



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:21 AM UTC

PDB ID : 1ZVL / pdb_00001zvl
Title : Rat Neuronal Nitric Oxide Synthase Oxygenase Domain complexed with natural substrate L-Arg.
Authors : Matter, H.; Kumar, H.S.; Fedorov, R.; Frey, A.; Kotsonis, P.; Hartmann, E.; Frohlich, L.G.; Reif, A.; Pfeleiderer, W.; Scheurer, P.; Ghosh, D.K.; Schlichting, I.; Schmidt, H.H.
Deposited on : 2005-06-02
Resolution : 2.50 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](#) ①) 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

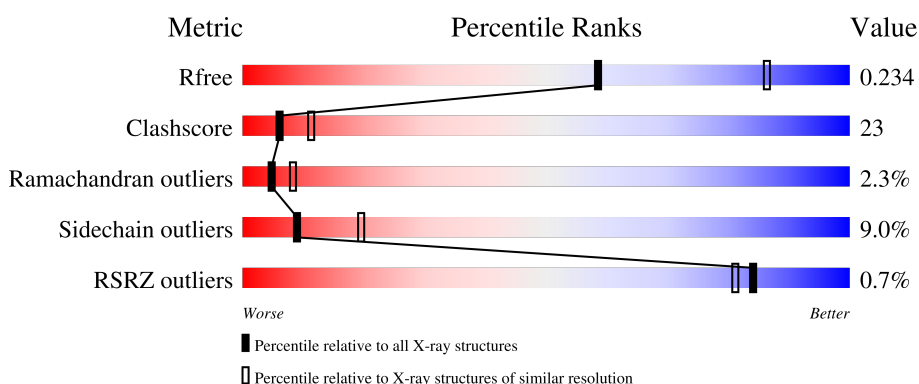
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	48% 44% 8%
1	B	420	58% 34% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7305 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	420	Total	C	N	O	S	0	0	0
			3418	2183	589	625	21			
1	B	420	Total	C	N	O	S	0	0	0
			3418	2183	589	625	21			

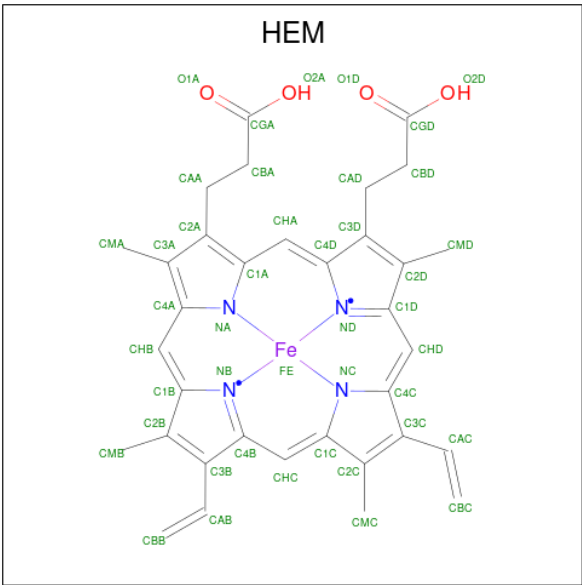
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	297	GLY	-	cloning artifact	UNP P29476
B	297	GLY	-	cloning artifact	UNP P29476

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

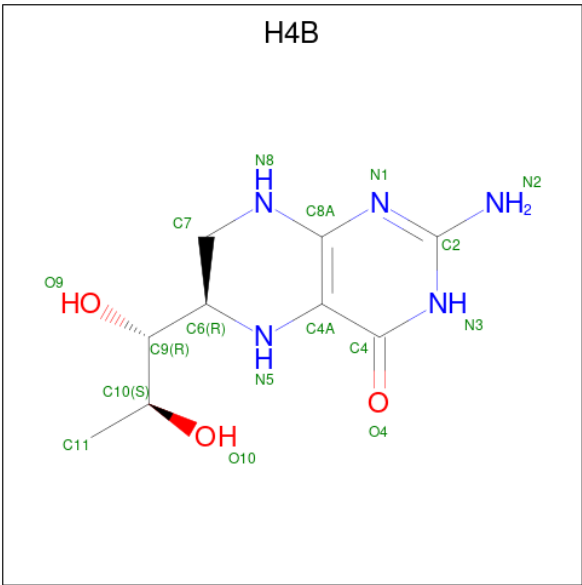
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



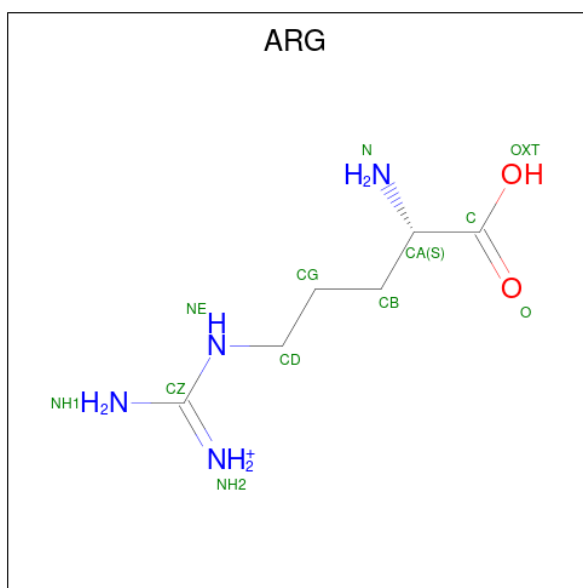
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



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

- Molecule 5 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



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		

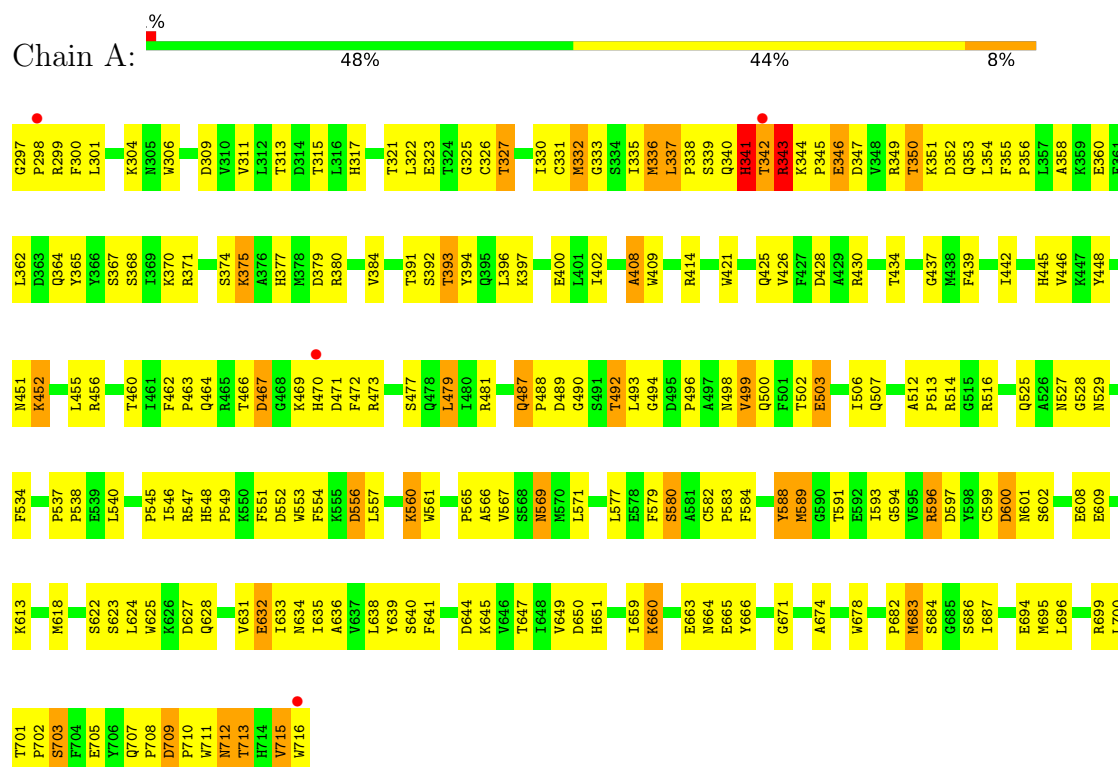
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	138	Total	O	0	0
			138	138		
6	B	186	Total	O	0	0
			186	186		

