



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:52 AM UTC

PDB ID : 2FLQ / pdb_00002flq
Title : Crystal Structure of Nitric Oxide Synthase from *Geobacillus Stearothermophilus* (ATCC 12980) complexed with L-arginine
Authors : Sudhamsu, J.; Crane, B.R.
Deposited on : 2006-01-06
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

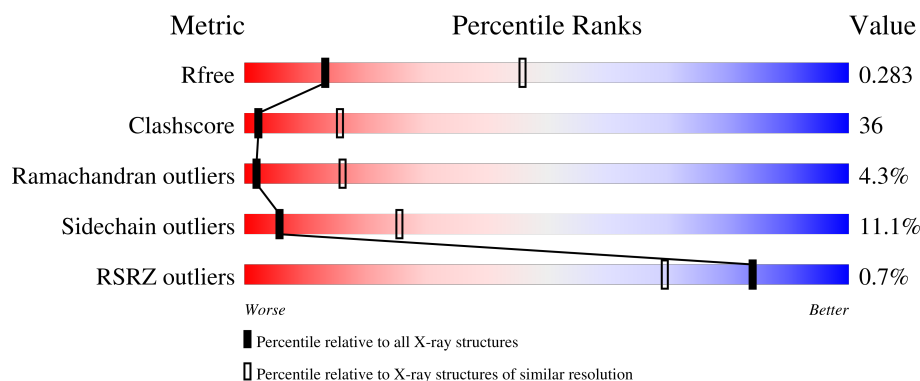
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

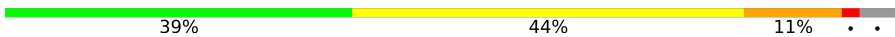
The reported resolution of this entry is 3.20 Å.

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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	375	
1	B	375	

2 Entry composition [i](#)

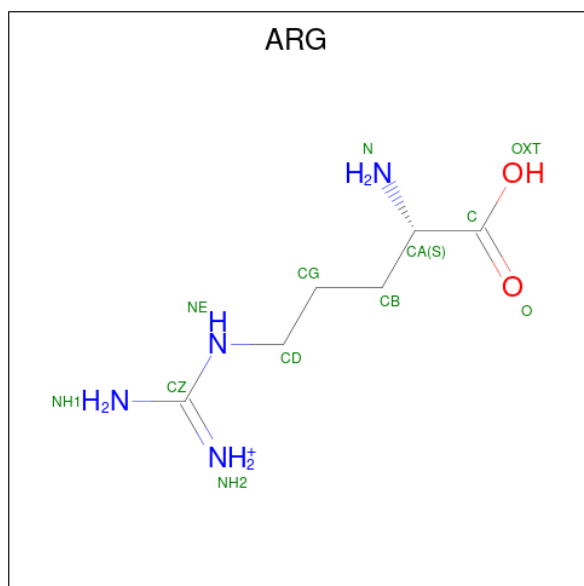
There are 4 unique types of molecules in this entry. The entry contains 6154 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	359	Total	C	N	O	S	0	0	0
			2933	1882	508	530	13			
1	B	358	Total	C	N	O	S	0	0	0
			2888	1854	496	525	13			

- Molecule 2 is ARGININE (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



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

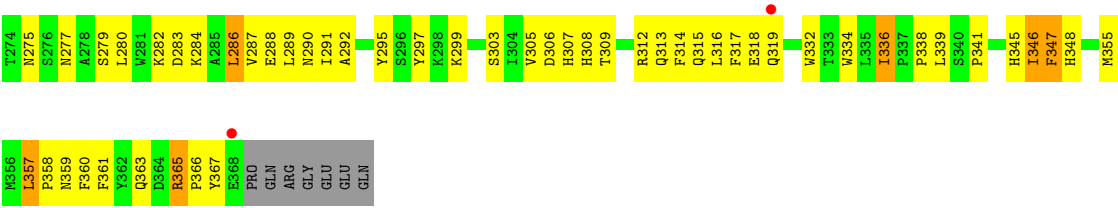
- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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 water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	113	Total O 113 113	0	0
4	B	110	Total O 110 110	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	154.01Å 118.72Å 49.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 30.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	87.7 (30.00-3.20) 87.6 (30.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.73 (at 3.18Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.295 0.211 , 0.283	Depositor DCC
R_{free} test set	724 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.842	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.2	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	0.91	EDS
Total number of atoms	6154	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.2778e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.53	1/3018 (0.0%)	1.11	25/4099 (0.6%)
1	B	0.50	0/2972	1.07	23/4040 (0.6%)
All	All	0.52	1/5990 (0.0%)	1.09	48/8139 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	ASN	C-N	-6.67	1.24	1.33

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	LYS	CA-C-N	-9.99	107.35	119.84
1	A	186	LYS	C-N-CA	-9.99	107.35	119.84
1	B	220	VAL	N-CA-C	9.31	117.56	107.60
1	A	134	HIS	N-CA-C	-8.42	101.68	111.03
1	A	12	HIS	N-CA-C	-7.79	103.38	113.12
1	A	220	VAL	N-CA-C	7.48	116.88	108.05
1	A	222	ILE	N-CA-C	7.11	113.82	106.21
1	A	137	ILE	N-CA-C	-6.98	98.31	108.71
1	A	192	ILE	CA-C-N	6.94	128.51	119.84
1	A	192	ILE	C-N-CA	6.94	128.51	119.84
1	B	185	GLN	N-CA-C	6.80	117.25	108.34
1	B	30	GLU	N-CA-C	6.71	119.20	111.02
1	B	234	ARG	CA-C-O	6.67	127.86	120.92
1	B	365	ARG	CA-C-N	6.63	128.12	119.84
1	B	365	ARG	C-N-CA	6.63	128.12	119.84
1	A	60	GLU	N-CA-C	-6.59	96.77	110.80
1	A	365	ARG	CA-C-N	6.58	127.10	119.47
1	A	365	ARG	C-N-CA	6.58	127.10	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	ASP	N-CA-C	-6.52	104.59	112.54
1	B	134	HIS	N-CA-C	-6.38	104.25	111.14
1	B	76	CYS	N-CA-C	6.37	118.79	108.41
1	A	271	GLY	N-CA-C	6.32	123.75	115.47
1	A	126	ASN	CA-C-O	-6.20	113.14	119.78
1	A	279	SER	N-CA-C	-6.02	105.97	113.38
1	A	242	GLY	N-CA-C	-5.99	101.25	110.77
1	B	204	HIS	CA-C-N	5.81	126.21	119.47
1	B	204	HIS	C-N-CA	5.81	126.21	119.47
1	B	336	ILE	CA-C-N	5.79	123.83	119.66
1	B	336	ILE	C-N-CA	5.79	123.83	119.66
1	A	171	THR	N-CA-C	-5.74	101.78	110.50
1	B	34	SER	N-CA-C	5.68	117.31	107.93
1	B	23	PHE	N-CA-C	5.67	118.55	111.24
1	B	238	ALA	CA-C-N	5.67	125.60	119.76
1	B	238	ALA	C-N-CA	5.67	125.60	119.76
1	A	291	ILE	N-CA-C	-5.64	105.01	110.42
1	B	146	GLU	N-CA-C	-5.56	100.22	109.46
1	B	348	HIS	N-CA-C	5.53	119.66	113.02
1	B	40	ARG	N-CA-C	5.45	120.04	112.90
1	A	219	ALA	N-CA-C	5.39	118.20	111.24
1	A	196	LEU	N-CA-C	-5.33	107.32	113.88
1	A	119	THR	N-CA-C	5.31	118.08	109.06
1	B	42	VAL	N-CA-C	-5.27	105.85	113.07
1	A	61	GLU	N-CA-C	-5.26	104.54	111.96
1	B	14	GLU	N-CA-C	-5.23	105.25	111.69
1	A	160	ALA	N-CA-C	-5.15	107.13	113.41
1	A	185	GLN	N-CA-C	5.13	121.73	110.80
1	B	149	ILE	N-CA-C	5.04	115.16	108.11
1	B	128	GLU	N-CA-C	-5.01	106.43	112.54

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	2933	0	2835	202	0
1	B	2888	0	2763	224	0
2	A	12	0	12	3	0
2	B	12	0	12	0	0
3	A	43	0	30	7	0
3	B	43	0	30	2	0
4	A	113	0	0	3	0
4	B	110	0	0	1	0
All	All	6154	0	5682	417	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 36.

