



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:54 PM UTC

PDB ID : 1P6I / pdb_00001p6i
Title : Rat neuronal NOS heme domain with (4S)-N-(4-amino-5-[aminoethyl]aminopentyl)-N'-nitroguanidine bound
Authors : Flinspach, M.L.; Li, H.; Jamal, J.; Yang, W.; Huang, H.; Hah, J.-M.; Gomez-Vidal, J.A.; Litzinger, E.A.; Silverman, R.B.; Poulos, T.L.
Deposited on : 2003-04-29
Resolution : 1.90 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

<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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

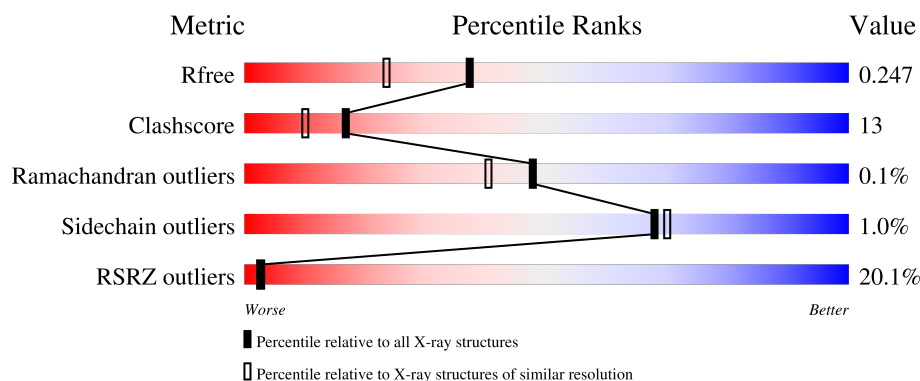
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	421	31% 64% 30% ..
1	B	421	8% 73% 23% ..

2 Entry composition [i](#)

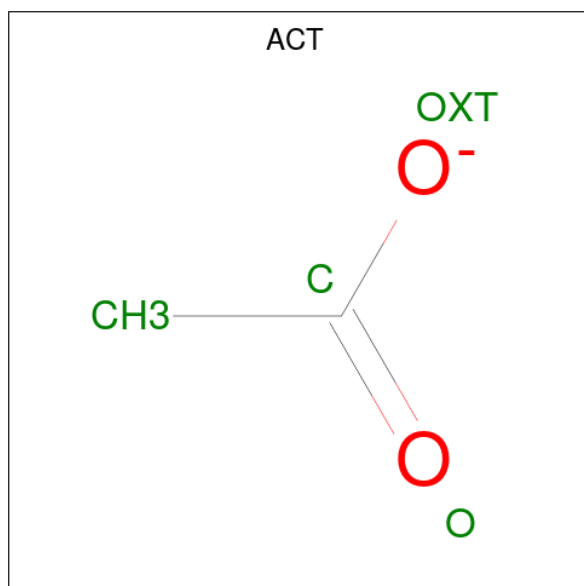
There are 7 unique types of molecules in this entry. The entry contains 7359 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	0	0	0
			3313	2121	566	605	21			
1	B	410	Total	C	N	O	S	0	0	0
			3341	2138	573	609	21			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).

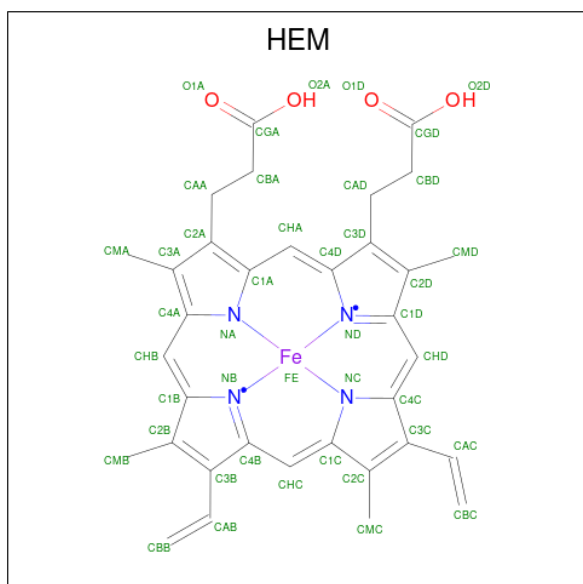


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

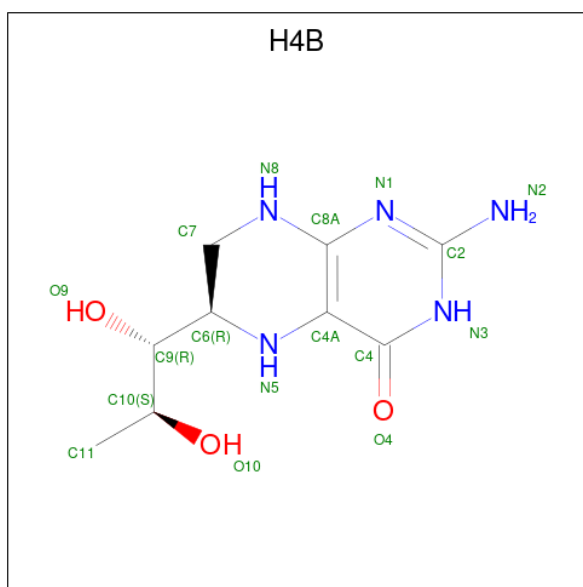
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



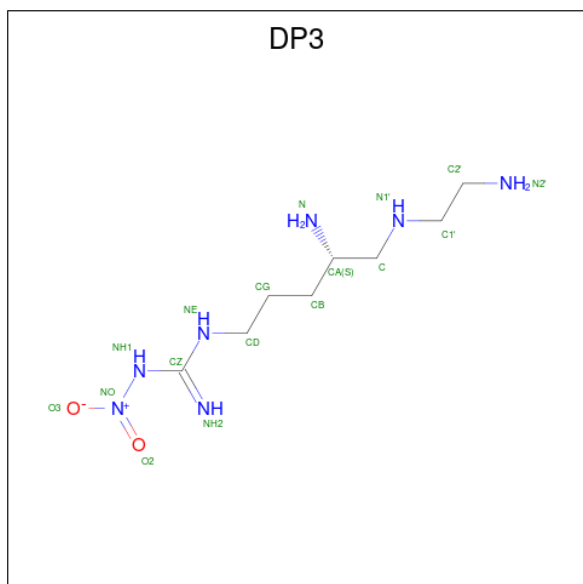
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: $\text{C}_9\text{H}_{15}\text{N}_5\text{O}_3$).



