



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:16 PM UTC

PDB ID : 3E68 / pdb_00003e68
Title : Structure of murine INOS oxygenase domain with inhibitor AR-C130232
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 : 2008-08-14
Resolution : 2.20 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](#) 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

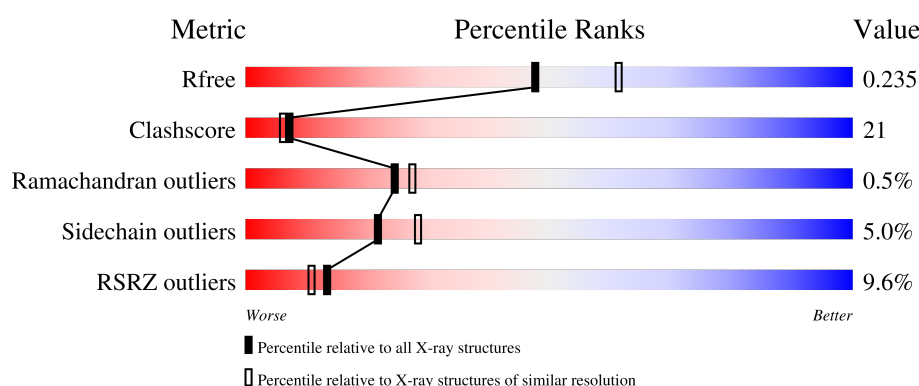
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	433	10% 60% 31% 5% .
1	B	433	8% 62% 28% 5% 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
6	H4B	A	902	X	-	-	-

2 Entry composition [i](#)

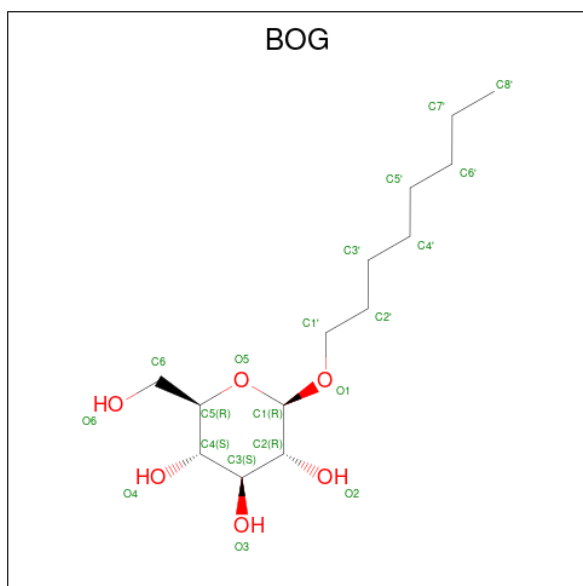
There are 8 unique types of molecules in this entry. The entry contains 7553 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	415	Total	C	N	O	S	0	0	0
			3385	2171	582	612	20			
1	B	410	Total	C	N	O	S	0	0	0
			3347	2148	577	602	20			

- Molecule 2 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).



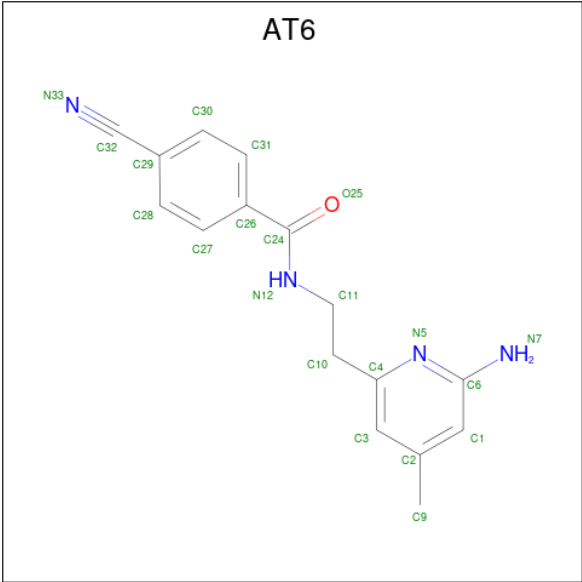
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



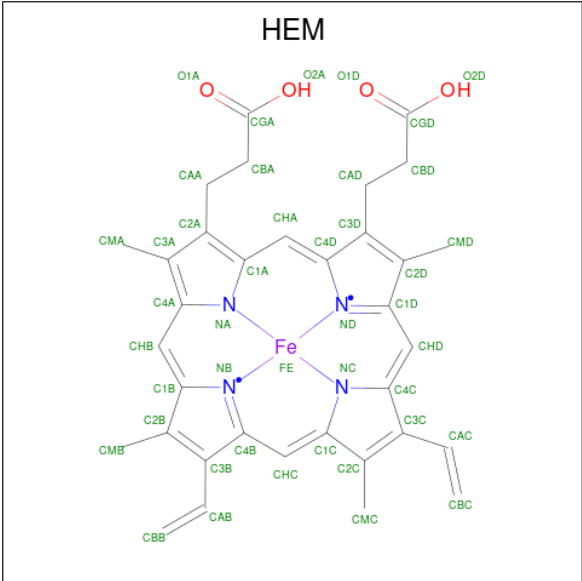
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is N-[2-(6-AMINO-4-METHYLPYRIDIN-2-YL)ETHYL]-4-CYANOBENZAMIDE (CCD ID: AT6) (formula: C₁₆H₁₆N₄O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			21	16	4	1		
4	B	1	Total	C	N	O	0	0
			21	16	4	1		

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



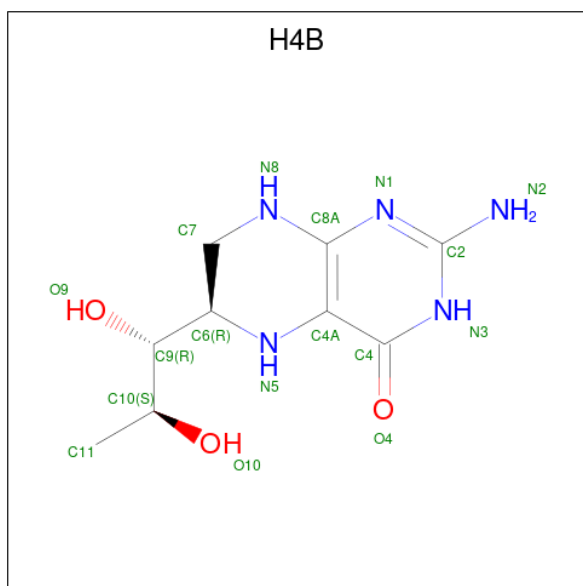
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 6 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: $C_9H_{15}N_5O_3$).



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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	279	Total	O	0	0
			279	279		
8	B	291	Total	O	0	0
			291	291		



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	213.78Å 213.78Å 115.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.63 – 2.20 19.63 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.8 (19.63-2.20) 96.7 (19.63-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.275 0.233 , 0.235	Depositor DCC
R_{free} test set	3880 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.821	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7553	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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, H4B, EDO, BOG, SO4, AT6

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	0.46	0/3484	0.97	17/4737 (0.4%)
1	B	0.45	0/3445	0.98	20/4684 (0.4%)
All	All	0.46	0/6929	0.97	37/9421 (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	B	348	ASN	N-CA-C	7.26	121.45	112.59
1	B	386	LEU	N-CA-C	7.16	118.78	110.97
1	A	348	ASN	N-CA-C	7.15	120.87	112.72
1	B	485	TYR	N-CA-C	-7.01	101.48	110.53
1	A	485	TYR	N-CA-C	-6.77	101.80	110.53
1	A	367	TYR	N-CA-C	6.71	119.96	110.50
1	A	176	THR	N-CA-C	-6.68	101.08	110.50
1	B	122	GLY	N-CA-C	6.64	119.97	112.00
1	A	122	GLY	CA-C-N	6.62	128.12	119.84
1	A	122	GLY	C-N-CA	6.62	128.12	119.84
1	A	386	LEU	N-CA-C	6.32	118.73	111.02
1	A	173	TYR	N-CA-C	6.26	116.71	107.88
1	B	316	PRO	CA-C-N	6.13	126.58	119.47
1	B	316	PRO	C-N-CA	6.13	126.58	119.47
1	B	251	PHE	N-CA-C	-5.98	99.91	109.96
1	A	368	MET	N-CA-C	-5.96	98.81	108.52
1	B	253	LEU	N-CA-C	-5.58	100.15	109.24
1	A	197	ARG	N-CA-C	5.55	119.53	112.87
1	B	197	ARG	N-CA-C	5.49	119.46	112.87
1	B	368	MET	N-CA-C	-5.49	99.46	108.41
1	A	316	PRO	CA-C-N	5.46	126.67	119.84
1	A	316	PRO	C-N-CA	5.46	126.67	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	CYS	N-CA-C	5.44	120.07	113.38
1	B	256	SER	N-CA-C	-5.43	105.27	111.14
1	B	122	GLY	CA-C-N	5.40	126.59	119.84
1	B	122	GLY	C-N-CA	5.40	126.59	119.84
1	B	488	GLU	CA-C-N	5.31	124.77	119.24
1	B	488	GLU	C-N-CA	5.31	124.77	119.24
1	A	234	ILE	N-CA-C	5.31	117.10	109.51
1	A	290	LYS	CA-C-N	5.28	125.19	119.76
1	A	290	LYS	C-N-CA	5.28	125.19	119.76
1	B	367	TYR	N-CA-C	5.19	117.38	110.53
1	B	435	GLU	N-CA-C	-5.17	105.82	111.82
1	B	176	THR	N-CA-C	-5.16	102.05	110.20
1	A	217	MET	N-CA-C	-5.09	105.62	111.07
1	A	466	ILE	N-CA-C	-5.07	105.45	112.50
1	B	325	MET	N-CA-C	5.06	116.99	109.25

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	3385	0	3277	154	0
1	B	3347	0	3247	126	0
2	A	20	0	28	1	0
2	B	20	0	28	0	0
3	A	15	0	0	0	0
3	B	10	0	0	0	0
4	A	21	0	16	1	0
4	B	21	0	16	0	0
5	A	43	0	30	1	0
5	B	43	0	30	2	0
6	A	17	0	14	1	0
6	B	17	0	14	0	0
7	A	12	0	18	1	0
7	B	12	0	18	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	279	0	0	11	1
8	B	291	0	0	6	1
All	All	7553	0	6736	284	2

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 21.

