



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:25 AM UTC

PDB ID : 6IQ5 / pdb_00006iq5
Title : Crystal Structure of CYP1B1 and Inhibitor Having Azide Group
Authors : Kubo, M.; Yamamoto, K.; Itoh, T.
Deposited on : 2018-11-06
Resolution : 3.70 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

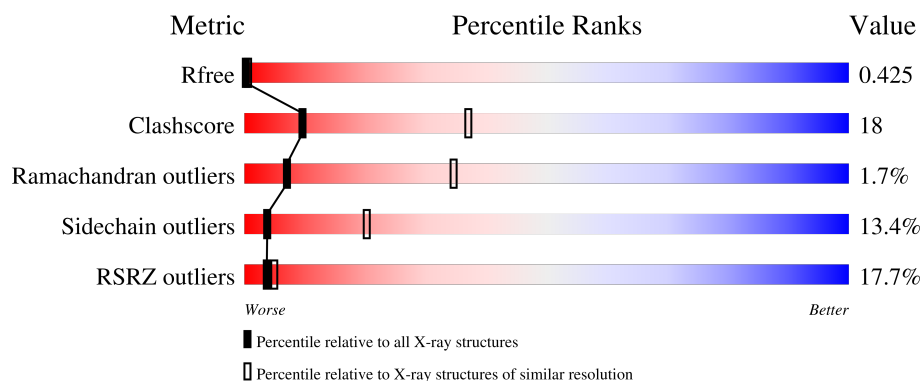
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	463	16% 62% 30% 7%
1	B	463	19% 59% 30% 5% 6%

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
3	AQ0	A	902	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7186 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.

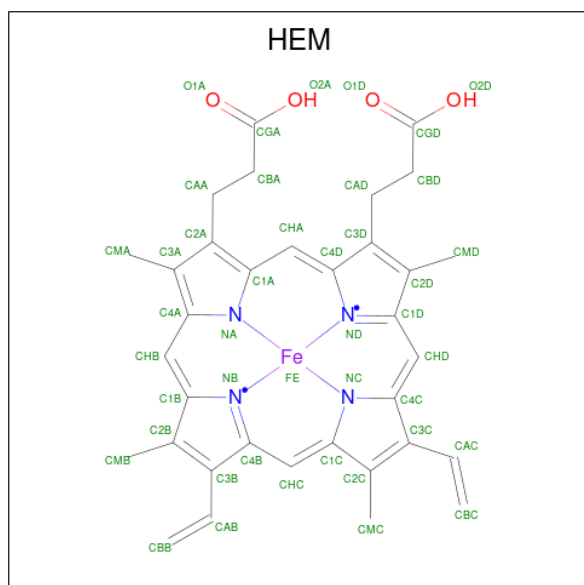
- Molecule 1 is a protein called Cytochrome P450 1B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	0	0
			3650	2322	656	652	20			
1	B	437	Total	C	N	O	S	0	0	0
			3423	2187	612	605	19			

There are 4 discrepancies between the modelled and reference sequences:

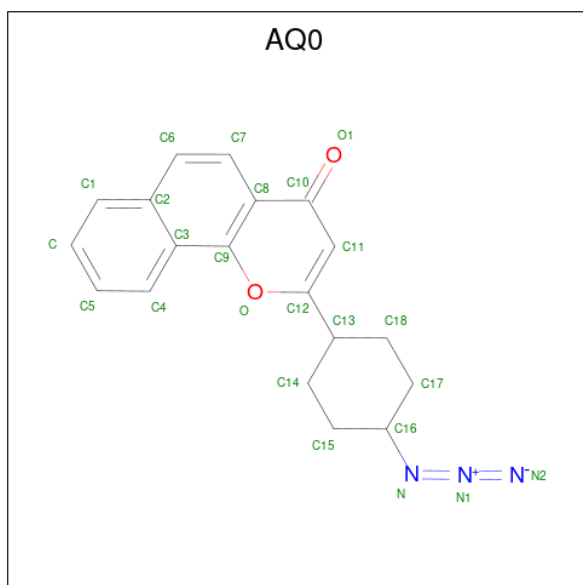
Chain	Residue	Modelled	Actual	Comment	Reference
A	119	SER	ALA	variant	UNP Q16678
A	432	VAL	LEU	variant	UNP Q16678
B	119	SER	ALA	variant	UNP Q16678
B	432	VAL	LEU	variant	UNP Q16678

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 3 is 2-(cis-4-azidocyclohexyl)-4H-naphtho[1,2-b]pyran-4-one (CCD ID: AQ0) (formula: C₁₉H₁₇N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	19	3	2		

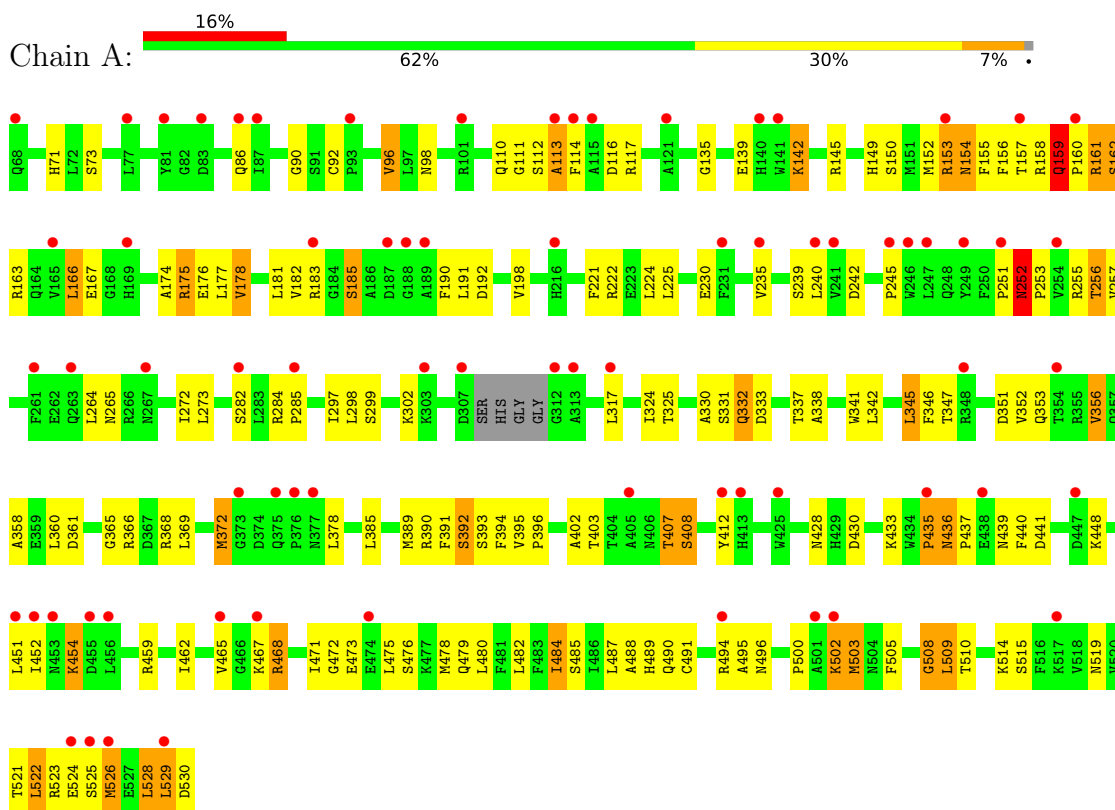
- Molecule 4 is water.