All (417) 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:186:LYS:HG3	1:A:187:PRO:HD3	1.22	1.15
1:A:182:VAL:HG12	1:A:183:GLY:H	1.18	1.04
1:A:243:TRP:H	3:A:901:HEM:HAB	1.24	1.02
1:B:132:TRP:HB2	1:B:179:VAL:HG13	1.46	0.98
1:B:359:ASN:HD22	1:B:360:PHE:H	1.03	0.96
1:B:21:GLU:HG3	1:B:22:GLN:H	1.32	0.94
1:B:359:ASN:ND2	1:B:360:PHE:H	1.66	0.94
1:A:133:ASN:H	1:A:133:ASN:ND2	1.61	0.93
1:B:95:THR:OG1	1:B:98:GLU:HB2	1.69	0.91
1:B:133:ASN:HD21	1:B:179:VAL:H	1.19	0.91
1:A:124:ARG:HG2	1:A:124:ARG:HH11	1.37	0.90
1:B:120:ILE:HD13	1:B:121:THR:N	1.87	0.89
1:A:193:PRO:HB2	1:A:196:LEU:HB2	1.53	0.89
1:A:186:LYS:CG	1:A:187:PRO:HD3	2.03	0.89
1:B:21:GLU:HG3	1:B:22:GLN:N	1.85	0.88
1:A:133:ASN:HD22	1:A:133:ASN:N	1.71	0.87
1:A:312:ARG:HH21	1:A:315:GLN:NE2	1.74	0.85
1:A:133:ASN:H	1:A:133:ASN:HD22	0.88	0.85
1:A:182:VAL:O	1:A:184:GLY:N	2.10	0.84
1:A:182:VAL:HG12	1:A:183:GLY:N	1.91	0.83
1:B:359:ASN:HD22	1:B:360:PHE:N	1.77	0.83
1:A:26:ALA:O	1:A:30:GLU:HG3	1.78	0.83
1:A:349:ARG:HD2	1:A:350:SER:H	1.43	0.81
1:A:22:GLN:O	1:A:25:ILE:HG22	1.83	0.79
1:A:223:ILE:HD11	2:A:376:ARG:HG2	1.64	0.78
1:A:182:VAL:CG1	1:A:183:GLY:H	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:THR:O	1:A:313:GLN:HG3	1.83	0.77
1:A:41:ARG:O	1:A:45:ILE:HG13	1.85	0.77
1:B:270:MET:HE2	1:B:272:LEU:HD11	1.66	0.76
1:A:280:LEU:HB2	1:B:291:ILE:HD11	1.66	0.75
1:A:107:ILE:HD13	1:A:192:ILE:HD11	1.68	0.75
1:B:82:TRP:CE2	1:B:83:GLN:HG3	2.22	0.75
1:A:266:VAL:HG12	1:A:270:MET:HE3	1.69	0.75
1:B:99:VAL:O	1:B:103:LEU:HG	1.85	0.75
1:B:262:MET:O	1:B:266:VAL:HG23	1.87	0.75
1:B:148:ILE:HD13	1:B:149:ILE:N	2.02	0.74
1:A:132:TRP:HE1	1:A:181:GLN:NE2	1.84	0.74
1:A:262:MET:O	1:A:266:VAL:HG23	1.88	0.74
1:B:315:GLN:HB2	1:B:345:HIS:CE1	2.22	0.73
1:B:309:THR:O	1:B:313:GLN:HG3	1.88	0.73
3:B:903:HEM:HBC2	3:B:903:HEM:HMC2	1.69	0.73
1:B:171:THR:HB	1:B:172:PRO:HD2	1.71	0.73
1:A:27:SER:O	1:A:31:LEU:HD23	1.90	0.72
1:B:241:ASN:O	3:B:903:HEM:HMC3	1.89	0.72
1:B:134:HIS:HA	1:B:225:ASP:OD2	1.91	0.71
1:B:37:GLU:O	1:B:38:ILE:C	2.34	0.71
1:A:41:ARG:HH21	1:A:58:THR:HG23	1.57	0.70
1:A:156:THR:HG21	1:A:368:GLU:HG3	1.73	0.70
1:A:17:MET:HE3	1:A:46:ARG:HA	1.73	0.70
1:B:148:ILE:HD13	1:B:148:ILE:C	2.16	0.70
1:A:227:CYS:SG	1:A:234:ARG:HG2	2.32	0.70
1:B:25:ILE:O	1:B:29:ARG:HG3	1.91	0.69
1:A:357:LEU:HD12	1:A:358:PRO:HA	1.74	0.69
3:A:901:HEM:HBC2	3:A:901:HEM:HMC2	1.74	0.69
1:B:80:LEU:HD22	1:B:313:GLN:HB3	1.75	0.69
1:B:359:ASN:ND2	1:B:360:PHE:N	2.39	0.69
1:B:38:ILE:O	1:B:42:VAL:HB	1.94	0.68
1:B:106:HIS:CE1	1:B:119:THR:HG23	2.27	0.68
1:B:244:TYR:CD1	1:B:249:ILE:HD11	2.28	0.68
1:A:124:ARG:HG2	1:A:124:ARG:NH1	2.06	0.68
1:B:13:ASP:OD2	1:B:49:VAL:HG22	1.93	0.68
1:A:286:LEU:HD13	1:A:339:LEU:HD13	1.75	0.68
1:A:45:ILE:O	1:A:49:VAL:HG23	1.94	0.67
1:B:193:PRO:HA	1:B:194:LYS:NZ	2.09	0.67
1:A:262:MET:HA	1:A:262:MET:HE2	1.75	0.67
1:B:193:PRO:HA	1:B:194:LYS:HZ2	1.57	0.67
1:A:133:ASN:ND2	1:A:133:ASN:N	2.35	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:HD21	1:A:187:PRO:HG2	1.77	0.66
1:B:332:TRP:CZ3	1:B:336:ILE:HD13	2.30	0.66
1:B:228:LEU:O	1:B:228:LEU:HD22	1.97	0.65
1:B:156:THR:HG23	1:B:157:PHE:N	2.12	0.65
1:A:90:ALA:HB3	1:A:122:ILE:O	1.96	0.65
1:A:167:LYS:C	1:A:167:LYS:HD2	2.22	0.65
1:B:235:TYR:O	1:B:237:ALA:N	2.30	0.65
1:A:199:GLU:OE2	1:A:216:LYS:HE3	1.98	0.64
1:B:228:LEU:O	1:B:228:LEU:HD13	1.97	0.64
1:B:87:VAL:HG12	1:B:88:ILE:N	2.13	0.64
1:B:96:GLU:HG2	1:B:182:VAL:HG11	1.78	0.64
1:A:131:ILE:HA	1:A:180:ILE:HG22	1.79	0.63
1:B:299:LYS:O	1:B:299:LYS:HG2	1.98	0.63
1:A:176:LEU:HD23	1:A:177:PRO:HD2	1.80	0.63
1:B:37:GLU:O	1:B:40:ARG:N	2.31	0.63
1:B:80:LEU:HG	1:B:80:LEU:O	2.00	0.62
1:A:223:ILE:HD11	2:A:376:ARG:CG	2.29	0.62
1:A:329:THR:HG22	1:A:352:ASP:O	2.00	0.61
1:B:21:GLU:O	1:B:25:ILE:HG12	2.00	0.61
1:A:103:LEU:HD11	1:A:131:ILE:HD12	1.81	0.61
1:B:23:PHE:O	1:B:27:SER:HB2	1.98	0.61
1:B:43:ASN:N	1:B:43:ASN:OD1	2.34	0.61
1:A:124:ARG:HD3	1:A:125:PRO:HD2	1.80	0.61
1:B:80:LEU:HD13	1:B:316:LEU:HB2	1.81	0.61
1:A:365:ARG:HB3	1:A:367:TYR:CE2	2.36	0.61
1:B:144:THR:O	1:B:145:GLU:C	2.43	0.61
1:B:116:ILE:HB	1:B:303:SER:HB2	1.84	0.60
1:B:256:ASP:HB2	1:B:259:ARG:HG2	1.83	0.60
1:B:357:LEU:HD12	1:B:357:LEU:C	2.26	0.60
1:A:57:HIS:HB3	1:A:61:GLU:HB3	1.83	0.60
1:A:355:MET:HE2	1:A:355:MET:C	2.27	0.60
1:B:120:ILE:HG12	1:B:239:PRO:O	2.02	0.60
1:B:41:ARG:HB2	1:B:41:ARG:CZ	2.30	0.59
1:B:254:PHE:O	1:B:262:MET:HB2	2.01	0.59
1:A:74:ASN:OD1	1:A:329:THR:HB	2.01	0.59
1:A:181:GLN:HG3	1:A:186:LYS:O	2.03	0.59
1:A:132:TRP:HE1	1:A:181:GLN:HE21	1.47	0.59
