



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:03 PM GMT

PDB ID : 4KCN
Title : Structure of neuronal nitric oxide synthase heme domain in complex with N-(3-(((3-fluorophenethyl)amino)methyl)phenyl)thiophene-2-carboximidamide
Authors : Li, H.; Poulos, T.L.
Deposited on : 2013-04-24
Resolution : 1.85 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.

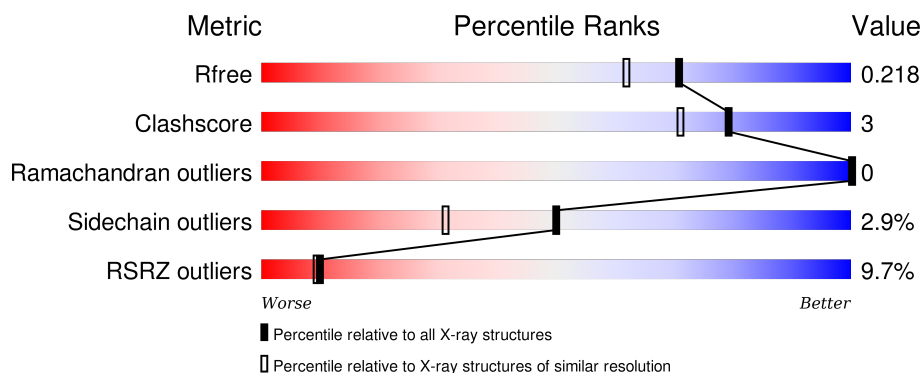
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

i

X-RAY DIFFRACTION

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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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	422	<div> <div>14%</div> <div>89%</div> <div>6%</div> </div>
1	B	422	<div> <div>5%</div> <div>89%</div> <div>8%</div> </div>

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	ACT	A	803	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7292 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	407	Total	C	N	O	S	6	2	0
			3322	2127	566	607	22			
1	B	411	Total	C	N	O	S	0	3	0
			3354	2146	574	612	22			

- 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: $C_9H_{15}N_5O_3$).



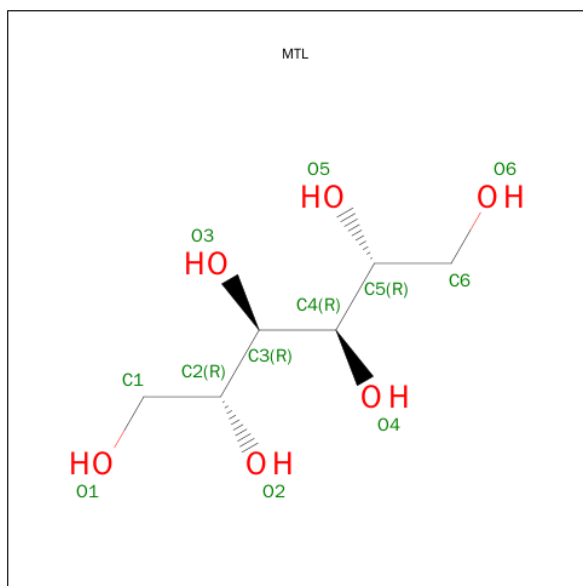
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 17	C 9	N 5	O 3	0	0
3	B	1	Total 17	C 9	N 5	O 3	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



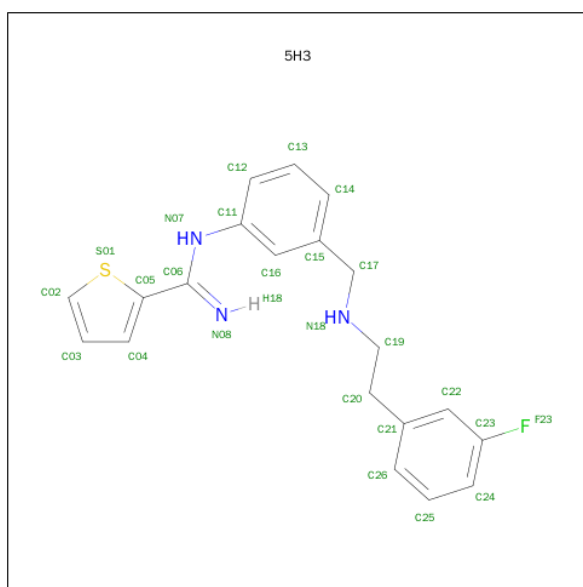
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is D-MANNITOL (three-letter code: MTL) (formula: $C_6H_{14}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			12	6	6		
5	B	1	Total	C	O	0	0
			12	6	6		
5	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 6 is N-[3-({[2-(3-FLUOROPHENYL)ETHYL]AMINO}METHYL)PHENYL]THIOPHENE-2-CARBOXIMIDAMIDE (three-letter code: 5H3) (formula: $C_{20}H_{20}FN_3S$).

