Full wwPDB X-ray Structure Validation Report (i)

Jun 2, 2016 – 04:52 PM EDT

PDB ID	:	5FVV
Title	:	Structure of human nNOS R354A G357D mutant heme domain in complex with 4-methyl-6-(2-(5-(1-methylpiperidin-4-yl)pyridin-3-yl)ethyl) pyridin-2-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2016-02-10
Resolution	:	2.05 Å(reported)

The following versions of software and data (see references (i)) 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-20027674
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-20027674

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 2.05 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	Percentile Ranks	Value
Rfree		0.246
Clashscore		5
Ramachandran outliers		0.2%
Sidechain outliers		4.0%
RSRZ outliers		1.3%

Worse — *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
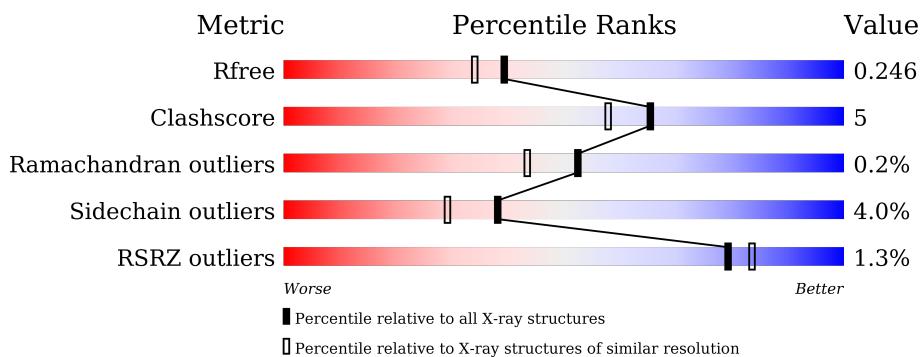
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	421	.% 85% 12% ‥
1	B	421	2% 83% 13% ‥
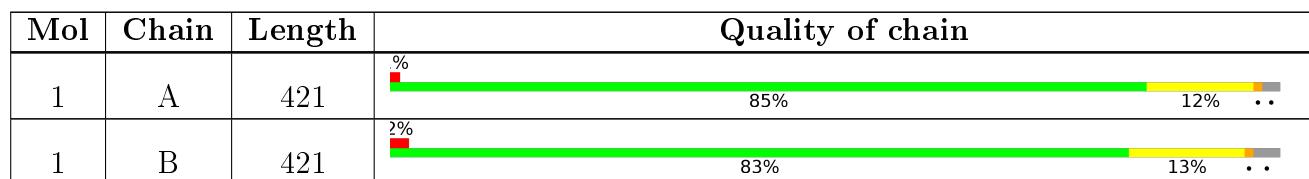
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	H65	A	800	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7272 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 NITRIC OXIDE SYNTHASE, BRAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total 3371	C 2159	N 574	O 616	S 22	0	2	0
1	B	408	Total 3333	C 2136	N 568	O 608	S 21	0	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ALA	ARG	ENGINEERED MUTATION	UNP P29475
A	357	ASP	GLY	ENGINEERED MUTATION	UNP P29475
B	354	ALA	ARG	ENGINEERED MUTATION	UNP P29475
B	357	ASP	GLY	ENGINEERED MUTATION	UNP P29475