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

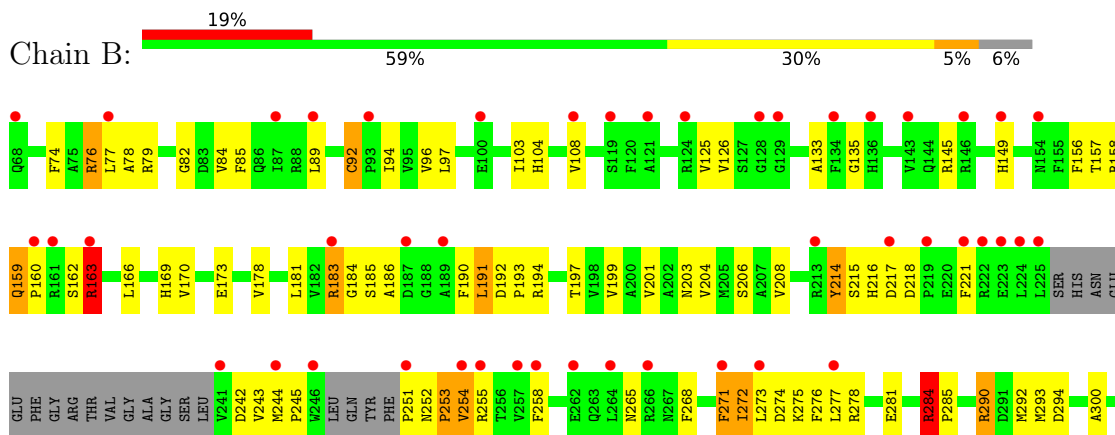
3 Residue-property plots

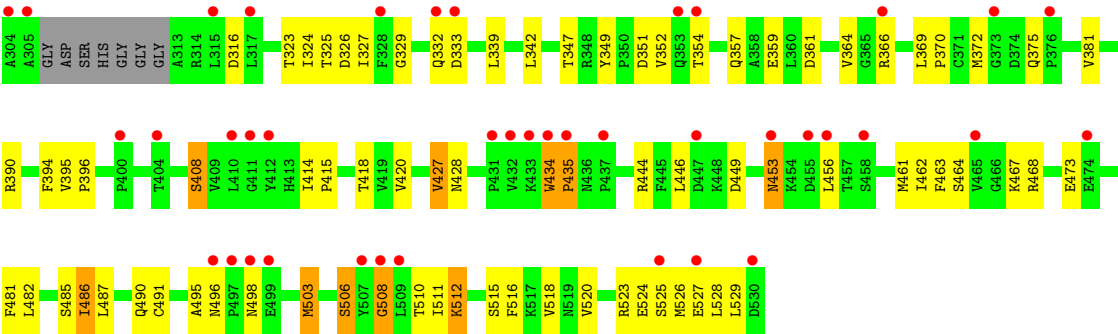
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cytochrome P450 1B1



• Molecule 1: Cytochrome P450 1B1





4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	135.19Å 135.19Å 302.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.80 – 3.70 47.80 – 3.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.80-3.70) 99.3 (47.80-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.06 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.356 , 0.396 0.419 , 0.425	Depositor DCC
R_{free} test set	1472 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	111.3	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 354.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	7186	wwPDB-VP
Average B, all atoms (Å ²)	316.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: HEM, AQ0

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	0.83	0/3739	1.11	16/5066 (0.3%)
1	B	0.88	0/3506	1.16	17/4759 (0.4%)
All	All	0.85	0/7245	1.13	33/9825 (0.3%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ALA	N-CA-C	-7.81	103.77	113.38
1	A	284	ARG	CA-C-N	7.50	129.21	119.84
1	A	284	ARG	C-N-CA	7.50	129.21	119.84
1	B	329	GLY	N-CA-C	7.17	121.33	112.73
1	B	183	ARG	N-CA-C	6.99	119.75	111.71
1	A	282	SER	N-CA-C	6.77	118.31	111.07
1	B	252	ASN	CA-C-N	6.59	127.12	119.47
1	B	252	ASN	C-N-CA	6.59	127.12	119.47
1	B	254	VAL	N-CA-C	-6.29	103.45	110.62
1	A	159	GLN	CA-C-N	-5.85	113.74	119.76
1	A	159	GLN	C-N-CA	-5.85	113.74	119.76
1	B	163	ARG	N-CA-C	-5.79	104.33	111.33
1	A	392	SER	N-CA-C	-5.78	104.67	110.97
1	A	488	ALA	N-CA-C	-5.66	104.75	111.03
1	A	356	VAL	N-CA-CB	5.62	118.19	110.54
1	B	486	ILE	N-CA-CB	5.62	116.75	110.62
1	B	503	MET	N-CA-C	5.54	118.35	110.10
1	A	502	LYS	N-CA-C	5.37	117.25	110.33
1	B	271	PHE	N-CA-C	5.35	119.43	113.01
1	B	253	PRO	CA-C-N	-5.32	113.03	120.53
1	B	253	PRO	C-N-CA	-5.32	113.03	120.53
1	B	284	ARG	CA-C-N	-5.26	113.61	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	284	ARG	C-N-CA	-5.26	113.61	119.19
1	B	332	GLN	CA-C-N	-5.26	113.28	120.44
1	B	332	GLN	C-N-CA	-5.26	113.28	120.44
1	B	408	SER	N-CA-C	5.24	116.61	107.49
1	A	441	ASP	CA-C-N	5.21	124.39	118.97
1	A	441	ASP	C-N-CA	5.21	124.39	118.97
1	A	353	GLN	N-CA-C	-5.21	105.50	111.07
1	B	300	ALA	N-CA-C	5.14	116.88	111.28
1	A	378	LEU	CA-C-N	5.11	125.39	119.47
1	A	378	LEU	C-N-CA	5.11	125.39	119.47
1	A	451	LEU	N-CA-C	5.02	117.00	110.43

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	3650	0	3606	137	0
1	B	3423	0	3349	115	0
2	A	43	0	30	4	0
2	B	43	0	30	5	0
3	A	24	0	0	1	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
All	All	7186	0	7015	252	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 18.

