



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:04 PM UTC

PDB ID : 3E6L / pdb_00003e6l
Title : Structure of murine INOS oxygenase domain with inhibitor AR-C132283
Authors : Garcin, E.D.; Arvai, A.S.; Rosenfeld, R.J.; Kroeger, M.D.; Crane, B.R.; Andersson, G.; Andrews, G.; Hamley, P.J.; Mallinder, P.R.; Nicholls, D.J.; St-Gallay, S.A.; Tinker, A.C.; Gensmantel, N.P.; Mete, A.; Cheshire, D.R.; Connolly, S.; Stueh, D.J.; Aberg, A.; Wallace, A.V.; Tainer, J.A.; Getzoff, E.D.
Deposited on : 2008-08-15
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) were used in the production of this report:

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

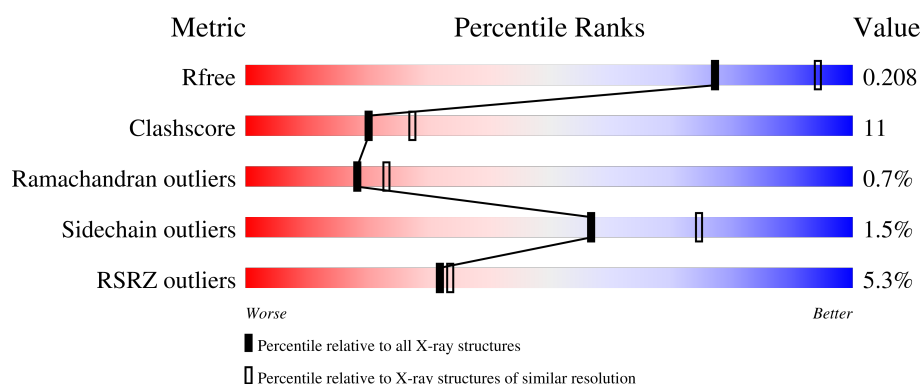
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	433	6% 69% 24% 5%
1	B	433	4% 71% 21% 5%

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	H4B	A	902	X	-	-	-
5	H4B	B	1902	X	-	-	-

2 Entry composition [i](#)

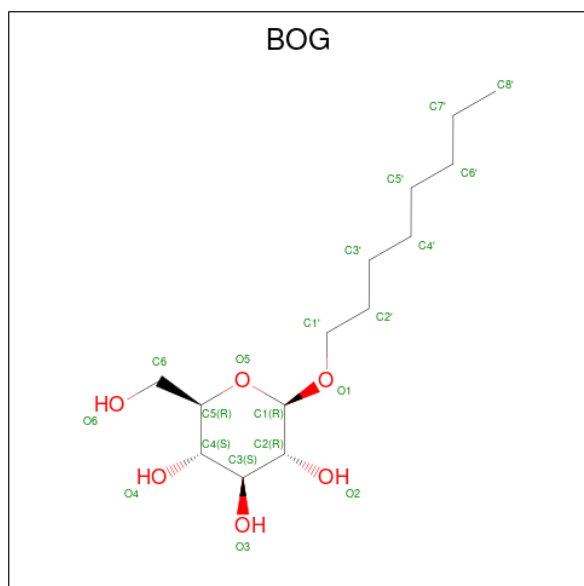
There are 7 unique types of molecules in this entry. The entry contains 7512 atoms, of which 0 are hydrogens and 0 are deuteriums.

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, inducible.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3364	2157	580	607	20			
1	B	413	Total	C	N	O	S	0	0	0
			3360	2155	579	606	20			

- Molecule 2 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



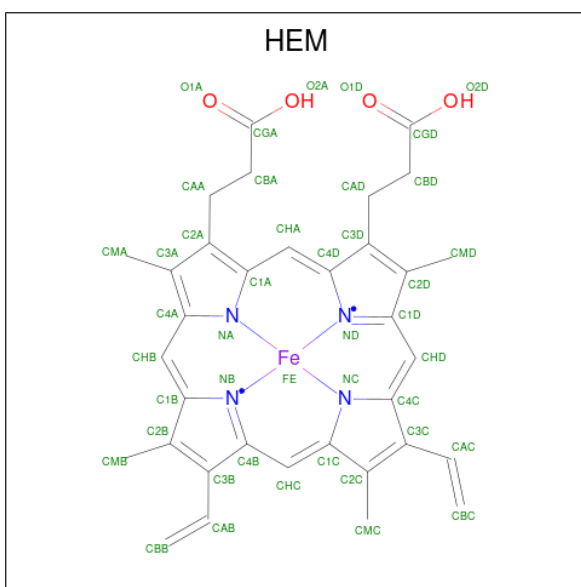
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



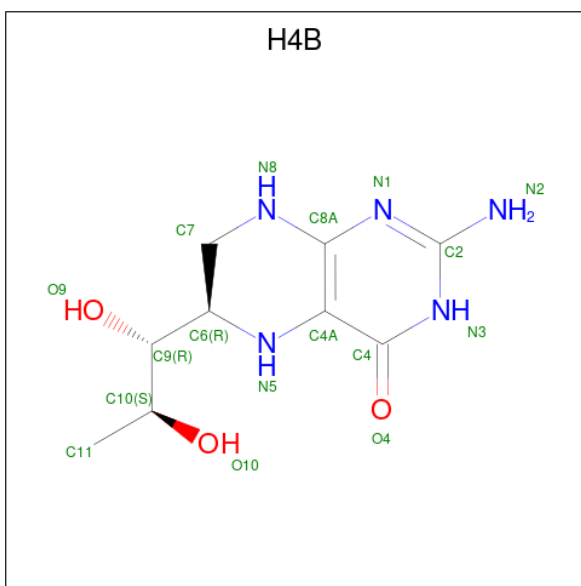
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



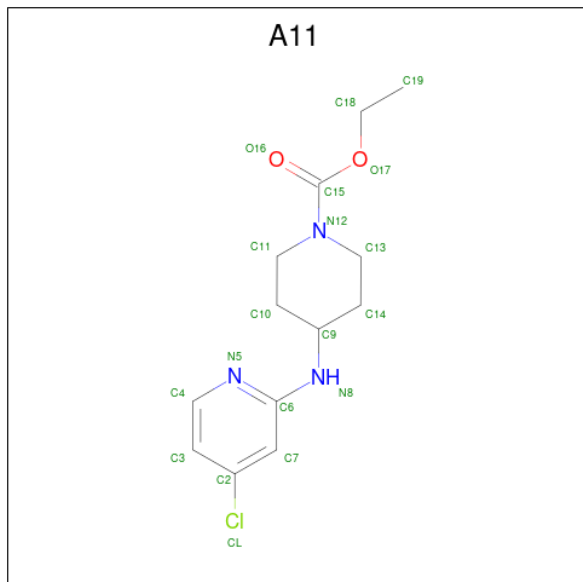
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: $\text{C}_9\text{H}_{15}\text{N}_5\text{O}_3$).



