



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:49 PM UTC

PDB ID : 1DMJ / pdb_00001dmj
Title : BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN
COMPLEXED WITH 5,6-CYCLIC-TETRAHYDROPTERIDINE
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Munch, U.; Schnabel, J.; Martasek, P.; Masters, B.S.; Strobel, H.; Poulos, T.;
Matter, H.; Pfeleiderer, W.; Schmidt, H.H.
Deposited on : 1999-12-14
Resolution : 2.35 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)

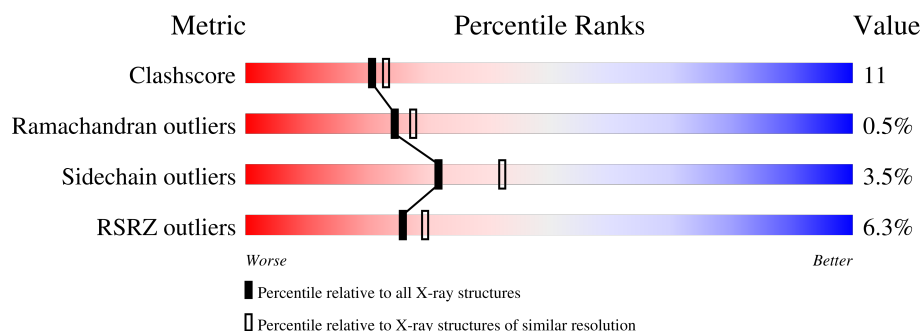
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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))
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	444	
1	B	444	

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7168 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3302	2099	584	603	16			
1	B	414	Total	C	N	O	S	0	0	0
			3291	2092	582	601	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	conflict	UNP P29473
B	100	ARG	CYS	conflict	UNP P29473

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



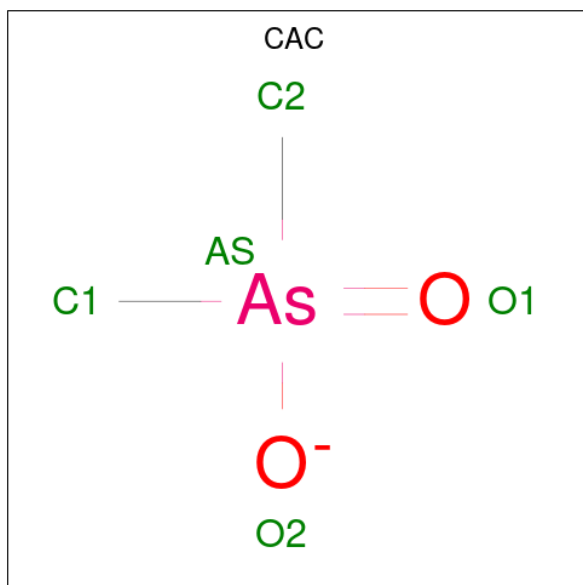
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

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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		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is CACODYLATE ION (CCD ID: CAC) (formula: $C_2H_6AsO_2$).



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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

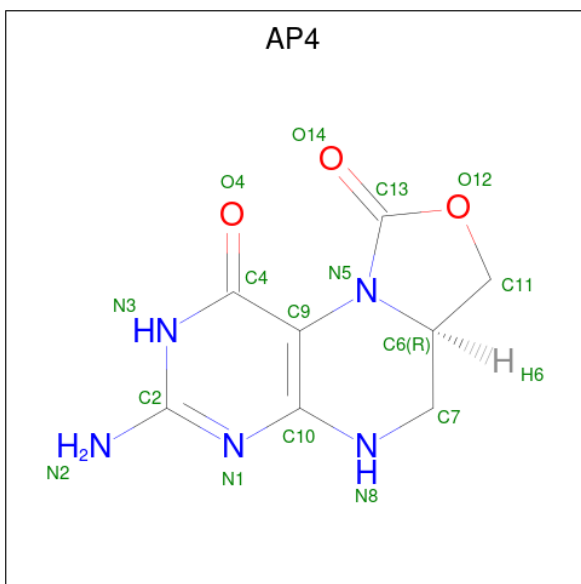
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 6 is 7-AMINO-3,3A,4,5-TETRAHYDRO-8H-2-OXA-5,6,8,9B-TETRAAZA-CYCLOPENTA[A]NAPHTHALENE-1,9-DIONE (CCD ID: AP4) (formula: C₈H₉N₅O₃).



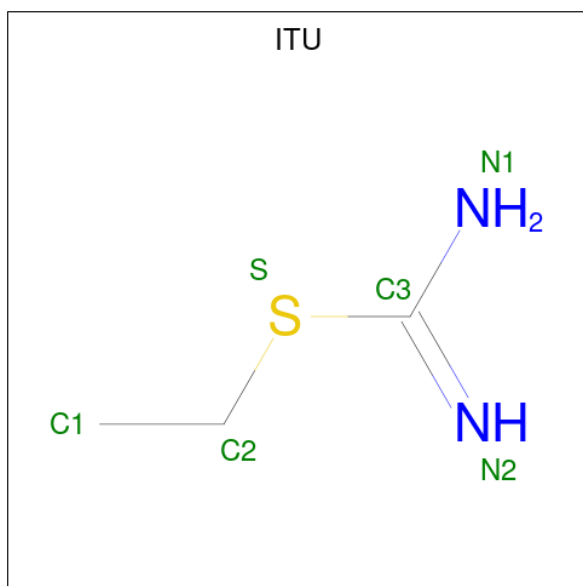
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			16	8	5	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			16	8	5	3		

- Molecule 7 is ETHYLISOTHIOUREA (CCD ID: ITU) (formula: $C_3H_8N_2S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	S	0	0
			6	3	2	1		
7	B	1	Total	C	N	S	0	0
			6	3	2	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