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
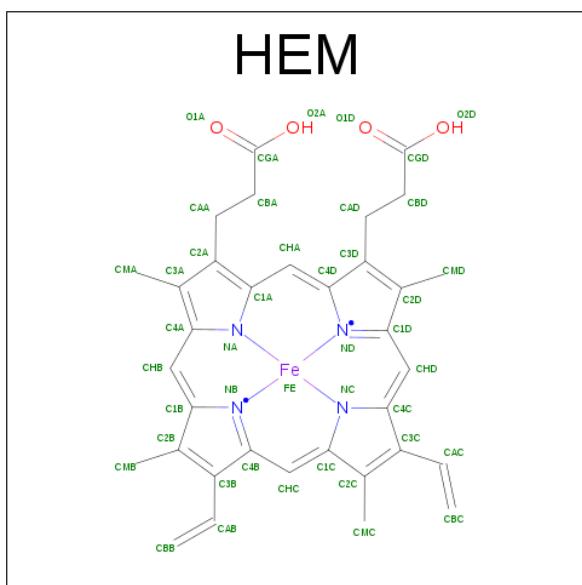
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).
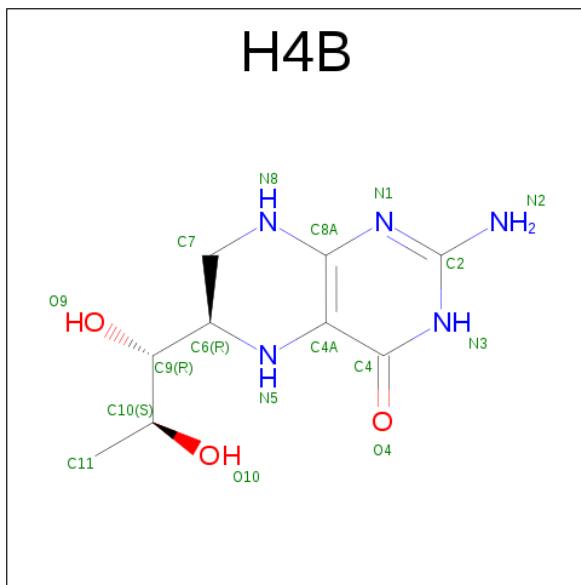
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 4-METHYL-6-(2-(5-(1-METHYLPIPERIDIN-4-YL)PYRIDIN-3-YL)ETHYL) PYRIDIN-2-AMINE (three-letter code: H65) (formula: $C_{19}H_{26}N_4$).
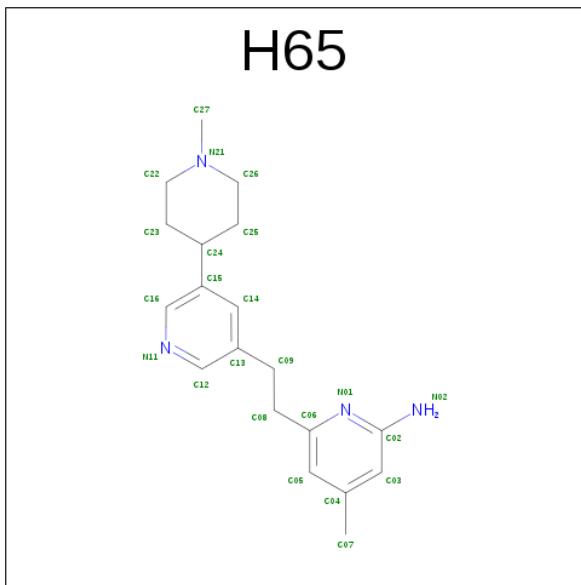
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 23	C 19	N 4	0	0
4	B	1	Total 23	C 19	N 4	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Zn 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	244	Total 244	O 244	0	0
6	B	157	Total 157	O 157	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: NITRIC OXIDE SYNTHASE, BRAIN
