



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:22 PM UTC

PDB ID : 2G6L / pdb_00002g6l
Title : Structure of rat nNOS heme domain (BH2 bound) complexed with NO
Authors : Li, H.; Igarashi, J.; Jamal, J.; Yang, W.; Poulos, T.L.
Deposited on : 2006-02-24
Resolution : 2.05 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

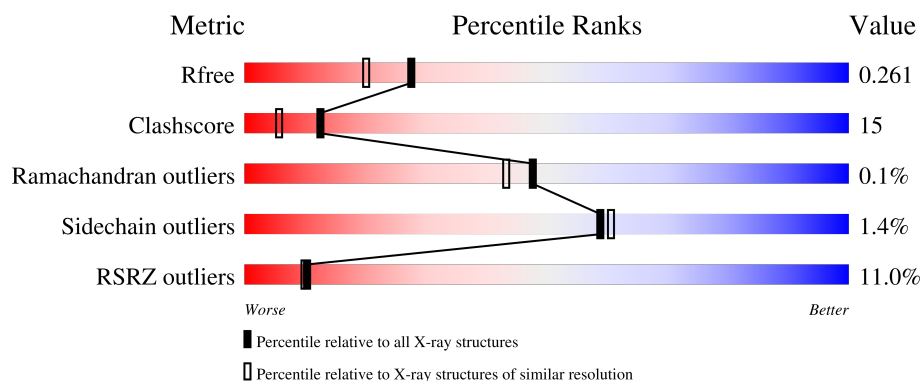
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	420	17% 60% 34% • •
1	B	420	4% 76% 21% • •

2 Entry composition [i](#)

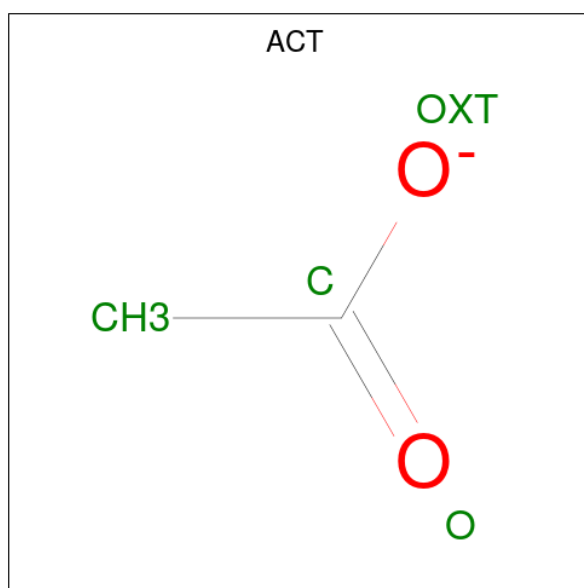
There are 8 unique types of molecules in this entry. The entry contains 7221 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	409	Total	C	N	O	S	0	0	0
			3331	2132	571	607	21			
1	B	411	Total	C	N	O	S	0	0	0
			3345	2140	574	610	21			

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

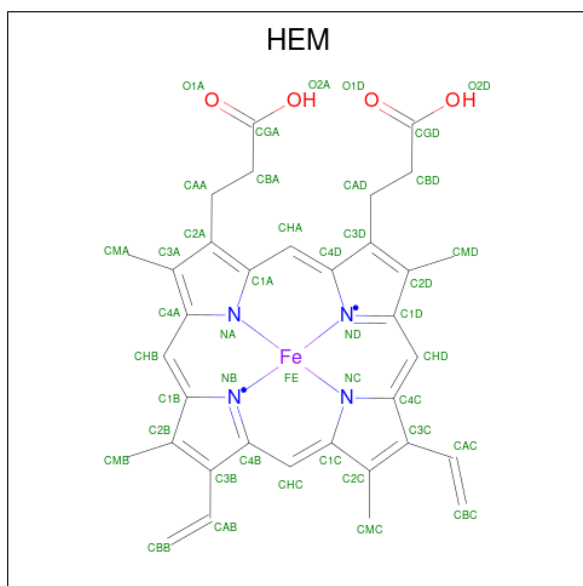


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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

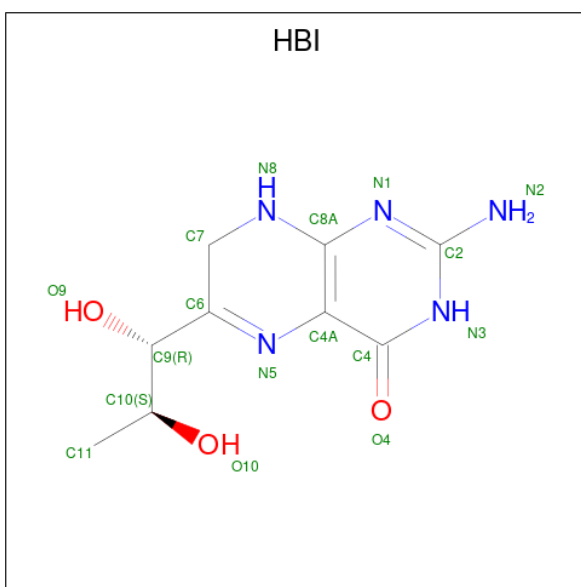
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

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



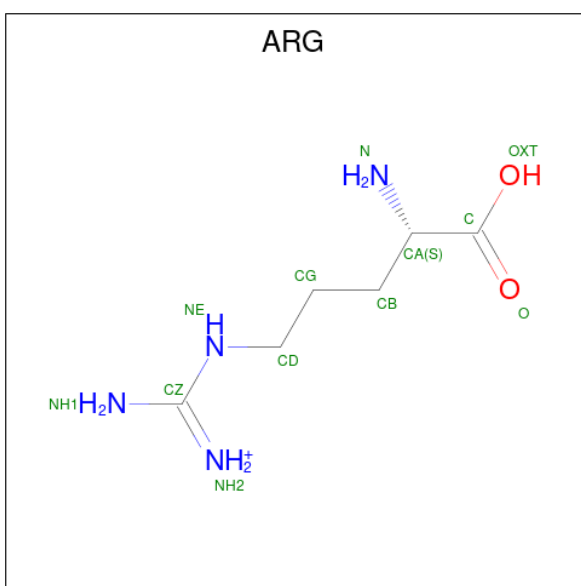
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is 7,8-DIHYDROBIOPTERIN (CCD ID: HBI) (formula: $\text{C}_9\text{H}_{13}\text{N}_5\text{O}_3$).



