



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:50 AM GMT

PDB ID : 3N5Q
Title : Structure of endothelial nitric oxide synthase heme domain complexed with 6,6'-(2,2'-(5-amino-1,3-phenylene)bis(ethane-2,1-diyl))bis(4-methylpyridin-2-amine)
Authors : Delker, S.L.; Li, H.; Poulos, T.L.
Deposited on : 2010-05-25
Resolution : 2.90 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

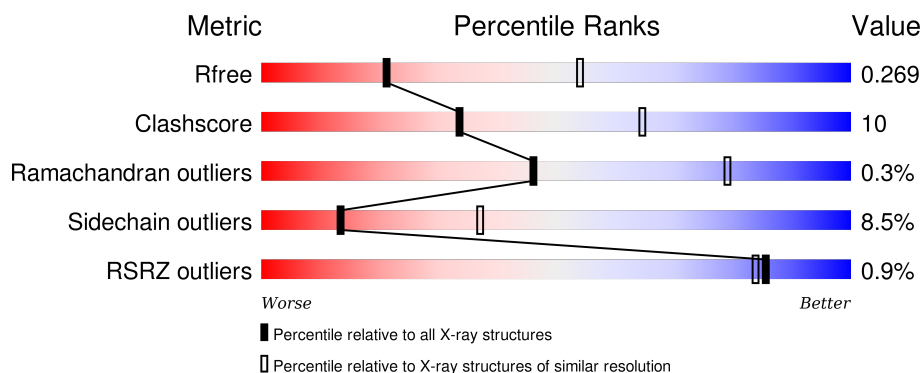
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	444	<div> <div></div> <div>73% 16% • 9%</div> </div>
1	B	444	<div> <div></div> <div>66% 21% • 9%</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
5	XFN	A	800	-	-	-	X
5	XFN	B	800	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6623 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.

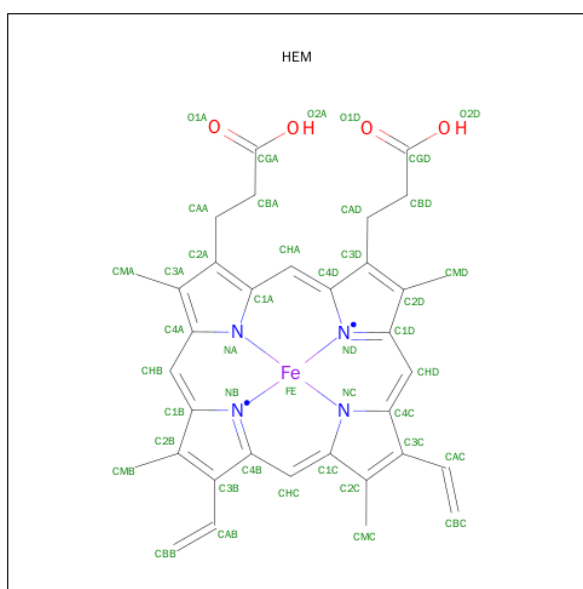
- Molecule 1 is a protein called Nitric oxide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	0	0
			3202	2036	563	587	16			
1	B	403	Total	C	N	O	S	0	0	0
			3211	2041	567	587	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	SEE REMARK 999	UNP P29473
B	100	ARG	CYS	SEE REMARK 999	UNP P29473

