



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 05:36 AM BST

PDB ID : 1EQH
Title : THE 2.7 ANGSTROM MODEL OF OVINE COX-1 COMPLEXED WITH FLURBIPROFEN
Authors : Loll, P.J.; Selinsky, B.S.; Gupta, K.; Sharkey, C.T.
Deposited on : 2000-04-04
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

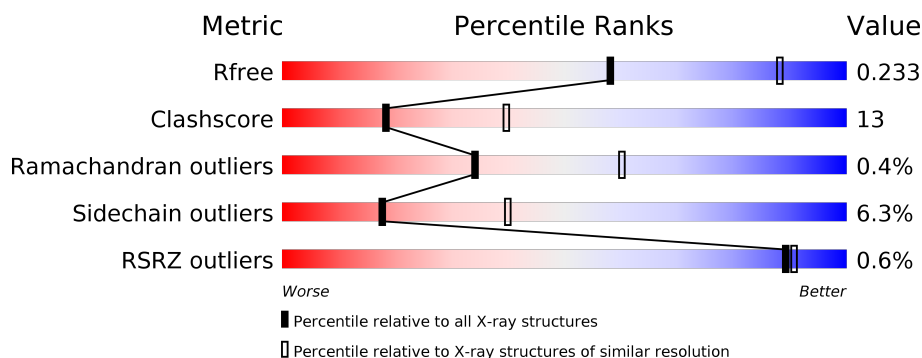
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>22%</div> <div>• 5%</div> </div> </div>
1	B	580	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>22%</div> <div>• 5%</div> </div> </div>

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
2	NAG	A	662	-	-	-	X
2	NAG	B	1662	-	-	-	X
3	BOG	B	1802	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9530 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 (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



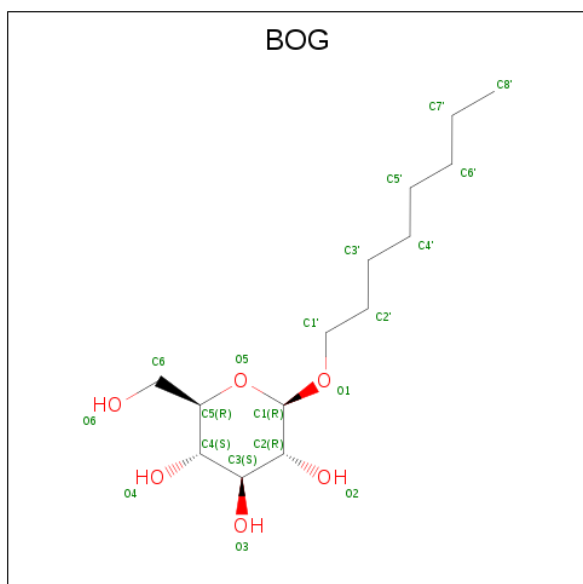
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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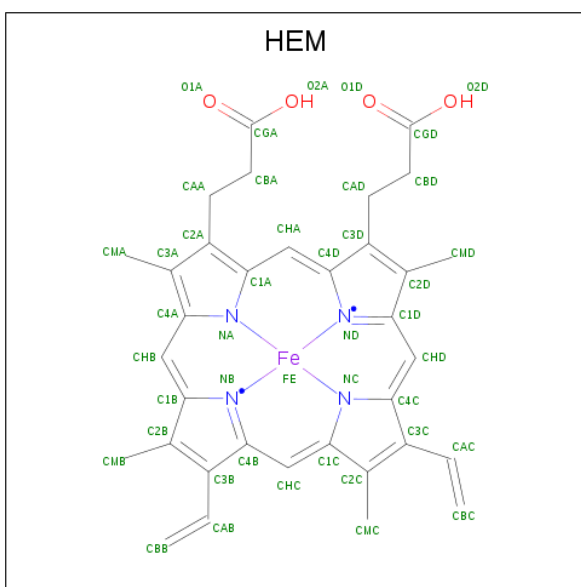
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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



