



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2023 – 10:54 AM EDT

PDB ID : 3FC5  
Title : G586S mutant nNOSoxy  
Authors : Bruckmann, C.; Mowat, C.G.  
Deposited on : 2008-11-21  
Resolution : 2.59 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

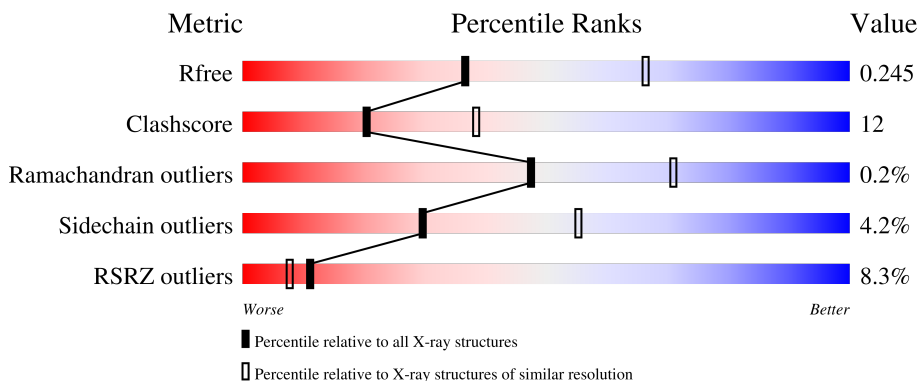
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	
1	B	422	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7003 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
			Total	C	N	O	S			
1	A	407	Total 3315	C 2122	N 566	O 606	S 21	0	0	0
1	B	411	Total 3347	C 2141	N 574	O 611	S 21	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	586	SER	GLY	engineered mutation	UNP P29476
B	586	SER	GLY	engineered mutation	UNP P29476

- 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
			Total	C	Fe	N	O		
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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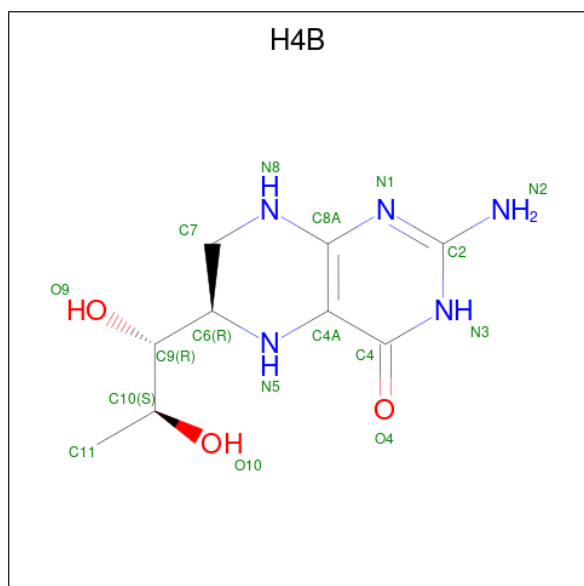
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	B	1	43	34	1	4	4	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

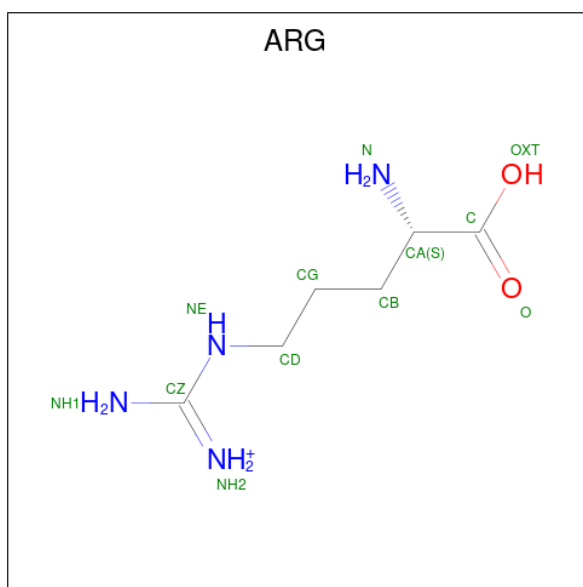
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0

- Molecule 4 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: C<sub>9</sub>H<sub>15</sub>N<sub>5</sub>O<sub>3</sub>).



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

- Molecule 5 is ARGININE (three-letter code: ARG) (formula: C<sub>6</sub>H<sub>15</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			12	6	4	2		
5	B	1	Total	C	N	O	0	0
			12	6	4	2		

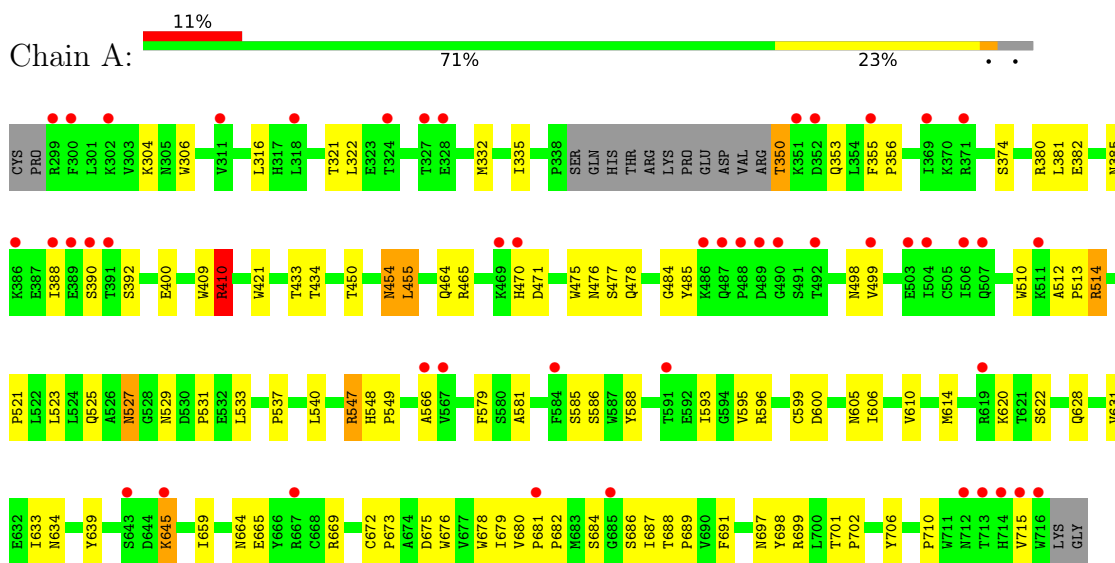
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	96	Total	O	0	0
			96	96		
6	B	100	Total	O	0	0
			100	100		