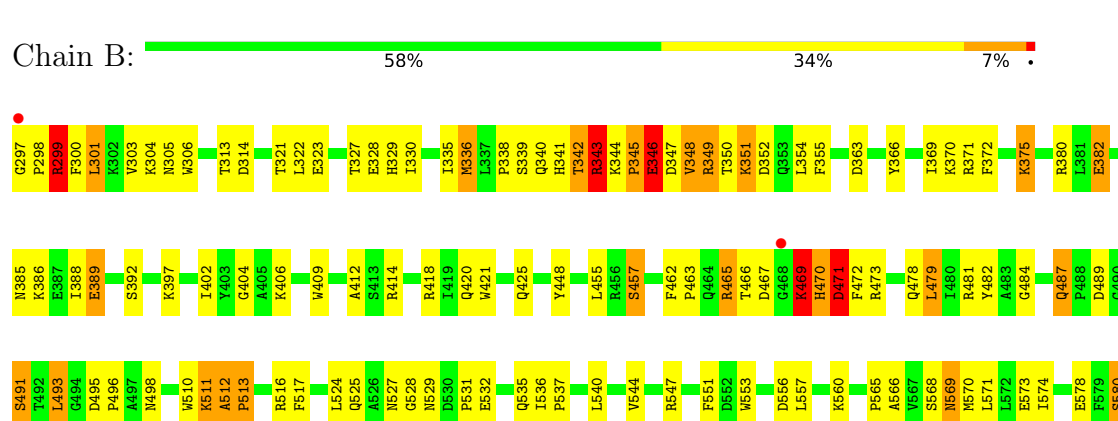
3 Residue-property plots

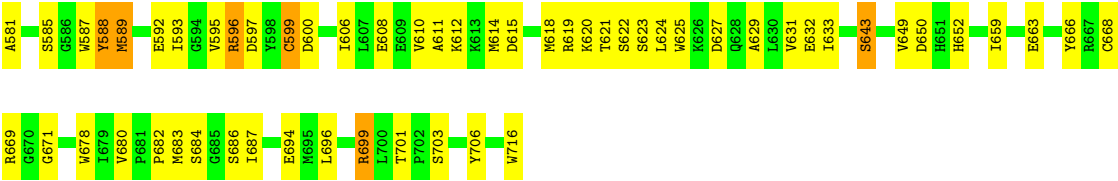
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	52.36Å 111.29Å 165.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 8.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.50) 92.4 (8.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 2.30Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.201 , 0.249 0.188 , 0.234	Depositor DCC
R_{free} test set	2048 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.656	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 100.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7305	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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: 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	0.48	0/3515	0.99	13/4770 (0.3%)
1	B	0.47	0/3515	1.01	19/4770 (0.4%)
All	All	0.48	0/7030	1.00	32/9540 (0.3%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	THR	N-CA-C	-10.33	100.94	112.72
1	B	354	LEU	N-CA-C	9.71	121.63	111.14
1	A	471	ASP	N-CA-C	8.38	120.67	108.86
1	A	589	MET	N-CA-C	-8.12	96.00	109.07
1	B	471	ASP	N-CA-C	7.99	121.22	110.35
1	B	680	VAL	CA-C-N	7.20	124.92	119.66
1	B	680	VAL	C-N-CA	7.20	124.92	119.66
1	B	469	LYS	N-CA-C	-7.15	103.42	111.07
1	A	354	LEU	N-CA-C	7.14	119.06	111.28
1	A	596	ARG	N-CA-C	7.04	118.75	111.14
1	B	512	ALA	N-CA-C	6.94	118.40	109.65
1	B	606	ILE	N-CA-C	6.90	118.78	112.29
1	B	589	MET	N-CA-C	-6.51	99.09	109.76
1	A	408	ALA	N-CA-C	-6.09	105.34	112.89
1	B	491	SER	N-CA-C	6.03	118.11	110.33
1	A	499	VAL	N-CA-C	6.01	116.19	110.42
1	B	472	PHE	N-CA-C	-5.97	99.00	108.73
1	B	557	LEU	N-CA-C	-5.93	104.76	112.23
1	A	588	TYR	N-CA-C	5.90	118.82	110.50
1	B	588	TYR	N-CA-C	5.79	119.04	110.48
1	B	599	CYS	N-CA-C	5.75	120.30	113.28
1	A	709	ASP	N-CA-C	-5.52	102.69	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	546	ILE	N-CA-C	5.49	116.13	108.89
1	A	712	ASN	N-CA-C	-5.32	105.64	113.61
1	B	513	PRO	N-CA-C	-5.31	106.94	113.84
1	B	596	ARG	N-CA-C	5.23	116.84	111.03
1	B	623	SER	N-CA-C	-5.14	106.52	112.89
1	B	699	ARG	N-CA-C	5.14	117.10	108.73
1	B	344	LYS	CA-C-N	5.12	126.25	119.84
1	B	344	LYS	C-N-CA	5.12	126.25	119.84
1	A	703	SER	N-CA-C	5.12	116.86	109.07
1	A	437	GLY	N-CA-C	-5.02	106.34	112.77

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	3418	0	3324	179	0
1	B	3418	0	3324	148	0
2	A	1	0	0	0	0
3	A	43	0	30	0	0
3	B	43	0	30	1	0
4	A	17	0	15	1	0
4	B	17	0	15	1	0
5	A	12	0	12	1	0
5	B	12	0	12	1	0
6	A	138	0	0	4	0
6	B	186	0	0	5	0
All	All	7305	0	6762	311	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 23.

