



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:10 AM UTC

PDB ID : 1EQG / pdb_00001eqg
Title : THE 2.6 ANGSTROM MODEL OF OVINE COX-1 COMPLEXED WITH IBUPROFEN
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Deposited on : 2000-04-04
Resolution : 2.61 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

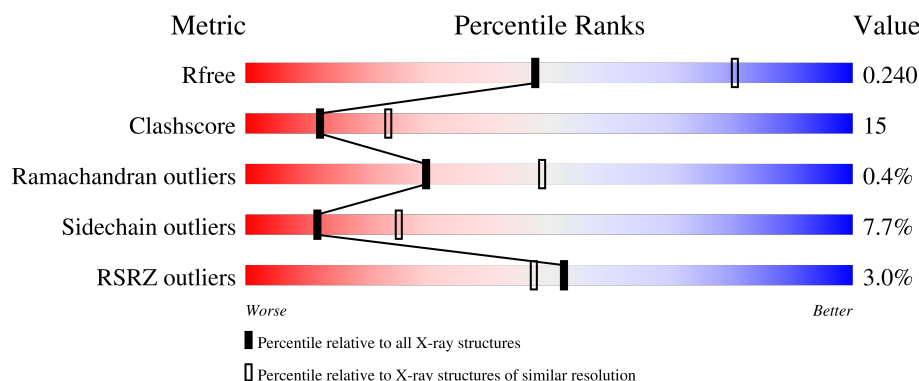
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	580	3% 66% 25% • 5%
1	B	580	3% 66% 24% • 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
3	BOG	A	802	-	-	X	-
3	BOG	B	1802	-	-	X	-

2 Entry composition [i](#)

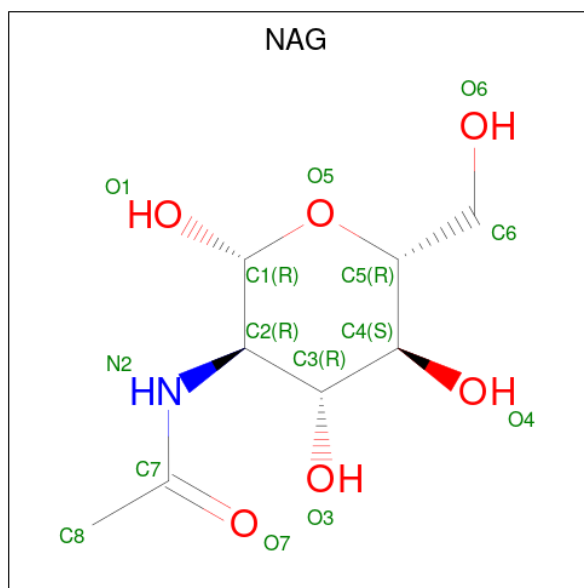
There are 6 unique types of molecules in this entry. The entry contains 9521 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROSTAGLANDIN H2 SYNTHASE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	0	0
			4477	2903	758	788	28			
1	B	551	Total	C	N	O	S	0	0	0
			4477	2903	758	788	28			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



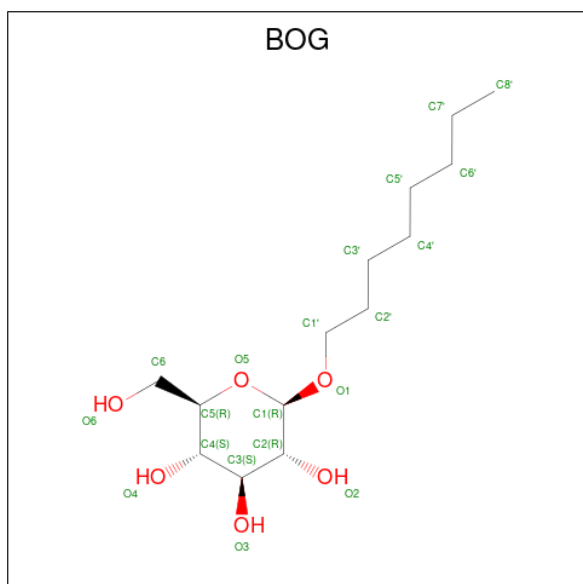
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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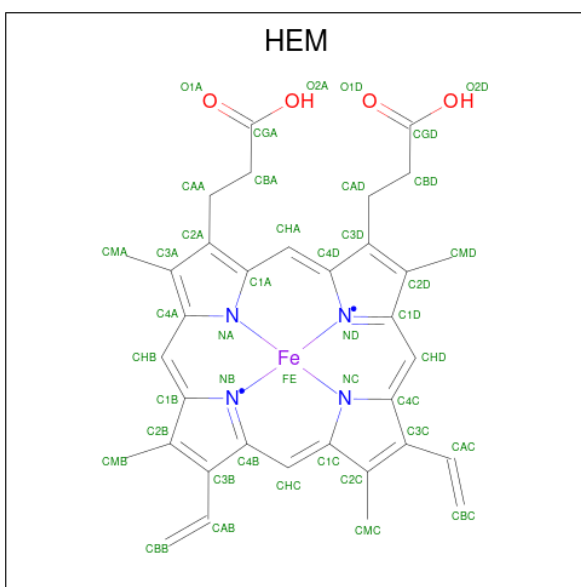
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



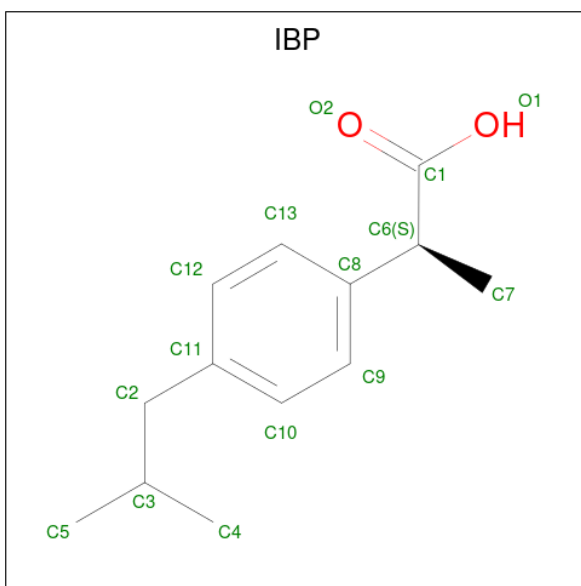
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	14	6		
3	A	1	Total	C	O	0	0
			20	14	6		
3	B	1	Total	C	O	0	0
			20	14	6		

- 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 IBUPROFEN (CCD ID: IBP) (formula: $C_{13}H_{18}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 15 13 2	0	0
5	B	1	Total C O 15 13 2	0	0

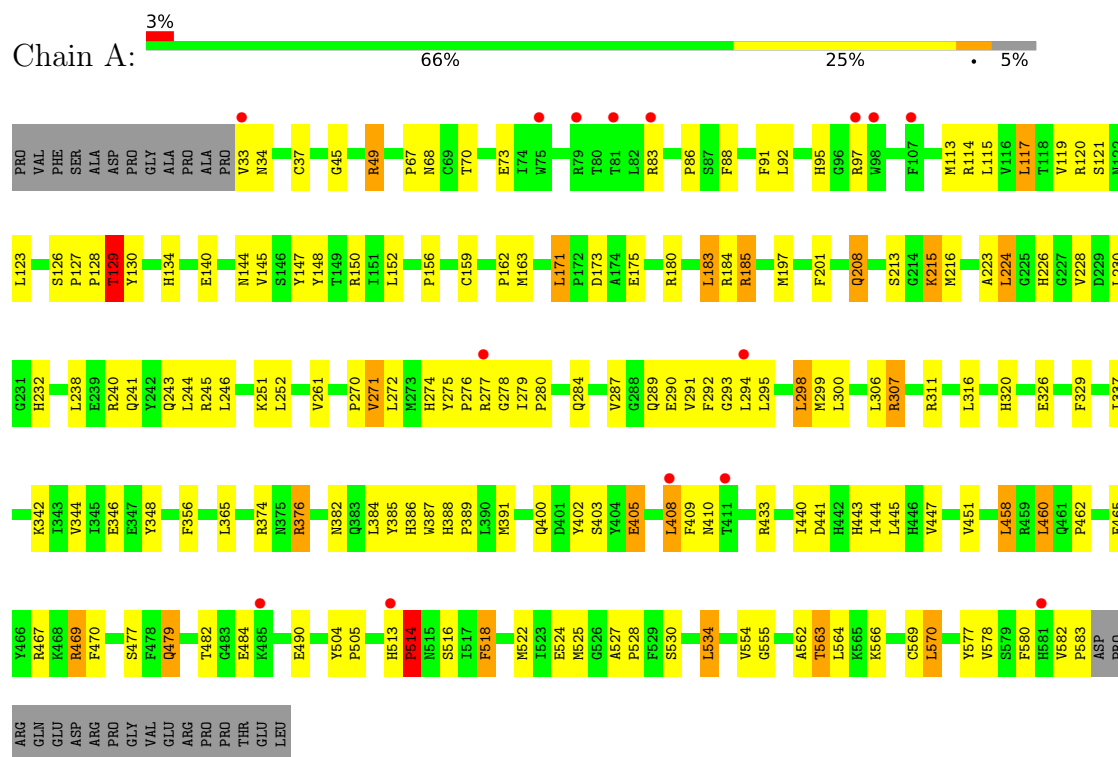
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	131	Total 131	O 131	0	0
6	B	120	Total 120	O 120	0	0