All (284) 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:217:MET:HE3	1:A:303:LEU:HB3	1.52	0.92
1:B:438:MET:HE3	1:B:469:VAL:HG12	1.57	0.87
1:A:213:THR:HG22	1:A:216:GLU:OE1	1.76	0.86
1:A:186:MET:HE1	1:A:189:ARG:HH11	1.42	0.84
1:A:134:LEU:O	1:A:138:ILE:HG12	1.79	0.83
1:B:464:GLY:O	1:B:467:THR:HG22	1.78	0.81
1:B:221:ILE:HG21	1:B:301:LEU:HD21	1.65	0.79
1:A:304:GLN:O	1:A:304:GLN:HG3	1.83	0.78
1:A:438:MET:HE3	1:A:469:VAL:HG12	1.64	0.78
1:B:215:GLN:HG2	8:B:2152:HOH:O	1.84	0.77
1:B:252:ARG:HB2	1:B:304:GLN:HG2	1.67	0.77
1:B:285:ILE:HD12	1:B:291:PRO:HD3	1.68	0.75
1:B:441:MET:HE1	1:B:472:GLN:HG2	1.66	0.75
1:B:292:ARG:NH1	1:B:292:ARG:HB3	2.02	0.74
1:A:176:THR:OG1	1:A:179:GLU:HG3	1.88	0.74
1:B:321:LEU:HD11	7:B:4101:EDO:H11	1.69	0.74
1:B:292:ARG:HB3	1:B:292:ARG:HH11	1.53	0.73
1:B:304:GLN:O	1:B:304:GLN:HG3	1.90	0.72
1:B:494:ILE:H	1:B:494:ILE:HD12	1.54	0.72
1:A:223:ARG:HD2	8:A:2045:HOH:O	1.89	0.71
1:A:153:ILE:HD12	1:A:154:GLU:H	1.55	0.71
1:B:303:LEU:HD23	1:B:313:PHE:CD2	2.26	0.71
1:B:130:LEU:CD2	1:B:167:ILE:HG22	2.20	0.70
1:B:130:LEU:HD21	1:B:167:ILE:HG22	1.73	0.70
1:A:467:THR:CG2	1:A:469:VAL:HG22	2.20	0.70
1:A:153:ILE:O	1:A:157:LEU:HD13	1.92	0.70
1:A:438:MET:HA	1:A:438:MET:HE2	1.72	0.70
1:A:141:ILE:CD1	1:A:163:VAL:HG21	2.23	0.69
1:A:217:MET:CE	1:A:303:LEU:HB3	2.20	0.69
1:B:244:ARG:HA	8:B:2161:HOH:O	1.91	0.69
1:A:159:ARG:O	1:A:163:VAL:HG23	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:PRO:HG2	1:B:132:GLU:HG2	1.73	0.69
1:A:264:TYR:HB2	1:A:266:MET:HE3	1.76	0.68
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.29	0.68
1:B:266:MET:HE2	1:B:272:ARG:CZ	2.23	0.68
1:A:138:ILE:HG22	1:A:142:ASN:HD21	1.58	0.67
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.31	0.66
1:A:467:THR:HG22	1:A:469:VAL:HG22	1.78	0.65
1:A:271:ILE:HD13	1:A:278:LEU:HD11	1.78	0.65
1:B:386:LEU:HB2	8:B:2193:HOH:O	1.96	0.65
1:A:132:GLU:O	1:A:135:PRO:HD2	1.97	0.65
1:A:209:ARG:O	1:A:242:PRO:HG3	1.98	0.64
1:A:163:VAL:O	1:A:167:ILE:HG13	1.97	0.64
1:A:132:GLU:C	1:A:135:PRO:HD2	2.22	0.64
1:A:213:THR:HG23	1:A:216:GLU:H	1.61	0.64
1:A:283:LEU:O	1:A:287:LEU:HG	1.96	0.64
1:B:249:HIS:C	1:B:306:ASP:O	2.40	0.64
1:B:159:ARG:O	1:B:163:VAL:HG23	1.99	0.63
1:B:163:VAL:O	1:B:167:ILE:HG13	1.98	0.63
1:A:77:GLN:O	1:A:96:HIS:HE1	1.82	0.63
1:A:429:ASP:OD2	1:A:432:THR:HG23	1.99	0.63
1:B:467:THR:HG23	1:B:469:VAL:HG22	1.80	0.63
1:A:99:THR:CG2	1:A:100:SER:N	2.61	0.62
1:B:80:ARG:NH2	1:B:89:ILE:HD13	2.14	0.62
1:B:223:ARG:HG3	1:B:223:ARG:HH11	1.63	0.62
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.35	0.62
1:A:186:MET:HE1	1:A:189:ARG:NH1	2.14	0.61
1:A:249:HIS:C	1:A:306:ASP:O	2.44	0.61
1:B:327:HIS:CG	1:B:328:PRO:HD2	2.36	0.60
1:A:439:LYS:O	1:A:442:GLN:HG2	2.01	0.60
1:A:123:PRO:HD3	1:A:487:ILE:HD12	1.83	0.60
1:A:78:TYR:CE1	1:A:91:HIS:ND1	2.69	0.60
1:A:141:ILE:HD11	1:A:163:VAL:HG21	1.84	0.60
1:A:254:TRP:CZ3	1:A:490:TRP:HB3	2.37	0.60
1:A:221:ILE:HD12	1:A:303:LEU:HD21	1.84	0.60
1:A:138:ILE:HG23	1:A:160:LEU:HD22	1.85	0.59
1:B:130:LEU:HD13	1:B:130:LEU:O	2.02	0.59
1:A:241:PHE:HB3	1:A:242:PRO:CD	2.33	0.59
1:A:285:ILE:HD12	1:A:291:PRO:HD3	1.84	0.59
1:A:138:ILE:HG22	1:A:142:ASN:ND2	2.17	0.58
1:A:141:ILE:HD13	1:A:163:VAL:HG21	1.85	0.58
1:B:494:ILE:HD12	1:B:494:ILE:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:THR:O	1:A:285:ILE:HG12	2.04	0.58
1:B:215:GLN:O	1:B:219:GLN:HG3	2.04	0.58
1:A:252:ARG:HD3	1:A:359:PRO:HB2	1.86	0.58
1:A:433:ALA:O	1:A:436:SER:HB3	2.04	0.58
1:B:252:ARG:HH21	1:B:489:PRO:HD3	1.68	0.57
1:A:465:SER:O	1:A:471:HIS:HE1	1.88	0.57
1:A:266:MET:HE1	1:A:293:TYR:HD1	1.70	0.57
1:B:134:LEU:O	1:B:138:ILE:HG13	2.04	0.57
1:A:264:TYR:HB2	1:A:266:MET:CE	2.34	0.57
5:B:1901:HEM:HMC1	5:B:1901:HEM:HBC2	1.87	0.57
1:A:285:ILE:HD11	1:A:291:PRO:HB3	1.87	0.57
1:A:99:THR:HG22	1:A:100:SER:N	2.20	0.57
1:B:271:ILE:HD13	1:B:278:LEU:HD11	1.87	0.57
1:B:303:LEU:O	1:B:310:PRO:HA	2.04	0.57
1:A:303:LEU:O	1:A:310:PRO:HA	2.04	0.56
1:B:78:TYR:CD1	1:B:78:TYR:C	2.84	0.56
1:B:303:LEU:HD23	1:B:313:PHE:HD2	1.70	0.56
1:A:480:SER:HA	1:A:481:PRO:C	2.30	0.56
1:A:215:GLN:HG3	1:A:219:GLN:NE2	2.21	0.55
1:A:215:GLN:NE2	8:A:2044:HOH:O	2.39	0.55
1:A:434:SER:CB	1:A:467:THR:HG23	2.37	0.55
1:B:266:MET:HB3	1:B:267:PRO:HD2	1.87	0.55
1:A:145:TYR:HA	1:A:148:PHE:CE2	2.42	0.54
1:B:132:GLU:C	1:B:135:PRO:HD2	2.32	0.54
1:A:149:LYS:HD3	1:A:150:GLU:HG3	1.89	0.54
1:A:161:GLU:HB3	8:A:2470:HOH:O	2.06	0.54
1:B:301:LEU:HB3	1:B:303:LEU:HD21	1.89	0.54
1:A:243:GLN:HB3	1:A:358:PHE:CE2	2.43	0.54
1:A:328:PRO:C	1:A:329:LYS:HD2	2.32	0.54
1:A:124:ARG:NH1	1:A:128:THR:OG1	2.42	0.53
1:B:332:TRP:O	1:B:335:GLU:HB2	2.08	0.53
1:A:78:TYR:C	1:A:78:TYR:CD1	2.86	0.53
1:B:303:LEU:N	1:B:303:LEU:HD22	2.22	0.53
1:A:429:ASP:CG	1:A:432:THR:HG23	2.34	0.53
5:A:901:HEM:HBC2	5:A:901:HEM:HMC2	1.91	0.53
1:A:153:ILE:CD1	1:A:154:GLU:H	2.21	0.53
1:B:453:ALA:HB3	1:B:474:MET:HB3	1.90	0.53
1:B:77:GLN:HE21	1:B:78:TYR:HD2	1.57	0.53
1:B:224:HIS:HD2	1:B:239:THR:OG1	1.93	0.52
1:B:190:ASN:O	1:B:192:PRO:HD3	2.09	0.52
1:A:467:THR:HG21	1:A:469:VAL:HG22	1.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:TYR:HE2	1:B:159:ARG:HG2	1.73	0.52
1:B:252:ARG:NH1	1:B:486:GLN:CD	2.68	0.52
1:B:285:ILE:HD11	1:B:291:PRO:HB3	1.92	0.52
1:A:84:TRP:CE2	1:A:114:MET:HG3	2.45	0.52
1:A:251:PHE:O	1:A:360:ALA:HB2	2.10	0.52
1:A:145:TYR:HA	1:A:148:PHE:HE2	1.72	0.52
1:B:244:ARG:NH1	1:B:357:GLU:OE2	2.43	0.52
1:A:244:ARG:HD2	1:A:357:GLU:OE2	2.10	0.51
1:B:252:ARG:HB2	1:B:304:GLN:CG	2.38	0.51
1:A:350:LEU:C	1:A:350:LEU:HD23	2.35	0.51
4:A:905:AT6:H27	8:A:2320:HOH:O	2.09	0.51
1:A:202:ASN:C	1:A:202:ASN:HD22	2.19	0.51
1:A:332:TRP:O	1:A:335:GLU:HB2	2.09	0.51
1:A:302:VAL:C	1:A:303:LEU:HD12	2.36	0.51
1:B:177:LEU:C	1:B:177:LEU:HD13	2.35	0.51
1:A:128:THR:O	1:A:129:PRO:C	2.54	0.51
1:A:134:LEU:HB3	1:A:135:PRO:HD3	1.93	0.51
1:B:251:PHE:O	1:B:252:ARG:HG2	2.11	0.51
1:A:129:PRO:HG3	8:A:2016:HOH:O	2.11	0.51
1:A:213:THR:CG2	1:A:216:GLU:HG3	2.40	0.51
1:B:241:PHE:HB3	1:B:242:PRO:CD	2.41	0.51
1:A:213:THR:HG22	1:A:216:GLU:CD	2.36	0.51
1:B:153:ILE:O	1:B:156:HIS:HB3	2.10	0.51
1:A:145:TYR:HE2	1:A:159:ARG:HG2	1.76	0.51
1:A:252:ARG:HB2	1:A:304:GLN:HG2	1.91	0.51
1:A:253:LEU:HD12	1:A:253:LEU:N	2.25	0.51
1:B:433:ALA:O	1:B:436:SER:HB3	2.10	0.51
1:A:327:HIS:CG	1:A:328:PRO:HD2	2.46	0.50