All (311) 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:470:HIS:HB3	1:A:528:GLY:HA3	1.41	1.03
1:A:608:GLU:HG3	1:A:618:MET:HE1	1.46	0.97
1:A:350:THR:HG22	1:A:352:ASP:H	1.26	0.96
1:A:344:LYS:HD3	1:A:346:GLU:HG3	1.54	0.88
1:B:343:ARG:HA	1:B:343:ARG:CZ	2.08	0.84
1:A:340:GLN:O	1:A:341:HIS:HB2	1.77	0.82
1:A:686:SER:HB2	1:B:682:PRO:HB2	1.63	0.80
1:B:298:PRO:C	1:B:299:ARG:HD3	2.09	0.78
1:B:343:ARG:HG3	1:B:571:LEU:HD13	1.64	0.78
1:B:469:LYS:O	1:B:470:HIS:HB2	1.83	0.77
1:B:525:GLN:HG3	1:B:529:ASN:O	1.85	0.77
1:A:470:HIS:CB	1:A:528:GLY:HA3	2.14	0.77
1:A:322:LEU:HB3	1:A:699:ARG:HH21	1.50	0.76
1:B:587:TRP:H	3:B:800:HEM:HAB	1.51	0.75
1:A:466:THR:OG1	1:A:469:LYS:HB3	1.85	0.75
1:A:487:GLN:OE1	1:A:493:LEU:HB2	1.88	0.74
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.02	0.73
1:A:350:THR:HG22	1:A:352:ASP:N	2.03	0.73
1:A:694:GLU:HG2	1:B:335:ILE:HD13	1.70	0.72
1:B:343:ARG:HA	1:B:343:ARG:NH1	2.04	0.72
1:A:297:GLY:N	1:A:300:PHE:HB2	2.05	0.71
1:B:537:PRO:HG2	1:B:540:LEU:HD12	1.73	0.70
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.75	0.69
1:A:500:GLN:HE21	1:A:500:GLN:HA	1.58	0.69
1:A:634:ASN:HB3	6:A:1023:HOH:O	1.92	0.69
1:B:404:GLY:HA3	1:B:574:ILE:HD13	1.75	0.69
1:A:380:ARG:O	1:A:384:VAL:HG23	1.93	0.68
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.76	0.67
1:B:345:PRO:C	1:B:346:GLU:HG2	2.19	0.67
1:A:344:LYS:CD	1:A:346:GLU:HG3	2.23	0.67
1:A:439:PHE:CD2	1:A:534:PHE:HB3	2.30	0.66
1:B:342:THR:O	1:B:343:ARG:HG2	1.95	0.66
1:A:350:THR:HB	1:A:353:GLN:HG3	1.79	0.65
1:B:524:LEU:O	1:B:531:PRO:HA	1.96	0.65
1:A:322:LEU:HB3	1:A:699:ARG:NH2	2.10	0.65
1:A:594:GLY:HA3	1:A:634:ASN:ND2	2.12	0.65
1:B:487:GLN:HE22	1:B:493:LEU:HB2	1.62	0.65
1:A:304:LYS:HB2	1:A:311:VAL:HG22	1.79	0.64
1:A:500:GLN:HA	1:A:500:GLN:NE2	2.12	0.64
1:A:343:ARG:HH12	1:A:349:ARG:HH22	1.45	0.64
1:A:351:LYS:HG2	1:A:392:SER:HA	1.79	0.64
1:B:297:GLY:HA3	1:B:299:ARG:HH12	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:GLU:HG2	1:B:335:ILE:HA	1.81	0.63
1:B:479:LEU:HD13	1:B:568:SER:HB3	1.81	0.63
1:A:506:ILE:HD13	1:A:514:ARG:HH12	1.63	0.62
1:A:525:GLN:HG3	1:A:529:ASN:O	1.99	0.62
1:A:367:SER:O	1:A:370:LYS:HE2	2.00	0.62
1:A:674:ALA:HB3	1:A:695:MET:HB3	1.80	0.62
1:A:298:PRO:HD2	1:A:299:ARG:HH11	1.65	0.62
1:B:363:ASP:HB3	1:B:372:PHE:HE1	1.65	0.62
1:B:297:GLY:HA3	1:B:299:ARG:NH1	2.15	0.61
1:B:465:ARG:HD3	1:B:471:ASP:OD2	2.00	0.61
1:A:352:ASP:O	1:A:356:PRO:HD2	2.00	0.61
1:A:341:HIS:HD2	1:A:705:GLU:HG3	1.64	0.61
1:B:551:PHE:HB3	1:B:553:TRP:NE1	2.15	0.61
1:A:306:TRP:NE1	1:B:336:MET:HG3	2.16	0.61
1:B:382:GLU:OE2	1:B:386:LYS:HG2	2.00	0.61
1:A:299:ARG:H	1:A:299:ARG:HD3	1.66	0.60
1:B:470:HIS:CB	1:B:528:GLY:HA3	2.31	0.60
1:B:511:LYS:HD3	1:B:511:LYS:C	2.26	0.60
1:A:487:GLN:HG3	1:A:488:PRO:HD2	1.84	0.60
1:B:593:ILE:HA	1:B:597:ASP:HB2	1.83	0.60
1:A:492:THR:HG21	1:A:496:PRO:HG3	1.84	0.59
1:B:684:SER:HB3	1:B:687:ILE:HD11	1.85	0.59
1:A:596:ARG:O	1:A:600:ASP:HB2	2.03	0.58
1:A:345:PRO:C	1:A:346:GLU:HG2	2.26	0.58
1:A:618:MET:HE3	1:A:625:TRP:CZ3	2.39	0.58
1:A:627:ASP:OD1	1:B:683:MET:HE2	2.02	0.58
1:A:684:SER:HB3	1:A:687:ILE:HD11	1.85	0.58
1:B:462:PHE:HB3	1:B:463:PRO:CD	2.33	0.58
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.39	0.58
1:B:338:PRO:O	1:B:340:GLN:N	2.37	0.58
1:B:349:ARG:NH1	1:B:578:GLU:OE1	2.37	0.58
1:A:571:LEU:HB2	1:A:707:GLN:NE2	2.19	0.58
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.39	0.57
1:A:696:LEU:HD22	1:B:330:ILE:HD11	1.84	0.57
1:B:684:SER:HB3	1:B:687:ILE:CD1	2.35	0.57
1:B:349:ARG:O	1:B:350:THR:HG23	2.05	0.57
1:B:473:ARG:HD2	1:B:580:SER:HB2	1.86	0.57
1:A:588:TYR:HE1	5:A:901:ARG:O	1.87	0.57
1:B:371:ARG:NH1	6:B:1032:HOH:O	2.37	0.56
1:A:425:GLN:HG2	1:A:448:TYR:CE2	2.41	0.56
1:B:610:VAL:O	1:B:614:MET:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:VAL:HG11	1:B:465:ARG:HG2	1.88	0.56
1:B:481:ARG:NH2	1:B:498:ASN:HD21	2.03	0.56
1:A:506:ILE:HD13	1:A:514:ARG:NH1	2.21	0.56
1:A:470:HIS:HB3	1:A:528:GLY:CA	2.26	0.55
1:A:397:LYS:HB2	1:A:400:GLU:HG3	1.88	0.55
1:A:551:PHE:HB3	1:A:553:TRP:NE1	2.22	0.55
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.42	0.55
1:B:478:GLN:HB2	1:B:481:ARG:CD	2.37	0.55
1:A:340:GLN:O	1:A:341:HIS:CB	2.51	0.55
1:A:414:ARG:HD3	1:A:678:TRP:CD2	2.41	0.55
1:A:608:GLU:HG3	1:A:618:MET:CE	2.30	0.54
1:B:382:GLU:O	1:B:386:LYS:HG2	2.07	0.54
1:B:304:LYS:HG2	1:B:305:ASN:N	2.21	0.54
1:B:699:ARG:HG2	1:B:699:ARG:HH11	1.72	0.54
1:A:300:PHE:CD2	1:A:313:THR:HG21	2.43	0.54
1:B:369:ILE:O	1:B:370:LYS:HB2	2.07	0.54
1:A:299:ARG:H	1:A:299:ARG:CD	2.19	0.54
1:B:478:GLN:HB2	1:B:481:ARG:CG	2.37	0.54
1:B:716:TRP:O	1:B:716:TRP:CG	2.61	0.54
1:B:482:TYR:CE2	1:B:517:PHE:HB3	2.43	0.53
1:B:328:GLU:OE1	1:B:328:GLU:N	2.38	0.53
1:B:479:LEU:HB2	1:B:566:ALA:HB3	1.91	0.53
1:A:394:TYR:CE2	1:A:577:LEU:HD21	2.44	0.53
1:A:350:THR:CG2	1:A:352:ASP:H	2.11	0.53
1:A:462:PHE:HB3	1:A:463:PRO:HD2	1.90	0.52
1:A:609:GLU:O	1:A:613:LYS:HG2	2.09	0.52
1:B:462:PHE:HB3	1:B:463:PRO:HD2	1.90	0.52
1:A:686:SER:CB	1:B:682:PRO:HB2	2.38	0.52
1:B:627:ASP:O	1:B:631:VAL:HG23	2.09	0.52
1:A:393:THR:OG1	1:A:394:TYR:N	2.42	0.52
1:A:460:THR:O	1:A:582:CYS:HA	2.10	0.52
1:B:478:GLN:HB2	1:B:481:ARG:HD2	1.91	0.51
1:A:306:TRP:CE2	1:B:336:MET:HG3	2.45	0.51
1:A:589:MET:HE3	1:A:591:THR:OG1	2.10	0.51
1:B:425:GLN:HG2	1:B:448:TYR:CE2	2.44	0.51
1:A:481:ARG:CZ	1:A:498:ASN:HD21	2.23	0.51
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.45	0.51
1:A:571:LEU:HD12	1:A:707:GLN:NE2	2.25	0.51
1:B:470:HIS:HB2	1:B:528:GLY:HA3	1.92	0.51
1:B:703:SER:HB3	6:B:1079:HOH:O	2.11	0.51
1:A:342:THR:HG22	1:A:342:THR:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:GLU:HB3	1:A:671:GLY:O	2.11	0.51
1:A:660:LYS:HE3	1:A:664:ASN:OD1	2.11	0.51
1:B:618:MET:HE3	1:B:625:TRP:CZ3	2.45	0.51
1:A:473:ARG:HD2	1:A:580:SER:O	2.10	0.50
1:B:298:PRO:HD2	1:B:299:ARG:CZ	2.41	0.50
1:B:300:PHE:O	1:B:313:THR:HG23	2.11	0.50
1:A:323:GLU:OE2	1:A:323:GLU:HA	2.12	0.50
1:A:325:GLY:O	1:A:332:MET:HG3	2.11	0.50
1:B:343:ARG:HA	1:B:343:ARG:NE	2.23	0.50
1:B:300:PHE:O	1:B:301:LEU:C	2.54	0.50
1:B:327:THR:OG1	1:B:330:ILE:HG22	2.12	0.50
1:A:507:GLN:O	1:A:507:GLN:HG2	2.13	0.49
1:B:304:LYS:O	1:B:694:GLU:HG3	2.11	0.49
1:A:336:MET:HG3	1:B:306:TRP:NE1	2.26	0.49
1:A:593:ILE:HA	1:A:597:ASP:OD2	2.13	0.49
1:B:469:LYS:O	1:B:470:HIS:CB	2.58	0.49
1:A:715:VAL:O	1:A:716:TRP:HB3	2.13	0.49
1:A:492:THR:CG2	1:A:496:PRO:HG3	2.42	0.48
1:B:470:HIS:HB3	1:B:528:GLY:HA3	1.94	0.48
1:A:301:LEU:CD1	1:B:330:ILE:HD13	2.43	0.48
1:B:462:PHE:HB2	1:B:581:ALA:HB3	1.94	0.48
1:B:481:ARG:HH21	1:B:498:ASN:HD21	1.61	0.48
1:B:659:ILE:O	1:B:663:GLU:HG3	2.13	0.48
1:A:599:CYS:O	1:A:600:ASP:C	2.56	0.48
1:A:341:HIS:CE1	1:A:343:ARG:NH2	2.82	0.48
1:A:360:GLU:O	1:A:364:GLN:HG3	2.14	0.48
1:A:299:ARG:HD3	1:A:300:PHE:H	1.79	0.48
1:B:323:GLU:HG3	1:B:340:GLN:OE1	2.13	0.48
1:B:349:ARG:HG2	1:B:349:ARG:HH11	1.79	0.48
1:A:342:THR:O	1:A:708:PRO:HD3	2.13	0.47
1:A:375:LYS:HE2	1:A:379:ASP:OD2	2.13	0.47
1:B:314:ASP:HB2	1:B:666:TYR:HE1	1.79	0.47