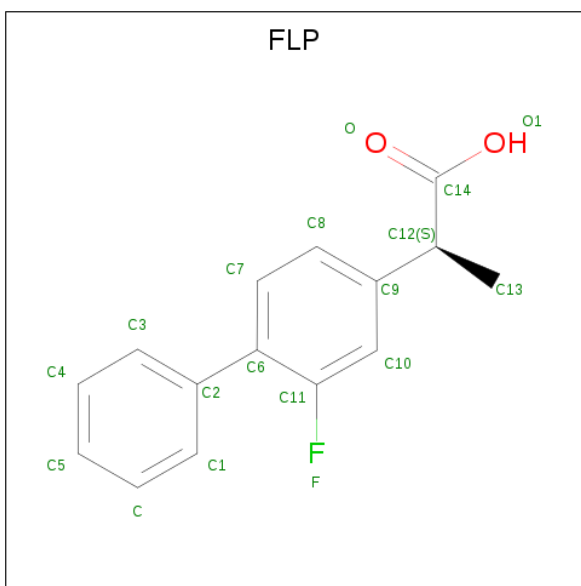
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	14	6		
3	A	1	Total	C	O	0	0
			20	14	6		
3	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: 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 FLURBIPROFEN (three-letter code: FLP) (formula: $C_{15}H_{13}FO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 18	C 15	F 1	O 2	0	0
5	B	1	Total 18	C 15	F 1	O 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	128	Total 128	O 128	0	0
6	B	126	Total 126	O 126	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.69Å 206.52Å 220.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.79 – 2.70 44.79 – 2.58	Depositor EDS
% Data completeness (in resolution range)	97.3 (44.79-2.70) 96.3 (44.79-2.58)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.29 (at 2.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.242 0.202 , 0.233	Depositor DCC
R_{free} test set	4638 reflections (6.76%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9530	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FLP, NAG, HEM, BOG

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	0.38	0/4615	0.62	0/6264
1	B	0.38	0/4615	0.62	1/6264 (0.0%)
All	All	0.38	0/9230	0.62	1/12528 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	LEU	N-CA-C	-5.07	97.31	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	120	0
1	B	4477	0	4386	127	0
2	A	70	0	65	5	0
2	B	70	0	65	5	0
3	A	40	0	56	5	0
3	B	20	0	28	11	0
4	A	43	0	30	4	0
4	B	43	0	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	18	0	12	0	0
5	B	18	0	12	0	0
6	A	128	0	0	4	0
6	B	126	0	0	3	0
All	All	9530	0	9070	243	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 13.