1:A:241:PHE:HB3	1:A:242:PRO:HD2	1.93	0.50
1:B:353:VAL:HG23	1:B:481:PRO:HG3	1.93	0.50
1:A:231:ASN:ND2	8:A:2405:HOH:O	2.44	0.50
1:B:283:LEU:O	1:B:287:LEU:HG	2.12	0.50
1:A:328:PRO:O	1:A:329:LYS:HD2	2.12	0.50
1:A:386:LEU:HB2	8:A:2084:HOH:O	2.12	0.49
1:B:301:LEU:HD13	1:B:315:ILE:HD11	1.94	0.49
1:B:281:THR:O	1:B:285:ILE:HG12	2.12	0.49
1:A:134:LEU:HD11	1:A:138:ILE:HD11	1.93	0.49
1:B:171:GLY:O	1:B:172:THR:HB	2.12	0.49
1:B:149:LYS:O	1:B:150:GLU:HB2	2.13	0.49
1:B:397:THR:HG22	1:B:397:THR:O	2.11	0.49
1:B:441:MET:HE1	1:B:472:GLN:CG	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:THR:CG2	1:B:469:VAL:HG22	2.41	0.49
1:B:153:ILE:O	1:B:157:LEU:HG	2.13	0.49
1:A:133:LEU:C	1:A:133:LEU:HD23	2.38	0.49
1:A:221:ILE:HG21	1:A:301:LEU:HD21	1.94	0.49
1:B:138:ILE:O	1:B:142:ASN:ND2	2.45	0.49
1:A:80:ARG:NH1	1:A:89:ILE:HG21	2.28	0.48
1:B:137:ALA:O	1:B:141:ILE:HD13	2.12	0.48
1:B:241:PHE:HB3	1:B:242:PRO:HD2	1.95	0.48
1:A:188:TRP:CZ3	1:A:200:TRP:HA	2.49	0.48
1:B:258:LEU:HD22	1:B:345:ALA:HB1	1.96	0.48
1:A:140:PHE:HE2	1:A:175:LEU:HD22	1.78	0.48
1:A:434:SER:HB3	1:A:467:THR:HG23	1.95	0.48
1:B:132:GLU:O	1:B:135:PRO:HD2	2.14	0.48
1:B:252:ARG:NH1	1:B:486:GLN:OE1	2.47	0.47
1:B:350:LEU:HB2	1:B:486:GLN:CD	2.38	0.47
1:B:384:ASN:CG	1:B:384:ASN:O	2.58	0.47
1:A:99:THR:CG2	1:A:100:SER:H	2.27	0.47
1:A:138:ILE:O	1:A:142:ASN:ND2	2.48	0.47
1:B:488:GLU:OE2	1:B:491:LYS:HE2	2.15	0.47
1:B:251:PHE:C	1:B:252:ARG:HG2	2.40	0.47
1:B:438:MET:HE2	1:B:438:MET:HA	1.97	0.47
1:A:285:ILE:CD1	1:A:291:PRO:HD3	2.45	0.46
1:A:321:LEU:HD11	7:A:3101:EDO:H22	1.96	0.46
1:B:209:ARG:O	1:B:242:PRO:HG3	2.16	0.46
1:B:407:ARG:HG3	8:B:2202:HOH:O	2.14	0.46
1:B:487:ILE:N	1:B:487:ILE:HD12	2.30	0.46
1:A:79:VAL:HG23	1:A:95:HIS:CE1	2.50	0.46
1:A:304:GLN:O	1:A:304:GLN:CG	2.61	0.46
1:A:133:LEU:CD2	1:A:167:ILE:HD13	2.45	0.46
1:A:133:LEU:HD22	1:A:167:ILE:HD13	1.98	0.46
1:A:303:LEU:N	1:A:303:LEU:CD1	2.79	0.46
1:B:346:VAL:O	1:B:362:PRO:HA	2.16	0.46
1:B:488:GLU:O	1:B:491:LYS:HB2	2.15	0.46
1:A:202:ASN:C	1:A:202:ASN:ND2	2.73	0.46
1:A:330:TYR:HB3	1:A:332:TRP:CE2	2.51	0.46
1:B:215:GLN:CG	8:B:2152:HOH:O	2.55	0.46
1:A:123:PRO:CD	1:A:487:ILE:HD12	2.44	0.46
1:B:258:LEU:HB2	1:B:345:ALA:HB3	1.97	0.46
1:B:224:HIS:HE1	1:B:364:ASN:OD1	1.98	0.45
1:B:256:SER:HB2	1:B:257:GLN:OE1	2.16	0.45
1:A:264:TYR:CE1	1:A:293:TYR:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:LEU:C	1:B:283:LEU:HD23	2.41	0.45
1:A:124:ARG:HD2	1:A:244:ARG:HD3	1.98	0.45
1:A:264:TYR:CD1	1:A:293:TYR:HA	2.52	0.45
1:B:124:ARG:HG3	1:B:124:ARG:HH11	1.82	0.45
1:A:134:LEU:CD1	1:A:138:ILE:HD11	2.47	0.45
1:B:145:TYR:CD1	1:B:148:PHE:HZ	2.35	0.45
1:B:285:ILE:CD1	1:B:291:PRO:HB3	2.47	0.45
1:B:414:VAL:HG13	7:B:4104:EDO:O2	2.16	0.45
1:B:480:SER:HA	1:B:481:PRO:C	2.42	0.45
1:A:92:ASP:O	1:A:95:HIS:CE1	2.70	0.45
1:A:239:THR:O	1:A:361:CYS:HA	2.17	0.45
1:A:248:LYS:O	1:A:248:LYS:HG3	2.17	0.45
1:A:398:HIS:HB2	8:A:2088:HOH:O	2.17	0.45
1:A:129:PRO:O	1:A:132:GLU:HG3	2.17	0.44
1:A:214:ALA:O	1:A:217:MET:HB2	2.17	0.44
1:A:368:MET:HE3	1:A:370:THR:OG1	2.16	0.44
1:B:123:PRO:HD3	1:B:487:ILE:HD13	1.99	0.44
1:B:133:LEU:C	1:B:133:LEU:HD13	2.42	0.44
1:A:99:THR:HG23	1:A:100:SER:H	1.83	0.44
1:A:494:ILE:HD12	1:A:495:TRP:H	1.83	0.44
1:B:149:LYS:HG2	1:B:150:GLU:HG3	1.99	0.44
1:A:217:MET:HE2	1:A:305:ALA:HB2	2.00	0.44
1:A:290:LYS:HA	1:A:291:PRO:HD2	1.85	0.44
1:A:350:LEU:HD21	1:A:357:GLU:HB2	2.00	0.44
1:A:441:MET:HE1	1:A:474:MET:HG2	2.00	0.44
1:B:494:ILE:H	1:B:494:ILE:CD1	2.10	0.44
1:A:258:LEU:HB2	1:A:345:ALA:HB3	2.00	0.44
1:B:213:THR:OG1	1:B:216:GLU:HG3	2.17	0.44
1:A:445:TYR:HA	1:A:450:GLY:H	1.82	0.43
1:A:84:TRP:NE1	1:A:114:MET:HG3	2.33	0.43
1:A:464:GLY:O	1:A:467:THR:HB	2.19	0.43
1:B:330:TYR:HB3	1:B:332:TRP:CE2	2.53	0.43
1:A:250:ASP:HB2	8:A:2344:HOH:O	2.19	0.43
1:A:358:PHE:CD1	1:A:358:PHE:N	2.86	0.43
1:B:84:TRP:NE1	1:B:114:MET:HG3	2.33	0.43
1:B:175:LEU:HD13	1:B:356:LEU:CD1	2.49	0.43
1:B:188:TRP:CZ3	1:B:200:TRP:HA	2.53	0.43
1:A:213:THR:HG22	1:A:216:GLU:CG	2.48	0.43
1:B:141:ILE:N	1:B:141:ILE:HD12	2.33	0.43
1:B:223:ARG:HG3	1:B:223:ARG:NH1	2.30	0.43
1:B:289:TRP:HE1	1:B:314:GLU:CD	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ASP:OD1	1:A:432:THR:HG23	2.19	0.43
1:A:457:TRP:HA	6:A:902:H4B:N1	2.34	0.43
1:A:301:LEU:HG	1:A:303:LEU:HD11	2.01	0.42
1:A:487:ILE:O	1:A:488:GLU:C	2.61	0.42
1:A:358:PHE:HB3	8:A:2080:HOH:O	2.19	0.42
1:A:165:LYS:O	1:A:169:THR:HG23	2.19	0.42
1:B:133:LEU:HD13	1:B:133:LEU:O	2.20	0.42
1:B:139:GLU:HG3	8:B:2382:HOH:O	2.20	0.42
1:B:330:TYR:HB3	1:B:332:TRP:NE1	2.34	0.42
1:B:309:ASP:HB3	1:B:495:TRP:CZ3	2.55	0.42
1:B:177:LEU:HD11	1:B:181:ILE:HD11	2.02	0.42
1:B:302:VAL:CG1	1:B:310:PRO:HB2	2.50	0.42
1:A:82:LYS:HD3	1:A:84:TRP:CE2	2.55	0.42
1:A:221:ILE:O	1:A:224:HIS:HB3	2.20	0.42
1:A:191:ALA:O	1:A:197:ARG:CZ	2.67	0.42
1:B:218:PHE:CE1	1:B:313:PHE:HB3	2.55	0.42
1:A:153:ILE:HD12	1:A:153:ILE:N	2.35	0.41
1:A:242:PRO:HG2	1:A:251:PHE:CZ	2.55	0.41
1:B:252:ARG:NH2	1:B:489:PRO:HD3	2.33	0.41
1:B:257:GLN:OE1	1:B:260:ARG:NH1	2.54	0.41
1:A:99:THR:O	1:A:100:SER:C	2.64	0.41
1:A:129:PRO:HB2	1:A:132:GLU:HG3	2.02	0.41
1:A:244:ARG:NH1	1:A:357:GLU:OE2	2.48	0.41
1:B:282:GLN:O	1:B:283:LEU:C	2.61	0.41
1:A:257:GLN:CB	1:A:345:ALA:O	2.68	0.41
1:A:393:MET:HB2	1:A:395:LEU:HD22	2.03	0.41
1:A:165:LYS:HB2	1:A:165:LYS:HE3	1.87	0.41
1:A:494:ILE:HD12	1:A:495:TRP:N	2.36	0.41
1:A:116:PRO:C	1:A:118:SER:N	2.78	0.41
1:A:172:THR:HG23	1:A:173:TYR:N	2.36	0.41
1:A:163:VAL:HG13	1:A:173:TYR:CD2	2.56	0.41
1:A:174:GLN:HA	8:A:2020:HOH:O	2.21	0.41
1:B:130:LEU:HD13	1:B:130:LEU:C	2.46	0.41
1:B:254:TRP:CZ3	1:B:490:TRP:HB3	2.55	0.41
1:B:453:ALA:O	1:B:476:ASN:HB2	2.21	0.41
1:B:489:PRO:C	1:B:491:LYS:H	2.29	0.41
1:B:304:GLN:O	1:B:304:GLN:CG	2.65	0.41
1:B:417:LEU:HB3	7:B:4104:EDO:H12	2.02	0.41
1:B:431:HIS:O	1:B:435:GLU:HG3	2.21	0.41
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.93	0.40
1:B:84:TRP:CE2	1:B:114:MET:HG3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:HIS:CD2	1:B:239:THR:OG1	2.74	0.40
1:B:470:PHE:CD1	1:B:470:PHE:C	2.99	0.40
5:B:1901:HEM:HBC2	5:B:1901:HEM:CMC	2.52	0.40
1:A:134:LEU:N	1:A:135:PRO:CD	2.84	0.40
1:B:124:ARG:HH21	1:B:128:THR:HB	1.87	0.40
1:B:397:THR:O	1:B:397:THR:CG2	2.70	0.40
1:A:138:ILE:HG21	2:A:3100:BOG:H7'1	2.02	0.40