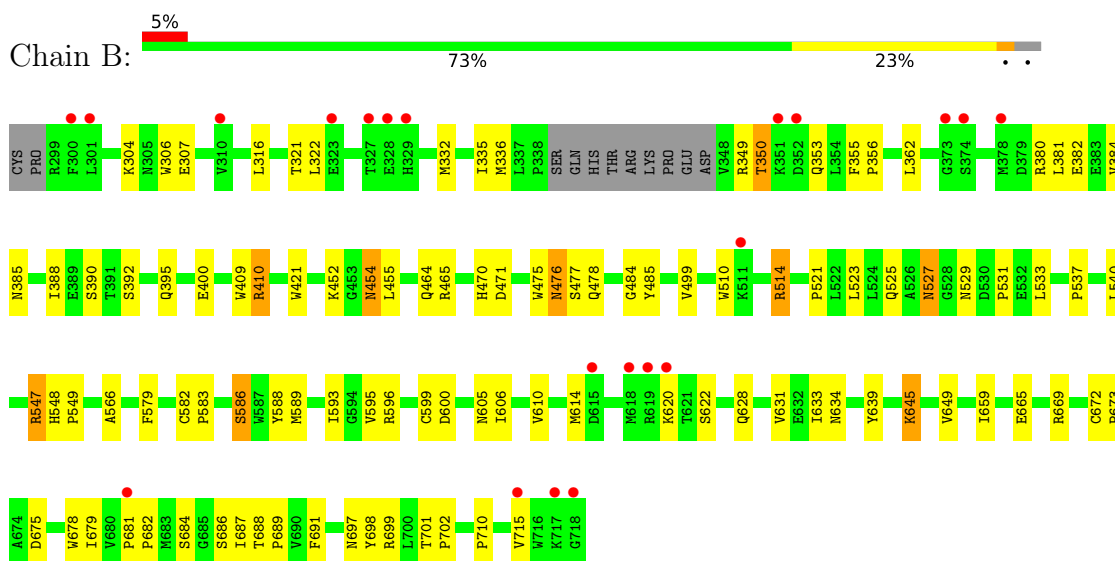
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.62Å 110.28Å 164.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.27 – 2.59 34.27 – 2.59	Depositor EDS
% Data completeness (in resolution range)	92.4 (34.27-2.59) 92.4 (34.27-2.59)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 2.57Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.199 , 0.254 0.190 , 0.245	Depositor DCC
$R_{free}$ test set	2000 reflections (7.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.6	Xtrriage
Anisotropy	1.089	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 54.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7003	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: ZN, H4B, 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	0.36	0/3408	0.68	9/4624 (0.2%)
1	B	0.36	0/3440	0.65	9/4664 (0.2%)
All	All	0.36	0/6848	0.66	18/9288 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	514	ARG	NE-CZ-NH1	-13.20	113.70	120.30
1	A	410	ARG	NE-CZ-NH2	12.32	126.46	120.30
1	A	514	ARG	NE-CZ-NH2	12.14	126.37	120.30
1	B	514	ARG	NE-CZ-NH2	-12.08	114.26	120.30
1	A	547	ARG	NE-CZ-NH1	-11.96	114.32	120.30
1	B	547	ARG	NE-CZ-NH2	-11.92	114.34	120.30
1	A	410	ARG	NE-CZ-NH1	-11.70	114.45	120.30
1	B	514	ARG	NE-CZ-NH1	11.52	126.06	120.30
1	A	547	ARG	NE-CZ-NH2	11.51	126.05	120.30
1	B	547	ARG	NE-CZ-NH1	10.73	125.66	120.30
1	B	410	ARG	NE-CZ-NH2	-10.31	115.14	120.30
1	B	410	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	A	514	ARG	CD-NE-CZ	6.36	132.50	123.60
1	A	410	ARG	CD-NE-CZ	5.99	131.99	123.60
1	B	514	ARG	CD-NE-CZ	5.91	131.88	123.60
1	A	547	ARG	CD-NE-CZ	5.58	131.42	123.60
1	B	547	ARG	CD-NE-CZ	5.48	131.28	123.60
1	B	410	ARG	CD-NE-CZ	5.33	131.07	123.60

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	3315	0	3223	85	0
1	B	3347	0	3261	76	0
2	A	43	0	30	6	0
2	B	43	0	30	3	0
3	A	1	0	0	0	0
4	A	17	0	15	1	0
4	B	17	0	15	2	0
5	A	12	0	12	0	0
5	B	12	0	12	0	0
6	A	96	0	0	7	0
6	B	100	0	0	2	0
All	All	7003	0	6598	166	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 12.

