NHE	C1-C2-S	-2.02	107.65	113.66
4	B	503	NHE	C1-C2-S	-2.01	107.67	113.66
4	B	504	NHE	C6'-C1'-C2'	2.09	114.36	110.87
2	B	501	HEM	CMB-C2B-C3B	2.24	129.48	125.09
4	A	504	NHE	C5'-C6'-C1'	2.74	115.35	111.15
4	A	504	NHE	O2-S-C2	2.75	108.81	106.87
4	B	503	NHE	O3-S-O1	2.79	117.45	111.26
2	A	501	HEM	CMB-C2B-C3B	2.89	130.75	125.09
2	A	501	HEM	CBA-CAA-C2A	3.18	118.08	112.49
4	B	503	NHE	O3-S-C2	3.35	111.94	104.99
4	A	504	NHE	O1-S-C2	3.47	109.32	106.87
2	B	501	HEM	CBA-CAA-C2A	3.59	118.81	112.49
4	B	504	NHE	O2-S-C2	3.75	109.52	106.87
3	B	502	PIM	C4-N3-C2	4.63	113.53	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	503	NHE	O2-S-C2	5.77	110.94	106.87
4	B	504	NHE	O1-S-C2	11.14	114.74	106.87
4	A	503	NHE	O2-S-C2	16.51	118.54	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	4	0
3	A	502	PIM	2	0
2	B	501	HEM	2	0
3	B	502	PIM	2	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	375/406 (92%)	-0.23	5 (1%)	79	84	18, 30, 52, 129	0
1	B	374/406 (92%)	-0.22	6 (1%)	74	80	19, 32, 55, 77	0
All	All	749/812 (92%)	-0.23	11 (1%)	76	82	18, 31, 54, 129	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	GLY	15.0
1	A	402	GLU	8.4
1	A	401	LYS	5.3
1	B	382	THR	3.6
1	B	140	ASN	3.6
1	A	362	PRO	3.6
1	B	381	GLY	3.5
1	B	359	SER	3.2
1	A	189	GLN	2.5
1	B	139	PRO	2.2
1	B	358	ALA	2.2

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	NHE	B	503	13/13	0.94	0.15	1.49	30,33,57,62	0
4	NHE	A	504	13/13	0.92	0.15	1.22	31,38,55,58	0
4	NHE	A	503	13/13	0.94	0.17	1.20	26,32,46,51	0
3	PIM	B	502	11/11	0.99	0.15	0.68	16,19,20,20	0
2	HEM	A	501	43/43	0.99	0.13	0.36	17,20,22,23	0
2	HEM	B	501	43/43	0.98	0.12	0.17	18,22,25,26	0
3	PIM	A	502	11/11	0.99	0.16	-0.15	15,18,21,22	0
4	NHE	B	504	13/13	0.98	0.09	-0.96	33,35,41,44	0

6.5 Other polymers

There are no such residues in this entry.