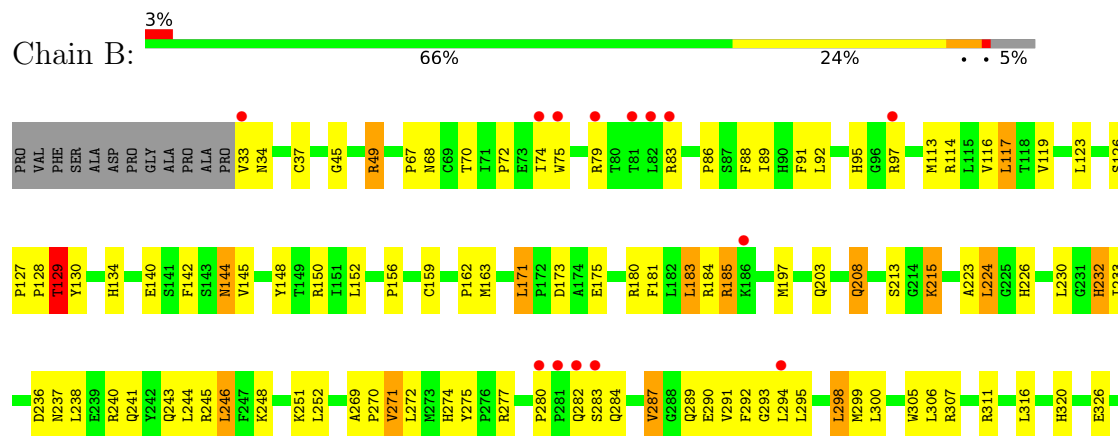
3 Residue-property plots

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: PROSTAGLANDIN H2 SYNTHASE-1



• Molecule 1: PROSTAGLANDIN H2 SYNTHASE-1





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.65Å 204.99Å 221.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.87 – 2.61 36.87 – 2.61	Depositor EDS
% Data completeness (in resolution range)	90.9 (36.87-2.61) 90.9 (36.87-2.61)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.12 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.250 0.212 , 0.240	Depositor DCC
R_{free} test set	5107 reflections (7.82%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9521	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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: BOG, IBP, NAG, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	1/4615 (0.0%)	0.94	22/6264 (0.4%)
1	B	0.44	1/4615 (0.0%)	0.95	17/6264 (0.3%)
All	All	0.43	2/9230 (0.0%)	0.95	39/12528 (0.3%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	129	THR	CA-C	6.17	1.56	1.52
1	A	129	THR	CA-C	5.32	1.55	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	LEU	N-CA-C	-10.79	96.30	110.43
1	B	408	LEU	N-CA-C	9.70	122.75	111.11
1	B	224	LEU	N-CA-C	-9.01	98.09	110.35
1	B	148	TYR	N-CA-C	-8.03	98.60	110.48
1	A	148	TYR	N-CA-C	-7.82	98.91	110.48
1	A	408	LEU	N-CA-C	7.72	124.10	111.37
1	A	287	VAL	N-CA-C	6.83	123.53	109.34
1	A	185	ARG	N-CA-C	-6.79	102.83	112.13
1	B	287	VAL	N-CA-C	6.70	123.28	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	LYS	N-CA-C	6.25	118.99	110.55
1	B	569	CYS	N-CA-C	6.01	118.62	111.71
1	A	569	CYS	N-CA-C	5.97	118.58	111.71
1	A	197	MET	N-CA-C	-5.88	104.87	111.28
1	B	129	THR	N-CA-C	5.81	118.07	108.48
1	A	129	THR	N-CA-C	5.71	117.90	108.48
1	B	197	MET	N-CA-C	-5.68	105.09	111.28
1	A	292	PHE	N-CA-C	5.63	119.77	113.01
1	B	292	PHE	N-CA-C	5.61	119.75	113.01
1	A	346	GLU	N-CA-C	5.54	119.88	113.18
1	A	201	PHE	N-CA-C	-5.54	105.16	111.14
1	B	185	ARG	N-CA-C	-5.51	102.64	111.02
1	A	580	PHE	N-CA-C	-5.43	106.33	113.17
1	A	356	PHE	N-CA-C	-5.43	106.61	113.18
1	A	337	ILE	N-CA-C	-5.26	105.37	110.42
1	B	251	LYS	N-CA-C	5.26	117.32	110.53
1	A	73	GLU	N-CA-C	-5.25	102.75	110.52
1	B	580	PHE	N-CA-C	-5.25	106.56	113.17
1	A	208	GLN	N-CA-C	-5.23	106.75	113.23
1	B	269	ALA	CA-C-N	5.22	126.37	119.84
1	B	269	ALA	C-N-CA	5.22	126.37	119.84
1	A	121	SER	N-CA-C	5.18	116.92	111.28
1	B	45	GLY	N-CA-C	-5.16	105.48	112.14
1	A	45	GLY	N-CA-C	-5.11	105.55	112.14
1	B	208	GLN	N-CA-C	-5.05	106.96	113.23
1	B	484	GLU	N-CA-C	5.05	114.96	108.34
1	B	144	ASN	N-CA-C	5.05	117.51	108.17
1	A	467	ARG	N-CA-C	-5.03	105.69	111.07
1	A	280	PRO	CA-C-N	5.02	124.62	119.05
1	A	280	PRO	C-N-CA	5.02	124.62	119.05

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	348	TYR	Sidechain

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	4477	0	4386	144	0
1	B	4477	0	4386	146	0
2	A	70	0	65	10	0
2	B	70	0	65	11	0
3	A	40	0	56	15	0
3	B	20	0	28	10	0
4	A	43	0	30	6	0
4	B	43	0	30	4	0
5	A	15	0	17	0	0
5	B	15	0	17	0	0
6	A	131	0	0	3	0
6	B	120	0	0	3	0
All	All	9521	0	9080	284	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 15.