All (252) 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:526:MET:CE	1:A:529:LEU:HD21	1.69	1.22
1:B:327:ILE:HG23	2:B:900:HEM:HBC1	1.17	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:MET:HE1	1:A:529:LEU:HD21	1.23	1.06
1:A:526:MET:CE	1:A:529:LEU:CD2	2.38	1.00
1:A:489:HIS:HA	1:A:523:ARG:NH1	1.77	0.99
1:A:490:GLN:HE21	1:A:528:LEU:CD2	1.77	0.96
1:B:159:GLN:HB3	1:B:162:SER:HB2	1.44	0.96
1:A:175:ARG:HA	1:A:528:LEU:HD12	1.48	0.95
1:B:327:ILE:HG23	2:B:900:HEM:CBC	1.96	0.95
1:A:526:MET:HE3	1:A:529:LEU:CD2	1.97	0.94
1:B:159:GLN:CB	1:B:162:SER:HB2	1.98	0.93
1:B:323:THR:O	1:B:327:ILE:HG13	1.69	0.93
1:B:199:VAL:HG13	1:B:221:PHE:CZ	2.04	0.93
1:A:157:THR:H	1:A:162:SER:HB3	1.32	0.92
1:B:366:ARG:HH21	1:B:524:GLU:CB	1.84	0.89
1:A:490:GLN:HE21	1:A:528:LEU:HD21	1.38	0.88
1:B:159:GLN:HB2	1:B:162:SER:CB	2.03	0.88
1:A:158:ARG:CZ	1:A:159:GLN:NE2	2.38	0.86
1:B:159:GLN:CB	1:B:162:SER:CB	2.53	0.85
1:A:175:ARG:HB2	1:A:528:LEU:HB3	1.59	0.85
1:A:489:HIS:HA	1:A:523:ARG:HH11	1.40	0.84
1:B:199:VAL:HG13	1:B:221:PHE:HZ	1.40	0.83
1:A:175:ARG:HA	1:A:528:LEU:CD1	2.09	0.81
1:A:150:SER:O	1:A:154:ASN:HB2	1.81	0.81
1:B:243:VAL:O	1:B:245:PRO:HD3	1.81	0.80
1:A:158:ARG:CZ	1:A:159:GLN:HE22	1.97	0.78
1:B:275:LYS:HA	1:B:278:ARG:HB2	1.66	0.76
1:B:126:VAL:HA	1:B:265:ASN:HD21	1.53	0.74
1:A:528:LEU:HD23	1:A:528:LEU:N	2.01	0.74
1:A:490:GLN:HE21	1:A:528:LEU:HD23	1.51	0.73
1:A:468:ARG:NH1	2:A:901:HEM:O1D	2.22	0.72
1:B:92:CYS:HB2	1:B:243:VAL:HG12	1.73	0.70
1:A:116:ASP:O	1:A:402:ALA:N	2.25	0.69
1:A:366:ARG:HH22	1:A:523:ARG:NH1	1.90	0.69
1:A:508:GLY:O	1:A:510:THR:N	2.25	0.69
1:A:110:GLN:NE2	1:A:408:SER:O	2.26	0.69
1:A:158:ARG:NH1	1:A:159:GLN:NE2	2.40	0.69
1:A:489:HIS:CA	1:A:523:ARG:HH11	2.05	0.69
1:B:159:GLN:HB2	1:B:162:SER:HB3	1.74	0.69
1:A:149:HIS:HA	1:A:152:MET:HB2	1.75	0.68
1:A:526:MET:CE	1:A:529:LEU:CG	2.71	0.68
1:A:175:ARG:HB2	1:A:528:LEU:CB	2.22	0.68
1:A:111:GLY:O	1:A:112:SER:HB3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:SER:HB3	1:B:191:LEU:HD12	1.75	0.67
1:A:526:MET:HE3	1:A:529:LEU:CG	2.23	0.67
1:B:159:GLN:HB3	1:B:162:SER:CB	2.19	0.66
1:B:243:VAL:C	1:B:245:PRO:HD3	2.20	0.65
1:A:522:LEU:HD22	1:A:525:SER:O	1.98	0.64
1:B:126:VAL:HA	1:B:265:ASN:ND2	2.14	0.63
1:B:526:MET:O	1:B:529:LEU:HD12	1.99	0.63
1:B:159:GLN:CB	1:B:162:SER:HB3	2.29	0.63
2:B:900:HEM:HBB2	2:B:900:HEM:HMB1	1.81	0.63
1:A:158:ARG:HG3	1:A:159:GLN:HG3	1.80	0.62
1:A:160:PRO:O	1:A:161:ARG:HB2	1.99	0.62
1:A:372:MET:HG2	1:A:482:LEU:HD21	1.79	0.62
1:A:526:MET:HE3	1:A:529:LEU:HG	1.79	0.62
1:A:490:GLN:HG3	1:A:528:LEU:HD21	1.82	0.62
1:A:407:THR:OG1	1:A:408:SER:N	2.31	0.62
1:B:156:PHE:O	1:B:157:THR:HG22	1.99	0.62
1:A:117:ARG:HH21	1:A:468:ARG:NH1	1.98	0.62
1:A:524:GLU:O	1:A:525:SER:HB3	1.99	0.62
1:A:490:GLN:NE2	1:A:528:LEU:HD21	2.12	0.61
1:A:361:ASP:CG	1:A:523:ARG:HH22	2.08	0.60
1:B:390:ARG:HD3	1:B:428:ASN:O	2.01	0.60
1:B:104:HIS:CE1	1:B:108:VAL:HG11	2.36	0.60
1:B:503:MET:HE1	1:B:516:PHE:CB	2.31	0.60
1:B:284:ARG:CB	1:B:285:PRO:HD2	2.32	0.60
1:B:482:LEU:O	1:B:486:ILE:HG12	2.00	0.59
1:A:366:ARG:NH2	1:A:523:ARG:CZ	2.65	0.59
1:A:360:LEU:HD21	1:A:485:SER:HA	1.83	0.59
1:A:157:THR:HG22	1:A:157:THR:O	2.03	0.58
1:A:489:HIS:C	1:A:523:ARG:HH11	2.10	0.58
1:B:253:PRO:O	1:B:254:VAL:C	2.42	0.58
1:B:281:GLU:O	1:B:284:ARG:CZ	2.51	0.58
1:B:414:ILE:HG22	1:B:418:THR:HG21	1.85	0.58
1:B:390:ARG:HD2	1:B:390:ARG:C	2.29	0.57
1:A:149:HIS:NE2	1:A:153:ARG:NH2	2.53	0.56
1:A:297:ILE:HG23	1:A:317:LEU:HD21	1.88	0.56
1:B:183:ARG:N	1:B:184:GLY:HA3	2.20	0.56
1:B:503:MET:HE1	1:B:516:PHE:HB3	1.85	0.56
1:B:215:SER:O	1:B:216:HIS:HB2	2.06	0.56
1:B:258:PHE:CD1	1:B:258:PHE:C	2.83	0.56
1:A:158:ARG:NH1	1:A:159:GLN:HE21	2.03	0.56
1:A:157:THR:H	1:A:162:SER:CB	2.13	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:PHE:O	1:A:157:THR:CB	2.55	0.55
1:B:369:LEU:HD21	1:B:528:LEU:HD22	1.88	0.55
1:B:347:THR:HB	1:B:495:ALA:HB2	1.89	0.55
1:A:366:ARG:HH22	1:A:523:ARG:CZ	2.20	0.55
1:A:526:MET:CE	1:A:529:LEU:HG	2.37	0.55
1:A:139:GLU:HA	1:A:142:LYS:HB2	1.89	0.54
1:A:392:SER:OG	1:A:394:PHE:HB3	2.07	0.54
1:A:494:ARG:HB2	1:A:519:ASN:HB3	1.89	0.54
1:B:364:VAL:HG21	1:B:370:PRO:HG3	1.87	0.54
1:A:361:ASP:O	1:A:365:GLY:N	2.40	0.54
1:A:454:LYS:HE2	1:B:186:ALA:HB3	1.90	0.54
1:A:178:VAL:HB	1:A:491:CYS:SG	2.47	0.54
1:B:251:PRO:HB3	1:B:255:ARG:NH2	2.23	0.54
1:B:77:LEU:HB2	1:B:85:PHE:CZ	2.44	0.53
1:A:389:MET:CG	1:A:462:ILE:HG21	2.38	0.53
1:B:192:ASP:OD1	1:B:194:ARG:HG3	2.09	0.53
1:B:508:GLY:C	1:B:510:THR:H	2.16	0.53
1:A:389:MET:HG3	1:A:462:ILE:HD13	1.89	0.53
1:B:268:PHE:CE1	1:B:325:THR:HG23	2.43	0.53
1:A:71:HIS:CB	1:A:396:PRO:HB2	2.39	0.53
1:A:489:HIS:CA	1:A:523:ARG:NH1	2.61	0.53
1:B:506:SER:O	1:B:511:ILE:HA	2.09	0.53
1:A:110:GLN:O	1:A:113:ALA:HB3	2.08	0.53
1:B:193:PRO:HG3	1:B:518:VAL:HG11	1.91	0.52
1:A:489:HIS:HA	1:A:523:ARG:HH12	1.68	0.52
1:B:181:LEU:HD22	1:B:520:VAL:HG21	1.91	0.52
1:B:284:ARG:HB3	1:B:285:PRO:HD2	1.91	0.52
1:A:149:HIS:O	1:A:153:ARG:N	2.41	0.52
1:A:166:LEU:HD11	1:A:475:LEU:HD13	1.92	0.52
1:B:290:ARG:O	1:B:294:ASP:HB2	2.10	0.52
1:A:156:PHE:O	1:A:157:THR:HB	2.10	0.51
1:A:330:ALA:HA	3:A:902:AQ0:C14	2.40	0.51
1:A:372:MET:HG2	1:A:482:LEU:CD2	2.41	0.51
1:B:208:VAL:O	1:B:292:MET:HG2	2.10	0.51
1:A:181:LEU:O	1:A:185:SER:HB2	2.10	0.51
1:A:346:PHE:CZ	1:A:356:VAL:HG21	2.46	0.50
1:A:152:MET:HG2	1:A:471:ILE:HD12	1.93	0.50
1:A:96:VAL:O	1:A:98:ASN:ND2	2.45	0.50
1:B:434:TRP:CE3	1:B:444:ARG:HD3	2.47	0.50
1:A:525:SER:OG	1:A:526:MET:N	2.45	0.50
1:A:117:ARG:NH2	1:A:468:ARG:NH1	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:LEU:O	1:A:529:LEU:C	2.55	0.50
1:B:215:SER:C	1:B:217:ASP:H	2.18	0.50