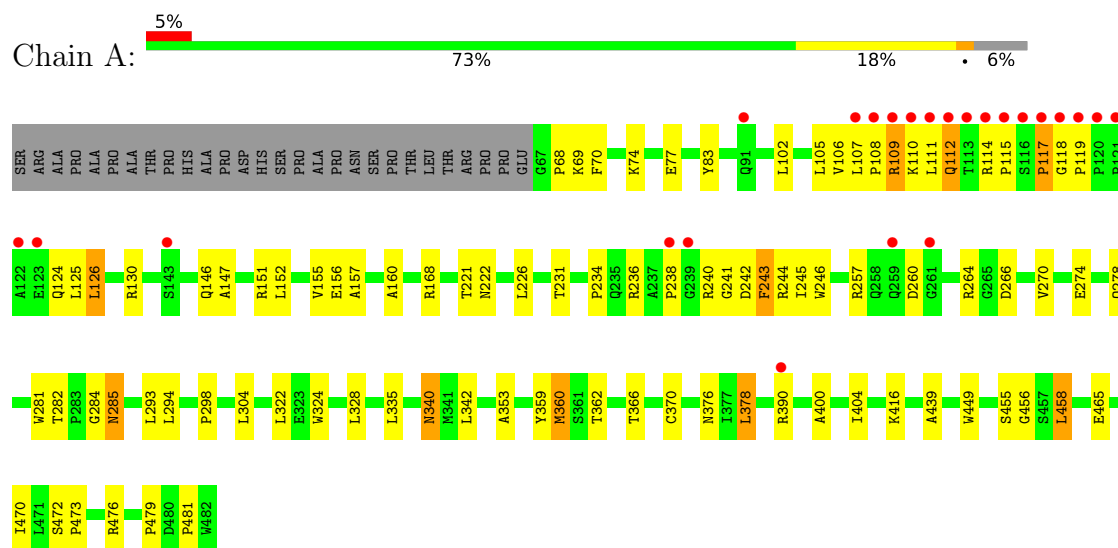
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	214	Total	O	0	0
			214	214		
9	B	196	Total	O	0	0
			196	196		

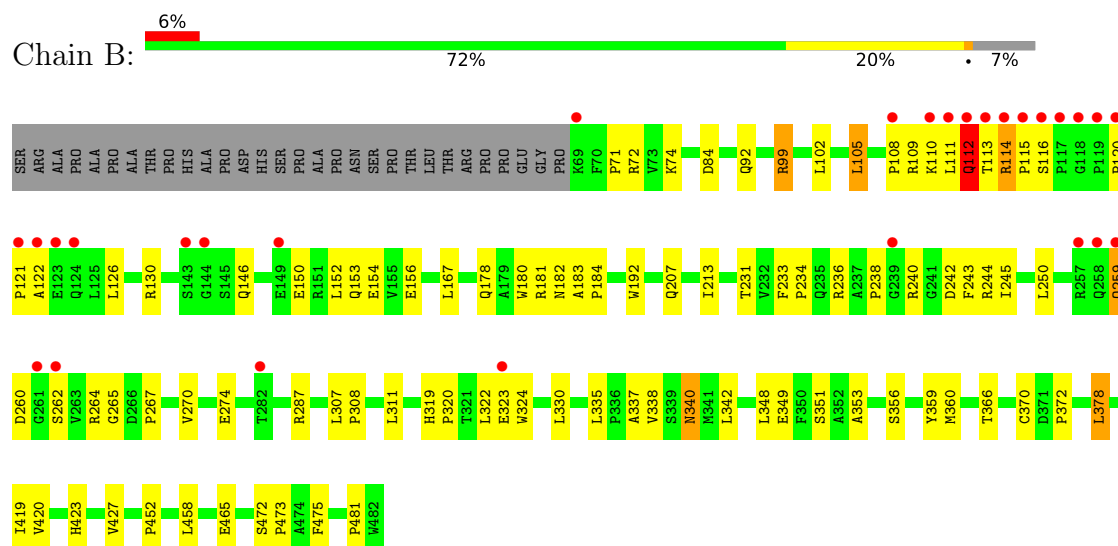
3 Residue-property plots [i](#)

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



• Molecule 1: NITRIC OXIDE SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.90Å 106.49Å 156.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.38 – 2.35 48.38 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.6 (48.38-2.35) 93.8 (48.38-2.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.43 (at 2.34Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.187 , 0.228 0.188 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7168	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 4.38% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, ZN, AP4, GOL, HEM, ITU, ACT

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	0.42	0/3397	0.94	13/4631 (0.3%)
1	B	0.45	1/3385 (0.0%)	0.95	10/4614 (0.2%)
All	All	0.44	1/6782 (0.0%)	0.94	23/9245 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	122	ALA	CA-CB	-9.50	1.38	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	MET	N-CA-C	-7.84	96.46	109.24
1	A	360	MET	N-CA-C	-7.46	97.05	109.07
1	A	109	ARG	N-CA-C	7.42	121.18	109.39
1	B	243	PHE	N-CA-C	-6.96	97.90	109.46
1	A	439	ALA	N-CA-C	6.86	118.83	111.36
1	B	452	PRO	N-CA-C	6.39	116.60	110.47
1	A	245	ILE	N-CA-C	-6.37	98.56	107.80
1	A	284	GLY	N-CA-C	-6.34	105.18	112.79
1	A	335	LEU	N-CA-C	6.23	119.91	108.69
1	B	240	ARG	N-CA-C	6.13	117.54	108.60
1	B	335	LEU	N-CA-C	6.13	119.72	108.69
1	B	245	ILE	N-CA-C	-6.05	98.41	107.37
1	B	475	PHE	N-CA-C	-5.77	99.83	109.24
1	A	226	LEU	N-CA-C	5.69	117.64	110.24
1	A	243	PHE	N-CA-C	-5.67	100.04	109.46
1	B	183	ALA	CA-C-N	5.61	125.45	119.28
1	B	183	ALA	C-N-CA	5.61	125.45	119.28
1	B	359	TYR	N-CA-C	5.21	117.85	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	TYR	N-CA-C	5.18	118.14	110.48
1	A	282	THR	CA-C-N	5.16	125.14	120.03
1	A	282	THR	C-N-CA	5.16	125.14	120.03
1	A	266	ASP	CA-C-N	5.05	125.33	119.47
1	A	266	ASP	C-N-CA	5.05	125.33	119.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3302	0	3215	80	0
1	B	3291	0	3205	68	0
2	A	8	0	6	1	0
2	B	8	0	6	0	0
3	A	3	0	0	1	0
3	B	3	0	0	0	0
4	A	1	0	0	0	0
5	A	43	0	30	1	0
5	B	43	0	30	0	0
6	A	16	0	8	1	0
6	B	16	0	8	0	0
7	A	6	0	7	0	0
7	B	6	0	7	1	0
8	A	6	0	8	1	0
8	B	6	0	8	1	0
9	A	214	0	0	4	0
9	B	196	0	0	10	0
All	All	7168	0	6538	147	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 11.