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:B:119:VAL:HG12	3:B:1802:BOG:O2	1.47	1.12
1:A:119:VAL:HG12	3:A:802:BOG:O2	1.47	1.12
1:B:563:THR:HG22	1:B:566:LYS:H	1.26	1.01
1:A:563:THR:HG22	1:A:566:LYS:H	1.26	0.98
1:A:129:THR:HG22	1:A:130:TYR:H	1.33	0.93
1:B:129:THR:HG22	1:B:130:TYR:H	1.33	0.92
1:B:144:ASN:HD21	2:B:1671:NAG:C1	1.87	0.87
1:A:144:ASN:HD21	2:A:671:NAG:C1	1.88	0.86
1:B:462:PRO:HG2	1:B:465:GLU:HG2	1.58	0.84
1:B:294:LEU:HD22	1:B:409:PHE:CE2	2.14	0.82
1:B:410:ASN:HD21	2:B:1681:NAG:C1	1.94	0.81
1:A:462:PRO:HG2	1:A:465:GLU:HG2	1.61	0.79
1:A:129:THR:CG2	1:A:130:TYR:N	2.46	0.78
1:B:163:MET:HE3	1:B:171:LEU:HD21	1.66	0.78
1:A:129:THR:CG2	1:A:130:TYR:H	1.96	0.78
1:A:163:MET:HE3	1:A:171:LEU:HD21	1.65	0.78
1:B:129:THR:CG2	1:B:130:TYR:H	1.96	0.77
1:A:150:ARG:HD3	1:A:152:LEU:O	1.85	0.76
1:B:129:THR:CG2	1:B:130:TYR:N	2.48	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ASN:HD21	2:A:681:NAG:C1	1.99	0.75
1:B:150:ARG:HD3	1:B:152:LEU:O	1.87	0.75
1:B:113:MET:HE3	1:B:117:LEU:HD13	1.69	0.74
1:A:120:ARG:HH11	3:A:802:BOG:H3	1.52	0.73
1:B:144:ASN:ND2	2:B:1671:NAG:C1	2.52	0.73
1:A:144:ASN:ND2	2:A:671:NAG:C1	2.52	0.72
1:A:113:MET:HE3	1:A:117:LEU:HD13	1.73	0.71
1:A:240:ARG:HG3	1:A:271:VAL:HG21	1.71	0.71
1:A:240:ARG:HG3	1:A:271:VAL:CG2	2.20	0.71
1:A:120:ARG:NH1	3:A:802:BOG:H3	2.06	0.70
1:A:276:PRO:HD2	1:A:279:ILE:HD12	1.72	0.70
1:A:208:GLN:NE2	1:A:230:LEU:H	1.89	0.70
1:B:119:VAL:CG1	3:B:1802:BOG:O2	2.34	0.69
1:B:145:VAL:HG12	1:B:224:LEU:HD22	1.74	0.69
1:B:563:THR:CG2	1:B:566:LYS:H	2.05	0.69
1:A:374:ARG:HD2	6:A:1791:HOH:O	1.93	0.69
1:B:208:GLN:NE2	1:B:230:LEU:H	1.91	0.68
1:A:294:LEU:HD22	1:A:409:PHE:CE2	2.29	0.68
1:B:410:ASN:HD21	2:B:1681:NAG:C2	2.07	0.67
1:A:277:ARG:HE	1:A:278:GLY:N	1.92	0.66
1:B:527:ALA:HB3	1:B:528:PRO:HD3	1.78	0.66
1:A:49:ARG:O	1:B:320:HIS:HD2	1.78	0.65
1:A:208:GLN:HE21	1:A:230:LEU:H	1.43	0.65
1:A:144:ASN:HD21	2:A:671:NAG:C2	2.10	0.65
1:A:410:ASN:HD21	2:A:681:NAG:C2	2.10	0.65
1:A:524:GLU:OE1	3:A:802:BOG:H5	1.97	0.65
1:A:563:THR:CG2	1:A:566:LYS:H	2.05	0.64
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.80	0.64
1:A:86:PRO:HA	3:A:802:BOG:O6	1.99	0.63
1:A:119:VAL:HG12	3:A:802:BOG:C2	2.28	0.63
1:B:144:ASN:HD21	2:B:1671:NAG:C2	2.11	0.63
1:A:320:HIS:HD2	1:B:49:ARG:O	1.82	0.63
1:A:530:SER:O	1:A:534:LEU:HD22	1.99	0.63
1:B:86:PRO:HG3	3:B:1802:BOG:H62	1.80	0.63
1:A:277:ARG:HE	1:A:278:GLY:H	1.46	0.62
1:A:113:MET:HE3	1:A:117:LEU:CD1	2.29	0.62
1:A:344:VAL:O	1:A:348:TYR:HB3	1.99	0.62
1:A:129:THR:HG23	1:A:130:TYR:CD2	2.35	0.62
1:A:114:ARG:HD3	1:A:365:LEU:O	1.99	0.61
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.82	0.61
1:A:129:THR:HG23	1:A:130:TYR:CG	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ARG:HH11	1:B:83:ARG:HG3	1.64	0.61
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.66	0.60
1:B:129:THR:HG23	1:B:130:TYR:CD2	2.36	0.60
1:B:129:THR:HG23	1:B:130:TYR:CG	2.37	0.60
1:B:208:GLN:HE21	1:B:230:LEU:H	1.48	0.60
1:B:477:SER:OG	1:B:479:GLN:HG2	2.02	0.60
1:B:280:PRO:HG2	1:B:283:SER:OG	2.01	0.60
1:A:213:SER:OG	1:A:215:LYS:HG2	2.01	0.60
1:B:119:VAL:HG12	3:B:1802:BOG:C2	2.33	0.59
1:B:183:LEU:HG	1:B:445:LEU:HD22	1.84	0.59
1:B:402:TYR:OH	2:B:1681:NAG:H62	2.04	0.58
1:A:119:VAL:CG1	3:A:802:BOG:O2	2.38	0.58
1:A:290:GLU:CD	1:A:290:GLU:H	2.09	0.58
1:B:213:SER:OG	1:B:215:LYS:HG2	2.04	0.58
1:A:183:LEU:HG	1:A:445:LEU:HD22	1.85	0.58
1:B:290:GLU:H	1:B:290:GLU:CD	2.11	0.58
1:B:294:LEU:O	1:B:408:LEU:O	2.22	0.57
1:A:387:TRP:HB2	4:A:601:HEM:HAC	1.87	0.56
1:B:294:LEU:HD22	1:B:409:PHE:CD2	2.41	0.56
1:B:479:GLN:O	1:B:482:THR:O	2.22	0.56
1:A:582:VAL:HG13	1:A:583:PRO:HD2	1.89	0.55
1:B:530:SER:O	1:B:534:LEU:HD22	2.06	0.55
2:A:661:NAG:H61	2:A:662:NAG:H3	1.89	0.55
1:A:477:SER:OG	1:A:479:GLN:HG2	2.06	0.55
1:A:479:GLN:O	1:A:482:THR:O	2.25	0.55
1:A:384:LEU:C	1:A:384:LEU:HD23	2.32	0.55
1:A:208:GLN:HE22	1:A:230:LEU:HD12	1.72	0.55
1:B:344:VAL:O	1:B:348:TYR:HB3	2.07	0.54
2:B:1661:NAG:H61	2:B:1662:NAG:H3	1.88	0.54
1:B:145:VAL:HG13	1:B:226:HIS:CD2	2.41	0.54
1:B:241:GLN:HE21	1:B:245:ARG:HH11	1.55	0.54
1:A:145:VAL:HG13	1:A:226:HIS:CD2	2.42	0.54
1:B:241:GLN:NE2	1:B:245:ARG:HH11	2.04	0.54
1:A:115:LEU:HD23	3:A:802:BOG:H4'2	1.88	0.54
1:B:513:HIS:HB3	1:B:514:PRO:HD2	1.90	0.54
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.90	0.54
1:B:245:ARG:HD2	1:B:329:PHE:CZ	2.42	0.54
1:B:232:HIS:H	1:B:232:HIS:CD2	2.25	0.54
1:A:291:VAL:HG13	1:A:294:LEU:HD12	1.90	0.53
1:B:114:ARG:HD3	1:B:365:LEU:O	2.08	0.53
1:B:291:VAL:HG13	1:B:294:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:MET:HE2	4:B:601:HEM:HAB	1.90	0.53
1:B:294:LEU:HD22	1:B:409:PHE:HE2	1.69	0.53
1:B:49:ARG:HG3	6:B:1803:HOH:O	2.08	0.53
1:B:295:LEU:HB2	1:B:298:LEU:HD22	1.89	0.53
1:A:479:GLN:CD	1:A:479:GLN:H	2.16	0.53
1:A:513:HIS:HB3	1:A:514:PRO:HD2	1.89	0.53
1:B:291:VAL:HG12	1:B:291:VAL:O	2.09	0.53
1:A:566:LYS:O	1:A:570:LEU:HB2	2.09	0.53
1:B:181:PHE:HZ	1:B:490:GLU:HG2	1.73	0.53
1:B:86:PRO:HA	3:B:1802:BOG:O6	2.09	0.53
1:A:180:ARG:HD3	1:A:490:GLU:OE2	2.08	0.52
1:B:566:LYS:O	1:B:570:LEU:HB2	2.10	0.52
1:A:49:ARG:HG3	1:A:49:ARG:HH11	1.74	0.52
1:A:91:PHE:O	1:A:95:HIS:HD2	1.92	0.52
1:A:119:VAL:CG1	3:A:802:BOG:C2	2.87	0.52
1:A:140:GLU:OE2	1:A:144:ASN:ND2	2.41	0.52
1:A:241:GLN:HE21	1:A:245:ARG:HH11	1.57	0.52
1:A:216:MET:HE1	6:A:1725:HOH:O	2.08	0.52
1:A:295:LEU:HB2	1:A:298:LEU:HD22	1.91	0.52
1:B:405:GLU:CD	1:B:405:GLU:H	2.16	0.52
1:B:408:LEU:HB3	1:B:409:PHE:CD1	2.45	0.52
1:B:150:ARG:HB3	1:B:379:MET:HE3	1.91	0.52
1:A:410:ASN:ND2	2:A:681:NAG:N2	2.58	0.52
1:B:49:ARG:HG3	1:B:49:ARG:HH11	1.74	0.52
1:B:582:VAL:HG13	1:B:583:PRO:HD2	1.92	0.52
1:B:208:GLN:HE22	1:B:230:LEU:HD12	1.75	0.51
1:B:280:PRO:HB2	1:B:282:GLN:CD	2.36	0.51
1:A:86:PRO:HG3	3:A:802:BOG:H62	1.92	0.51
1:A:185:ARG:HH11	1:A:185:ARG:HG2	1.75	0.51
1:B:89:ILE:HD12	3:B:1802:BOG:O6	2.11	0.51
1:B:162:PRO:O	1:B:163:MET:HE2	2.11	0.51
1:B:479:GLN:CD	1:B:479:GLN:H	2.19	0.51
1:A:223:ALA:C	1:A:224:LEU:O	2.47	0.51
1:A:130:TYR:HB3	1:A:134:HIS:O	2.11	0.51
1:A:245:ARG:HD2	1:A:329:PHE:CZ	2.47	0.50
1:A:447:VAL:O	1:A:451:VAL:HG23	2.12	0.50
1:B:387:TRP:HB2	4:B:601:HEM:HAC	1.94	0.50
1:B:185:ARG:HG2	1:B:185:ARG:HH11	1.76	0.50
1:B:306:LEU:C	1:B:306:LEU:HD23	2.36	0.50
1:A:391:MET:HE2	4:A:601:HEM:HAB	1.92	0.50
1:A:402:TYR:OH	2:A:681:NAG:H62	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:MET:HE3	1:B:117:LEU:CD1	2.40	0.50
1:B:142:PHE:C	1:B:376:ARG:HH22	2.19	0.50
1:A:294:LEU:HD22	1:A:409:PHE:HE2	1.76	0.50
1:A:388:HIS:N	1:A:389:PRO:CD	2.75	0.49