1:A:223:ILE:HD11	2:A:376:ARG:CD	2.33	0.59
1:A:367:TYR:H	1:A:367:TYR:HD2	1.50	0.58
1:B:46:ARG:O	1:B:49:VAL:HG12	2.04	0.58
1:A:25:ILE:HG23	1:A:26:ALA:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:LEU:HD12	1:B:228:LEU:H	1.67	0.58
1:B:251:ALA:O	1:B:255:ALA:HB3	2.03	0.58
1:A:185:GLN:HA	1:A:185:GLN:OE1	2.04	0.58
1:A:82:TRP:CE2	1:A:83:GLN:HG3	2.39	0.58
1:B:247:THR:HB	1:B:338:PRO:CG	2.34	0.58
1:B:266:VAL:O	1:B:270:MET:HG2	2.04	0.58
1:B:247:THR:HG22	1:B:339:LEU:HD21	1.86	0.57
1:B:204:HIS:ND1	1:B:205:PRO:HD2	2.19	0.57
1:A:115:LYS:HA	1:A:303:SER:OG	2.04	0.57
1:B:277:ASN:C	1:B:279:SER:H	2.11	0.57
1:A:160:ALA:O	1:A:164:LEU:HD13	2.04	0.57
1:B:35:GLU:O	1:B:37:GLU:N	2.38	0.57
1:A:63:SER:O	1:A:67:LYS:HG3	2.04	0.57
1:A:62:LEU:HD13	1:A:122:ILE:HG13	1.87	0.57
1:B:25:ILE:HD13	1:B:25:ILE:N	2.20	0.57
1:B:95:THR:HG1	1:B:98:GLU:HB2	1.69	0.57
1:B:194:LYS:CD	1:B:194:LYS:H	2.17	0.57
1:A:62:LEU:HD21	1:A:235:TYR:OH	2.05	0.56
1:A:337:PRO:O	1:A:341:PRO:HB3	2.04	0.56
1:B:290:ASN:ND2	1:B:339:LEU:HD13	2.19	0.56
1:A:144:THR:O	1:A:145:GLU:C	2.47	0.56
1:A:156:THR:HG21	1:A:368:GLU:CG	2.34	0.56
1:B:37:GLU:C	1:B:39:LYS:N	2.58	0.56
1:A:259:ARG:HG3	1:A:259:ARG:HH11	1.70	0.56
1:A:349:ARG:HD2	1:A:350:SER:N	2.16	0.56
1:B:117:ARG:O	1:B:119:THR:HG22	2.06	0.56
1:A:75:ARG:HD2	4:A:1092:HOH:O	2.05	0.56
1:B:70:TRP:CE3	1:B:82:TRP:HA	2.41	0.56
1:A:58:THR:HG23	1:A:61:GLU:OE2	2.06	0.56
1:B:162:GLU:HA	1:B:166:TRP:O	2.06	0.56
1:A:114:GLY:O	1:A:116:ILE:HG13	2.06	0.55
1:A:279:SER:O	1:B:291:ILE:HD11	2.06	0.55
1:A:331:ASP:OD1	1:A:333:THR:OG1	2.23	0.55
1:B:63:SER:HA	1:B:87:VAL:HG21	1.88	0.55
1:A:207:PHE:HB3	1:A:209:TRP:CE2	2.42	0.55
1:B:312:ARG:O	1:B:315:GLN:HB3	2.07	0.55
1:B:18:THR:HG22	1:B:19:LYS:N	2.21	0.55
1:B:27:SER:HA	1:B:68:MET:HE1	1.89	0.55
1:B:69:ALA:HA	1:B:358:PRO:O	2.06	0.55
1:A:145:GLU:H	1:A:145:GLU:CD	2.15	0.54
1:B:87:VAL:HG12	1:B:88:ILE:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:PHE:O	1:B:160:ALA:HB3	2.07	0.54
1:A:156:THR:HG21	1:A:368:GLU:CD	2.32	0.54
1:B:176:LEU:HD23	1:B:177:PRO:HD2	1.89	0.54
1:A:105:HIS:CE1	1:A:109:VAL:HG21	2.42	0.54
1:B:230:ILE:CG2	1:B:235:TYR:HE2	2.21	0.54
1:A:58:THR:OG1	1:A:61:GLU:HB2	2.08	0.54
1:B:341:PRO:O	1:B:347:PHE:HB2	2.08	0.54
1:B:92:GLU:OE1	1:B:92:GLU:HA	2.07	0.53
1:A:127:GLY:N	1:A:236:MET:HE3	2.23	0.53
1:A:130:ARG:NH2	1:A:363:GLN:HG3	2.23	0.53
1:A:148:ILE:HG23	1:A:148:ILE:O	2.09	0.53
1:B:38:ILE:O	1:B:42:VAL:CG2	2.57	0.53
1:B:96:GLU:CG	1:B:182:VAL:HG11	2.38	0.53
1:B:205:PRO:HB3	1:B:295:TYR:CD1	2.44	0.53
1:A:136:LEU:CD1	1:A:222:ILE:HG21	2.39	0.53
1:A:254:PHE:O	1:A:262:MET:HB2	2.08	0.53
1:B:56:ARG:HD2	1:B:57:HIS:O	2.08	0.53
1:B:137:ILE:HD13	1:B:197:VAL:HG13	1.89	0.52
1:B:39:LYS:O	1:B:43:ASN:OD1	2.27	0.52
1:A:308:HIS:CD2	1:B:282:LYS:HD2	2.44	0.52
1:B:247:THR:HB	1:B:338:PRO:HG2	1.92	0.52
1:B:59:TYR:CD1	1:B:60:GLU:N	2.77	0.52
1:B:286:LEU:HD22	1:B:290:ASN:HD21	1.75	0.52
1:A:59:TYR:OH	1:A:87:VAL:O	2.26	0.52
1:A:242:GLY:HA3	3:A:901:HEM:HHC	1.92	0.52
1:B:11:GLN:N	1:B:14:GLU:OE1	2.43	0.52
1:A:114:GLY:O	1:A:116:ILE:N	2.42	0.52
1:A:337:PRO:HG3	1:A:344:THR:HG21	1.91	0.52
1:A:45:ILE:HG23	1:A:55:TYR:CG	2.45	0.51
1:B:30:GLU:C	1:B:32:GLY:N	2.66	0.51
1:B:168:GLY:C	1:B:170:LYS:H	2.19	0.51
1:A:103:LEU:HD22	1:A:136:LEU:HD22	1.92	0.51
1:A:179:VAL:HB	1:A:189:TRP:HB3	1.93	0.51
1:A:245:MET:HE2	3:A:901:HEM:CMA	2.40	0.51
1:A:322:LYS:HG3	1:A:323:ALA:N	2.25	0.51
1:A:59:TYR:HD1	1:A:59:TYR:O	1.93	0.51
1:B:156:THR:HG23	1:B:157:PHE:H	1.75	0.51
1:A:258:TYR:HD1	1:A:258:TYR:H	1.59	0.51
1:B:204:HIS:HB2	1:B:210:PHE:CG	2.46	0.51
1:B:332:TRP:CH2	1:B:336:ILE:HD13	2.46	0.51
1:B:120:ILE:HD13	1:B:121:THR:C	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ILE:HD13	1:B:238:ALA:CB	2.41	0.51
1:B:228:LEU:HB3	1:B:360:PHE:CD1	2.46	0.51
1:A:22:GLN:C	1:A:25:ILE:HG22	2.36	0.50
1:B:110:ALA:HB2	1:B:119:THR:CG2	2.41	0.50
1:B:235:TYR:O	1:B:236:MET:C	2.54	0.50
1:B:148:ILE:C	1:B:148:ILE:CD1	2.84	0.50
1:A:191:PRO:HG2	4:A:1090:HOH:O	2.10	0.50
1:B:34:SER:O	1:B:35:GLU:C	2.55	0.50
1:B:176:LEU:CD2	1:B:177:PRO:HD2	2.42	0.50
1:A:106:HIS:HE1	1:A:241:ASN:OD1	1.95	0.50
1:B:94:VAL:HG22	1:B:94:VAL:O	2.10	0.50
1:B:95:THR:O	1:B:99:VAL:HG23	2.12	0.50
1:A:131:ILE:HG13	1:A:180:ILE:HG22	1.93	0.50
1:B:52:THR:OG1	1:B:53:GLY:N	2.45	0.50
1:B:204:HIS:HB2	1:B:210:PHE:CB	2.41	0.50
1:B:235:TYR:C	1:B:237:ALA:N	2.69	0.50
1:B:14:GLU:HG3	1:B:15:GLN:N	2.26	0.50
1:B:38:ILE:O	1:B:42:VAL:CB	2.59	0.50
1:B:134:HIS:O	1:B:224:SER:N	2.39	0.50