All (166) 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)
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.63	0.80
1:B:510:TRP:CD1	1:B:521:PRO:HG3	2.24	0.73
1:A:510:TRP:CD1	1:A:521:PRO:HG3	2.26	0.70
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.71	0.70
1:B:475:TRP:HE1	1:B:525:GLN:NE2	1.89	0.70
1:A:673:PRO:HG3	1:A:698:TYR:CE1	2.27	0.69
1:B:678:TRP:HA	4:B:761:H4B:N1	2.08	0.69
1:A:475:TRP:HE1	1:A:525:GLN:NE2	1.89	0.68
1:B:673:PRO:HG3	1:B:698:TYR:CE1	2.29	0.68
1:A:485:TYR:CE1	1:A:514:ARG:HA	2.31	0.65
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.31	0.65
1:A:475:TRP:HE1	1:A:525:GLN:HE21	1.45	0.63
1:A:410:ARG:HG3	1:A:421:TRP:CD2	2.33	0.63
1:B:475:TRP:HE1	1:B:525:GLN:HE21	1.46	0.62
1:A:595:VAL:HG11	1:A:682:PRO:HB2	1.80	0.62
1:B:595:VAL:HG11	1:B:682:PRO:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:HIS:ND1	1:B:549:PRO:HD2	2.16	0.60
1:A:548:HIS:ND1	1:A:549:PRO:HD2	2.16	0.59
1:B:586:SER:HB2	2:B:750:HEM:CBB	2.32	0.59
1:B:350:THR:HB	1:B:353:GLN:OE1	2.02	0.59
1:B:452:LYS:HA	6:B:159:HOH:O	2.02	0.59
2:A:750:HEM:HBC2	2:A:750:HEM:CMC	2.32	0.59
1:A:678:TRP:HA	4:A:760:H4B:N1	2.18	0.58
1:A:374:SER:HB2	6:A:42:HOH:O	2.05	0.57
1:A:410:ARG:HD3	1:A:665:GLU:OE1	2.05	0.56
1:B:510:TRP:NE1	1:B:521:PRO:HG3	2.21	0.56
1:A:588:TYR:CD1	1:A:593:ILE:HD11	2.41	0.55
1:B:701:THR:HA	1:B:702:PRO:C	2.27	0.55
1:A:350:THR:HB	1:A:353:GLN:OE1	2.07	0.54
1:A:701:THR:HA	1:A:702:PRO:C	2.28	0.54
1:B:595:VAL:HG23	1:B:634:ASN:HD21	1.72	0.54
1:A:581:ALA:HA	6:A:96:HOH:O	2.08	0.54
1:A:322:LEU:HD13	1:A:699:ARG:HH21	1.72	0.54
1:B:588:TYR:CD1	1:B:593:ILE:HD11	2.43	0.54
1:A:388:ILE:O	1:A:392:SER:HA	2.08	0.53
6:A:186:HOH:O	1:B:307:GLU:HG3	2.09	0.53
1:A:537:PRO:HB2	1:A:540:LEU:HG	1.90	0.52
1:B:388:ILE:O	1:B:392:SER:HA	2.09	0.52
1:A:675:ASP:O	1:A:679:ILE:HG12	2.09	0.52
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.74	0.52
1:A:549:PRO:HG3	1:A:639:TYR:CG	2.45	0.52
1:A:304:LYS:HD3	1:A:306:TRP:CE2	2.44	0.52
1:A:510:TRP:NE1	1:A:521:PRO:HG3	2.25	0.51
1:A:610:VAL:O	1:A:614:MET:HG3	2.10	0.51
1:B:304:LYS:HD3	1:B:306:TRP:CE2	2.45	0.51
1:A:628:GLN:HG3	1:B:631:VAL:HG11	1.93	0.51
1:A:485:TYR:CZ	1:A:514:ARG:HA	2.46	0.50
1:A:595:VAL:HG23	1:A:634:ASN:HD21	1.76	0.50
1:A:631:VAL:HG11	1:B:628:GLN:HG3	1.93	0.50
1:A:510:TRP:CE2	1:A:521:PRO:HG3	2.47	0.50
1:B:549:PRO:HG3	1:B:639:TYR:CG	2.47	0.50
1:B:510:TRP:CE2	1:B:521:PRO:HG3	2.47	0.49
1:A:523:LEU:HD13	1:A:533:LEU:HD23	1.94	0.49
1:B:316:LEU:HD22	1:B:669:ARG:HG2	1.94	0.49
1:B:523:LEU:HD13	1:B:533:LEU:HD23	1.93	0.49
1:A:350:THR:HB	1:A:353:GLN:CD	2.33	0.49
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.13	0.49
1:B:475:TRP:CZ2	1:B:531:PRO:HG3	2.48	0.49
1:A:410:ARG:HD2	1:A:669:ARG:NH1	2.28	0.49
1:B:350:THR:HB	1:B:353:GLN:CD	2.32	0.49
2:B:750:HEM:CMC	2:B:750:HEM:HBC2	2.43	0.49
1:A:355:PHE:HD1	1:A:388:ILE:HD12	1.77	0.48
1:A:332:MET:HE3	1:A:335:ILE:HG13	1.95	0.48
1:B:610:VAL:O	1:B:614:MET:HG3	2.13	0.48
1:B:675:ASP:O	1:B:679:ILE:HG12	2.13	0.48
1:B:537:PRO:HB2	1:B:540:LEU:HG	1.94	0.48
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.49	0.48
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.48	0.48
2:A:750:HEM:HBC2	2:A:750:HEM:HMC1	1.95	0.48
1:A:454:ASN:C	1:A:454:ASN:HD22	2.18	0.47
1:B:620:LYS:HE3	1:B:622:SER:OG	2.14	0.47
1:A:353:GLN:O	1:A:356:PRO:HD2	2.14	0.47
1:A:610:VAL:HG21	1:A:633:ILE:HD11	1.96	0.47
1:B:470:HIS:HB3	1:B:527:ASN:ND2	2.30	0.47
1:B:684:SER:HB3	1:B:687:ILE:HG12	1.95	0.47
1:A:525:GLN:HG3	1:A:529:ASN:O	2.14	0.47
1:B:454:ASN:C	1:B:454:ASN:HD22	2.18	0.47
1:A:510:TRP:CG	1:A:521:PRO:HG3	2.50	0.47
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.49	0.47
1:A:523:LEU:HD11	1:A:531:PRO:HB2	1.97	0.46
1:A:548:HIS:CE1	1:A:549:PRO:HD2	2.49	0.46
1:A:659:ILE:HG13	1:A:689:PRO:HB2	1.97	0.46
1:B:478:GLN:HA	1:B:566:ALA:O	2.15	0.46
1:A:682:PRO:HG3	6:A:53:HOH:O	2.15	0.46
1:B:380:ARG:HD3	1:B:400:GLU:OE1	2.16	0.45
1:B:523:LEU:HD11	1:B:531:PRO:HB2	1.98	0.45