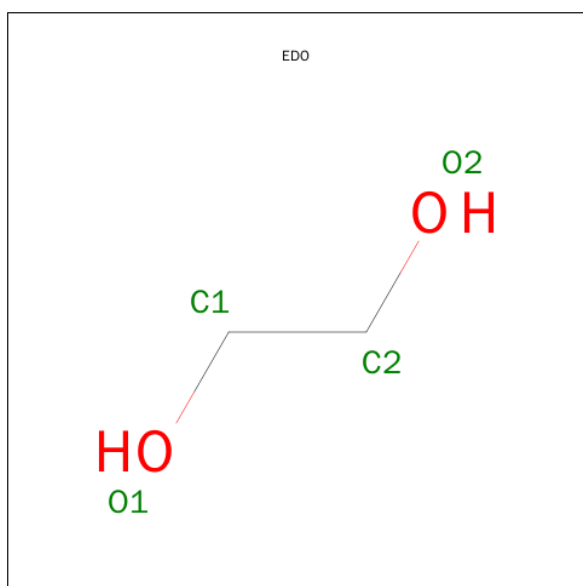


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	F	N	S	0	0
			25	20	1	3	1		
6	B	1	Total	C	F	N	S	0	0
			25	20	1	3	1		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		

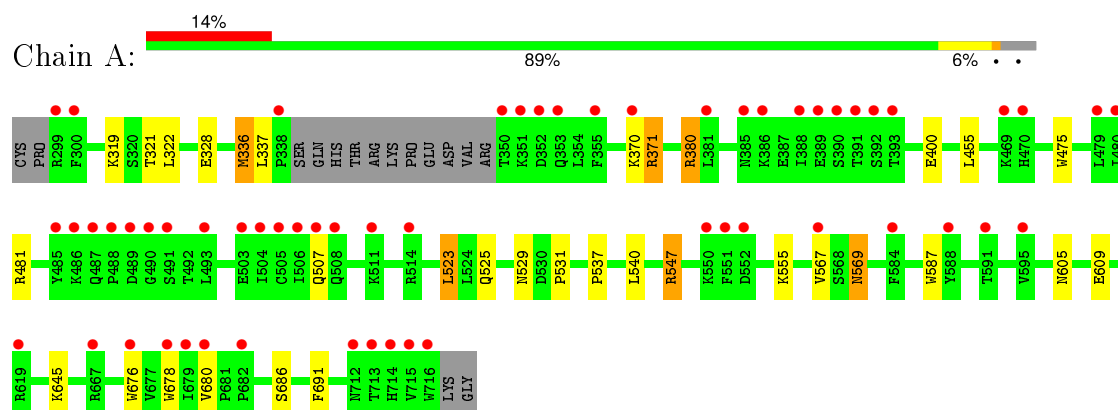
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	161	Total	O	0	0
			161	161		
9	B	236	Total	O	0	0
			236	236		

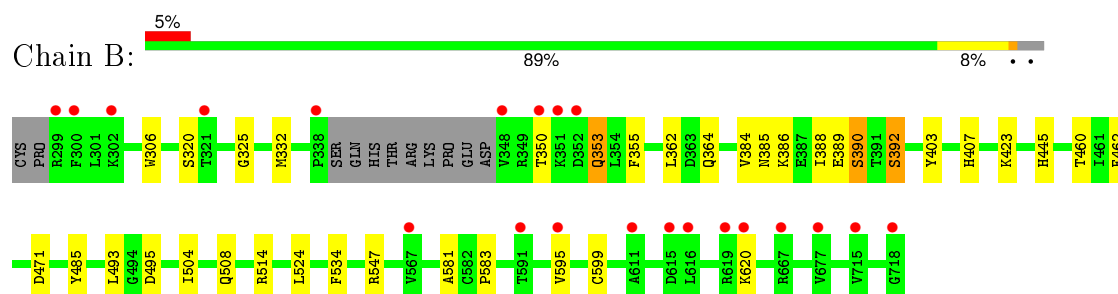
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.08Å 110.96Å 165.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.00 – 1.85 37.97 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.3 (38.00-1.85) 99.0 (37.97-1.85)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.185 , 0.217 0.186 , 0.218	Depositor DCC
R_{free} test set	4058 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.709	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 82281 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7292	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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, 0.375 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: ZN, H4B, EDO, 5H3, MTL, ACT, 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	0.56	0/3421	0.67	1/4641 (0.0%)
1	B	0.67	0/3456	0.73	2/4685 (0.0%)
All	All	0.62	0/6877	0.70	3/9326 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	471	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	495	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	547	ARG	NE-CZ-NH1	-5.00	117.80	120.30