1:B:109:VAL:HG13	1:B:110:ALA:N	2.26	0.49
1:A:64:TYR:CD1	1:A:68:MET:HE2	2.48	0.49
1:A:148:ILE:O	1:A:148:ILE:CG2	2.60	0.49
1:A:243:TRP:H	3:A:901:HEM:CAB	2.11	0.49
1:B:195:GLU:OE2	1:B:195:GLU:N	2.45	0.49
1:A:166:TRP:HD1	1:A:189:TRP:CZ3	2.30	0.49
1:A:228:LEU:HD13	1:A:360:PHE:CE1	2.48	0.49
1:A:341:PRO:HD2	1:B:338:PRO:O	2.13	0.49
1:B:57:HIS:HE1	1:B:230:ILE:HG12	1.78	0.49
1:A:62:LEU:HD21	1:A:235:TYR:CZ	2.48	0.49
1:A:176:LEU:CD2	1:A:177:PRO:HD2	2.41	0.49
1:B:190:THR:O	1:B:190:THR:HG23	2.13	0.49
1:B:71:ARG:HH21	1:B:72:HIS:HE1	1.60	0.49
1:B:133:ASN:HD21	1:B:179:VAL:N	1.99	0.49
1:A:230:ILE:HG22	1:A:358:PRO:HB3	1.93	0.49
1:A:355:MET:HE1	1:A:357:LEU:HD22	1.94	0.49
1:A:240:PHE:CD1	1:A:240:PHE:C	2.91	0.49
1:A:287:VAL:O	1:A:291:ILE:HG12	2.13	0.49
1:B:307:HIS:ND1	1:B:307:HIS:N	2.57	0.49
1:A:253:ASN:HA	1:A:259:ARG:NH1	2.28	0.48
1:B:120:ILE:CD1	1:B:121:THR:N	2.70	0.48
1:B:160:ALA:O	1:B:163:GLN:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ALA:HA	1:A:270:MET:HG2	1.95	0.48
1:B:194:LYS:NZ	1:B:194:LYS:H	2.11	0.48
1:B:260:TYR:O	1:B:261:ASN:C	2.56	0.48
1:A:245:MET:HA	1:A:305:VAL:O	2.13	0.48
1:B:96:GLU:HG2	1:B:182:VAL:CG1	2.42	0.48
1:B:122:ILE:CD1	1:B:228:LEU:HD11	2.43	0.48
1:B:158:THR:O	1:B:159:ARG:C	2.55	0.48
1:A:25:ILE:O	1:A:29:ARG:HB2	2.13	0.48
1:A:125:PRO:HB3	1:A:235:TYR:CD1	2.48	0.48
1:A:186:LYS:CB	1:A:187:PRO:CD	2.91	0.48
1:A:270:MET:HE1	1:A:288:GLU:HB2	1.95	0.48
1:B:228:LEU:H	1:B:228:LEU:CD1	2.26	0.48
1:B:23:PHE:HE2	1:B:57:HIS:HE2	1.61	0.48
1:A:178:LEU:O	1:A:189:TRP:HA	2.14	0.48
1:B:240:PHE:CD1	1:B:240:PHE:C	2.91	0.48
1:A:242:GLY:HA3	3:A:901:HEM:CHC	2.43	0.48
1:A:361:PHE:N	1:A:361:PHE:CD1	2.81	0.48
1:B:289:LEU:O	1:B:292:ALA:HB3	2.13	0.48
1:A:103:LEU:O	1:A:107:ILE:HG13	2.13	0.48
1:A:283:ASP:OD1	1:B:308:HIS:CE1	2.67	0.48
1:B:225:ASP:C	1:B:363:GLN:HE21	2.21	0.47
1:B:357:LEU:HA	1:B:358:PRO:C	2.39	0.47
1:A:225:ASP:C	1:A:363:GLN:HE21	2.22	0.47
1:A:314:PHE:O	1:A:318:GLU:HG3	2.13	0.47
1:B:245:MET:HA	1:B:305:VAL:O	2.14	0.47
1:A:169:GLU:HB2	1:A:171:THR:HG23	1.97	0.47
1:A:365:ARG:HD3	4:A:1056:HOH:O	2.13	0.47
1:B:179:VAL:HG13	1:B:179:VAL:O	2.14	0.47
1:A:291:ILE:HD11	1:B:280:LEU:HB2	1.97	0.47
1:B:247:THR:OG1	1:B:248:GLU:N	2.46	0.47
1:A:157:PHE:O	1:A:160:ALA:HB3	2.14	0.47
1:A:25:ILE:CG2	1:A:26:ALA:N	2.78	0.47
1:A:180:ILE:C	1:A:180:ILE:HD12	2.39	0.47
1:A:245:MET:O	1:A:246:GLY:C	2.56	0.47
1:B:36:GLN:O	1:B:37:GLU:CB	2.62	0.47
1:B:171:THR:CB	1:B:172:PRO:HD2	2.42	0.47
1:B:206:GLU:O	1:B:208:PRO:HD3	2.14	0.47
1:B:247:THR:HG22	1:B:339:LEU:CD2	2.45	0.47
1:A:122:ILE:HG22	1:A:235:TYR:CD1	2.50	0.47
1:B:156:THR:CG2	1:B:157:PHE:N	2.77	0.47
1:A:59:TYR:CE1	1:A:63:SER:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:THR:CG2	1:B:19:LYS:N	2.78	0.47
1:B:178:LEU:HG	1:B:192:ILE:HD11	1.96	0.47
1:A:134:HIS:HA	1:A:225:ASP:HB3	1.97	0.46
1:A:367:TYR:CD2	1:A:367:TYR:N	2.78	0.46
1:A:205:PRO:HD3	1:A:295:TYR:CG	2.50	0.46
1:A:256:ASP:HB3	1:A:258:TYR:CE1	2.50	0.46
1:B:160:ALA:O	1:B:164:LEU:HD13	2.15	0.46
1:A:59:TYR:O	1:A:59:TYR:CD1	2.68	0.46
1:A:69:ALA:HA	1:A:358:PRO:O	2.16	0.46
1:A:360:PHE:C	1:A:361:PHE:CD1	2.93	0.46
1:B:21:GLU:O	1:B:23:PHE:N	2.49	0.46
1:A:260:TYR:O	1:A:261:ASN:C	2.59	0.46
1:B:63:SER:O	1:B:67:LYS:HG3	2.16	0.46
1:B:21:GLU:O	1:B:22:GLN:C	2.58	0.46
1:B:114:GLY:O	1:B:116:ILE:N	2.47	0.46
1:B:205:PRO:HB3	1:B:295:TYR:CE1	2.51	0.46
1:A:15:GLN:O	1:A:18:THR:N	2.48	0.46
1:A:186:LYS:CB	1:A:187:PRO:HD3	2.45	0.46
1:B:23:PHE:HE2	1:B:57:HIS:NE2	2.14	0.46
1:A:80:LEU:HD22	1:A:313:GLN:HB3	1.98	0.46
1:B:228:LEU:HB3	1:B:360:PHE:CE1	2.51	0.46
1:B:247:THR:O	1:B:248:GLU:C	2.59	0.46
1:B:263:LEU:N	1:B:264:PRO:HD2	2.30	0.46
1:A:158:THR:C	1:A:160:ALA:H	2.23	0.46
1:A:257:ASP:O	1:A:261:ASN:HB2	2.16	0.46
1:B:277:ASN:C	1:B:279:SER:N	2.72	0.46
1:A:64:TYR:HD1	1:A:68:MET:HE2	1.81	0.45
1:A:23:PHE:O	1:A:27:SER:OG	2.28	0.45
1:B:21:GLU:C	1:B:23:PHE:N	2.72	0.45
1:A:41:ARG:NH1	1:A:45:ILE:HG12	2.31	0.45
1:A:205:PRO:HD3	1:A:295:TYR:CD2	2.51	0.45
1:B:23:PHE:O	1:B:27:SER:CB	2.65	0.45
1:B:100:PHE:CE1	1:B:190:THR:HG22	2.51	0.45
1:A:249:ILE:HA	1:A:253:ASN:HD22	1.82	0.45
1:B:30:GLU:C	1:B:32:GLY:H	2.25	0.45
1:B:229:GLU:HG2	4:B:1057:HOH:O	2.17	0.45
1:B:34:SER:O	1:B:36:GLN:N	2.49	0.45
1:B:240:PHE:CD2	1:B:360:PHE:CE1	3.04	0.45
1:B:288:GLU:OE1	1:B:288:GLU:HA	2.16	0.45
1:A:283:ASP:OD1	1:B:308:HIS:HE1	2.00	0.45
1:B:106:HIS:HE1	1:B:241:ASN:OD1	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:LEU:HD23	1:B:339:LEU:H	1.82	0.45
1:A:19:LYS:H	1:A:19:LYS:HG2	1.42	0.45