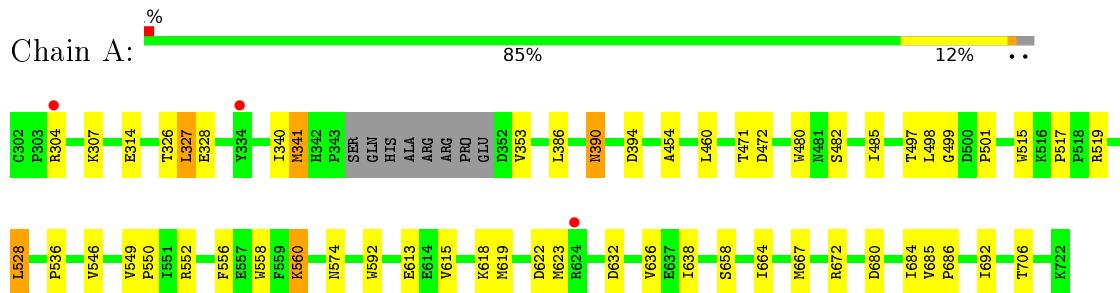
- Molecule 1: NITRIC OXIDE SYNTHASE, BRAIN
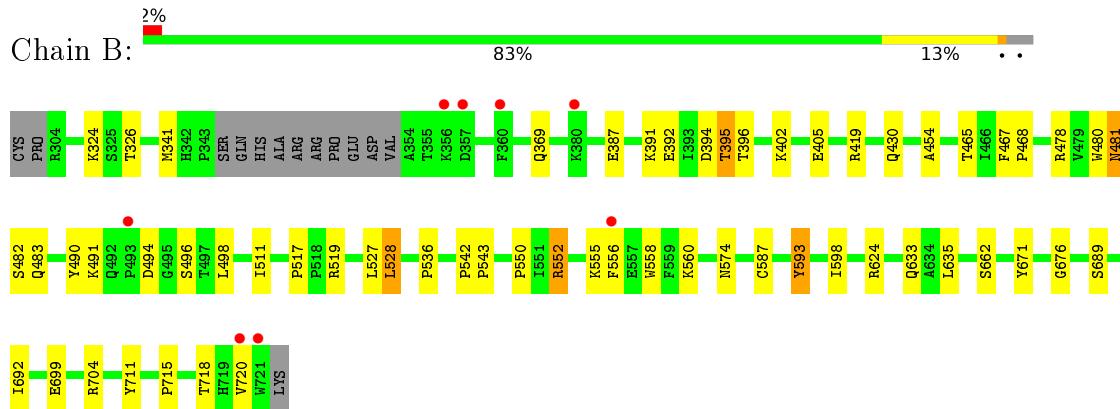
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.48Å 121.86Å 164.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.78 – 2.05 82.07 – 2.05	Depositor EDS
% Data completeness (in resolution range)	67.5 (35.78-2.05) 67.5 (82.07-2.05)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.05Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.183 , 0.247 0.177 , 0.246	Depositor DCC
R_{free} test set	2211 reflections (4.89%)	DCC
Wilson B-factor (Å^2)	22.2	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.8	EDS
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7272	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ZN, H65, H4B