1:B:130:TYR:HB3	1:B:134:HIS:O	2.12	0.49
1:A:306:LEU:HD23	1:A:306:LEU:C	2.37	0.49
1:A:129:THR:HG23	1:A:130:TYR:N	2.25	0.49
1:A:403:SER:OG	1:A:405:GLU:HG2	2.12	0.49
1:B:119:VAL:CG1	3:B:1802:BOG:C2	2.90	0.49
1:B:524:GLU:OE1	3:B:1802:BOG:H5	2.13	0.49
1:B:74:ILE:HG22	6:B:1877:HOH:O	2.12	0.49
1:B:180:ARG:NH2	1:B:490:GLU:OE1	2.46	0.49
1:A:162:PRO:O	1:A:163:MET:HE2	2.13	0.49
1:B:470:PHE:CD2	1:B:525:MET:HG2	2.47	0.49
1:A:291:VAL:HG12	1:A:291:VAL:O	2.12	0.49
1:A:518:PHE:CD1	1:A:522:MET:HG2	2.48	0.49
1:B:240:ARG:NH1	1:B:271:VAL:HG13	2.28	0.48
1:A:563:THR:HG22	1:A:566:LYS:N	2.10	0.48
1:A:67:PRO:C	1:A:68:ASN:HD22	2.22	0.48
1:A:374:ARG:HB3	1:B:374:ARG:NH1	2.29	0.48
1:B:388:HIS:N	1:B:389:PRO:CD	2.77	0.48
1:B:447:VAL:O	1:B:451:VAL:HG23	2.13	0.48
1:A:119:VAL:CG1	3:A:802:BOG:H2	2.43	0.48
1:B:441:ASP:OD2	1:B:443:HIS:HB2	2.14	0.48
1:B:518:PHE:CD1	1:B:522:MET:HG2	2.48	0.48
1:A:470:PHE:CD2	1:A:525:MET:HG2	2.48	0.48
1:B:126:SER:HA	1:B:127:PRO:C	2.38	0.48
1:B:67:PRO:C	1:B:68:ASN:HD22	2.22	0.48
1:B:388:HIS:CE1	1:B:447:VAL:HG11	2.49	0.48
1:B:145:VAL:O	1:B:145:VAL:CG1	2.61	0.47
1:B:563:THR:HG22	1:B:566:LYS:N	2.10	0.47
1:A:294:LEU:O	1:A:408:LEU:O	2.33	0.47
1:B:140:GLU:OE2	1:B:144:ASN:ND2	2.42	0.47
1:B:554:VAL:HG13	1:B:555:GLY:N	2.29	0.47
1:B:391:MET:HE2	4:B:601:HEM:CAB	2.45	0.47
1:A:145:VAL:HG13	1:A:226:HIS:NE2	2.30	0.47
1:B:513:HIS:O	1:B:514:PRO:C	2.58	0.46
1:A:513:HIS:O	1:A:514:PRO:C	2.59	0.46
1:B:70:THR:O	1:B:72:PRO:HD3	2.15	0.46
1:B:237:ASN:ND2	1:B:240:ARG:H	2.14	0.46
1:A:388:HIS:CE1	1:A:447:VAL:HG11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:PRO:HB2	1:B:159:CYS:SG	2.56	0.46
1:A:126:SER:HA	1:A:127:PRO:C	2.40	0.46
1:A:441:ASP:OD2	1:A:443:HIS:HB2	2.15	0.46
1:A:389:PRO:HG3	1:A:440:ILE:HG12	1.98	0.46
1:B:91:PHE:O	1:B:95:HIS:HD2	1.99	0.46
1:B:246:LEU:HD13	1:B:248:LYS:HB3	1.98	0.46
1:B:382:ASN:OD1	1:B:386:HIS:HE1	1.99	0.46
1:B:410:ASN:ND2	2:B:1681:NAG:N2	2.63	0.46
1:B:410:ASN:ND2	2:B:1681:NAG:C1	2.72	0.46
1:A:120:ARG:CZ	3:A:802:BOG:H1	2.46	0.45
1:A:458:LEU:HB3	1:A:460:LEU:HD13	1.98	0.45
1:B:129:THR:HG23	1:B:130:TYR:N	2.27	0.45
1:B:458:LEU:HB3	1:B:460:LEU:HD13	1.98	0.45
1:B:232:HIS:CD2	1:B:232:HIS:N	2.85	0.45
1:A:342:LYS:HG2	1:A:562:ALA:HB3	1.99	0.45
1:A:554:VAL:HG13	1:A:555:GLY:N	2.31	0.45
1:A:156:PRO:HB2	1:A:159:CYS:SG	2.57	0.45
1:A:391:MET:HE2	4:A:601:HEM:CAB	2.46	0.45
1:A:145:VAL:O	1:A:145:VAL:CG1	2.65	0.45
1:A:173:ASP:OD2	1:A:175:GLU:HB3	2.17	0.45
1:A:272:LEU:HD11	1:A:274:HIS:CE1	2.52	0.45
1:B:68:ASN:OD1	2:B:1661:NAG:C1	2.65	0.45
1:A:49:ARG:HH11	1:A:49:ARG:CG	2.30	0.44
1:A:469:ARG:HA	1:A:469:ARG:HD2	1.85	0.44
1:B:389:PRO:HG3	1:B:440:ILE:CG1	2.46	0.44
1:A:68:ASN:OD1	2:A:661:NAG:C1	2.66	0.44
1:A:374:ARG:NH1	1:B:374:ARG:HB3	2.33	0.44
1:A:134:HIS:CE1	1:B:326:GLU:OE1	2.70	0.44
1:B:223:ALA:O	1:B:224:LEU:C	2.61	0.44
1:A:134:HIS:HE1	1:B:326:GLU:OE1	1.99	0.44
1:A:145:VAL:HG12	1:A:224:LEU:HD22	2.00	0.44
1:A:277:ARG:NE	1:A:278:GLY:H	2.15	0.44
1:A:223:ALA:O	1:A:224:LEU:C	2.61	0.43
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.59	0.43
1:A:171:LEU:HD12	1:A:171:LEU:HA	1.90	0.43
1:B:245:ARG:HD2	1:B:329:PHE:CE1	2.54	0.43
1:A:382:ASN:OD1	1:A:386:HIS:HE1	2.02	0.43
1:B:49:ARG:HH11	1:B:49:ARG:CG	2.31	0.43
1:B:293:GLY:HA2	1:B:299:MET:HE2	1.99	0.43
1:B:389:PRO:HG3	1:B:440:ILE:HG12	2.01	0.43
1:A:311:ARG:NH2	1:A:570:LEU:HD23	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ALA:C	1:B:224:LEU:O	2.59	0.43
1:A:240:ARG:HG3	1:A:271:VAL:HG22	1.98	0.43
1:B:119:VAL:CG1	3:B:1802:BOG:H2	2.49	0.42
1:B:173:ASP:OD2	1:B:175:GLU:HB3	2.18	0.42
1:B:340:THR:O	1:B:344:VAL:HG23	2.19	0.42
1:A:91:PHE:O	1:A:95:HIS:CD2	2.72	0.42
1:B:513:HIS:HB2	1:B:516:SER:OG	2.20	0.42
1:A:128:PRO:HG3	1:A:376:ARG:NH1	2.35	0.42
1:A:295:LEU:HD12	1:A:298:LEU:HD22	2.02	0.42
1:A:293:GLY:HA2	1:A:299:MET:HE2	2.02	0.42
1:B:272:LEU:HD11	1:B:274:HIS:CE1	2.54	0.42
1:B:240:ARG:HG3	1:B:271:VAL:HG22	2.01	0.42
1:B:295:LEU:HD12	1:B:298:LEU:HD22	2.00	0.42
1:B:485:LYS:HA	1:B:485:LYS:HD3	1.92	0.42
1:A:144:ASN:CG	2:A:671:NAG:C1	2.92	0.42
1:A:513:HIS:HB2	1:A:516:SER:OG	2.19	0.42
1:B:128:PRO:HG3	1:B:376:ARG:NH1	2.35	0.42
1:A:386:HIS:CE1	4:A:601:HEM:HAD2	2.54	0.42
1:B:287:VAL:HA	6:B:1889:HOH:O	2.20	0.42
1:A:129:THR:HG22	1:A:130:TYR:N	2.07	0.42
1:B:233:ILE:HD13	1:B:305:TRP:HB3	2.01	0.42
1:A:261:VAL:HB	1:A:307:ARG:HD2	2.02	0.41
1:B:34:ASN:HB3	1:B:37:CYS:SG	2.59	0.41
1:B:74:ILE:HG23	1:B:75:TRP:N	2.35	0.41
1:B:275:TYR:CD2	1:B:284:GLN:HG2	2.55	0.41
1:B:311:ARG:NH2	1:B:570:LEU:HD23	2.34	0.41
1:A:391:MET:HG3	4:A:601:HEM:CBB	2.50	0.41
1:A:243:GLN:OE1	1:A:243:GLN:HA	2.19	0.41
1:B:79:ARG:O	1:B:83:ARG:HB3	2.21	0.41
1:B:144:ASN:CG	2:B:1671:NAG:C1	2.93	0.41
1:B:236:ASP:OD1	1:B:236:ASP:C	2.62	0.41
1:A:70:THR:HB	3:A:801:BOG:H5	2.02	0.41
1:B:482:THR:C	1:B:484:GLU:H	2.29	0.41
1:B:577:TYR:CE2	1:B:583:PRO:HD3	2.55	0.41
1:A:275:TYR:CE2	1:A:284:GLN:HB3	2.56	0.41
1:A:326:GLU:OE1	1:B:134:HIS:HE1	2.04	0.41
1:A:405:GLU:CD	1:A:405:GLU:H	2.28	0.41
1:B:183:LEU:HD23	1:B:184:ARG:H	1.85	0.41
1:A:183:LEU:HD22	1:A:184:ARG:O	2.20	0.41
1:A:577:TYR:CE2	1:A:583:PRO:HD3	2.56	0.41
1:B:129:THR:HG22	1:B:130:TYR:N	2.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ARG:NH1	1:B:326:GLU:OE2	2.48	0.41
1:B:469:ARG:HA	1:B:469:ARG:HD2	1.85	0.41
1:A:183:LEU:HD23	1:A:184:ARG:H	1.85	0.41
1:A:208:GLN:NE2	1:A:228:VAL:HA	2.36	0.41
1:B:145:VAL:HG13	1:B:226:HIS:NE2	2.36	0.41
1:A:120:ARG:HH12	3:A:802:BOG:H5	1.86	0.40
1:A:147:TYR:HB2	6:A:1722:HOH:O	2.21	0.40
1:B:203:GLN:HA	4:B:601:HEM:HBC2	2.02	0.40
1:A:145:VAL:HG13	1:A:226:HIS:HE2	1.85	0.40
1:A:444:ILE:HG21	4:A:601:HEM:HBB2	2.02	0.40
1:B:88:PHE:CZ	1:B:92:LEU:HD11	2.56	0.40
1:A:120:ARG:NH1	3:A:802:BOG:H1	2.37	0.40
1:B:116:VAL:HG22	3:B:1802:BOG:H2'1	2.03	0.40
1:B:145:VAL:HG12	1:B:145:VAL:O	2.21	0.40
1:A:400:GLN:CA	1:A:400:GLN:HE21	2.33	0.40
1:A:88:PHE:CZ	1:A:92:LEU:HD11	2.56	0.40
1:A:162:PRO:C	1:A:163:MET:HE2	2.47	0.40
1:A:326:GLU:OE1	1:B:134:HIS:CE1	2.74	0.40
1:B:162:PRO:C	1:B:163:MET:HE2	2.46	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	549/580 (95%)	523 (95%)	24 (4%)	2 (0%)	30	49
1	B	549/580 (95%)	524 (95%)	23 (4%)	2 (0%)	30	49
All	All	1098/1160 (95%)	1047 (95%)	47 (4%)	4 (0%)	30	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	PRO
1	B	514	PRO
1	A	270	PRO
1	B	270	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	486/510 (95%)	450 (93%)	36 (7%)	13	27
1	B	486/510 (95%)	447 (92%)	39 (8%)	11	23
All	All	972/1020 (95%)	897 (92%)	75 (8%)	12	25