All (147) 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:115:PRO:HD3	1:A:479:PRO:HG2	1.16	1.15
1:A:105:LEU:HB2	1:A:108:PRO:HG3	1.47	0.96
1:B:108:PRO:HB3	1:B:111:LEU:HD13	1.54	0.89
1:A:119:PRO:HG3	1:A:238:PRO:HB2	1.57	0.86
1:B:250:LEU:HD22	9:B:2962:HOH:O	1.77	0.84
1:B:116:SER:O	1:B:238:PRO:HA	1.80	0.81
1:A:111:LEU:HD21	1:A:470:ILE:HD13	1.64	0.80
1:A:111:LEU:HD22	1:A:476:ARG:NH1	1.95	0.80
1:B:114:ARG:HA	1:B:114:ARG:HH11	1.46	0.78
1:A:115:PRO:HD3	1:A:479:PRO:CG	2.10	0.72
1:A:119:PRO:HG3	1:A:238:PRO:CB	2.20	0.71
1:A:111:LEU:CD2	1:A:470:ILE:HD13	2.22	0.69
1:B:152:LEU:O	1:B:156:GLU:HG3	1.94	0.67
1:B:366:THR:O	1:B:370:CYS:HB2	1.95	0.67
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.78	0.65
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.61	0.65
1:B:338:VAL:HG23	7:B:2800:ITU:H11	1.78	0.65
1:A:69:LYS:O	1:A:69:LYS:HG2	1.95	0.65
1:A:126:LEU:HD11	1:A:156:GLU:HB3	1.78	0.65
1:A:126:LEU:HD12	1:A:130:ARG:HE	1.61	0.65
1:B:114:ARG:HH11	1:B:115:PRO:HD3	1.61	0.64
1:A:378:LEU:HB2	9:A:2083:HOH:O	1.97	0.64
1:B:236:ARG:HD2	1:B:242:ASP:OD2	1.98	0.64
1:A:146:GLN:NE2	1:A:147:ALA:H	1.96	0.63
1:A:105:LEU:CB	1:A:108:PRO:HG3	2.26	0.63
1:B:423:HIS:O	1:B:427:VAL:HG23	2.00	0.62
1:A:77:GLU:HG3	1:B:372:PRO:HG2	1.81	0.61
1:A:274:GLU:O	1:A:278:GLN:HG3	1.98	0.61
1:B:378:LEU:HB2	9:B:3020:HOH:O	1.99	0.61
1:A:168:ARG:HD2	9:A:2002:HOH:O	2.01	0.60
1:A:111:LEU:CD2	1:A:476:ARG:HH12	2.15	0.60
1:B:113:THR:HG21	1:B:342:LEU:CD1	2.33	0.59
1:A:111:LEU:CD2	1:A:476:ARG:NH1	2.64	0.59
1:B:126:LEU:O	1:B:130:ARG:HG3	2.02	0.59
1:B:114:ARG:HA	1:B:114:ARG:NH1	2.16	0.58
1:B:308:PRO:HD2	1:B:311:LEU:HD12	1.86	0.58
1:A:465:GLU:HB3	1:B:105:LEU:HD22	1.84	0.58
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.44	0.58
1:A:115:PRO:C	1:A:117:PRO:HD3	2.29	0.57
2:A:1860:ACT:H2	5:A:1500:HEM:HMB3	1.87	0.56
1:B:114:ARG:HD3	1:B:115:PRO:CD	2.35	0.56
1:A:70:PHE:O	1:B:109:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PRO:O	1:A:117:PRO:HD3	2.07	0.55
1:B:207:GLN:HB2	9:B:3056:HOH:O	2.07	0.55
8:B:2880:GOL:H32	9:B:2968:HOH:O	2.07	0.55
1:A:106:VAL:C	1:A:108:PRO:HD3	2.31	0.55
1:A:151:ARG:HD3	1:A:168:ARG:HE	1.72	0.55
1:B:260:ASP:C	1:B:262:SER:H	2.15	0.54
1:A:472:SER:HA	1:A:473:PRO:C	2.33	0.54
1:A:340:ASN:H	1:A:340:ASN:HD22	1.56	0.53
1:A:111:LEU:HD21	1:A:470:ILE:HG21	1.88	0.53
1:B:108:PRO:CB	1:B:111:LEU:HB2	2.39	0.53
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.91	0.53
1:B:182:ASN:O	1:B:184:PRO:HD3	2.10	0.52
1:A:257:ARG:HG3	1:A:257:ARG:NH1	2.24	0.52
1:B:472:SER:HA	1:B:473:PRO:C	2.34	0.52
1:A:240:ARG:HD2	1:A:241:GLY:O	2.10	0.52
1:A:342:LEU:C	1:A:342:LEU:HD23	2.35	0.52
1:B:114:ARG:NH1	1:B:115:PRO:HD3	2.24	0.52
1:B:72:ARG:NH1	9:B:3010:HOH:O	2.42	0.51
1:B:99:ARG:HB2	1:B:99:ARG:HH11	1.74	0.51
1:A:108:PRO:HG2	9:A:1906:HOH:O	2.10	0.51
1:A:111:LEU:O	1:A:112:GLN:C	2.53	0.51
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.93	0.51
1:A:109:ARG:O	1:A:110:LYS:HD2	2.11	0.50
1:A:376:ASN:ND2	9:A:2083:HOH:O	2.34	0.50
1:A:115:PRO:CD	1:A:479:PRO:HG2	2.11	0.50
1:A:152:LEU:O	1:A:156:GLU:HG2	2.11	0.50
1:B:340:ASN:HD22	1:B:340:ASN:H	1.58	0.50
1:A:244:ARG:NH2	1:A:481:PRO:HD3	2.27	0.50
1:A:324:TRP:HB2	3:A:950:CAC:C2	2.41	0.50
1:A:146:GLN:H	1:A:146:GLN:CD	2.19	0.50
1:A:360:MET:HE3	1:A:362:THR:OG1	2.12	0.50
1:A:270:VAL:O	1:A:274:GLU:HG3	2.12	0.49
1:B:114:ARG:HD3	1:B:115:PRO:HD2	1.93	0.49
1:A:111:LEU:HD22	1:A:476:ARG:HH11	1.73	0.48
1:B:231:THR:O	1:B:353:ALA:HA	2.14	0.48
