



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 12:12 PM EDT

PDB ID : 1DF1 / pdb_00001df1
Title : MURINE INOSOXY DIMER WITH ISOTHIOUREA BOUND IN THE ACTIVE SITE
Authors : Crane, B.R.; Rosenfeld, R.J.; Arvai, A.S.; Ghosh, D.K.; Ghosh, S.; Tainer, J.A.; Stuehr, D.J.; Getzoff, E.D.
Deposited on : 1999-11-16
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

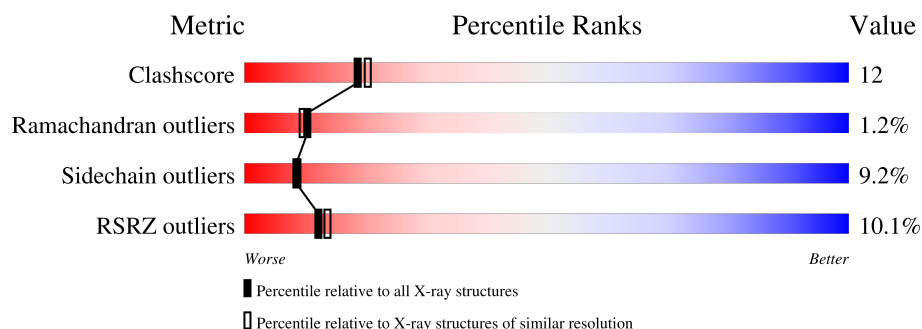
1 Overall quality at a glance

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	423	
1	B	423	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ITU	B	1899	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7198 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.

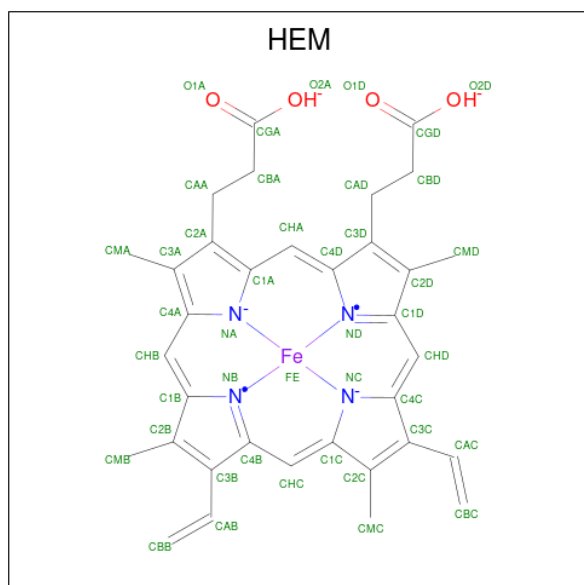
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3423	2194	590	618	21			
1	B	420	Total	C	N	O	S	0	0	0
			3423	2194	590	618	21			

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

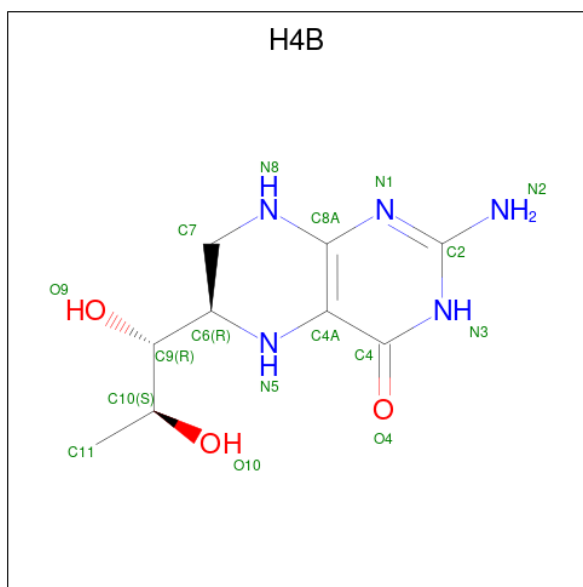
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



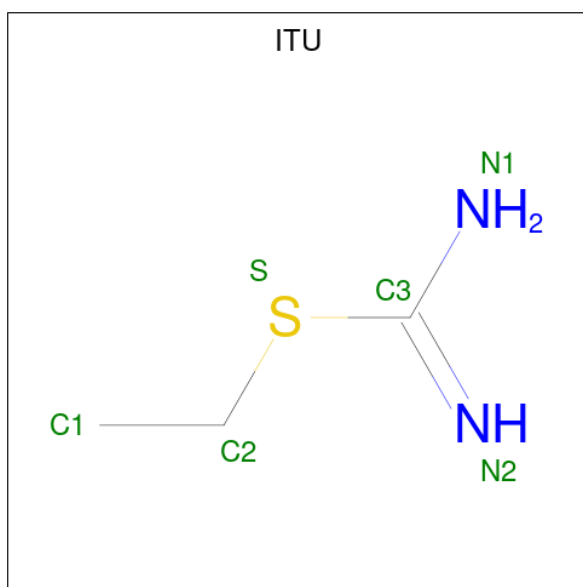
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



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

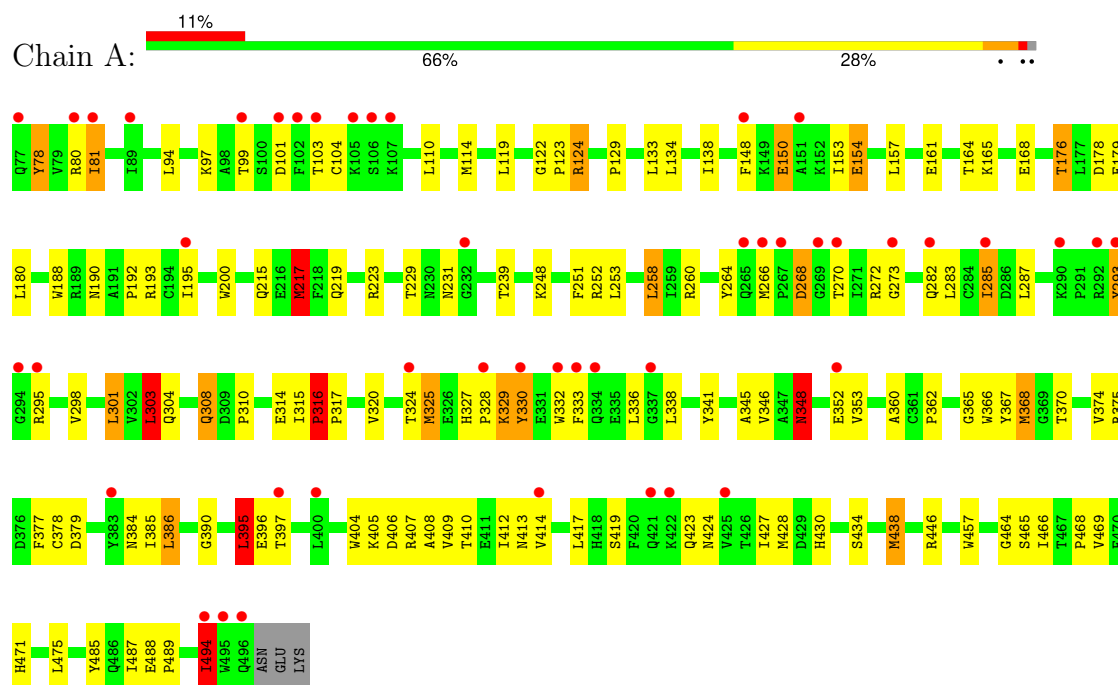
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	107	Total	O	0	0
			107	107		
6	B	111	Total	O	0	0
			111	111		