1:B:271:PHE:CG	1:B:271:PHE:O	2.65	0.50
1:B:357:GLN:NE2	1:B:523:ARG:HD2	2.27	0.49
1:A:190:PHE:CE1	1:A:496:ASN:HA	2.48	0.49
1:A:528:LEU:O	1:A:530:ASP:N	2.46	0.49
1:B:181:LEU:HB3	1:B:520:VAL:HG21	1.95	0.49
1:B:135:GLY:O	1:B:468:ARG:NH2	2.40	0.49
1:B:284:ARG:CB	1:B:285:PRO:CD	2.91	0.49
1:B:395:VAL:HG11	2:B:900:HEM:HMA3	1.94	0.49
1:A:436:ASN:HB3	1:A:439:ASN:HB2	1.95	0.48
1:B:427:VAL:HG21	1:B:461:MET:HE3	1.94	0.48
1:A:190:PHE:CZ	1:A:496:ASN:HA	2.48	0.48
1:A:111:GLY:O	1:A:112:SER:CB	2.60	0.48
1:A:239:SER:OG	1:A:240:LEU:N	2.47	0.48
1:A:366:ARG:NH2	1:A:523:ARG:NH2	2.61	0.48
1:B:190:PHE:HA	1:B:518:VAL:O	2.14	0.48
1:A:341:TRP:CZ2	1:A:505:PHE:CE1	3.01	0.48
1:A:242:ASP:O	1:A:245:PRO:HD3	2.13	0.47
1:B:490:GLN:CD	1:B:528:LEU:HD21	2.39	0.47
1:A:145:ARG:NH1	2:A:901:HEM:O2D	2.48	0.47
1:A:156:PHE:CD1	1:A:166:LEU:HD12	2.50	0.47
1:A:389:MET:HG2	1:A:462:ILE:HG21	1.97	0.47
1:A:272:ILE:HD13	1:A:325:THR:HA	1.97	0.47
1:B:97:LEU:HD13	1:B:103:ILE:HA	1.96	0.47
1:A:508:GLY:O	1:A:509:LEU:HB3	2.14	0.46
1:B:104:HIS:CD2	1:B:108:VAL:HG21	2.50	0.46
1:B:284:ARG:HB2	1:B:285:PRO:HD2	1.97	0.46
1:B:349:TYR:O	1:B:352:VAL:HG22	2.15	0.46
1:A:167:GLU:HG3	1:A:482:LEU:HD11	1.97	0.46
1:B:145:ARG:O	1:B:149:HIS:N	2.45	0.46
1:B:394:PHE:O	1:B:510:THR:HA	2.14	0.46
1:A:435:PRO:O	1:A:437:PRO:HD3	2.15	0.46
1:B:255:ARG:O	1:B:255:ARG:HG2	2.15	0.46
1:A:508:GLY:C	1:A:510:THR:N	2.73	0.46
1:B:293:MET:HE2	1:B:324:ILE:HG21	1.98	0.46
1:A:522:LEU:HD11	1:A:526:MET:HG3	1.96	0.46
1:B:76:ARG:HA	1:B:79:ARG:HD3	1.98	0.46
1:A:153:ARG:HG2	1:B:523:ARG:O	2.15	0.46
1:A:358:ALA:O	1:A:361:ASP:N	2.49	0.45
1:A:528:LEU:CD2	1:A:528:LEU:N	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:HIS:O	1:A:152:MET:N	2.49	0.45
1:B:215:SER:C	1:B:217:ASP:N	2.73	0.45
1:B:496:ASN:ND2	1:B:498:ASN:HB2	2.32	0.45
1:A:225:LEU:HD22	1:A:332:GLN:HG3	1.98	0.45
1:B:197:THR:HG22	1:B:339:LEU:HD23	1.99	0.45
1:B:284:ARG:HB3	1:B:285:PRO:CD	2.46	0.45
1:A:113:ALA:O	1:A:403:THR:HG22	2.17	0.45
1:A:174:ALA:O	1:A:178:VAL:HG13	2.17	0.45
1:B:293:MET:HE2	1:B:324:ILE:HD13	1.99	0.45
1:B:92:CYS:CB	1:B:243:VAL:HG12	2.43	0.44
1:A:157:THR:N	1:A:162:SER:HB3	2.16	0.44
1:B:481:PHE:O	1:B:485:SER:OG	2.34	0.44
1:B:357:GLN:HE21	1:B:523:ARG:HD2	1.82	0.44
1:B:511:ILE:O	1:B:511:ILE:HG22	2.17	0.44
1:B:197:THR:O	1:B:201:VAL:HG23	2.18	0.44
1:B:272:ILE:HA	1:B:275:LYS:HG2	1.99	0.44
1:A:135:GLY:O	1:A:468:ARG:NH2	2.50	0.44
1:B:78:ALA:HA	1:B:82:GLY:O	2.17	0.44
1:A:472:GLY:O	1:A:473:GLU:C	2.60	0.44
1:A:352:VAL:O	1:A:356:VAL:HG13	2.17	0.44
1:A:251:PRO:O	1:A:252:ASN:HB3	2.18	0.43
1:A:252:ASN:O	1:A:253:PRO:C	2.61	0.43
1:B:206:SER:OG	1:B:214:TYR:CE2	2.70	0.43
1:A:235:VAL:HG23	1:A:509:LEU:HD23	1.99	0.43
1:A:503:MET:HA	1:A:503:MET:HE2	1.99	0.43
1:A:338:ALA:HB3	1:A:480:LEU:HD21	2.00	0.43
1:A:342:LEU:HB3	1:A:484:ILE:HD12	2.00	0.43
1:B:394:PHE:CE1	1:B:462:ILE:HD11	2.53	0.43
1:A:347:THR:HB	1:A:495:ALA:HB2	2.00	0.43
1:A:158:ARG:NH2	1:A:159:GLN:HE22	2.17	0.43
1:A:390:ARG:HA	1:A:428:ASN:ND2	2.33	0.43
1:A:361:ASP:OD2	1:A:523:ARG:NH2	2.51	0.43
1:A:526:MET:HE2	1:A:529:LEU:HD11	2.01	0.43
1:B:463:PHE:CG	1:B:473:GLU:HG3	2.54	0.43
1:A:149:HIS:CD2	1:A:153:ARG:CZ	3.02	0.43
1:A:331:SER:O	1:A:332:GLN:C	2.62	0.43
1:A:333:ASP:OD1	1:A:333:ASP:C	2.62	0.43
1:B:169:HIS:O	1:B:170:VAL:C	2.62	0.43
1:B:369:LEU:HD21	1:B:528:LEU:CD2	2.49	0.43
2:A:901:HEM:HBB2	2:A:901:HEM:HMB2	2.01	0.42
1:A:114:PHE:CE1	1:A:407:THR:HG21	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:THR:O	1:A:338:ALA:C	2.62	0.42
1:B:268:PHE:HE1	1:B:325:THR:HG23	1.84	0.42
1:B:372:MET:HE1	1:B:375:GLN:CD	2.44	0.42
1:B:74:PHE:CD2	1:B:96:VAL:HG11	2.54	0.42
1:B:255:ARG:HA	1:B:258:PHE:HB3	2.02	0.42
1:B:366:ARG:NH2	1:B:524:GLU:CB	2.67	0.42
1:A:489:HIS:O	1:A:523:ARG:HD3	2.20	0.42
1:A:508:GLY:O	1:A:509:LEU:CB	2.66	0.42
1:B:491:CYS:HB3	1:B:520:VAL:CG1	2.50	0.42
1:B:84:VAL:HG22	1:B:97:LEU:HD23	2.01	0.42
1:A:178:VAL:O	1:A:182:VAL:HG23	2.20	0.42
1:A:366:ARG:HA	1:A:366:ARG:NE	2.35	0.42
1:A:472:GLY:O	1:A:475:LEU:N	2.53	0.42
1:B:162:SER:O	1:B:163:ARG:C	2.63	0.42
1:A:177:LEU:HD23	1:A:487:LEU:HD21	2.02	0.41
1:B:89:LEU:O	1:B:243:VAL:HB	2.20	0.41
1:B:414:ILE:CG2	1:B:418:THR:HG21	2.49	0.41
1:B:427:VAL:HG21	1:B:461:MET:CE	2.50	0.41
1:A:514:LYS:O	1:A:515:SER:C	2.64	0.41
1:B:508:GLY:C	1:B:510:THR:N	2.79	0.41
1:A:389:MET:HG3	1:A:462:ILE:HG21	2.03	0.41
1:B:268:PHE:O	1:B:271:PHE:N	2.53	0.41
1:A:152:MET:CG	1:A:471:ILE:HD12	2.50	0.41
1:A:391:PHE:CD1	1:A:391:PHE:C	2.99	0.41
1:B:242:ASP:C	1:B:244:MET:N	2.77	0.41
1:B:366:ARG:HH12	1:B:490:GLN:NE2	2.19	0.41
1:B:217:ASP:O	1:B:218:ASP:C	2.62	0.41
1:B:276:PHE:CD1	1:B:276:PHE:C	2.99	0.41
1:B:333:ASP:OD1	1:B:512:LYS:NZ	2.50	0.41
1:B:415:PRO:O	1:B:418:THR:HG22	2.20	0.41
1:B:133:ALA:HB2	2:B:900:HEM:CAD	2.50	0.41
1:B:204:VAL:O	1:B:208:VAL:HG23	2.20	0.41
1:B:435:PRO:HD2	1:B:444:ARG:HH12	1.86	0.41
1:B:453:ASN:ND2	1:B:456:LEU:HD12	2.35	0.41
1:A:225:LEU:HD22	1:A:332:GLN:CG	2.51	0.40
1:A:256:THR:HG22	1:A:257:VAL:N	2.36	0.40
1:A:221:PHE:CE2	1:A:225:LEU:HD11	2.55	0.40
1:A:395:VAL:HG11	2:A:901:HEM:HMA2	2.02	0.40
1:B:158:ARG:NH2	1:B:162:SER:OG	2.54	0.40
1:A:345:LEU:HG	1:A:440:PHE:CE1	2.56	0.40
1:A:490:GLN:NE2	1:A:528:LEU:CD2	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:LEU:O	1:A:530:ASP:C	2.65	0.40
1:B:208:VAL:HG12	1:B:292:MET:CG	2.52	0.40
1:B:277:LEU:O	1:B:281:GLU:HG3	2.21	0.40
1:B:396:PRO:HG3	1:B:511:ILE:HD11	2.04	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	455/463 (98%)	393 (86%)	54 (12%)	8 (2%)	6	34
1	B	429/463 (93%)	367 (86%)	55 (13%)	7 (2%)	7	35
All	All	884/926 (96%)	760 (86%)	109 (12%)	15 (2%)	7	34