1:B:544:VAL:O	1:B:560:LYS:HA	2.14	0.47
1:A:451:ASN:O	1:A:451:ASN:ND2	2.47	0.47
1:A:304:LYS:NZ	1:A:309:ASP:OD1	2.38	0.47
1:A:408:ALA:HA	1:A:702:PRO:O	2.14	0.47
1:A:481:ARG:NE	1:A:498:ASN:HD21	2.12	0.47
1:A:589:MET:HA	1:A:649:VAL:O	2.14	0.47
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.49	0.47
1:B:388:ILE:O	1:B:392:SER:HA	2.14	0.47
1:B:596:ARG:O	1:B:600:ASP:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:ILE:O	1:A:663:GLU:HG3	2.14	0.47
1:A:300:PHE:HD2	1:A:313:THR:HG21	1.80	0.47
1:A:304:LYS:O	1:A:694:GLU:HB2	2.15	0.47
1:A:430:ARG:O	1:A:463:PRO:HG3	2.14	0.47
1:A:466:THR:O	1:A:467:ASP:HB2	2.13	0.47
1:B:611:ALA:O	1:B:615:ASP:N	2.48	0.47
1:A:709:ASP:HB3	1:A:711:TRP:CE2	2.50	0.47
1:A:343:ARG:HD3	1:A:571:LEU:HD13	1.97	0.47
1:B:389:GLU:HA	1:B:389:GLU:OE1	2.14	0.47
1:A:327:THR:HG23	1:A:330:ILE:CG2	2.46	0.46
1:A:547:ARG:O	1:A:639:TYR:HD2	1.98	0.46
1:A:571:LEU:HD23	1:A:571:LEU:C	2.41	0.46
1:A:341:HIS:C	1:A:343:ARG:H	2.23	0.46
1:A:503:GLU:O	1:A:507:GLN:HB2	2.15	0.46
1:A:651:HIS:CE1	1:A:683:MET:HE2	2.50	0.46
1:A:623:SER:O	1:A:624:LEU:HB2	2.15	0.46
1:A:582:CYS:O	1:A:583:PRO:C	2.58	0.46
1:A:618:MET:HA	1:A:625:TRP:CD1	2.51	0.46
1:B:482:TYR:O	1:B:498:ASN:OD1	2.33	0.46
1:A:567:VAL:HB	1:A:584:PHE:CZ	2.50	0.46
1:B:369:ILE:HG13	1:B:371:ARG:HG2	1.97	0.46
1:B:629:ALA:O	1:B:633:ILE:HG13	2.16	0.46
1:B:571:LEU:C	1:B:571:LEU:HD23	2.40	0.46
1:A:694:GLU:CG	1:B:335:ILE:HA	2.45	0.46
1:A:298:PRO:HD2	1:A:299:ARG:NH1	2.30	0.46
1:B:484:GLY:HA3	1:B:495:ASP:O	2.15	0.46
1:A:462:PHE:HB3	1:A:463:PRO:CD	2.46	0.46
1:A:551:PHE:HE1	1:A:632:GLU:HG2	1.81	0.46
1:A:332:MET:HB3	1:A:335:ILE:HG13	1.98	0.45
1:B:366:TYR:HD2	1:B:371:ARG:HB2	1.80	0.45
1:A:549:PRO:HB3	1:A:639:TYR:CE1	2.51	0.45
1:B:370:LYS:O	1:B:371:ARG:HD3	2.16	0.45
1:B:510:TRP:HE1	1:B:535:GLN:HE22	1.63	0.45
1:A:349:ARG:HA	1:A:353:GLN:OE1	2.17	0.45
1:B:297:GLY:N	1:B:300:PHE:HB2	2.31	0.45
1:B:345:PRO:O	1:B:346:GLU:HG2	2.16	0.45
1:B:412:ALA:O	1:B:418:ARG:CZ	2.64	0.45
1:A:353:GLN:O	1:A:356:PRO:HG2	2.16	0.45
1:A:678:TRP:HA	4:A:900:H4B:N1	2.31	0.45
1:A:479:LEU:HD22	1:A:566:ALA:HB1	1.98	0.45
1:A:494:GLY:O	1:A:496:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:THR:O	1:A:506:ILE:HG13	2.17	0.45
1:A:358:ALA:O	1:A:362:LEU:HG	2.17	0.45
1:A:565:PRO:HG2	1:A:565:PRO:O	2.16	0.45
1:A:638:LEU:HD13	1:A:650:ASP:HB3	1.99	0.45
1:A:709:ASP:HB2	1:A:712:ASN:OD1	2.17	0.44
1:A:445:HIS:CD2	1:A:445:HIS:C	2.95	0.44
1:B:469:LYS:NZ	1:B:469:LYS:HB3	2.32	0.44
1:A:323:GLU:OE2	1:B:329:HIS:ND1	2.50	0.44
1:A:365:TYR:O	1:A:368:SER:OG	2.33	0.44
1:A:456:ARG:HD3	6:A:1053:HOH:O	2.18	0.44
1:A:548:HIS:HB2	1:A:554:PHE:CD1	2.53	0.44
1:B:402:ILE:O	1:B:406:LYS:HG3	2.18	0.44
1:B:619:ARG:HG2	1:B:620:LYS:HG3	1.99	0.44
1:A:451:ASN:O	1:A:452:LYS:HB2	2.17	0.44
1:B:348:VAL:HG21	1:B:466:THR:O	2.18	0.44
1:B:512:ALA:HA	1:B:513:PRO:HD3	1.82	0.44
1:A:470:HIS:HB2	1:A:527:ASN:O	2.17	0.44
1:B:565:PRO:HB3	1:B:588:TYR:CZ	2.53	0.44
1:A:569:ASN:H	1:A:569:ASN:HD22	1.65	0.44
1:B:322:LEU:HB2	1:B:699:ARG:HB2	1.99	0.44
1:B:551:PHE:HB3	1:B:553:TRP:CE2	2.52	0.44
1:A:335:ILE:HD13	1:B:694:GLU:HB3	2.00	0.44
1:B:569:ASN:H	1:B:569:ASN:HD22	1.66	0.44
1:A:341:HIS:NE2	1:A:343:ARG:NH1	2.66	0.43
1:A:355:PHE:N	1:A:356:PRO:HD2	2.33	0.43
1:A:548:HIS:ND1	1:A:549:PRO:HD2	2.33	0.43
1:A:428:ASP:OD1	1:A:428:ASP:C	2.62	0.43
1:A:553:TRP:HZ3	1:A:557:LEU:HD11	1.84	0.43
1:B:570:MET:HE3	1:B:706:TYR:CD1	2.53	0.43
1:A:472:PHE:O	1:A:473:ARG:HG2	2.18	0.43
1:B:678:TRP:HA	4:B:920:H4B:N1	2.33	0.43
1:A:545:PRO:HD2	1:A:644:ASP:OD1	2.18	0.43
1:A:682:PRO:HB2	1:B:686:SER:OG	2.17	0.43
1:A:442:ILE:O	1:A:446:VAL:HG23	2.19	0.43
1:A:344:LYS:HD3	1:A:346:GLU:CG	2.38	0.43
1:B:397:LYS:HD2	6:B:1096:HOH:O	2.18	0.43
1:A:341:HIS:NE2	1:A:343:ARG:CZ	2.82	0.42
1:A:339:SER:C	1:A:341:HIS:H	2.27	0.42
1:A:560:LYS:HG2	1:A:561:TRP:N	2.33	0.42
1:B:298:PRO:HG2	1:B:299:ARG:HD3	2.01	0.42
1:B:592:GLU:OE2	5:B:921:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:PRO:HG2	1:B:299:ARG:CD	2.49	0.42
1:B:668:CYS:SG	1:B:669:ARG:N	2.93	0.42
1:A:337:LEU:C	1:A:339:SER:H	2.26	0.42
1:A:384:VAL:HG13	1:A:394:TYR:CD1	2.54	0.42
1:A:633:ILE:O	1:A:636:ALA:HB3	2.20	0.42
1:B:375:LYS:HE2	1:B:375:LYS:HA	2.01	0.42
1:B:547:ARG:NH2	1:B:643:SER:HB3	2.34	0.42
1:B:470:HIS:HA	6:B:1075:HOH:O	2.19	0.42
1:B:479:LEU:HD22	1:B:566:ALA:HB1	2.00	0.42
1:B:487:GLN:NE2	1:B:493:LEU:HB2	2.33	0.42
1:B:551:PHE:CE1	1:B:614:MET:HE3	2.54	0.42
1:A:322:LEU:HD13	1:A:699:ARG:NH2	2.34	0.42
1:A:326:CYS:SG	1:A:331:CYS:HA	2.59	0.42
1:A:362:LEU:HD11	1:A:384:VAL:HG21	2.02	0.42
1:A:391:THR:O	1:A:392:SER:HB2	2.20	0.42
1:A:684:SER:HB3	1:A:687:ILE:CD1	2.50	0.42
1:B:589:MET:HA	1:B:649:VAL:O	2.19	0.42
1:A:402:ILE:HA	1:A:426:VAL:HG21	2.02	0.42
1:A:434:THR:HB	6:A:978:HOH:O	2.20	0.42
1:A:488:PRO:C	1:A:490:GLY:H	2.28	0.42
1:B:348:VAL:O	1:B:349:ARG:O	2.38	0.42
1:A:582:CYS:N	1:A:583:PRO:CD	2.82	0.41
1:B:366:TYR:CD2	1:B:369:ILE:HD11	2.55	0.41
1:B:478:GLN:HA	1:B:566:ALA:O	2.20	0.41
1:B:495:ASP:HA	1:B:496:PRO:HD3	1.92	0.41
1:A:512:ALA:HA	1:A:513:PRO:HD3	1.86	0.41
1:B:414:ARG:HD3	1:B:678:TRP:CD2	2.55	0.41
1:B:420:GLN:HB3	6:B:995:HOH:O	2.19	0.41
1:A:345:PRO:HB3	1:A:713:THR:HG22	2.02	0.41
1:A:455:LEU:HB2	1:A:647:THR:HB	2.01	0.41
1:B:380:ARG:HD2	1:B:380:ARG:O	2.20	0.41
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.50	0.41
1:B:536:ILE:O	1:B:537:PRO:C	2.63	0.41
1:B:388:ILE:O	1:B:392:SER:N	2.53	0.41
1:A:569:ASN:HD22	1:A:569:ASN:N	2.18	0.41
1:A:299:ARG:HG2	1:A:300:PHE:HD1	1.86	0.41
1:B:565:PRO:HG2	1:B:565:PRO:O	2.20	0.41
1:B:595:VAL:O	1:B:599:CYS:HB2	2.21	0.41
1:A:338:PRO:O	1:A:339:SER:HB2	2.21	0.41
1:A:700:LEU:O	1:A:703:SER:HB3	2.21	0.41
1:B:348:VAL:HB	1:B:349:ARG:H	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:ARG:HD3	1:B:517:PHE:CE1	2.56	0.41
1:B:556:ASP:OD1	1:B:556:ASP:N	2.54	0.41
1:B:614:MET:CE	1:B:632:GLU:HG3	2.51	0.41
1:A:299:ARG:O	1:A:317:HIS:HE1	2.04	0.41
1:A:396:LEU:HG	1:A:577:LEU:CD1	2.51	0.41
1:B:299:ARG:HD3	1:B:299:ARG:N	2.34	0.41
1:B:351:LYS:HE2	1:B:351:LYS:HB3	1.76	0.41
1:A:516:ARG:HG3	6:A:1083:HOH:O	2.21	0.40
1:B:650:ASP:OD2	1:B:652:HIS:HB2	2.21	0.40
1:A:631:VAL:O	1:A:635:ILE:HG13	2.22	0.40
1:A:694:GLU:CG	1:B:335:ILE:HD13	2.46	0.40
1:A:666:TYR:HA	1:A:671:GLY:H	1.86	0.40
1:B:342:THR:O	1:B:343:ARG:CG	2.67	0.40
1:B:457:SER:HA	1:B:585:SER:O	2.21	0.40
1:B:621:THR:O	1:B:624:LEU:HD23	2.20	0.40
1:B:666:TYR:CE1	1:B:671:GLY:HA2	2.56	0.40
1:A:537:PRO:O	1:A:540:LEU:HB2	2.22	0.40
1:A:556:ASP:N	1:A:556:ASP:OD1	2.54	0.40
1:A:374:SER:O	1:A:377:HIS:HB3	2.22	0.40
1:A:640:SER:O	1:A:641:PHE:C	2.63	0.40
1:B:347:ASP:OD1	1:B:348:VAL:N	2.55	0.40
1:B:536:ILE:HA	1:B:537:PRO:HD2	1.91	0.40
1:B:612:LYS:O	1:B:615:ASP:N	2.54	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	418/420 (100%)	373 (89%)	39 (9%)	6 (1%)	9 17
1	B	418/420 (100%)	366 (88%)	39 (9%)	13 (3%)	3 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	836/840 (100%)	739 (88%)	78 (9%)	19 (2%)	5 8