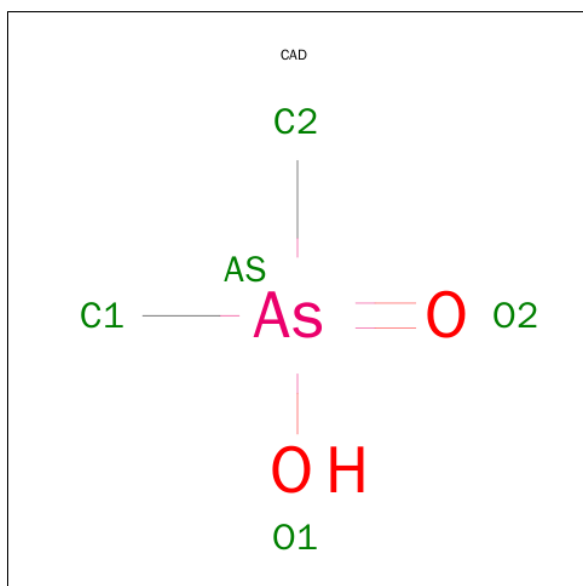
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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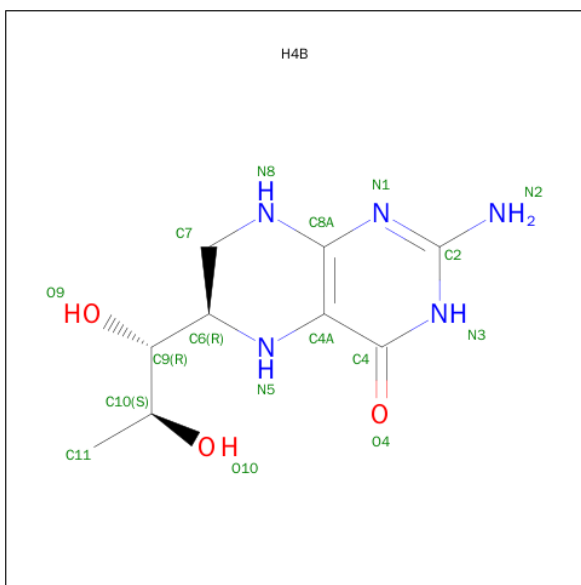
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

- Molecule 3 is CACODYLIC ACID (three-letter code: CAD) (formula: $C_2H_7AsO_2$).



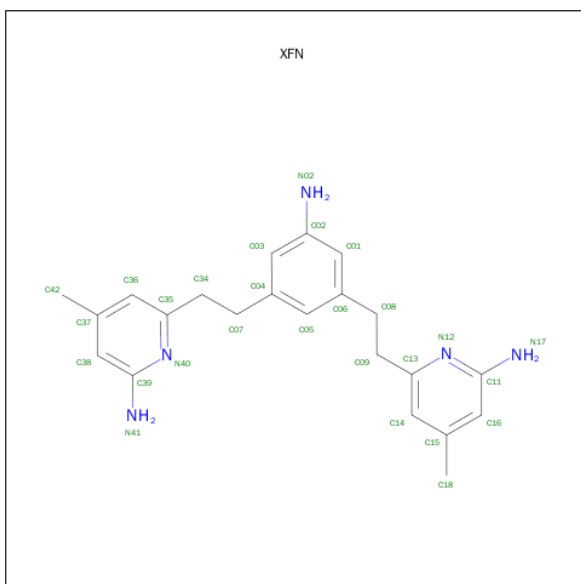
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	As	C		
			3	1	2	0	0
3	B	1	Total	As	C		
			3	1	2	0	0

- Molecule 4 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



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

- Molecule 5 is 6,6'-[(5-AMINOBENZENE-1,3-DIYL)DIETHANE-2,1-DIYL]BIS(4-METHYLPYRIDIN-2-AMINE) (three-letter code: XFN) (formula: $C_{22}H_{27}N_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			27	22	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	N	0	0
			27	22	5		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