1:A:156:THR:CG2	1:A:368:GLU:HG3	2.45	0.45
1:A:314:PHE:O	1:A:317:PHE:HB3	2.17	0.45
1:A:158:THR:C	1:A:160:ALA:N	2.74	0.45
1:A:310:ALA:O	1:A:311:ALA:C	2.59	0.45
1:B:64:TYR:CD1	1:B:68:MET:HE2	2.51	0.45
1:B:305:VAL:HG22	1:B:306:ASP:N	2.32	0.45
1:A:75:ARG:HD3	1:A:334:TRP:CD2	2.51	0.44
1:B:122:ILE:HD13	1:B:238:ALA:HB2	2.00	0.44
1:A:38:ILE:O	1:A:42:VAL:HG23	2.17	0.44
1:B:87:VAL:CG1	1:B:88:ILE:N	2.80	0.44
1:A:281:TRP:H	1:A:281:TRP:CD1	2.36	0.44
1:A:359:ASN:HB3	1:A:361:PHE:CE1	2.52	0.44
1:B:144:THR:O	1:B:145:GLU:O	2.34	0.44
1:B:220:VAL:HG12	1:B:222:ILE:CG1	2.48	0.44
1:B:359:ASN:O	1:B:361:PHE:CE1	2.71	0.44
1:A:230:ILE:CG2	1:A:358:PRO:HB3	2.48	0.44
1:B:279:SER:O	1:B:280:LEU:C	2.60	0.44
1:A:89:ASP:OD2	1:A:91:ARG:NH2	2.42	0.44
1:B:87:VAL:O	1:B:88:ILE:HG13	2.18	0.44
1:B:21:GLU:CG	1:B:22:GLN:H	2.17	0.44
1:B:120:ILE:HD13	1:B:121:THR:CA	2.46	0.44
1:B:120:ILE:HA	1:B:239:PRO:O	2.18	0.44
1:B:243:TRP:CD1	1:B:243:TRP:O	2.71	0.44
1:B:151:ASP:O	1:B:153:SER:N	2.51	0.43
1:A:136:LEU:HD12	1:A:222:ILE:HG21	1.99	0.43
1:A:355:MET:O	1:A:355:MET:SD	2.76	0.43
1:A:45:ILE:HG23	1:A:55:TYR:CD2	2.54	0.43
1:A:123:PHE:O	1:A:124:ARG:C	2.61	0.43
1:A:287:VAL:HG11	1:B:284:LYS:CG	2.49	0.43
1:B:145:GLU:H	1:B:145:GLU:CD	2.25	0.43
1:B:103:LEU:O	1:B:107:ILE:HG13	2.19	0.43
1:B:230:ILE:HA	1:B:358:PRO:HB3	2.01	0.43
1:B:305:VAL:HG22	1:B:306:ASP:O	2.18	0.43
1:B:130:ARG:HE	1:B:130:ARG:HA	1.83	0.43
1:A:126:ASN:C	1:A:236:MET:HE3	2.44	0.43
1:B:139:TYR:CE1	1:B:173:PHE:HB3	2.53	0.43
1:B:151:ASP:C	1:B:153:SER:N	2.74	0.43
1:B:315:GLN:O	1:B:318:GLU:HB2	2.18	0.43
1:B:21:GLU:CG	1:B:22:GLN:N	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LEU:HD22	1:A:285:ALA:HB3	2.00	0.43
3:A:901:HEM:HMC2	3:A:901:HEM:CBC	2.47	0.43
1:A:16:LEU:HA	1:A:19:LYS:HG3	2.01	0.42
1:A:151:ASP:OD1	1:A:153:SER:OG	2.37	0.42
1:B:64:TYR:HD1	1:B:68:MET:HE2	1.84	0.42
1:A:70:TRP:CD1	1:A:70:TRP:O	2.72	0.42
1:A:266:VAL:O	1:A:270:MET:HG2	2.19	0.42
1:B:157:PHE:HD2	1:B:367:TYR:CE2	2.37	0.42
1:B:105:HIS:O	1:B:106:HIS:C	2.63	0.42
1:B:159:ARG:HA	1:B:159:ARG:HD3	1.81	0.42
1:A:98:GLU:O	1:A:99:VAL:C	2.62	0.42
1:A:108:GLU:O	1:A:109:VAL:C	2.63	0.42
1:A:190:THR:O	1:A:191:PRO:C	2.59	0.42
1:A:112:ASN:O	1:A:113:GLY:C	2.62	0.42
1:B:130:ARG:HB2	1:B:181:GLN:HB3	2.01	0.42
1:A:196:LEU:HD12	1:A:196:LEU:HA	1.83	0.42
1:A:298:LYS:O	1:A:301:GLY:N	2.51	0.42
1:B:220:VAL:HG12	1:B:222:ILE:HG13	2.02	0.42
1:B:286:LEU:HD22	1:B:290:ASN:ND2	2.34	0.42
1:A:179:VAL:HG23	1:A:187:PRO:HB2	2.01	0.41
1:A:204:HIS:CD2	1:A:207:PHE:HD2	2.37	0.41
1:B:228:LEU:CD1	1:B:228:LEU:N	2.83	0.41
1:A:134:HIS:ND1	1:A:225:ASP:OD1	2.53	0.41
1:B:273:ASP:OD2	1:B:275:ASN:HB2	2.20	0.41
1:B:336:ILE:O	1:B:336:ILE:HG13	2.20	0.41
1:A:317:PHE:O	1:A:321:GLU:HG2	2.20	0.41
1:A:319:GLN:HE21	1:A:319:GLN:HB3	1.64	0.41
1:A:108:GLU:O	1:A:111:THR:N	2.53	0.41
1:A:282:LYS:HD2	1:B:308:HIS:CD2	2.56	0.41
1:A:284:LYS:HG2	1:B:287:VAL:HG11	2.02	0.41
1:A:287:VAL:HG11	1:B:284:LYS:HG3	2.00	0.41
1:A:332:TRP:CZ3	1:A:336:ILE:HD13	2.56	0.41
1:B:75:ARG:NH1	1:B:334:TRP:CE2	2.89	0.41
1:B:218:TYR:O	1:B:297:TYR:OH	2.27	0.41
1:B:57:HIS:HE1	1:B:230:ILE:CD1	2.33	0.41
1:A:15:GLN:O	1:A:16:LEU:C	2.64	0.41
1:B:193:PRO:O	1:B:194:LYS:C	2.64	0.41
1:A:48:GLU:OE1	1:A:56:ARG:HG2	2.21	0.41
1:A:156:THR:HG21	1:A:368:GLU:OE1	2.20	0.41
1:A:164:LEU:CD2	1:A:187:PRO:HG2	2.45	0.41
1:A:79:ARG:O	1:A:80:LEU:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ASP:CG	1:A:91:ARG:HE	2.29	0.41
1:B:204:HIS:ND1	1:B:205:PRO:CD	2.82	0.41
1:A:308:HIS:HE1	1:B:283:ASP:OD1	2.04	0.41
1:B:144:THR:CG2	1:B:145:GLU:N	2.83	0.41
1:B:145:GLU:N	1:B:145:GLU:OE1	2.39	0.41
1:B:314:PHE:O	1:B:317:PHE:HB3	2.21	0.41
1:B:365:ARG:HA	1:B:366:PRO:HD3	1.81	0.41
1:B:346:ILE:O	1:B:347:PHE:C	2.65	0.40
1:A:224:SER:C	1:A:226:MET:H	2.29	0.40
1:B:37:GLU:O	1:B:39:LYS:N	2.53	0.40
1:B:70:TRP:CZ2	1:B:78:GLY:O	2.75	0.40
1:B:110:ALA:O	1:B:116:ILE:HA	2.21	0.40
1:A:51:GLN:HE21	1:A:51:GLN:HB2	1.58	0.40
1:A:212:ASP:C	1:A:214:GLN:H	2.30	0.40
1:A:332:TRP:O	1:A:336:ILE:HG12	2.22	0.40
1:B:79:ARG:NH2	1:B:314:PHE:CZ	2.88	0.40
1:A:57:HIS:ND1	1:A:61:GLU:HG2	2.36	0.40
1:B:120:ILE:CD1	1:B:122:ILE:HG12	2.52	0.40
1:A:59:TYR:CD1	1:A:59:TYR:C	3.00	0.40
1:B:30:GLU:O	1:B:32:GLY:N	2.53	0.40
1:B:58:THR:H	1:B:61:GLU:HB2	1.86	0.40
1:B:226:MET:C	1:B:363:GLN:NE2	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	357/375 (95%)	290 (81%)	53 (15%)	14 (4%)	2	18
1	B	356/375 (95%)	285 (80%)	54 (15%)	17 (5%)	2	14
All	All	713/750 (95%)	575 (81%)	107 (15%)	31 (4%)	2	16