1:A:231:THR:O	1:A:353:ALA:HA	2.14	0.48
1:B:74:LYS:O	1:B:465:GLU:HG3	2.13	0.48
1:B:244:ARG:NH2	1:B:481:PRO:HD3	2.28	0.48
1:A:74:LYS:O	1:A:465:GLU:HG3	2.13	0.48
1:B:337:ALA:HB2	1:B:356:SER:HB3	1.96	0.48
1:B:113:THR:HG21	1:B:342:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HB3	1:A:130:ARG:NH2	2.29	0.47
1:B:111:LEU:O	1:B:112:GLN:O	2.31	0.47
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.50	0.47
1:A:264:ARG:HH11	1:A:264:ARG:HG3	1.79	0.47
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.50	0.47
1:B:114:ARG:HD3	1:B:115:PRO:HD3	1.95	0.47
1:B:213:ILE:HG21	9:B:2962:HOH:O	2.14	0.47
1:A:69:LYS:O	1:A:69:LYS:CG	2.63	0.47
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.98	0.46
1:B:178:GLN:HE22	1:B:181:ARG:HH11	1.63	0.46
1:A:114:ARG:HD2	1:A:479:PRO:HG3	1.97	0.46
1:B:113:THR:HG21	1:B:342:LEU:HD13	1.97	0.46
1:A:117:PRO:O	1:A:118:GLY:C	2.59	0.45
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.46	0.45
1:A:400:ALA:O	1:A:404:ILE:HG13	2.17	0.45
1:B:307:LEU:HD11	9:B:2971:HOH:O	2.16	0.45
1:A:340:ASN:HD22	1:A:340:ASN:N	2.14	0.45
1:B:259:GLN:HG3	1:B:260:ASP:H	1.81	0.45
1:B:419:ILE:HG13	1:B:420:VAL:N	2.32	0.45
1:B:342:LEU:C	1:B:342:LEU:HD23	2.42	0.45
1:B:270:VAL:O	1:B:274:GLU:HG3	2.16	0.45
1:B:113:THR:HG23	1:B:349:GLU:OE2	2.17	0.44
1:A:126:LEU:HB3	1:A:130:ARG:HH21	1.83	0.44
1:B:150:GLU:O	1:B:154:GLU:HG3	2.17	0.44
1:A:236:ARG:HG2	1:A:242:ASP:OD2	2.18	0.44
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.58	0.43
1:A:77:GLU:HG3	1:B:372:PRO:CG	2.46	0.43
1:B:71:PRO:HG2	1:B:84:ASP:HB3	1.99	0.43
1:B:213:ILE:CG2	9:B:2962:HOH:O	2.66	0.43
1:B:108:PRO:HB3	1:B:111:LEU:HB2	2.01	0.43
1:B:264:ARG:HH11	1:B:287:ARG:HG3	1.83	0.43
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.53	0.43
1:B:236:ARG:HD2	1:B:242:ASP:CG	2.44	0.43
1:A:366:THR:O	1:A:370:CYS:HB2	2.19	0.43
8:A:1880:GOL:H32	9:B:2961:HOH:O	2.17	0.43
1:B:323:GLU:HG2	1:B:324:TRP:N	2.34	0.43
1:A:294:LEU:HD13	1:A:304:LEU:HD13	2.00	0.43
1:B:120:PRO:HA	1:B:121:PRO:HD3	1.93	0.43
1:B:319:HIS:CG	1:B:320:PRO:HD2	2.54	0.42
1:A:111:LEU:HD22	1:A:476:ARG:HH12	1.70	0.42
1:B:340:ASN:HD22	1:B:340:ASN:N	2.13	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ASN:H	1:B:340:ASN:ND2	2.17	0.42
1:A:126:LEU:HD12	1:A:130:ARG:NE	2.30	0.42
1:B:105:LEU:HD23	1:B:105:LEU:N	2.34	0.42
1:B:109:ARG:O	1:B:110:LYS:HG3	2.20	0.42
1:B:109:ARG:C	1:B:110:LYS:HG3	2.45	0.42
1:A:109:ARG:HD3	1:A:109:ARG:HA	1.86	0.42
1:A:236:ARG:HH11	1:A:236:ARG:HG3	1.84	0.42
1:A:157:ALA:O	1:A:160:ALA:HB3	2.20	0.41
1:A:68:PRO:HD2	1:A:83:TYR:CZ	2.55	0.41
1:B:233:PHE:HB3	1:B:234:PRO:HD2	2.01	0.41
1:B:265:GLY:O	1:B:267:PRO:HD3	2.20	0.41
1:A:281:TRP:HB2	1:A:304:LEU:HD21	2.01	0.41
1:A:107:LEU:N	1:A:108:PRO:HD3	2.36	0.41
1:A:285:ASN:N	1:A:285:ASN:HD22	2.18	0.41
1:A:455:SER:O	1:A:458:LEU:HB2	2.21	0.41
1:A:151:ARG:O	1:A:155:VAL:HG23	2.21	0.40
1:A:110:LYS:O	1:A:111:LEU:C	2.64	0.40
1:A:234:PRO:HB2	1:A:243:PHE:CE1	2.57	0.40
1:A:236:ARG:HG3	1:A:236:ARG:NH1	2.37	0.40
1:A:449:TRP:HA	6:A:1650:AP4:N1	2.37	0.40
1:A:221:THR:O	1:A:222:ASN:C	2.63	0.40
1:A:264:ARG:HG3	1:A:264:ARG:NH1	2.36	0.40
1:A:456:GLY:HA3	9:B:3076:HOH:O	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	414/444 (93%)	390 (94%)	22 (5%)	2 (0%)	24	27
1	B	412/444 (93%)	384 (93%)	26 (6%)	2 (0%)	24	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	826/888 (93%)	774 (94%)	48 (6%)	4 (0%)	24 27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	PRO
1	B	112	GLN
1	B	259	GLN
1	A	112	GLN