All (2) 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)
8:B:2368:HOH:O	8:B:2499:HOH:O[9_766]	1.99	0.21
8:A:2473:HOH:O	8:A:2473:HOH:O[9_765]	2.00	0.20

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	411/433 (95%)	368 (90%)	41 (10%)	2 (0%)	24	27
1	B	406/433 (94%)	373 (92%)	31 (8%)	2 (0%)	24	27
All	All	817/866 (94%)	741 (91%)	72 (9%)	4 (0%)	24	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	172	THR
1	B	306	ASP
1	A	306	ASP
1	A	123	PRO

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	363/381 (95%)	344 (95%)	19 (5%)	21	26
1	B	358/381 (94%)	341 (95%)	17 (5%)	23	31
All	All	721/762 (95%)	685 (95%)	36 (5%)	22	28

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	LEU
1	A	114	MET
1	A	118	SER
1	A	121	ARG
1	A	129	PRO
1	A	132	GLU
1	A	153	ILE
1	A	180	LEU
1	A	257	GLN
1	A	258	LEU
1	A	292	ARG
1	A	301	LEU
1	A	303	LEU
1	A	338	LEU
1	A	348	ASN
1	A	380	THR
1	A	395	LEU
1	A	417	LEU
1	A	432	THR
1	B	114	MET
1	B	119	LEU
1	B	128	THR
1	B	133	LEU
1	B	175	LEU
1	B	215	GLN
1	B	226	LEU
1	B	257	GLN

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Mol	Chain	Res	Type
1	B	258	LEU
1	B	292	ARG
1	B	301	LEU
1	B	303	LEU
1	B	348	ASN
1	B	407	ARG
1	B	417	LEU
1	B	467	THR
1	B	494	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	96	HIS
1	A	202	ASN
1	A	204	GLN
1	A	215	GLN
1	A	219	GLN
1	A	220	HIS
1	A	233	ASN
1	A	243	GLN
1	A	249	HIS
1	A	265	GLN
1	A	348	ASN
1	A	364	ASN
1	A	384	ASN
1	A	442	GLN
1	A	471	HIS
1	A	476	ASN
1	B	77	GLN
1	B	142	ASN
1	B	143	GLN
1	B	199	GLN
1	B	202	ASN
1	B	215	GLN
1	B	220	HIS
1	B	224	HIS
1	B	233	ASN
1	B	282	GLN
1	B	334	GLN
1	B	348	ASN

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Mol	Chain	Res	Type
1	B	364	ASN
1	B	421	GLN
1	B	476	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 ⓘ