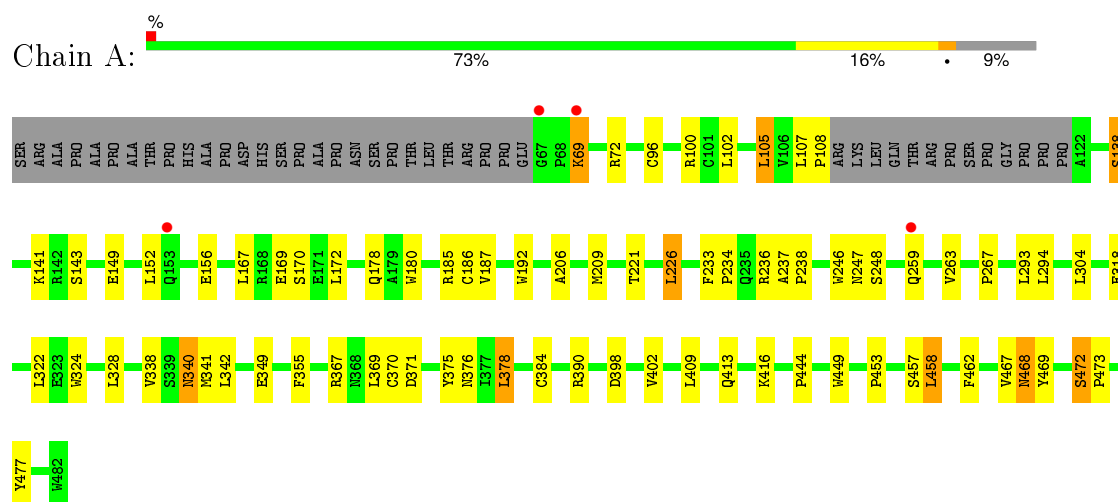
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	14	Total	O	0	0
			14	14		
7	B	15	Total	O	0	0
			15	15		

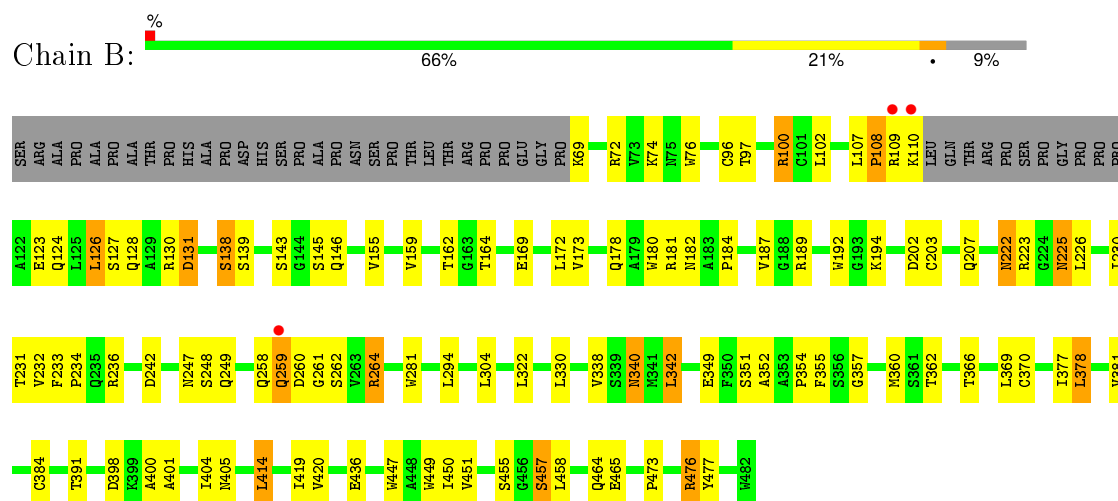
3 Residue-property plots

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



• Molecule 1: Nitric oxide synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.85Å 107.09Å 157.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.73 – 2.90 42.73 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (42.73-2.90) 97.9 (42.73-2.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.192 , 0.269 0.189 , 0.269	Depositor DCC
R_{free} test set	1097 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 36.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 21908 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6623	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.62	0/3291	0.69	0/4483
1	B	0.61	1/3299 (0.0%)	0.72	1/4491 (0.0%)
All	All	0.62	1/6590 (0.0%)	0.70	1/8974 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	CYS	CB-SG	-5.42	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	414	LEU	CA-CB-CG	6.11	129.35	115.30

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	3202	0	3107	44	0
1	B	3211	0	3123	69	0
2	A	43	0	30	11	0
2	B	43	0	30	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3	0	0	1	0
3	B	3	0	0	2	0
4	A	17	0	15	1	0
4	B	17	0	15	4	0
5	A	27	0	27	8	0
5	B	27	0	27	4	0
6	A	1	0	0	0	0
7	A	14	0	0	0	0
7	B	15	0	0	1	0
All	All	6623	0	6374	132	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 10.