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	49	ARG
1	A	97	ARG
1	A	117	LEU
1	A	123	LEU
1	A	129	THR
1	A	171	LEU
1	A	183	LEU
1	A	215	LYS
1	A	232	HIS
1	A	238	LEU
1	A	244	LEU
1	A	246	LEU
1	A	252	LEU
1	A	271	VAL
1	A	289	GLN
1	A	298	LEU
1	A	300	LEU
1	A	307	ARG
1	A	316	LEU

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Mol	Chain	Res	Type
1	A	376	ARG
1	A	385	TYR
1	A	405	GLU
1	A	433	ARG
1	A	458	LEU
1	A	460	LEU
1	A	469	ARG
1	A	479	GLN
1	A	484	GLU
1	A	514	PRO
1	A	518	PHE
1	A	534	LEU
1	A	563	THR
1	A	564	LEU
1	A	570	LEU
1	A	578	VAL
1	B	33	VAL
1	B	49	ARG
1	B	97	ARG
1	B	117	LEU
1	B	123	LEU
1	B	129	THR
1	B	171	LEU
1	B	183	LEU
1	B	215	LYS
1	B	232	HIS
1	B	238	LEU
1	B	243	GLN
1	B	244	LEU
1	B	246	LEU
1	B	252	LEU
1	B	271	VAL
1	B	277	ARG
1	B	289	GLN
1	B	298	LEU
1	B	300	LEU
1	B	307	ARG
1	B	316	LEU
1	B	376	ARG
1	B	385	TYR
1	B	400	GLN
1	B	405	GLU

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Mol	Chain	Res	Type
1	B	433	ARG
1	B	458	LEU
1	B	460	LEU
1	B	469	ARG
1	B	479	GLN
1	B	484	GLU
1	B	514	PRO
1	B	518	PHE
1	B	534	LEU
1	B	563	THR
1	B	564	LEU
1	B	570	LEU
1	B	578	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	43	HIS
1	A	56	GLN
1	A	68	ASN
1	A	95	HIS
1	A	134	HIS
1	A	144	ASN
1	A	170	GLN
1	A	208	GLN
1	A	237	ASN
1	A	241	GLN
1	A	255	GLN
1	A	274	HIS
1	A	320	HIS
1	A	358	GLN
1	A	386	HIS
1	A	400	GLN
1	A	442	HIS
1	A	443	HIS
1	A	446	HIS
1	B	42	GLN
1	B	43	HIS
1	B	56	GLN
1	B	68	ASN
1	B	95	HIS

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Mol	Chain	Res	Type
1	B	134	HIS
1	B	144	ASN
1	B	170	GLN
1	B	204	HIS
1	B	208	GLN
1	B	232	HIS
1	B	241	GLN
1	B	320	HIS
1	B	358	GLN
1	B	375	ASN
1	B	386	HIS
1	B	400	GLN
1	B	410	ASN
1	B	442	HIS
1	B	443	HIS
1	B	446	HIS
1	B	571	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](#)

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
2	NAG	A	662	-	14,14,15	1.23	2 (14%)	17,19,21	0.70	0
2	NAG	A	1672	-	14,14,15	1.33	2 (14%)	17,19,21	0.90	2 (11%)
3	BOG	B	1802	-	20,20,20	1.52	5 (25%)	25,25,25	0.95	2 (8%)
5	IBP	A	701	-	15,15,15	1.28	2 (13%)	20,20,20	0.41	0
2	NAG	B	1662	-	14,14,15	1.29	2 (14%)	17,19,21	0.74	0
2	NAG	A	681	-	14,14,15	1.33	2 (14%)	17,19,21	0.84	0
2	NAG	A	661	-	14,14,15	0.95	0	17,19,21	0.91	1 (5%)
2	NAG	A	671	-	14,14,15	0.70	0	17,19,21	0.71	0
2	NAG	B	672	-	14,14,15	1.23	1 (7%)	17,19,21	0.84	1 (5%)
2	NAG	B	1681	-	14,14,15	1.40	2 (14%)	17,19,21	0.86	1 (5%)
3	BOG	A	802	-	20,20,20	1.48	5 (25%)	25,25,25	0.97	2 (8%)
2	NAG	B	1661	-	14,14,15	0.94	0	17,19,21	0.93	1 (5%)
3	BOG	A	801	-	20,20,20	1.57	5 (25%)	25,25,25	0.75	0
4	HEM	B	601	1	50,50,50	1.41	5 (10%)	67,82,82	1.16	7 (10%)
5	IBP	B	1701	-	15,15,15	1.23	2 (13%)	20,20,20	0.42	0
4	HEM	A	601	1	50,50,50	1.41	5 (10%)	67,82,82	1.18	7 (10%)
2	NAG	B	1671	-	14,14,15	0.61	0	17,19,21	0.71	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	NAG	A	662	-	-	4/6/23/26	0/1/1/1
2	NAG	A	1672	-	-	4/6/23/26	0/1/1/1
3	BOG	B	1802	-	-	4/11/31/31	0/1/1/1
5	IBP	A	701	-	-	2/12/12/12	0/1/1/1
2	NAG	B	1662	-	-	4/6/23/26	0/1/1/1
2	NAG	A	681	-	-	3/6/23/26	0/1/1/1
2	NAG	A	661	-	-	2/6/23/26	0/1/1/1
2	NAG	A	671	-	-	4/6/23/26	0/1/1/1
2	NAG	B	672	-	-	4/6/23/26	0/1/1/1
2	NAG	B	1681	-	-	3/6/23/26	0/1/1/1
3	BOG	A	802	-	-	4/11/31/31	0/1/1/1
2	NAG	B	1661	-	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BOG	A	801	-	-	2/11/31/31	0/1/1/1
4	HEM	B	601	1	-	4/14/54/54	-
5	IBP	B	1701	-	-	2/12/12/12	0/1/1/1
4	HEM	A	601	1	-	4/14/54/54	-
2	NAG	B	1671	-	-	4/6/23/26	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	HEM	CBB-CAB	4.75	1.53	1.30
4	A	601	HEM	CBB-CAB	4.71	1.53	1.30
4	B	601	HEM	CBC-CAC	4.54	1.52	1.30
4	A	601	HEM	CBC-CAC	4.51	1.52	1.30
3	A	801	BOG	O5-C1	3.13	1.49	1.41
2	B	1681	NAG	C1-C2	3.08	1.56	1.52
3	A	801	BOG	C3'-C2'	-3.01	1.36	1.51
3	A	801	BOG	C4-C5	-2.93	1.46	1.53
3	B	1802	BOG	C3'-C2'	-2.79	1.37	1.51
3	A	802	BOG	O5-C1	2.79	1.49	1.41
3	B	1802	BOG	O5-C1	2.78	1.49	1.41
3	A	802	BOG	C3'-C2'	-2.74	1.38	1.51
2	A	681	NAG	C1-C2	2.69	1.56	1.52
4	A	601	HEM	CMB-C2B	2.67	1.56	1.50
3	B	1802	BOG	C4-C5	-2.66	1.47	1.53
2	B	1662	NAG	O5-C5	2.62	1.48	1.43
4	A	601	HEM	CAB-C3B	2.59	1.54	1.47
4	B	601	HEM	CAB-C3B	2.56	1.54	1.47
4	B	601	HEM	CAC-C3C	2.56	1.54	1.47
4	A	601	HEM	CAC-C3C	2.54	1.54	1.47
3	A	802	BOG	C4-C5	-2.52	1.47	1.53
4	B	601	HEM	CMB-C2B	2.50	1.55	1.50
3	A	801	BOG	C7'-C6'	-2.47	1.36	1.51
2	A	681	NAG	O5-C5	2.44	1.48	1.43
2	A	662	NAG	O5-C5	2.41	1.48	1.43
3	A	801	BOG	O5-C5	2.40	1.50	1.44
2	A	1672	NAG	C1-C2	2.40	1.55	1.52
3	B	1802	BOG	O5-C5	2.39	1.50	1.44
3	A	802	BOG	O5-C5	2.31	1.50	1.44
2	B	1681	NAG	O5-C5	2.27	1.47	1.43
5	A	701	IBP	C13-C12	2.25	1.42	1.38
2	B	1662	NAG	C1-C2	2.22	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	BOG	C7'-C6'	-2.22	1.37	1.51
2	A	662	NAG	C1-C2	2.22	1.55	1.52
2	B	672	NAG	O5-C5	2.21	1.47	1.43
3	B	1802	BOG	C7'-C6'	-2.21	1.38	1.51
2	A	1672	NAG	O5-C5	2.17	1.47	1.43
5	B	1701	IBP	C13-C8	2.11	1.42	1.39
5	A	701	IBP	C10-C9	2.10	1.42	1.38
5	B	1701	IBP	C13-C12	2.06	1.42	1.38

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	HEM	C2B-C1B-NB	3.59	113.97	109.84
4	B	601	HEM	C2B-C1B-NB	3.41	113.76	109.84
3	B	1802	BOG	O1-C1-C2	2.97	112.79	108.27
3	A	802	BOG	O1-C1-C2	2.97	112.78	108.27
4	B	601	HEM	CBA-CAA-C2A	-2.87	104.59	112.53
3	A	802	BOG	C1'-O1-C1	2.87	118.58	113.68
4	A	601	HEM	CBA-CAA-C2A	-2.86	104.64	112.53
3	B	1802	BOG	C1'-O1-C1	2.70	118.30	113.68
4	A	601	HEM	C3B-C4B-NB	2.54	111.29	109.47
4	B	601	HEM	C3B-C4B-NB	2.54	111.29	109.47
4	B	601	HEM	CBB-CAB-C3B	-2.45	115.28	127.53
4	A	601	HEM	CBB-CAB-C3B	-2.44	115.33	127.53
4	A	601	HEM	C3B-C2B-C1B	-2.40	104.61	106.41
2	B	1661	NAG	C1-O5-C5	2.36	115.35	112.19
4	B	601	HEM	C2D-C1D-ND	2.28	112.54	109.90
4	B	601	HEM	C3B-C2B-C1B	-2.22	104.75	106.41
4	A	601	HEM	C1D-C2D-C3D	-2.21	104.66	106.98
2	A	661	NAG	C1-O5-C5	2.21	115.14	112.19
2	A	1672	NAG	O7-C7-C8	-2.18	118.17	122.05
4	B	601	HEM	C1D-C2D-C3D	-2.13	104.74	106.98
2	B	1681	NAG	O7-C7-C8	-2.11	118.30	122.05
2	A	1672	NAG	C1-O5-C5	2.10	115.00	112.19
2	B	672	NAG	C1-O5-C5	2.08	114.98	112.19
4	A	601	HEM	C2D-C1D-ND	2.06	112.29	109.90