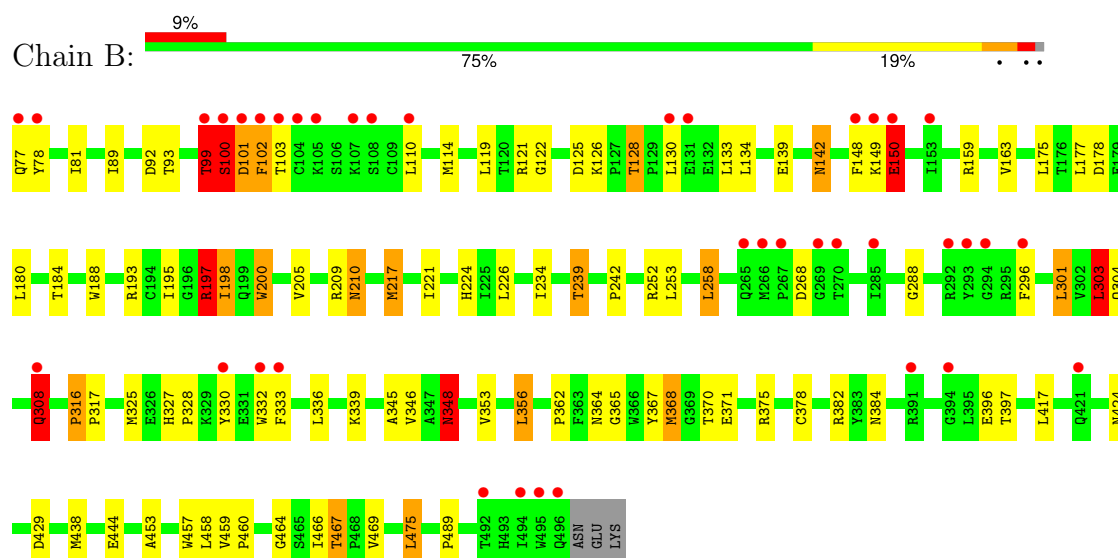
3 Residue-property plots

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



• Molecule 1: NITRIC OXIDE SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	214.46Å 214.46Å 112.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.35 20.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-2.35) 92.2 (20.00-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.35Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.223 , 0.298 0.238 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.881	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.2	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	0.93	EDS
Total number of atoms	7198	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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, ITU, HEM, H4B

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	0.70	4/3523 (0.1%)	1.16	29/4789 (0.6%)
1	B	0.70	1/3523 (0.0%)	1.16	30/4789 (0.6%)
All	All	0.70	5/7046 (0.1%)	1.16	59/9578 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	438	MET	SD-CE	-5.98	1.64	1.79
1	A	368	MET	SD-CE	5.89	1.94	1.79
1	A	217	MET	SD-CE	-5.17	1.66	1.79
1	B	205	VAL	CA-CB	5.10	1.60	1.54
1	A	494	ILE	CA-CB	5.08	1.59	1.53

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	488	GLU	CA-C-N	8.08	128.53	119.32
1	A	488	GLU	C-N-CA	8.08	128.53	119.32
1	A	104	CYS	N-CA-C	7.93	122.65	110.36
1	B	378	CYS	N-CA-C	7.51	122.62	113.38
1	A	365	GLY	N-CA-C	-7.27	101.09	111.20
1	B	197	ARG	N-CA-C	7.23	121.80	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	THR	N-CA-C	7.07	119.59	111.11
1	A	122	GLY	CA-C-N	7.06	126.99	120.21
1	A	122	GLY	C-N-CA	7.06	126.99	120.21
1	B	348	ASN	N-CA-C	6.96	121.48	112.92
1	B	122	GLY	CA-C-N	6.86	126.82	120.03
1	B	122	GLY	C-N-CA	6.86	126.82	120.03
1	A	378	CYS	N-CA-C	6.82	121.60	113.28
1	B	234	ILE	N-CA-C	6.74	118.14	109.30
1	A	348	ASN	N-CA-C	6.72	120.38	112.72
1	B	424	ASN	N-CA-C	6.70	120.41	111.30
1	B	99	THR	N-CA-C	-6.63	96.68	110.80
1	A	386	LEU	N-CA-C	6.58	119.01	111.11
1	A	153	ILE	N-CA-C	6.49	117.23	110.62
1	A	303	LEU	N-CA-C	6.49	119.81	109.24
1	A	430	HIS	N-CA-C	6.34	119.00	111.71
1	A	485	TYR	N-CA-C	-6.28	102.07	110.55
1	B	303	LEU	N-CA-C	6.25	120.00	109.76
1	A	293	TYR	N-CA-C	6.14	123.88	110.80
1	B	101	ASP	CA-C-N	5.94	132.88	121.54
1	B	101	ASP	C-N-CA	5.94	132.88	121.54
1	A	316	PRO	CA-C-N	5.93	126.35	119.47
1	A	316	PRO	C-N-CA	5.93	126.35	119.47
1	B	198	ILE	N-CA-C	-5.83	103.87	112.04
1	A	377	PHE	N-CA-C	5.81	118.83	111.69
1	A	101	ASP	N-CA-C	5.69	118.57	110.10
1	B	100	SER	CA-C-N	-5.60	114.89	123.07
1	B	100	SER	C-N-CA	-5.60	114.89	123.07
1	A	308	GLN	N-CA-C	5.55	122.62	110.80
1	B	253	LEU	N-CA-C	-5.44	99.66	108.52
1	B	368	MET	N-CA-C	-5.43	99.56	108.41
1	B	384	ASN	N-CA-C	5.41	118.85	111.39
1	B	308	GLN	N-CA-C	5.41	122.32	110.80
1	A	390	GLY	N-CA-C	-5.39	105.97	112.49
1	B	460	PRO	CA-C-N	5.39	126.57	119.84
1	B	460	PRO	C-N-CA	5.39	126.57	119.84
1	B	92	ASP	N-CA-C	5.36	117.05	108.41
1	B	466	ILE	N-CA-C	-5.36	105.78	113.07
1	B	325	MET	N-CA-C	5.33	118.23	109.76
1	A	325	MET	N-CA-C	5.32	118.61	110.20
1	A	253	LEU	N-CA-C	-5.29	99.89	108.52
1	B	288	GLY	N-CA-C	5.29	123.70	115.72
1	A	384	ASN	N-CA-C	5.29	118.54	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	316	PRO	CA-C-N	5.29	125.60	119.47
1	B	316	PRO	C-N-CA	5.29	125.60	119.47
1	A	424	ASN	N-CA-C	5.20	118.61	111.54
1	A	176	THR	N-CA-C	-5.20	103.54	110.55
1	B	114	MET	N-CA-C	5.13	116.68	111.14
1	B	200	TRP	N-CA-C	5.12	121.70	110.80
1	A	217	MET	N-CA-C	-5.10	105.62	111.07
1	B	102	PHE	N-CA-CB	-5.08	101.90	110.49
1	A	395	LEU	N-CA-C	5.04	121.53	110.80
1	B	103	THR	N-CA-C	5.03	119.67	111.37
1	A	368	MET	N-CA-C	-5.02	100.23	108.41