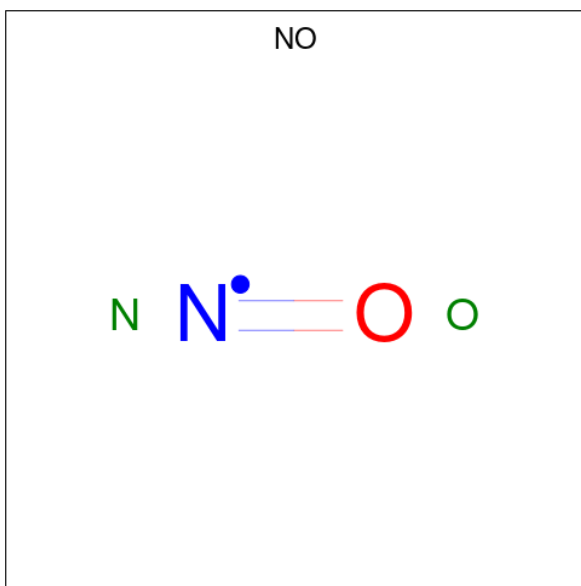
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			17	9	5	3		
5	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 6 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



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

- Molecule 7 is NITRIC OXIDE (CCD ID: NO) (formula: NO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	N	O	0	0
			2	1	1		
7	B	1	Total	N	O	0	0
			2	1	1		

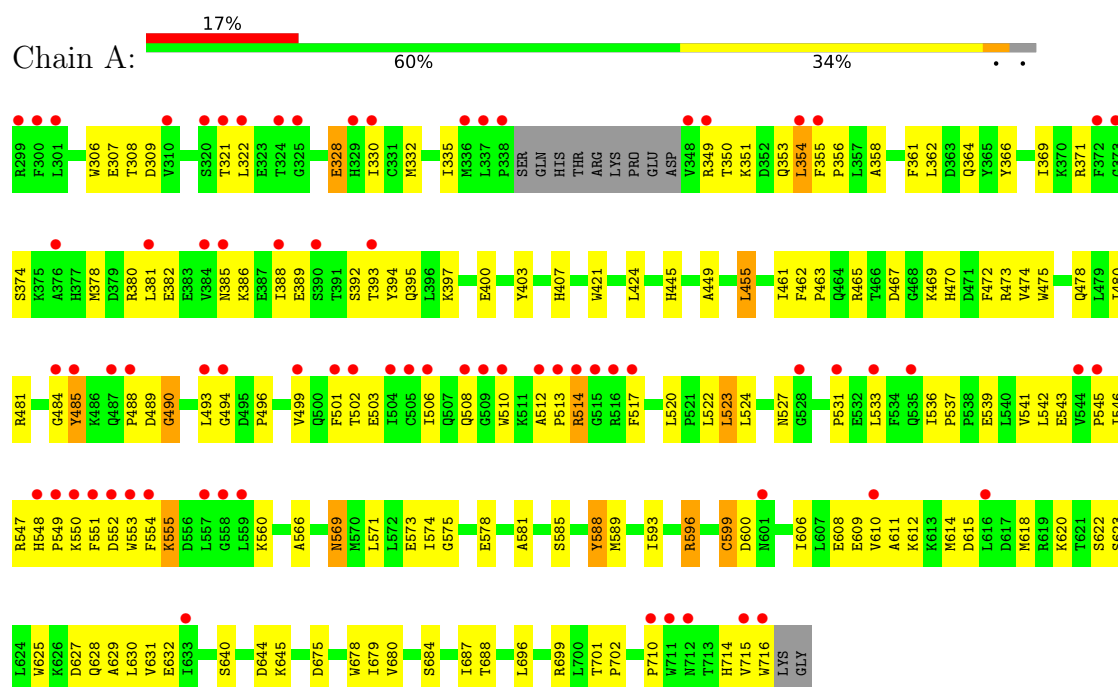
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	148	Total	O	0	0
			148	148		
8	B	240	Total	O	0	0
			240	240		

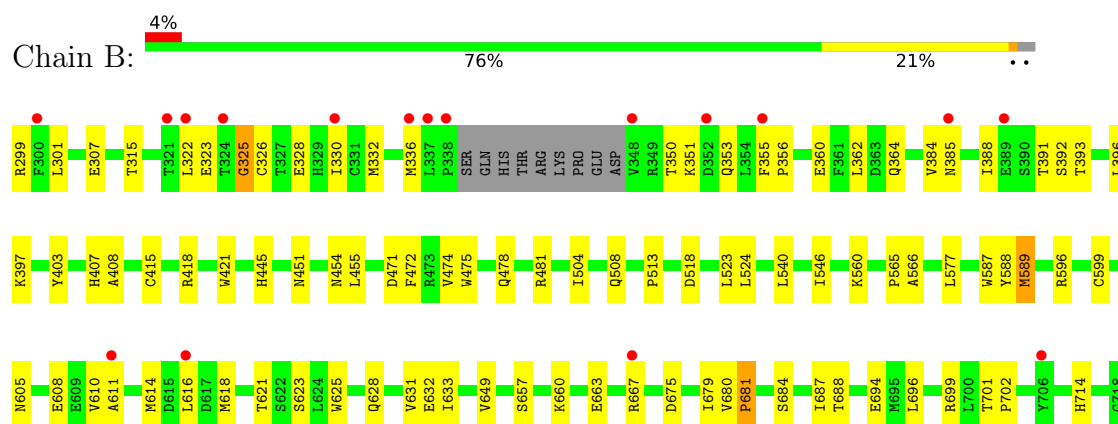
3 Residue-property plots [i](#)

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



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.03Å 111.16Å 164.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.61 – 2.05 49.61 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.61-2.05) 97.4 (49.61-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.272 0.217 , 0.261	Depositor DCC
R_{free} test set	2951 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7221	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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, 0.333 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, NO, HEM, HBI, ZN

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	0.48	0/3424	0.98	17/4645 (0.4%)
1	B	0.53	0/3438	0.99	19/4661 (0.4%)
All	All	0.51	0/6862	0.99	36/9306 (0.4%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	589	MET	N-CA-C	-9.16	94.33	109.07
1	A	397	LYS	N-CA-C	-8.05	100.50	110.41
1	A	589	MET	N-CA-C	-7.82	96.49	109.24
1	A	354	LEU	N-CA-C	7.72	119.60	111.03
1	B	421	TRP	N-CA-C	7.31	120.18	111.33
1	B	714	HIS	N-CA-C	7.06	120.62	110.10
1	A	606	ILE	N-CA-C	7.05	118.86	112.17
1	A	421	TRP	N-CA-C	6.86	119.63	111.33
1	B	455	LEU	N-CA-C	6.79	119.82	110.24
1	B	681	PRO	CA-C-N	6.74	127.60	120.12
1	B	681	PRO	C-N-CA	6.74	127.60	120.12
1	B	471	ASP	N-CA-C	6.34	118.97	110.35
1	B	408	ALA	N-CA-C	-6.24	104.56	111.36
1	B	596	ARG	N-CA-C	6.19	117.90	111.03
1	A	490	GLY	N-CA-C	-6.15	106.25	114.25
1	B	599	CYS	N-CA-C	5.90	121.39	113.72
1	A	688	THR	N-CA-C	-5.79	101.24	110.10
1	B	623	SER	N-CA-C	-5.74	105.77	112.89
1	B	474	VAL	N-CA-C	-5.69	99.04	107.51
1	B	472	PHE	N-CA-C	-5.41	100.89	109.76
1	B	315	THR	N-CA-C	-5.40	107.35	114.31
1	B	418	ARG	N-CA-C	5.34	119.27	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	680	VAL	CA-C-N	5.31	123.54	119.66
1	A	680	VAL	C-N-CA	5.31	123.54	119.66
1	A	596	ARG	N-CA-C	5.26	117.82	111.40
1	A	588	TYR	N-CA-C	5.22	117.44	110.35
1	A	623	SER	N-CA-C	-5.21	106.88	113.18
1	A	599	CYS	N-CA-C	5.20	119.68	113.23
1	A	455	LEU	N-CA-C	5.16	117.52	110.24
1	B	688	THR	N-CA-C	-5.16	102.35	110.14
1	B	397	LYS	N-CA-C	-5.11	103.65	110.55
1	B	325	GLY	N-CA-C	-5.11	108.61	114.69
1	A	424	LEU	N-CA-C	5.07	117.65	110.10
1	B	524	LEU	N-CA-C	5.06	117.22	109.07
1	A	461	ILE	N-CA-C	5.03	114.82	107.37
1	A	474	VAL	N-CA-C	-5.02	100.66	107.99