All (132) 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:B:384:CYS:SG	3:B:950:CAD:AS	2.50	1.29
1:A:384:CYS:SG	3:A:950:CAD:AS	2.55	1.25
2:B:500:HEM:HBB2	2:B:500:HEM:HHC	1.26	1.08
1:B:476:ARG:HH11	1:B:476:ARG:HG3	1.27	0.99
2:A:500:HEM:HMC1	2:A:500:HEM:HBC2	1.45	0.95
2:B:500:HEM:CBB	2:B:500:HEM:HHC	2.07	0.84
1:B:476:ARG:NH1	1:B:476:ARG:HG3	1.91	0.83
1:B:236:ARG:HD2	1:B:242:ASP:OD1	1.79	0.83
1:B:476:ARG:CG	1:B:476:ARG:HH11	1.92	0.82
2:B:500:HEM:HBB2	2:B:500:HEM:CHC	2.07	0.78
2:A:500:HEM:CMC	2:A:500:HEM:HBC2	2.13	0.78
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.67	0.77
1:A:105:LEU:N	1:A:105:LEU:HD23	2.00	0.77
1:B:370:CYS:HB3	1:B:378:LEU:HD22	1.67	0.75
1:B:258:GLN:HE21	1:B:264:ARG:HB3	1.51	0.73
1:A:186:CYS:HB2	2:A:500:HEM:ND	2.05	0.72
1:B:178:GLN:HB3	1:B:473:PRO:HG2	1.72	0.72
1:B:182:ASN:O	1:B:184:PRO:HD3	1.90	0.72
1:B:340:ASN:HD22	1:B:340:ASN:C	1.95	0.70
1:B:178:GLN:HE22	1:B:181:ARG:HH11	1.42	0.67
2:B:500:HEM:HBC2	2:B:500:HEM:HMC1	1.76	0.67
1:B:258:GLN:NE2	1:B:264:ARG:HB3	2.09	0.67
2:B:500:HEM:HBA1	5:B:800:XFN:H34	1.79	0.65
1:A:338:VAL:HG22	5:A:800:XFN:H03	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:ALA:O	1:B:404:ILE:HG13	1.96	0.64
2:B:500:HEM:HBC2	2:B:500:HEM:CMC	2.29	0.62
2:A:500:HEM:O2A	5:A:800:XFN:H08A	1.99	0.62
1:B:222:ASN:HB3	1:B:225:ASN:O	2.00	0.61
1:B:230:ILE:HG13	1:B:355:PHE:HB3	1.83	0.61
2:B:500:HEM:CGA	4:B:600:H4B:HN3	2.14	0.60
1:A:409:LEU:O	1:A:413:GLN:HG3	2.02	0.59
1:A:178:GLN:HB3	1:A:473:PRO:HG2	1.82	0.59
1:B:247:ASN:ND2	7:B:1024:HOH:O	2.35	0.59
5:A:800:XFN:C13	5:A:800:XFN:H01	2.33	0.59
1:A:468:ASN:HD22	1:A:469:TYR:N	2.02	0.58
1:A:96:CYS:HB3	1:B:96:CYS:HB3	1.86	0.58
1:B:126:LEU:O	1:B:130:ARG:HG3	2.04	0.57
1:B:377:ILE:O	1:B:381:VAL:HG23	2.05	0.57
1:A:167:LEU:HD12	1:A:172:LEU:HD12	1.88	0.56
1:A:187:VAL:O	1:A:187:VAL:HG22	2.06	0.55
1:A:221:THR:O	1:A:226:LEU:HD12	2.06	0.55
5:A:800:XFN:C14	5:A:800:XFN:H01	2.37	0.55
1:A:477:TYR:CE1	5:A:800:XFN:N17	2.75	0.54
1:A:105:LEU:N	1:A:105:LEU:CD2	2.69	0.54
1:B:342:LEU:HD23	1:B:342:LEU:C	2.28	0.54