All (243) 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:563:THR:HG22	1:A:566:LYS:H	1.25	1.01
1:B:391:MET:HG3	4:B:601:HEM:HAB	1.43	0.99
1:B:563:THR:HG22	1:B:566:LYS:H	1.26	0.99
1:A:391:MET:HG3	4:A:601:HEM:HAB	1.45	0.96
1:B:410:ASN:HD21	2:B:1681:NAG:C1	1.80	0.94
1:A:410:ASN:HD21	2:A:681:NAG:C1	1.81	0.94
1:B:144:ASN:HD21	2:B:1671:NAG:C1	1.81	0.93
1:A:144:ASN:HD21	2:A:671:NAG:C1	1.81	0.93
1:B:208:GLN:NE2	1:B:230:LEU:H	1.65	0.93
1:B:86:PRO:HG3	3:B:1802:BOG:H61	1.56	0.88
1:A:208:GLN:NE2	1:A:230:LEU:H	1.72	0.87
1:A:276:PRO:HD2	1:A:279:ILE:HD12	1.54	0.87
1:B:294:LEU:HD22	1:B:409:PHE:CE2	2.08	0.87
1:B:215:LYS:H	1:B:215:LYS:HE2	1.40	0.86
1:B:215:LYS:CE	1:B:215:LYS:H	1.92	0.83
1:A:150:ARG:HD3	1:A:152:LEU:O	1.80	0.81
1:A:185:ARG:HH21	1:A:438:ARG:HH11	1.28	0.81
1:A:215:LYS:H	1:A:215:LYS:CE	1.94	0.80
1:B:145:VAL:HG12	1:B:224:LEU:HD22	1.65	0.79
1:B:150:ARG:HD3	1:B:152:LEU:O	1.82	0.79
1:B:144:ASN:ND2	2:B:1671:NAG:C1	2.47	0.78
1:B:116:VAL:HG22	3:B:1802:BOG:H2'1	1.64	0.78
1:A:144:ASN:ND2	2:A:671:NAG:C1	2.46	0.78
1:A:215:LYS:H	1:A:215:LYS:HE2	1.49	0.77
1:A:185:ARG:HH21	1:A:438:ARG:NH1	1.81	0.77
1:B:185:ARG:HH21	1:B:438:ARG:NH1	1.81	0.77
1:A:294:LEU:HD22	1:A:409:PHE:CE2	2.21	0.75
1:B:462:PRO:HG2	1:B:465:GLU:HG2	1.71	0.73
1:B:185:ARG:HH21	1:B:438:ARG:HH11	1.35	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:PRO:HG2	1:A:465:GLU:HG2	1.70	0.72
1:B:240:ARG:NH1	1:B:271:VAL:HG13	2.05	0.71
1:B:208:GLN:HE21	1:B:230:LEU:H	1.36	0.71
1:B:518:PHE:CD1	1:B:522:MET:HG2	2.26	0.70
1:A:208:GLN:HE21	1:A:230:LEU:H	1.40	0.69
1:B:294:LEU:HD22	1:B:409:PHE:CD2	2.28	0.69
1:B:582:VAL:HG22	1:B:583:PRO:HD2	1.74	0.68
1:A:114:ARG:HD3	1:A:365:LEU:O	1.93	0.68
1:A:582:VAL:HG22	1:A:583:PRO:HD2	1.74	0.67
1:A:144:ASN:HD21	2:A:671:NAG:C2	2.07	0.67
1:A:86:PRO:HG3	3:A:802:BOG:H61	1.76	0.67
1:A:241:GLN:HE21	1:A:245:ARG:HH11	1.41	0.67
1:A:387:TRP:HB2	4:A:601:HEM:HAC	1.77	0.67
1:B:144:ASN:HD21	2:B:1671:NAG:C2	2.07	0.66
1:A:180:ARG:HD3	1:A:490:GLU:OE2	1.96	0.66
1:A:518:PHE:CD1	1:A:522:MET:HG2	2.31	0.66
1:B:514:PRO:HB2	6:B:1854:HOH:O	1.96	0.65
1:A:240:ARG:NH1	1:A:271:VAL:HG13	2.13	0.64
1:A:49:ARG:O	1:B:320:HIS:HD2	1.81	0.63
1:B:185:ARG:NH2	1:B:438:ARG:NH1	2.46	0.63
1:B:89:ILE:HD12	3:B:1802:BOG:H62	1.79	0.63
1:B:387:TRP:HB2	4:B:601:HEM:HAC	1.81	0.63
1:B:454:GLU:HG2	1:B:458:LEU:HD22	1.81	0.63
1:A:145:VAL:HG12	1:A:224:LEU:HD22	1.81	0.62
1:B:527:ALA:HB3	1:B:528:PRO:HD3	1.83	0.61
1:A:454:GLU:HG2	1:A:458:LEU:HD22	1.83	0.61
1:A:132:ILE:HD13	1:A:458:LEU:HD12	1.83	0.61
1:B:458:LEU:HB3	1:B:460:LEU:HD13	1.82	0.61
1:A:458:LEU:HB3	1:A:460:LEU:HD13	1.83	0.60
1:A:165:THR:HB	6:A:1763:HOH:O	2.02	0.60
1:B:132:ILE:HD13	1:B:458:LEU:HD12	1.83	0.60
1:A:91:PHE:O	1:A:95:HIS:HD2	1.85	0.59
1:B:165:THR:HB	6:B:1850:HOH:O	2.01	0.59