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	341	HIS
1	A	347	ASP
1	A	467	ASP
1	B	299	ARG
1	B	339	SER
1	B	343	ARG
1	B	349	ARG
1	B	301	LEU
1	B	341	HIS
1	B	345	PRO
1	B	467	ASP
1	B	470	HIS
1	A	333	GLY
1	A	343	ARG
1	A	393	THR
1	B	346	GLU
1	B	455	LEU
1	B	608	GLU
1	B	348	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	375/375 (100%)	337 (90%)	38 (10%)	7 15
1	B	375/375 (100%)	345 (92%)	30 (8%)	11 24
All	All	750/750 (100%)	682 (91%)	68 (9%)	9 19

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	315	THR
1	A	321	THR
1	A	327	THR
1	A	332	MET
1	A	336	MET
1	A	337	LEU
1	A	341	HIS
1	A	343	ARG
1	A	346	GLU
1	A	350	THR
1	A	371	ARG
1	A	375	LYS
1	A	452	LYS
1	A	477	SER
1	A	479	LEU
1	A	487	GLN
1	A	489	ASP
1	A	492	THR
1	A	499	VAL
1	A	503	GLU
1	A	538	PRO
1	A	552	ASP
1	A	556	ASP
1	A	560	LYS
1	A	569	ASN
1	A	580	SER
1	A	600	ASP
1	A	601	ASN
1	A	602	SER
1	A	622	SER
1	A	628	GLN
1	A	632	GLU
1	A	645	LYS
1	A	660	LYS
1	A	683	MET
1	A	701	THR
1	A	713	THR
1	A	715	VAL
1	B	299	ARG
1	B	303	VAL
1	B	321	THR
1	B	336	MET
1	B	342	THR