1:B:248:SER:HA	1:B:340:ASN:HB3	1.89	0.54
1:B:233:PHE:HB3	1:B:234:PRO:HD2	1.90	0.53
1:B:369:LEU:HB3	1:B:377:ILE:HD11	1.90	0.53
1:A:370:CYS:HB3	1:A:378:LEU:HD22	1.91	0.53
1:B:72:ARG:NH2	1:B:74:LYS:HD2	2.24	0.53
1:A:369:LEU:HA	1:A:375:TYR:HB2	1.91	0.52
1:B:178:GLN:O	1:B:182:ASN:ND2	2.42	0.52
2:A:500:HEM:CBC	2:A:500:HEM:HMC1	2.31	0.52
1:A:180:TRP:CE3	1:A:192:TRP:HA	2.44	0.52
1:B:447:TRP:CZ2	1:B:451:VAL:HG21	2.45	0.52
1:B:381:VAL:HG21	1:B:404:ILE:HD11	1.93	0.51
1:B:130:ARG:HB3	1:B:130:ARG:NH1	2.25	0.51
1:B:138:SER:HA	1:B:143:SER:HB2	1.91	0.51
1:A:138:SER:O	1:A:141:LYS:HD3	2.11	0.51
1:B:360:MET:HA	1:B:420:VAL:O	2.11	0.51
1:B:74:LYS:HD3	1:B:76:TRP:CE2	2.45	0.51
2:A:500:HEM:HBA1	5:A:800:XFN:H34	1.93	0.51
1:B:384:CYS:CB	3:B:950:CAD:AS	3.19	0.50
5:B:800:XFN:C14	5:B:800:XFN:H01	2.41	0.50
1:A:180:TRP:CZ3	1:A:192:TRP:HA	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:CYS:HB2	2:A:500:HEM:C4D	2.46	0.50
1:B:464:GLN:HG3	1:B:465:GLU:O	2.11	0.49
1:A:453:PRO:HB2	1:B:457:SER:HB3	1.93	0.49
1:B:72:ARG:HH22	1:B:74:LYS:HD2	1.77	0.49
1:B:155:VAL:O	1:B:159:VAL:HG23	2.13	0.49
1:A:468:ASN:HD22	1:A:468:ASN:C	2.16	0.49
1:B:338:VAL:O	1:B:354:PRO:HA	2.13	0.49
1:A:105:LEU:HD22	1:B:465:GLU:HB3	1.94	0.48
1:B:181:ARG:NE	1:B:436:GLU:OE2	2.42	0.48
1:B:247:ASN:HB3	1:B:249:GLN:O	2.14	0.48
1:A:367:ARG:NH2	1:A:371:ASP:OD2	2.38	0.47
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.95	0.47
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.50	0.47
1:B:189:ARG:O	1:B:192:TRP:HD1	1.98	0.47
1:A:248:SER:HA	1:A:340:ASN:HB3	1.96	0.47
1:A:206:ALA:O	1:A:209:MET:HB2	2.16	0.46
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.50	0.46
1:B:162:THR:OG1	1:B:164:THR:O	2.33	0.46
1:A:233:PHE:HB3	1:A:234:PRO:CD	2.46	0.46
1:B:233:PHE:HB2	1:B:352:ALA:HB3	1.98	0.46
1:A:338:VAL:HB	1:A:355:PHE:CZ	2.51	0.46
1:B:108:PRO:HB2	1:B:110:LYS:HG3	1.97	0.46
1:B:340:ASN:ND2	1:B:340:ASN:C	2.67	0.45
1:A:398:ASP:O	1:A:402:VAL:HG23	2.15	0.45
1:B:124:GLN:O	1:B:128:GLN:HG3	2.17	0.45
1:A:263:VAL:HG11	1:A:267:PRO:HA	1.98	0.45