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

- Molecule 6 is N-{(4S)-4-AMINO-5-[(2-AMINOETHYL)AMINO]PENTYL}-N'-NITROGUANIDINE (CCD ID: DP3) (formula: C₈H₂₁N₇O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			17	8	7	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			17	8	7	2		

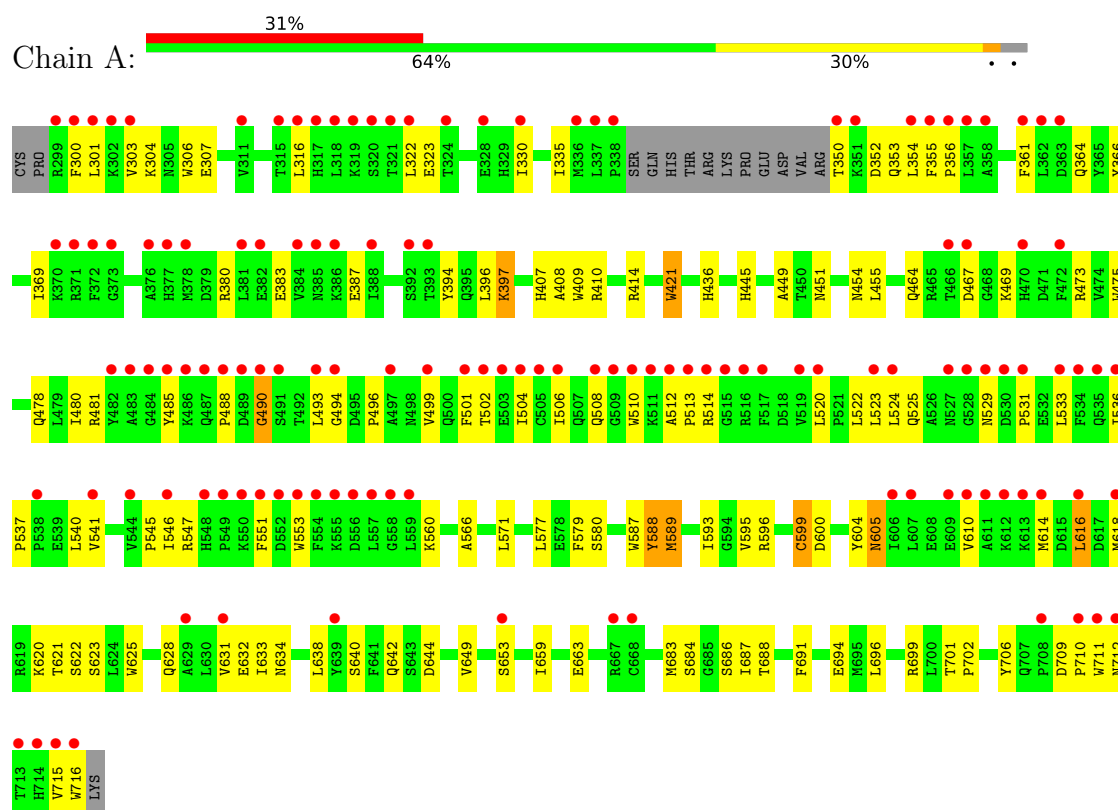
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	232	Total	O	0	0
			232	232		
7	B	310	Total	O	0	0
			310	310		

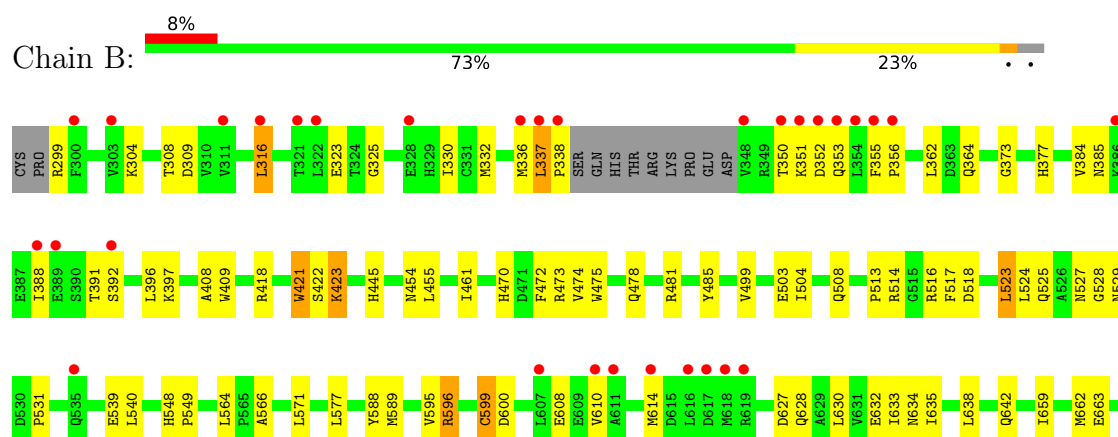
3 Residue-property plots

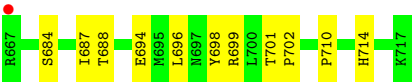
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, α , β , γ	51.11Å 110.69Å 164.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.03 – 1.90 32.03 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.1 (32.03-1.90) 97.2 (32.03-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 1.87Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.256 0.222 , 0.247	Depositor DCC
R_{free} test set	3695 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7359	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: ACT, ZN, DP3, 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	0/3406	0.90	10/4621 (0.2%)
1	B	0.38	0/3434	0.91	16/4656 (0.3%)
All	All	0.37	0/6840	0.91	26/9277 (0.3%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	589	MET	N-CA-C	-8.68	95.52	109.76
1	B	589	MET	N-CA-C	-8.01	96.19	109.24
1	B	421	TRP	N-CA-C	7.06	119.87	111.33
1	A	354	LEU	N-CA-C	6.77	118.45	111.14
1	A	490	GLY	N-CA-C	-6.77	106.63	114.69
1	B	588	TYR	N-CA-C	6.63	120.30	110.48
1	B	474	VAL	N-CA-C	-6.50	97.75	107.37
1	A	623	SER	N-CA-C	-6.47	105.35	113.18
1	A	588	TYR	N-CA-C	6.24	119.71	110.48
1	B	397	LYS	N-CA-C	-6.00	102.61	110.53
1	A	599	CYS	N-CA-C	5.84	120.56	113.38
1	A	397	LYS	N-CA-C	-5.75	102.39	110.50
1	B	472	PHE	N-CA-C	-5.66	100.01	109.24
1	A	408	ALA	N-CA-C	-5.64	105.13	111.28
1	B	688	THR	N-CA-C	-5.39	102.18	110.32
1	B	418	ARG	N-CA-C	5.32	119.25	112.87
1	A	421	TRP	N-CA-C	5.31	120.14	111.37
1	B	408	ALA	N-CA-C	-5.28	105.52	111.28
1	B	455	LEU	N-CA-C	5.26	117.65	110.24
1	B	461	ILE	N-CA-C	5.24	115.12	107.37
1	B	599	CYS	N-CA-C	5.24	119.82	113.38
1	B	596	ARG	N-CA-C	5.23	117.98	111.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	564	LEU	N-CA-C	5.20	118.79	108.59
1	A	688	THR	N-CA-C	-5.15	103.04	110.40
1	B	635	ILE	N-CA-C	-5.10	105.57	110.72
1	B	714	HIS	N-CA-C	5.06	117.57	110.23

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	3313	0	3221	108	0
1	B	3341	0	3256	69	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
3	A	1	0	0	0	0
4	A	43	0	30	2	0
4	B	43	0	30	0	0
5	A	17	0	15	0	0
5	B	17	0	15	0	0
6	A	17	0	21	2	0
6	B	17	0	21	1	0
7	A	232	0	0	6	0
7	B	310	0	0	8	0
All	All	7359	0	6615	172	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 13.