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	101	ASP	Mainchain

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	3423	0	3320	88	0
1	B	3423	0	3320	65	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	43	0	30	3	0
3	B	43	0	30	2	0
4	A	17	0	14	0	0
4	B	17	0	14	0	0
5	A	6	0	7	1	0
5	B	6	0	7	7	0
6	A	107	0	0	20	0
6	B	111	0	0	28	0
All	All	7198	0	6742	163	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 12.

All (163) 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:438:MET:HE3	1:A:469:VAL:HG12	1.49	0.91
5:B:1899:ITU:S	6:B:1125:HOH:O	2.30	0.89
1:B:364:ASN:HA	6:B:1124:HOH:O	1.74	0.86
1:A:195:ILE:HG13	6:A:1031:HOH:O	1.83	0.79
1:A:404:TRP:HE3	6:A:1063:HOH:O	1.67	0.76
1:B:438:MET:HE3	1:B:469:VAL:HG12	1.67	0.75
1:B:217:MET:HB3	1:B:303:LEU:HD23	1.68	0.74
1:A:239:THR:HB	6:A:909:HOH:O	1.88	0.72
3:B:901:HEM:HHC	6:B:1090:HOH:O	1.90	0.72
5:B:1899:ITU:H12	6:B:1124:HOH:O	1.89	0.70
1:B:301:LEU:HB3	1:B:303:LEU:HD11	1.73	0.70
1:A:438:MET:HG3	1:A:468:PRO:HB2	1.78	0.66
1:A:457:TRP:CE3	6:A:1131:HOH:O	2.49	0.66
1:A:80:ARG:NH2	6:A:1121:HOH:O	2.29	0.65
1:B:239:THR:HG23	1:B:362:PRO:HG2	1.78	0.65
1:B:327:HIS:ND1	1:B:328:PRO:HD2	2.11	0.65
3:B:901:HEM:HMC2	6:B:1090:HOH:O	1.97	0.64
5:B:1899:ITU:H13	6:B:1123:HOH:O	1.98	0.64
1:A:215:GLN:HE21	1:A:219:GLN:HE21	1.45	0.63
1:B:438:MET:HA	1:B:438:MET:HE2	1.79	0.63
1:A:405:LYS:O	1:A:409:VAL:HG23	1.99	0.63
1:A:154:GLU:H	1:A:154:GLU:CD	2.06	0.63
1:A:348:ASN:HD22	1:A:348:ASN:H	1.47	0.62
1:A:408:ALA:HB2	6:A:1063:HOH:O	1.99	0.62
1:B:303:LEU:HD12	1:B:303:LEU:N	2.15	0.62
1:A:348:ASN:H	1:A:348:ASN:ND2	1.97	0.61
1:A:266:MET:SD	1:A:272:ARG:HD3	2.41	0.61
1:A:368:MET:HE3	1:A:370:THR:OG1	2.01	0.61
1:A:457:TRP:HE3	6:A:1131:HOH:O	1.83	0.60
3:A:901:HEM:HHA	6:A:1131:HOH:O	2.01	0.60
1:A:327:HIS:ND1	1:A:328:PRO:HD2	2.16	0.60
1:A:223:ARG:HD3	6:A:993:HOH:O	2.01	0.60
1:A:438:MET:HA	1:A:438:MET:HE2	1.83	0.60
1:B:195:ILE:HG13	6:B:1002:HOH:O	2.02	0.60
1:B:346:VAL:HB	6:B:945:HOH:O	2.01	0.59
1:A:258:LEU:HB2	1:A:345:ALA:HB3	1.85	0.58
1:A:465:SER:O	1:A:471:HIS:HE1	1.87	0.58
1:B:345:ALA:HA	6:B:1124:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ASN:HD22	1:A:348:ASN:N	2.00	0.57
1:B:239:THR:HB	6:B:1105:HOH:O	2.05	0.57
1:A:124:ARG:HH11	1:A:124:ARG:HG3	1.71	0.56
1:B:99:THR:O	1:B:100:SER:O	2.24	0.56
1:A:298:VAL:HG21	1:A:320:VAL:HG11	1.88	0.55
1:A:81:ILE:HD11	1:A:475:LEU:HD13	1.88	0.55
1:B:365:GLY:HA3	6:B:1090:HOH:O	2.08	0.54
1:B:81:ILE:HD11	1:B:475:LEU:HD13	1.88	0.54
1:B:89:ILE:HD11	6:B:1122:HOH:O	2.07	0.54
1:A:301:LEU:HD22	1:A:315:ILE:HG12	1.90	0.54
1:B:195:ILE:HD13	6:B:1137:HOH:O	2.08	0.54
5:B:1899:ITU:H11	6:B:1000:HOH:O	2.06	0.54
1:B:258:LEU:HB2	1:B:345:ALA:HB3	1.89	0.54
1:B:368:MET:HE3	1:B:370:THR:OG1	2.08	0.53
1:A:494:ILE:H	1:A:494:ILE:HD12	1.73	0.53
1:B:149:LYS:O	1:B:150:GLU:HG2	2.08	0.53
1:B:459:VAL:HG22	1:B:469:VAL:HG23	1.90	0.53
5:B:1899:ITU:C1	6:B:1123:HOH:O	2.54	0.53
1:B:128:THR:HG23	6:B:1080:HOH:O	2.09	0.53
1:A:239:THR:HG23	1:A:362:PRO:HG2	1.91	0.53
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.45	0.53
1:B:209:ARG:O	1:B:242:PRO:HG3	2.09	0.52
1:B:346:VAL:HG21	6:B:1000:HOH:O	2.09	0.52
5:B:1899:ITU:H21	6:B:999:HOH:O	2.10	0.51
1:A:217:MET:HE1	1:A:304:GLN:C	2.36	0.51
1:A:148:PHE:HB2	6:A:995:HOH:O	2.11	0.51
1:B:159:ARG:O	1:B:163:VAL:HG23	2.10	0.51
1:A:410:THR:O	1:A:414:VAL:HG23	2.11	0.51
1:B:365:GLY:N	6:B:1125:HOH:O	2.42	0.51
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.46	0.51
1:B:348:ASN:ND2	1:B:348:ASN:H	2.08	0.50
1:B:356:LEU:HG	6:B:1106:HOH:O	2.10	0.50
1:A:124:ARG:HG3	1:A:124:ARG:NH1	2.26	0.50
1:B:304:GLN:HG3	1:B:308:GLN:O	2.11	0.50
1:B:382:ARG:NH2	6:B:1126:HOH:O	2.45	0.49
1:A:134:LEU:O	1:A:138:ILE:HG12	2.13	0.49
1:A:272:ARG:HG2	1:A:295:ARG:HE	1.78	0.49
1:B:467:THR:HG23	1:B:469:VAL:HG22	1.94	0.49
1:A:78:TYR:CD1	1:A:78:TYR:C	2.90	0.48
1:A:150:GLU:HG2	1:A:150:GLU:O	2.14	0.47