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	PRO
1	A	436	ASN
1	A	500	PRO
1	B	284	ARG
1	B	435	PRO
1	B	464	SER
1	A	252	ASN
1	A	529	LEU
1	B	214	TYR
1	B	508	GLY
1	A	90	GLY
1	A	435	PRO
1	B	160	PRO
1	B	434	TRP

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Mol	Chain	Res	Type
1	A	508	GLY

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	394/397 (99%)	329 (84%)	65 (16%)	2	14
1	B	362/397 (91%)	326 (90%)	36 (10%)	7	30
All	All	756/794 (95%)	655 (87%)	101 (13%)	4	20

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	SER
1	A	86	GLN
1	A	92	CYS
1	A	96	VAL
1	A	142	LYS
1	A	153	ARG
1	A	154	ASN
1	A	155	PHE
1	A	159	GLN
1	A	161	ARG
1	A	162	SER
1	A	163	ARG
1	A	166	LEU
1	A	175	ARG
1	A	176	GLU
1	A	178	VAL
1	A	183	ARG
1	A	185	SER
1	A	191	LEU
1	A	192	ASP
1	A	198	VAL
1	A	222	ARG

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Mol	Chain	Res	Type
1	A	224	LEU
1	A	230	GLU
1	A	252	ASN
1	A	255	ARG
1	A	256	THR
1	A	264	LEU
1	A	265	ASN
1	A	273	LEU
1	A	298	LEU
1	A	299	SER
1	A	302	LYS
1	A	324	ILE
1	A	332	GLN
1	A	345	LEU
1	A	351	ASP
1	A	368	ARG
1	A	369	LEU
1	A	372	MET
1	A	385	LEU
1	A	393	SER
1	A	407	THR
1	A	408	SER
1	A	412	TYR
1	A	430	ASP
1	A	433	LYS
1	A	448	LYS
1	A	452	ILE
1	A	454	LYS
1	A	459	ARG
1	A	465	VAL
1	A	467	LYS
1	A	468	ARG
1	A	476	SER
1	A	478	MET
1	A	479	GLN
1	A	484	ILE
1	A	502	LYS
1	A	503	MET
1	A	509	LEU
1	A	521	THR
1	A	522	LEU
1	A	526	MET

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Mol	Chain	Res	Type
1	A	528	LEU
1	B	76	ARG
1	B	92	CYS
1	B	94	ILE
1	B	125	VAL
1	B	159	GLN
1	B	163	ARG
1	B	166	LEU
1	B	173	GLU
1	B	178	VAL
1	B	191	LEU
1	B	203	ASN
1	B	272	ILE
1	B	273	LEU
1	B	274	ASP
1	B	290	ARG
1	B	316	ASP
1	B	326	ASP
1	B	342	LEU
1	B	351	ASP
1	B	354	THR
1	B	359	GLU
1	B	361	ASP
1	B	381	VAL
1	B	408	SER
1	B	420	VAL
1	B	427	VAL
1	B	446	LEU
1	B	449	ASP
1	B	453	ASN
1	B	467	LYS
1	B	487	LEU
1	B	506	SER
1	B	512	LYS
1	B	515	SER
1	B	525	SER
1	B	527	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN

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Mol	Chain	Res	Type
1	A	159	GLN
1	A	248	GLN
1	A	263	GLN
1	A	375	GLN
1	A	423	ASN
1	A	429	HIS
1	A	479	GLN
1	A	490	GLN
1	B	71	HIS
1	B	104	HIS
1	B	149	HIS
1	B	265	ASN
1	B	279	HIS
1	B	319	ASN
1	B	357	GLN
1	B	423	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	HEM	A	901	1	50,50,50	1.61	8 (16%)	67,82,82	1.63	15 (22%)
2	HEM	B	900	1	50,50,50	1.60	8 (16%)	67,82,82	1.60	15 (22%)
3	AQ0	A	902	-	27,27,27	1.49	4 (14%)	31,38,38	2.31	7 (22%)

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	HEM	A	901	1	-	2/14/54/54	-
2	HEM	B	900	1	-	1/14/54/54	-
3	AQ0	A	902	-	-	4/7/17/17	1/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	HEM	FE-NB	5.13	2.10	1.94
2	B	900	HEM	FE-NB	4.99	2.10	1.94
2	B	900	HEM	FE-NC	4.89	2.11	1.95
2	A	901	HEM	FE-NC	4.75	2.10	1.95
3	A	902	AQ0	C8-C9	4.19	1.48	1.39
2	B	900	HEM	C1B-NB	-3.76	1.33	1.40
2	A	901	HEM	C1B-NB	-3.70	1.33	1.40
2	A	901	HEM	C4D-ND	-3.21	1.34	1.40
3	A	902	AQ0	C3-C2	3.15	1.48	1.43
2	B	900	HEM	C4B-NB	-2.88	1.33	1.38
2	A	901	HEM	C4B-NB	-2.72	1.33	1.38
2	B	900	HEM	C1C-C2C	-2.72	1.40	1.45
2	A	901	HEM	C1C-C2C	-2.70	1.40	1.45
3	A	902	AQ0	C9-C3	2.59	1.48	1.43
2	B	900	HEM	C4D-ND	-2.49	1.35	1.40
2	B	900	HEM	C3B-C4B	2.32	1.49	1.44
3	A	902	AQ0	C11-C10	-2.28	1.39	1.44
2	A	901	HEM	O2D-CGD	-2.10	1.23	1.30
2	A	901	HEM	C1C-NC	-2.05	1.35	1.39
2	B	900	HEM	C1D-C2D	2.03	1.48	1.44

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	AQ0	C16-N-N1	8.39	133.12	115.10
3	A	902	AQ0	O-C9-C3	5.03	122.79	114.77
3	A	902	AQ0	C9-C8-C10	-4.46	115.84	119.55
2	A	901	HEM	CHA-C4D-ND	4.12	129.47	124.37
2	A	901	HEM	CHC-C4B-NB	4.07	128.80	124.42
2	B	900	HEM	CHC-C4B-NB	4.01	128.74	124.42
2	A	901	HEM	CHD-C1D-ND	3.87	128.59	124.42
2	B	900	HEM	CAC-C3C-C4C	3.85	134.02	124.82
2	B	900	HEM	C1B-NB-C4B	3.79	109.70	105.21
2	B	900	HEM	CHA-C4D-ND	3.67	128.91	124.37
2	B	900	HEM	CHD-C1D-ND	3.50	128.19	124.42
2	A	901	HEM	C1B-NB-C4B	3.11	108.89	105.21
2	A	901	HEM	CBC-CAC-C3C	-3.11	112.01	127.53
2	A	901	HEM	CMD-C2D-C1D	3.03	129.76	125.03
2	B	900	HEM	CHA-C4D-C3D	-2.95	119.78	125.23
2	B	900	HEM	CAC-C3C-C2C	-2.88	119.06	128.43
2	A	901	HEM	O2A-CGA-CBA	2.74	122.66	114.00
2	B	900	HEM	CMD-C2D-C1D	2.69	129.23	125.03
2	A	901	HEM	CHD-C1D-C2D	-2.54	121.02	125.03
3	A	902	AQ0	C17-C18-C13	2.46	115.51	111.18
2	B	900	HEM	C4B-C3B-C2B	-2.34	105.13	107.28
2	B	900	HEM	O2D-CGD-O1D	-2.32	117.37	123.33
2	A	901	HEM	C4B-C3B-C2B	-2.32	105.15	107.28
2	A	901	HEM	O2D-CGD-CBD	2.29	121.23	114.00
3	A	902	AQ0	O-C9-C8	-2.26	119.61	121.63
2	B	900	HEM	CHD-C1D-C2D	-2.24	121.49	125.03
2	A	901	HEM	CHB-C1B-NB	2.22	127.12	124.37
2	A	901	HEM	CHA-C4D-C3D	-2.21	121.16	125.23
3	A	902	AQ0	C7-C8-C9	2.19	121.04	118.42
2	B	900	HEM	CHD-C4C-C3C	2.17	128.87	125.21
2	B	900	HEM	CHB-C1B-NB	2.16	127.04	124.37
2	B	900	HEM	O2A-CGA-CBA	2.10	120.62	114.00
2	A	901	HEM	CAD-CBD-CGD	-2.09	108.13	113.67
3	A	902	AQ0	C14-C15-C16	2.08	115.24	111.20
2	B	900	HEM	C1A-CHA-C4D	-2.07	121.38	126.25
2	A	901	HEM	CAC-C3C-C4C	2.04	129.68	124.82
2	A	901	HEM	O2A-CGA-O1A	-2.03	118.12	123.33