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	0.39	0/3473	0.55	0/4712
1	B	0.35	0/3434	0.53	0/4660
All	All	0.37	0/6907	0.54	0/9372

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 (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	3371	0	3282	31	0
1	B	3333	0	3244	32	0
2	A	43	0	30	2	0
2	B	43	0	30	4	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	23	0	0	1	0
4	B	23	0	0	1	0
5	A	1	0	0	0	0
6	A	244	0	0	5	0
6	B	157	0	0	4	0
All	All	7272	0	6616	67	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 (67) 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:528:LEU:HD22	1:A:536:PRO:HB2	1.58	0.84
1:A:519:ARG:NH2	6:A:2144:HOH:O	2.18	0.77
2:B:750:HEM:HBB2	2:B:750:HEM:HHC	1.67	0.76
1:B:528:LEU:HD22	1:B:536:PRO:HB2	1.68	0.75
2:B:750:HEM:HBC2	2:B:750:HEM:HMC2	1.75	0.68
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.75	0.67
1:A:390:ASN:ND2	6:A:2024:HOH:O	2.29	0.65
1:B:482:SER:HA	1:B:574:ASN:HB3	1.79	0.63
1:A:480:TRP:HB2	1:A:528:LEU:HB3	1.84	0.59
1:A:485:ILE:HD13	1:A:546:VAL:HG13	1.85	0.59
1:A:326:THR:HG21	1:A:706:THR:HG22	1.83	0.58
1:B:662[B]:SER:OG	6:B:2035:HOH:O	2.17	0.57
1:B:704:ARG:NH1	6:B:2008:HOH:O	2.37	0.57
1:B:392:GLU:O	1:B:396:THR:OG1	2.16	0.56
1:A:482:SER:HA	1:A:574:ASN:HB3	1.88	0.55
1:B:391:LYS:O	1:B:395:THR:OG1	2.26	0.54
1:B:387:GLU:OE2	1:B:391:LYS:NZ	2.38	0.52
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.92	0.52
1:A:340:ILE:HD13	1:B:699:GLU:HB3	1.92	0.51
1:B:550:PRO:HG2	1:B:552:ARG:NH1	2.25	0.51
1:A:636:VAL:HG11	1:B:633:GLN:HG3	1.92	0.51
1:B:480:TRP:CE2	1:B:715:PRO:HB2	2.46	0.50
4:A:800:H65:N21	6:A:2244:HOH:O	2.34	0.50
1:A:556:PHE:HB3	1:A:558:TRP:CE2	2.46	0.50
1:A:471:THR:OG1	1:A:472:ASP:N	2.45	0.50
1:A:622:ASP:N	6:A:2196:HOH:O	2.40	0.49
1:B:511:ILE:HG12	1:B:517:PRO:HG3	1.95	0.49
1:A:515:TRP:O	1:A:517:PRO:HD3	2.13	0.48
1:B:480:TRP:HB2	1:B:528:LEU:HB3	1.96	0.48
1:A:327:LEU:HD13	1:A:328:GLU:H	1.79	0.48
1:B:430:GLN:NE2	6:B:2041:HOH:O	2.47	0.47
1:A:664:ILE:HD13	1:A:667:MET:HE3	1.96	0.47
1:A:692:ILE:HD13	1:B:635:LEU:HD22	1.96	0.47
1:A:615:VAL:HG21	1:A:638:ILE:HD11	1.96	0.47
1:A:556:PHE:HB3	1:A:558:TRP:NE1	2.30	0.46
1:B:490:TYR:CE2	1:B:519:ARG:HA	2.50	0.46
1:B:671:TYR:CE1	1:B:676:GLY:HA2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:689:SER:HB3	1:B:692:ILE:HD11	1.98	0.45
1:A:615:VAL:O	1:A:619:MET:HG3	2.16	0.45
1:A:680:ASP:O	1:A:684:ILE:HG12	2.16	0.45
1:A:460:LEU:HD12	1:A:592:TRP:HB3	1.99	0.45
1:B:481:ASN:HD21	1:B:527:LEU:HA	1.82	0.44
1:B:467:PHE:HB3	1:B:468:PRO:HD2	2.00	0.43
1:A:497:THR:HG21	1:A:501:PRO:HA	1.99	0.43
1:B:454:ALA:HB1	6:B:2069:HOH:O	2.19	0.43
1:A:498:LEU:HD12	1:A:499:GLY:H	1.83	0.43
1:B:483:GLN:HG2	4:B:800:H65:C12	2.49	0.43
1:B:556:PHE:HB3	1:B:558:TRP:CE2	2.53	0.42
1:B:465:THR:O	1:B:587:CYS:HA	2.19	0.42
2:B:750:HEM:HBB2	2:B:750:HEM:CHC	2.43	0.42
1:A:353:VAL:HG11	1:A:471:THR:O	2.19	0.42
1:B:402:LYS:HB2	1:B:405:GLU:HG3	2.01	0.42
1:A:613:GLU:HG3	1:A:623:MET:HE1	2.01	0.42
1:B:542:PRO:HA	1:B:543:PRO:HD3	1.82	0.42
1:A:560:LYS:N	6:A:2166:HOH:O	2.49	0.42
1:B:481:ASN:N	1:B:481:ASN:OD1	2.43	0.42
1:B:490:TYR:HB2	1:B:498:LEU:HB3	2.02	0.41
1:B:593:TYR:CD2	1:B:598:ILE:HD11	2.55	0.41
1:B:419:ARG:NH1	1:B:711:TYR:OH	2.54	0.41
1:A:558:TRP:CE3	1:A:618:LYS:HD3	2.56	0.41
1:B:491:LYS:HA	1:B:491:LYS:HD2	1.88	0.41
2:B:750:HEM:HHC	2:B:750:HEM:CBB	2.44	0.41
1:B:478:ARG:HA	1:B:478:ARG:HD2	1.93	0.41
1:A:685:VAL:HA	1:A:686:PRO:HD3	1.90	0.40
1:A:549:VAL:HA	1:A:550:PRO:HD3	1.91	0.40
1:A:341:MET:HB2	1:A:341:MET:HE2	1.91	0.40
1:A:454:ALA:O	1:A:460:LEU:HA	2.21	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	411/421 (98%)	399 (97%)	12 (3%)	0	100	100
1	B	406/421 (96%)	390 (96%)	14 (3%)	2 (0%)	34	22
All	All	817/842 (97%)	789 (97%)	26 (3%)	2 (0%)	52	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	494	ASP
1	B	496	SER