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	3331	0	3243	145	0
1	B	3345	0	3259	70	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	1	0
4	B	43	0	30	3	0
5	A	17	0	13	1	0
5	B	17	0	13	0	0
6	A	12	0	12	0	0
6	B	12	0	12	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
8	A	148	0	0	22	0
8	B	240	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7221	0	6618	206	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 15.

All (206) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.39	1.04
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.41	0.86
1:A:560:LYS:HG3	8:A:992:HOH:O	1.80	0.82
1:A:355:PHE:HB2	8:A:1001:HOH:O	1.81	0.81
1:A:555:LYS:NZ	1:A:555:LYS:HB3	1.98	0.79
1:B:699:ARG:HG2	8:B:1023:HOH:O	1.82	0.79
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.68	0.76
1:A:371:ARG:HH21	1:A:371:ARG:HG3	1.52	0.75
1:A:545:PRO:HG2	1:A:547:ARG:NH2	2.02	0.74
1:A:546:ILE:HG12	1:A:560:LYS:HA	1.68	0.74
1:A:696:LEU:HD22	1:B:330:ILE:HD11	1.69	0.74
1:A:322:LEU:HD13	1:A:699:ARG:NH2	2.03	0.73
1:A:493:LEU:HA	8:A:963:HOH:O	1.90	0.72
1:A:574:ILE:HG22	8:A:1017:HOH:O	1.91	0.71
1:A:322:LEU:HB2	1:A:699:ARG:HB2	1.73	0.70
1:B:356:PRO:O	1:B:360:GLU:HG3	1.92	0.69
1:B:299:ARG:HB3	1:B:299:ARG:NH1	2.09	0.67
1:A:701:THR:HG22	1:A:702:PRO:HA	1.74	0.67
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.10	0.66
1:A:684:SER:HB3	1:A:687:ILE:HD11	1.77	0.66
1:B:299:ARG:HB3	1:B:299:ARG:HH11	1.60	0.65
1:A:321:THR:HG23	1:A:322:LEU:HG	1.78	0.64
1:A:517:PHE:HB3	8:A:992:HOH:O	1.98	0.63
1:A:716:TRP:H	1:A:716:TRP:CD1	2.15	0.63
1:A:551:PHE:HB3	1:A:553:TRP:NE1	2.15	0.62
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.81	0.62
1:A:496:PRO:HA	1:A:499:VAL:HG23	1.82	0.62
1:A:610:VAL:O	1:A:614:MET:HG3	2.00	0.61
1:A:514:ARG:HH21	1:A:514:ARG:HG3	1.65	0.61
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.81	0.61
1:A:701:THR:HG22	8:A:971:HOH:O	2.00	0.61
1:B:391:THR:O	1:B:392:SER:HB2	2.01	0.61
1:A:382:GLU:HG3	1:A:386:LYS:HE3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:657:SER:HA	8:B:1087:HOH:O	2.01	0.61
1:B:322:LEU:HD13	1:B:699:ARG:NH2	2.14	0.60
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.82	0.60
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.32	0.60
1:B:621:THR:HG22	8:B:1143:HOH:O	2.02	0.60
1:A:510:TRP:HZ2	8:A:1015:HOH:O	1.84	0.59
1:A:322:LEU:CB	1:A:699:ARG:HE	2.14	0.59
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.37	0.59
1:B:322:LEU:HB2	1:B:699:ARG:HB2	1.83	0.59
1:A:545:PRO:HG2	1:A:547:ARG:HH21	1.68	0.59
1:A:350:THR:OG1	1:A:353:GLN:HG3	2.03	0.59
1:B:660:LYS:HD2	8:B:1087:HOH:O	2.02	0.59
1:A:308:THR:O	1:A:309:ASP:HB2	2.03	0.59
1:B:323:GLU:O	1:B:699:ARG:HD3	2.02	0.58
1:A:328:GLU:HA	1:B:326:CYS:O	2.04	0.58
1:A:378:MET:HA	1:A:378:MET:HE2	1.86	0.58
1:A:361:PHE:O	1:A:364:GLN:HG2	2.04	0.57
8:A:955:HOH:O	1:B:307:GLU:HG3	2.03	0.57
1:A:539:GLU:HG3	8:A:979:HOH:O	2.03	0.57
1:A:555:LYS:HB3	1:A:555:LYS:HZ3	1.69	0.57
1:A:627:ASP:O	1:A:631:VAL:HG23	2.04	0.57
1:A:552:ASP:HB3	8:A:1014:HOH:O	2.04	0.56
1:A:467:ASP:OD2	1:A:469:LYS:HB2	2.06	0.56
1:A:485:TYR:HE2	1:A:512:ALA:HB1	1.71	0.56
1:B:350:THR:OG1	1:B:353:GLN:HG2	2.06	0.56
1:A:506:ILE:C	1:A:508:GLN:H	2.12	0.56
1:A:555:LYS:HB3	1:A:555:LYS:HZ2	1.69	0.56
1:A:322:LEU:HB2	1:A:699:ARG:HE	1.69	0.56
1:A:322:LEU:HD13	1:A:699:ARG:HH21	1.71	0.56
1:A:620:LYS:HE3	1:A:622:SER:OG	2.05	0.56
1:A:612:LYS:O	1:A:615:ASP:N	2.32	0.55
1:A:506:ILE:C	1:A:508:GLN:N	2.64	0.55
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.07	0.55
1:A:555:LYS:HE2	8:A:1014:HOH:O	2.06	0.55
1:B:546:ILE:HG12	1:B:560:LYS:HA	1.89	0.55
1:A:560:LYS:HE3	8:A:992:HOH:O	2.07	0.54
1:A:335:ILE:HD13	1:B:694:GLU:HB3	1.89	0.54
1:A:321:THR:HG23	1:A:322:LEU:H	1.73	0.54
1:A:332:MET:HE1	1:B:301:LEU:HD22	1.90	0.54
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.33	0.54
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:TRP:H	4:B:750:HEM:HAB	1.73	0.54
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.90	0.53
1:A:684:SER:HB3	1:A:687:ILE:CD1	2.39	0.53
4:A:750:HEM:HMC2	4:A:750:HEM:HBC2	1.89	0.53
1:A:382:GLU:O	1:A:386:LYS:HG3	2.08	0.53
1:A:569:ASN:ND2	1:A:569:ASN:H	2.07	0.53
1:B:355:PHE:HD2	1:B:385:ASN:ND2	2.07	0.52
1:A:701:THR:CG2	1:A:702:PRO:HA	2.39	0.52
1:A:371:ARG:HH21	1:A:371:ARG:CG	2.22	0.52
1:A:508:GLN:NE2	1:A:508:GLN:HA	2.25	0.52
1:A:499:VAL:O	1:A:503:GLU:HG3	2.09	0.52
1:B:608:GLU:HG2	1:B:618:MET:CE	2.40	0.52
1:A:355:PHE:N	1:A:356:PRO:HD2	2.26	0.51
1:A:542:LEU:HD12	1:A:543:GLU:N	2.26	0.51
1:A:306:TRP:CD1	1:B:336:MET:HE2	2.46	0.51
1:A:366:TYR:HA	1:A:369:ILE:HG12	1.93	0.51
1:A:470:HIS:HB3	1:A:527:ASN:ND2	2.25	0.51
1:A:478:GLN:HB2	1:A:481:ARG:CG	2.40	0.51
1:B:355:PHE:N	1:B:356:PRO:HD2	2.26	0.50
1:A:546:ILE:HA	1:A:640:SER:OG	2.10	0.50
1:A:351:LYS:HE2	1:A:392:SER:HB3	1.93	0.50
1:A:629:ALA:O	1:A:630:LEU:C	2.55	0.50
1:B:336:MET:HE1	8:B:1101:HOH:O	2.11	0.50
1:A:569:ASN:HD22	1:A:569:ASN:N	2.10	0.50
1:A:484:GLY:O	1:A:499:VAL:HA	2.12	0.50