All (172) 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:373:GLY:H	1:B:377:HIS:HD2	1.17	0.93
1:B:523:LEU:HD22	1:B:531:PRO:HB2	1.49	0.91
1:B:350:THR:HB	1:B:353:GLN:OE1	1.79	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:PRO:HG2	1:A:547:ARG:NH1	2.01	0.75
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.68	0.73
1:A:350:THR:HB	1:A:353:GLN:HG3	1.69	0.73
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.08	0.69
1:A:350:THR:HG22	1:A:352:ASP:H	1.58	0.69
1:A:616:LEU:HD13	1:A:625:TRP:HB2	1.75	0.68
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.74	0.68
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.18	0.68
1:A:684:SER:HB3	1:A:687:ILE:HD11	1.77	0.67
4:A:750:HEM:HMC2	4:A:750:HEM:HBC2	1.77	0.67
1:B:373:GLY:H	1:B:377:HIS:CD2	2.07	0.66
1:A:380:ARG:NH1	1:A:397:LYS:HE2	2.11	0.65
1:A:546:ILE:HA	1:A:640:SER:OG	1.97	0.65
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.31	0.63
1:B:659:ILE:O	1:B:663:GLU:HG3	1.98	0.63
1:A:537:PRO:HB2	1:A:540:LEU:HG	1.81	0.62
1:A:307:GLU:HG3	7:B:935:HOH:O	1.97	0.62
1:A:620:LYS:HE3	1:A:622:SER:OG	1.99	0.62
1:A:361:PHE:O	1:A:364:GLN:HG2	1.98	0.62
1:A:304:LYS:O	1:A:694:GLU:HG3	1.99	0.61
1:B:684:SER:HB3	1:B:687:ILE:HD11	1.82	0.61
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.83	0.61
1:A:545:PRO:HG2	1:A:547:ARG:HH11	1.65	0.61
1:B:355:PHE:N	1:B:356:PRO:HD2	2.16	0.61
1:B:337:LEU:N	1:B:337:LEU:HD23	2.16	0.61
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.31	0.60
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.30	0.60
1:B:336:MET:HB3	1:B:337:LEU:HD23	1.83	0.60
1:A:595:VAL:HG23	1:A:634:ASN:HD21	1.67	0.59
1:B:323:GLU:O	1:B:699:ARG:HD3	2.03	0.59
1:B:350:THR:HG22	1:B:352:ASP:H	1.67	0.59
1:B:325:GLY:O	1:B:332:MET:HE2	2.03	0.59
1:A:684:SER:HB3	1:A:687:ILE:CD1	2.33	0.59
1:B:391:THR:O	1:B:392:SER:HB2	2.03	0.58
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.86	0.58
1:A:350:THR:HB	1:A:353:GLN:CG	2.32	0.58
1:B:499:VAL:O	1:B:503:GLU:HG3	2.04	0.58
1:A:322:LEU:HD13	1:A:699:ARG:NH2	2.20	0.57
1:A:610:VAL:O	1:A:614:MET:HG3	2.04	0.57
1:B:422:SER:OG	1:B:423:LYS:HD2	2.05	0.56
1:A:524:LEU:O	1:A:531:PRO:HA	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ILE:HD11	1:A:512:ALA:HB2	1.89	0.55
1:A:396:LEU:HG	1:A:577:LEU:HD12	1.88	0.55
1:A:502:THR:O	1:A:506:ILE:HG12	2.07	0.55
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.42	0.55
1:B:396:LEU:HG	1:B:577:LEU:HD12	1.89	0.55
1:A:355:PHE:N	1:A:356:PRO:HD2	2.23	0.54
1:A:366:TYR:HA	1:A:369:ILE:HG12	1.90	0.54
1:B:701:THR:HA	1:B:702:PRO:C	2.33	0.54
1:A:335:ILE:HD13	1:B:694:GLU:HB3	1.89	0.53
1:A:621:THR:HG23	7:A:1123:HOH:O	2.09	0.53
1:A:618:MET:HE3	1:A:625:TRP:CZ3	2.43	0.53
1:A:618:MET:HE2	7:A:1052:HOH:O	2.09	0.53
1:B:638:LEU:O	1:B:642:GLN:HG3	2.09	0.53
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.91	0.52
1:A:684:SER:HB3	1:A:687:ILE:HG12	1.89	0.52
1:A:659:ILE:O	1:A:663:GLU:HG3	2.09	0.52
1:A:596:ARG:O	1:A:600:ASP:HB2	2.10	0.52
1:B:304:LYS:O	1:B:694:GLU:HG3	2.10	0.51
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.91	0.51
1:A:322:LEU:HB3	1:A:699:ARG:NH1	2.25	0.51
1:B:684:SER:HB3	1:B:687:ILE:CD1	2.40	0.51
1:B:364:GLN:HG3	7:B:1135:HOH:O	2.10	0.51
1:A:621:THR:HG22	7:A:1058:HOH:O	2.11	0.51
1:B:504:ILE:O	1:B:508:GLN:HG2	2.11	0.51
1:B:595:VAL:HG23	1:B:634:ASN:HD21	1.75	0.50
1:A:350:THR:HG22	1:A:352:ASP:N	2.26	0.50
1:B:308:THR:O	1:B:309:ASP:HB2	2.11	0.50
1:A:701:THR:HA	1:A:702:PRO:C	2.37	0.50
1:B:316:LEU:HB3	1:B:698:TYR:OH	2.12	0.50
1:A:614:MET:CE	1:A:632:GLU:HG3	2.42	0.49
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.47	0.49
1:A:604:TYR:O	1:A:605:ASN:C	2.56	0.49
1:A:504:ILE:O	1:A:508:GLN:HB2	2.13	0.49
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.48	0.49
1:B:596:ARG:O	1:B:600:ASP:HB2	2.13	0.49
1:A:506:ILE:C	1:A:508:GLN:H	2.21	0.48
1:A:451:ASN:HB3	1:A:454:ASN:O	2.13	0.48
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.96	0.48
1:A:436:HIS:HB2	7:A:1040:HOH:O	2.13	0.48
1:A:696:LEU:HD22	1:B:330:ILE:HD11	1.96	0.48
1:B:362:LEU:HD11	1:B:384:VAL:HG21	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:LEU:C	1:A:571:LEU:HD23	2.39	0.48