1:A:320:HIS:HD2	1:B:49:ARG:O	1.85	0.59
1:B:185:ARG:NH2	1:B:438:ARG:HH11	1.99	0.59
1:A:180:ARG:O	1:A:438:ARG:NH1	2.37	0.58
1:B:410:ASN:ND2	2:B:1681:NAG:C1	2.61	0.58
1:B:208:GLN:NE2	1:B:230:LEU:N	2.45	0.58
1:A:185:ARG:NH2	1:A:438:ARG:NH1	2.51	0.58
1:B:88:PHE:O	1:B:92:LEU:HD13	2.04	0.57
1:B:215:LYS:N	1:B:215:LYS:HE2	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ARG:HE	1:B:438:ARG:HD3	1.68	0.57
1:A:410:ASN:ND2	2:A:681:NAG:C1	2.60	0.57
1:A:88:PHE:O	1:A:92:LEU:HD13	2.05	0.56
1:A:230:LEU:HG	1:A:233:ILE:HD12	1.86	0.56
1:B:208:GLN:HE22	1:B:230:LEU:H	1.52	0.56
1:B:34:ASN:HB3	1:B:37:CYS:SG	2.45	0.56
1:B:241:GLN:HE21	1:B:245:ARG:HH11	1.52	0.56
1:A:49:ARG:HG3	1:A:49:ARG:HH11	1.71	0.56
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.88	0.56
1:A:120:ARG:NH1	3:A:802:BOG:H3	2.20	0.56
1:B:267:GLU:OE1	1:B:282:GLN:HG3	2.07	0.55
1:A:577:TYR:CE2	1:A:583:PRO:HD3	2.42	0.55
1:B:49:ARG:HH11	1:B:49:ARG:HG3	1.71	0.55
1:B:70:THR:O	1:B:72:PRO:HD3	2.06	0.55
1:A:295:LEU:HD12	1:A:298:LEU:HD22	1.89	0.55
1:A:88:PHE:CZ	1:A:92:LEU:HD11	2.42	0.55
1:B:344:VAL:O	1:B:348:TYR:HB3	2.06	0.55
1:A:294:LEU:HD22	1:A:409:PHE:CD2	2.42	0.54
1:B:123:LEU:O	1:B:469:ARG:NH2	2.40	0.54
1:B:294:LEU:O	1:B:408:LEU:O	2.25	0.54
1:B:577:TYR:CE2	1:B:583:PRO:HD3	2.42	0.54
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.48	0.54
1:A:246:LEU:HD13	1:A:248:LYS:HB3	1.90	0.53
1:B:524:GLU:OE1	3:B:1802:BOG:H5	2.09	0.53
1:A:306:LEU:HD23	1:A:306:LEU:C	2.29	0.53
1:A:389:PRO:HG3	1:A:440:ILE:HG12	1.91	0.53
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.91	0.53
1:B:295:LEU:HB2	1:B:298:LEU:HD22	1.90	0.53
1:B:306:LEU:HD23	1:B:306:LEU:C	2.30	0.53
1:A:120:ARG:HD3	3:A:802:BOG:O2	2.10	0.52
1:B:233:ILE:HD13	1:B:305:TRP:HB3	1.91	0.52
1:B:88:PHE:CZ	1:B:92:LEU:HD11	2.44	0.52
1:A:185:ARG:NH2	1:A:438:ARG:HH11	2.02	0.52
1:A:470:PHE:CD2	1:A:525:MET:HG2	2.44	0.52
1:B:241:GLN:NE2	1:B:245:ARG:HH11	2.07	0.52
1:B:530:SER:O	1:B:534:LEU:HD22	2.10	0.51
1:B:295:LEU:HD12	1:B:298:LEU:HD22	1.91	0.51
1:A:295:LEU:HB2	1:A:298:LEU:HD22	1.92	0.51
1:A:185:ARG:HE	1:A:438:ARG:HD3	1.76	0.51
1:B:186:LYS:HB2	1:B:186:LYS:NZ	2.26	0.51
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LYS:HB2	1:A:186:LYS:NZ	2.26	0.51
1:A:479:GLN:H	1:A:479:GLN:CD	2.14	0.51
1:B:389:PRO:HG3	1:B:440:ILE:HG12	1.93	0.50
1:A:74:ILE:HG23	1:A:75:TRP:N	2.26	0.50
1:B:375:ASN:HD22	1:B:532:LYS:HG3	1.76	0.50
1:A:403:SER:OG	1:A:405:GLU:HG2	2.11	0.50
1:A:123:LEU:O	1:A:469:ARG:NH2	2.44	0.50
1:A:291:VAL:CG2	1:A:294:LEU:HD12	2.41	0.50
1:A:208:GLN:NE2	1:A:230:LEU:N	2.52	0.50
1:A:241:GLN:NE2	1:A:245:ARG:HH11	2.07	0.50
1:A:116:VAL:HG22	3:A:802:BOG:H2'1	1.94	0.49
1:A:175:GLU:HB2	6:A:1790:HOH:O	2.12	0.49
1:B:291:VAL:CG2	1:B:294:LEU:HD12	2.42	0.49
1:B:384:LEU:C	1:B:384:LEU:HD23	2.32	0.49