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	371/376 (99%)	356 (96%)	15 (4%)	38	29
1	B	366/376 (97%)	351 (96%)	15 (4%)	37	28
All	All	737/752 (98%)	707 (96%)	30 (4%)	38	28

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	ARG
1	A	307	LYS
1	A	314	GLU
1	A	327	LEU
1	A	341	MET
1	A	386	LEU
1	A	390	ASN
1	A	394	ASP
1	A	528	LEU
1	A	552	ARG
1	A	560	LYS

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Mol	Chain	Res	Type
1	A	632	ASP
1	A	658[A]	SER
1	A	658[B]	SER
1	A	672	ARG
1	B	324	LYS
1	B	326	THR
1	B	341	MET
1	B	369	GLN
1	B	394	ASP
1	B	395	THR
1	B	481	ASN
1	B	528	LEU
1	B	552	ARG
1	B	555	LYS
1	B	560	LYS
1	B	593	TYR
1	B	624	ARG
1	B	718	THR
1	B	720	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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	750	1	24,50,50	2.27	5 (20%)	16,82,82	2.20	2 (12%)
3	H4B	A	760	-	15,18,18	0.84	0	12,26,26	2.36	5 (41%)
4	H65	A	800	-	25,25,25	0.49	0	34,34,34	1.92	6 (17%)
2	HEM	B	750	1	24,50,50	2.26	6 (25%)	16,82,82	1.99	5 (31%)
3	H4B	B	760	-	15,18,18	0.66	0	12,26,26	2.38	5 (41%)
4	H65	B	800	-	25,25,25	0.51	0	34,34,34	1.87	8 (23%)