1:A:328:GLU:H	1:A:328:GLU:CD	2.19	0.50
1:A:381:LEU:HB2	8:A:1000:HOH:O	2.11	0.49
1:B:605:ASN:ND2	8:B:1142:HOH:O	2.29	0.49
1:B:299:ARG:NH1	1:B:299:ARG:CB	2.75	0.49
1:A:678:TRP:HA	5:A:760:HBI:N1	2.27	0.49
1:B:350:THR:H	1:B:353:GLN:CG	2.26	0.48
1:B:415:CYS:HB2	4:B:750:HEM:ND	2.28	0.48
1:B:388:ILE:O	1:B:392:SER:N	2.35	0.48
1:A:374:SER:O	1:A:378:MET:HG2	2.13	0.48
1:A:551:PHE:CD2	1:A:551:PHE:N	2.81	0.48
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.49	0.48
1:A:371:ARG:HG3	1:A:371:ARG:NH2	2.26	0.48
1:A:548:HIS:ND1	1:A:549:PRO:HD2	2.28	0.47
1:B:701:THR:HA	1:B:702:PRO:C	2.38	0.47
1:A:502:THR:O	1:A:506:ILE:HG13	2.13	0.47
1:A:481:ARG:NE	8:A:1044:HOH:O	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:THR:HG23	1:A:322:LEU:N	2.29	0.47
1:A:349:ARG:NH2	1:A:573:GLU:OE2	2.48	0.47
1:A:571:LEU:C	1:A:571:LEU:HD23	2.40	0.47
1:B:504:ILE:O	1:B:508:GLN:HG2	2.14	0.47
1:A:382:GLU:CG	1:A:386:LYS:HE3	2.45	0.47
1:B:336:MET:HG3	8:B:1024:HOH:O	2.14	0.46
1:A:701:THR:HA	1:A:702:PRO:C	2.40	0.46
1:A:354:LEU:C	1:A:356:PRO:HD2	2.41	0.46
1:B:663:GLU:HB3	1:B:667:ARG:NH1	2.31	0.46
1:A:551:PHE:O	1:A:554:PHE:HB2	2.14	0.46
1:B:445:HIS:C	1:B:445:HIS:CD2	2.94	0.46
1:B:565:PRO:HB3	1:B:588:TYR:CZ	2.51	0.46
1:A:332:MET:HE2	1:B:696:LEU:HD21	1.98	0.46
1:A:449:ALA:O	1:A:455:LEU:HA	2.16	0.46
1:B:610:VAL:O	1:B:614:MET:HG3	2.16	0.46
1:A:524:LEU:O	1:A:531:PRO:HA	2.17	0.46
1:A:566:ALA:HB2	1:A:585:SER:HB3	1.98	0.46
1:A:608:GLU:N	8:A:1053:HOH:O	2.12	0.46
1:B:608:GLU:HG2	1:B:618:MET:HE1	1.99	0.45
1:B:364:GLN:NE2	8:B:1112:HOH:O	2.49	0.45
1:A:489:ASP:OD2	1:A:489:ASP:O	2.35	0.45
1:A:494:GLY:O	1:A:496:PRO:HD3	2.16	0.45
1:A:542:LEU:HD12	1:A:543:GLU:H	1.81	0.45
1:A:548:HIS:CG	1:A:549:PRO:HD2	2.52	0.45
1:A:569:ASN:H	1:A:569:ASN:HD22	1.62	0.45
1:A:632:GLU:OE2	1:B:628:GLN:NE2	2.48	0.45
1:A:463:PRO:HB2	1:A:472:PHE:CE1	2.52	0.45
1:A:596:ARG:O	1:A:600:ASP:HB2	2.17	0.44
1:A:501:PHE:HD2	1:A:520:LEU:HD13	1.81	0.44
1:A:522:LEU:O	1:A:533:LEU:HA	2.17	0.44
1:A:393:THR:OG1	1:A:394:TYR:N	2.50	0.44
1:B:478:GLN:HA	1:B:566:ALA:O	2.18	0.44
1:B:610:VAL:HG21	1:B:633:ILE:HD11	1.98	0.44
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.99	0.44
1:A:512:ALA:HA	1:A:513:PRO:HD3	1.86	0.44
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.05	0.44
1:A:475:TRP:CE3	1:A:523:LEU:HD13	2.53	0.44
1:A:696:LEU:HD22	1:B:330:ILE:CD1	2.42	0.44
4:B:750:HEM:HMC1	4:B:750:HEM:HBC2	2.00	0.44
1:A:599:CYS:O	1:A:600:ASP:C	2.61	0.44
1:A:395:GLN:HA	8:A:1034:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:GLN:CA	1:A:508:GLN:HE21	2.30	0.43
1:A:569:ASN:ND2	1:A:569:ASN:N	2.65	0.43
1:A:715:VAL:O	1:A:715:VAL:HG23	2.18	0.43
1:A:545:PRO:HD2	1:A:644:ASP:OD2	2.19	0.43
1:A:378:MET:HE2	1:A:378:MET:CA	2.46	0.43
1:A:609:GLU:HB3	8:A:982:HOH:O	2.17	0.43
1:A:480:ILE:HD13	1:A:541:VAL:HG13	2.01	0.43
1:A:335:ILE:CD1	1:B:694:GLU:HB3	2.49	0.43
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.91	0.43
1:A:307:GLU:HG3	8:B:927:HOH:O	2.18	0.43
1:A:358:ALA:O	1:A:362:LEU:HG	2.19	0.43
1:B:322:LEU:HD12	1:B:699:ARG:HB3	2.00	0.42
1:A:445:HIS:CD2	1:A:445:HIS:C	2.97	0.42
1:A:489:ASP:N	8:A:969:HOH:O	2.47	0.42
1:B:325:GLY:O	1:B:332:MET:HE2	2.18	0.42
1:B:355:PHE:HB2	1:B:356:PRO:HD3	2.01	0.42
1:B:396:LEU:HG	1:B:577:LEU:HD12	2.02	0.42
1:A:608:GLU:O	1:A:611:ALA:HB3	2.19	0.42
1:A:714:HIS:HA	8:A:1047:HOH:O	2.20	0.42
1:B:388:ILE:HA	1:B:393:THR:O	2.20	0.42
1:A:575:GLY:HA3	8:A:1017:HOH:O	2.20	0.42
1:A:618:MET:HE3	1:A:625:TRP:CH2	2.55	0.42
1:B:618:MET:HG2	1:B:625:TRP:CD2	2.55	0.42
1:A:330:ILE:O	1:A:330:ILE:HG23	2.20	0.42
1:B:299:ARG:CB	1:B:299:ARG:CZ	2.98	0.42
1:B:355:PHE:HB2	1:B:356:PRO:CD	2.50	0.42
1:B:362:LEU:HD11	1:B:384:VAL:HG21	2.02	0.42
1:B:675:ASP:O	1:B:679:ILE:HG12	2.20	0.41
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.80	0.41
1:A:388:ILE:O	1:A:392:SER:N	2.50	0.41
1:B:451:ASN:HB3	1:B:454:ASN:O	2.21	0.41
1:A:588:TYR:CD1	1:A:593:ILE:HD11	2.56	0.41
1:B:684:SER:HB3	1:B:687:ILE:HD11	2.03	0.41
1:B:684:SER:HB3	1:B:687:ILE:HG12	2.02	0.41
1:A:351:LYS:HE2	1:A:392:SER:CB	2.51	0.41
1:A:381:LEU:HD22	8:A:1000:HOH:O	2.20	0.41
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.09	0.41
1:B:351:LYS:HE3	1:B:392:SER:OG	2.21	0.41
1:B:589:MET:HA	1:B:649:VAL:O	2.21	0.41
1:B:611:ALA:HA	1:B:616:LEU:HD12	2.02	0.41
1:B:614:MET:CE	1:B:632:GLU:HG3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:ARG:NH1	1:A:578:GLU:OE1	2.54	0.41
1:A:536:ILE:O	1:A:537:PRO:C	2.63	0.41
1:A:625:TRP:HA	8:A:985:HOH:O	2.20	0.41
1:A:462:PHE:HB2	1:A:581:ALA:HB3	2.02	0.40
1:A:614:MET:CE	1:A:632:GLU:HG3	2.51	0.40
1:A:488:PRO:C	1:A:490:GLY:N	2.78	0.40
1:A:355:PHE:CE1	1:A:385:ASN:HB2	2.57	0.40
1:A:620:LYS:HE3	1:A:620:LYS:HB2	1.92	0.40
1:A:675:ASP:O	1:A:679:ILE:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	405/420 (96%)	368 (91%)	36 (9%)	1 (0%)	43	37
1	B	407/420 (97%)	385 (95%)	22 (5%)	0	100	100
All	All	812/840 (97%)	753 (93%)	58 (7%)	1 (0%)	48	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	550	LYS