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	3322	0	3232	27	0
1	B	3354	0	3274	19	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	3	0	0
4	B	4	0	3	0	0
5	A	12	0	14	0	0
5	B	24	0	28	0	0
6	A	25	0	19	2	0
6	B	25	0	19	0	0
7	A	1	0	0	0	0
8	B	4	0	6	0	0
9	A	161	0	0	4	0
9	B	236	0	0	1	0
All	All	7292	0	6688	47	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 (47) 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:336:MET:CE	1:A:678:TRP:HZ2	1.79	0.95
1:A:336:MET:HE3	1:A:678:TRP:CZ2	2.08	0.88
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.65	0.79
1:A:336:MET:HE3	1:A:678:TRP:HZ2	1.43	0.78
1:A:336:MET:HE1	1:A:678:TRP:HZ2	1.50	0.75
1:A:336:MET:CE	1:A:678:TRP:CZ2	2.65	0.72
1:B:364:GLN:NE2	9:B:1093:HOH:O	2.27	0.65
1:A:371:ARG:HH21	1:A:371:ARG:CG	2.12	0.63
1:A:371:ARG:HH21	1:A:371:ARG:HG3	1.65	0.61
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.00	0.61
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.83	0.59
1:B:325:GLY:O	1:B:332:MET:HG3	2.05	0.56
2:B:801:HEM:HBB2	2:B:801:HEM:HHC	1.87	0.55
1:B:524:LEU:HD12	1:B:534:PHE:CD1	2.42	0.55
1:A:609:GLU:HG3	9:A:927:HOH:O	2.07	0.55
1:A:336:MET:HA	1:A:336:MET:HE2	1.88	0.54
2:A:801:HEM:HHC	2:A:801:HEM:HBB2	1.91	0.53
1:A:328:GLU:CD	1:A:328:GLU:H	2.12	0.52
1:A:525:GLN:HG3	1:A:529:ASN:O	2.10	0.52
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.72	0.50
1:A:569:ASN:HD22	1:A:569:ASN:H	1.59	0.50
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.47	0.49
1:A:321:THR:HG23	1:A:322:LEU:HG	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:MET:HG3	1:B:306:TRP:CE2	2.48	0.48
1:B:504:ILE:O	1:B:508:GLN:HG2	2.14	0.48
1:B:362:LEU:HD11	1:B:384:VAL:HG21	1.97	0.47
1:A:686:SER:HA	1:A:691:PHE:CG	2.49	0.47
1:A:336:MET:HG3	1:B:306:TRP:NE1	2.30	0.47
1:A:481:ARG:HG2	9:A:913:HOH:O	2.15	0.46
1:B:353:GLN:HG2	1:B:353:GLN:H	1.58	0.46
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.99	0.44
6:A:805:5H3:C05	6:A:805:5H3:C12	2.94	0.44
1:B:386:LYS:O	1:B:390:SER:HB3	2.18	0.44
1:A:567:VAL:HG21	6:A:805:5H3:C14	2.48	0.43
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.53	0.43
1:A:605:ASN:ND2	9:A:926:HOH:O	2.45	0.43
1:A:537:PRO:HB2	1:A:540:LEU:HG	2.01	0.43
1:B:388:ILE:O	1:B:392:SER:N	2.49	0.43
1:B:595:VAL:O	1:B:599:CYS:HB2	2.19	0.42
1:A:321:THR:HG22	9:A:1025:HOH:O	2.20	0.42
1:B:445:HIS:C	1:B:445:HIS:CD2	2.93	0.41
1:B:388:ILE:O	1:B:392:SER:HA	2.21	0.41
1:B:460:THR:O	1:B:583:PRO:HD2	2.19	0.41
1:B:462:PHE:HB2	1:B:581:ALA:HB3	2.02	0.41
1:B:493:LEU:HD21	1:B:514:ARG:O	2.21	0.40
1:A:676:TRP:CE2	1:A:680:VAL:HG21	2.55	0.40
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.09	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	405/422 (96%)	396 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	410/422 (97%)	401 (98%)	9 (2%)	0	100	100
All	All	815/844 (97%)	797 (98%)	18 (2%)	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	365/377 (97%)	353 (97%)	12 (3%)	45	25
1	B	369/377 (98%)	360 (98%)	9 (2%)	57	39
All	All	734/754 (97%)	713 (97%)	21 (3%)	50	31