1:A:407:HIS:CE1	1:A:410:ARG:HH11	2.32	0.48
1:A:475:TRP:CZ3	1:A:711:TRP:HB3	2.49	0.48
6:A:793:DP3:H2	7:A:1130:HOH:O	2.14	0.48
1:B:478:GLN:HB2	1:B:481:ARG:CG	2.40	0.48
1:B:608:GLU:HG3	7:B:1163:HOH:O	2.13	0.48
1:A:709:ASP:HB2	1:A:712:ASN:ND2	2.29	0.47
1:A:536:ILE:O	1:A:537:PRO:C	2.56	0.47
1:B:332:MET:HE3	1:B:338:PRO:HB2	1.95	0.47
1:A:301:LEU:CD1	1:B:330:ILE:HD13	2.44	0.47
1:A:449:ALA:O	1:A:455:LEU:HA	2.15	0.47
1:A:715:VAL:O	1:A:715:VAL:HG23	2.15	0.47
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.50	0.47
6:B:794:DP3:H1'1	7:B:1008:HOH:O	2.15	0.47
1:B:351:LYS:HE2	1:B:392:SER:OG	2.15	0.47
1:B:445:HIS:C	1:B:445:HIS:CD2	2.93	0.47
1:A:545:PRO:HD2	1:A:644:ASP:OD2	2.15	0.46
1:A:478:GLN:HB2	1:A:481:ARG:CG	2.44	0.46
1:A:467:ASP:OD1	1:A:469:LYS:HB2	2.15	0.46
1:A:610:VAL:HG21	1:A:633:ILE:HD11	1.96	0.46
1:A:496:PRO:O	1:A:499:VAL:HG23	2.16	0.46
1:A:473:ARG:HD3	1:A:580:SER:HB2	1.98	0.46
1:A:687:ILE:HD13	1:B:630:LEU:HD22	1.98	0.46
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.50	0.46
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.51	0.46
1:B:684:SER:HB3	1:B:687:ILE:HG12	1.97	0.45
1:A:323:GLU:O	1:A:699:ARG:HD3	2.15	0.45
1:A:350:THR:HB	1:A:353:GLN:CD	2.41	0.45
1:A:387:GLU:OE2	1:A:394:TYR:HA	2.17	0.45
1:A:506:ILE:C	1:A:508:GLN:N	2.74	0.45
1:B:539:GLU:HG2	1:B:540:LEU:HD13	1.98	0.45
1:A:716:TRP:H	1:A:716:TRP:CD1	2.33	0.45
1:A:485:TYR:HB3	1:A:514:ARG:NH1	2.32	0.45
1:A:512:ALA:HA	1:A:513:PRO:HD3	1.85	0.45
1:B:388:ILE:O	1:B:392:SER:N	2.44	0.45
1:A:522:LEU:O	1:A:533:LEU:HA	2.17	0.44
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.52	0.44
1:A:709:ASP:HB2	1:A:712:ASN:HD22	1.82	0.44
1:A:494:GLY:O	1:A:496:PRO:HD3	2.18	0.44
1:A:551:PHE:HB3	1:A:553:TRP:NE1	2.33	0.44
1:B:299:ARG:HB3	1:B:299:ARG:HH11	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:GLN:HG3	1:B:529:ASN:O	2.17	0.44
1:B:614:MET:CE	1:B:632:GLU:HG3	2.48	0.44
1:B:473:ARG:NH2	1:B:710:PRO:HD3	2.33	0.44
1:A:525:GLN:HG3	1:A:529:ASN:O	2.18	0.44
1:A:614:MET:HE3	1:A:632:GLU:HG3	2.00	0.43
1:B:470:HIS:HB3	1:B:527:ASN:ND2	2.32	0.43
1:A:445:HIS:CD2	1:A:445:HIS:C	2.96	0.43
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.99	0.43
1:B:470:HIS:HA	1:B:528:GLY:HA3	2.01	0.43
1:A:488:PRO:C	1:A:490:GLY:N	2.76	0.43
1:A:595:VAL:O	1:A:599:CYS:HB2	2.18	0.43
1:B:548:HIS:CG	1:B:549:PRO:HD2	2.52	0.43
1:B:662:MET:HE3	7:B:896:HOH:O	2.17	0.43
1:B:699:ARG:HG2	7:B:974:HOH:O	2.18	0.43
1:B:516:ARG:HD3	1:B:517:PHE:CE1	2.54	0.42
1:A:683:MET:HE2	1:B:627:ASP:OD2	2.19	0.42
1:A:501:PHE:HD2	1:A:520:LEU:HD13	1.83	0.42
1:A:303:VAL:CG1	1:A:696:LEU:HG	2.49	0.42
1:A:618:MET:HE3	1:A:625:TRP:CH2	2.54	0.42
1:A:686:SER:HA	1:A:691:PHE:CG	2.54	0.42
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.55	0.42
1:A:300:PHE:CD1	1:A:300:PHE:N	2.87	0.42
1:B:355:PHE:N	1:B:356:PRO:CD	2.82	0.42
1:B:524:LEU:O	1:B:531:PRO:HA	2.19	0.42
1:A:322:LEU:HB3	1:A:699:ARG:CZ	2.50	0.41
1:A:383:GLU:HG3	7:A:1094:HOH:O	2.20	0.41
1:A:551:PHE:HE1	1:A:614:MET:HE3	1.85	0.41
1:A:414:ARG:NH1	1:A:706:TYR:OH	2.52	0.41
1:A:510:TRP:HB2	1:A:533:LEU:HD13	2.01	0.41
1:A:638:LEU:O	1:A:642:GLN:HG3	2.20	0.41
1:A:595:VAL:HG23	1:A:634:ASN:ND2	2.33	0.41
1:B:454:ASN:ND2	7:B:875:HOH:O	2.53	0.41
1:A:589:MET:HA	1:A:649:VAL:O	2.20	0.41
4:A:750:HEM:HBA2	6:A:793:DP3:HD1	2.02	0.41
1:B:478:GLN:HA	1:B:566:ALA:O	2.20	0.41
1:B:571:LEU:C	1:B:571:LEU:HD23	2.45	0.41
1:A:306:TRP:CD1	1:B:336:MET:HE2	2.56	0.41
1:A:588:TYR:CD1	1:A:593:ILE:HD11	2.56	0.40
1:A:653:SER:HB2	7:B:1016:HOH:O	2.20	0.40
1:A:478:GLN:HA	1:A:566:ALA:O	2.21	0.40
1:A:618:MET:HA	1:A:625:TRP:CD1	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:VAL:O	1:B:599:CYS:HB2	2.21	0.40
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.50	0.40
1:A:480:ILE:HD13	1:A:541:VAL:HG13	2.03	0.40
1:A:546:ILE:HG12	1:A:560:LYS:HA	2.04	0.40
1:B:610:VAL:HG21	1:B:633:ILE:HD11	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	403/421 (96%)	378 (94%)	24 (6%)	1 (0%)	43	36
1	B	406/421 (96%)	393 (97%)	13 (3%)	0	100	100
All	All	809/842 (96%)	771 (95%)	37 (5%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	605	ASN