1:A:252:ARG:NH2	1:A:489:PRO:HD3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ILE:HG21	1:B:301:LEU:HD21	1.96	0.47
1:B:348:ASN:H	1:B:348:ASN:HD22	1.63	0.47
1:A:366:TRP:HB2	6:A:907:HOH:O	2.14	0.47
1:B:210:ASN:ND2	1:B:210:ASN:H	2.11	0.47
1:A:434:SER:HB3	1:A:468:PRO:HD2	1.97	0.47
1:A:330:TYR:HB3	1:A:332:TRP:NE1	2.29	0.47
1:B:210:ASN:N	1:B:210:ASN:HD22	2.12	0.47
1:B:195:ILE:N	6:B:1002:HOH:O	2.49	0.46
1:A:324:THR:H	1:A:423:GLN:HE22	1.63	0.46
1:B:180:LEU:O	1:B:184:THR:HG23	2.16	0.46
1:B:356:LEU:HA	1:B:356:LEU:HD13	1.74	0.46
1:B:464:GLY:O	1:B:467:THR:HG22	2.16	0.46
1:A:154:GLU:CD	1:A:154:GLU:N	2.74	0.46
1:A:367:TYR:HD2	6:A:1071:HOH:O	1.99	0.45
1:A:413:ASN:O	1:A:417:LEU:HD13	2.17	0.45
1:B:367:TYR:HD2	6:B:1053:HOH:O	1.99	0.45
1:B:371:GLU:OE2	5:B:1899:ITU:N2	2.49	0.45
1:A:248:LYS:HB2	6:A:990:HOH:O	2.16	0.45
1:B:417:LEU:HD21	1:B:429:ASP:HB3	1.97	0.45
1:A:346:VAL:HG23	5:A:899:ITU:H11	1.99	0.45
1:B:197:ARG:H	1:B:197:ARG:HG2	1.61	0.45
1:B:210:ASN:H	1:B:210:ASN:HD22	1.65	0.45
1:A:374:VAL:CG2	1:A:413:ASN:HD21	2.29	0.44
1:A:272:ARG:HG2	1:A:295:ARG:NE	2.32	0.44
1:A:385:ILE:HD11	1:A:412:ILE:HD13	1.98	0.44
1:A:303:LEU:O	1:A:310:PRO:HA	2.16	0.44
1:B:78:TYR:C	1:B:78:TYR:CD1	2.96	0.44
1:B:371:GLU:HB3	6:B:1021:HOH:O	2.16	0.44
1:A:466:ILE:HG22	1:A:466:ILE:O	2.18	0.44
1:B:348:ASN:HD22	1:B:348:ASN:N	2.14	0.44
1:A:283:LEU:O	1:A:287:LEU:HG	2.16	0.44
3:A:901:HEM:HAA1	6:A:1131:HOH:O	2.18	0.44
1:B:77:GLN:HG3	1:B:78:TYR:H	1.83	0.44
1:B:193:ARG:HB3	1:B:457:TRP:CE3	2.52	0.43
1:B:224:HIS:HB2	6:B:1105:HOH:O	2.17	0.43
1:A:215:GLN:HE21	1:A:219:GLN:NE2	2.14	0.43
1:A:258:LEU:HD12	1:A:258:LEU:HA	1.82	0.43
1:A:176:THR:OG1	1:A:179:GLU:HG3	2.18	0.43
1:A:408:ALA:CB	6:A:1063:HOH:O	2.62	0.43
1:B:121:ARG:HA	1:B:121:ARG:HD3	1.78	0.43
1:A:188:TRP:CZ3	1:A:200:TRP:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ASN:O	1:A:192:PRO:HD3	2.19	0.43
1:A:407:ARG:HH11	1:A:407:ARG:HG3	1.83	0.43
1:B:258:LEU:HD12	1:B:258:LEU:HA	1.90	0.43
1:A:333:PHE:O	1:A:336:LEU:HB2	2.19	0.43
1:A:397:THR:O	1:A:397:THR:HG22	2.18	0.43
1:B:330:TYR:HB3	1:B:332:TRP:NE1	2.34	0.43
1:A:272:ARG:HE	1:A:295:ARG:HG3	1.84	0.43
1:A:329:LYS:HB3	1:A:330:TYR:HD1	1.84	0.43
1:B:333:PHE:O	1:B:336:LEU:HB2	2.19	0.43
1:A:375:ARG:NH1	1:A:379:ASP:OD2	2.53	0.42
1:B:296:PHE:HB2	1:B:339:LYS:HE3	2.01	0.42
1:A:266:MET:HE3	1:A:272:ARG:HB2	2.02	0.42
1:A:193:ARG:HD2	6:A:1033:HOH:O	2.19	0.42
1:A:341:TYR:HB2	6:A:1070:HOH:O	2.20	0.42
1:B:252:ARG:NH2	1:B:489:PRO:HD3	2.35	0.42
1:A:94:LEU:HD12	1:A:97:LYS:HD2	2.01	0.42
1:A:325:MET:HA	1:A:419:SER:OG	2.19	0.42
1:A:386:LEU:HD21	1:A:409:VAL:HG22	2.02	0.42
1:B:330:TYR:HD2	1:B:332:TRP:HE1	1.66	0.42
1:A:78:TYR:C	1:A:78:TYR:HD1	2.28	0.42
1:A:165:LYS:HE3	1:A:165:LYS:HB2	1.88	0.41
1:A:248:LYS:HD2	6:A:990:HOH:O	2.20	0.41
1:A:164:THR:O	1:A:168:GLU:HG2	2.20	0.41
1:A:251:PHE:O	1:A:360:ALA:HB2	2.21	0.41
1:A:273:GLY:HA3	6:A:1060:HOH:O	2.20	0.41
1:B:375:ARG:HB2	6:B:1055:HOH:O	2.20	0.41
1:A:366:TRP:H	3:A:901:HEM:HAB	1.85	0.41
1:A:282:GLN:O	1:A:285:ILE:HG22	2.21	0.41
1:A:316:PRO:HA	1:A:317:PRO:HD3	1.89	0.41
1:B:195:ILE:O	1:B:195:ILE:HG22	2.20	0.41
1:B:198:ILE:HG22	6:B:953:HOH:O	2.20	0.41
1:B:453:ALA:HB1	1:B:458:LEU:CD1	2.51	0.41
1:B:142:ASN:HD22	1:B:142:ASN:N	2.18	0.41
1:A:123:PRO:HD3	1:A:487:ILE:HD12	2.02	0.40
1:A:229:THR:HG22	1:A:231:ASN:H	1.86	0.40
1:A:217:MET:HE1	1:A:304:GLN:O	2.21	0.40
1:A:272:ARG:NE	1:A:295:ARG:HG3	2.36	0.40
1:A:325:MET:HB3	1:A:333:PHE:HE2	1.87	0.40
1:A:352:GLU:HG3	1:A:353:VAL:N	2.36	0.40
1:B:102:PHE:HB2	6:B:1135:HOH:O	2.22	0.40
1:B:316:PRO:HA	1:B:317:PRO:HD3	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:HB	6:A:975:HOH:O	2.22	0.40
1:A:427:ILE:HG13	1:A:428:MET:N	2.37	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	418/423 (99%)	381 (91%)	30 (7%)	7 (2%)	7	6
1	B	418/423 (99%)	385 (92%)	30 (7%)	3 (1%)	18	20
All	All	836/846 (99%)	766 (92%)	60 (7%)	10 (1%)	10	9