1:A:379:MET:SD	1:A:458:LEU:HG	2.52	0.49
1:B:479:GLN:H	1:B:479:GLN:CD	2.15	0.49
1:B:183:LEU:HG	1:B:445:LEU:HD22	1.94	0.49
1:A:134:HIS:HD2	1:A:138:SER:OG	1.95	0.49
1:A:530:SER:O	1:A:534:LEU:HD22	2.13	0.49
1:B:294:LEU:HD22	1:B:409:PHE:HE2	1.70	0.49
1:B:150:ARG:NH2	1:B:458:LEU:O	2.46	0.48
1:B:203:GLN:HA	4:B:601:HEM:HBC2	1.95	0.48
1:B:86:PRO:CG	3:B:1802:BOG:H61	2.37	0.48
1:B:388:HIS:N	1:B:389:PRO:CD	2.77	0.48
1:A:183:LEU:HG	1:A:445:LEU:HD22	1.96	0.48
1:A:150:ARG:NH2	1:A:458:LEU:O	2.46	0.48
1:B:120:ARG:NH1	3:B:1802:BOG:H3	2.29	0.48
1:B:323:TRP:CE3	1:B:327:GLN:HG2	2.49	0.47
1:B:119:VAL:HG12	3:B:1802:BOG:O2	2.13	0.47
1:B:208:GLN:HE22	1:B:230:LEU:HD12	1.80	0.47
1:A:49:ARG:CG	1:A:49:ARG:HH11	2.27	0.47
1:B:134:HIS:HD2	1:B:138:SER:OG	1.97	0.47
1:A:388:HIS:N	1:A:389:PRO:CD	2.78	0.47
1:A:382:ASN:OD1	1:A:386:HIS:HE1	1.97	0.47
1:B:237:ASN:ND2	1:B:240:ARG:H	2.13	0.47
1:A:293:GLY:HA2	1:A:299:MET:HE3	1.97	0.47
1:B:208:GLN:HE21	1:B:230:LEU:N	2.09	0.47
1:A:479:GLN:O	1:A:482:THR:O	2.31	0.47
1:A:240:ARG:HG3	1:A:271:VAL:HG22	1.97	0.46
1:A:163:MET:CE	1:A:171:LEU:HD21	2.45	0.46
1:B:403:SER:OG	1:B:405:GLU:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LYS:N	1:A:215:LYS:HE2	2.23	0.46
1:B:243:GLN:HG3	1:B:270:PRO:HD2	1.97	0.46
1:B:49:ARG:HH11	1:B:49:ARG:CG	2.27	0.46
1:B:213:SER:OG	1:B:215:LYS:HE3	2.15	0.46
1:A:294:LEU:HD22	1:A:409:PHE:HE2	1.77	0.46
1:B:275:TYR:CD2	1:B:284:GLN:HG2	2.51	0.46
1:A:185:ARG:HH11	1:A:185:ARG:HG2	1.81	0.46
1:A:295:LEU:HD21	4:A:601:HEM:HBB2	1.97	0.46
1:A:374:ARG:NH1	1:B:374:ARG:HB3	2.31	0.46
1:A:323:TRP:CE3	1:A:327:GLN:HG2	2.51	0.45
1:A:119:VAL:HG12	3:A:802:BOG:O2	2.17	0.45
1:B:459:ARG:HG2	1:B:459:ARG:HH21	1.82	0.45
1:A:215:LYS:H	1:A:215:LYS:HE3	1.76	0.45
1:B:293:GLY:HA2	1:B:299:MET:HE3	1.97	0.45
1:A:374:ARG:HB3	1:B:374:ARG:NH1	2.31	0.45
1:B:339:GLU:HG2	1:B:562:ALA:HB2	1.98	0.45
1:A:344:VAL:O	1:A:348:TYR:HB3	2.16	0.45
1:B:156:PRO:HB2	1:B:159:CYS:SG	2.57	0.45
1:B:295:LEU:HD21	4:B:601:HEM:HBB2	1.97	0.45
1:B:274:HIS:O	1:B:294:LEU:HD21	2.17	0.45
1:A:546:LYS:HE3	6:B:1845:HOH:O	2.17	0.44
1:B:291:VAL:HG22	1:B:294:LEU:HD12	1.99	0.44
1:A:290:GLU:H	1:A:290:GLU:CD	2.21	0.44
1:A:459:ARG:HG2	1:A:459:ARG:HH21	1.82	0.44
1:B:340:THR:O	1:B:344:VAL:HG23	2.18	0.44
1:A:91:PHE:O	1:A:95:HIS:CD2	2.69	0.44
1:B:290:GLU:CD	1:B:290:GLU:H	2.20	0.44
1:B:163:MET:CE	1:B:171:LEU:HD21	2.48	0.44
1:B:185:ARG:HH11	1:B:185:ARG:HG2	1.82	0.44
1:B:64:TYR:CE1	1:B:76:THR:HG21	2.53	0.44
1:A:291:VAL:HG22	1:A:294:LEU:HD12	2.00	0.44
1:B:382:ASN:OD1	1:B:386:HIS:HE1	2.00	0.44
1:B:481:LEU:HD22	1:B:501:LEU:HD22	1.99	0.44
1:A:213:SER:OG	1:A:215:LYS:HE3	2.17	0.43
1:B:120:ARG:CZ	3:B:1802:BOG:H1	2.48	0.43
1:B:206:THR:HB	1:B:210:PHE:CD2	2.53	0.43
1:B:485:LYS:HD3	1:B:485:LYS:HA	1.84	0.43