1:B:599:CYS:O	1:B:600:ASP:C	2.54	0.45
1:A:606:ILE:O	1:A:610:VAL:HG23	2.17	0.45
1:A:498:ASN:HA	6:A:68:HOH:O	2.16	0.45
1:A:409:TRP:CZ3	2:A:750:HEM:HMC3	2.51	0.45
1:A:527:ASN:HD22	1:A:527:ASN:HA	1.60	0.45
1:B:645:LYS:HE3	1:B:645:LYS:HB2	1.80	0.45
1:B:395:GLN:HA	6:B:1:HOH:O	2.16	0.45
1:A:350:THR:HG22	1:A:353:GLN:H	1.81	0.45
1:A:410:ARG:HG3	1:A:421:TRP:CE2	2.51	0.45
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.46	0.45
1:A:478:GLN:HA	1:A:566:ALA:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:GLY:O	1:B:499:VAL:HA	2.16	0.45
1:B:548:HIS:CE1	1:B:549:PRO:HD2	2.51	0.45
1:A:684:SER:HB3	1:A:687:ILE:HG12	1.98	0.45
1:B:353:GLN:O	1:B:356:PRO:HD2	2.17	0.45
1:A:355:PHE:CE1	1:A:385:ASN:HA	2.52	0.45
1:A:599:CYS:O	1:A:600:ASP:C	2.55	0.45
1:B:606:ILE:O	1:B:610:VAL:HG23	2.17	0.45
1:A:665:GLU:CB	1:A:672:CYS:HB2	2.47	0.44
1:B:665:GLU:CB	1:B:672:CYS:HB2	2.48	0.44
1:B:355:PHE:CE1	1:B:385:ASN:HA	2.53	0.44
1:A:620:LYS:HE3	1:A:622:SER:OG	2.18	0.44
1:B:355:PHE:HD1	1:B:388:ILE:HD12	1.81	0.44
1:A:684:SER:O	1:A:687:ILE:HG12	2.17	0.43
1:B:686:SER:HA	1:B:691:PHE:CG	2.53	0.43
1:A:686:SER:HA	1:A:691:PHE:CG	2.53	0.43
1:A:706:TYR:HB3	6:A:161:HOH:O	2.18	0.43
1:B:659:ILE:HG13	1:B:689:PRO:HB2	2.00	0.43
1:B:525:GLN:HG3	1:B:529:ASN:O	2.18	0.43
1:B:610:VAL:HG21	1:B:633:ILE:HD11	2.00	0.43
1:A:665:GLU:HB3	1:A:672:CYS:HB2	1.99	0.43
1:B:684:SER:HB3	1:B:687:ILE:HD11	2.01	0.43
1:B:350:THR:HG22	1:B:353:GLN:H	1.82	0.43
1:A:512:ALA:HA	1:A:513:PRO:HD3	1.91	0.43
1:B:464:GLN:HB3	1:B:579:PHE:CE2	2.54	0.43
1:B:527:ASN:HD22	1:B:527:ASN:HA	1.64	0.43
1:A:382:GLU:O	1:A:385:ASN:HB3	2.19	0.43
1:A:645:LYS:HE3	1:A:645:LYS:HB2	1.82	0.42
2:A:750:HEM:HMC1	2:A:750:HEM:CBC	2.49	0.42
1:A:664:ASN:HB2	6:A:121:HOH:O	2.18	0.42
1:B:410:ARG:HG3	1:B:421:TRP:CD2	2.54	0.42
1:A:470:HIS:HB3	1:A:527:ASN:ND2	2.34	0.42
1:B:322:LEU:HB2	1:B:699:ARG:HB2	2.01	0.42
1:A:484:GLY:O	1:A:499:VAL:HA	2.20	0.42
1:B:382:GLU:O	1:B:385:ASN:HB3	2.19	0.42
1:A:450:THR:HA	1:A:455:LEU:HD12	2.02	0.42
1:A:355:PHE:N	1:A:356:PRO:CD	2.82	0.42
1:A:410:ARG:NH2	1:A:669:ARG:HD2	2.34	0.42
1:A:332:MET:CE	1:A:335:ILE:HG13	2.49	0.42
1:A:596:ARG:O	1:A:600:ASP:HB2	2.20	0.42
1:B:510:TRP:CG	1:B:521:PRO:HG3	2.53	0.42
1:B:476:ASN:OD1	1:B:476:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:665:GLU:HB3	1:B:672:CYS:HB2	2.01	0.42
1:A:523:LEU:HD13	1:A:533:LEU:CD2	2.50	0.41
1:A:676:TRP:CZ2	1:A:680:VAL:HG21	2.55	0.41
1:B:523:LEU:HD13	1:B:533:LEU:CD2	2.50	0.41
1:A:681:PRO:HG2	1:A:688:THR:HG21	2.01	0.41
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.49	0.41
1:B:465:ARG:HG3	1:B:471:ASP:OD2	2.20	0.41
1:B:475:TRP:CE2	1:B:710:PRO:HB2	2.55	0.41
1:A:322:LEU:HB2	1:A:699:ARG:HB2	2.02	0.41
1:B:582:CYS:O	1:B:583:PRO:C	2.56	0.41
1:A:316:LEU:HD22	1:A:669:ARG:HG2	2.02	0.41
1:B:681:PRO:HG2	1:B:688:THR:HG21	2.03	0.41
1:A:322:LEU:HD12	1:A:699:ARG:HB3	2.02	0.41
1:A:433:THR:OG1	1:A:434:THR:HG23	2.21	0.41
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.56	0.41
2:A:750:HEM:CMC	2:A:750:HEM:CBC	2.98	0.41
1:B:596:ARG:HH12	4:B:761:H4B:C4	2.33	0.41
1:A:465:ARG:HG3	1:A:471:ASP:OD2	2.22	0.41
1:A:684:SER:HB3	1:A:687:ILE:HD11	2.03	0.41
1:B:362:LEU:HD11	1:B:384:VAL:HG21	2.02	0.40
1:B:589:MET:HA	1:B:649:VAL:O	2.21	0.40
1:B:684:SER:O	1:B:687:ILE:HG12	2.21	0.40
1:A:475:TRP:CE2	1:A:710:PRO:HB2	2.57	0.40
1:B:349:ARG:HB3	1:B:350:THR:H	1.56	0.40
1:B:681:PRO:HA	1:B:682:PRO:HD3	1.84	0.40
1:B:332:MET:HE3	1:B:335:ILE:HG13	2.02	0.40
1:A:681:PRO:HA	1:A:682:PRO:HD3	1.84	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	403/422 (96%)	380 (94%)	22 (6%)	1 (0%)	47	71
1	B	407/422 (96%)	379 (93%)	27 (7%)	1 (0%)	47	71
All	All	810/844 (96%)	759 (94%)	49 (6%)	2 (0%)	47	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	586	SER
1	B	586	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	364/378 (96%)	348 (96%)	16 (4%)	28	53
1	B	367/378 (97%)	352 (96%)	15 (4%)	30	56
All	All	731/756 (97%)	700 (96%)	31 (4%)	30	55