1:A:444:PRO:HA	1:A:467:VAL:O	2.17	0.45
1:B:230:ILE:HG13	1:B:354:PRO:O	2.17	0.44
2:B:500:HEM:HMC1	2:B:500:HEM:CBC	2.46	0.44
1:A:237:ALA:HB1	1:A:238:PRO:HD2	2.00	0.44
1:A:338:VAL:HG11	1:A:341:MET:HG3	1.99	0.43
1:B:281:TRP:HB2	1:B:304:LEU:HD21	2.00	0.43
1:A:458:LEU:HD21	1:B:401:ALA:HB2	2.01	0.43
2:A:500:HEM:O2A	5:A:800:XFN:H05	2.18	0.43
1:B:172:LEU:HD11	1:B:232:VAL:HG11	2.01	0.43
2:B:500:HEM:HAA2	4:B:600:H4B:HN22	1.84	0.43
1:A:185:ARG:HD3	1:A:449:TRP:CD2	2.54	0.43
1:B:231:THR:O	1:B:354:PRO:HD2	2.19	0.43
1:B:362:THR:HA	1:B:405:ASN:HD21	1.83	0.43
1:B:455:SER:HB3	1:B:458:LEU:HD22	2.01	0.43
1:B:342:LEU:HD11	1:B:349:GLU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:500:HEM:CGA	4:A:600:H4B:HN22	2.32	0.42
1:A:152:LEU:HD23	1:A:152:LEU:HA	1.92	0.42
5:B:800:XFN:C13	5:B:800:XFN:H01	2.50	0.42
2:A:500:HEM:HBB2	2:A:500:HEM:HHC	2.01	0.42
1:A:96:CYS:HB3	1:B:96:CYS:CB	2.48	0.42
1:B:169:GLU:O	1:B:173:VAL:HG23	2.20	0.42
1:B:366:THR:O	1:B:370:CYS:HB2	2.20	0.42
1:B:226:LEU:HD23	1:B:357:GLY:O	2.20	0.41
5:A:800:XFN:C13	5:A:800:XFN:C01	2.99	0.41
1:B:260:ASP:HB2	1:B:262:SER:HB2	2.02	0.41
1:B:127:SER:O	1:B:131:ASP:HB3	2.20	0.41
1:B:259:GLN:C	1:B:261:GLY:H	2.23	0.41
1:B:110:LYS:H	1:B:110:LYS:HG2	1.69	0.41
2:B:500:HEM:CAA	4:B:600:H4B:HN22	2.33	0.41
1:B:97:THR:HG23	1:B:100:ARG:NH1	2.36	0.41
1:A:107:LEU:HA	1:A:108:PRO:HD3	1.92	0.41
1:A:342:LEU:HD21	1:A:349:GLU:HG2	2.03	0.41
1:A:69:LYS:HA	1:A:69:LYS:NZ	2.36	0.41
1:B:338:VAL:HB	1:B:355:PHE:CZ	2.57	0.40
2:A:500:HEM:CBC	2:A:500:HEM:CMC	2.91	0.40
1:B:449:TRP:HA	4:B:600:H4B:N1	2.36	0.40
1:B:477:TYR:CE1	5:B:800:XFN:N17	2.89	0.40
1:A:457:SER:HA	1:A:462:PHE:CG	2.56	0.40
1:A:338:VAL:HB	1:A:355:PHE:CE1	2.56	0.40
1:A:472:SER:HA	1:A:473:PRO:C	2.42	0.40
1:B:187:VAL:HG23	1:B:450:ILE:HG23	2.03	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	399/444 (90%)	366 (92%)	33 (8%)	0	100	100
1	B	399/444 (90%)	370 (93%)	27 (7%)	2 (0%)	34	71
All	All	798/888 (90%)	736 (92%)	60 (8%)	2 (0%)	46	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	145	SER
1	B	108	PRO