1:A:59:CYS:O	1:A:62:THR:HG23	2.19	0.43
1:B:246:LEU:O	1:B:247:PHE:HB2	2.19	0.43
1:B:59:CYS:O	1:B:62:THR:HG23	2.18	0.43
1:A:226:HIS:CE1	1:A:376:ARG:HD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:MET:O	1:A:257:LEU:HD23	2.19	0.43
1:B:206:THR:HB	1:B:210:PHE:HD2	1.83	0.43
1:B:388:HIS:CE1	1:B:447:VAL:HG11	2.53	0.43
1:A:384:LEU:HD23	1:A:384:LEU:C	2.39	0.43
1:A:215:LYS:NZ	1:A:222:LYS:HD2	2.32	0.43
1:B:148:TYR:CZ	1:B:221:THR:HB	2.54	0.43
6:A:1722:HOH:O	1:B:546:LYS:HE3	2.17	0.43
1:B:389:PRO:HG3	1:B:440:ILE:CG1	2.49	0.43
1:A:130:TYR:HB2	1:A:150:ARG:HG3	2.01	0.42
1:A:481:LEU:HD22	1:A:501:LEU:HD22	2.00	0.42
1:A:389:PRO:HG3	1:A:440:ILE:CG1	2.49	0.42
1:A:230:LEU:CD2	1:A:336:LEU:HB3	2.49	0.42
1:B:215:LYS:H	1:B:215:LYS:HE3	1.79	0.42
1:A:126:SER:HA	1:A:127:PRO:C	2.39	0.42
1:B:582:VAL:CG2	1:B:583:PRO:HD2	2.48	0.42
1:B:74:ILE:HG23	1:B:75:TRP:N	2.35	0.42
1:A:420:GLU:HG3	1:A:572:THR:HB	2.02	0.42
1:B:130:TYR:HB2	1:B:150:ARG:HG3	2.00	0.42
1:A:163:MET:HE2	1:A:171:LEU:HD21	2.01	0.42
1:B:83:ARG:HD3	3:B:1802:BOG:O6	2.20	0.42
1:A:472:MET:HG3	6:A:1705:HOH:O	2.20	0.41
1:B:126:SER:HA	1:B:127:PRO:C	2.40	0.41
1:B:176:PHE:CZ	1:B:180:ARG:HG3	2.56	0.41
1:B:441:ASP:OD2	1:B:443:HIS:HD2	2.03	0.41
1:B:238:LEU:HD23	1:B:238:LEU:HA	1.83	0.41
1:B:420:GLU:HG3	1:B:572:THR:HB	2.01	0.41
1:A:208:GLN:HE22	1:A:230:LEU:HD12	1.85	0.41
1:B:120:ARG:HD3	3:B:1802:BOG:O2	2.20	0.41
1:B:120:ARG:NH1	3:B:1802:BOG:H1	2.35	0.41
1:A:441:ASP:OD2	1:A:443:HIS:CD2	2.74	0.41
1:A:49:ARG:CG	1:A:49:ARG:NH1	2.83	0.41
1:A:513:HIS:O	1:A:514:PRO:C	2.58	0.41
1:B:441:ASP:OD2	1:B:443:HIS:CD2	2.73	0.41
1:A:156:PRO:HB2	1:A:159:CYS:SG	2.61	0.41
1:A:247:PHE:HA	1:A:325:ASP:OD2	2.20	0.41
1:A:374:ARG:O	1:A:532:LYS:HE3	2.21	0.41
1:A:275:TYR:CD2	1:A:284:GLN:HG2	2.56	0.41
1:B:230:LEU:CD2	1:B:336:LEU:HB3	2.51	0.41
1:A:210:PHE:HB3	4:A:601:HEM:HBD1	2.02	0.41
1:A:479:GLN:HG3	1:A:485:LYS:NZ	2.37	0.41
1:A:88:PHE:O	1:A:91:PHE:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ARG:HD3	1:B:490:GLU:OE2	2.21	0.41
1:B:513:HIS:O	1:B:514:PRO:C	2.60	0.41
1:A:180:ARG:NH2	1:A:490:GLU:OE1	2.54	0.40
1:A:479:GLN:CB	1:A:485:LYS:NZ	2.84	0.40
1:B:180:ARG:O	1:B:438:ARG:NH1	2.54	0.40
1:A:223:ALA:C	1:A:224:LEU:O	2.58	0.40
1:A:275:TYR:CE2	1:A:284:GLN:HB3	2.56	0.40
1:B:344:VAL:HA	1:B:348:TYR:HB3	2.03	0.40
1:B:180:ARG:NH2	1:B:490:GLU:OE1	2.50	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%)	34	60
1	B	549/580 (95%)	521 (95%)	26 (5%)	2 (0%)	34	60
All	All	1098/1160 (95%)	1044 (95%)	50 (5%)	4 (0%)	34	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	PRO
1	B	514	PRO
1	B	270	PRO
1	A	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%)	457 (94%)	29 (6%)	19	42
1	B	486/510 (95%)	454 (93%)	32 (7%)	16	38
All	All	972/1020 (95%)	911 (94%)	61 (6%)	18	40