19 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	$\# Z > 2$
7	EDO	B	4104	-	3,3,3	0.48	0	2,2,2	0.67	0
3	SO4	B	4003	-	4,4,4	0.44	0	6,6,6	0.05	0
6	H4B	A	902	-	17,18,18	2.61	4 (23%)	14,26,26	2.02	4 (28%)
7	EDO	A	3104	-	3,3,3	0.48	0	2,2,2	0.66	0
4	AT6	A	905	-	22,22,22	1.32	4 (18%)	28,29,29	1.54	4 (14%)
7	EDO	B	4101	-	3,3,3	0.63	0	2,2,2	0.49	0
7	EDO	A	3102	-	3,3,3	0.42	0	2,2,2	0.68	0
3	SO4	A	3004	-	4,4,4	0.37	0	6,6,6	0.12	0
3	SO4	B	4004	-	4,4,4	0.42	0	6,6,6	0.13	0
5	HEM	B	1901	1	50,50,50	1.51	8 (16%)	67,82,82	1.13	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	3005	-	4,4,4	0.42	0	6,6,6	0.12	0
5	HEM	A	901	-	50,50,50	1.55	7 (14%)	67,82,82	0.92	3 (4%)
2	BOG	B	4100	-	20,20,20	0.92	1 (5%)	25,25,25	0.65	0
2	BOG	A	3100	-	20,20,20	0.95	2 (10%)	25,25,25	0.61	0
7	EDO	A	3101	-	3,3,3	0.59	0	2,2,2	0.54	0
4	AT6	B	1905	-	22,22,22	1.51	4 (18%)	28,29,29	1.69	6 (21%)
6	H4B	B	1902	-	17,18,18	2.70	4 (23%)	14,26,26	2.01	4 (28%)
3	SO4	A	3003	-	4,4,4	0.43	0	6,6,6	0.05	0
7	EDO	B	4102	-	3,3,3	0.42	0	2,2,2	0.70	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	A	3100	-	-	1/11/31/31	0/1/1/1
6	H4B	A	902	-	1/1/3/5	4/8/17/17	0/2/2/2
7	EDO	B	4101	-	-	0/1/1/1	-
7	EDO	A	3101	-	-	0/1/1/1	-
7	EDO	A	3102	-	-	0/1/1/1	-
7	EDO	A	3104	-	-	0/1/1/1	-
4	AT6	A	905	-	-	2/12/12/12	0/2/2/2
4	AT6	B	1905	-	-	2/12/12/12	0/2/2/2
6	H4B	B	1902	-	-	0/8/17/17	0/2/2/2
7	EDO	B	4102	-	-	0/1/1/1	-
7	EDO	B	4104	-	-	0/1/1/1	-
5	HEM	B	1901	1	-	2/14/54/54	-
5	HEM	A	901	-	-	1/14/54/54	-
2	BOG	B	4100	-	-	1/11/31/31	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1902	H4B	C7-N8	-7.69	1.38	1.46
6	A	902	H4B	C7-N8	-7.33	1.39	1.46
6	B	1902	H4B	C7-C6	-6.47	1.46	1.52
6	A	902	H4B	C7-C6	-6.03	1.46	1.52
5	A	901	HEM	FE-NC	4.64	2.10	1.95
5	B	1901	HEM	FE-NB	4.16	2.07	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1901	HEM	FE-NC	4.11	2.08	1.95
5	A	901	HEM	FE-ND	3.82	2.06	1.94
5	A	901	HEM	FE-NB	3.64	2.06	1.94
5	B	1901	HEM	FE-ND	3.50	2.05	1.94
5	A	901	HEM	FE-NA	3.09	2.05	1.95
6	A	902	H4B	C4-N3	-3.01	1.33	1.38
5	B	1901	HEM	CAB-C3B	-2.89	1.39	1.47
5	B	1901	HEM	FE-NA	2.81	2.04	1.95
6	B	1902	H4B	C4-N3	-2.78	1.33	1.38
2	B	4100	BOG	O1-C1	2.76	1.44	1.40
5	A	901	HEM	C3C-C2C	2.72	1.42	1.37
4	B	1905	AT6	C1-C2	2.67	1.43	1.39
2	A	3100	BOG	O1-C1	2.61	1.44	1.40
5	A	901	HEM	CAB-C3B	-2.60	1.40	1.47
4	B	1905	AT6	C31-C26	2.57	1.43	1.39
4	A	905	AT6	C31-C30	2.32	1.42	1.38
6	A	902	H4B	C4A-N5	-2.31	1.32	1.37
4	B	1905	AT6	C27-C26	2.29	1.42	1.39
4	A	905	AT6	C1-C2	2.26	1.42	1.39
2	A	3100	BOG	O5-C1	2.26	1.47	1.41
5	B	1901	HEM	C3B-C4B	2.20	1.49	1.44
5	B	1901	HEM	CBC-CAC	2.18	1.40	1.30
4	A	905	AT6	C31-C26	2.13	1.42	1.39
4	A	905	AT6	C4-N5	2.13	1.38	1.34
6	B	1902	H4B	C4A-C8A	2.11	1.42	1.38
4	B	1905	AT6	C31-C30	2.10	1.42	1.38
5	B	1901	HEM	CBB-CAB	2.03	1.40	1.30
5	A	901	HEM	CBC-CAC	2.01	1.40	1.30

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1905	AT6	C6-N5-C4	5.68	122.32	118.07
4	A	905	AT6	C6-N5-C4	5.18	121.94	118.07
6	B	1902	H4B	C2-N1-C8A	4.26	120.88	113.36
6	A	902	H4B	O4-C4-C4A	-4.12	117.33	127.26
6	A	902	H4B	C2-N1-C8A	4.10	120.59	113.36
6	B	1902	H4B	O4-C4-C4A	-3.93	117.77	127.26
5	B	1901	HEM	CMD-C2D-C1D	3.07	129.84	125.03
5	B	1901	HEM	C4C-C3C-C2C	-2.93	104.27	106.81
6	A	902	H4B	C4A-C4-N3	2.87	120.02	112.13
6	B	1902	H4B	C4A-C4-N3	2.79	119.80	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1901	HEM	CAD-C3D-C2D	-2.67	122.87	127.87
4	A	905	AT6	N7-C6-N5	2.63	120.82	116.59
4	A	905	AT6	C10-C4-N5	2.62	120.03	116.06
4	B	1905	AT6	C10-C4-N5	2.57	119.95	116.06
6	A	902	H4B	C2-N3-C4	-2.56	120.47	125.11
4	B	1905	AT6	N7-C6-N5	2.52	120.64	116.59
6	B	1902	H4B	C2-N3-C4	-2.51	120.56	125.11
5	A	901	HEM	CAA-C2A-C1A	2.38	129.59	124.94
4	B	1905	AT6	O25-C24-C26	-2.36	116.23	120.90
5	B	1901	HEM	CHC-C4B-NB	-2.32	121.92	124.42
4	B	1905	AT6	C26-C24-N12	2.32	121.94	117.12
5	A	901	HEM	C4C-C3C-C2C	-2.26	104.85	106.81
4	B	1905	AT6	C3-C4-N5	-2.21	120.22	122.73
5	A	901	HEM	C4B-C3B-C2B	-2.11	105.34	107.28
5	B	1901	HEM	CAD-C3D-C4D	2.05	128.26	124.70
5	B	1901	HEM	C1D-C2D-C3D	-2.05	104.83	106.98
4	A	905	AT6	C3-C4-N5	-2.02	120.43	122.73

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	902	H4B	C6

All (13) torsion outliers are listed below:

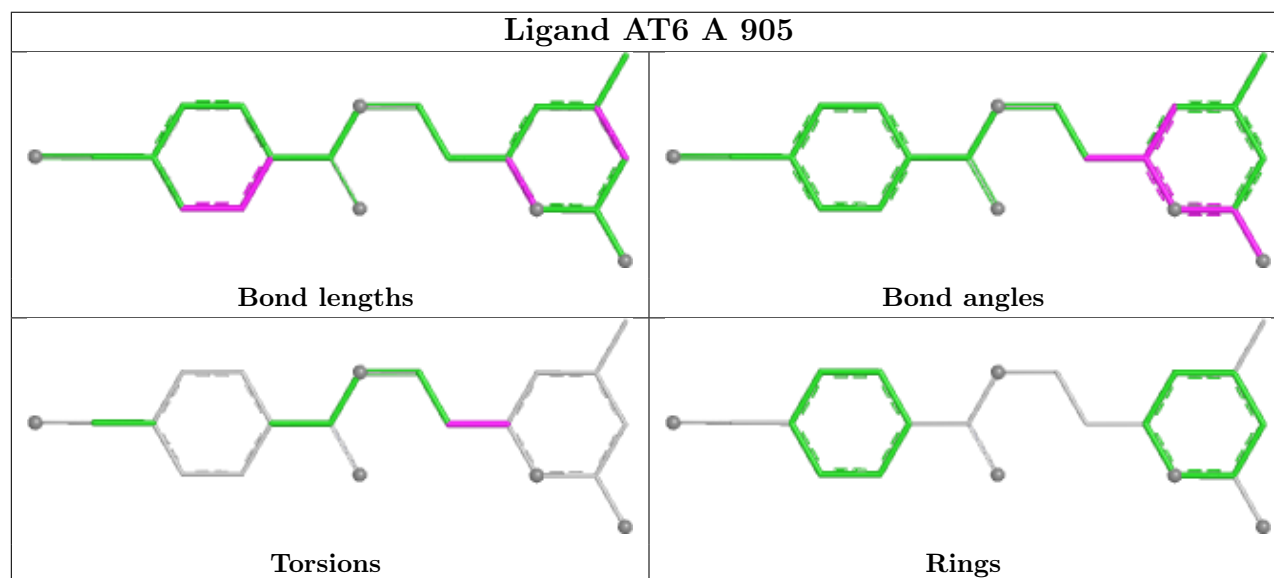
Mol	Chain	Res	Type	Atoms
6	A	902	H4B	C7-C6-C9-O9
6	A	902	H4B	C7-C6-C9-C10
4	B	1905	AT6	C11-C10-C4-N5
2	B	4100	BOG	O1-C1'-C2'-C3'
2	A	3100	BOG	O1-C1'-C2'-C3'
4	B	1905	AT6	C11-C10-C4-C3
4	A	905	AT6	C11-C10-C4-N5
6	A	902	H4B	N5-C6-C9-O9
4	A	905	AT6	C11-C10-C4-C3
5	A	901	HEM	C1A-C2A-CAA-CBA
6	A	902	H4B	N5-C6-C9-C10
5	B	1901	HEM	C2C-C3C-CAC-CBC
5	B	1901	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