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	662	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	B	1662	NAG	O5-C5-C6-O6
2	A	1672	NAG	C4-C5-C6-O6
2	B	672	NAG	O5-C5-C6-O6
2	A	1672	NAG	O5-C5-C6-O6
2	B	672	NAG	C4-C5-C6-O6
2	A	661	NAG	C8-C7-N2-C2
2	A	662	NAG	C8-C7-N2-C2
2	A	671	NAG	C8-C7-N2-C2
2	A	681	NAG	C8-C7-N2-C2
2	A	1672	NAG	C8-C7-N2-C2
2	B	672	NAG	C8-C7-N2-C2
2	B	1661	NAG	C8-C7-N2-C2
2	B	1662	NAG	C8-C7-N2-C2
2	B	1671	NAG	C8-C7-N2-C2
2	B	1681	NAG	C8-C7-N2-C2
3	B	1802	BOG	O1-C1'-C2'-C3'
2	A	662	NAG	C4-C5-C6-O6
2	B	1662	NAG	C4-C5-C6-O6
3	A	802	BOG	O1-C1'-C2'-C3'
5	A	701	IBP	C11-C2-C3-C5
5	B	1701	IBP	C11-C2-C3-C5
2	A	661	NAG	O7-C7-N2-C2
2	A	662	NAG	O7-C7-N2-C2
2	A	671	NAG	O7-C7-N2-C2
2	A	681	NAG	O7-C7-N2-C2
2	A	1672	NAG	O7-C7-N2-C2
2	B	672	NAG	O7-C7-N2-C2
2	B	1661	NAG	O7-C7-N2-C2
2	B	1662	NAG	O7-C7-N2-C2
2	B	1671	NAG	O7-C7-N2-C2
2	B	1681	NAG	O7-C7-N2-C2
3	B	1802	BOG	C1'-C2'-C3'-C4'
3	A	802	BOG	C2'-C3'-C4'-C5'
3	A	802	BOG	C3'-C4'-C5'-C6'
5	A	701	IBP	C11-C2-C3-C4
3	B	1802	BOG	C3'-C4'-C5'-C6'
5	B	1701	IBP	C11-C2-C3-C4
3	B	1802	BOG	C2'-C3'-C4'-C5'
4	A	601	HEM	C2C-C3C-CAC-CBC
4	B	601	HEM	C2C-C3C-CAC-CBC
2	B	1681	NAG	O5-C5-C6-O6
2	A	681	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	802	BOG	C1'-C2'-C3'-C4'
3	A	801	BOG	C3'-C4'-C5'-C6'
2	A	671	NAG	C4-C5-C6-O6
2	B	1671	NAG	C4-C5-C6-O6
2	A	671	NAG	O5-C5-C6-O6
3	A	801	BOG	C2'-C3'-C4'-C5'
4	A	601	HEM	C2B-C3B-CAB-CBB
4	B	601	HEM	C2B-C3B-CAB-CBB
2	B	1671	NAG	O5-C5-C6-O6
4	A	601	HEM	C4C-C3C-CAC-CBC
4	B	601	HEM	C4C-C3C-CAC-CBC
4	A	601	HEM	C4B-C3B-CAB-CBB
4	B	601	HEM	C4B-C3B-CAB-CBB

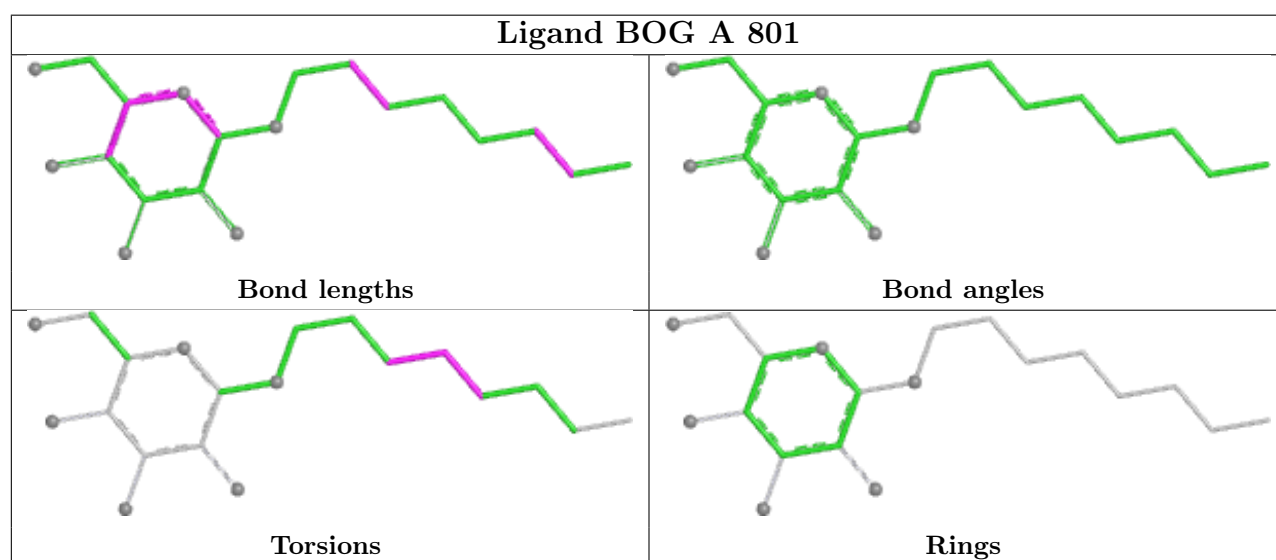
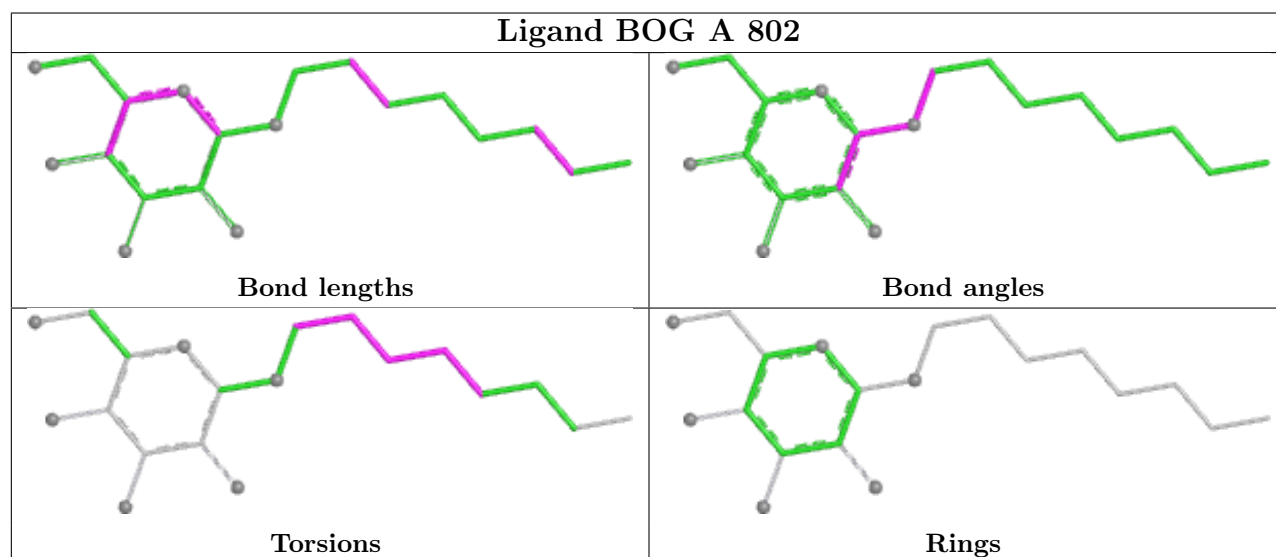
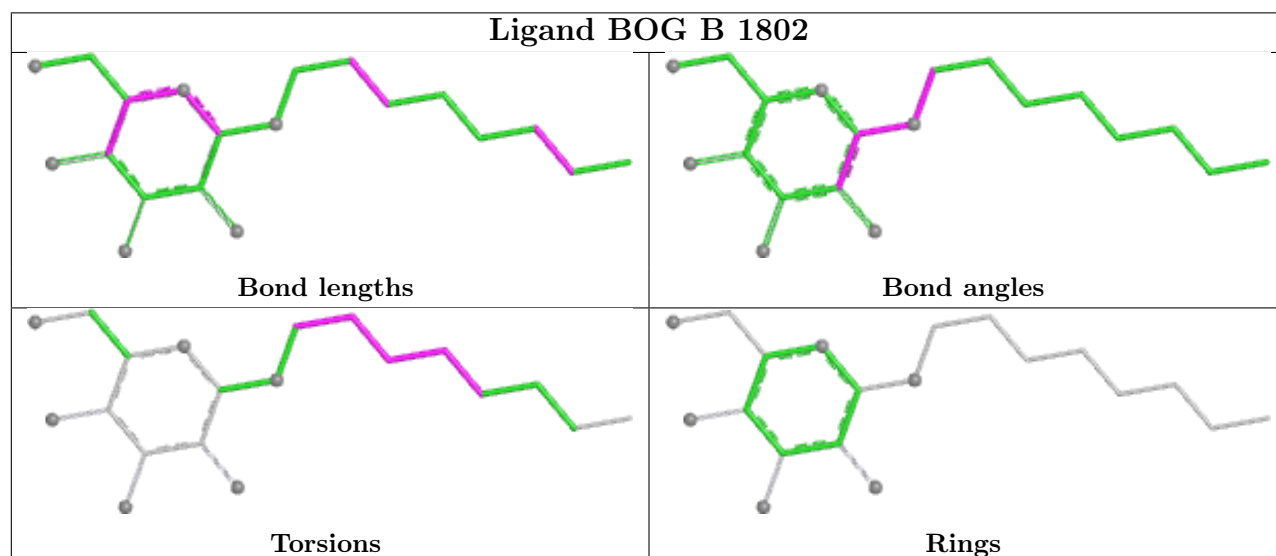
There are no ring outliers.