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Mol	Chain	Res	Type
1	B	343	ARG
1	B	346	GLU
1	B	351	LYS
1	B	352	ASP
1	B	375	LYS
1	B	382	GLU
1	B	389	GLU
1	B	457	SER
1	B	465	ARG
1	B	469	LYS
1	B	471	ASP
1	B	479	LEU
1	B	487	GLN
1	B	489	ASP
1	B	491	SER
1	B	493	LEU
1	B	511	LYS
1	B	527	ASN
1	B	532	GLU
1	B	569	ASN
1	B	573	GLU
1	B	580	SER
1	B	622	SER
1	B	643	SER
1	B	701	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	HIS
1	A	341	HIS
1	A	364	GLN
1	A	440	ASN
1	A	451	ASN
1	A	470	HIS
1	A	478	GLN
1	A	498	ASN
1	A	500	GLN
1	A	569	ASN
1	A	628	GLN
1	A	634	ASN
1	A	707	GLN

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Mol	Chain	Res	Type
1	B	353	GLN
1	B	451	ASN
1	B	478	GLN
1	B	487	GLN
1	B	498	ASN
1	B	529	ASN
1	B	535	GLN
1	B	569	ASN
1	B	634	ASN
1	B	661	HIS
1	B	664	ASN
1	B	707	GLN
1	B	712	ASN
1	B	714	HIS

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 oligosaccharides 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
3	HEM	A	800	1	50,50,50	1.50	4 (8%)	67,82,82	1.16	7 (10%)
5	ARG	A	901	-	10,11,11	0.61	0	9,13,13	0.25	0
4	H4B	A	900	-	17,18,18	1.67	5 (29%)	14,26,26	1.89	3 (21%)
3	HEM	B	800	1	50,50,50	1.56	7 (14%)	67,82,82	1.29	7 (10%)
5	ARG	B	921	-	10,11,11	0.66	0	9,13,13	0.38	0
4	H4B	B	920	-	17,18,18	1.48	4 (23%)	14,26,26	1.92	2 (14%)

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
3	HEM	A	800	1	-	6/14/54/54	-
5	ARG	A	901	-	-	0/11/11/11	-
4	H4B	A	900	-	-	0/8/17/17	0/2/2/2
3	HEM	B	800	1	-	7/14/54/54	-
5	ARG	B	921	-	-	0/11/11/11	-
4	H4B	B	920	-	-	0/8/17/17	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	HEM	FE-NC	6.72	2.17	1.95
3	B	800	HEM	FE-NC	5.83	2.14	1.95
4	A	900	H4B	C4A-N5	3.87	1.46	1.37
3	B	800	HEM	FE-NA	3.18	2.05	1.95
3	A	800	HEM	FE-NA	3.15	2.05	1.95
4	B	920	H4B	C4A-N5	2.95	1.44	1.37
3	B	800	HEM	CAB-C3B	-2.89	1.39	1.47
3	A	800	HEM	CAB-C3B	-2.84	1.39	1.47
4	A	900	H4B	C8A-N1	2.77	1.40	1.36
4	A	900	H4B	C6-N5	2.64	1.52	1.47
3	B	800	HEM	CAC-C3C	-2.53	1.40	1.47
4	B	920	H4B	C8A-N1	2.51	1.40	1.36
4	B	920	H4B	C6-N5	2.48	1.51	1.47
3	B	800	HEM	C4C-NC	-2.46	1.35	1.39
3	B	800	HEM	C1D-C2D	2.39	1.49	1.44
3	A	800	HEM	CAC-C3C	-2.27	1.41	1.47
4	A	900	H4B	C7-N8	2.27	1.48	1.46
4	A	900	H4B	C4-N3	2.20	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	800	HEM	C4B-NB	2.13	1.43	1.38
4	B	920	H4B	C4-N3	2.03	1.42	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	920	H4B	C2-N1-C8A	5.18	122.50	113.36
4	A	900	H4B	C2-N1-C8A	5.18	122.50	113.36
3	A	800	HEM	CHD-C4C-NC	-3.64	120.49	124.45
3	B	800	HEM	C3B-C2B-C1B	3.39	108.96	106.41
4	B	920	H4B	N3-C2-N1	-3.35	117.20	123.32
3	B	800	HEM	CMC-C2C-C1C	3.28	130.51	124.73
4	A	900	H4B	N3-C2-N1	-3.21	117.45	123.32
3	B	800	HEM	C3B-C4B-NB	3.15	111.73	109.47
3	A	800	HEM	CAA-C2A-C1A	3.07	130.94	124.94
3	B	800	HEM	CHD-C4C-NC	-3.00	121.18	124.45
3	B	800	HEM	C4B-C3B-C2B	-2.95	104.57	107.28
3	B	800	HEM	C3C-C2C-C1C	-2.82	104.38	107.05
3	A	800	HEM	CAD-C3D-C4D	2.63	129.28	124.70
3	A	800	HEM	CMA-C3A-C4A	2.58	129.34	125.42
3	B	800	HEM	CHC-C1C-NC	-2.50	121.73	124.45
4	A	900	H4B	O10-C10-C9	-2.43	105.76	109.77
3	A	800	HEM	CAA-C2A-C3A	-2.35	121.81	127.07
3	A	800	HEM	CAD-C3D-C2D	-2.10	123.92	127.87
3	A	800	HEM	CHD-C4C-C3C	2.08	128.72	125.21

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	800	HEM	C1A-C2A-CAA-CBA
3	A	800	HEM	C2B-C3B-CAB-CBB
3	A	800	HEM	C4B-C3B-CAB-CBB
3	B	800	HEM	C2B-C3B-CAB-CBB
3	B	800	HEM	C1A-C2A-CAA-CBA
3	B	800	HEM	C4B-C3B-CAB-CBB
3	A	800	HEM	C4D-C3D-CAD-CBD
3	B	800	HEM	CAD-CBD-CGD-O2D
3	B	800	HEM	CAD-CBD-CGD-O1D
3	B	800	HEM	CAA-CBA-CGA-O2A
3	B	800	HEM	CAA-CBA-CGA-O1A
3	A	800	HEM	CAD-CBD-CGD-O2D