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

- Molecule 6 is ETHYL 4-[(4-CHLOROPYRIDIN-2-YL)AMINO]PIPERIDINE-1-CARBOXYLATE (CCD ID: A11) (formula: $C_{13}H_{18}ClN_3O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Cl	N	O	0	0
			19	13	1	3	2		
6	B	1	Total	C	Cl	N	O	0	0
			19	13	1	3	2		

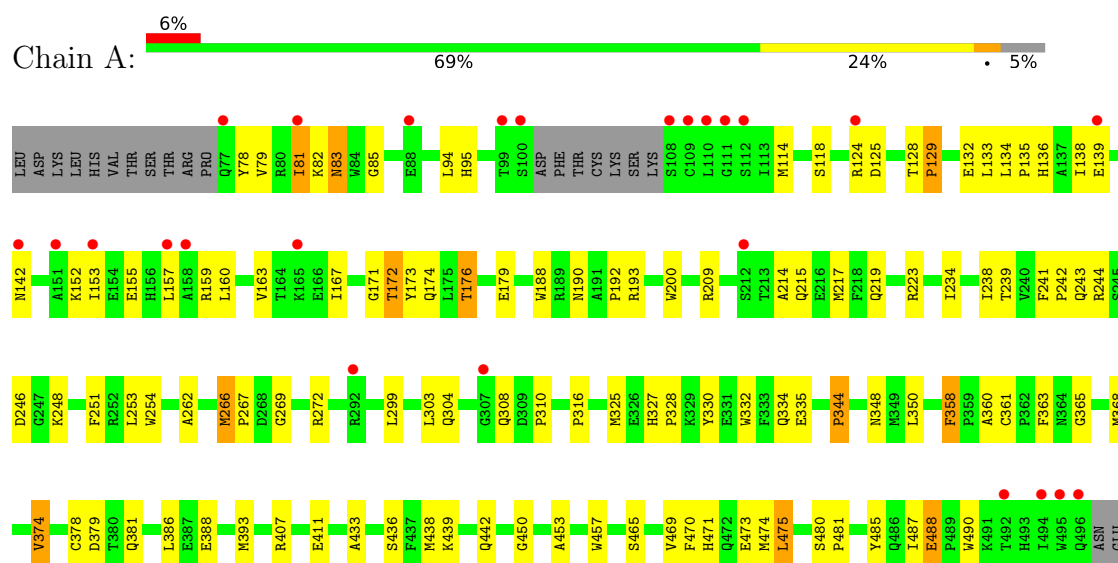
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	274	Total	O	0	0
			274	274		
7	B	271	Total	O	0	0
			271	271		

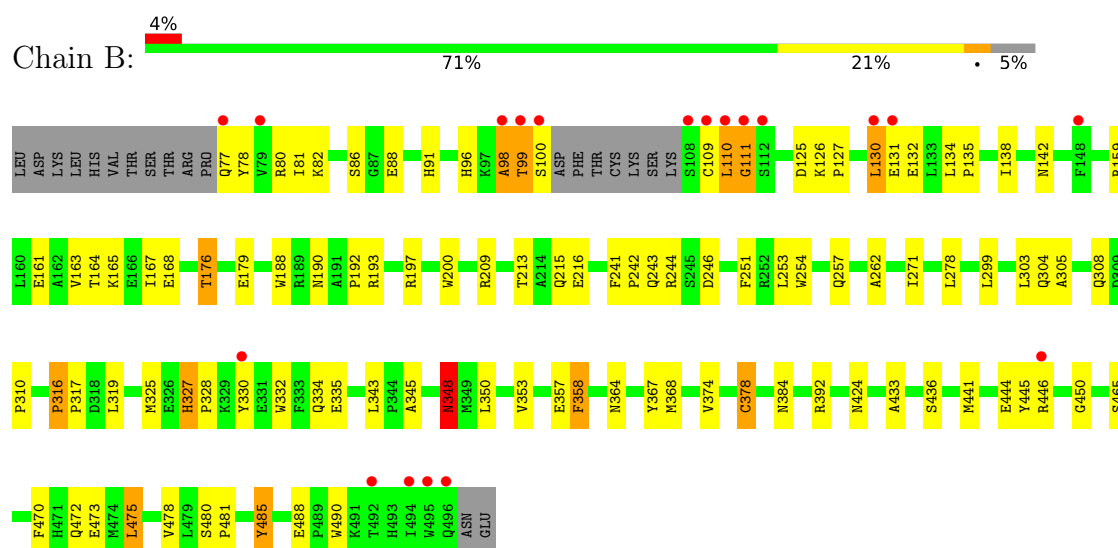
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Nitric oxide synthase, inducible



- Molecule 1: Nitric oxide synthase, inducible



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	213.90Å 213.90Å 116.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.98 – 2.30 29.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.5 (29.98-2.30) 92.5 (29.98-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.50 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.244 0.205 , 0.208	Depositor DCC
R_{free} test set	3464 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7512	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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: SO4, BOG, H4B, HEM, A11

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	0.44	0/3462	0.98	18/4707 (0.4%)
1	B	0.45	0/3458	0.98	19/4702 (0.4%)
All	All	0.44	0/6920	0.98	37/9409 (0.4%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	ASN	N-CA-C	7.44	121.20	112.72
1	A	485	TYR	N-CA-C	-7.29	101.13	110.53
1	B	98	ALA	N-CA-C	6.99	118.86	110.19
1	B	485	TYR	N-CA-C	-6.75	100.81	110.59
1	A	176	THR	N-CA-C	-6.67	101.10	110.50
1	B	358	PHE	CA-C-N	6.54	126.17	119.56
1	B	358	PHE	C-N-CA	6.54	126.17	119.56
1	A	365	GLY	N-CA-C	-6.47	100.48	110.77
1	B	367	TYR	N-CA-C	6.44	119.03	110.53
1	B	316	PRO	CA-C-N	6.38	126.60	119.32
1	B	316	PRO	C-N-CA	6.38	126.60	119.32
1	B	348	ASN	N-CA-C	6.37	121.10	112.88
1	B	176	THR	N-CA-C	-6.31	102.04	110.55
1	B	253	LEU	N-CA-C	-6.30	98.97	109.24
1	B	368	MET	N-CA-C	-5.75	99.53	108.90
1	A	368	MET	N-CA-C	-5.72	99.20	108.52
1	A	488	GLU	CA-C-N	5.72	125.84	119.32
1	A	488	GLU	C-N-CA	5.72	125.84	119.32
1	B	197	ARG	N-CA-C	5.68	119.68	112.87
1	A	266	MET	CA-C-N	5.63	124.83	118.97
1	A	266	MET	C-N-CA	5.63	124.83	118.97
1	A	386	LEU	N-CA-C	5.54	117.76	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	PRO	CA-C-N	5.47	125.81	119.47
1	A	316	PRO	C-N-CA	5.47	125.81	119.47
1	B	325	MET	N-CA-C	5.46	117.60	109.25
1	B	444	GLU	N-CA-C	5.46	117.22	111.28
1	A	253	LEU	N-CA-C	-5.40	99.92	108.73
1	A	325	MET	N-CA-C	5.40	117.51	109.25
1	B	251	PHE	N-CA-C	-5.40	100.50	109.46
1	B	378	CYS	N-CA-C	5.36	120.10	113.50
1	A	374	VAL	CB-CA-C	-5.26	107.24	111.71
1	A	358	PHE	CA-C-N	5.17	125.25	119.87
1	A	358	PHE	C-N-CA	5.17	125.25	119.87
1	B	327	HIS	CA-C-N	5.09	125.16	119.87
1	B	327	HIS	C-N-CA	5.09	125.16	119.87
1	B	424	ASN	N-CA-C	5.06	118.57	111.74
1	A	234	ILE	N-CA-C	5.05	116.73	109.51