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	321	THR
1	A	350	THR
1	A	381	LEU
1	A	390	SER
1	A	410	ARG
1	A	454	ASN
1	A	455	LEU
1	A	476	ASN
1	A	477	SER
1	A	527	ASN
1	A	547	ARG
1	A	585	SER
1	A	605	ASN
1	A	645	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	697	ASN
1	A	715	VAL
1	B	321	THR
1	B	336	MET
1	B	350	THR
1	B	381	LEU
1	B	390	SER
1	B	454	ASN
1	B	455	LEU
1	B	476	ASN
1	B	477	SER
1	B	527	ASN
1	B	547	ARG
1	B	605	ASN
1	B	645	LYS
1	B	697	ASN
1	B	715	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	364	GLN
1	A	451	ASN
1	A	454	ASN
1	A	487	GLN
1	A	507	GLN
1	A	525	GLN
1	A	527	ASN
1	A	535	GLN
1	A	605	ASN
1	A	634	ASN
1	A	697	ASN
1	B	364	GLN
1	B	451	ASN
1	B	454	ASN
1	B	487	GLN
1	B	507	GLN
1	B	525	GLN
1	B	527	ASN
1	B	535	GLN
1	B	605	ASN
1	B	634	ASN

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Mol	Chain	Res	Type
1	B	697	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 monosaccharides 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	B	750	1	41,50,50	1.97	6 (14%)	45,82,82	1.84	10 (22%)
4	H4B	A	760	-	16,18,18	5.97	11 (68%)	11,26,26	2.74	7 (63%)
5	ARG	B	771	-	10,11,11	0.72	1 (10%)	11,13,13	0.92	1 (9%)
5	ARG	A	770	-	10,11,11	0.72	1 (10%)	11,13,13	0.89	1 (9%)
2	HEM	A	750	1	41,50,50	1.93	7 (17%)	45,82,82	2.03	11 (24%)
4	H4B	B	761	-	16,18,18	5.96	11 (68%)	11,26,26	2.83	5 (45%)

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	B	750	1	-	1/12/54/54	-
4	H4B	A	760	-	-	0/8/17/17	0/2/2/2
5	ARG	B	771	-	-	0/11/11/11	-
5	ARG	A	770	-	-	0/11/11/11	-
2	HEM	A	750	1	-	1/12/54/54	-
4	H4B	B	761	-	-	1/8/17/17	0/2/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	760	H4B	C4-N3	10.42	1.51	1.33
4	B	761	H4B	C4-N3	10.24	1.50	1.33
4	B	761	H4B	C2-N1	9.79	1.52	1.35
4	A	760	H4B	C8A-N1	9.52	1.52	1.34
4	B	761	H4B	C8A-N1	9.50	1.52	1.34
4	A	760	H4B	C2-N1	9.24	1.51	1.35
4	A	760	H4B	C4A-C4	8.67	1.53	1.41
4	B	761	H4B	C4A-C4	8.32	1.52	1.41
2	B	750	HEM	C3D-C2D	8.07	1.53	1.36
4	B	761	H4B	C2-N3	7.98	1.49	1.35
4	A	760	H4B	C2-N3	7.90	1.49	1.35
2	A	750	HEM	C3D-C2D	7.70	1.53	1.36
4	A	760	H4B	O4-C4	6.53	1.41	1.24
4	B	761	H4B	O4-C4	6.50	1.40	1.24
4	A	760	H4B	C2-N2	6.46	1.46	1.33
4	B	761	H4B	C2-N2	6.18	1.46	1.33
4	A	760	H4B	C4A-N5	4.82	1.47	1.38
2	A	750	HEM	C3C-C2C	-4.65	1.33	1.40
2	B	750	HEM	C3C-C2C	-4.65	1.33	1.40
4	B	761	H4B	C4A-N5	4.53	1.47	1.38
4	A	760	H4B	C7-C6	4.20	1.56	1.52
4	B	761	H4B	C7-C6	4.16	1.56	1.52
4	B	761	H4B	C4A-C8A	3.86	1.48	1.41
4	A	760	H4B	C4A-C8A	3.81	1.48	1.41
2	B	750	HEM	C3C-CAC	3.35	1.54	1.47
2	A	750	HEM	C3C-CAC	3.26	1.54	1.47
2	B	750	HEM	CAB-C3B	3.01	1.55	1.47
2	A	750	HEM	CAB-C3B	2.78	1.55	1.47
2	B	750	HEM	FE-ND	2.74	2.10	1.96
2	A	750	HEM	FE-ND	2.69	2.10	1.96
4	B	761	H4B	C7-N8	2.59	1.49	1.44
2	A	750	HEM	FE-NB	2.19	2.07	1.96
2	B	750	HEM	CMD-C2D	2.17	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	CMB-C2B	2.13	1.55	1.50
4	A	760	H4B	C7-N8	2.08	1.48	1.44
5	B	771	ARG	OXT-C	-2.05	1.23	1.30
5	A	770	ARG	OXT-C	-2.01	1.24	1.30