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	LYS
1	A	336	MET
1	A	337	LEU
1	A	370	LYS
1	A	371	ARG
1	A	380	ARG
1	A	507	GLN
1	A	523	LEU
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	645	LYS
1	B	320	SER
1	B	350	THR
1	B	353	GLN
1	B	389	GLU
1	B	390	SER
1	B	392	SER

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Mol	Chain	Res	Type
1	B	423	LYS
1	B	547	ARG
1	B	620	LYS

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	353	GLN
1	A	385	ASN
1	A	436	HIS
1	A	454	ASN
1	A	507	GLN
1	A	527	ASN
1	A	569	ASN
1	A	605	ASN
1	A	628	GLN
1	A	697	ASN
1	B	425	GLN
1	B	454	ASN
1	B	507	GLN
1	B	508	GLN
1	B	601	ASN
1	B	605	ASN
1	B	697	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

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	801	1	30,50,50	2.20	9 (30%)	24,82,82	2.27	8 (33%)
3	H4B	A	802	-	13,18,18	1.44	3 (23%)	11,26,26	2.54	5 (45%)
4	ACT	A	803	-	1,3,3	1.42	0	0,3,3	0.00	-
5	MTL	A	804	-	11,11,11	0.81	0	14,14,14	0.78	0
6	5H3	A	805	-	26,27,27	1.49	6 (23%)	27,35,35	2.18	5 (18%)
2	HEM	B	801	1	30,50,50	2.16	6 (20%)	24,82,82	2.49	10 (41%)
3	H4B	B	802	-	13,18,18	1.47	2 (15%)	11,26,26	2.66	4 (36%)
6	5H3	B	803	-	26,27,27	1.58	6 (23%)	27,35,35	1.94	6 (22%)
4	ACT	B	804	-	1,3,3	0.90	0	0,3,3	0.00	-
5	MTL	B	805	-	11,11,11	0.90	0	14,14,14	1.14	0
5	MTL	B	806	-	11,11,11	0.70	0	14,14,14	0.77	0
8	EDO	B	807	-	3,3,3	0.71	0	2,2,2	0.44	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	801	1	-	0/10/54/54	0/0/8/8
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2
4	ACT	A	803	-	-	0/0/0/0	0/0/0/0
5	MTL	A	804	-	-	0/16/16/16	0/0/0/0
6	5H3	A	805	-	-	0/11/15/15	0/3/3/3
2	HEM	B	801	1	-	0/10/54/54	0/0/8/8
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2
6	5H3	B	803	-	-	0/11/15/15	0/3/3/3
4	ACT	B	804	-	-	0/0/0/0	0/0/0/0
5	MTL	B	805	-	-	0/16/16/16	0/0/0/0
5	MTL	B	806	-	-	0/16/16/16	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	B	807	-	-	0/1/1/1	0/0/0/0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C2D-C3D	-6.78	1.34	1.54
2	A	801	HEM	C2D-C3D	-6.51	1.35	1.54
2	B	801	HEM	C2C-C1C	-6.44	1.40	1.52
2	A	801	HEM	C2C-C1C	-5.60	1.41	1.52
2	A	801	HEM	C3B-C4B	-3.67	1.48	1.51
2	B	801	HEM	C3B-C4B	-3.24	1.49	1.51
2	A	801	HEM	C3D-C4D	-3.20	1.47	1.51
6	A	805	5H3	C11-N07	-3.04	1.35	1.41
2	B	801	HEM	C3D-C4D	-2.87	1.47	1.51
2	B	801	HEM	C2B-C1B	-2.85	1.42	1.51
6	B	803	5H3	C06-N07	-2.60	1.33	1.39
2	A	801	HEM	C2B-C1B	-2.42	1.43	1.51
6	A	805	5H3	C06-N07	-2.40	1.34	1.39
6	B	803	5H3	C11-N07	-2.20	1.37	1.41
2	A	801	HEM	CHD-C4C	2.13	1.41	1.36
6	A	805	5H3	C05-S01	2.18	1.75	1.72
3	A	802	H4B	C7-N8	2.19	1.49	1.46
2	A	801	HEM	FE-NB	2.20	2.09	1.97
6	B	803	5H3	C05-C06	2.31	1.48	1.45
3	B	802	H4B	C8A-N1	2.33	1.38	1.34
6	B	803	5H3	C22-C23	2.33	1.41	1.37
6	A	805	5H3	C22-C23	2.41	1.41	1.37
3	A	802	H4B	C4-N3	2.53	1.37	1.33
2	A	801	HEM	C1C-NC	2.54	1.39	1.36
2	B	801	HEM	FE-NC	2.70	2.06	1.95
6	A	805	5H3	C13-C14	2.94	1.45	1.38
3	A	802	H4B	C2-N2	3.35	1.40	1.34
2	A	801	HEM	FE-NC	3.36	2.09	1.95
3	B	802	H4B	C7-N8	3.52	1.50	1.46
6	A	805	5H3	C05-C06	3.53	1.50	1.45
6	B	803	5H3	C13-C14	3.67	1.46	1.38
6	B	803	5H3	C05-S01	3.93	1.77	1.72