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	3364	0	3259	81	0
1	B	3360	0	3253	72	0
2	A	20	0	28	1	0
2	B	20	0	28	0	0
3	A	30	0	0	0	0
3	B	15	0	0	0	0
4	A	43	0	30	1	0
4	B	43	0	30	0	0
5	A	17	0	14	0	0
5	B	17	0	14	0	0
6	A	19	0	18	0	0
6	B	19	0	18	1	0
7	A	274	0	0	7	0
7	B	271	0	0	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7512	0	6692	154	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (154) 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:B:81:ILE:HD11	1:B:475:LEU:HD13	1.37	1.05
1:A:83:ASN:C	1:A:83:ASN:HD22	1.91	0.79
1:A:83:ASN:ND2	1:A:85:GLY:H	1.82	0.78
1:A:83:ASN:HD22	1:A:85:GLY:H	1.31	0.77
1:A:215:GLN:O	1:A:219:GLN:HG3	1.83	0.77
1:A:469:VAL:HG13	1:A:474:MET:HE1	1.64	0.77
1:B:125:ASP:O	1:B:126:LYS:HD2	1.84	0.77
1:A:244:ARG:HA	7:A:2095:HOH:O	1.87	0.74
1:B:125:ASP:C	1:B:126:LYS:HD2	2.12	0.74
1:A:129:PRO:HB2	1:A:132:GLU:HG3	1.71	0.71
1:A:132:GLU:O	1:A:135:PRO:HD2	1.90	0.70
1:A:215:GLN:HE21	1:A:219:GLN:HE21	1.39	0.68
1:A:176:THR:OG1	1:A:179:GLU:HG3	1.95	0.66
1:A:438:MET:HE3	1:A:469:VAL:HG22	1.79	0.65
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.33	0.64
1:B:81:ILE:HD11	1:B:475:LEU:CD1	2.22	0.63
1:B:130:LEU:HD23	1:B:167:ILE:HG22	1.80	0.62
1:A:223:ARG:HD2	7:A:2156:HOH:O	1.99	0.62
1:A:133:LEU:HD22	1:A:167:ILE:HD13	1.81	0.62
1:A:81:ILE:HD11	1:A:475:LEU:HD13	1.80	0.62
1:A:215:GLN:HE21	1:A:219:GLN:NE2	1.98	0.61
1:B:332:TRP:CE3	1:B:392:ARG:HD2	2.35	0.61
4:A:901:HEM:HMC2	4:A:901:HEM:HBC2	1.82	0.61
1:A:124:ARG:HD2	7:A:2420:HOH:O	2.00	0.61
1:B:78:TYR:C	1:B:78:TYR:CD1	2.78	0.61
1:A:438:MET:HA	1:A:438:MET:HE2	1.84	0.60
1:A:388:GLU:HG3	7:A:2359:HOH:O	1.99	0.60
1:A:241:PHE:HB3	1:A:242:PRO:CD	2.32	0.59
1:A:266:MET:HE2	1:A:272:ARG:CZ	2.32	0.59
1:A:159:ARG:O	1:A:163:VAL:HG23	2.02	0.59
1:B:327:HIS:CG	1:B:328:PRO:HD2	2.38	0.58
1:A:138:ILE:HG22	1:A:142:ASN:HD21	1.67	0.58
1:B:209:ARG:O	1:B:242:PRO:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:PHE:HB3	1:A:242:PRO:HD2	1.88	0.56
1:B:441:MET:HE1	1:B:472:GLN:HG2	1.88	0.56
1:B:98:ALA:O	1:B:99:THR:HG23	2.06	0.56
1:B:110:LEU:HD12	1:B:110:LEU:N	2.22	0.55
1:B:82:LYS:O	1:B:473:GLU:HG3	2.07	0.54
1:B:80:ARG:NH1	7:B:2523:HOH:O	2.40	0.54
1:B:110:LEU:HD12	1:B:110:LEU:H	1.71	0.54
1:A:304:GLN:HG3	1:A:308:GLN:O	2.08	0.54
1:B:332:TRP:O	1:B:335:GLU:HB2	2.07	0.54
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.43	0.53
1:A:132:GLU:C	1:A:135:PRO:HD2	2.34	0.52
1:B:254:TRP:CZ3	1:B:490:TRP:HB3	2.43	0.52
1:A:134:LEU:O	1:A:138:ILE:HG12	2.10	0.52
1:A:163:VAL:O	1:A:167:ILE:HG13	2.09	0.52
1:A:465:SER:O	1:A:471:HIS:HE1	1.93	0.52
1:A:83:ASN:C	1:A:83:ASN:ND2	2.62	0.52
1:B:304:GLN:HG3	1:B:308:GLN:O	2.10	0.52
1:B:488:GLU:HB3	1:B:490:TRP:CE2	2.45	0.51
1:A:487:ILE:O	1:A:488:GLU:C	2.54	0.51
1:B:190:ASN:O	1:B:192:PRO:HD3	2.11	0.51
1:A:330:TYR:HB3	1:A:332:TRP:CE2	2.46	0.51
1:B:130:LEU:CD2	1:B:167:ILE:HG22	2.41	0.50
1:B:213:THR:OG1	1:B:216:GLU:HG3	2.11	0.50
1:B:374:VAL:O	1:B:378:CYS:HB2	2.11	0.50
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.47	0.50
1:A:209:ARG:O	1:A:242:PRO:HG3	2.11	0.50
1:A:133:LEU:HD23	1:A:133:LEU:C	2.36	0.50
1:A:94:LEU:HB3	1:A:450:GLY:HA3	1.93	0.50
1:A:303:LEU:O	1:A:310:PRO:HA	2.11	0.49
1:B:176:THR:OG1	1:B:179:GLU:HG3	2.12	0.49
1:A:153:ILE:O	1:A:157:LEU:HD23	2.11	0.49
1:B:445:TYR:CZ	1:B:450:GLY:HA2	2.46	0.49
1:A:344:PRO:HG2	1:A:344:PRO:O	2.12	0.49
1:A:153:ILE:HG22	1:A:157:LEU:HD23	1.94	0.49
1:A:78:TYR:CD1	1:A:78:TYR:C	2.91	0.48
1:A:124:ARG:NH2	1:A:128:THR:OG1	2.46	0.48
1:A:138:ILE:O	1:A:142:ASN:ND2	2.46	0.48
1:B:130:LEU:HD13	1:B:130:LEU:C	2.38	0.48
1:B:109:CYS:O	1:B:111:GLY:N	2.43	0.48
1:B:241:PHE:HB3	1:B:242:PRO:CD	2.43	0.48
1:A:138:ILE:HG22	1:A:142:ASN:ND2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:ARG:CZ	1:B:446:ARG:HB3	2.44	0.48
1:B:163:VAL:O	1:B:167:ILE:HG13	2.14	0.47
1:B:480:SER:HA	1:B:481:PRO:C	2.40	0.47
1:A:246:ASP:OD2	1:A:248:LYS:HB2	2.14	0.47
1:A:374:VAL:O	1:A:378:CYS:HB2	2.14	0.47
1:B:262:ALA:HB2	1:B:299:LEU:CD2	2.44	0.47
1:A:262:ALA:HB2	1:A:299:LEU:CD2	2.45	0.47
1:B:134:LEU:HB3	1:B:135:PRO:HD3	1.97	0.47
1:A:379:ASP:HB3	1:A:381:GLN:NE2	2.29	0.47
1:B:77:GLN:O	1:B:96:HIS:HE1	1.98	0.47
1:B:110:LEU:H	1:B:110:LEU:CD1	2.28	0.47
1:B:241:PHE:HB3	1:B:242:PRO:HD2	1.95	0.47
1:B:445:TYR:HA	1:B:450:GLY:H	1.79	0.47
1:B:100:SER:HA	1:B:478:VAL:HG11	1.97	0.46
1:A:243:GLN:HB3	1:A:358:PHE:CE2	2.50	0.46
1:A:214:ALA:O	1:A:217:MET:HB2	2.16	0.46
1:A:350:LEU:C	1:A:350:LEU:HD23	2.40	0.46
1:B:127:PRO:HG3	1:B:246:ASP:HA	1.98	0.46
1:B:348:ASN:ND2	1:B:348:ASN:H	2.14	0.46
1:A:480:SER:HA	1:A:481:PRO:C	2.41	0.46
1:B:244:ARG:NH1	1:B:357:GLU:OE2	2.48	0.46
1:A:439:LYS:O	1:A:442:GLN:HB3	2.16	0.45
1:A:407:ARG:HD2	7:A:2117:HOH:O	2.15	0.45
1:B:193:ARG:NH1	1:B:485:TYR:OH	2.49	0.45
1:A:193:ARG:HD3	1:A:457:TRP:CD2	2.51	0.45
1:A:453:ALA:HB3	1:A:474:MET:HB3	1.99	0.45
1:A:172:THR:HG23	1:A:173:TYR:N	2.31	0.45
1:A:239:THR:O	1:A:361:CYS:HA	2.17	0.45
1:A:334:GLN:HG3	1:A:335:GLU:N	2.29	0.45
1:A:267:PRO:C	1:A:269:GLY:H	2.24	0.44
1:A:469:VAL:HG13	1:A:474:MET:CE	2.41	0.44
1:B:441:MET:HE1	1:B:472:GLN:CD	2.43	0.44
1:A:136:HIS:O	1:A:139:GLU:HB3	2.17	0.44
1:A:160:LEU:HD13	2:A:4001:BOG:H5'1	2.00	0.44
1:B:445:TYR:CE2	1:B:450:GLY:HA2	2.53	0.44
1:A:82:LYS:O	1:A:473:GLU:HG3	2.18	0.44
1:B:350:LEU:C	1:B:350:LEU:HD23	2.43	0.44
1:A:238:ILE:HG13	1:A:363:PHE:HB3	1.99	0.44
1:A:327:HIS:CG	1:A:328:PRO:HD2	2.53	0.43
1:A:470:PHE:C	1:A:470:PHE:CD1	2.97	0.43
1:B:138:ILE:O	1:B:142:ASN:ND2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLN:HA	7:A:2052:HOH:O	2.18	0.43
1:B:348:ASN:H	1:B:348:ASN:HD22	1.65	0.43
1:A:79:VAL:HG23	1:A:95:HIS:CE1	2.53	0.43
1:B:215:GLN:NE2	7:B:2540:HOH:O	2.51	0.43
1:A:125:ASP:O	1:A:248:LYS:HE3	2.19	0.42
1:A:407:ARG:HG2	7:A:2149:HOH:O	2.18	0.42
1:A:215:GLN:NE2	1:A:219:GLN:HE21	2.14	0.42
1:B:257:GLN:HG2	6:B:1906:A11:O16	2.19	0.42
1:B:316:PRO:O	1:B:319:LEU:HB2	2.19	0.42
1:B:348:ASN:HD22	1:B:348:ASN:N	2.18	0.42
1:A:332:TRP:O	1:A:335:GLU:HB2	2.19	0.42
1:B:132:GLU:O	1:B:135:PRO:HD2	2.19	0.42
1:B:305:ALA:O	1:B:308:GLN:HG2	2.19	0.42
1:B:433:ALA:O	1:B:436:SER:HB3	2.19	0.42
1:B:257:GLN:HA	1:B:345:ALA:O	2.20	0.42
1:B:159:ARG:O	1:B:163:VAL:HG23	2.20	0.42
1:A:433:ALA:O	1:A:436:SER:HB3	2.19	0.42
1:B:271:ILE:HD12	1:B:278:LEU:HD11	2.02	0.42
1:A:171:GLY:O	1:A:172:THR:HB	2.20	0.41
1:B:188:TRP:CZ3	1:B:200:TRP:HA	2.54	0.41
1:A:251:PHE:O	1:A:360:ALA:HB2	2.20	0.41
1:B:78:TYR:CE1	1:B:91:HIS:ND1	2.88	0.41
1:A:393:MET:CE	1:A:411:GLU:HG3	2.50	0.41
1:A:81:ILE:HD13	1:A:81:ILE:HA	1.78	0.41
1:B:86:SER:C	1:B:88:GLU:H	2.28	0.41
1:B:164:THR:O	1:B:168:GLU:HG3	2.21	0.41
1:B:303:LEU:O	1:B:310:PRO:HA	2.20	0.41
1:B:441:MET:HE1	1:B:472:GLN:CG	2.49	0.41
1:A:190:ASN:O	1:A:192:PRO:HD3	2.21	0.41
1:A:217:MET:HB3	1:A:303:LEU:HD13	2.03	0.41
1:B:161:GLU:HG2	1:B:165:LYS:HE3	2.03	0.41
1:B:343:LEU:HD11	1:B:364:ASN:ND2	2.35	0.41
1:B:78:TYR:C	1:B:78:TYR:HD1	2.28	0.41
1:B:131:GLU:HG3	1:B:132:GLU:N	2.36	0.41
1:B:316:PRO:HA	1:B:317:PRO:HD3	1.88	0.41
1:B:330:TYR:HB3	1:B:332:TRP:CE2	2.56	0.41
1:A:152:LYS:HD2	1:A:155:GLU:OE2	2.21	0.40
1:A:254:TRP:CZ3	1:A:490:TRP:HB3	2.56	0.40
1:B:465:SER:HA	1:B:470:PHE:CG	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:2227:HOH:O	7:B:2259:HOH:O[9_766]	2.13	0.07