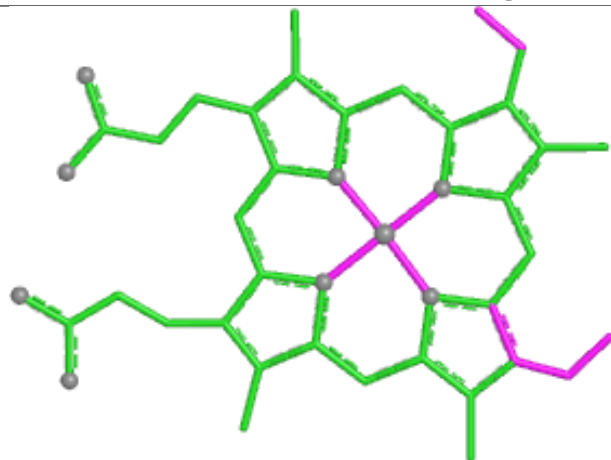
8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	4104	EDO	2	0
6	A	902	H4B	1	0
4	A	905	AT6	1	0
7	B	4101	EDO	1	0
5	B	1901	HEM	2	0
5	A	901	HEM	1	0
2	A	3100	BOG	1	0
7	A	3101	EDO	1	0

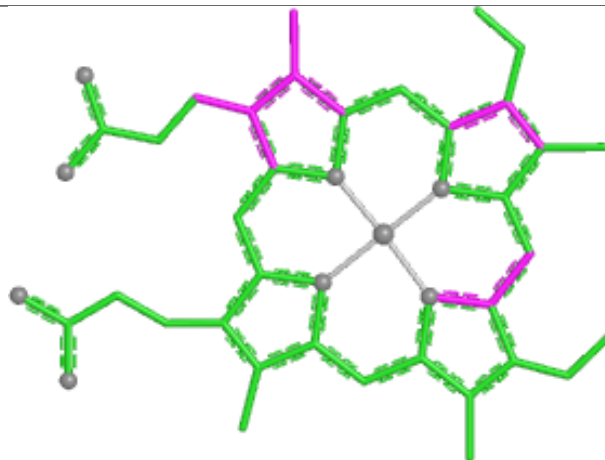
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