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	THR
1	A	293	TYR
1	A	308	GLN
1	A	395	LEU
1	B	100	SER
1	B	308	GLN
1	A	464	GLY
1	A	270	THR
1	A	268	ASP
1	B	150	GLU

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	368/371 (99%)	335 (91%)	33 (9%)	9	9
1	B	368/371 (99%)	333 (90%)	35 (10%)	8	7
All	All	736/742 (99%)	668 (91%)	68 (9%)	8	9

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

Mol	Chain	Res	Type
1	A	78	TYR
1	A	81	ILE
1	A	110	LEU
1	A	114	MET
1	A	119	LEU
1	A	124	ARG
1	A	129	PRO
1	A	133	LEU
1	A	150	GLU
1	A	154	GLU
1	A	157	LEU
1	A	161	GLU
1	A	178	ASP
1	A	180	LEU
1	A	217	MET
1	A	258	LEU
1	A	260	ARG
1	A	264	TYR
1	A	268	ASP
1	A	285	ILE
1	A	301	LEU
1	A	303	LEU
1	A	314	GLU
1	A	316	PRO
1	A	329	LYS
1	A	330	TYR
1	A	338	LEU
1	A	348	ASN
1	A	395	LEU
1	A	396	GLU
1	A	406	ASP
1	A	446	ARG
1	A	494	ILE

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Mol	Chain	Res	Type
1	B	93	THR
1	B	99	THR
1	B	100	SER
1	B	110	LEU
1	B	119	LEU
1	B	125	ASP
1	B	126	LYS
1	B	128	THR
1	B	130	LEU
1	B	133	LEU
1	B	134	LEU
1	B	139	GLU
1	B	142	ASN
1	B	148	PHE
1	B	150	GLU
1	B	175	LEU
1	B	177	LEU
1	B	178	ASP
1	B	197	ARG
1	B	210	ASN
1	B	217	MET
1	B	226	LEU
1	B	239	THR
1	B	258	LEU
1	B	268	ASP
1	B	301	LEU
1	B	303	LEU
1	B	348	ASN
1	B	353	VAL
1	B	356	LEU
1	B	396	GLU
1	B	397	THR
1	B	444	GLU
1	B	467	THR
1	B	475	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	HIS
1	A	202	ASN
1	A	219	GLN

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Mol	Chain	Res	Type
1	A	231	ASN
1	A	233	ASN
1	A	257	GLN
1	A	265	GLN
1	A	308	GLN
1	A	348	ASN
1	A	413	ASN
1	A	443	ASN
1	A	471	HIS
1	A	486	GLN
1	B	95	HIS
1	B	142	ASN
1	B	143	GLN
1	B	156	HIS
1	B	199	GLN
1	B	210	ASN
1	B	219	GLN
1	B	220	HIS
1	B	224	HIS
1	B	231	ASN
1	B	233	ASN
1	B	348	ASN
1	B	364	ASN
1	B	486	GLN
1	B	493	HIS

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 8 ligands modelled in this entry, 2 are 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
5	ITU	B	1899	-	4,5,5	2.07	1 (25%)	3,5,5	5.19	1 (33%)
4	H4B	B	1902	-	17,18,18	2.61	3 (17%)	14,26,26	1.97	4 (28%)
3	HEM	B	901	1	50,50,50	1.47	6 (12%)	67,82,82	1.33	7 (10%)
5	ITU	A	899	-	4,5,5	1.99	1 (25%)	3,5,5	1.96	1 (33%)
3	HEM	A	901	1	50,50,50	1.66	8 (16%)	67,82,82	1.40	11 (16%)
4	H4B	A	902	-	17,18,18	2.43	4 (23%)	14,26,26	2.03	4 (28%)

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	ITU	B	1899	-	-	0/3/3/3	-
4	H4B	B	1902	-	-	0/8/17/17	0/2/2/2
3	HEM	B	901	1	-	2/14/54/54	-
5	ITU	A	899	-	-	0/3/3/3	-
3	HEM	A	901	1	-	2/14/54/54	-
4	H4B	A	902	-	-	2/8/17/17	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1902	H4B	C7-C6	-6.91	1.45	1.52
4	B	1902	H4B	C7-N8	-6.81	1.39	1.46
4	A	902	H4B	C7-N8	-6.62	1.39	1.46
4	A	902	H4B	C7-C6	-6.03	1.46	1.52
3	A	901	HEM	FE-ND	5.68	2.12	1.94
3	B	901	HEM	FE-ND	4.12	2.07	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	HEM	FE-NC	3.82	2.07	1.95
5	A	899	ITU	C3-S	3.74	1.79	1.75
3	A	901	HEM	CAB-C3B	-3.50	1.38	1.47
5	B	1899	ITU	C3-S	3.47	1.79	1.75
3	B	901	HEM	CAB-C3B	-3.26	1.38	1.47
3	A	901	HEM	C4D-C3D	2.86	1.49	1.45
3	A	901	HEM	C3C-C2C	2.83	1.42	1.37
4	B	1902	H4B	C4-N3	-2.72	1.33	1.38
3	A	901	HEM	C1A-C2A	2.66	1.49	1.44
4	A	902	H4B	C4-N3	-2.64	1.33	1.38
3	B	901	HEM	CAC-C3C	-2.59	1.40	1.47
3	B	901	HEM	C3C-C2C	2.59	1.42	1.37
3	B	901	HEM	C4B-NB	-2.34	1.34	1.38
3	B	901	HEM	FE-NC	2.26	2.02	1.95
3	A	901	HEM	C4D-ND	-2.16	1.36	1.40
3	A	901	HEM	CBC-CAC	2.11	1.40	1.30
4	A	902	H4B	C4A-C8A	2.03	1.42	1.38