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	CBA-CAA-C2A	-6.76	101.08	112.62
4	B	761	H4B	C8A-C4A-C4	6.69	120.52	114.57
2	B	750	HEM	CBA-CAA-C2A	-6.45	101.61	112.62
2	A	750	HEM	C4D-ND-C1D	5.71	110.97	105.07
2	B	750	HEM	C4D-ND-C1D	5.59	110.85	105.07
4	A	760	H4B	C8A-C4A-C4	5.57	119.52	114.57
4	A	760	H4B	N1-C2-N3	-3.54	119.87	125.42
2	A	750	HEM	C4C-CHD-C1D	3.20	126.78	122.56
4	B	761	H4B	C2-N3-C4	3.12	120.89	115.93
4	A	760	H4B	C4-C4A-N5	3.03	121.66	119.12
4	B	761	H4B	N1-C2-N3	-3.02	120.67	125.42
2	A	750	HEM	C2C-C3C-C4C	2.91	108.93	106.90
4	A	760	H4B	C2-N3-C4	2.85	120.45	115.93
2	A	750	HEM	CBD-CAD-C3D	-2.81	104.82	112.63
4	B	761	H4B	C4-C4A-N5	2.67	121.36	119.12
4	A	760	H4B	C4A-N5-C6	-2.65	113.96	121.16
2	A	750	HEM	CHA-C4D-ND	2.53	127.51	124.38
4	B	761	H4B	C4A-N5-C6	-2.50	114.34	121.16
2	A	750	HEM	CAD-CBD-CGD	-2.50	108.23	113.60
2	B	750	HEM	CHB-C1B-NB	2.48	127.45	124.38
2	A	750	HEM	C1B-NB-C4B	2.48	107.63	105.07
2	B	750	HEM	CBD-CAD-C3D	-2.47	105.76	112.63
2	A	750	HEM	C4B-CHC-C1C	2.42	125.75	122.56
4	A	760	H4B	C2-N1-C8A	2.31	119.72	114.54
2	A	750	HEM	CMD-C2D-C1D	2.30	128.55	125.04
2	B	750	HEM	C3B-C2B-C1B	2.25	108.16	106.49
2	B	750	HEM	CAD-C3D-C4D	2.21	128.53	124.66
5	B	771	ARG	OXT-C-O	-2.21	119.08	124.09
5	A	770	ARG	OXT-C-O	-2.19	119.12	124.09
2	B	750	HEM	C1D-C2D-C3D	-2.17	104.68	106.96
2	A	750	HEM	C3C-C4C-NC	-2.16	106.87	110.94
2	B	750	HEM	CHD-C1D-ND	2.11	126.72	124.43
2	B	750	HEM	C1B-NB-C4B	2.10	107.24	105.07
2	B	750	HEM	C4B-CHC-C1C	2.07	125.29	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	760	H4B	N2-C2-N1	2.02	120.39	117.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

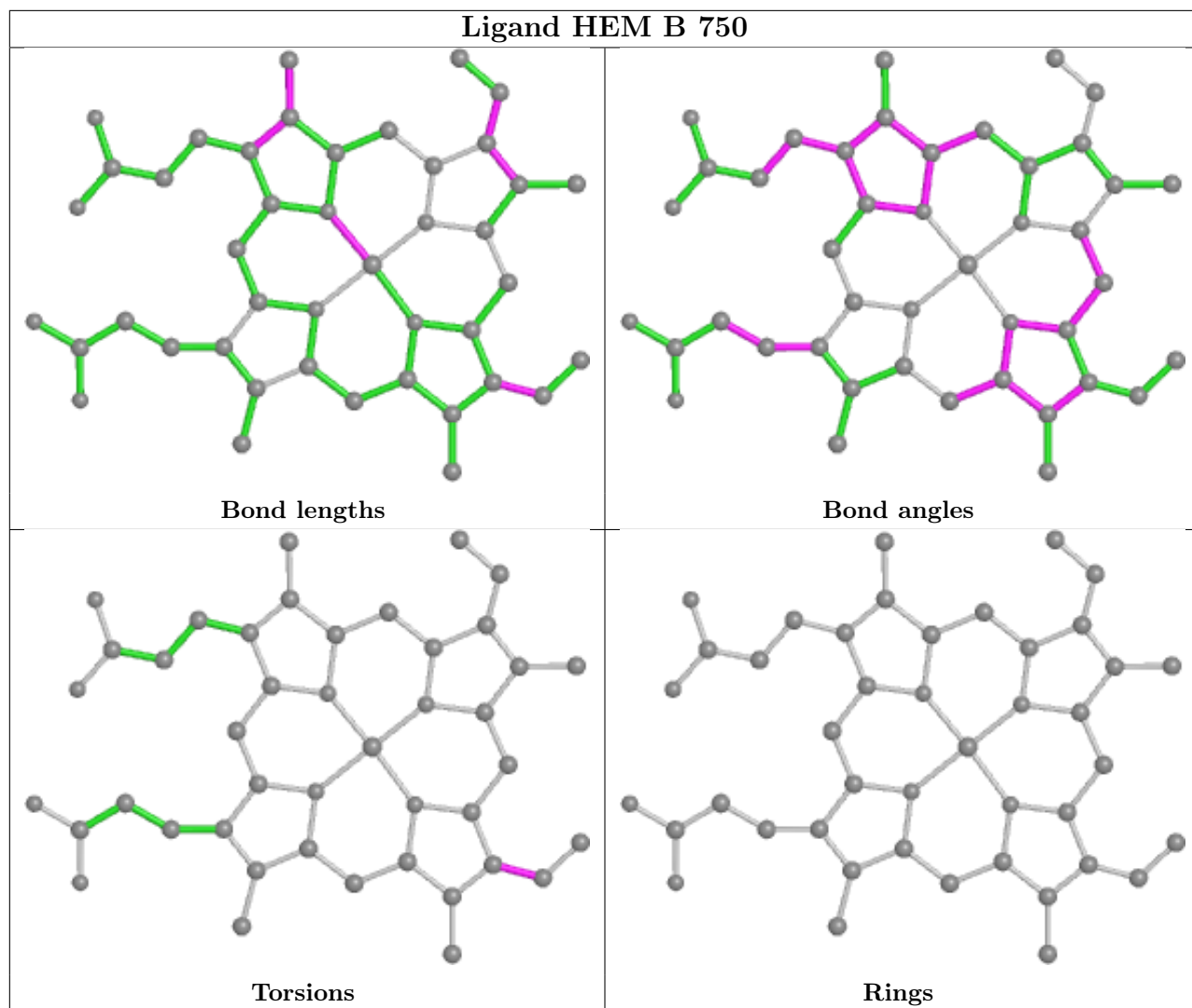
Mol	Chain	Res	Type	Atoms
2	A	750	HEM	C4B-C3B-CAB-CBB
2	B	750	HEM	C4B-C3B-CAB-CBB
4	B	761	H4B	N5-C6-C9-O9