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	805	5H3	C03-C02-S01	-7.76	104.64	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	C1D-CHD-C4C	-4.72	117.93	125.82
6	B	803	5H3	C14-C13-C12	-4.04	114.47	120.24
3	A	802	H4B	N3-C2-N1	-3.59	119.65	125.53
2	A	801	HEM	C1D-CHD-C4C	-3.56	119.87	125.82
6	A	805	5H3	C11-N07-C06	-3.06	120.79	128.32
6	B	803	5H3	C11-C16-C15	-3.02	116.08	120.81
3	B	802	H4B	N3-C2-N1	-2.86	120.84	125.53
6	B	803	5H3	C03-C02-S01	-2.85	110.08	113.23
2	B	801	HEM	CBA-CAA-C2A	-2.65	107.79	112.53
2	B	801	HEM	CMA-C3A-C4A	-2.53	124.18	128.36
6	A	805	5H3	C17-C15-C16	-2.19	116.73	120.62
2	A	801	HEM	C3B-C4B-NB	-2.11	107.60	111.63
2	B	801	HEM	C3B-C4B-NB	-2.08	107.64	111.63
6	B	803	5H3	C17-C15-C14	-2.07	116.30	120.90
2	B	801	HEM	C2D-C3D-C4D	2.03	104.95	101.50
2	B	801	HEM	CMD-C2D-C3D	2.23	124.21	114.35
2	A	801	HEM	C2D-C3D-C4D	2.52	105.78	101.50
3	B	802	H4B	C2-N1-C8A	2.97	121.22	114.54
2	A	801	HEM	CMB-C2B-C3B	3.01	124.04	116.53
2	A	801	HEM	CMD-C2D-C3D	3.11	128.11	114.35
6	A	805	5H3	C13-C12-C11	3.11	123.67	119.72
3	A	802	H4B	C4-N3-C2	3.17	120.34	115.94
3	A	802	H4B	C4-C4A-C8A	3.49	117.72	114.56
3	B	802	H4B	C4-N3-C2	3.52	120.83	115.94
3	A	802	H4B	C4A-C8A-N8	3.60	122.67	118.43
6	A	805	5H3	C14-C15-C16	3.61	123.89	118.55
3	A	802	H4B	C2-N1-C8A	3.88	123.27	114.54
2	A	801	HEM	CAD-C3D-C4D	3.94	126.38	112.47
2	B	801	HEM	CMB-C2B-C3B	4.37	127.45	116.53
2	B	801	HEM	CAD-C3D-C4D	4.39	127.95	112.47
2	B	801	HEM	CMC-C2C-C3C	4.63	128.08	116.53
6	B	803	5H3	C14-C15-C16	4.72	125.53	118.55
2	B	801	HEM	CAD-C3D-C2D	4.83	127.10	113.22
2	A	801	HEM	CMC-C2C-C3C	4.85	128.64	116.53
2	A	801	HEM	CAD-C3D-C2D	5.09	127.84	113.22
6	B	803	5H3	C13-C12-C11	5.20	126.32	119.72
3	B	802	H4B	C4-C4A-C8A	6.34	120.30	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	HEM	1	0
6	A	805	5H3	2	0
2	B	801	HEM	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, 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	407/422 (96%)	0.68	58 (14%) 4 3	21, 43, 78, 107	0
1	B	411/422 (97%)	0.16	21 (5%) 32 30	21, 33, 58, 85	0
All	All	818/844 (96%)	0.42	79 (9%) 10 9	21, 38, 74, 107	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	8.4