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	365/375 (97%)	357 (98%)	8 (2%)	45	44
1	B	366/375 (98%)	364 (100%)	2 (0%)	81	85
All	All	731/750 (98%)	721 (99%)	10 (1%)	59	60

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	328	GLU
1	A	389	GLU
1	A	485	TYR
1	A	514	ARG
1	A	523	LEU
1	A	555	LYS
1	A	569	ASN
1	A	645	LYS
1	B	328	GLU
1	B	540	LEU

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

Mol	Chain	Res	Type
1	A	420	GLN
1	A	425	GLN
1	A	454	ASN
1	A	507	GLN
1	A	508	GLN
1	A	527	ASN
1	A	569	ASN
1	A	601	ASN
1	A	605	ASN
1	A	697	ASN
1	A	712	ASN
1	B	364	GLN
1	B	385	ASN
1	B	407	HIS
1	B	425	GLN
1	B	440	ASN
1	B	454	ASN
1	B	507	GLN

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Mol	Chain	Res	Type
1	B	527	ASN
1	B	535	GLN
1	B	601	ASN
1	B	642	GLN

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 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	ACT	B	861	-	3,3,3	1.04	0	3,3,3	0.75	0
5	HBI	A	760	-	15,18,18	2.46	6 (40%)	14,26,26	2.13	3 (21%)
4	HEM	A	750	7,1	50,50,50	1.46	9 (18%)	67,82,82	0.94	3 (4%)
6	ARG	A	770	-	10,11,11	0.99	0	9,13,13	0.73	0
7	NO	B	910	4	0,1,1	-	-	-	-	-
6	ARG	B	771	-	10,11,11	0.76	0	9,13,13	0.67	0
4	HEM	B	750	7,1	50,50,50	1.35	5 (10%)	67,82,82	0.97	2 (2%)
2	ACT	A	860	-	3,3,3	0.95	0	3,3,3	0.77	0
5	HBI	B	761	-	15,18,18	2.35	4 (26%)	14,26,26	2.02	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NO	A	910	4	0,1,1	-	-	-		