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1899	ITU	C2-S-C3	-8.91	93.88	103.15
4	B	1902	H4B	C2-N1-C8A	4.52	121.33	113.36
4	A	902	H4B	C2-N1-C8A	4.30	120.96	113.36
3	A	901	HEM	C4C-C3C-C2C	-4.07	103.28	106.81
4	A	902	H4B	O4-C4-C4A	-3.92	117.82	127.26
4	B	1902	H4B	O4-C4-C4A	-3.58	118.63	127.26
3	A	901	HEM	CMD-C2D-C1D	3.49	130.50	125.03
3	B	901	HEM	C1D-C2D-C3D	-3.48	103.31	106.98
3	B	901	HEM	CMD-C2D-C1D	3.42	130.37	125.03
5	A	899	ITU	C2-S-C3	-3.37	99.64	103.15
3	A	901	HEM	CHD-C1D-ND	-3.32	120.85	124.42
3	B	901	HEM	C4C-C3C-C2C	-3.22	104.03	106.81
3	B	901	HEM	CAD-C3D-C2D	-3.13	122.01	127.87
3	A	901	HEM	C2D-C1D-ND	2.90	113.26	109.90
4	A	902	H4B	C4A-C4-N3	2.89	120.06	112.13
4	B	1902	H4B	C4A-C4-N3	2.83	119.89	112.13
4	A	902	H4B	C2-N3-C4	-2.65	120.31	125.11
4	B	1902	H4B	C2-N3-C4	-2.50	120.59	125.11
3	B	901	HEM	C2B-C1B-NB	2.49	112.71	109.84
3	A	901	HEM	CMC-C2C-C1C	-2.49	120.34	124.73
3	B	901	HEM	C4D-C3D-C2D	2.37	110.34	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	HEM	C2B-C1B-NB	2.36	112.55	109.84
3	A	901	HEM	C4D-ND-C1D	-2.29	102.49	105.21
3	A	901	HEM	CAD-C3D-C4D	2.28	128.68	124.70
3	B	901	HEM	C2D-C1D-ND	2.12	112.36	109.90
3	A	901	HEM	CHA-C4D-ND	-2.12	121.74	124.37
3	A	901	HEM	CAD-C3D-C2D	-2.07	123.99	127.87
3	A	901	HEM	CAB-C3B-C2B	-2.01	121.89	128.43

There are no chirality outliers.

All (6) torsion outliers are listed below:

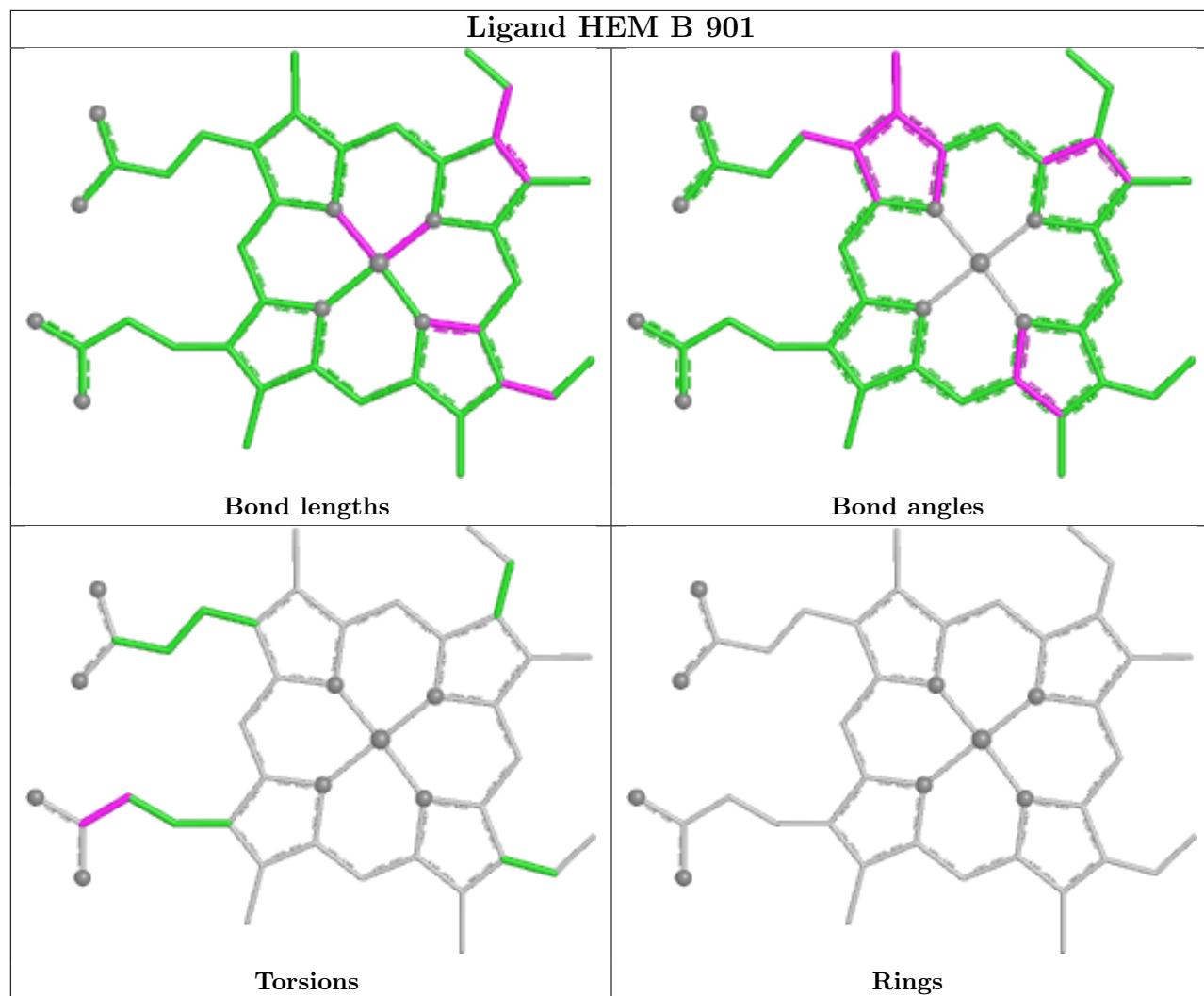
Mol	Chain	Res	Type	Atoms
4	A	902	H4B	C7-C6-C9-O9
4	A	902	H4B	C7-C6-C9-C10
3	B	901	HEM	CAA-CBA-CGA-O1A
3	A	901	HEM	CAA-CBA-CGA-O1A
3	A	901	HEM	CAA-CBA-CGA-O2A
3	B	901	HEM	CAA-CBA-CGA-O2A