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	HEM	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
3	A	902	AQ0	O-C12-C13-C14
3	A	902	AQ0	C11-C12-C13-C14
3	A	902	AQ0	C15-C16-N-N1
2	B	900	HEM	C4C-C3C-CAC-CBC
2	A	901	HEM	C4C-C3C-CAC-CBC
3	A	902	AQ0	O-C12-C13-C18

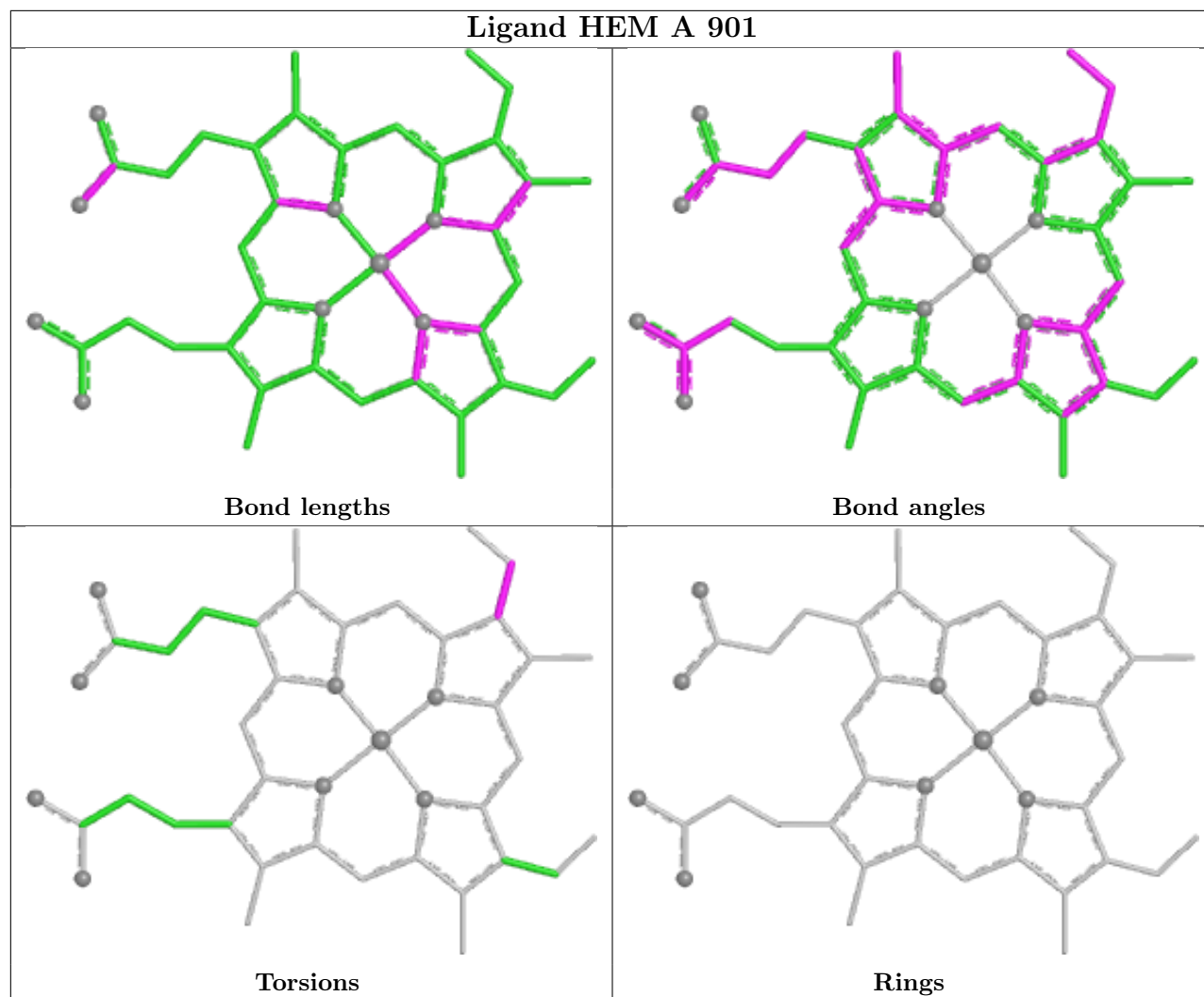
All (1) ring outliers are listed below:

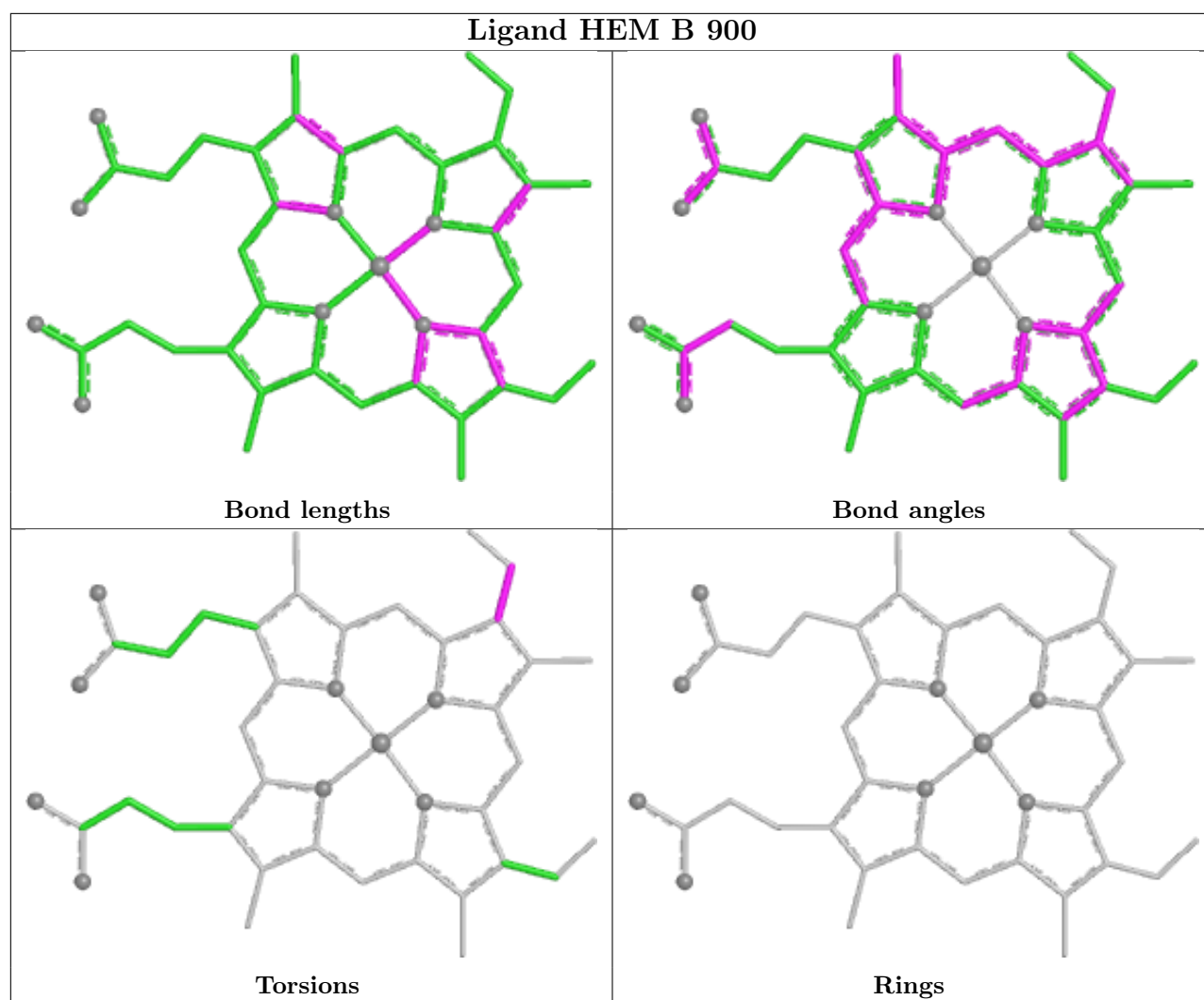
Mol	Chain	Res	Type	Atoms
3	A	902	AQ0	C13-C14-C15-C16-C17-C18