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	GLU
1	A	108	GLU
1	A	183	GLY
1	A	185	GLN
1	A	186	LYS
1	B	37	GLU
1	B	145	GLU
1	B	236	MET
1	A	187	PRO
1	A	193	PRO
1	A	246	GLY
1	B	35	GLU
1	B	54	THR
1	B	244	TYR
1	B	259	ARG
1	B	346	ILE
1	A	115	LYS
1	A	261	ASN
1	B	36	GLN
1	B	90	ALA
1	B	126	ASN
1	B	184	GLY
1	B	347	PHE
1	A	145	GLU
1	A	155	LEU
1	B	63	SER
1	B	152	SER
1	B	186	LYS
1	A	33	LYS
1	A	109	VAL
1	B	25	ILE

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	308/327 (94%)	274 (89%)	34 (11%)	6	26
1	B	300/327 (92%)	266 (89%)	34 (11%)	5	24
All	All	608/654 (93%)	540 (89%)	68 (11%)	6	25

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

Mol	Chain	Res	Type
1	A	13	ASP
1	A	15	GLN
1	A	17	MET
1	A	19	LYS
1	A	21	GLU
1	A	31	LEU
1	A	37	GLU
1	A	51	GLN
1	A	56	ARG
1	A	61	GLU
1	A	108	GLU
1	A	115	LYS
1	A	119	THR
1	A	122	ILE
1	A	133	ASN
1	A	148	ILE
1	A	163	GLN
1	A	179	VAL
1	A	185	GLN
1	A	188	VAL
1	A	193	PRO
1	A	230	ILE
1	A	244	TYR
1	A	258	TYR
1	A	316	LEU
1	A	322	LYS
1	A	327	HIS
1	A	329	THR
1	A	349	ARG
1	A	355	MET
1	A	357	LEU
1	A	361	PHE
1	A	367	TYR
1	A	368	GLU
1	B	12	HIS

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Mol	Chain	Res	Type
1	B	13	ASP
1	B	17	MET
1	B	18	THR
1	B	25	ILE
1	B	31	LEU
1	B	41	ARG
1	B	43	ASN
1	B	57	HIS
1	B	83	GLN
1	B	92	GLU
1	B	102	TYR
1	B	117	ARG
1	B	120	ILE
1	B	126	ASN
1	B	130	ARG
1	B	144	THR
1	B	146	GLU
1	B	148	ILE
1	B	153	SER
1	B	154	SER
1	B	159	ARG
1	B	169	GLU
1	B	175	VAL
1	B	194	LYS
1	B	209	TRP
1	B	228	LEU
1	B	230	ILE
1	B	236	MET
1	B	273	ASP
1	B	286	LEU
1	B	319	GLN
1	B	355	MET
1	B	357	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	22	GLN
1	A	51	GLN
1	A	86	HIS
1	A	106	HIS

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Mol	Chain	Res	Type
1	A	133	ASN
1	A	181	GLN
1	A	261	ASN
1	A	308	HIS
1	A	315	GLN
1	A	319	GLN
1	A	320	GLN
1	A	327	HIS
1	A	348	HIS
1	A	363	GLN
1	B	11	GLN
1	B	57	HIS
1	B	72	HIS
1	B	86	HIS
1	B	105	HIS
1	B	106	HIS
1	B	133	ASN
1	B	181	GLN
1	B	185	GLN
1	B	261	ASN
1	B	290	ASN
1	B	308	HIS
1	B	315	GLN
1	B	320	GLN
1	B	348	HIS
1	B	359	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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	ARG	A	376	-	10,11,11	0.72	0	9,13,13	0.47	0
3	HEM	B	903	1	50,50,50	1.82	9 (18%)	67,82,82	1.04	2 (2%)
2	ARG	B	376	-	10,11,11	0.79	1 (10%)	9,13,13	0.50	0
3	HEM	A	901	1	50,50,50	1.45	6 (12%)	67,82,82	0.94	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ARG	A	376	-	-	0/11/11/11	-
3	HEM	B	903	1	-	2/14/54/54	-
2	ARG	B	376	-	-	1/11/11/11	-
3	HEM	A	901	1	-	4/14/54/54	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	903	HEM	FE-NA	5.30	2.12	1.95
3	B	903	HEM	FE-ND	5.06	2.10	1.94
3	A	901	HEM	FE-NC	4.43	2.09	1.95
3	A	901	HEM	FE-NB	4.10	2.07	1.94
3	B	903	HEM	FE-NB	3.91	2.06	1.94
3	A	901	HEM	CAB-C3B	-3.63	1.37	1.47
3	B	903	HEM	CHD-C4C	3.58	1.45	1.38
3	A	901	HEM	FE-ND	3.45	2.05	1.94
3	B	903	HEM	CAB-C3B	-3.10	1.39	1.47
3	B	903	HEM	CAC-C3C	-2.94	1.39	1.47
3	B	903	HEM	CHD-C1D	2.89	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	HEM	FE-NA	2.75	2.04	1.95
3	A	901	HEM	CAC-C3C	-2.60	1.40	1.47
3	B	903	HEM	FE-NC	2.53	2.03	1.95
3	B	903	HEM	C1A-C2A	2.21	1.49	1.44
2	B	376	ARG	OXT-C	-2.06	1.24	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	903	HEM	CBA-CAA-C2A	-3.09	104.00	112.53
3	B	903	HEM	CAA-C2A-C1A	2.30	129.43	124.94
3	A	901	HEM	CAA-C2A-C1A	2.06	128.96	124.94

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	HEM	C2B-C3B-CAB-CBB
3	B	903	HEM	C2B-C3B-CAB-CBB
3	A	901	HEM	C4B-C3B-CAB-CBB
3	B	903	HEM	C4B-C3B-CAB-CBB
2	B	376	ARG	O-C-CA-N
3	A	901	HEM	CAA-CBA-CGA-O2A
3	A	901	HEM	CAA-CBA-CGA-O1A