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	409/433 (94%)	379 (93%)	28 (7%)	2 (0%)	24	31
1	B	409/433 (94%)	375 (92%)	30 (7%)	4 (1%)	12	15
All	All	818/866 (94%)	754 (92%)	58 (7%)	6 (1%)	18	23

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	99	THR
1	B	110	LEU
1	B	111	GLY
1	A	172	THR
1	B	384	ASN
1	A	344	PRO

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	360/381 (94%)	354 (98%)	6 (2%)	53	72
1	B	359/381 (94%)	354 (99%)	5 (1%)	59	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	719/762 (94%)	708 (98%)	11 (2%)	57	75

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ILE
1	A	83	ASN
1	A	114	MET
1	A	118	SER
1	A	129	PRO
1	A	475	LEU
1	B	130	LEU
1	B	334	GLN
1	B	348	ASN
1	B	353	VAL
1	B	475	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	96	HIS
1	A	115	ASN
1	A	142	ASN
1	A	219	GLN
1	A	308	GLN
1	A	334	GLN
1	A	421	GLN
1	A	442	GLN
1	A	471	HIS
1	A	496	GLN
1	B	96	HIS
1	B	115	ASN
1	B	142	ASN
1	B	219	GLN
1	B	334	GLN
1	B	348	ASN
1	B	384	ASN
1	B	418	HIS
1	B	421	GLN
1	B	486	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

17 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	$\# Z > 2$
3	SO4	A	3002	-	4,4,4	0.43	0	6,6,6	0.06	0
3	SO4	A	3007	-	4,4,4	0.45	0	6,6,6	0.08	0
3	SO4	A	3006	-	4,4,4	0.39	0	6,6,6	0.10	0
3	SO4	A	3008	-	4,4,4	0.48	0	6,6,6	0.09	0
3	SO4	B	3009	-	4,4,4	0.42	0	6,6,6	0.08	0
2	BOG	B	4002	-	20,20,20	1.47	3 (15%)	25,25,25	0.78	1 (4%)
3	SO4	B	3004	-	4,4,4	0.45	0	6,6,6	0.05	0
6	A11	A	906	-	20,20,20	1.66	3 (15%)	24,26,26	1.42	4 (16%)
5	H4B	A	902	-	17,18,18	2.58	4 (23%)	14,26,26	1.99	4 (28%)
6	A11	B	1906	-	20,20,20	1.70	4 (20%)	24,26,26	1.36	3 (12%)
4	HEM	A	901	-	50,50,50	1.41	8 (16%)	67,82,82	1.17	5 (7%)
3	SO4	A	3003	-	4,4,4	0.40	0	6,6,6	0.08	0
3	SO4	A	3001	-	4,4,4	0.41	0	6,6,6	0.09	0
4	HEM	B	1901	1	50,50,50	1.36	7 (14%)	67,82,82	1.11	4 (5%)
2	BOG	A	4001	-	20,20,20	1.51	4 (20%)	25,25,25	0.79	1 (4%)
5	H4B	B	1902	-	17,18,18	2.83	4 (23%)	14,26,26	2.04	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	3005	-	4,4,4	0.40	0	6,6,6	0.08	0