1	A	488	PRO	7.1
1	A	715	VAL	6.3
1	A	352	ASP	6.1
1	A	716	TRP	6.0
1	A	351	LYS	6.0
1	B	348	VAL	5.7
1	A	355	PHE	5.7
1	B	338	PRO	5.3
1	A	300	PHE	5.0
1	A	338	PRO	5.0
1	A	486	LYS	4.8
1	B	350	THR	4.6
1	B	619	ARG	4.6
1	A	392	SER	4.2
1	A	299	ARG	4.0
1	A	388	ILE	4.0
1	A	491	SER	3.9
1	A	490	GLY	3.8
1	B	620	LYS	3.8
1	A	350	THR	3.7
1	A	506	ILE	3.7
1	A	390	SER	3.7
1	A	391	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	470	HIS	3.4
1	A	389	GLU	3.4
1	A	714	HIS	3.3
1	A	489	ASP	3.3
1	A	507	GLN	3.3
1	A	713	THR	3.2
1	B	718	GLY	3.1
1	A	504	ILE	3.0
1	A	552	ASP	3.0
1	A	567	VAL	3.0
1	A	503	GLU	3.0
1	A	619	ARG	2.9
1	A	353	GLN	2.9
1	B	615	ASP	2.8
1	A	679	ILE	2.7
1	A	386	LYS	2.7
1	A	508	GLN	2.7
1	B	616	LEU	2.6
1	B	351	LYS	2.5
1	A	682	PRO	2.5
1	A	485	TYR	2.5
1	A	469	LYS	2.5
1	A	385	ASN	2.5
1	A	514	ARG	2.5
1	A	487	GLN	2.5
1	B	352	ASP	2.5
1	A	712	ASN	2.4
1	A	678	TRP	2.4
1	A	480	ILE	2.4
1	A	667	ARG	2.4
1	B	667	ARG	2.4
1	A	550	LYS	2.4
1	A	511	LYS	2.4
1	A	584	PHE	2.4
1	A	505	CYS	2.3
1	A	588	TYR	2.3
1	A	393	THR	2.3
1	B	611	ALA	2.3
1	A	370	LYS	2.2
1	B	677	VAL	2.2
1	A	591	THR	2.2
1	B	591	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	381	LEU	2.1
1	A	595	VAL	2.1
1	A	680	VAL	2.1
1	B	567	VAL	2.1
1	B	715	VAL	2.1
1	A	493	LEU	2.1
1	B	299	ARG	2.1
1	B	302	LYS	2.1
1	A	676	TRP	2.1
1	B	321	THR	2.1
1	A	551	PHE	2.0
1	A	479	LEU	2.0
1	B	595	VAL	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	ACT	A	803	4/4	0.96	0.14	5.84	59,59,61,61	0
5	MTL	B	805	12/12	0.87	0.17	1.10	34,39,42,43	0
7	ZN	A	806	1/1	1.00	0.10	0.97	31,31,31,31	0
3	H4B	A	802	17/17	0.97	0.16	0.85	23,25,27,29	0
5	MTL	B	806	12/12	0.85	0.12	0.83	32,48,49,53	0
2	HEM	B	801	43/43	0.98	0.14	0.70	21,23,27,30	0
3	H4B	B	802	17/17	0.97	0.15	0.68	22,24,28,28	0
6	5H3	B	803	25/25	0.94	0.16	0.63	21,25,47,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	HEM	A	801	43/43	0.97	0.17	0.52	23,26,30,33	0
4	ACT	B	804	4/4	0.97	0.09	0.38	44,45,48,49	0
5	MTL	A	804	12/12	0.87	0.17	0.12	39,43,45,47	0
6	5H3	A	805	25/25	0.90	0.16	-0.45	13,17,43,52	0
8	EDO	B	807	4/4	0.86	0.29	-	40,44,50,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.