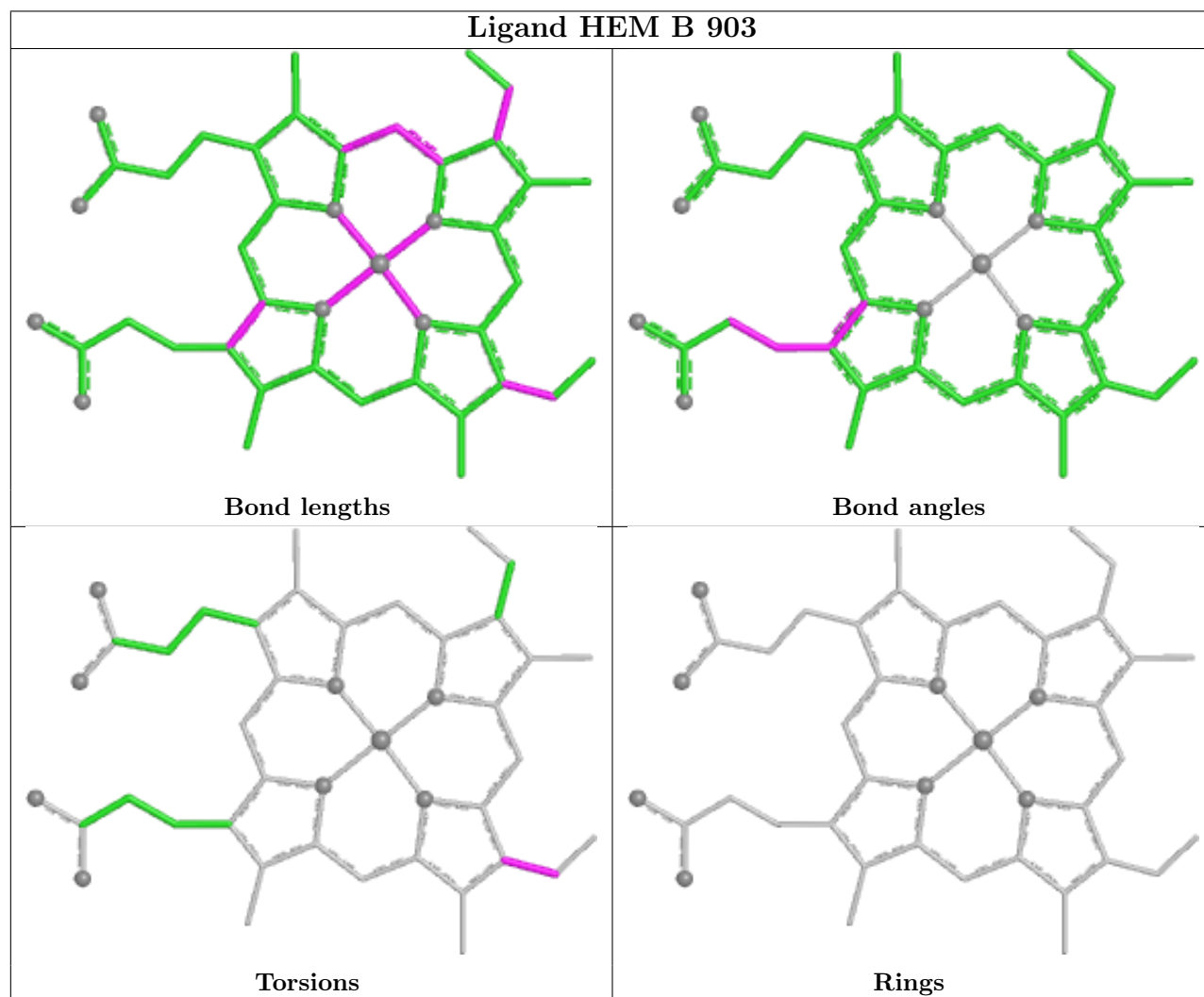
There are no ring outliers.

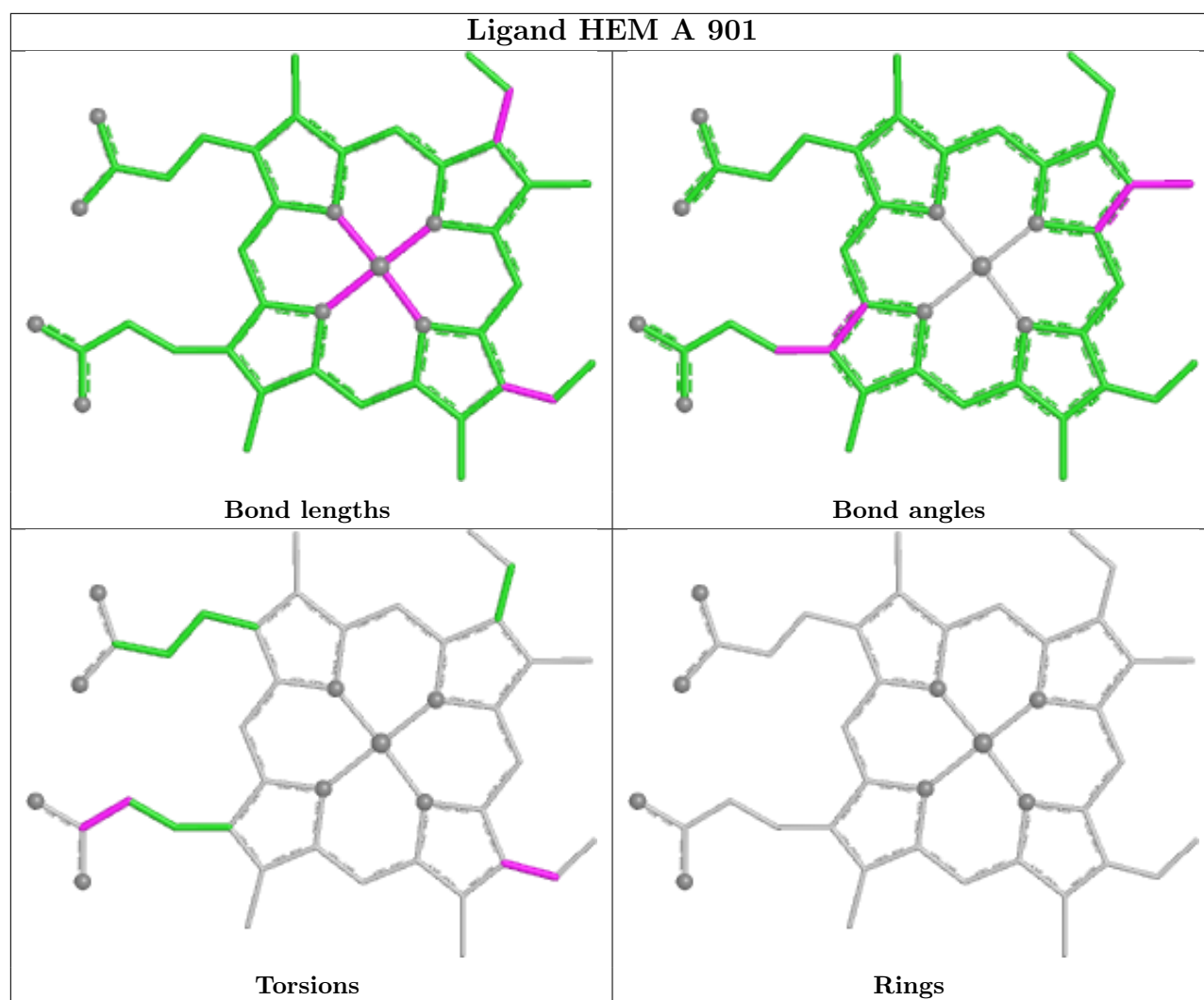
3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	376	ARG	3	0
3	B	903	HEM	2	0
3	A	901	HEM	7	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	359/375 (95%)	-0.20	1 (0%) 90 81	5, 11, 54, 87	0
1	B	358/375 (95%)	-0.07	4 (1%) 78 61	5, 15, 74, 103	0
All	All	717/750 (95%)	-0.13	5 (0%) 84 69	5, 13, 64, 103	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	209	TRP	3.0
1	B	86	HIS	2.7
1	B	319	GLN	2.6
1	A	186	LYS	2.2
1	B	368	GLU	2.1