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	BOG	B	4002	-	-	2/11/31/31	0/1/1/1
6	A11	A	906	-	-	0/11/21/21	0/2/2/2
5	H4B	A	902	-	1/1/3/5	3/8/17/17	0/2/2/2
6	A11	B	1906	-	-	0/11/21/21	0/2/2/2
4	HEM	A	901	-	-	1/14/54/54	-
4	HEM	B	1901	1	-	1/14/54/54	-
2	BOG	A	4001	-	-	4/11/31/31	0/1/1/1
5	H4B	B	1902	-	1/1/3/5	4/8/17/17	0/2/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1902	H4B	C7-N8	-8.13	1.38	1.46
5	A	902	H4B	C7-N8	-7.66	1.38	1.46
5	B	1902	H4B	C7-C6	-6.60	1.45	1.52
5	A	902	H4B	C7-C6	-5.59	1.46	1.52
2	B	4002	BOG	C3-C2	-4.29	1.41	1.52
6	A	906	A11	O16-C15	4.21	1.27	1.21
6	B	1906	A11	O16-C15	4.10	1.27	1.21
2	A	4001	BOG	C3-C2	-3.97	1.42	1.52
4	B	1901	HEM	FE-ND	3.90	2.06	1.94
6	A	906	A11	C6-N5	3.87	1.41	1.34
6	B	1906	A11	C6-N5	3.85	1.41	1.34
4	A	901	HEM	FE-NC	3.61	2.07	1.95
2	B	4002	BOG	C4-C3	-3.51	1.43	1.52
4	B	1901	HEM	FE-NC	3.38	2.06	1.95
6	B	1906	A11	C4-N5	3.12	1.41	1.34
2	A	4001	BOG	C4-C3	-3.11	1.44	1.52
4	A	901	HEM	FE-NB	3.01	2.04	1.94
6	A	906	A11	C4-N5	2.91	1.40	1.34
2	A	4001	BOG	O1-C1	2.90	1.45	1.40
5	A	902	H4B	C4-N3	-2.83	1.33	1.38
5	B	1902	H4B	C4-N3	-2.78	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1901	HEM	FE-NB	2.56	2.02	1.94
4	B	1901	HEM	C3B-C4B	2.56	1.49	1.44
4	A	901	HEM	FE-ND	2.55	2.02	1.94
4	A	901	HEM	C4A-C3A	2.50	1.49	1.43
4	A	901	HEM	CAB-C3B	-2.47	1.40	1.47
2	A	4001	BOG	O5-C1	2.45	1.48	1.41
4	A	901	HEM	C1A-C2A	2.31	1.49	1.44
4	A	901	HEM	FE-NA	2.26	2.02	1.95
4	B	1901	HEM	C2A-C3A	-2.25	1.33	1.38
2	B	4002	BOG	O1-C1	2.23	1.43	1.40
4	A	901	HEM	CBC-CAC	2.13	1.40	1.30
5	A	902	H4B	C4A-N5	-2.07	1.33	1.37
4	B	1901	HEM	CAC-C3C	-2.06	1.41	1.47
6	B	1906	A11	C3-C4	2.05	1.42	1.38
5	B	1902	H4B	C4A-N5	-2.03	1.33	1.37
4	B	1901	HEM	CBC-CAC	2.00	1.40	1.30

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1902	H4B	C2-N1-C8A	4.38	121.09	113.36
5	A	902	H4B	C2-N1-C8A	4.08	120.56	113.36
5	A	902	H4B	O4-C4-C4A	-4.04	117.52	127.26
5	B	1902	H4B	O4-C4-C4A	-4.01	117.60	127.26
4	A	901	HEM	C4B-C3B-C2B	-3.72	103.86	107.28
6	A	906	A11	C3-C4-N5	-3.33	119.89	123.97
4	A	901	HEM	C3B-C2B-C1B	3.32	108.91	106.41
4	A	901	HEM	CMD-C2D-C1D	3.16	129.97	125.03
6	B	1906	A11	C3-C4-N5	-3.12	120.14	123.97
4	B	1901	HEM	CAA-C2A-C1A	2.86	130.53	124.94
5	B	1902	H4B	C4A-C4-N3	2.86	119.99	112.13
5	A	902	H4B	C4A-C4-N3	2.79	119.79	112.13
4	B	1901	HEM	CMD-C2D-C1D	2.65	129.18	125.03
5	B	1902	H4B	C2-N3-C4	-2.63	120.34	125.11
5	A	902	H4B	C2-N3-C4	-2.42	120.72	125.11
6	A	906	A11	O16-C15-N12	-2.42	119.82	124.30
6	B	1906	A11	C7-C6-N5	-2.41	119.75	122.92
4	A	901	HEM	C3B-C4B-NB	2.38	111.18	109.47
6	B	1906	A11	O16-C15-N12	-2.33	119.98	124.30
4	A	901	HEM	CAA-C2A-C1A	2.31	129.44	124.94
6	A	906	A11	C7-C6-N5	-2.30	119.90	122.92
4	B	1901	HEM	C4B-C3B-C2B	-2.15	105.31	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4001	BOG	C4-C3-C2	2.10	114.52	110.83
4	B	1901	HEM	C4C-C3C-C2C	-2.04	105.05	106.81
6	A	906	A11	C4-N5-C6	2.03	120.11	117.21
2	B	4002	BOG	C4-C3-C2	2.01	114.36	110.83

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	902	H4B	C6
5	B	1902	H4B	C6

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	902	H4B	C7-C6-C9-O9
5	A	902	H4B	C7-C6-C9-C10
5	B	1902	H4B	N5-C6-C9-O9
5	B	1902	H4B	C7-C6-C9-O9
5	B	1902	H4B	C7-C6-C9-C10
2	A	4001	BOG	C4-C5-C6-O6
2	A	4001	BOG	O5-C5-C6-O6
2	A	4001	BOG	O1-C1'-C2'-C3'
4	A	901	HEM	C1A-C2A-CAA-CBA
2	B	4002	BOG	C2-C1-O1-C1'
2	A	4001	BOG	C3'-C4'-C5'-C6'
2	B	4002	BOG	O5-C1-O1-C1'
5	B	1902	H4B	N5-C6-C9-C10
5	A	902	H4B	N5-C6-C9-O9
4	B	1901	HEM	CAD-CBD-CGD-O2D

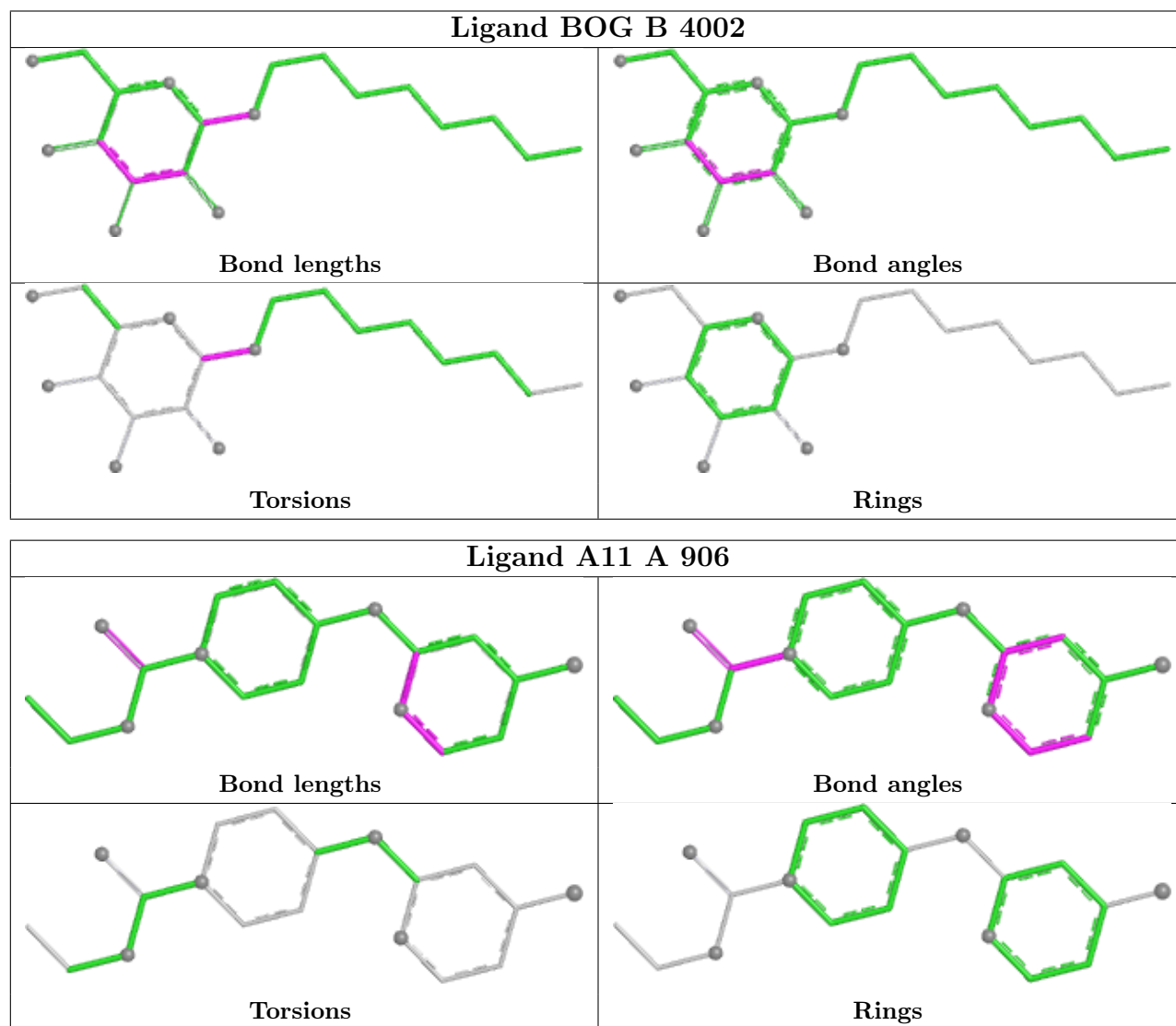
There are no ring outliers.