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	117	LEU
1	A	123	LEU
1	A	171	LEU
1	A	183	LEU
1	A	186	LYS
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	289	GLN
1	A	298	LEU
1	A	300	LEU
1	A	316	LEU
1	A	376	ARG
1	A	385	TYR
1	A	405	GLU
1	A	458	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	556	PHE

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Mol	Chain	Res	Type
1	A	563	THR
1	A	564	LEU
1	B	49	ARG
1	B	97	ARG
1	B	117	LEU
1	B	123	LEU
1	B	171	LEU
1	B	180	ARG
1	B	183	LEU
1	B	186	LYS
1	B	215	LYS
1	B	238	LEU
1	B	244	LEU
1	B	246	LEU
1	B	252	LEU
1	B	271	VAL
1	B	289	GLN
1	B	298	LEU
1	B	300	LEU
1	B	316	LEU
1	B	352	LEU
1	B	376	ARG
1	B	385	TYR
1	B	405	GLU
1	B	458	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	556	PHE
1	B	563	THR
1	B	564	LEU

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

Mol	Chain	Res	Type
1	A	56	GLN
1	A	95	HIS
1	A	134	HIS
1	A	144	ASN

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Mol	Chain	Res	Type
1	A	203	GLN
1	A	204	HIS
1	A	207	HIS
1	A	208	GLN
1	A	237	ASN
1	A	241	GLN
1	A	320	HIS
1	A	375	ASN
1	A	386	HIS
1	A	400	GLN
1	A	443	HIS
1	A	479	GLN
1	B	56	GLN
1	B	95	HIS
1	B	134	HIS
1	B	144	ASN
1	B	203	GLN
1	B	208	GLN
1	B	237	ASN
1	B	241	GLN
1	B	274	HIS
1	B	320	HIS
1	B	375	ASN
1	B	386	HIS
1	B	400	GLN
1	B	443	HIS
1	B	479	GLN
1	B	513	HIS

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 monosaccharides 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
2	NAG	A	661	-	14,14,15	0.95	0	17,19,21	0.81	1 (5%)
2	NAG	B	1661	-	14,14,15	0.93	0	17,19,21	0.84	1 (5%)
4	HEM	A	601	1	27,50,50	1.87	7 (25%)	17,82,82	1.67	4 (23%)
5	FLP	A	701	-	16,19,19	2.34	7 (43%)	22,26,26	1.04	1 (4%)
2	NAG	B	1681	-	14,14,15	0.97	0	17,19,21	0.91	1 (5%)
2	NAG	B	1671	-	14,14,15	0.66	0	17,19,21	0.66	0
4	HEM	B	601	1	27,50,50	1.88	7 (25%)	17,82,82	1.65	4 (23%)
2	NAG	A	1672	-	14,14,15	1.17	1 (7%)	17,19,21	0.83	1 (5%)
2	NAG	B	1662	-	14,14,15	1.21	1 (7%)	17,19,21	0.77	1 (5%)
3	BOG	A	802	-	20,20,20	1.53	5 (25%)	25,25,25	0.89	2 (8%)
2	NAG	B	672	-	14,14,15	1.24	2 (14%)	17,19,21	0.83	1 (5%)
3	BOG	B	1802	-	20,20,20	1.52	5 (25%)	25,25,25	0.92	2 (8%)
2	NAG	A	671	-	14,14,15	0.82	0	17,19,21	0.69	0
5	FLP	B	1701	-	16,19,19	2.45	8 (50%)	22,26,26	1.04	1 (4%)
2	NAG	A	662	-	14,14,15	1.25	1 (7%)	17,19,21	0.74	1 (5%)
3	BOG	A	801	-	20,20,20	1.47	4 (20%)	25,25,25	0.78	2 (8%)
2	NAG	A	681	-	14,14,15	1.04	0	17,19,21	0.91	1 (5%)