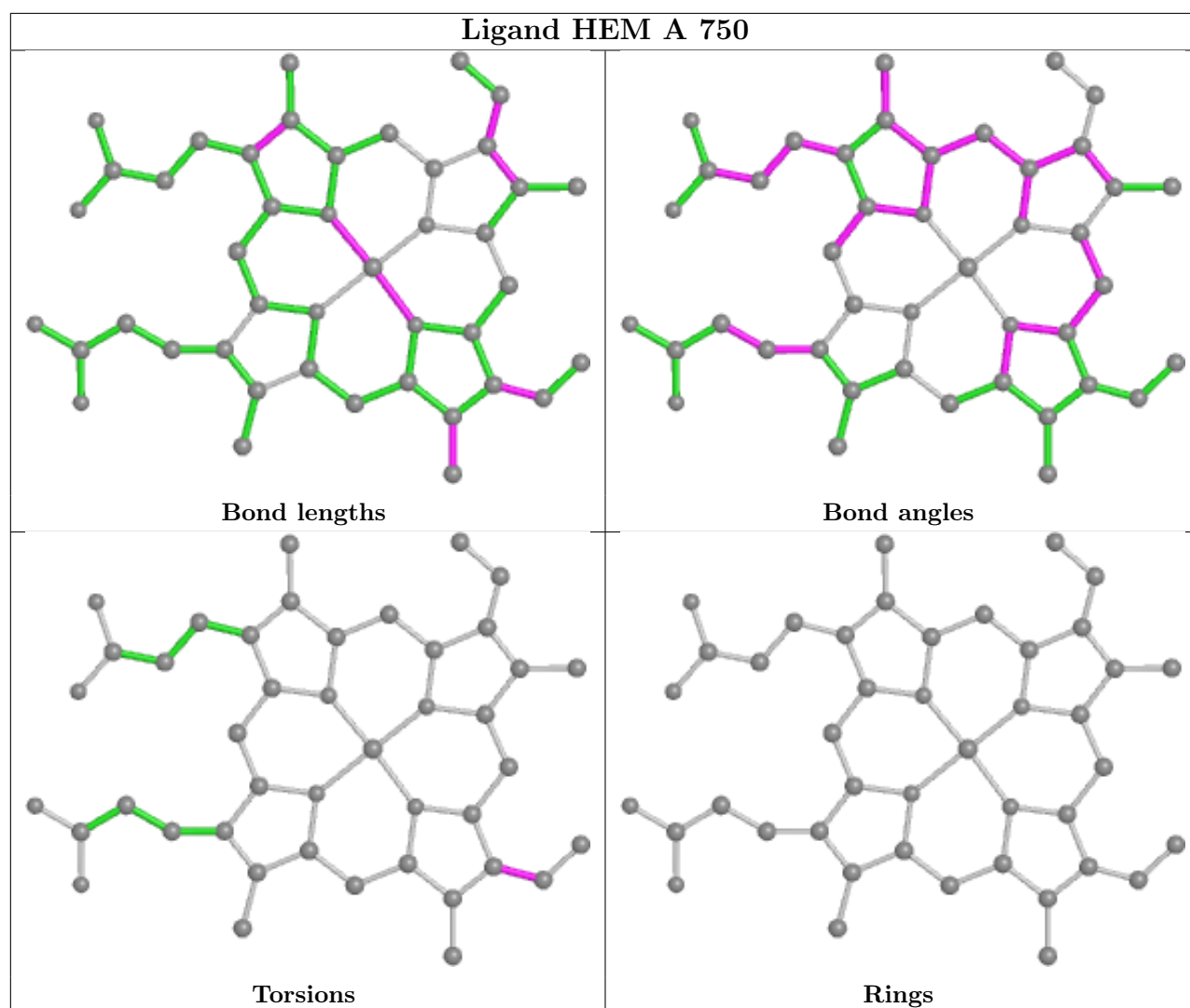
There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	750	HEM	3	0
4	A	760	H4B	1	0
2	A	750	HEM	6	0
4	B	761	H4B	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	407/422 (96%)	0.60	47 (11%) 4 3	31, 49, 75, 89	0
1	B	411/422 (97%)	0.32	21 (5%) 28 22	30, 48, 75, 87	0
All	All	818/844 (96%)	0.46	68 (8%) 11 8	30, 48, 75, 89	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	488	PRO	6.3
1	A	716	TRP	5.9
1	A	715	VAL	5.4
1	B	373	GLY	5.0
1	A	299	ARG	5.0
1	B	300	PHE	4.9
1	A	371	ARG	4.5
1	B	352	ASP	4.5
1	A	390	SER	4.4
1	B	301	LEU	4.2
1	A	300	PHE	4.1
1	A	487	GLN	4.0
1	A	355	PHE	3.8
1	A	352	ASP	3.7
1	A	712	ASN	3.7
1	A	667	ARG	3.6
1	A	714	HIS	3.6
1	A	324	THR	3.6
1	B	378	MET	3.5
1	A	389	GLU	3.5
1	B	619	ARG	3.3
1	A	351	LYS	3.3
1	A	486	LYS	3.3
1	B	328	GLU	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	328	GLU	3.1
1	A	489	ASP	3.1
1	B	329	HIS	3.0
1	A	619	ARG	3.0
1	B	374	SER	3.0
1	A	318	LEU	3.0
1	B	715	VAL	2.9
1	B	511	LYS	2.9
1	A	388	ILE	2.8
1	B	310	VAL	2.8
1	A	490	GLY	2.7
1	A	713	THR	2.7
1	A	302	LYS	2.6
1	A	566	ALA	2.6
1	B	351	LYS	2.5
1	A	507	GLN	2.5
1	A	511	LYS	2.5
1	A	469	LYS	2.5
1	B	620	LYS	2.4
1	A	567	VAL	2.3
1	A	591	THR	2.3
1	B	618	MET	2.3
1	A	311	VAL	2.3
1	B	323	GLU	2.3
1	A	470	HIS	2.3
1	B	681	PRO	2.3
1	A	327	THR	2.3
1	A	391	THR	2.2
1	B	327	THR	2.2
1	B	718	GLY	2.2
1	A	681	PRO	2.2
1	A	685	GLY	2.2
1	A	369	ILE	2.2
1	A	506	ILE	2.2
1	A	499	VAL	2.2
1	A	504	ILE	2.2
1	A	492	THR	2.1
1	A	645	LYS	2.1
1	A	643	SER	2.1
1	A	503	GLU	2.1
1	B	717	LYS	2.1
1	A	386	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	584	PHE	2.1
1	B	615	ASP	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 monosaccharides 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