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	363/377 (96%)	360 (99%)	3 (1%)	73	75
1	B	366/377 (97%)	362 (99%)	4 (1%)	65	67
All	All	729/754 (97%)	722 (99%)	7 (1%)	68	70

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	LEU
1	A	493	LEU
1	A	616	LEU
1	B	316	LEU
1	B	337	LEU
1	B	423	LYS
1	B	523	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	HIS
1	A	420	GLN
1	A	425	GLN
1	A	451	ASN
1	A	454	ASN
1	A	500	GLN
1	A	634	ASN
1	A	697	ASN
1	B	364	GLN
1	B	377	HIS
1	B	425	GLN
1	B	451	ASN
1	B	454	ASN
1	B	478	GLN
1	B	507	GLN
1	B	527	ASN
1	B	535	GLN
1	B	634	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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$
4	HEM	A	750	1	50,50,50	1.16	4 (8%)	67,82,82	1.08	3 (4%)
4	HEM	B	750	1	50,50,50	1.14	2 (4%)	67,82,82	1.10	3 (4%)
2	ACT	B	861	-	3,3,3	0.97	0	3,3,3	0.81	0
6	DP3	A	793	-	11,16,16	1.69	3 (27%)	11,18,18	1.36	3 (27%)
5	H4B	B	761	-	17,18,18	1.72	3 (17%)	14,26,26	1.94	4 (28%)
5	H4B	A	760	-	17,18,18	1.63	2 (11%)	14,26,26	1.97	4 (28%)
6	DP3	B	794	-	11,16,16	1.53	2 (18%)	11,18,18	1.34	3 (27%)
2	ACT	A	860	-	3,3,3	0.94	0	3,3,3	0.79	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
4	HEM	A	750	1	-	1/14/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	B	750	1	-	2/14/54/54	-
6	DP3	A	793	-	-	5/13/16/16	-
5	H4B	B	761	-	-	0/8/17/17	0/2/2/2
5	H4B	A	760	-	-	0/8/17/17	0/2/2/2
6	DP3	B	794	-	-	4/13/16/16	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	761	H4B	C4A-N5	4.18	1.47	1.37
5	A	760	H4B	C4A-N5	4.13	1.47	1.37
5	B	761	H4B	C6-N5	4.09	1.54	1.47
5	A	760	H4B	C6-N5	3.77	1.54	1.47
6	A	793	DP3	C-CA	3.31	1.56	1.53
6	B	794	DP3	C-CA	3.10	1.56	1.53
6	A	793	DP3	CB-CA	2.91	1.57	1.53
4	B	750	HEM	CAB-C3B	-2.86	1.39	1.47
4	A	750	HEM	CAB-C3B	-2.66	1.40	1.47
6	B	794	DP3	CB-CA	2.64	1.57	1.53
4	A	750	HEM	FE-NA	2.50	2.03	1.95
4	A	750	HEM	CAC-C3C	-2.42	1.40	1.47
4	A	750	HEM	FE-NB	2.40	2.02	1.94
6	A	793	DP3	CD-NE	2.21	1.51	1.46
5	B	761	H4B	C4-N3	2.14	1.42	1.38
4	B	750	HEM	CAC-C3C	-2.06	1.41	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	760	H4B	C2-N1-C8A	5.36	122.83	113.36
5	B	761	H4B	C2-N1-C8A	5.23	122.59	113.36
5	A	760	H4B	N3-C2-N1	-2.98	117.86	123.32
5	B	761	H4B	O10-C10-C9	-2.97	104.86	109.77
5	B	761	H4B	N3-C2-N1	-2.86	118.08	123.32
6	A	793	DP3	CB-CA-C	2.77	114.20	109.47
6	B	794	DP3	CB-CA-C	2.75	114.17	109.47
5	A	760	H4B	O10-C10-C9	-2.66	105.38	109.77
4	A	750	HEM	CMA-C3A-C4A	2.60	129.37	125.42
4	B	750	HEM	CBD-CAD-C3D	-2.42	105.85	112.53
4	A	750	HEM	CBD-CAD-C3D	-2.31	106.14	112.53
4	B	750	HEM	C4A-C3A-C2A	-2.15	104.35	106.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	794	DP3	NE-CZ-NH2	-2.14	116.31	120.26
4	B	750	HEM	C1D-C2D-C3D	-2.14	104.73	106.98
6	B	794	DP3	CD-NE-CZ	2.13	127.36	123.46
6	A	793	DP3	NE-CZ-NH2	-2.11	116.37	120.26
6	A	793	DP3	CD-NE-CZ	2.10	127.32	123.46
5	A	760	H4B	O9-C9-C6	2.10	114.32	109.28
4	A	750	HEM	CAB-C3B-C2B	-2.05	121.77	128.43
5	B	761	H4B	O9-C9-C6	2.04	114.16	109.28

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	793	DP3	N1'-C1'-C2'-N2'
6	A	793	DP3	N1'-C-CA-CB
6	B	794	DP3	N1'-C-CA-N
6	B	794	DP3	N1'-C-CA-CB
6	A	793	DP3	N1'-C-CA-N
4	B	750	HEM	C2B-C3B-CAB-CBB
6	B	794	DP3	N-CA-CB-CG
4	A	750	HEM	C4B-C3B-CAB-CBB
4	B	750	HEM	C4B-C3B-CAB-CBB
6	A	793	DP3	C-CA-CB-CG
6	B	794	DP3	C-CA-CB-CG
6	A	793	DP3	N-CA-CB-CG