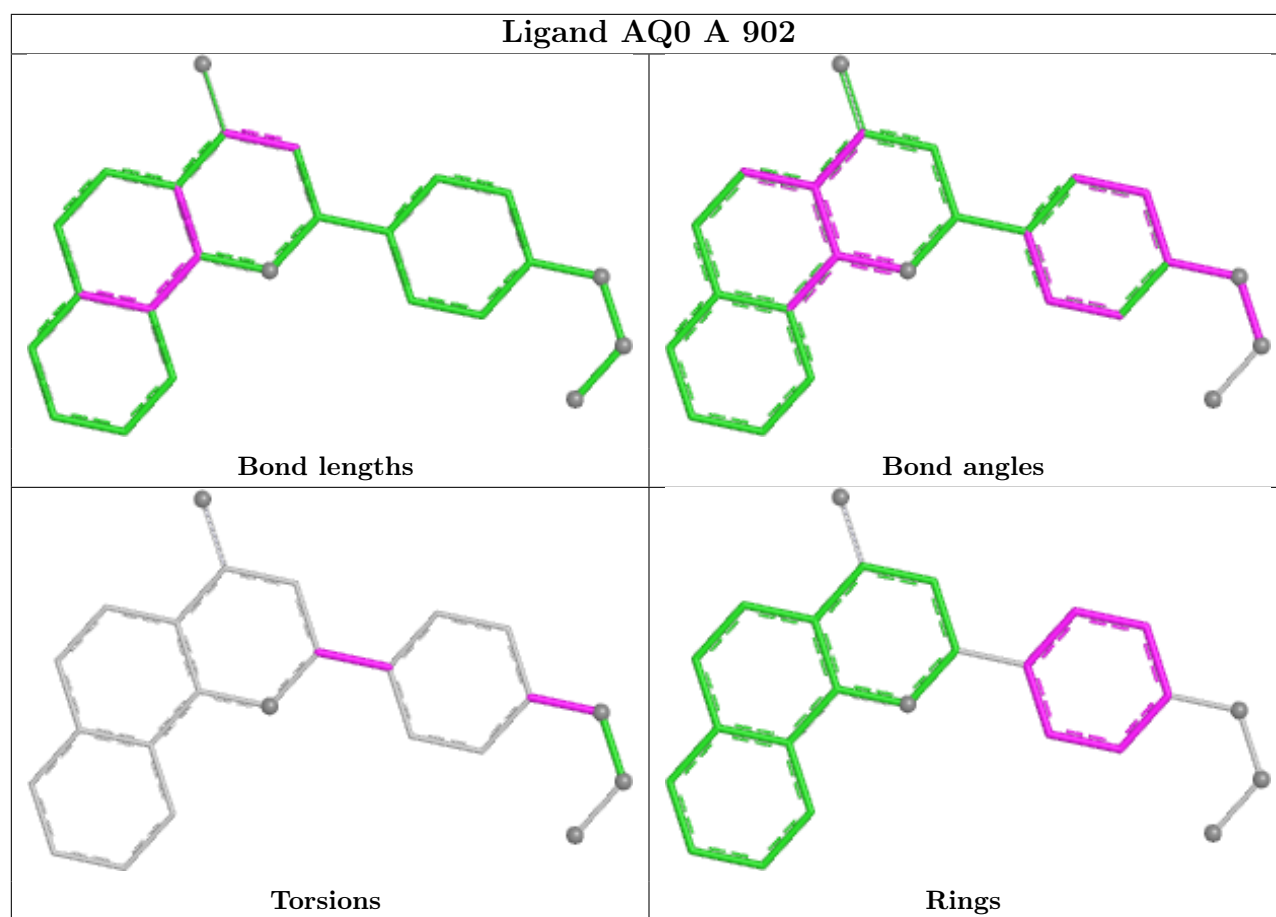
3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	HEM	4	0
2	B	900	HEM	5	0
3	A	902	AQ0	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	459/463 (99%)	1.17	73 (15%) 5 6	241, 305, 413, 474	0
1	B	437/463 (94%)	1.31	86 (19%) 3 3	213, 303, 392, 507	0
All	All	896/926 (96%)	1.24	159 (17%) 4 5	213, 304, 402, 507	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	508	GLY	7.3
1	B	254	VAL	6.4
1	B	509	LEU	6.4
1	B	241	VAL	5.4
1	B	251	PRO	5.1
1	B	498	ASN	4.7
1	B	154	ASN	4.5
1	A	87	ILE	4.5
1	A	77	LEU	4.4
1	B	89	LEU	4.3
1	A	451	LEU	4.3
1	B	317	LEU	4.2
1	B	273	LEU	4.1
1	B	225	LEU	4.1
1	B	224	LEU	3.9
1	A	216	HIS	3.8
1	A	246	TRP	3.8
1	B	221	PHE	3.8
1	B	143	VAL	3.8
1	B	160	PRO	3.8
1	A	412	TYR	3.7
1	A	501	ALA	3.6
1	A	376	PRO	3.6
1	B	496	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	455	ASP	3.5
1	A	377	ASN	3.4
1	B	223	GLU	3.3
1	A	81	TYR	3.2
1	B	497	PRO	3.2
1	B	525	SER	3.2
1	B	411	GLY	3.1
1	A	115	ALA	3.1
1	B	305	ALA	3.1
1	A	452	ILE	3.1
1	A	183	ARG	3.1
1	B	433	LYS	3.1
1	A	525	SER	3.1
1	A	455	ASP	3.1
1	A	235	VAL	3.0
1	B	507	TYR	3.0
1	B	277	LEU	3.0
1	A	101	ARG	3.0
1	A	153	ARG	3.0
1	B	146	ARG	3.0
1	B	447	ASP	3.0
1	B	474	GLU	3.0
1	B	87	ILE	3.0
1	A	86	GLN	2.9
1	B	257	VAL	2.9
1	A	160	PRO	2.9
1	B	246	TRP	2.9
1	A	93	PRO	2.9
1	B	435	PRO	2.8
1	B	217	ASP	2.8
1	A	141	TRP	2.7
1	A	121	ALA	2.7
1	A	467	LYS	2.7
1	A	474	GLU	2.7
1	B	527	GLU	2.7
1	B	222	ARG	2.7
1	B	333	ASP	2.7
1	B	262	GLU	2.7
1	A	261	PHE	2.7
1	A	68	GLN	2.7
1	A	405	ALA	2.7
1	A	456	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	267	ASN	2.6
1	A	169	HIS	2.6
1	A	354	THR	2.6
1	B	453	ASN	2.6
1	A	438	GLU	2.6
1	B	410	LEU	2.5
1	B	373	GLY	2.5
1	B	149	HIS	2.5
1	B	456	LEU	2.5
1	A	114	PHE	2.5
1	B	124	ARG	2.5
1	B	412	TYR	2.5
1	B	134	PHE	2.5
1	B	244	MET	2.5
1	A	140	HIS	2.4
1	A	524	GLU	2.4
1	A	240	LEU	2.4
1	B	183	ARG	2.4
1	A	465	VAL	2.4
1	B	77	LEU	2.4
1	B	129	GLY	2.4
1	A	249	TYR	2.4
1	A	526	MET	2.4
1	B	434	TRP	2.4
1	B	376	PRO	2.4
1	B	404	THR	2.4
1	B	304	ALA	2.4
1	B	328	PHE	2.4
1	B	161	ARG	2.4
1	A	245	PRO	2.3
1	B	219	PRO	2.3
1	A	187	ASP	2.3
1	A	313	ALA	2.3
1	B	68	GLN	2.3
1	B	264	LEU	2.3
1	B	189	ALA	2.3
1	A	165	VAL	2.3
1	B	255	ARG	2.3
1	A	263	GLN	2.3
1	B	431	PRO	2.3
1	B	213	ARG	2.3
1	B	458	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	163	ARG	2.3
1	A	317	LEU	2.3
1	B	432	VAL	2.3
1	A	282	SER	2.2
1	B	530	ASP	2.2
1	A	312	GLY	2.2
1	A	447	ASP	2.2
1	A	375	GLN	2.2
1	A	241	VAL	2.2
1	A	188	GLY	2.2
1	B	499	GLU	2.2
1	A	435	PRO	2.2
1	A	83	ASP	2.2
1	B	119	SER	2.2
1	B	400	PRO	2.2
1	A	517	LYS	2.2
1	A	413	HIS	2.2
1	B	353	GLN	2.2
1	A	502	LYS	2.2
1	A	425	TRP	2.1
1	A	529	LEU	2.1
1	B	258	PHE	2.1
1	B	271	PHE	2.1
1	A	251	PRO	2.1
1	B	93	PRO	2.1
1	B	266	ARG	2.1
1	A	453	ASN	2.1
1	A	231	PHE	2.1
1	A	285	PRO	2.1
1	A	348	ARG	2.1
1	B	121	ALA	2.1
1	B	332	GLN	2.1
1	A	254	VAL	2.1
1	B	136	HIS	2.1
1	B	354	THR	2.1
1	A	303	LYS	2.1
1	A	189	ALA	2.1
1	A	247	LEU	2.1
1	A	373	GLY	2.0
1	A	157	THR	2.0
1	B	315	LEU	2.0
1	B	465	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	494	ARG	2.0
1	B	437	PRO	2.0
1	B	100	GLU	2.0
1	B	187	ASP	2.0
1	B	128	GLY	2.0
1	B	366	ARG	2.0
1	A	113	ALA	2.0
1	A	307	ASP	2.0
1	B	108	VAL	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](#)