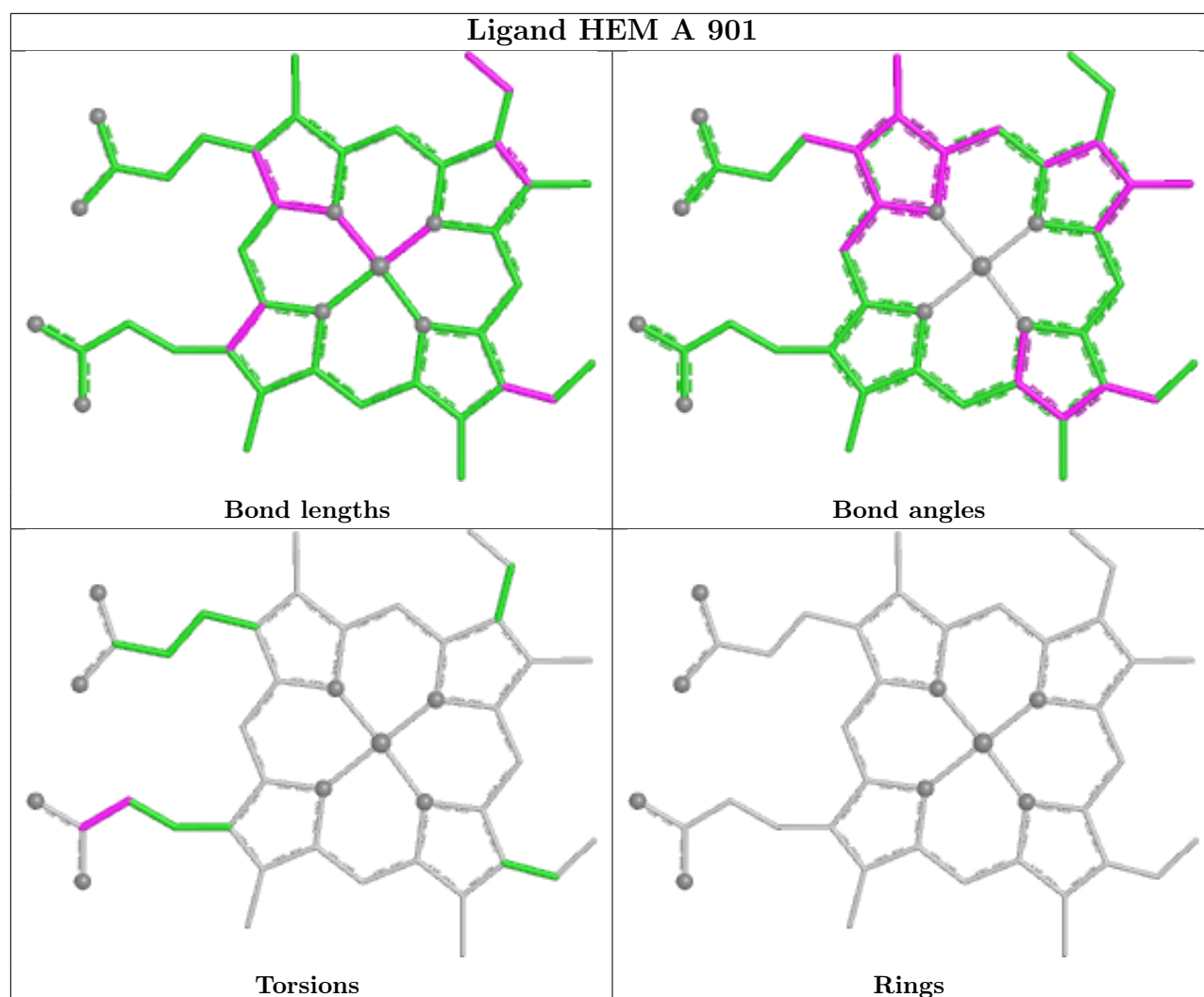
There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1899	ITU	7	0
3	B	901	HEM	2	0
5	A	899	ITU	1	0
3	A	901	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	420/423 (99%)	0.69	46 (10%) 10 12	9, 45, 78, 91	9 (2%)
1	B	420/423 (99%)	0.61	39 (9%) 14 17	17, 45, 76, 98	9 (2%)
All	All	840/846 (99%)	0.65	85 (10%) 12 14	9, 45, 77, 98	18 (2%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	495	TRP	6.3
1	B	496	GLN	6.0
1	A	496	GLN	5.4
1	A	148	PHE	5.4
1	B	100	SER	5.1
1	B	494	ILE	5.0
1	B	102	PHE	4.7
1	A	151	ALA	4.3
1	A	105	LYS	4.2
1	B	269	GLY	4.2
1	A	330	TYR	4.2
1	A	332	TRP	4.2
1	A	494	ILE	4.1
1	B	103	THR	4.0
1	B	267	PRO	3.9
1	A	265	GLN	3.8
1	A	292	ARG	3.8
1	A	383	TYR	3.7
1	A	285	ILE	3.7
1	B	105	LYS	3.5
1	A	294	GLY	3.5
1	B	292	ARG	3.4
1	A	267	PRO	3.4
1	A	89	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	391	ARG	3.3
1	B	330	TYR	3.3
1	A	397	THR	3.3
1	B	99	THR	3.3
1	B	266	MET	3.2
1	A	102	PHE	3.1
1	B	394	GLY	3.1
1	A	77	GLN	3.1
1	A	103	THR	3.0
1	B	108	SER	3.0
1	B	293	TYR	3.0
1	B	285	ILE	3.0
1	A	425	VAL	3.0
1	B	78	TYR	2.9
1	B	148	PHE	2.9
1	A	295	ARG	2.8
1	B	265	GLN	2.8
1	A	290	LYS	2.8
1	A	324	THR	2.8
1	A	269	GLY	2.8
1	A	495	TRP	2.7
1	A	333	PHE	2.7
1	A	266	MET	2.6
1	B	492	THR	2.6
1	A	99	THR	2.6
1	A	414	VAL	2.6
1	A	101	ASP	2.6
1	B	101	ASP	2.6
1	B	153	ILE	2.6
1	B	107	LYS	2.6
1	A	352	GLU	2.5
1	A	80	ARG	2.5
1	A	232	GLY	2.5
1	A	334	GLN	2.5
1	B	332	TRP	2.5
1	A	293	TYR	2.5
1	A	107	LYS	2.4
1	A	337	GLY	2.4
1	A	328	PRO	2.4
1	B	270	THR	2.4
1	B	149	LYS	2.3
1	A	270	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	421	GLN	2.3
1	B	333	PHE	2.2
1	B	294	GLY	2.2
1	A	106	SER	2.2
1	B	110	LEU	2.2
1	B	308	GLN	2.2
1	A	422	LYS	2.1
1	A	421	GLN	2.1
1	A	400	LEU	2.1
1	B	296	PHE	2.1
1	A	81	ILE	2.1
1	A	195	ILE	2.1
1	B	104	CYS	2.1
1	A	282	GLN	2.1
1	B	77	GLN	2.1
1	B	150	GLU	2.0
1	A	273	GLY	2.0
1	B	131	GLU	2.0
1	B	130	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
2	ZN	B	900	1/1	0.92	0.22	52,52,52,52	1
2	ZN	A	900	1/1	0.94	0.08	78,78,78,78	1
4	H4B	B	1902	17/17	0.95	0.06	20,24,33,34	0
5	ITU	A	899	6/6	0.95	0.10	22,24,27,34	0