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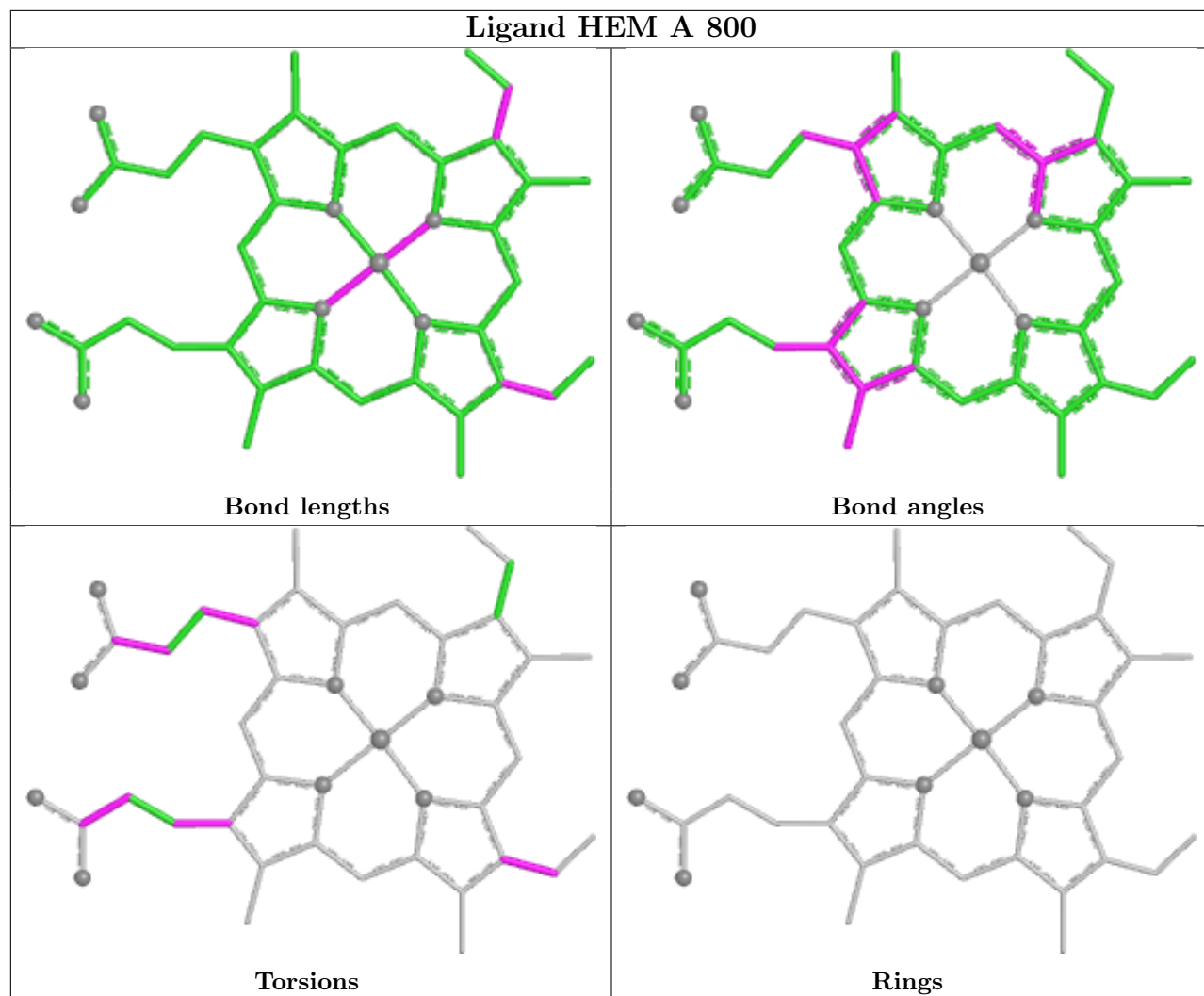
Mol	Chain	Res	Type	Atoms
3	A	800	HEM	CAA-CBA-CGA-O2A

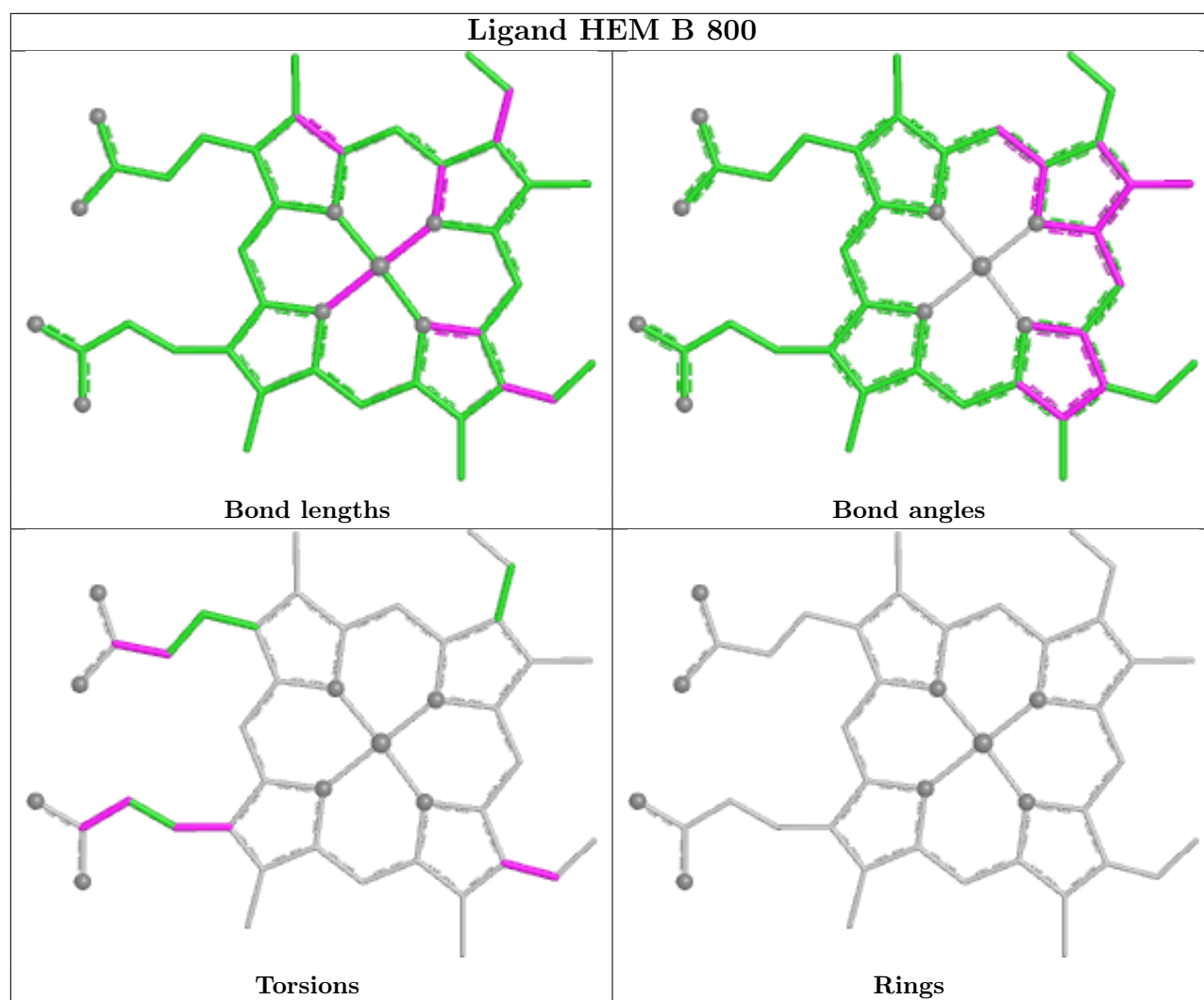
There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	901	ARG	1	0
4	A	900	H4B	1	0
3	B	800	HEM	1	0
5	B	921	ARG	1	0
4	B	920	H4B	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	420/420 (100%)	-0.47	4 (0%) 79 76	12, 33, 73, 136	0
1	B	420/420 (100%)	-0.57	2 (0%) 87 85	13, 30, 72, 130	0
All	All	840/840 (100%)	-0.52	6 (0%) 84 81	12, 32, 73, 136	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	298	PRO	4.7
1	B	468	GLY	3.1
1	A	716	TRP	2.3
1	A	342	THR	2.2
1	A	470	HIS	2.1
1	B	297	GLY	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](#)