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](#)

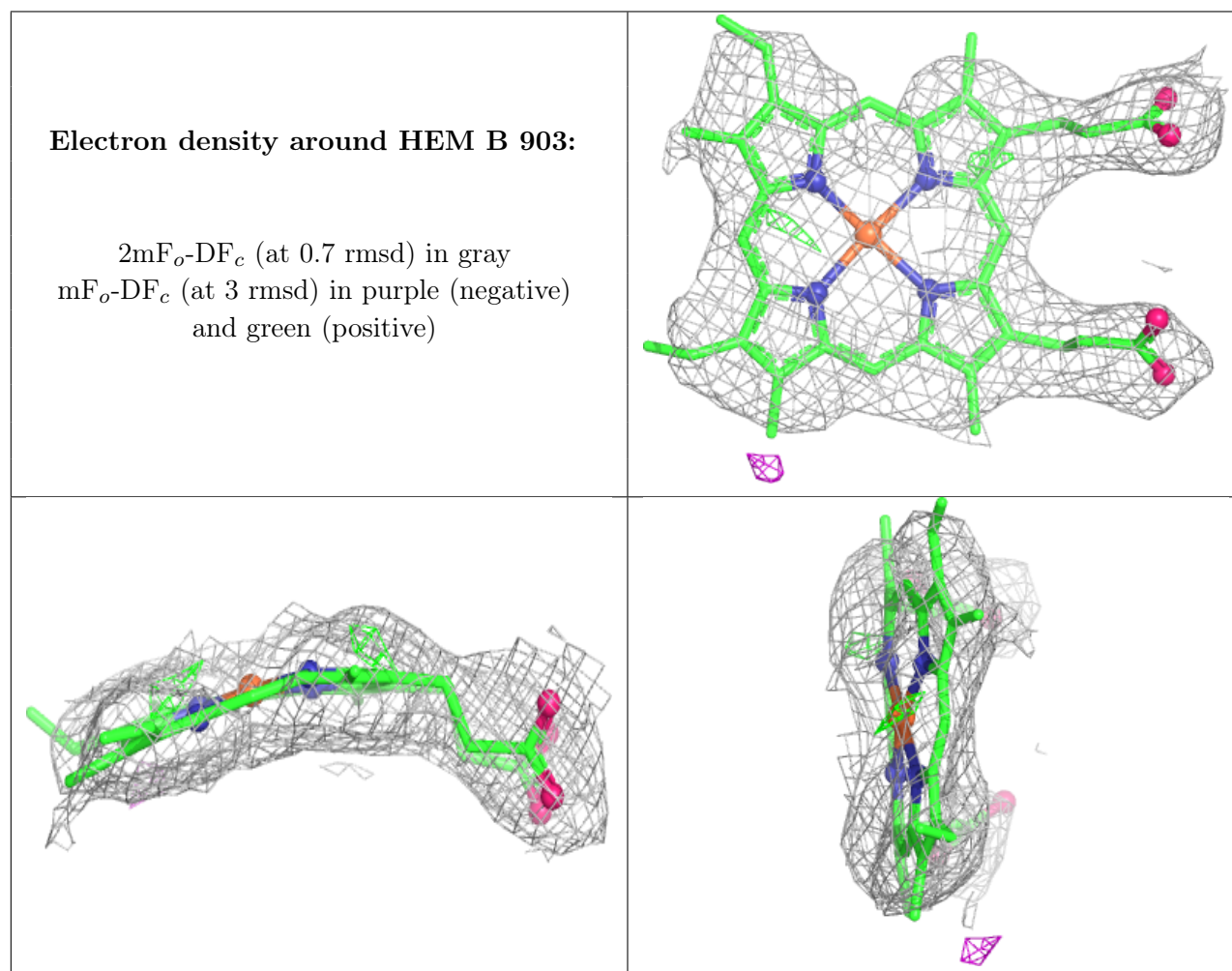
There are no oligosaccharides in this entry.

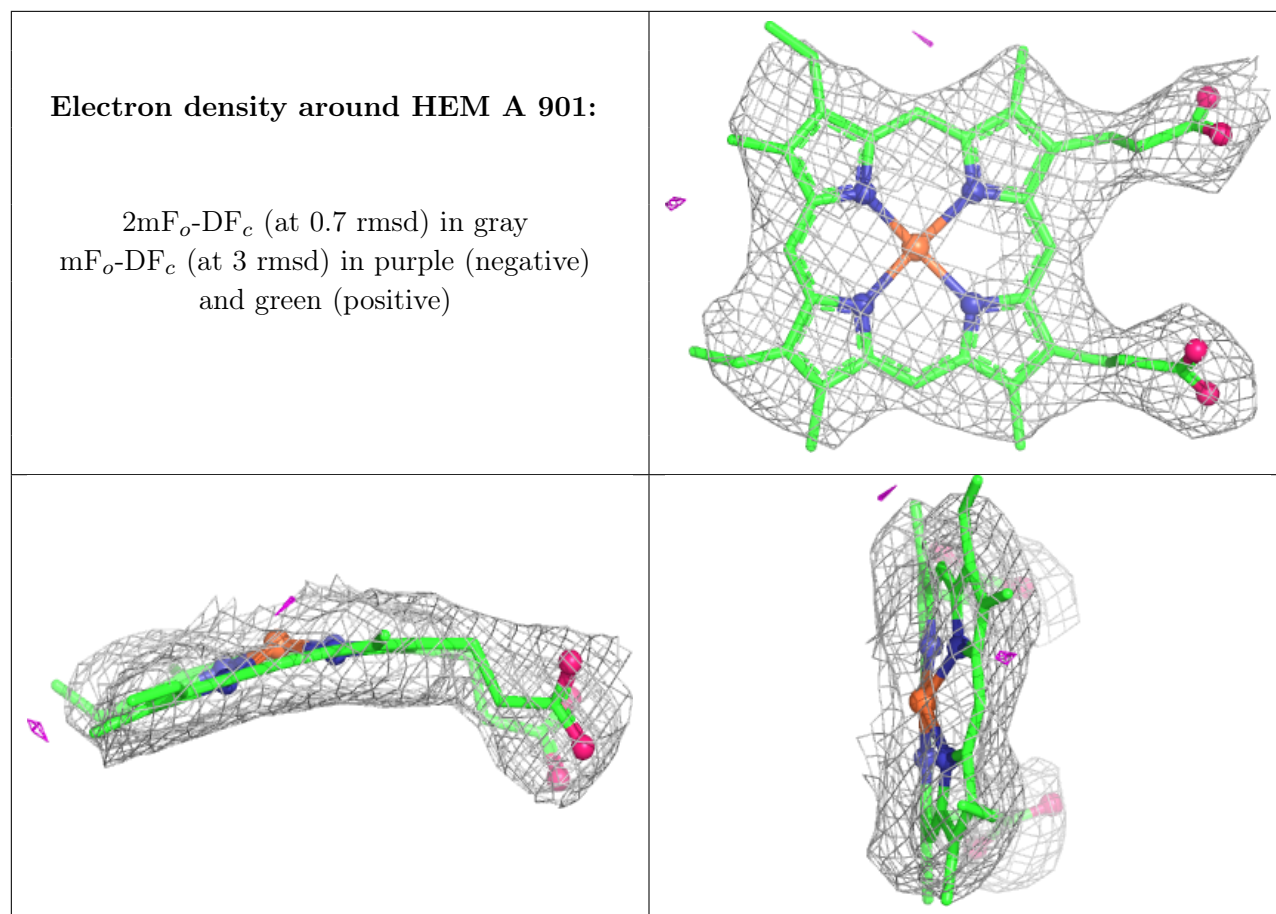
6.4 Ligands [i](#)

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	ARG	A	376	12/12	0.91	0.14	24,24,25,25	0
2	ARG	B	376	12/12	0.91	0.15	11,45,45,45	0
3	HEM	B	903	43/43	0.96	0.11	16,16,16,16	0
3	HEM	A	901	43/43	0.98	0.08	16,16,16,16	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 [i](#)

There are no such residues in this entry.