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
5	HBI	A	760	-	-	0/4/17/17	0/2/2/2
4	HEM	A	750	7,1	-	0/14/54/54	-
6	ARG	A	770	-	-	0/11/11/11	-
6	ARG	B	771	-	-	0/11/11/11	-
4	HEM	B	750	7,1	-	2/14/54/54	-
5	HBI	B	761	-	-	0/4/17/17	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	760	HBI	C6-N5	6.63	1.39	1.28
5	B	761	HBI	C6-N5	6.43	1.38	1.28
5	A	760	HBI	C7-N8	4.20	1.52	1.45
5	B	761	HBI	C7-N8	3.84	1.51	1.45
4	A	750	HEM	FE-NB	3.12	2.04	1.94
4	B	750	HEM	FE-ND	2.99	2.04	1.94
5	B	761	HBI	C7-C6	2.86	1.53	1.49
4	A	750	HEM	FE-NA	2.72	2.04	1.95
5	A	760	HBI	C7-C6	2.69	1.52	1.49
4	B	750	HEM	CAB-C3B	-2.58	1.40	1.47
4	B	750	HEM	C4C-NC	-2.57	1.34	1.39
4	A	750	HEM	FE-ND	2.55	2.02	1.94
4	A	750	HEM	CAB-C3B	-2.52	1.40	1.47
5	A	760	HBI	C8A-N1	2.49	1.40	1.36
5	A	760	HBI	C4-N3	2.45	1.43	1.38
4	A	750	HEM	CMD-C2D	2.43	1.55	1.50
4	B	750	HEM	CHC-C1C	2.26	1.42	1.38
4	A	750	HEM	CMC-C2C	2.22	1.55	1.50
4	A	750	HEM	CAC-C3C	-2.20	1.41	1.47
5	A	760	HBI	C2-N1	2.19	1.38	1.33
4	B	750	HEM	C2A-C3A	-2.16	1.33	1.38
4	A	750	HEM	CHC-C1C	2.12	1.42	1.38
5	B	761	HBI	C4-N3	2.11	1.42	1.38
4	A	750	HEM	C3C-C4C	-2.09	1.42	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	760	HBI	C2-N1-C8A	5.70	123.43	113.36
5	B	761	HBI	C2-N1-C8A	5.52	123.10	113.36
5	A	760	HBI	N3-C2-N1	-3.44	117.02	123.32
5	B	761	HBI	N3-C2-N1	-3.20	117.47	123.32
4	A	750	HEM	CAB-C3B-C2B	-2.43	120.52	128.43
5	A	760	HBI	C4A-N5-C6	2.43	121.29	116.08
4	B	750	HEM	C2D-C1D-ND	2.36	112.63	109.90
5	B	761	HBI	C4A-N5-C6	2.23	120.86	116.08
4	B	750	HEM	CBA-CAA-C2A	-2.16	106.55	112.53
4	A	750	HEM	CHC-C4B-NB	-2.12	122.14	124.42
4	A	750	HEM	C3C-C2C-C1C	-2.08	105.08	107.05

There are no chirality outliers.

All (2) torsion outliers are listed below:

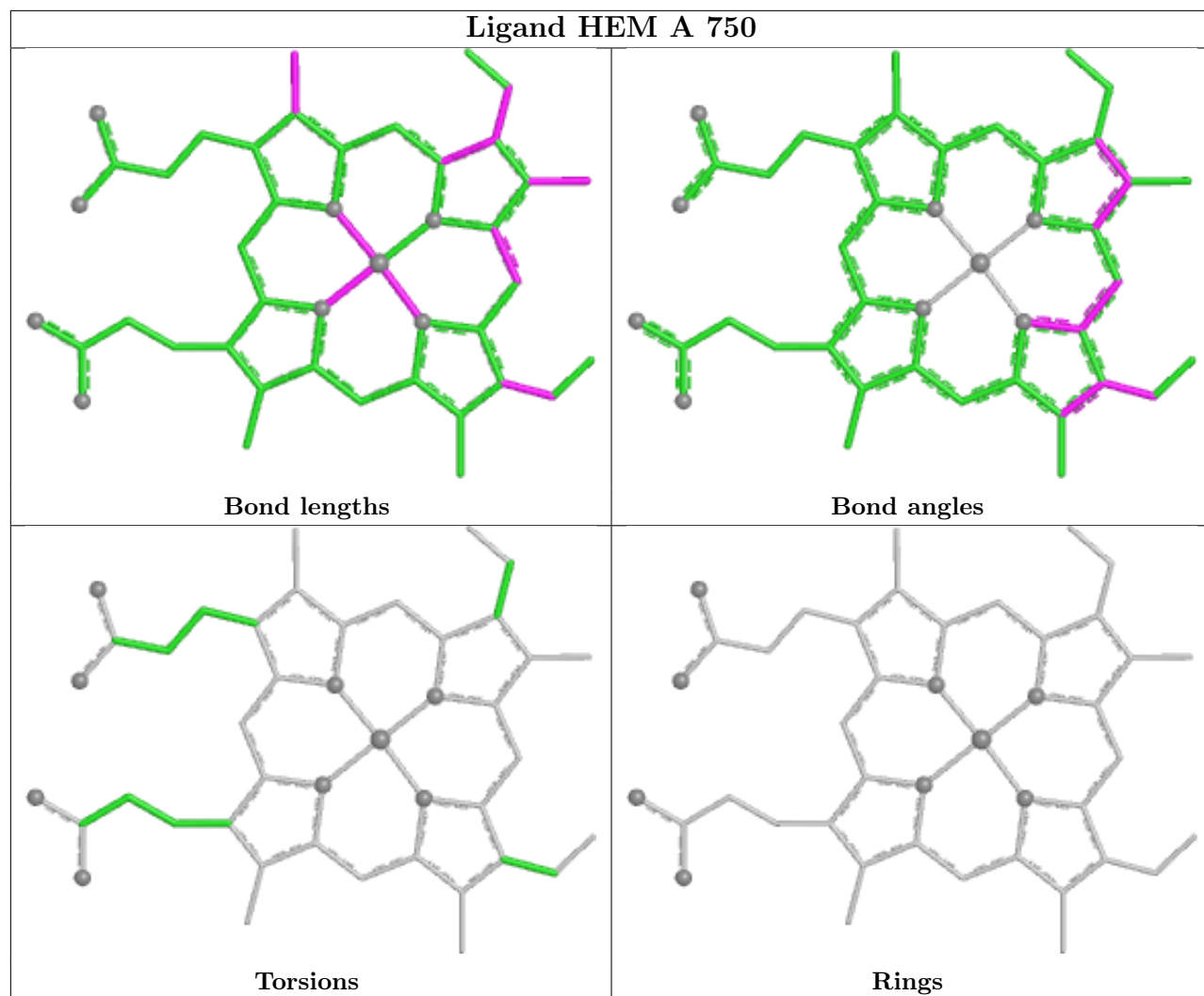
Mol	Chain	Res	Type	Atoms
4	B	750	HEM	C2B-C3B-CAB-CBB
4	B	750	HEM	C4B-C3B-CAB-CBB