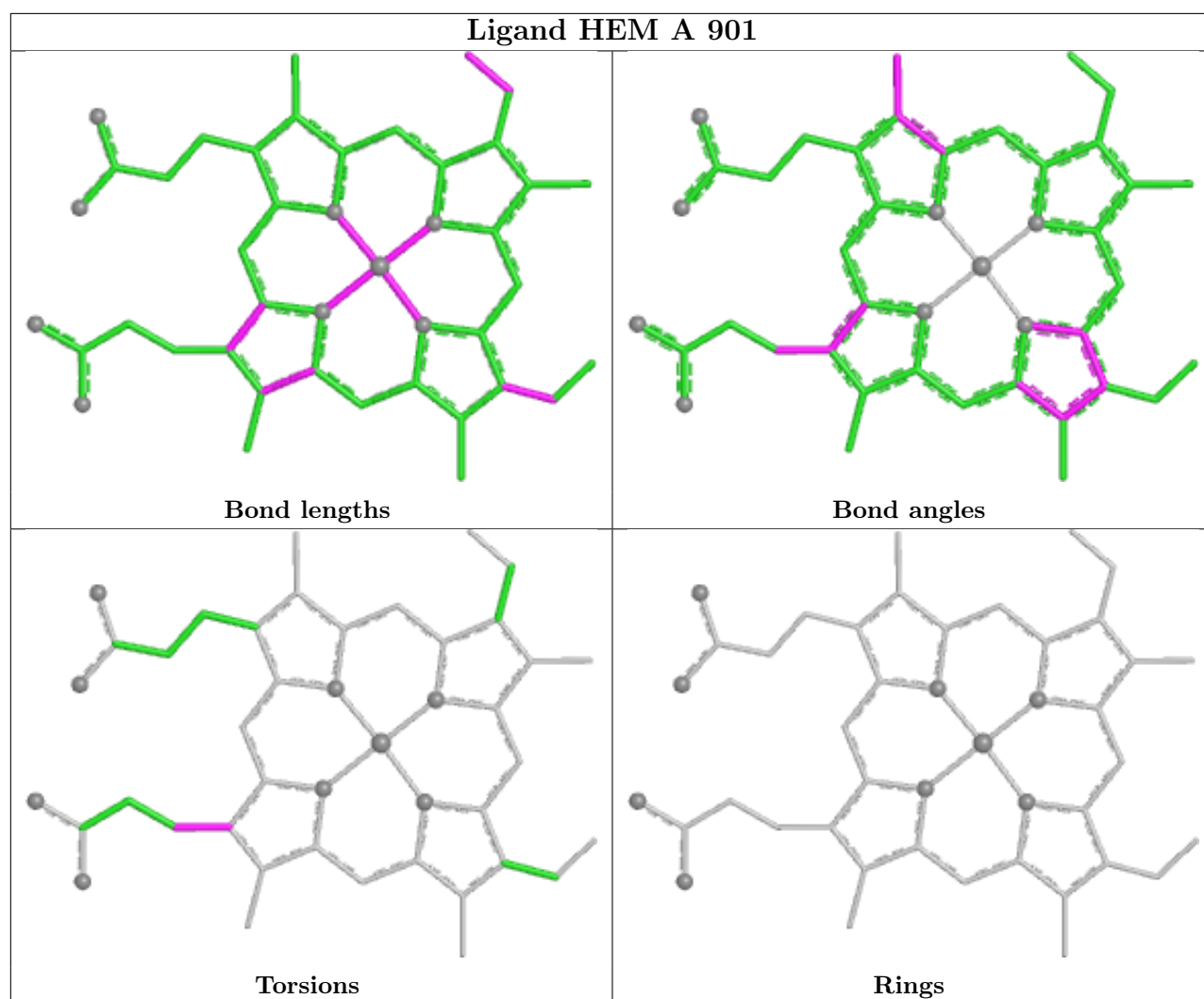
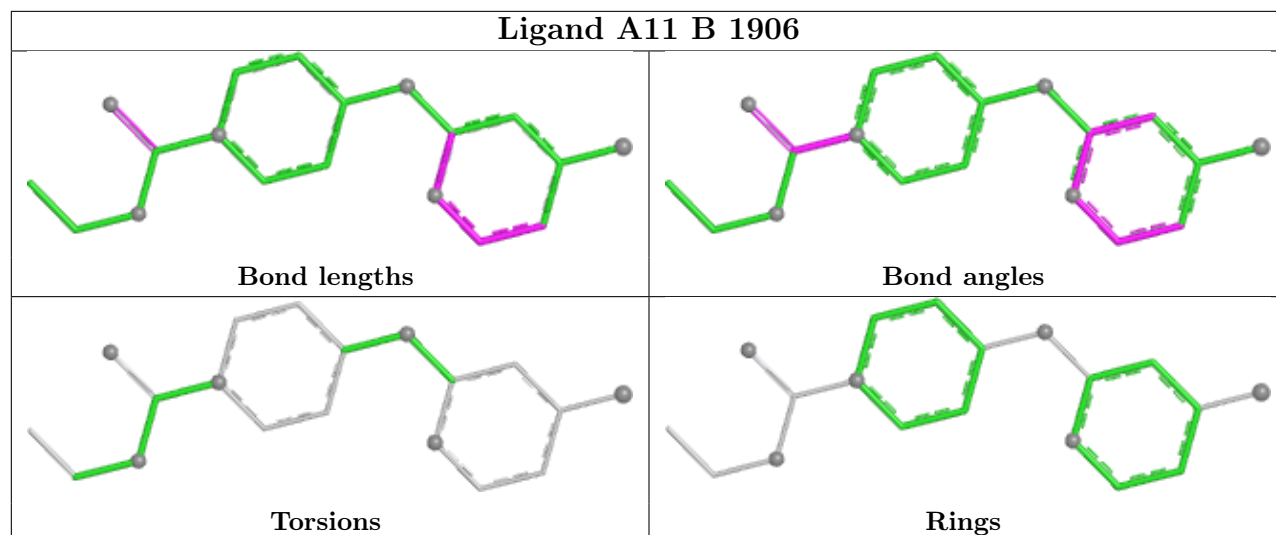
3 monomers are involved in 3 short contacts:

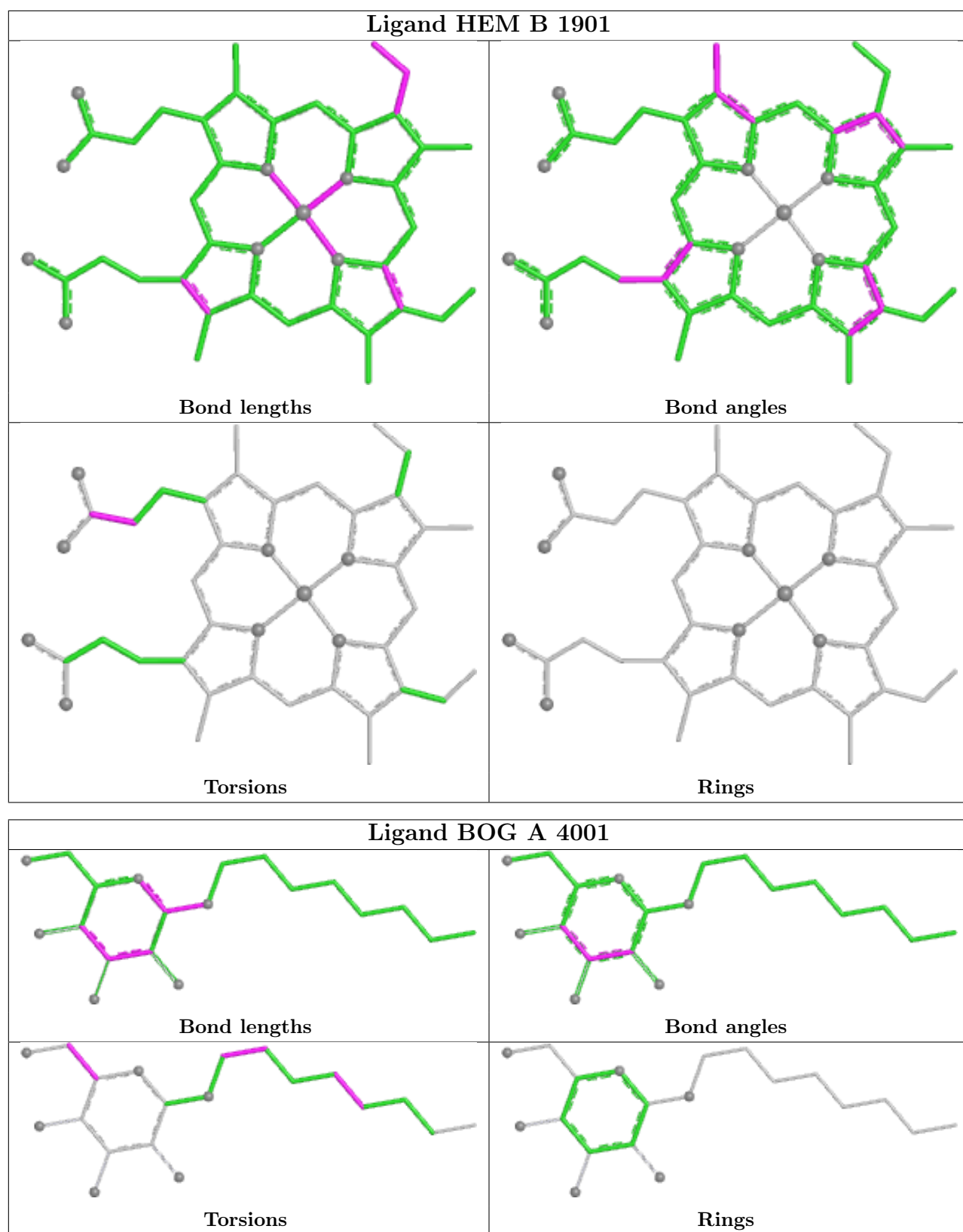
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1906	A11	1	0
4	A	901	HEM	1	0
2	A	4001	BOG	1	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	413/433 (95%)	0.40	25 (6%) 27 29	28, 44, 70, 95	0
1	B	413/433 (95%)	0.33	19 (4%) 37 39	26, 42, 67, 98	0
All	All	826/866 (95%)	0.37	44 (5%) 32 34	26, 43, 69, 98	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	496	GLN	5.6
1	B	110	LEU	4.9
1	A	110	LEU	4.6
1	A	77	GLN	4.2
1	B	131	GLU	4.1
1	A	496	GLN	4.0
1	A	111	GLY	4.0
1	B	111	GLY	4.0
1	B	109	CYS	3.7
1	B	112	SER	3.6
1	B	100	SER	3.4
1	A	165	LYS	3.4
1	A	492	THR	3.3
1	B	130	LEU	3.2
1	A	109	CYS	3.1
1	B	495	TRP	3.1
1	B	99	THR	3.1
1	A	153	ILE	2.9
1	A	88	GLU	2.8
1	A	151	ALA	2.8
1	B	77	GLN	2.8
1	B	79	VAL	2.6
1	A	99	THR	2.6
1	A	495	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	292	ARG	2.5
1	A	112	SER	2.5
1	B	494	ILE	2.4
1	A	212	SER	2.3
1	A	307	GLY	2.3
1	B	98	ALA	2.3
1	B	330	TYR	2.2
1	A	108	SER	2.2
1	A	157	LEU	2.2
1	A	494	ILE	2.2
1	A	124	ARG	2.2
1	A	81	ILE	2.2
1	A	158	ALA	2.2
1	B	492	THR	2.2
1	B	148	PHE	2.1
1	B	108	SER	2.1
1	A	142	ASN	2.1
1	A	139	GLU	2.0
1	A	100	SER	2.0
1	B	446	ARG	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
3	SO4	A	3008	5/5	0.61	0.19	123,123,124,124	0
2	BOG	A	4001	20/20	0.69	0.18	84,95,97,98	0
3	SO4	A	3002	5/5	0.75	0.14	112,112,113,113	0

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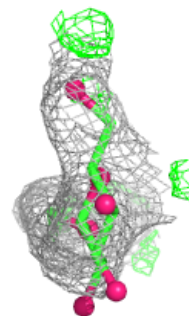
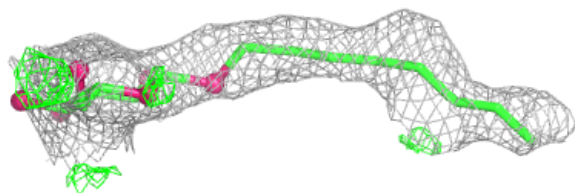
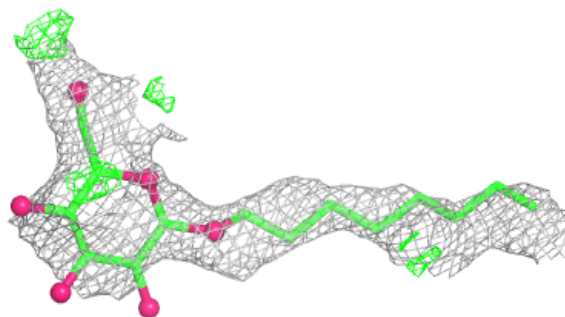
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	3009	5/5	0.79	0.14	118,119,119,120	0
3	SO4	A	3001	5/5	0.80	0.14	102,103,103,103	0
2	BOG	B	4002	20/20	0.80	0.18	83,87,88,89	0
3	SO4	B	3004	5/5	0.82	0.15	117,118,118,118	0
3	SO4	B	3005	5/5	0.86	0.11	97,97,98,99	0
3	SO4	A	3006	5/5	0.87	0.21	104,104,105,106	0
3	SO4	A	3007	5/5	0.87	0.14	115,115,116,116	0
3	SO4	A	3003	5/5	0.89	0.15	99,99,99,100	0
5	H4B	A	902	17/17	0.96	0.06	31,32,37,37	0
5	H4B	B	1902	17/17	0.96	0.08	30,32,38,40	0
6	A11	A	906	19/19	0.96	0.07	26,28,34,35	0
6	A11	B	1906	19/19	0.96	0.07	27,29,31,37	0
4	HEM	A	901	43/43	0.99	0.05	24,27,30,34	0
4	HEM	B	1901	43/43	0.99	0.06	22,27,29,29	0