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	354/377 (94%)	341 (96%)	13 (4%)	30 40
1	B	353/377 (94%)	341 (97%)	12 (3%)	32 43
All	All	707/754 (94%)	682 (96%)	25 (4%)	32 42

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	LEU
1	A	124	GLN
1	A	125	LEU
1	A	126	LEU
1	A	260	ASP
1	A	285	ASN
1	A	293	LEU
1	A	328	LEU
1	A	340	ASN
1	A	378	LEU
1	A	390	ARG
1	A	416	LYS
1	A	458	LEU
1	B	92	GLN

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Mol	Chain	Res	Type
1	B	99	ARG
1	B	102	LEU
1	B	105	LEU
1	B	112	GLN
1	B	114	ARG
1	B	146	GLN
1	B	153	GLN
1	B	330	LEU
1	B	340	ASN
1	B	378	LEU
1	B	458	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	112	GLN
1	A	128	GLN
1	A	146	GLN
1	A	207	GLN
1	A	278	GLN
1	A	285	ASN
1	A	296	GLN
1	A	340	ASN
1	A	376	ASN
1	A	410	HIS
1	A	413	GLN
1	A	437	GLN
1	A	468	ASN
1	B	178	GLN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	278	GLN
1	B	340	ASN
1	B	405	ASN
1	B	410	HIS
1	B	437	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 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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	A	1860	-	3,3,3	0.90	0	3,3,3	0.83	0
6	AP4	A	1650	-	16,18,18	4.24	7 (43%)	16,27,27	2.82	7 (43%)
6	AP4	B	2650	-	16,18,18	4.17	7 (43%)	16,27,27	2.86	7 (43%)
2	ACT	A	1850	-	3,3,3	1.06	0	3,3,3	0.73	0
8	GOL	A	1880	-	5,5,5	0.15	0	5,5,5	0.20	0
7	ITU	A	1800	-	4,5,5	2.00	1 (25%)	3,5,5	3.34	1 (33%)
2	ACT	B	2860	-	3,3,3	0.95	0	3,3,3	0.74	0
5	HEM	A	1500	1	50,50,50	1.09	3 (6%)	67,82,82	1.09	3 (4%)
3	CAC	A	950	1	0,2,4	-	-	0,1,6	-	-
7	ITU	B	2800	-	4,5,5	2.63	1 (25%)	3,5,5	3.08	1 (33%)
3	CAC	B	950	1	0,2,4	-	-	0,1,6	-	-
8	GOL	B	2880	-	5,5,5	0.20	0	5,5,5	0.20	0
2	ACT	B	2850	-	3,3,3	0.88	0	3,3,3	0.79	0
5	HEM	B	2500	1	50,50,50	1.09	3 (6%)	67,82,82	1.21	4 (5%)

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
6	AP4	A	1650	-	-	-	0/3/3/3
6	AP4	B	2650	-	-	-	0/3/3/3
8	GOL	A	1880	-	-	0/4/4/4	-
7	ITU	A	1800	-	-	0/3/3/3	-
5	HEM	A	1500	1	-	2/14/54/54	-
8	GOL	B	2880	-	-	0/4/4/4	-
7	ITU	B	2800	-	-	0/3/3/3	-
5	HEM	B	2500	1	-	2/14/54/54	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1650	AP4	C7-C6	-9.86	1.41	1.52
6	B	2650	AP4	C7-C6	-9.74	1.41	1.52
6	B	2650	AP4	C13-N5	8.45	1.52	1.39
6	A	1650	AP4	C13-N5	8.33	1.52	1.39
6	B	2650	AP4	O12-C13	6.65	1.43	1.35
6	A	1650	AP4	O12-C13	6.55	1.43	1.35
6	A	1650	AP4	C6-N5	5.21	1.53	1.47
7	B	2800	ITU	C3-S	5.19	1.81	1.75
6	A	1650	AP4	C7-N8	-4.62	1.41	1.46
6	B	2650	AP4	C6-N5	4.59	1.52	1.47
6	B	2650	AP4	C7-N8	-4.28	1.42	1.46
7	A	1800	ITU	C3-S	3.90	1.79	1.75
6	A	1650	AP4	C10-N1	3.11	1.41	1.36
6	B	2650	AP4	C10-N1	3.09	1.40	1.36
5	A	1500	HEM	CAB-C3B	-2.60	1.40	1.47
5	B	2500	HEM	FE-NB	2.47	2.02	1.94
6	B	2650	AP4	O12-C11	-2.43	1.41	1.45
5	A	1500	HEM	CAC-C3C	-2.41	1.41	1.47
6	A	1650	AP4	O12-C11	-2.28	1.41	1.45
5	B	2500	HEM	FE-NC	2.20	2.02	1.95
5	B	2500	HEM	CAB-C3B	-2.03	1.42	1.47
5	A	1500	HEM	FE-NC	2.02	2.01	1.95

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	2650	AP4	C6-N5-C13	-6.52	105.50	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1650	AP4	C6-N5-C13	-6.27	105.71	111.10
7	A	1800	ITU	C2-S-C3	5.77	109.15	103.15
7	B	2800	ITU	C2-S-C3	5.30	108.66	103.15
6	A	1650	AP4	C2-N1-C10	4.17	120.71	113.36
6	B	2650	AP4	C9-C4-N3	4.14	118.22	110.94
5	B	2500	HEM	C3B-C4B-NB	4.13	112.44	109.47
6	B	2650	AP4	C2-N1-C10	4.11	120.61	113.36
6	A	1650	AP4	C9-C4-N3	4.01	118.00	110.94
6	B	2650	AP4	O12-C11-C6	3.72	109.31	105.36
6	A	1650	AP4	O12-C11-C6	3.71	109.29	105.36
6	B	2650	AP4	O14-C13-N5	3.67	132.73	128.62
6	A	1650	AP4	O14-C13-N5	3.63	132.68	128.62
5	A	1500	HEM	C3B-C4B-NB	3.21	111.77	109.47
6	B	2650	AP4	O4-C4-C9	-2.78	120.78	127.62
5	A	1500	HEM	CMD-C2D-C1D	2.78	129.38	125.03
6	A	1650	AP4	O4-C4-C9	-2.73	120.91	127.62
6	A	1650	AP4	O12-C13-O14	-2.72	119.29	122.53
5	B	2500	HEM	CMC-C2C-C1C	2.63	129.36	124.73
5	B	2500	HEM	C4B-C3B-C2B	-2.59	104.89	107.28
6	B	2650	AP4	O12-C13-O14	-2.59	119.44	122.53
5	A	1500	HEM	C4D-ND-C1D	-2.02	102.81	105.21
5	B	2500	HEM	CMA-C3A-C4A	2.01	128.47	125.42