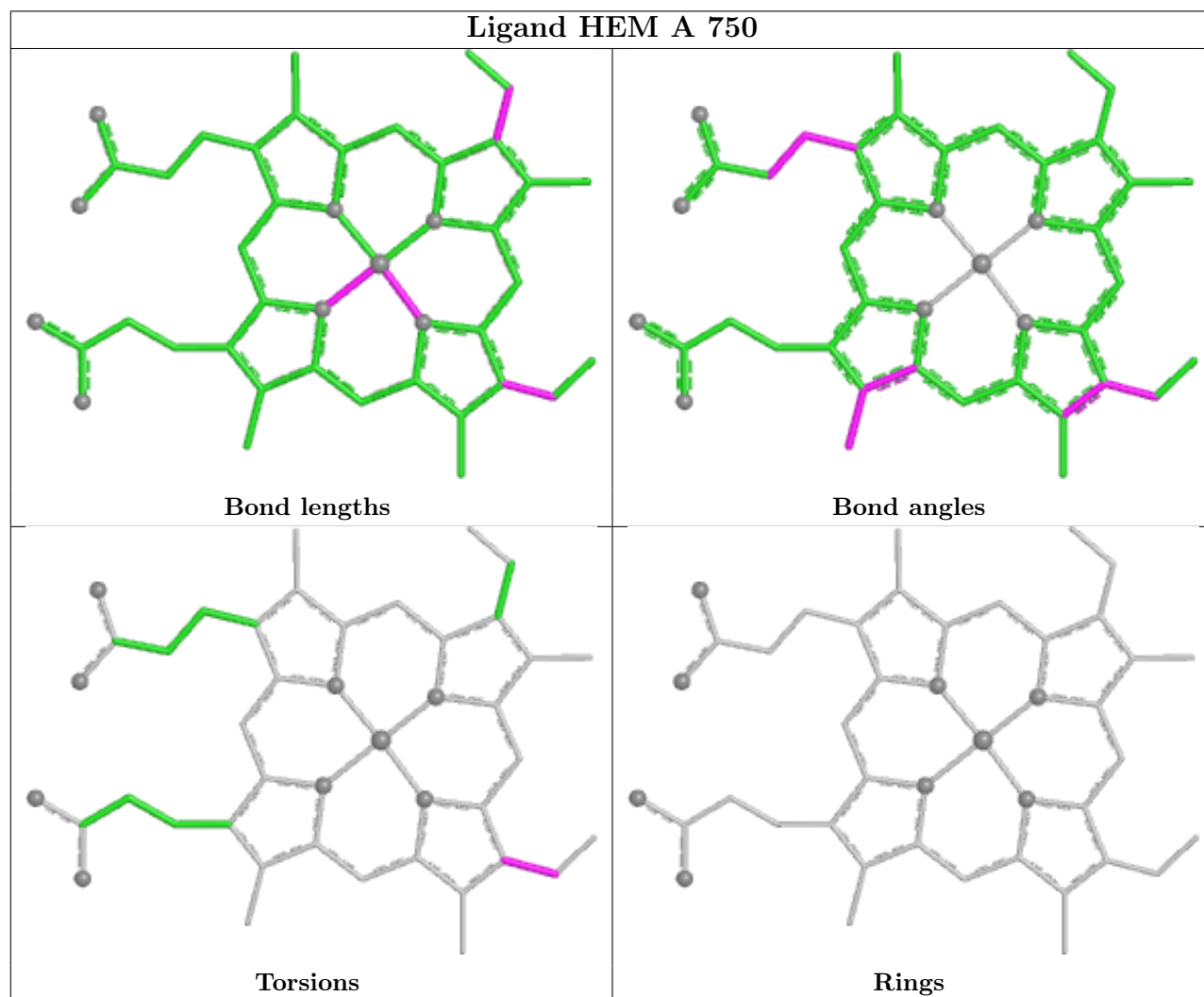
There are no ring outliers.