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	342/377 (91%)	315 (92%)	27 (8%)	15	41
1	B	343/377 (91%)	312 (91%)	31 (9%)	12	34
All	All	685/754 (91%)	627 (92%)	58 (8%)	13	37

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	72	ARG
1	A	100	ARG
1	A	102	LEU
1	A	105	LEU
1	A	138	SER
1	A	143	SER
1	A	149	GLU
1	A	156	GLU
1	A	169	GLU
1	A	170	SER
1	A	226	LEU
1	A	236	ARG
1	A	247	ASN

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Mol	Chain	Res	Type
1	A	259	GLN
1	A	293	LEU
1	A	304	LEU
1	A	318	GLU
1	A	328	LEU
1	A	340	ASN
1	A	376	ASN
1	A	378	LEU
1	A	390	ARG
1	A	416	LYS
1	A	458	LEU
1	A	468	ASN
1	A	472	SER
1	B	69	LYS
1	B	100	ARG
1	B	102	LEU
1	B	107	LEU
1	B	109	ARG
1	B	123	GLU
1	B	126	LEU
1	B	131	ASP
1	B	138	SER
1	B	139	SER
1	B	146	GLN
1	B	194	LYS
1	B	202	ASP
1	B	207	GLN
1	B	222	ASN
1	B	223	ARG
1	B	225	ASN
1	B	259	GLN
1	B	264	ARG
1	B	294	LEU
1	B	322	LEU
1	B	330	LEU
1	B	340	ASN
1	B	342	LEU
1	B	378	LEU
1	B	391	THR
1	B	398	ASP
1	B	414	LEU
1	B	419	ILE

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Mol	Chain	Res	Type
1	B	457	SER
1	B	476	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	340	ASN
1	A	376	ASN
1	A	468	ASN
1	B	146	GLN
1	B	178	GLN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	258	GLN
1	B	340	ASN
1	B	376	ASN
1	B	405	ASN

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 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	500	1	30,50,50	2.23	6 (20%)	24,82,82	2.23	8 (33%)
4	H4B	A	600	-	13,18,18	0.93	1 (7%)	11,26,26	2.50	4 (36%)
5	XFN	A	800	-	29,29,29	0.69	0	40,40,40	1.71	6 (15%)
3	CAD	A	950	-	0,2,4	0.00	-	0,1,6	0.00	-
2	HEM	B	500	1	30,50,50	2.27	6 (20%)	24,82,82	2.41	11 (45%)
4	H4B	B	600	-	13,18,18	0.89	0	11,26,26	2.51	3 (27%)
5	XFN	B	800	-	29,29,29	0.55	0	40,40,40	1.69	8 (20%)
3	CAD	B	950	-	0,2,4	0.00	-	0,1,6	0.00	-

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	500	1	-	0/10/54/54	0/0/8/8
4	H4B	A	600	-	-	0/8/17/17	0/2/2/2
5	XFN	A	800	-	-	0/10/10/10	0/3/3/3
3	CAD	A	950	-	-	0/0/0/0	0/0/0/0
2	HEM	B	500	1	-	0/10/54/54	0/0/8/8
4	H4B	B	600	-	-	0/8/17/17	0/2/2/2
5	XFN	B	800	-	-	0/10/10/10	0/3/3/3
3	CAD	B	950	-	-	0/0/0/0	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C3B-C4B	-8.48	1.44	1.51
2	A	500	HEM	C3B-C4B	-8.12	1.44	1.51
2	A	500	HEM	C3D-C4D	-4.89	1.45	1.51
2	B	500	HEM	C3D-C4D	-4.75	1.45	1.51
2	B	500	HEM	C2C-C1C	-4.34	1.44	1.52
2	A	500	HEM	C2C-C1C	-4.24	1.44	1.52
2	B	500	HEM	C2D-C1D	-2.38	1.44	1.51
2	A	500	HEM	C2D-C1D	-2.22	1.44	1.51
2	A	500	HEM	CMA-C3A	2.06	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	CAA-C2A	2.21	1.55	1.52
4	A	600	H4B	C4-N3	2.40	1.37	1.33
2	A	500	HEM	C3B-CAB	2.46	1.55	1.51
2	B	500	HEM	FE-NC	2.83	2.07	1.95