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1500	HEM	CAD-CBD-CGD-O2D
5	A	1500	HEM	CAD-CBD-CGD-O1D
5	B	2500	HEM	CAA-CBA-CGA-O2A
5	B	2500	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

7 monomers are involved in 6 short contacts:

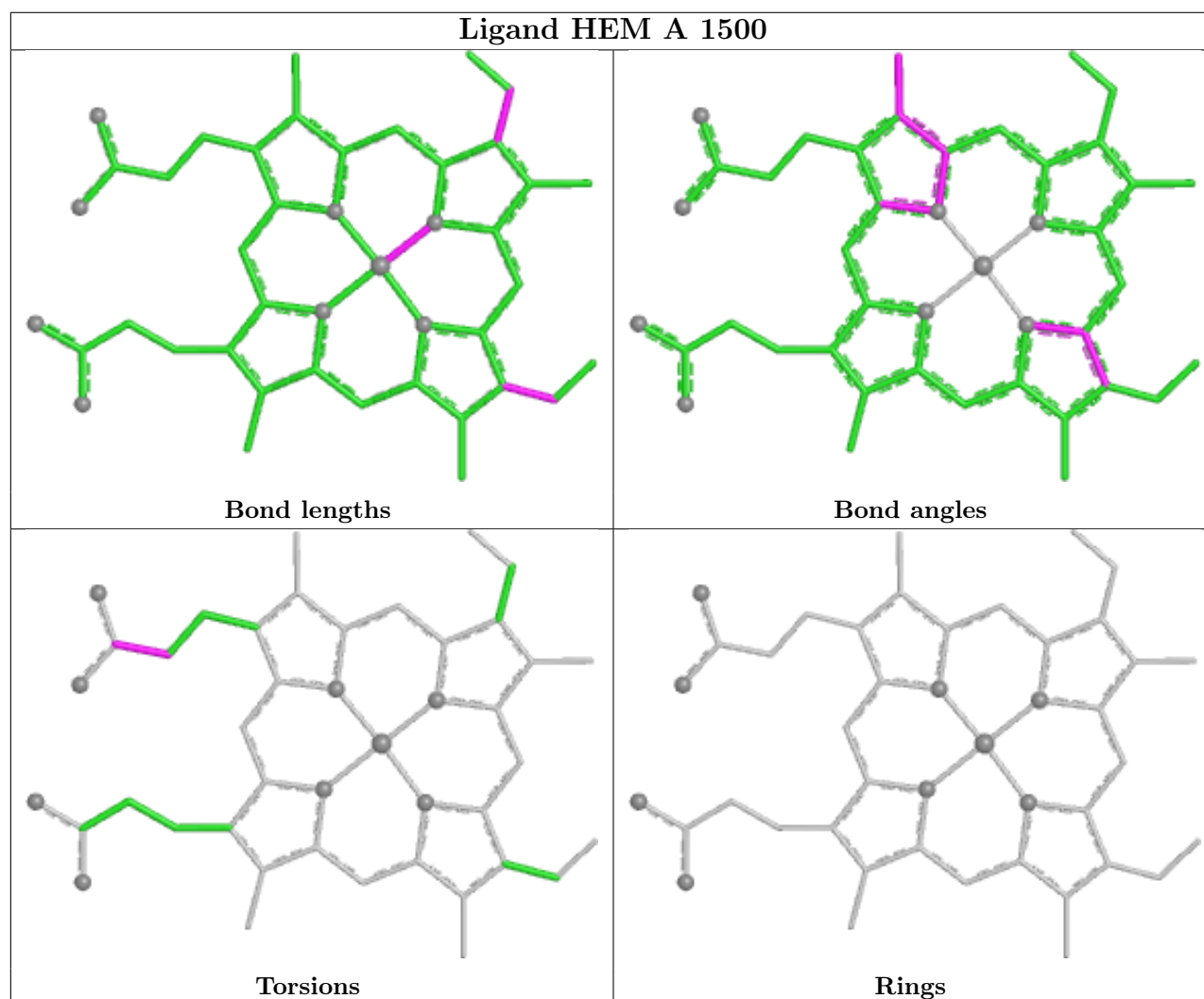
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1860	ACT	1	0
6	A	1650	AP4	1	0
8	A	1880	GOL	1	0
5	A	1500	HEM	1	0
3	A	950	CAC	1	0