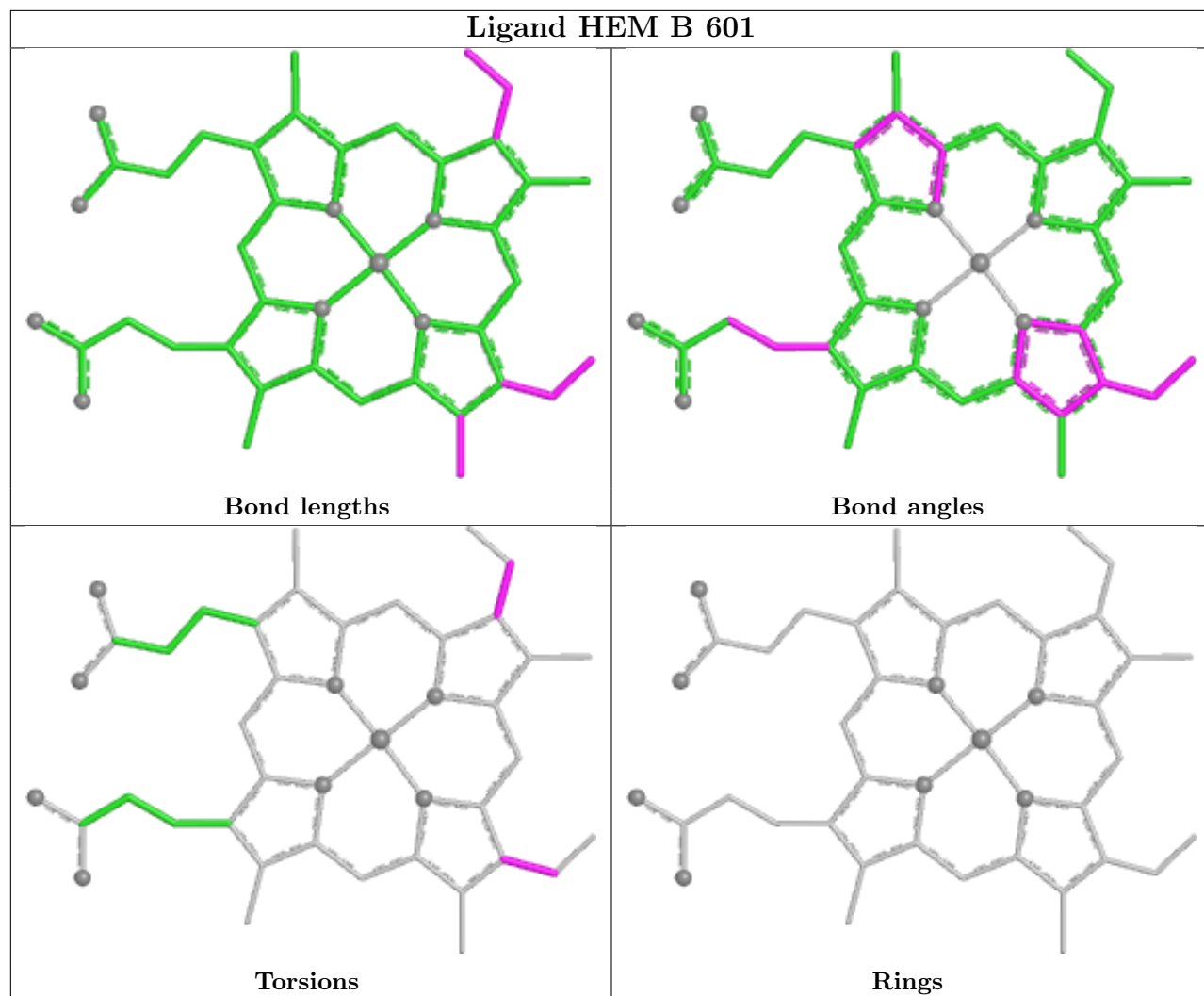
13 monomers are involved in 56 short contacts:

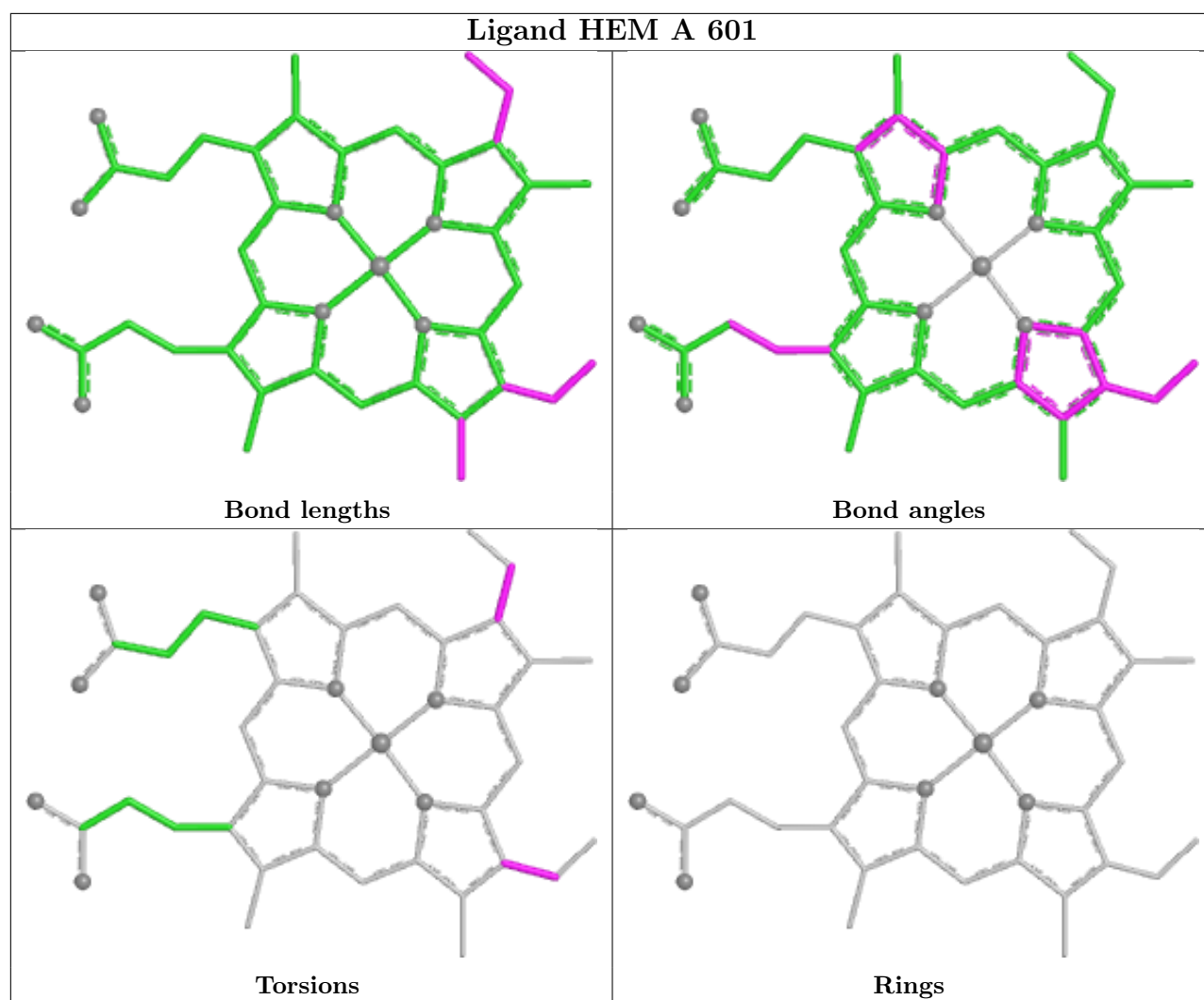
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	662	NAG	1	0
3	B	1802	BOG	10	0
2	B	1662	NAG	1	0
2	A	681	NAG	4	0
2	A	661	NAG	2	0
2	A	671	NAG	4	0
2	B	1681	NAG	5	0
3	A	802	BOG	14	0
2	B	1661	NAG	2	0
3	A	801	BOG	1	0
4	B	601	HEM	4	0
4	A	601	HEM	6	0
2	B	1671	NAG	4	0