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

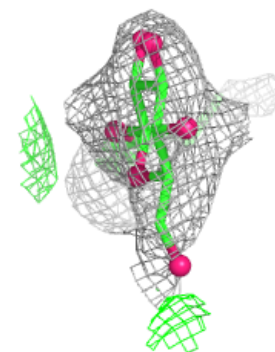
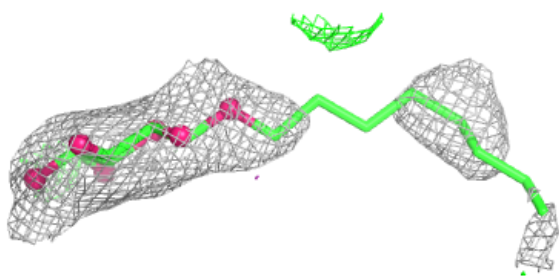
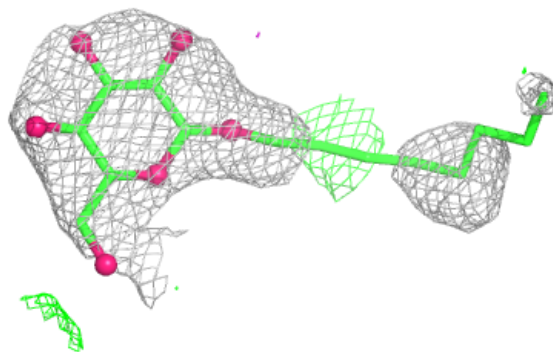
Electron density around BOG A 4001:

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

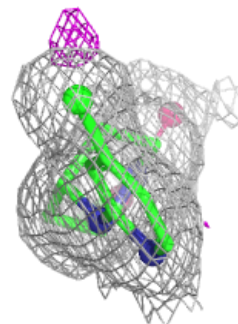
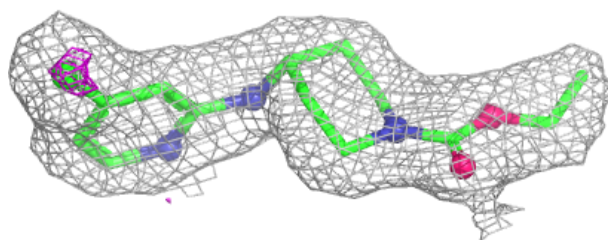
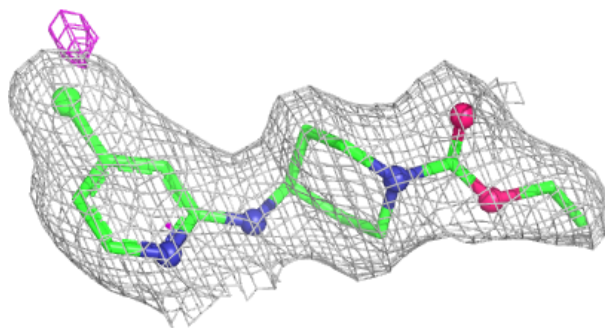


Electron density around BOG B 4002:

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

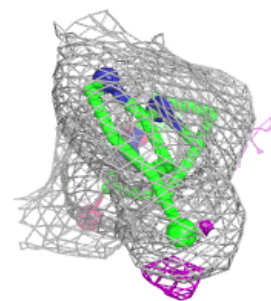
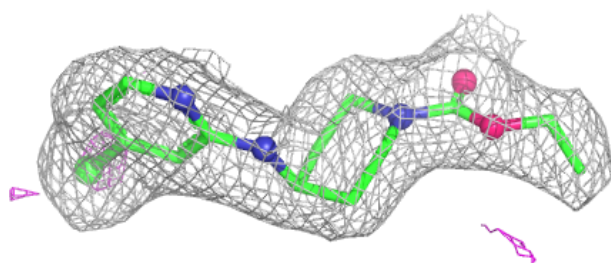
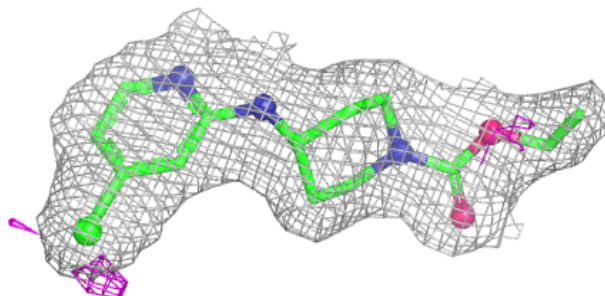
**Electron density around A11 A 906:**

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



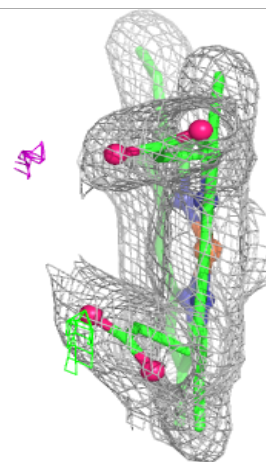
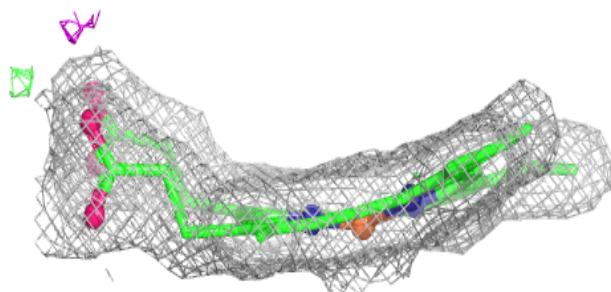
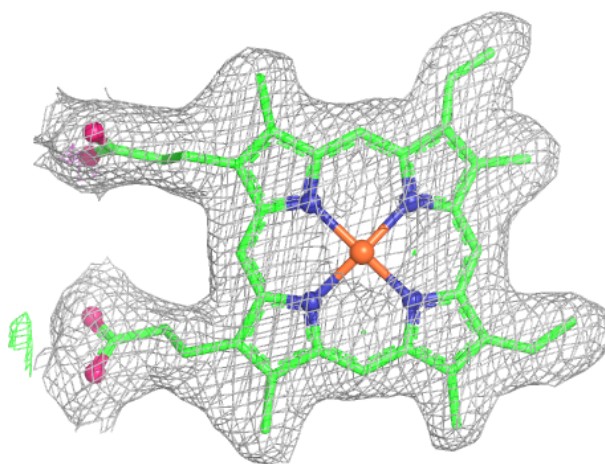
Electron density around A11 B 1906:

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



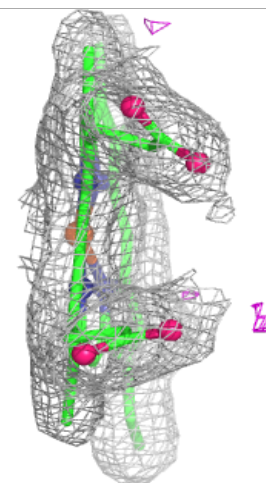
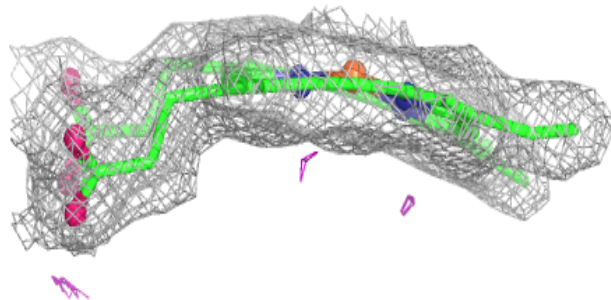
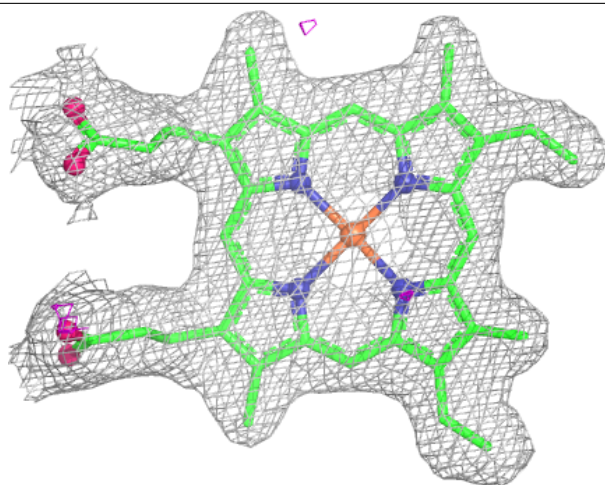
Electron density around HEM A 901:

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



Electron density around HEM B 1901:

$2mF_o-DF_c$ (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.