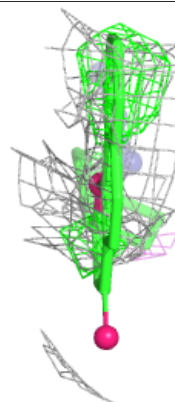
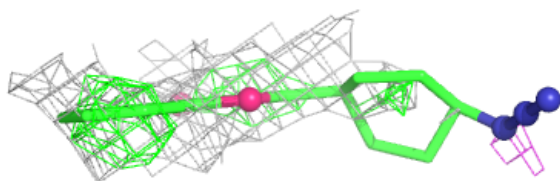
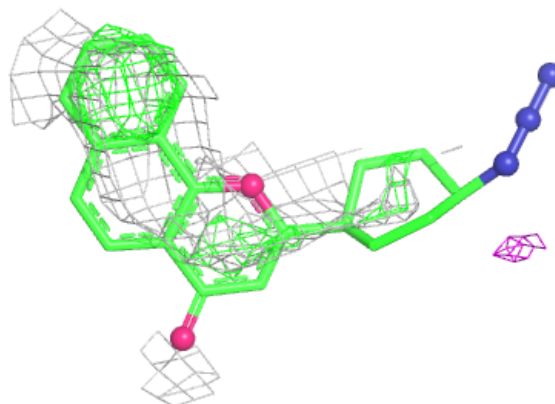
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AQ0	A	902	24/24	0.76	0.44	493,503,524,557	0
2	HEM	A	901	43/43	0.85	0.35	474,487,497,508	0
2	HEM	B	900	43/43	0.86	0.33	475,489,505,518	0

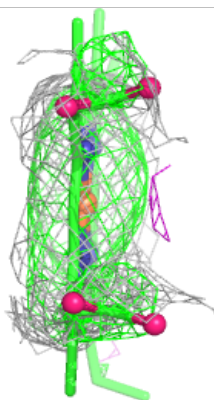
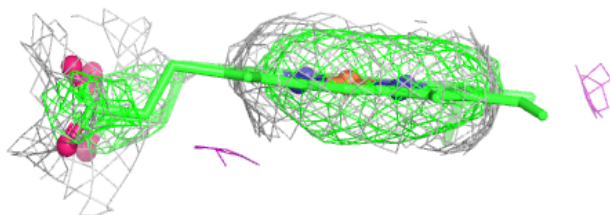
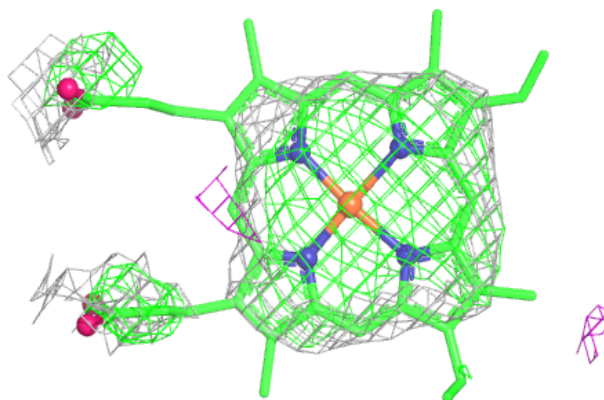
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

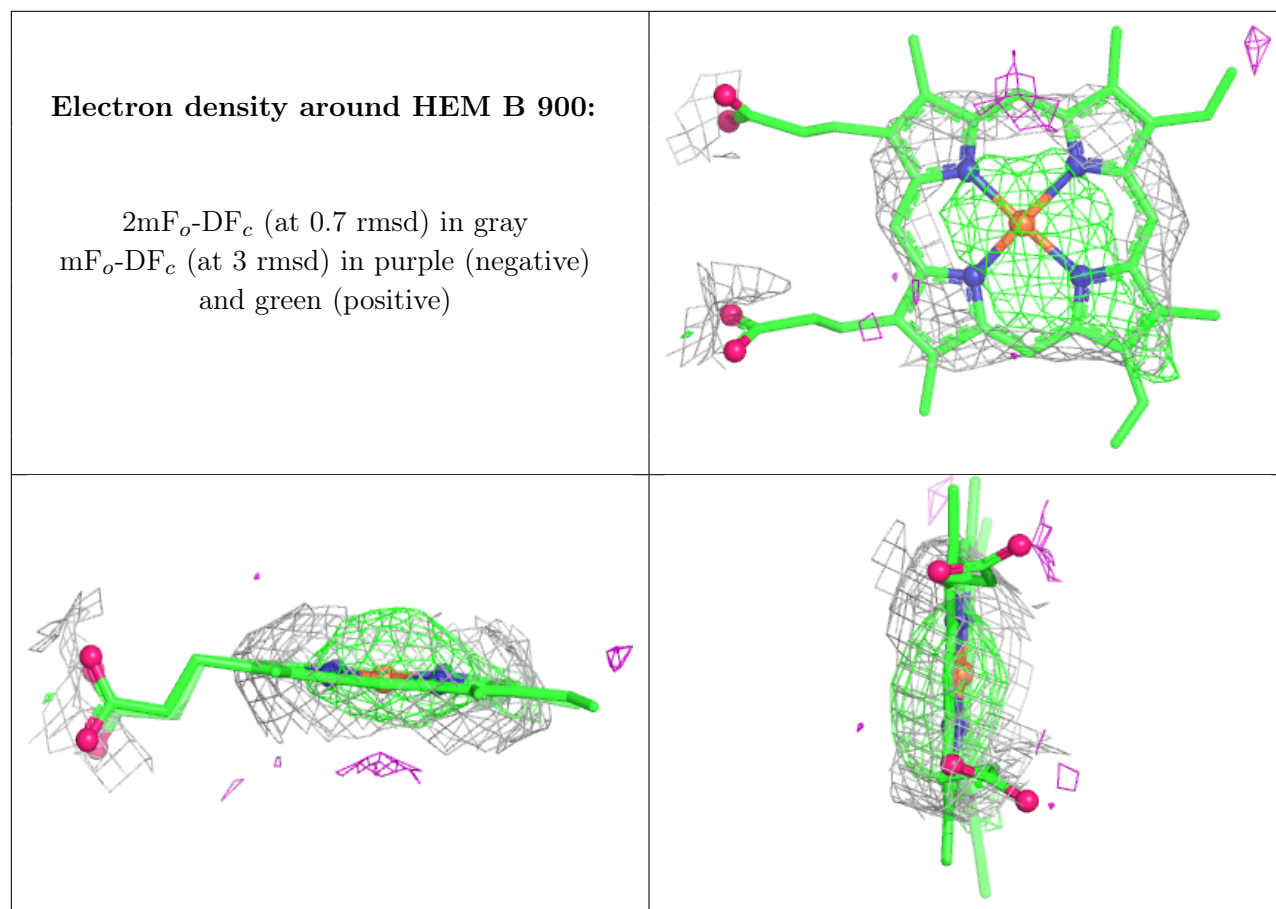
Electron density around AQ0 A 902:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**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 ⓘ

There are no such residues in this entry.