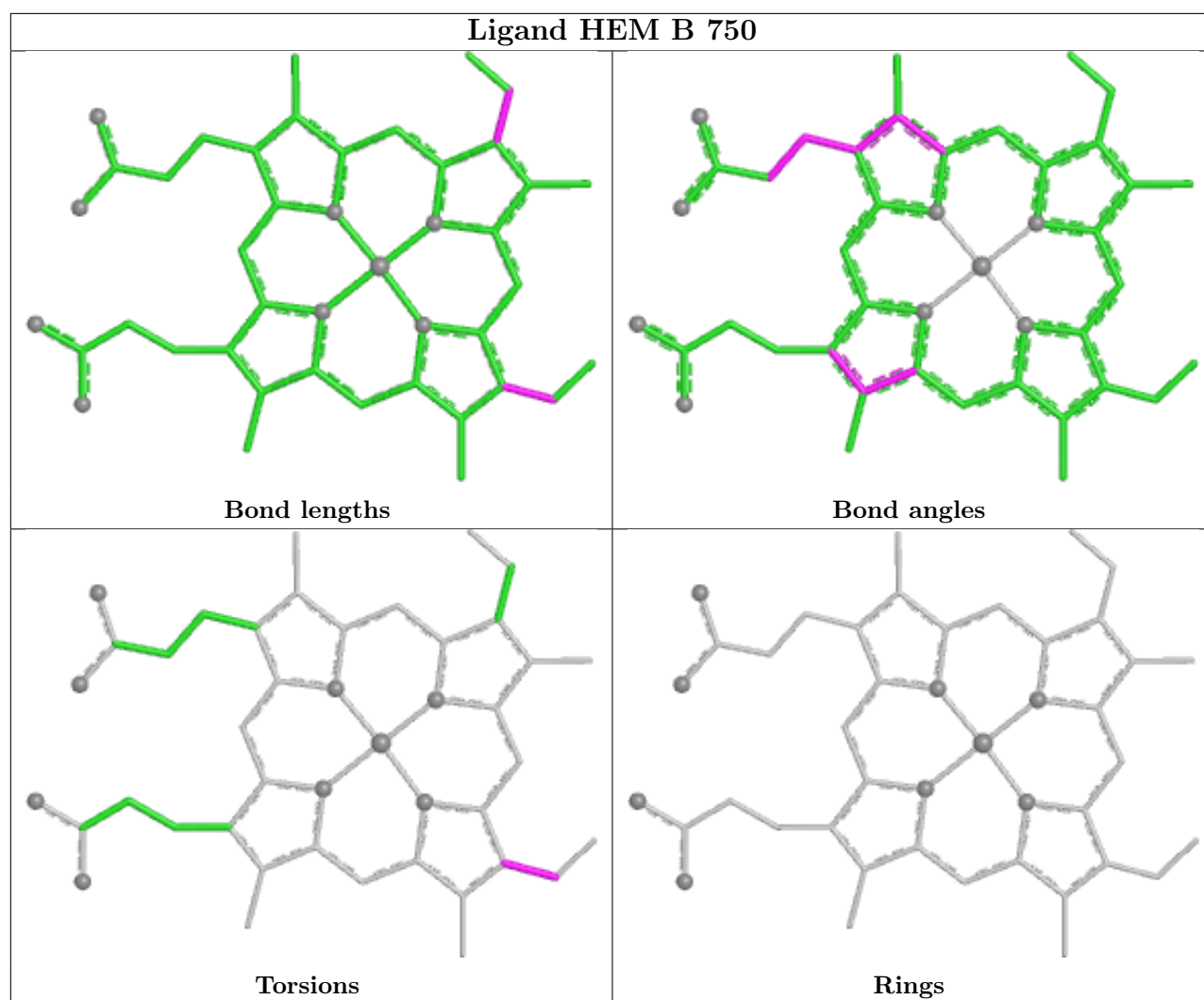
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	750	HEM	2	0
6	A	793	DP3	2	0
6	B	794	DP3	1	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, 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	407/421 (96%)	1.37	132 (32%) 1 1	16, 37, 60, 74	0
1	B	410/421 (97%)	0.51	32 (7%) 19 20	16, 27, 49, 62	0
All	All	817/842 (97%)	0.94	164 (20%) 3 2	16, 31, 57, 74	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	373	GLY	5.2
1	A	355	PHE	5.1
1	A	493	LEU	4.9
1	B	350	THR	4.8
1	A	300	PHE	4.7
1	A	554	PHE	4.6
1	A	715	VAL	4.6
1	A	488	PRO	4.6
1	A	716	TRP	4.5
1	A	303	VAL	4.4
1	A	513	PRO	4.4
1	A	510	TRP	4.4
1	A	486	LYS	4.3
1	B	348	VAL	4.3
1	B	321	THR	4.2
1	A	485	TYR	4.2
1	A	533	LEU	4.2
1	A	551	PHE	4.1
1	A	711	TRP	4.1
1	A	517	PHE	4.0
1	A	321	THR	4.0
1	A	384	VAL	4.0
1	A	338	PRO	3.8
1	A	301	LEU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	354	LEU	3.7
1	A	506	ILE	3.7
1	A	350	THR	3.7
1	A	512	ALA	3.5
1	A	504	ILE	3.5
1	A	501	PHE	3.5
1	A	557	LEU	3.4
1	A	552	ASP	3.4
1	A	376	ALA	3.4
1	A	546	ILE	3.4
1	A	318	LEU	3.4
1	A	322	LEU	3.4
1	B	616	LEU	3.3
1	B	300	PHE	3.3
1	A	531	PRO	3.3
1	A	499	VAL	3.3
1	B	389	GLU	3.3
1	B	611	ALA	3.2
1	A	470	HIS	3.2
1	A	668	CYS	3.2
1	A	534	PHE	3.1
1	B	392	SER	3.1
1	B	610	VAL	3.1
1	B	352	ASP	3.1
1	A	386	LYS	3.0
1	A	319	LYS	3.0
1	B	338	PRO	3.0
1	B	337	LEU	2.9
1	A	320	SER	2.9
1	A	490	GLY	2.9
1	A	713	THR	2.9
1	A	519	VAL	2.9
1	A	553	TRP	2.9
1	A	550	LYS	2.9
1	A	382	GLU	2.9
1	A	487	GLN	2.9
1	A	381	LEU	2.9
1	A	393	THR	2.8
1	A	714	HIS	2.8
1	A	549	PRO	2.8
1	A	610	VAL	2.8
1	B	303	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	355	PHE	2.8
1	A	505	CYS	2.8
1	A	559	LEU	2.8
1	A	356	PRO	2.8
1	A	535	GLN	2.8
1	A	528	GLY	2.8
1	A	357	LEU	2.8
1	B	322	LEU	2.7
1	A	378	MET	2.7
1	A	515	GLY	2.7
1	A	361	PHE	2.7
1	A	556	ASP	2.7
1	A	529	ASN	2.7
1	A	489	ASP	2.6
1	A	370	LYS	2.6
1	A	337	LEU	2.6
1	A	385	ASN	2.6
1	B	607	LEU	2.6
1	A	311	VAL	2.6
1	A	336	MET	2.6
1	A	494	GLY	2.6
1	A	358	ALA	2.6
1	A	520	LEU	2.6
1	A	629	ALA	2.6
1	A	354	LEU	2.6
1	A	653	SER	2.6
1	A	516	ARG	2.5
1	A	667	ARG	2.5
1	B	353	GLN	2.5
1	A	609	GLU	2.5
1	A	316	LEU	2.5
1	A	523	LEU	2.5
1	A	330	ILE	2.5
1	A	388	ILE	2.5
1	A	483	ALA	2.5
1	A	328	GLU	2.5
1	A	466	THR	2.5
1	A	548	HIS	2.5
1	A	611	ALA	2.5
1	A	530	ASP	2.5
1	A	712	ASN	2.4
1	A	524	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	336	MET	2.4
1	A	351	LYS	2.4
1	A	544	VAL	2.4
1	A	482	TYR	2.4
1	A	607	LEU	2.4
1	A	616	LEU	2.4
1	A	324	THR	2.4
1	A	377	HIS	2.4
1	A	555	LYS	2.4
1	A	511	LYS	2.4
1	B	386	LYS	2.4
1	A	299	ARG	2.3
1	A	708	PRO	2.3
1	B	356	PRO	2.3
1	A	484	GLY	2.3
1	A	509	GLY	2.3
1	A	467	ASP	2.3
1	A	614	MET	2.3
1	A	372	PHE	2.3
1	B	328	GLU	2.3
1	A	317	HIS	2.3
1	A	502	THR	2.3
1	B	667	ARG	2.2
1	A	536	ILE	2.2
1	B	388	ILE	2.2
1	A	612	LYS	2.2
1	A	362	LEU	2.2
1	A	363	ASP	2.2
1	A	392	SER	2.2
1	B	617	ASP	2.2
1	B	316	LEU	2.2
1	A	538	PRO	2.2
1	A	472	PHE	2.1
1	A	302	LYS	2.1
1	A	514	ARG	2.1
1	A	710	PRO	2.1
1	A	631	VAL	2.1
1	B	351	LYS	2.1
1	A	527	ASN	2.1
1	A	508	GLN	2.1
1	B	535	GLN	2.1
1	A	606	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	639	TYR	2.1
1	A	491	SER	2.1
1	B	619	ARG	2.1
1	A	558	GLY	2.1
1	A	618	MET	2.1
1	B	618	MET	2.1
1	B	311	VAL	2.1
1	A	503	GLU	2.0
1	A	613	LYS	2.0
1	A	315	THR	2.0
1	B	614	MET	2.0
1	A	541	VAL	2.0
1	A	371	ARG	2.0
1	A	497	ALA	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](#)