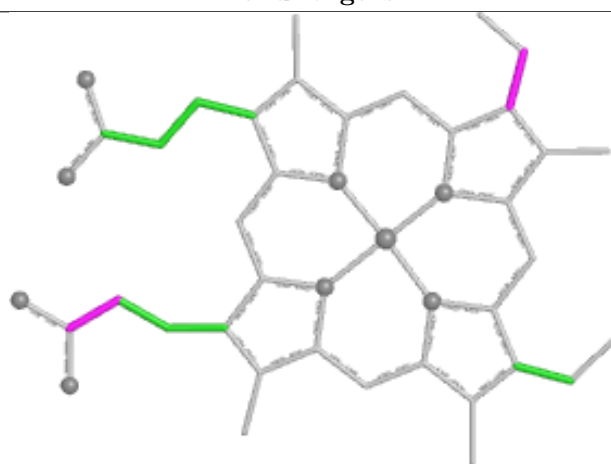
Ligand HEM B 1901



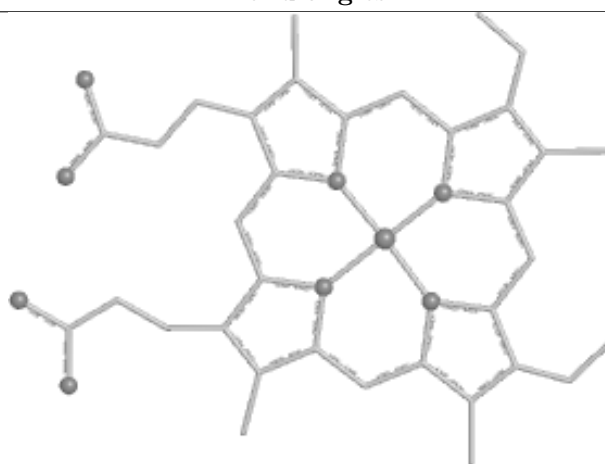
Bond lengths



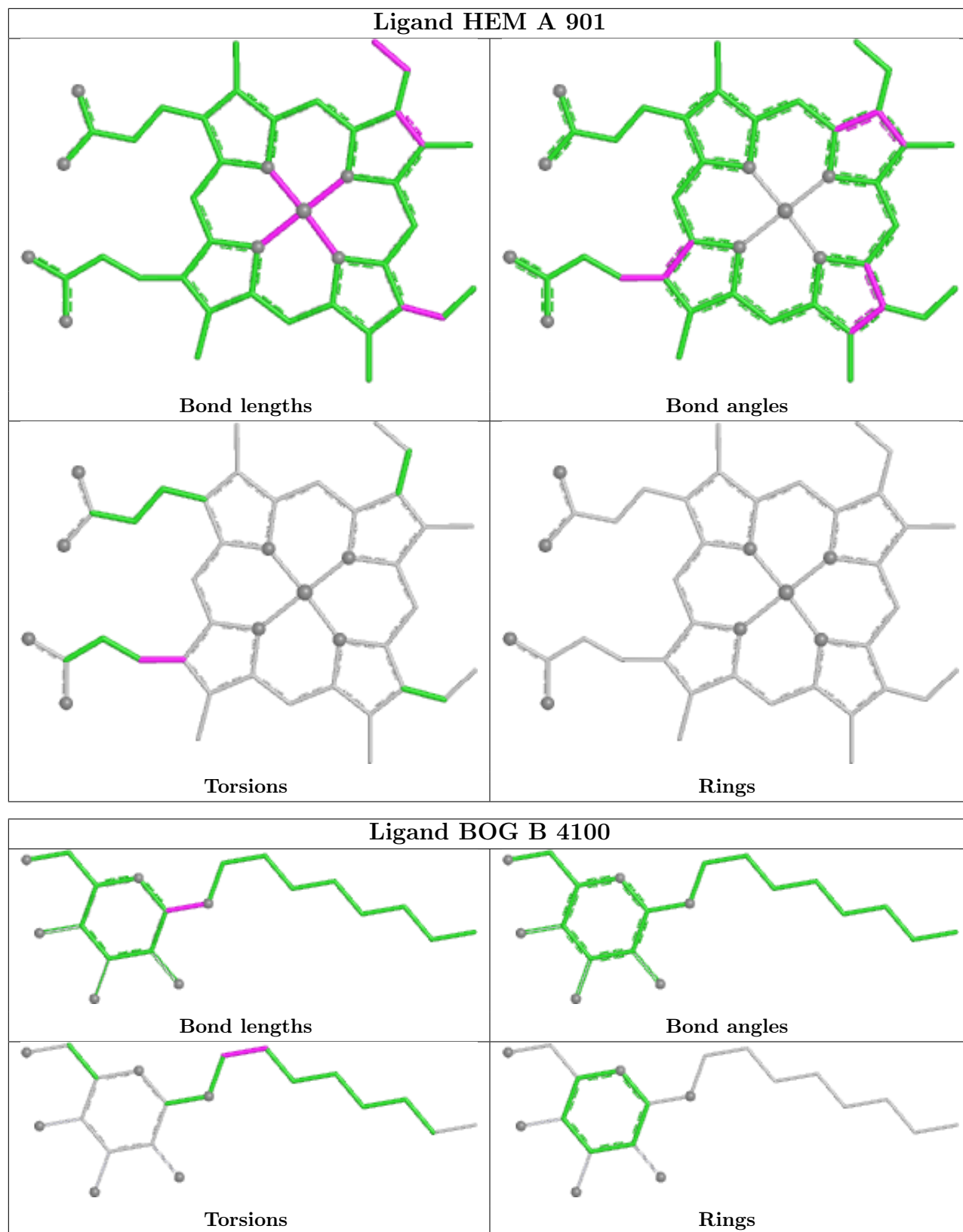
Bond angles

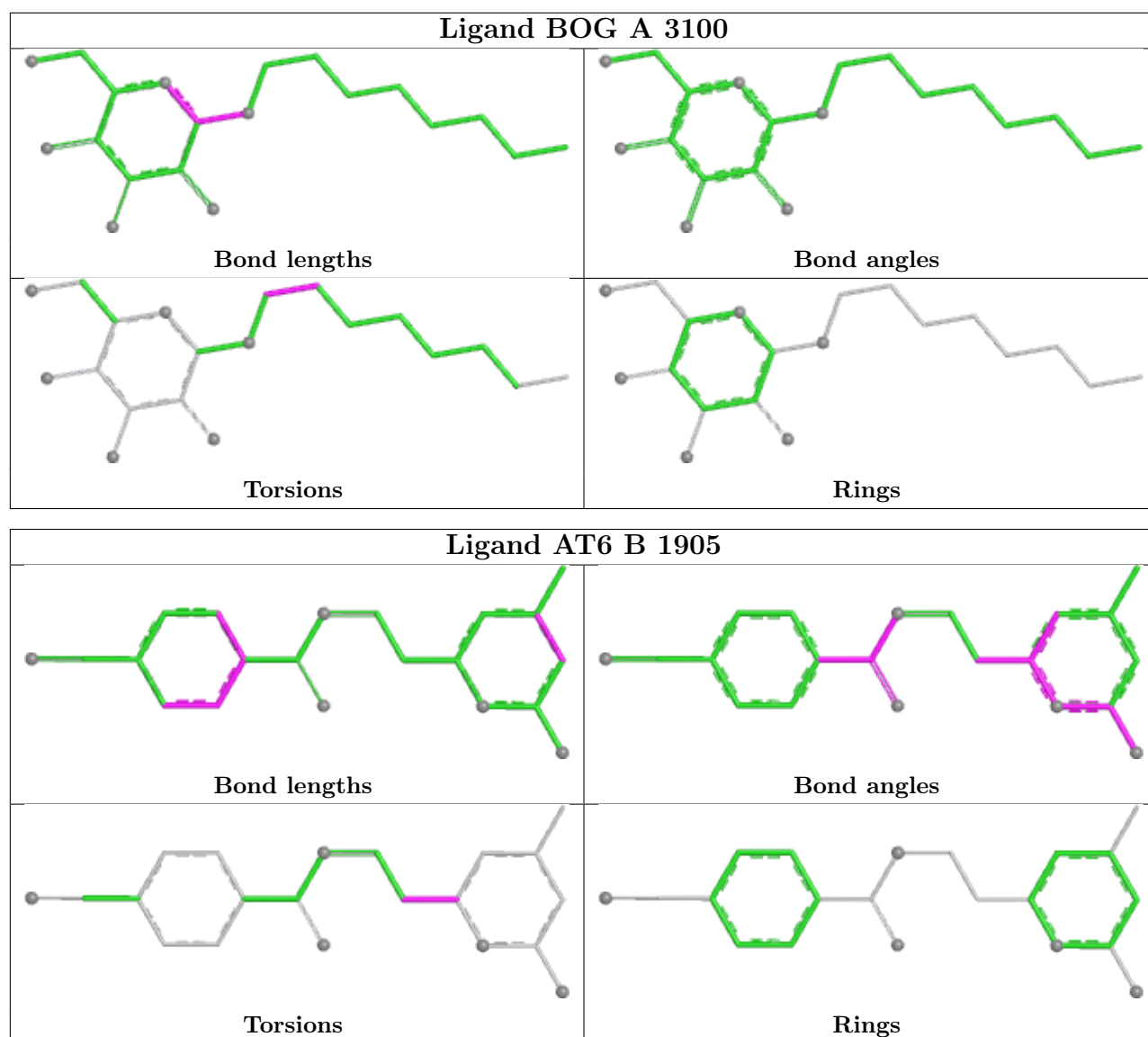


Torsions



Rings





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	415/433 (95%)	0.69	45 (10%) 11 8	25, 46, 78, 106	0
1	B	410/433 (94%)	0.57	34 (8%) 17 15	21, 45, 74, 91	0
All	All	825/866 (95%)	0.63	79 (9%) 13 11	21, 46, 75, 106	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	494	ILE	6.2
1	B	494	ILE	4.5
1	B	148	PHE	4.4
1	A	306	ASP	4.2
1	A	103	THR	4.2
1	A	153	ILE	4.2
1	B	307	GLY	3.9
1	A	99	THR	3.8
1	B	130	LEU	3.7
1	A	493	HIS	3.7
1	A	158	ALA	3.6
1	B	98	ALA	3.6
1	A	154	GLU	3.6
1	A	102	PHE	3.6
1	A	307	GLY	3.6
1	A	288	GLY	3.5
1	A	108	SER	3.4
1	B	157	LEU	3.4
1	B	495	TRP	3.4
1	A	495	TRP	3.3
1	A	269	GLY	3.2
1	B	288	GLY	3.2
1	A	81	ILE	3.1
1	A	127	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	492	THR	3.0
1	A	270	THR	2.9
1	B	151	ALA	2.8
1	B	99	THR	2.8
1	B	158	ALA	2.8
1	A	128	THR	2.7
1	A	492	THR	2.7
1	A	210	ASN	2.7
1	B	308	GLN	2.7
1	A	101	ASP	2.6
1	A	77	GLN	2.6
1	B	128	THR	2.6
1	A	78	TYR	2.6
1	A	292	ARG	2.5
1	B	110	LEU	2.5
1	A	142	ASN	2.5
1	B	129	PRO	2.5
1	B	139	GLU	2.4
1	A	109	CYS	2.4
1	A	178	ASP	2.4
1	B	131	GLU	2.4
1	A	212	SER	2.4
1	A	285	ILE	2.4
1	A	100	SER	2.4
1	A	98	ALA	2.3
1	B	149	LYS	2.3
1	A	112	SER	2.3
1	A	167	ILE	2.3
1	A	124	ARG	2.3
1	A	161	GLU	2.3
1	B	285	ILE	2.3
1	B	109	CYS	2.3
1	B	331	GLU	2.2
1	A	125	ASP	2.2
1	B	210	ASN	2.2
1	B	391	ARG	2.2
1	B	78	TYR	2.2
1	B	112	SER	2.2
1	B	442	GLN	2.2
1	A	137	ALA	2.2
1	A	141	ILE	2.2
1	B	153	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	171	GLY	2.2
1	A	446	ARG	2.1
1	B	96	HIS	2.1
1	A	147	SER	2.1
1	A	157	LEU	2.1
1	A	249	HIS	2.1
1	B	170	THR	2.1
1	A	250	ASP	2.1
1	B	81	ILE	2.1
1	A	169	THR	2.1
1	B	160	LEU	2.0
1	B	306	ASP	2.0
1	A	130	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BOG	A	3100	20/20	0.65	0.18	89,101,103,104	0
3	SO4	A	3004	5/5	0.69	0.19	111,112,112,113	0
3	SO4	A	3003	5/5	0.76	0.12	111,111,111,111	0
3	SO4	B	4003	5/5	0.76	0.13	107,108,109,109	0
2	BOG	B	4100	20/20	0.79	0.14	80,83,84,86	0
3	SO4	B	4004	5/5	0.81	0.14	98,99,100,101	0
3	SO4	A	3005	5/5	0.83	0.16	99,99,100,100	0
7	EDO	A	3101	4/4	0.85	0.17	63,65,66,68	0
7	EDO	B	4104	4/4	0.85	0.15	67,68,68,70	0
7	EDO	B	4101	4/4	0.90	0.12	64,65,66,66	0

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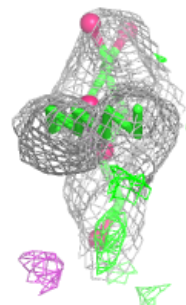
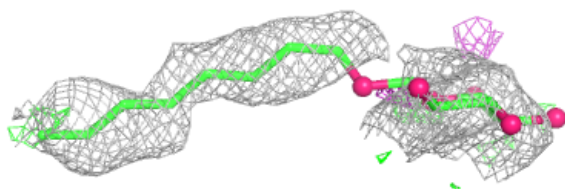
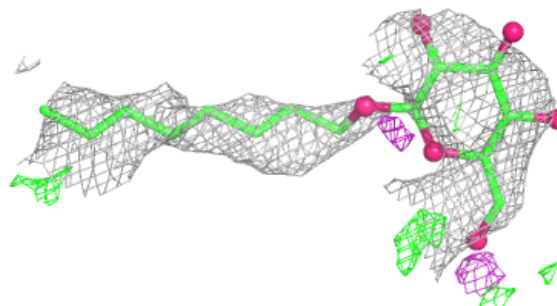
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	B	4102	4/4	0.91	0.09	42,42,43,43	0
7	EDO	A	3104	4/4	0.91	0.11	59,60,60,60	0
7	EDO	A	3102	4/4	0.93	0.09	42,42,44,45	0
4	AT6	B	1905	21/21	0.93	0.08	26,36,42,45	0
4	AT6	A	905	21/21	0.94	0.08	25,36,38,43	0
6	H4B	B	1902	17/17	0.95	0.07	29,31,36,38	0
6	H4B	A	902	17/17	0.96	0.06	28,30,37,37	0
5	HEM	A	901	43/43	0.98	0.06	24,28,31,35	0
5	HEM	B	1901	43/43	0.98	0.06	20,28,31,34	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.