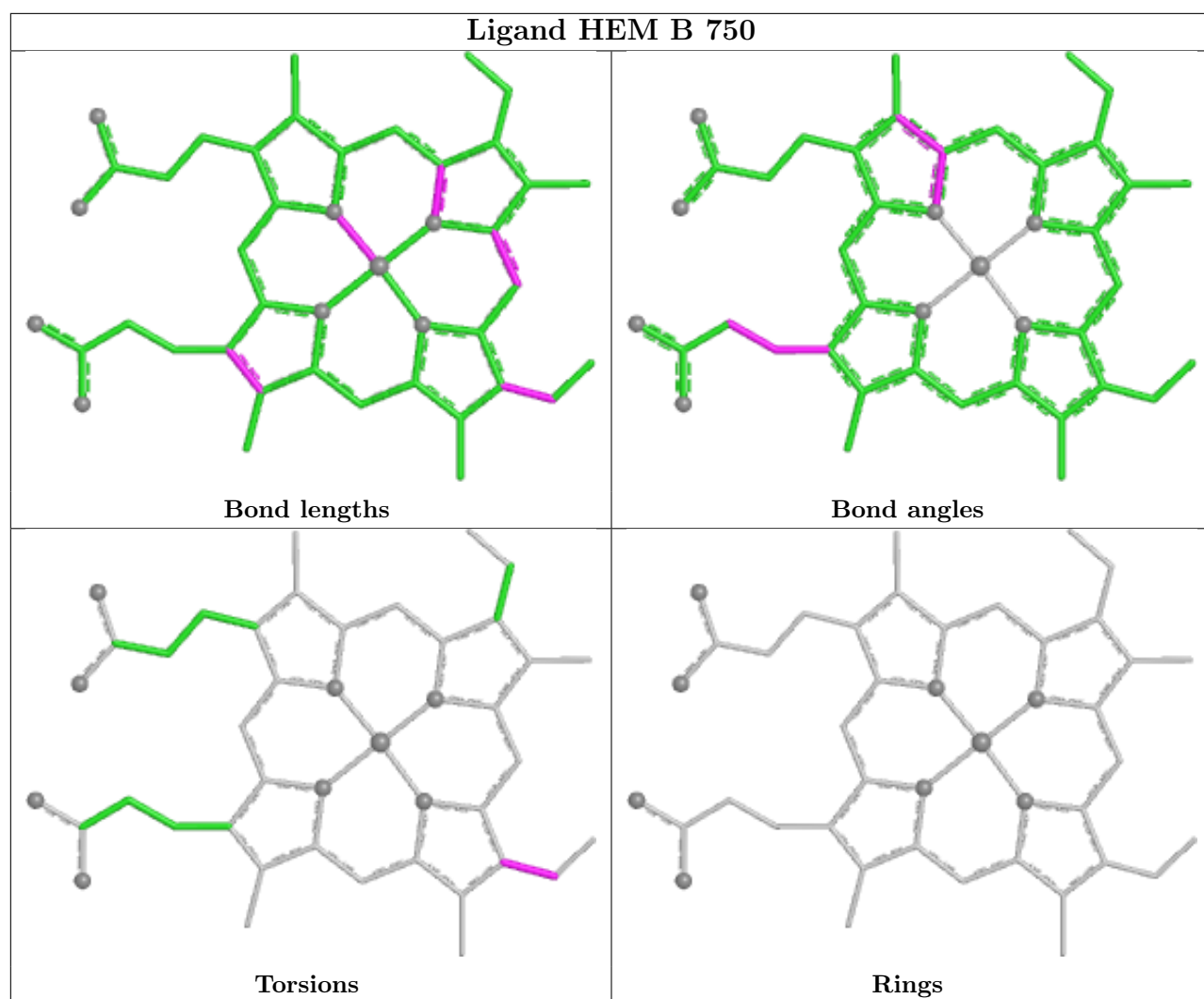
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	760	HBI	1	0
4	A	750	HEM	1	0
4	B	750	HEM	3	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	409/420 (97%)	0.97	73 (17%) 4 3	23, 45, 75, 90	0
1	B	411/420 (97%)	0.29	17 (4%) 41 41	24, 36, 63, 80	0
All	All	820/840 (97%)	0.63	90 (10%) 10 10	23, 40, 71, 90	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	322	LEU	5.1
1	A	300	PHE	4.7
1	A	554	PHE	4.4
1	B	322	LEU	4.3
1	A	355	PHE	4.3
1	A	338	PRO	4.1
1	B	321	THR	3.8
1	B	300	PHE	3.7
1	A	321	THR	3.7
1	A	553	TRP	3.6
1	A	513	PRO	3.6
1	A	373	GLY	3.6
1	A	512	ALA	3.5
1	A	324	THR	3.5
1	A	711	TRP	3.4
1	A	716	TRP	3.4
1	A	501	PHE	3.3
1	B	338	PRO	3.3
1	B	337	LEU	3.3
1	A	504	ILE	3.2
1	A	485	TYR	3.2
1	A	506	ILE	3.1
1	A	494	GLY	3.0
1	A	610	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	493	LEU	3.0
1	A	551	PHE	3.0
1	B	385	ASN	3.0
1	A	301	LEU	2.9
1	A	533	LEU	2.9
1	A	376	ALA	2.9
1	A	336	MET	2.9
1	B	611	ALA	2.9
1	A	337	LEU	2.8
1	A	715	VAL	2.8
1	B	324	THR	2.8
1	A	299	ARG	2.8
1	A	516	ARG	2.8
1	B	330	ILE	2.8
1	A	488	PRO	2.8
1	B	355	PHE	2.7
1	A	330	ILE	2.7
1	A	487	GLN	2.7
1	A	517	PHE	2.7
1	B	336	MET	2.6
1	A	484	GLY	2.6
1	A	558	GLY	2.6
1	A	505	CYS	2.6
1	B	352	ASP	2.5
1	B	348	VAL	2.5
1	A	710	PRO	2.5
1	A	354	LEU	2.5
1	A	557	LEU	2.5
1	A	510	TRP	2.5
1	A	544	VAL	2.5
1	A	508	GLN	2.4
1	A	535	GLN	2.4
1	A	348	VAL	2.4
1	A	550	LYS	2.4
1	A	528	GLY	2.4
1	A	559	LEU	2.4
1	A	320	SER	2.4
1	A	601	ASN	2.3
1	A	349	ARG	2.3
1	A	502	THR	2.3
1	A	515	GLY	2.3
1	A	388	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	384	VAL	2.2
1	A	499	VAL	2.2
1	A	549	PRO	2.2
1	A	329	HIS	2.2
1	A	509	GLY	2.2
1	A	381	LEU	2.2
1	A	393	THR	2.2
1	B	616	LEU	2.1
1	A	385	ASN	2.1
1	B	706	TYR	2.1
1	A	325	GLY	2.1
1	A	548	HIS	2.1
1	A	633	ILE	2.1
1	A	390	SER	2.1
1	A	616	LEU	2.1
1	A	514	ARG	2.1
1	A	531	PRO	2.1
1	A	545	PRO	2.1
1	A	712	ASN	2.0
1	A	310	VAL	2.0
1	A	372	PHE	2.0
1	B	389	GLU	2.0
1	A	552	ASP	2.0
1	B	667	ARG	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](#)