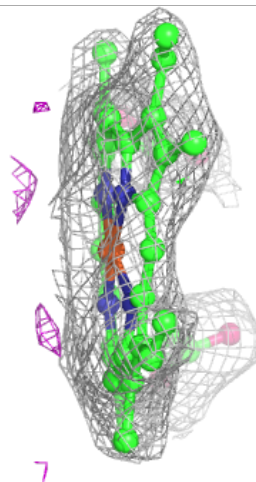
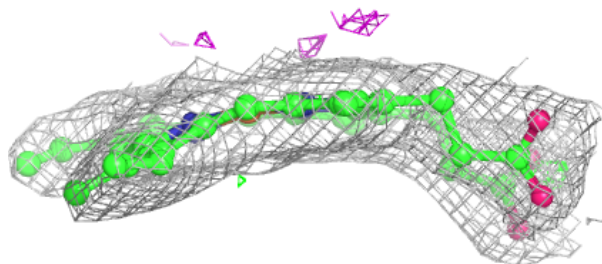
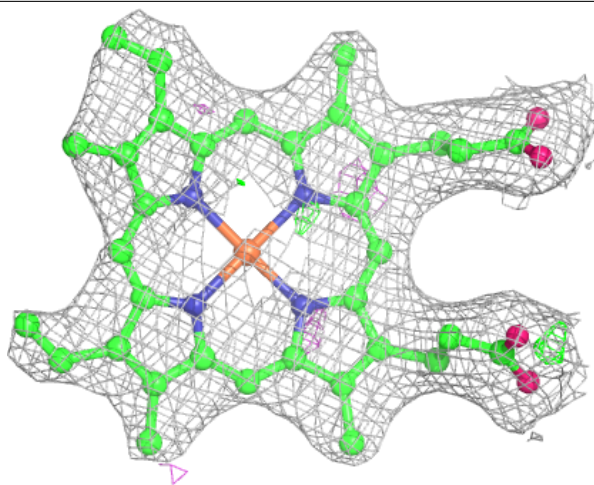
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	H4B	A	760	17/17	0.96	0.23	30,36,40,43	0
4	H4B	B	761	17/17	0.96	0.23	28,33,37,39	0
5	ARG	B	771	12/12	0.96	0.22	29,37,41,43	0
2	HEM	B	750	43/43	0.97	0.23	32,39,46,49	0
2	HEM	A	750	43/43	0.97	0.24	19,38,46,49	0
5	ARG	A	770	12/12	0.98	0.30	29,33,39,44	0
3	ZN	A	900	1/1	1.00	0.10	47,47,47,47	0

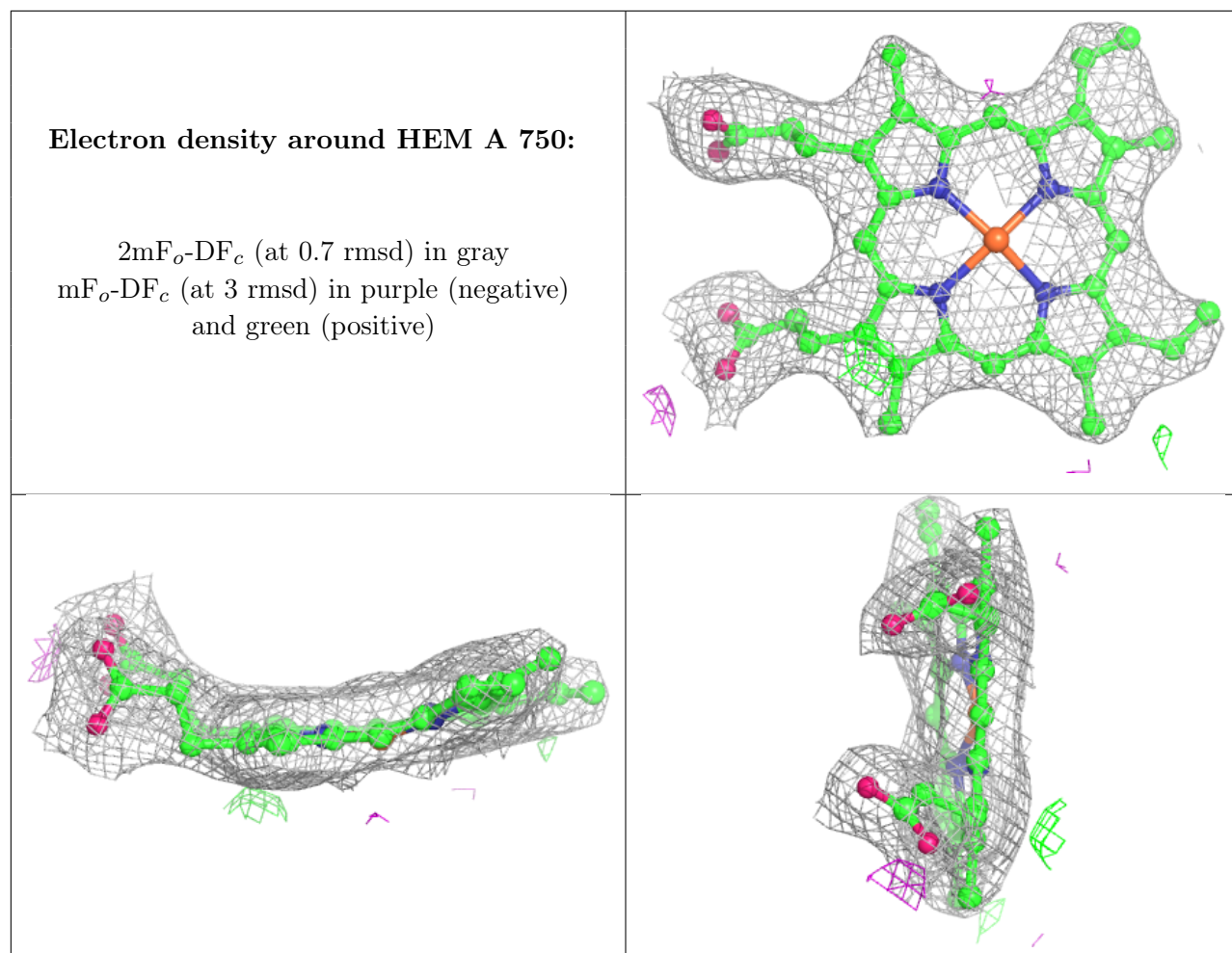
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around HEM B 750:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.