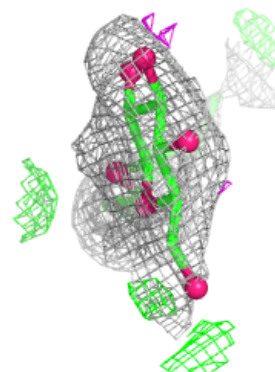
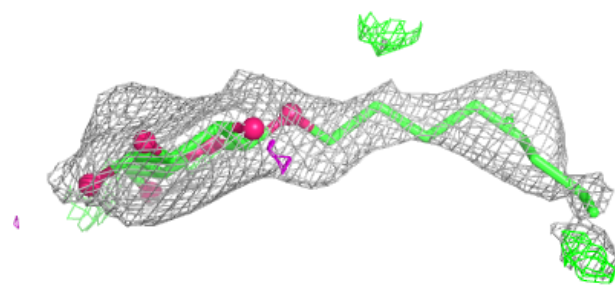
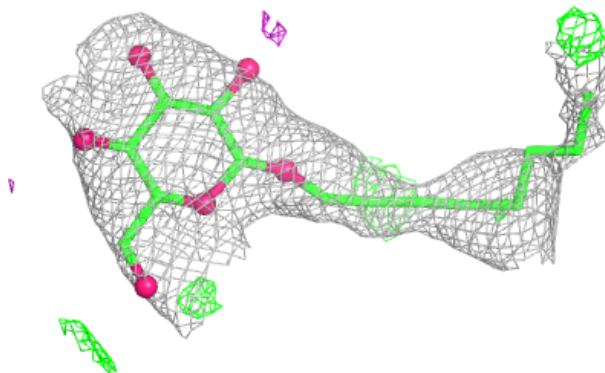
Electron density around BOG A 3100:

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

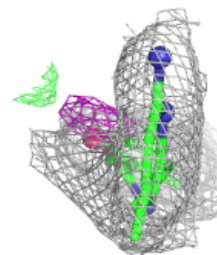
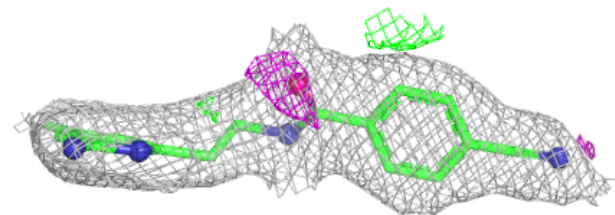
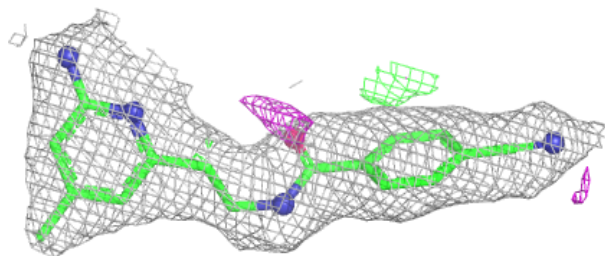


Electron density around BOG B 4100:

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

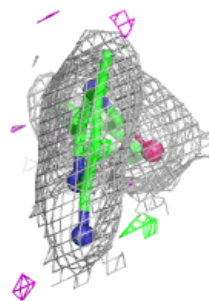
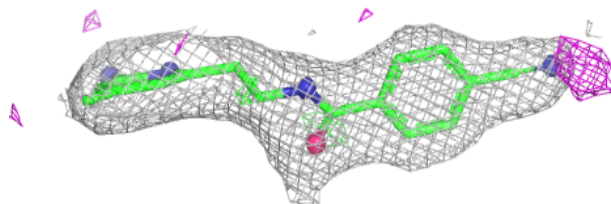
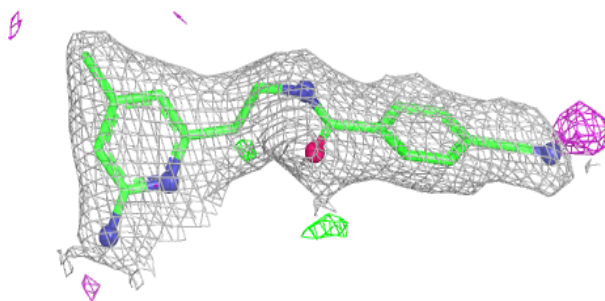
**Electron density around AT6 B 1905:**

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



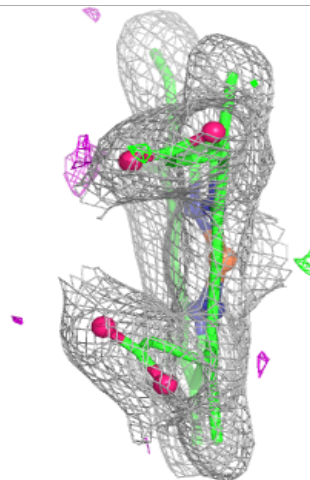
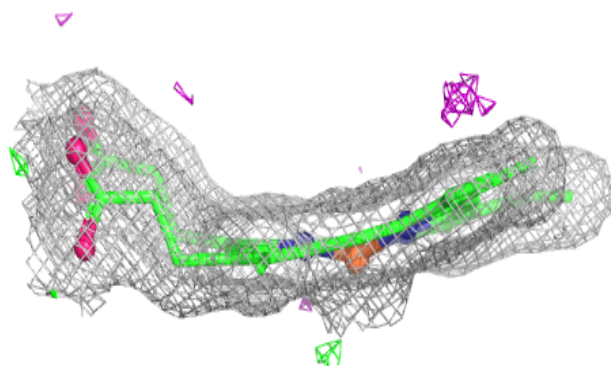
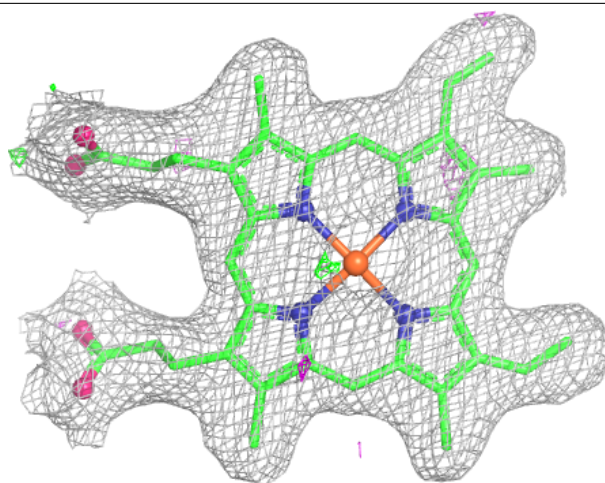
Electron density around AT6 A 905:

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



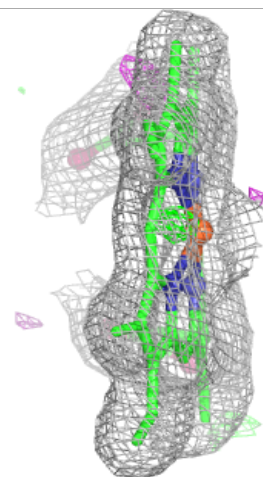
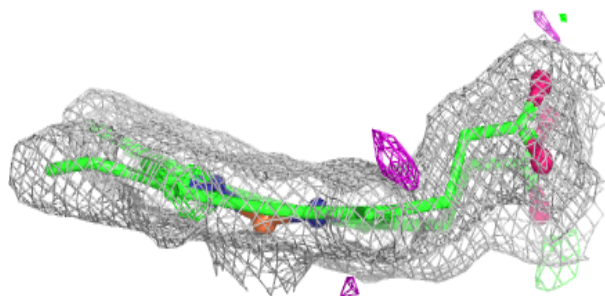
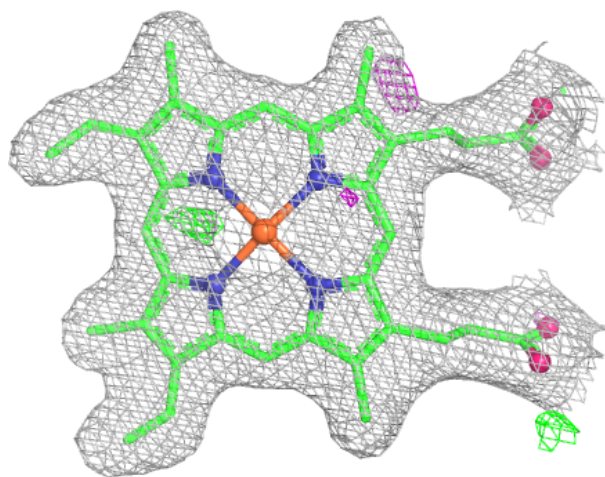
Electron density around HEM A 901:

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



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.