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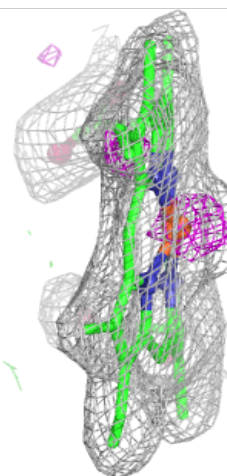
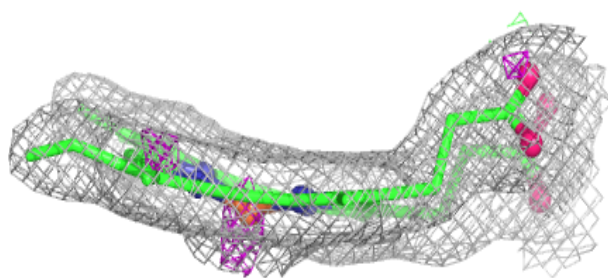
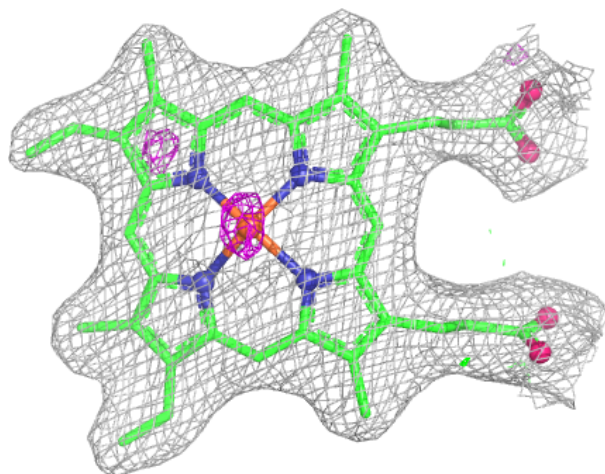
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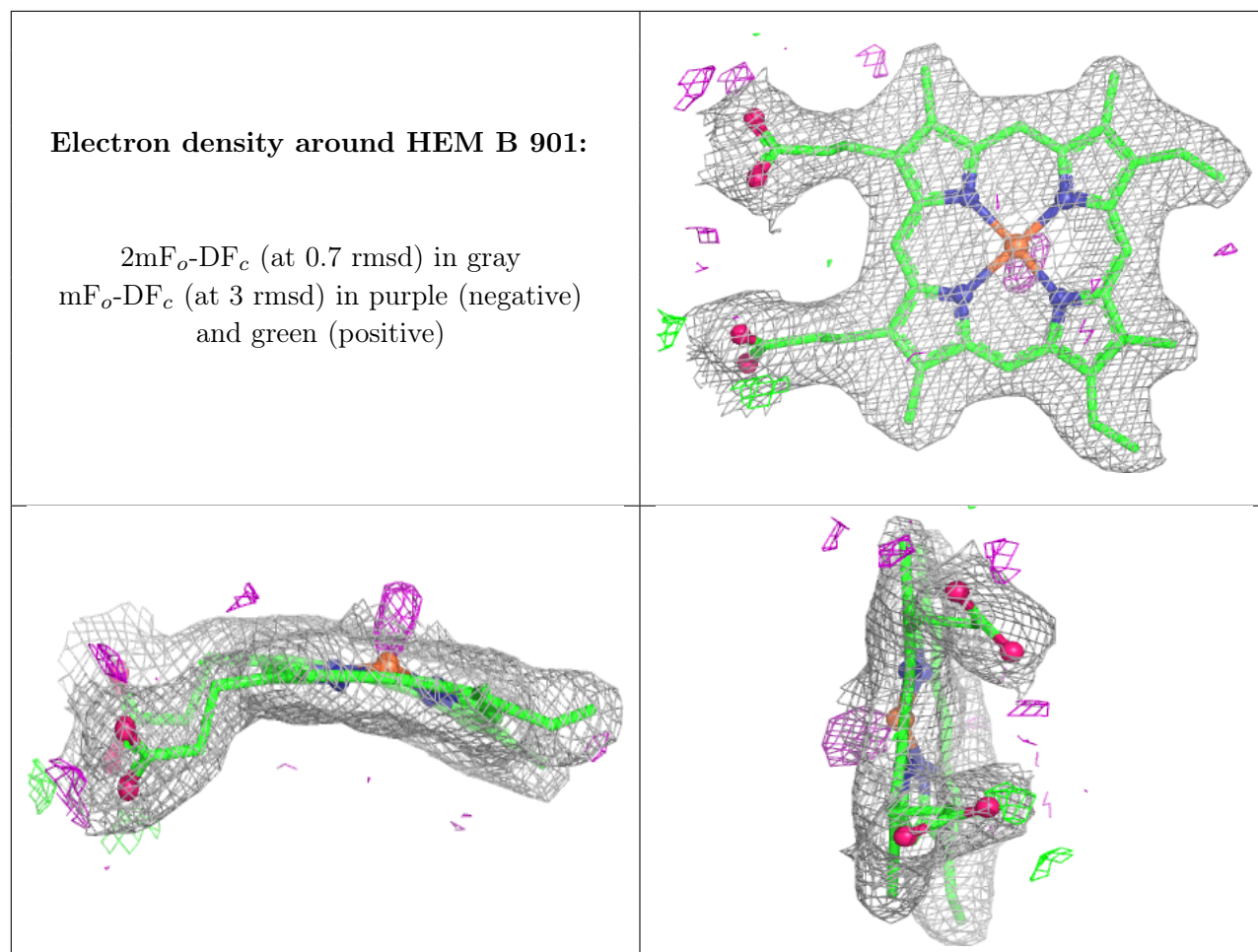
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	H4B	A	902	17/17	0.96	0.06	19,23,31,31	0
5	ITU	B	1899	6/6	0.96	0.10	19,29,35,39	0
3	HEM	A	901	43/43	0.97	0.06	17,24,30,34	0
3	HEM	B	901	43/43	0.98	0.06	18,24,30,36	0

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 901:

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.