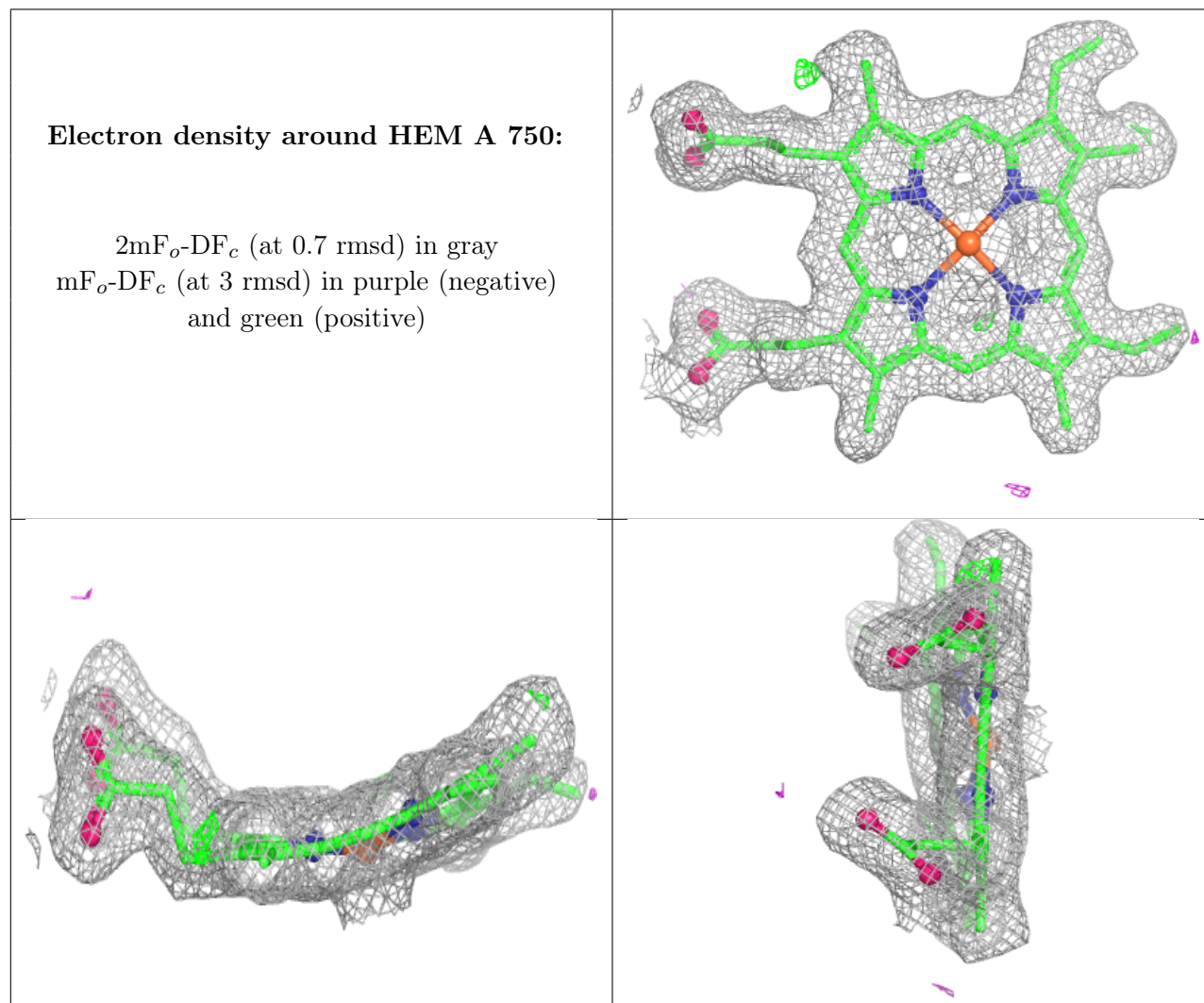
There are no oligosaccharides in this entry.

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, 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.

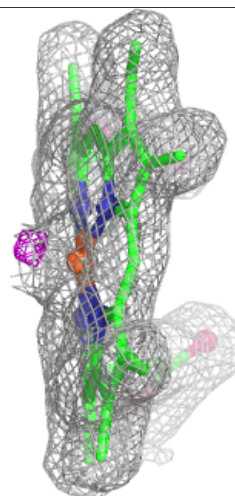
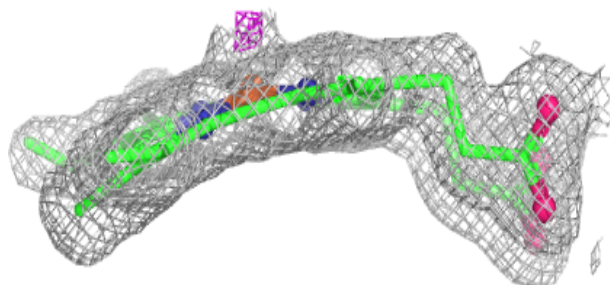
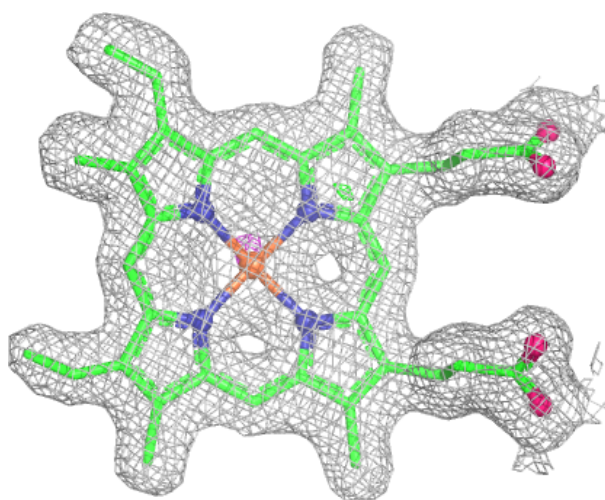
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACT	A	860	4/4	0.87	0.16	50,50,50,51	0
6	DP3	A	793	17/17	0.91	0.10	23,27,33,33	0
6	DP3	B	794	17/17	0.91	0.09	23,26,32,32	0
2	ACT	B	861	4/4	0.93	0.11	36,36,36,36	0
5	H4B	A	760	17/17	0.96	0.06	19,20,21,21	0
5	H4B	B	761	17/17	0.96	0.06	16,17,19,19	0
4	HEM	A	750	43/43	0.97	0.07	18,19,20,20	0
4	HEM	B	750	43/43	0.98	0.07	16,17,19,20	0
3	ZN	A	900	1/1	0.99	0.04	30,30,30,30	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 ⓘ

There are no such residues in this entry.