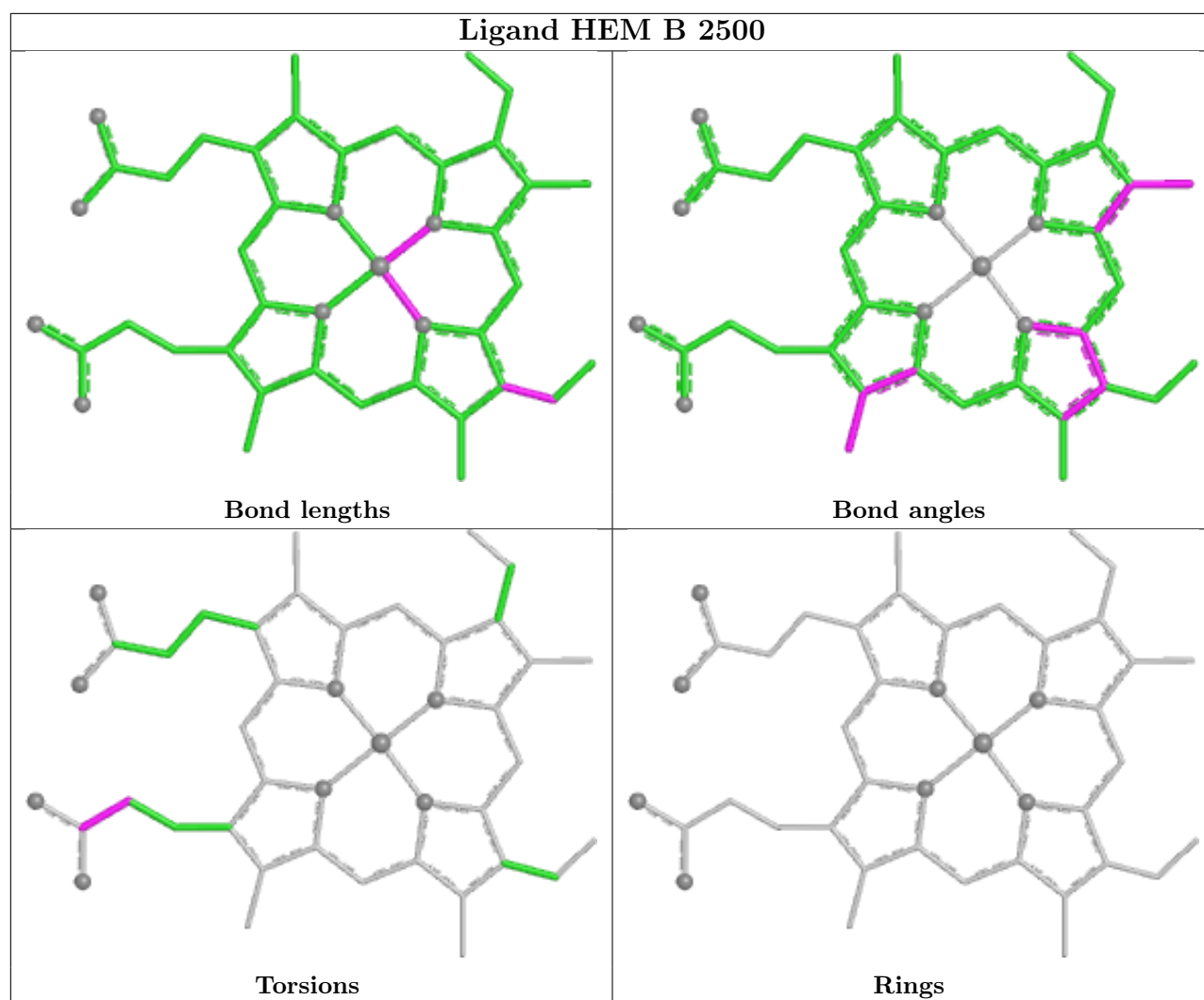
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	2800	ITU	1	0
8	B	2880	GOL	1	0

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	416/444 (93%)	0.15	24 (5%) 29 33	17, 28, 59, 100	0
1	B	414/444 (93%)	0.24	28 (6%) 23 26	16, 30, 63, 100	0
All	All	830/888 (93%)	0.19	52 (6%) 26 29	16, 29, 62, 100	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	115	PRO	9.4
1	A	119	PRO	7.8
1	A	113	THR	7.6
1	B	113	THR	7.1
1	A	111	LEU	7.0
1	B	111	LEU	6.9
1	B	117	PRO	6.4
1	B	121	PRO	6.0
1	A	110	LYS	5.9
1	A	120	PRO	5.8
1	B	119	PRO	5.8
1	A	114	ARG	5.6
1	B	115	PRO	5.5
1	B	120	PRO	5.2
1	B	118	GLY	5.1
1	A	117	PRO	4.8
1	B	116	SER	4.5
1	B	112	GLN	4.3
1	A	118	GLY	4.3
1	B	114	ARG	4.1
1	A	121	PRO	4.0
1	A	109	ARG	3.9
1	A	108	PRO	3.8
1	A	112	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	110	LYS	3.7
1	B	239	GLY	3.5
1	A	122	ALA	3.3
1	B	262	SER	3.1
1	A	239	GLY	3.0
1	A	238	PRO	3.0
1	B	122	ALA	2.8
1	B	123	GLU	2.7
1	B	258	GLN	2.7
1	B	261	GLY	2.7
1	A	116	SER	2.6
1	A	143	SER	2.6
1	B	257	ARG	2.3
1	A	261	GLY	2.3
1	A	390	ARG	2.3
1	B	143	SER	2.3
1	B	69	LYS	2.3
1	A	91	GLN	2.3
1	A	123	GLU	2.2
1	A	259	GLN	2.2
1	B	259	GLN	2.2
1	B	108	PRO	2.1
1	B	149	GLU	2.1
1	B	144	GLY	2.1
1	B	282	THR	2.1
1	B	323	GLU	2.0
1	B	124	GLN	2.0
1	A	107	LEU	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,

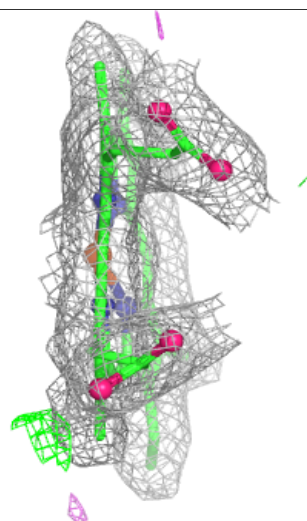
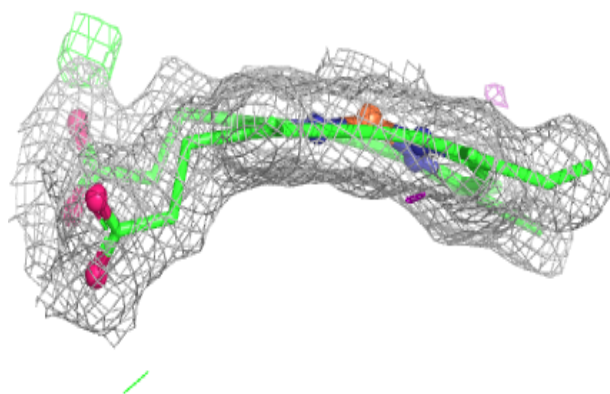
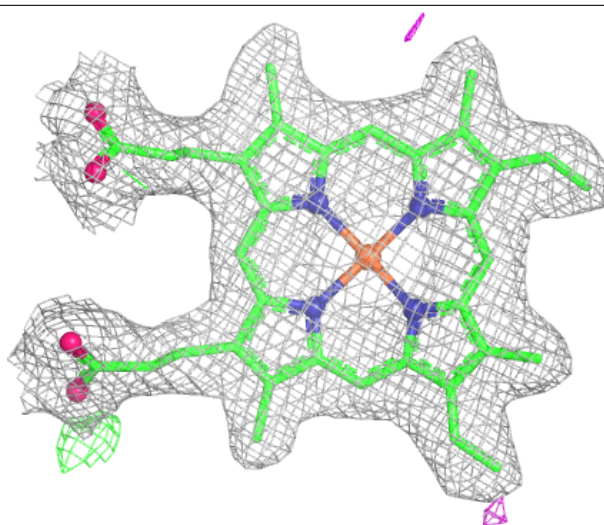
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