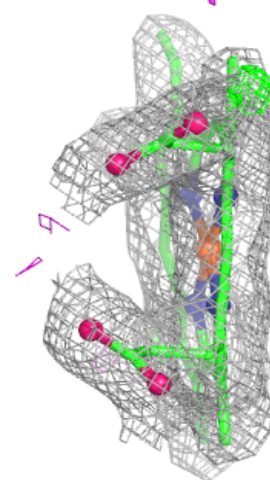
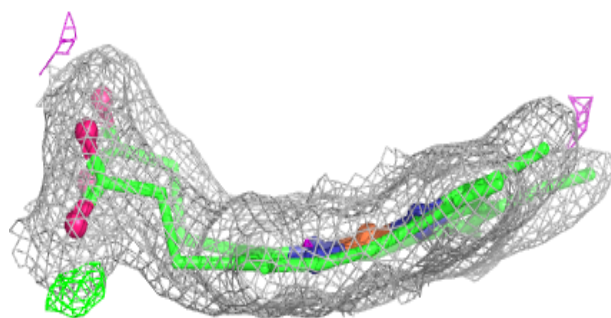
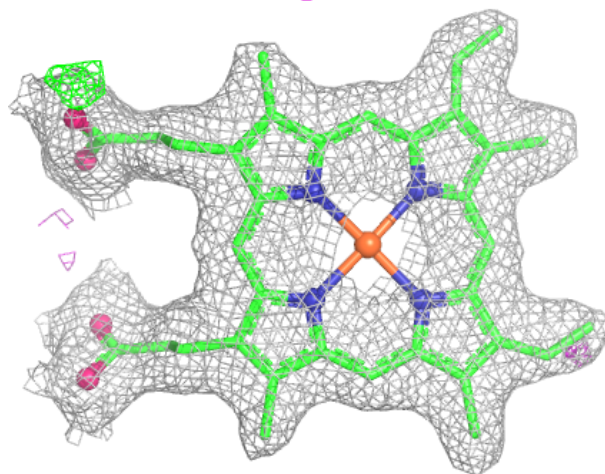
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

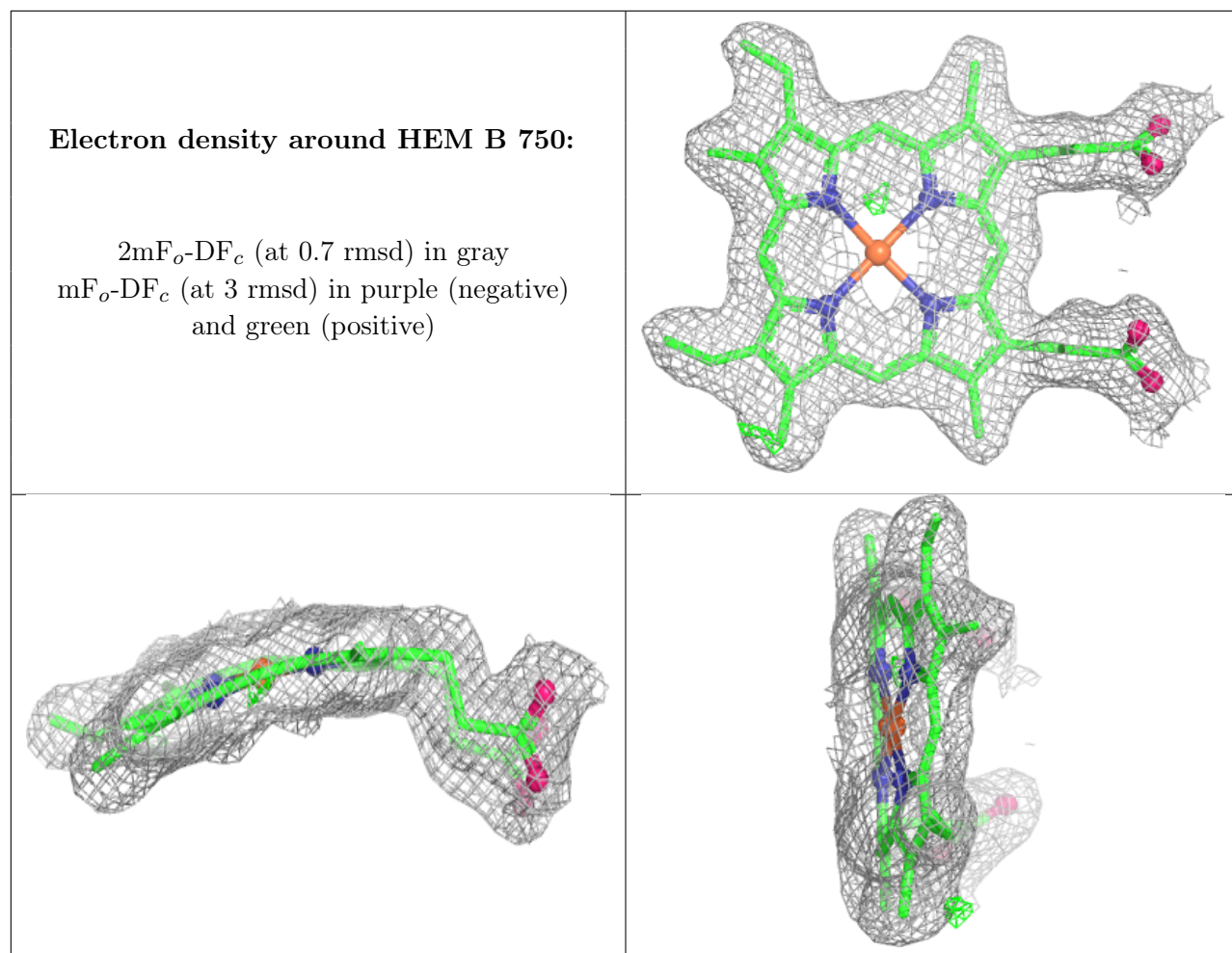
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACT	A	860	4/4	0.85	0.20	61,62,62,63	0
2	ACT	B	861	4/4	0.91	0.12	43,47,48,49	0
5	HBI	A	760	17/17	0.95	0.06	26,29,34,36	0
6	ARG	A	770	12/12	0.95	0.07	28,30,32,32	0
5	HBI	B	761	17/17	0.96	0.06	23,25,30,31	0
6	ARG	B	771	12/12	0.96	0.06	21,24,30,30	0
7	NO	A	910	2/2	0.97	0.05	29,29,29,31	0
7	NO	B	910	2/2	0.97	0.05	28,28,28,30	0
4	HEM	A	750	43/43	0.98	0.06	22,26,29,30	0
4	HEM	B	750	43/43	0.98	0.07	21,25,30,34	0
3	ZN	A	900	1/1	0.99	0.05	46,46,46,46	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 A 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.