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	800	XFN	C14-C13-N12	-3.74	118.75	122.96
2	A	500	HEM	C3C-CAC-CBC	-3.69	118.79	124.46
5	B	800	XFN	C36-C35-N40	-3.49	119.02	122.96
5	A	800	XFN	C36-C35-N40	-3.22	119.33	122.96
2	A	500	HEM	CBD-CAD-C3D	-3.03	104.75	113.55
2	B	500	HEM	CMA-C3A-C4A	-2.85	123.65	128.36
4	B	600	H4B	N3-C2-N1	-2.82	120.92	125.53
2	B	500	HEM	C3B-CAB-CBB	-2.75	120.23	124.46
4	A	600	H4B	N3-C2-N1	-2.60	121.27	125.53
5	B	800	XFN	C14-C13-N12	-2.46	120.18	122.96
5	B	800	XFN	C34-C07-C04	-2.43	105.26	113.27
2	B	500	HEM	CBD-CAD-C3D	-2.30	106.86	113.55
2	B	500	HEM	C3C-CAC-CBC	-2.11	121.22	124.46
5	B	800	XFN	C34-C35-N40	2.22	118.96	115.69
4	A	600	H4B	C2-N1-C8A	2.31	119.72	114.54
2	B	500	HEM	CAA-C2A-C1A	2.33	129.54	127.01
2	A	500	HEM	C2D-C3D-C4D	2.36	105.50	101.50
5	A	800	XFN	C09-C13-N12	2.61	119.55	115.69
2	A	500	HEM	CMD-C2D-C3D	2.65	126.06	114.35
5	B	800	XFN	C09-C13-N12	2.68	119.65	115.69
2	B	500	HEM	C2D-C3D-C4D	2.90	106.42	101.50
2	B	500	HEM	CMD-C2D-C3D	3.32	129.04	114.35
5	B	800	XFN	C07-C34-C35	3.53	119.33	112.53
4	A	600	H4B	C4-N3-C2	3.55	120.87	115.94
2	A	500	HEM	CMB-C2B-C3B	3.71	125.80	116.53
5	B	800	XFN	C11-N12-C13	3.80	120.93	118.23
4	B	600	H4B	C4-N3-C2	3.86	121.30	115.94
5	A	800	XFN	C11-N12-C13	3.92	121.02	118.23
5	A	800	XFN	C07-C34-C35	4.00	120.22	112.53
2	A	500	HEM	CAD-C3D-C2D	4.14	125.13	113.22
2	B	500	HEM	CAD-C3D-C4D	4.19	127.24	112.47
2	B	500	HEM	CMB-C2B-C3B	4.26	127.16	116.53
2	B	500	HEM	CMC-C2C-C3C	4.39	127.50	116.53
2	A	500	HEM	CMC-C2C-C3C	4.41	127.55	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	HEM	CAD-C3D-C2D	4.56	126.33	113.22
2	A	500	HEM	CAD-C3D-C4D	4.79	129.36	112.47
5	A	800	XFN	C39-N40-C35	5.22	121.94	118.23
5	B	800	XFN	C39-N40-C35	5.73	122.30	118.23
4	A	600	H4B	C4-C4A-C8A	5.98	119.98	114.56
4	B	600	H4B	C4-C4A-C8A	5.99	119.99	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	11	0
4	A	600	H4B	1	0
5	A	800	XFN	8	0
3	A	950	CAD	1	0
2	B	500	HEM	10	0
4	B	600	H4B	4	0
5	B	800	XFN	4	0
3	B	950	CAD	2	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	403/444 (90%)	-0.39	4 (0%) 84 82	27, 44, 68, 81	0
1	B	403/444 (90%)	-0.42	3 (0%) 89 88	27, 47, 68, 95	0
All	All	806/888 (90%)	-0.41	7 (0%) 85 84	27, 45, 68, 95	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	GLN	2.7
1	A	67	GLY	2.5
1	A	69	LYS	2.4
1	A	153	GLN	2.3
1	A	259	GLN	2.2
1	B	109	ARG	2.1
1	B	110	LYS	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. 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(\AA^2)	Q<0.9
5	XFN	A	800	27/27	0.84	0.33	9.66	55,76,102,103	0
5	XFN	B	800	27/27	0.91	0.26	3.63	46,68,86,87	0
2	HEM	B	500	43/43	0.97	0.17	0.98	26,34,51,53	0
4	H4B	B	600	17/17	0.95	0.17	0.96	50,51,53,54	0
4	H4B	A	600	17/17	0.94	0.16	0.93	41,46,48,49	0
2	HEM	A	500	43/43	0.97	0.17	0.76	31,36,45,50	0
6	ZN	A	900	1/1	0.99	0.08	-1.21	46,46,46,46	0
3	CAD	A	950	3/5	0.99	0.09	-3.11	68,68,69,70	0
3	CAD	B	950	3/5	0.98	0.11	-	72,72,73,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.