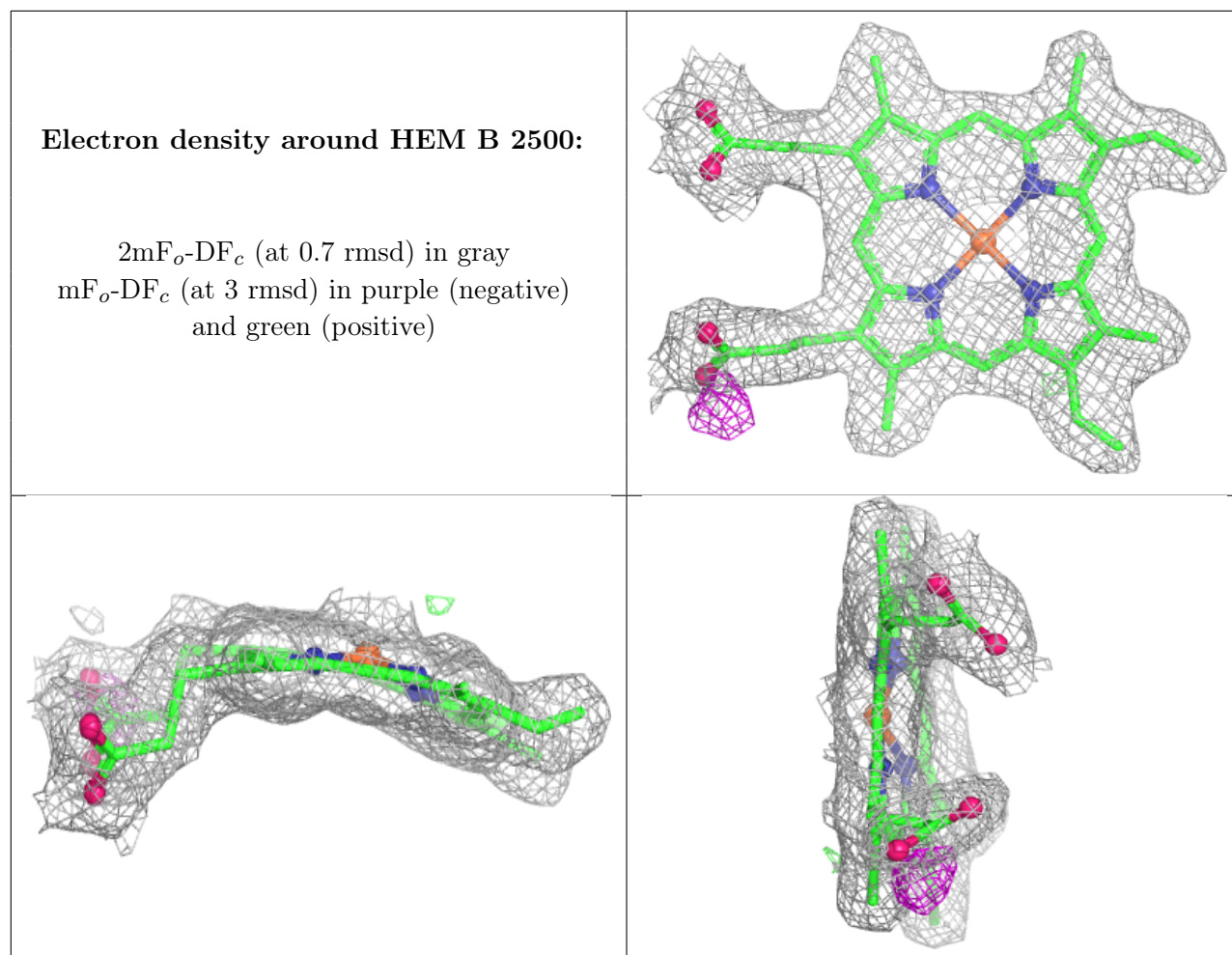
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	GOL	A	1880	6/6	0.86	0.22	51,52,53,55	0
8	GOL	B	2880	6/6	0.89	0.12	33,34,38,44	0
2	ACT	A	1860	4/4	0.93	0.08	32,34,34,35	0
3	CAC	A	950	3/5	0.93	0.14	41,41,47,52	0
2	ACT	B	2860	4/4	0.94	0.09	25,27,28,31	0
6	AP4	A	1650	16/16	0.95	0.06	16,21,23,23	0
6	AP4	B	2650	16/16	0.95	0.07	20,22,26,27	0
2	ACT	B	2850	4/4	0.96	0.10	23,24,25,26	0
2	ACT	A	1850	4/4	0.97	0.06	24,26,29,29	0
3	CAC	B	950	3/5	0.97	0.12	46,46,48,52	0
7	ITU	A	1800	6/6	0.98	0.07	21,23,24,25	0
5	HEM	A	1500	43/43	0.98	0.06	15,19,31,36	0
5	HEM	B	2500	43/43	0.98	0.07	17,22,28,37	0
4	ZN	A	900	1/1	0.99	0.02	23,23,23,23	0
7	ITU	B	2800	6/6	0.99	0.04	16,21,23,23	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 1500:

$2mF_o-DF_c$ (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.