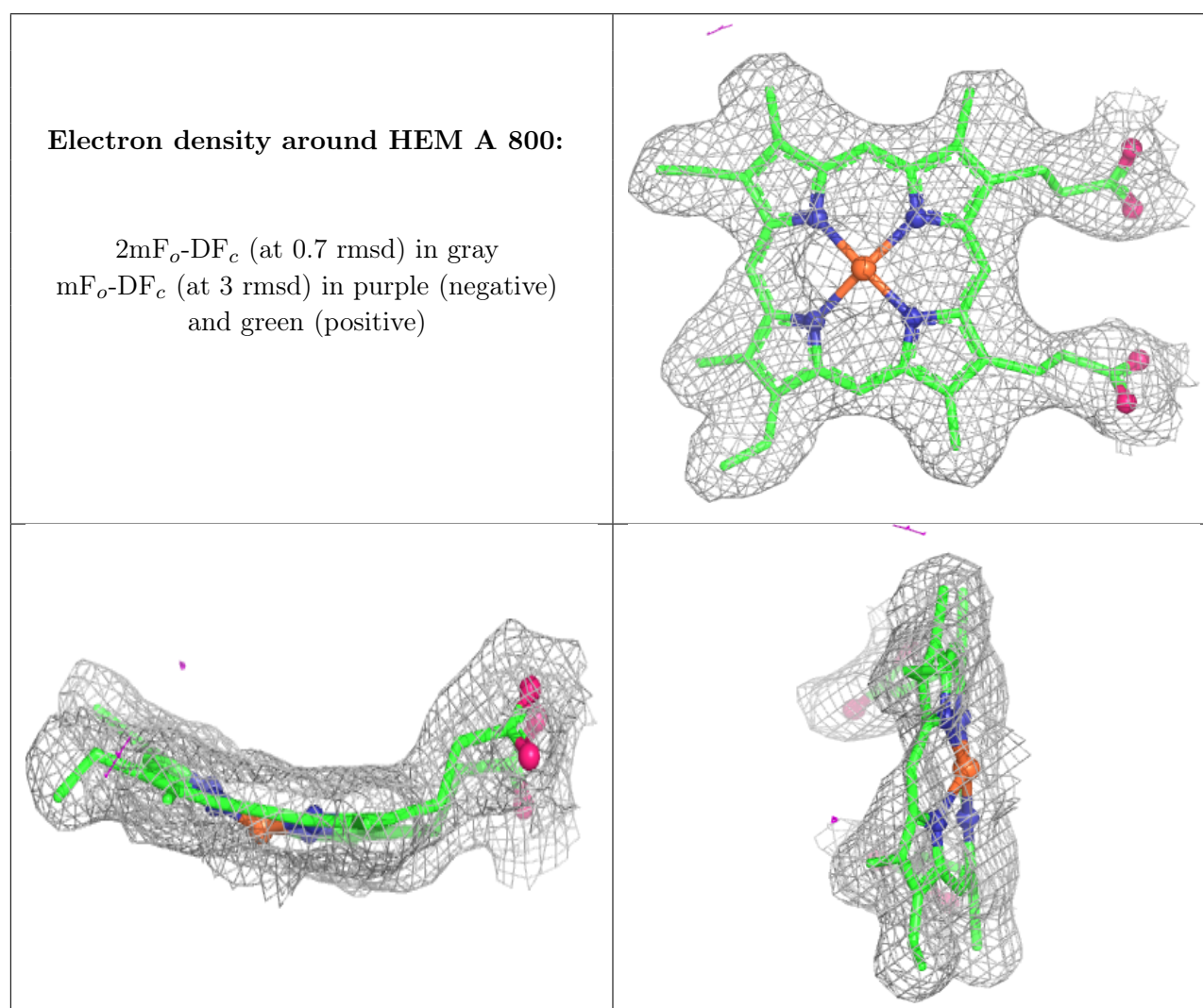
There are no oligosaccharides in this entry.

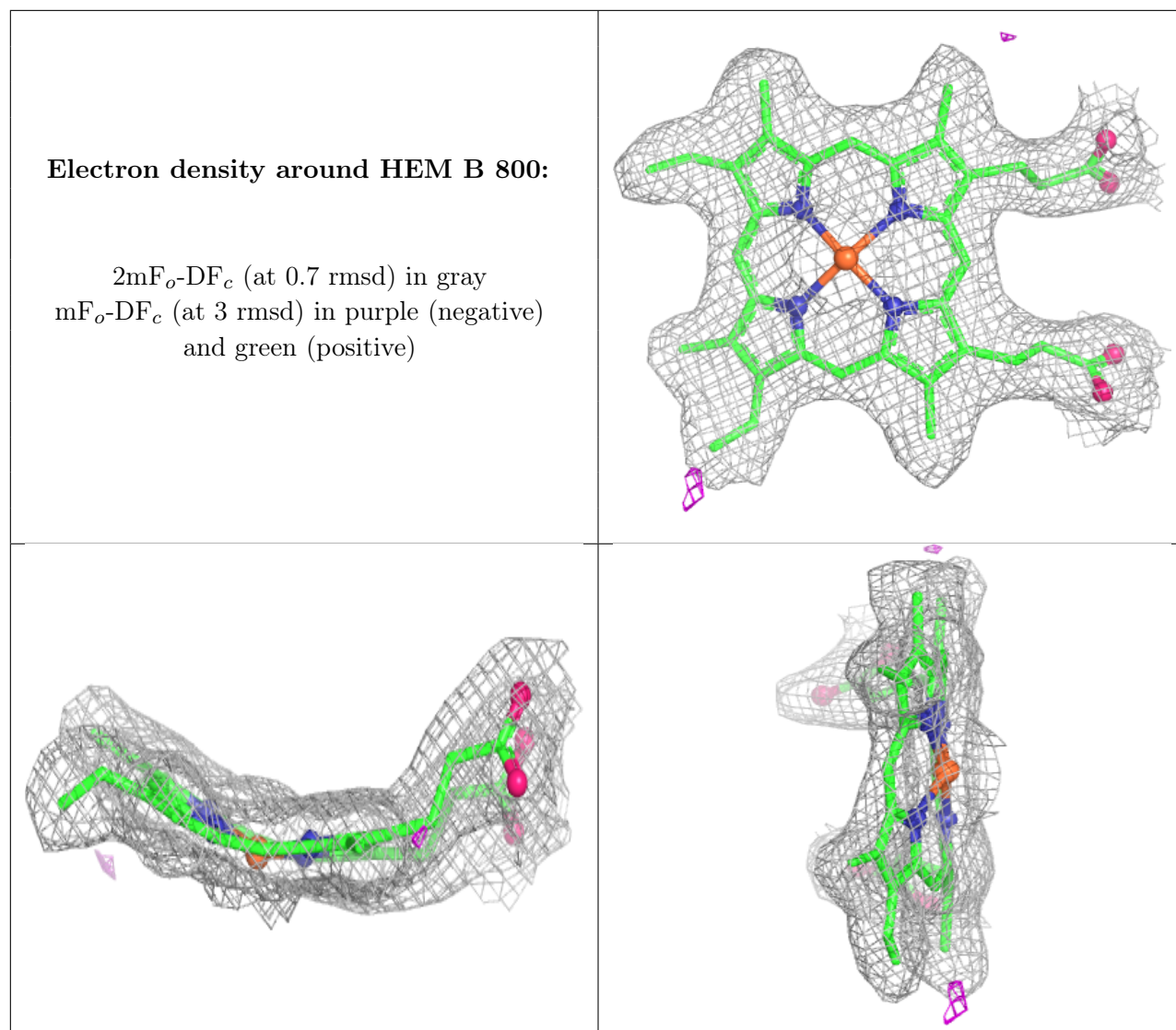
6.4 Ligands [i](#)

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
5	ARG	A	901	12/12	0.95	0.06	23,29,38,42	0
5	ARG	B	921	12/12	0.95	0.06	18,27,48,53	0
4	H4B	A	900	17/17	0.96	0.06	13,23,32,35	0
4	H4B	B	920	17/17	0.96	0.04	9,16,26,29	0
3	HEM	A	800	43/43	0.97	0.06	10,24,36,39	0
3	HEM	B	800	43/43	0.98	0.05	9,20,28,37	0
2	ZN	A	950	1/1	0.99	0.03	29,29,29,29	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.