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	551/580 (95%)	-0.06	15 (2%)	56 51	11, 23, 38, 52	0
1	B	551/580 (95%)	-0.07	18 (3%)	49 44	10, 22, 38, 52	0
All	All	1102/1160 (95%)	-0.07	33 (2%)	52 47	10, 23, 38, 52	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	75	TRP	5.0
1	B	283	SER	4.7
1	A	107	PHE	4.6
1	B	281	PRO	4.4
1	B	409	PHE	4.2
1	B	282	GLN	4.2
1	B	81	THR	4.1
1	B	75	TRP	3.7
1	A	294	LEU	3.4
1	B	82	LEU	3.3
1	B	294	LEU	3.3
1	A	81	THR	3.1
1	A	408	LEU	3.0
1	B	79	ARG	3.0
1	A	411	THR	3.0
1	A	79	ARG	2.9
1	A	581	HIS	2.9
1	B	581	HIS	2.9
1	B	485	LYS	2.8
1	B	479	GLN	2.7
1	A	277	ARG	2.7
1	A	513	HIS	2.7
1	B	280	PRO	2.6
1	A	83	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	186	LYS	2.5
1	A	485	LYS	2.3
1	A	98	TRP	2.2
1	A	97	ARG	2.2
1	B	83	ARG	2.1
1	A	33	VAL	2.1
1	B	33	VAL	2.1
1	B	74	ILE	2.0
1	B	97	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	BOG	A	802	20/20	0.61	0.29	45,64,65,67	0
2	NAG	A	1672	14/15	0.65	0.27	36,39,44,47	0
3	BOG	B	1802	20/20	0.67	0.36	45,64,66,66	0
2	NAG	B	1662	14/15	0.68	0.32	74,76,78,78	0
2	NAG	A	662	14/15	0.68	0.26	75,77,77,77	0
3	BOG	A	801	20/20	0.68	0.32	54,66,69,70	0
2	NAG	B	1661	14/15	0.68	0.26	55,57,58,58	0
2	NAG	A	661	14/15	0.70	0.26	55,57,59,60	0
2	NAG	B	1681	14/15	0.73	0.27	32,36,39,40	0
2	NAG	B	672	14/15	0.74	0.22	34,38,44,45	0
2	NAG	A	681	14/15	0.79	0.18	32,37,40,41	0
2	NAG	B	1671	14/15	0.88	0.12	9,16,19,19	0
2	NAG	A	671	14/15	0.91	0.10	10,16,19,20	0
5	IBP	A	701	15/15	0.93	0.10	27,27,29,29	0

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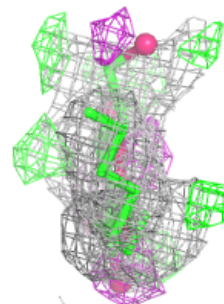
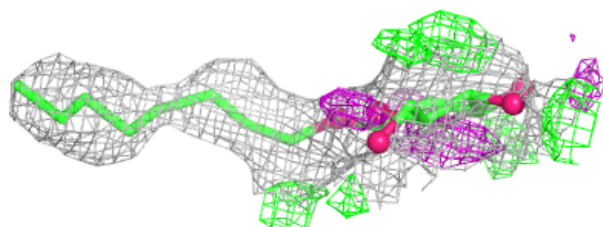
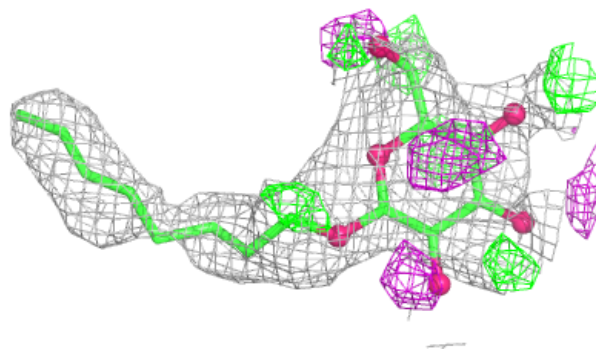
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	IBP	B	1701	15/15	0.93	0.11	26,28,30,31	0
4	HEM	A	601	43/43	0.95	0.10	20,23,37,43	0
4	HEM	B	601	43/43	0.96	0.11	21,25,38,43	0

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.

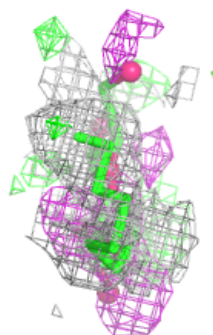
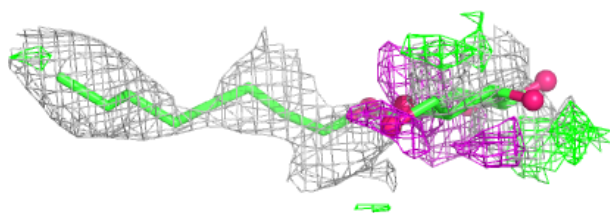
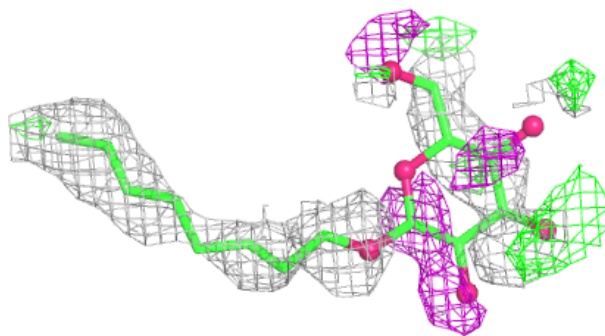
Electron density around BOG A 802:

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

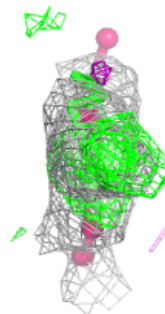
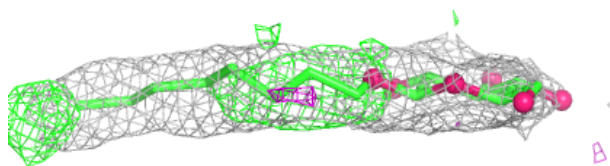
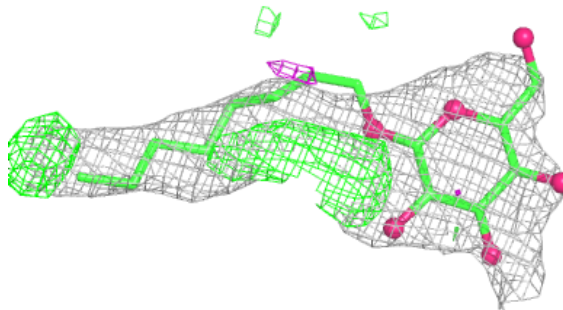


Electron density around BOG B 1802:

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

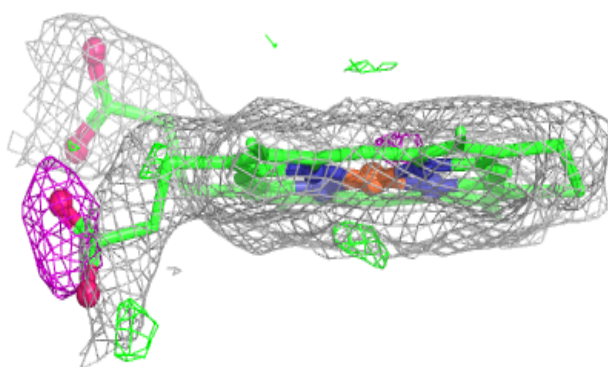
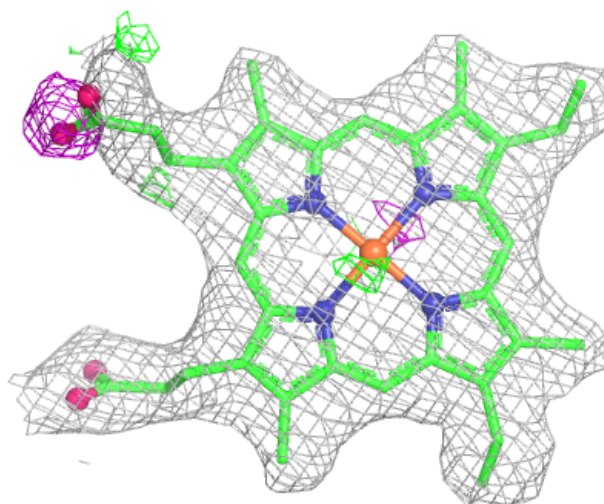
**Electron density around BOG A 801:**

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



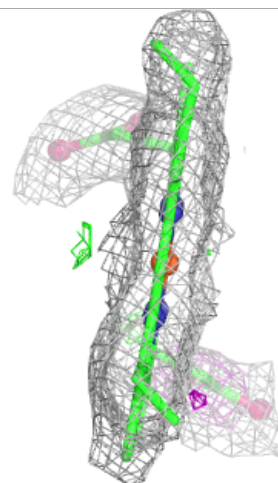
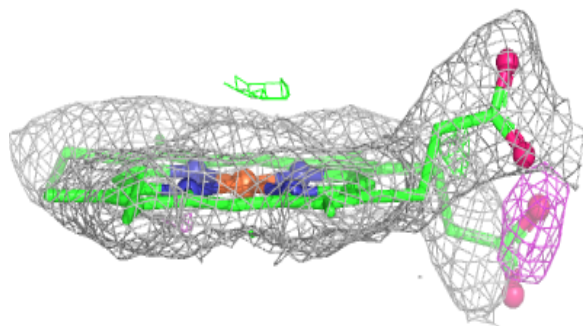
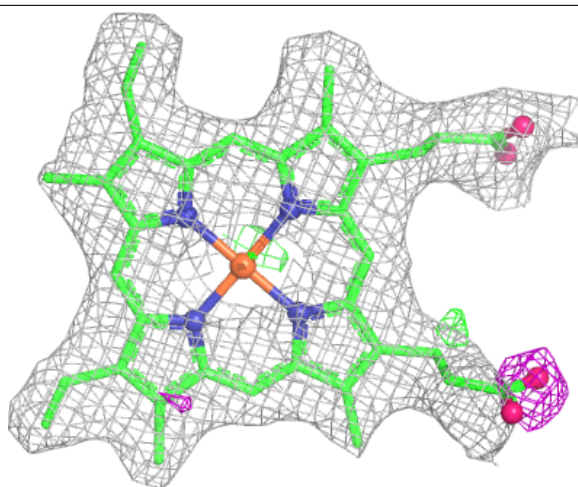
Electron density around HEM A 601:

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



Electron density around HEM B 601:

$2mF_o-DF_c$ (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.