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	750	1	-	0/6/54/54	0/0/8/8
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
4	H65	A	800	-	-	0/9/19/19	0/3/3/3
2	HEM	B	750	1	-	0/6/54/54	0/0/8/8
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
4	H65	B	800	-	-	0/9/19/19	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C3B-C2B	-5.52	1.33	1.40
2	A	750	HEM	C3B-C2B	-5.46	1.33	1.40
2	A	750	HEM	C3C-C2C	-4.36	1.34	1.40
2	B	750	HEM	C3C-C2C	-3.97	1.35	1.40
2	B	750	HEM	C4D-ND	2.22	1.39	1.36
2	A	750	HEM	C3C-CAC	3.26	1.54	1.47
2	B	750	HEM	C3B-CAB	3.40	1.55	1.47
2	B	750	HEM	C3C-CAC	3.54	1.55	1.47
2	A	750	HEM	C3B-CAB	3.65	1.55	1.47
2	A	750	HEM	C3D-C2D	5.02	1.52	1.37
2	B	750	HEM	C3D-C2D	5.05	1.52	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	H65	C09-C08-C06	-5.95	100.69	112.76
2	A	750	HEM	CBA-CAA-C2A	-5.68	102.50	112.49
2	A	750	HEM	CBD-CAD-C3D	-5.29	103.19	112.47
4	A	800	H65	C09-C08-C06	-5.25	102.11	112.76
2	B	750	HEM	CBD-CAD-C3D	-4.61	104.39	112.47
2	B	750	HEM	CBA-CAA-C2A	-3.99	105.47	112.49
3	A	760	H4B	N3-C2-N1	-3.25	120.20	125.51
4	A	800	H65	C05-C06-N01	-3.24	119.30	122.90
3	B	760	H4B	N3-C2-N1	-3.18	120.32	125.51
4	A	800	H65	C09-C13-C12	-3.10	116.64	121.63
4	B	800	H65	C09-C13-C12	-2.94	116.90	121.63
4	B	800	H65	C05-C06-N01	-2.89	119.69	122.90
2	B	750	HEM	CAD-CBD-CGD	-2.47	107.98	112.78
2	B	750	HEM	C3B-CAB-CBB	-2.07	122.23	126.40
4	B	800	H65	C08-C09-C13	2.01	119.93	113.27
4	A	800	H65	C14-C15-C16	2.04	119.06	116.82
3	A	760	H4B	C4A-C8A-N8	2.13	120.51	118.26
4	B	800	H65	C14-C15-C16	2.23	119.27	116.82
2	B	750	HEM	CMC-C2C-C3C	2.37	129.72	125.09
3	A	760	H4B	C2-N1-C8A	2.68	120.66	114.63
3	B	760	H4B	C2-N1-C8A	2.74	120.78	114.63
4	B	800	H65	C14-C13-C12	2.85	119.56	116.58
4	B	800	H65	C08-C06-N01	2.86	120.06	115.71
4	A	800	H65	C14-C13-C12	2.92	119.63	116.58
3	B	760	H4B	C4A-C8A-N8	3.10	121.55	118.26
3	B	760	H4B	C4-C4A-C8A	3.77	117.93	114.61
4	B	800	H65	C02-N01-C06	3.81	121.17	118.20
3	A	760	H4B	C4-N3-C2	3.99	120.56	115.88
3	B	760	H4B	C4-N3-C2	4.32	120.94	115.88
3	A	760	H4B	C4-C4A-C8A	4.76	118.80	114.61
4	A	800	H65	C02-N01-C06	5.01	122.10	118.20

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	750	HEM	2	0
4	A	800	H65	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	750	HEM	4	0
4	B	800	H65	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 (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(Å²)	Q<0.9
1	A	413/421 (98%)	-0.22	3 (0%)	89	91	14, 31, 61, 94	0
1	B	408/421 (96%)	0.02	8 (1%)	68	73	16, 39, 77, 97	0
All	All	821/842 (97%)	-0.10	11 (1%)	79	83	14, 34, 71, 97	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	721	TRP	3.6
1	A	624	ARG	2.7
1	B	357	ASP	2.5
1	B	556	PHE	2.3
1	B	360	PHE	2.3
1	A	334	TYR	2.3
1	B	356	LYS	2.2
1	A	304	ARG	2.2
1	B	380	LYS	2.0
1	B	720	VAL	2.0
1	B	493	PRO	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, 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	LLDF	B-factors($Å^2$)	Q<0.9
4	H65	A	800	23/23	0.96	0.14	3.31	19,28,49,52	0
2	HEM	B	750	43/43	0.99	0.11	0.85	11,28,35,49	0
4	H65	B	800	23/23	0.97	0.12	0.71	16,33,37,38	0
2	HEM	A	750	43/43	0.99	0.11	0.64	10,19,27,31	0
5	ZN	A	900	1/1	1.00	0.12	0.54	26,26,26,26	0
3	H4B	B	760	17/17	0.99	0.10	-0.41	11,24,36,37	0
3	H4B	A	760	17/17	0.98	0.10	-0.82	16,20,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.