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	661	-	-	2/6/23/26	0/1/1/1
2	NAG	B	1661	-	-	2/6/23/26	0/1/1/1
4	HEM	A	601	1	-	0/6/54/54	-
5	FLP	A	701	-	-	0/8/12/12	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1681	-	-	3/6/23/26	0/1/1/1
2	NAG	B	1671	-	-	4/6/23/26	0/1/1/1
4	HEM	B	601	1	-	0/6/54/54	-
2	NAG	A	1672	-	-	4/6/23/26	0/1/1/1
2	NAG	B	1662	-	-	2/6/23/26	0/1/1/1
3	BOG	A	802	-	-	3/11/31/31	0/1/1/1
2	NAG	B	672	-	-	4/6/23/26	0/1/1/1
3	BOG	B	1802	-	-	6/11/31/31	0/1/1/1
2	NAG	A	671	-	-	4/6/23/26	0/1/1/1
5	FLP	B	1701	-	-	0/8/12/12	0/2/2/2
2	NAG	A	662	-	-	2/6/23/26	0/1/1/1
3	BOG	A	801	-	-	3/11/31/31	0/1/1/1
2	NAG	A	681	-	-	3/6/23/26	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1701	FLP	C6-C11	4.44	1.45	1.39
5	A	701	FLP	C7-C6	4.13	1.46	1.40
5	A	701	FLP	C6-C11	4.08	1.44	1.39
5	B	1701	FLP	C7-C6	4.02	1.46	1.40
4	B	601	HEM	C3C-C2C	-3.94	1.34	1.40
5	B	1701	FLP	C8-C9	3.67	1.45	1.39
4	A	601	HEM	C3C-C2C	-3.64	1.35	1.40
4	B	601	HEM	CBB-CAB	3.58	1.53	1.29
4	A	601	HEM	CBC-CAC	3.56	1.52	1.29
4	B	601	HEM	CBC-CAC	3.56	1.52	1.29
5	A	701	FLP	C8-C9	3.51	1.44	1.39
4	B	601	HEM	C3B-CAB	3.50	1.55	1.47
4	A	601	HEM	C3C-CAC	3.50	1.55	1.47
4	A	601	HEM	CBB-CAB	3.49	1.52	1.29
5	B	1701	FLP	C1-C2	3.32	1.46	1.39
5	A	701	FLP	C1-C2	3.31	1.46	1.39
4	B	601	HEM	C3C-CAC	3.24	1.54	1.47
4	A	601	HEM	C3B-CAB	3.17	1.54	1.47
3	B	1802	BOG	O5-C1	3.15	1.49	1.41
5	B	1701	FLP	C8-C7	3.13	1.44	1.38
3	A	802	BOG	O5-C1	3.08	1.49	1.41
5	A	701	FLP	C8-C7	2.94	1.44	1.38
3	A	802	BOG	O5-C5	2.87	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	BOG	O5-C1	2.86	1.49	1.41
3	A	801	BOG	O5-C5	2.74	1.51	1.44
3	B	1802	BOG	O5-C5	2.73	1.51	1.44
3	A	801	BOG	C4-C5	-2.69	1.47	1.53
3	A	801	BOG	C3'-C2'	-2.59	1.37	1.51
5	B	1701	FLP	C-C1	2.56	1.44	1.38
4	A	601	HEM	C1C-C2C	2.54	1.48	1.42
3	A	802	BOG	C4-C5	-2.51	1.47	1.53
3	A	802	BOG	C3'-C2'	-2.48	1.37	1.51
5	B	1701	FLP	C4-C3	2.42	1.44	1.38
3	B	1802	BOG	C3'-C2'	-2.39	1.38	1.51
2	A	662	NAG	O5-C5	2.38	1.48	1.43
3	B	1802	BOG	C4-C5	-2.24	1.48	1.53
2	B	1662	NAG	O5-C5	2.24	1.48	1.43
4	B	601	HEM	C1C-C2C	2.20	1.47	1.42
5	A	701	FLP	C4-C3	2.16	1.43	1.38
2	A	1672	NAG	O5-C5	2.13	1.47	1.43
4	A	601	HEM	CMB-C2B	2.12	1.56	1.51
5	A	701	FLP	C-C1	2.10	1.43	1.38
2	B	672	NAG	O5-C5	2.04	1.47	1.43
2	B	672	NAG	C1-C2	2.03	1.55	1.52
3	B	1802	BOG	C4-C3	2.03	1.57	1.52
3	A	802	BOG	C4-C3	2.02	1.57	1.52
5	B	1701	FLP	C5-C4	2.01	1.43	1.38
4	B	601	HEM	CAA-C2A	2.01	1.55	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	HEM	C1D-C2D-C3D	-3.31	104.69	107.00
4	B	601	HEM	C1D-C2D-C3D	-3.23	104.75	107.00
5	B	1701	FLP	C10-C9-C12	-2.87	115.50	120.97
5	A	701	FLP	C10-C9-C12	-2.80	115.63	120.97
3	A	802	BOG	C1'-O1-C1	2.78	118.45	113.84
4	B	601	HEM	CMB-C2B-C3B	2.76	129.84	124.68
4	A	601	HEM	CMB-C2B-C3B	2.75	129.83	124.68
3	B	1802	BOG	O1-C1-C2	2.67	112.47	108.30
4	A	601	HEM	CBA-CAA-C2A	-2.66	107.58	112.49
4	B	601	HEM	CBA-CAA-C2A	-2.63	107.64	112.49
4	A	601	HEM	CAA-CBA-CGA	2.60	117.03	112.67
3	B	1802	BOG	C1'-O1-C1	2.57	118.10	113.84
4	B	601	HEM	CAA-CBA-CGA	2.56	116.96	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1662	NAG	C1-O5-C5	2.24	115.23	112.19
3	A	802	BOG	O1-C1-C2	2.23	111.78	108.30
2	B	1661	NAG	C1-O5-C5	2.22	115.20	112.19
3	A	801	BOG	O1-C1-C2	2.19	111.72	108.30
2	A	1672	NAG	O7-C7-C8	-2.17	118.03	122.06
2	A	662	NAG	C1-O5-C5	2.14	115.09	112.19
3	A	801	BOG	C1'-O1-C1	2.11	117.34	113.84
2	A	681	NAG	C1-O5-C5	2.08	115.02	112.19
2	B	1681	NAG	C1-O5-C5	2.07	115.00	112.19
2	B	672	NAG	O7-C7-C8	-2.06	118.22	122.06
2	A	661	NAG	C1-O5-C5	2.06	114.98	112.19

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1672	NAG	O5-C5-C6-O6
2	B	672	NAG	O5-C5-C6-O6
2	A	1672	NAG	C4-C5-C6-O6
2	B	672	NAG	C4-C5-C6-O6
2	A	661	NAG	C8-C7-N2-C2
2	B	1661	NAG	C8-C7-N2-C2
2	B	1671	NAG	C8-C7-N2-C2
2	B	1681	NAG	C8-C7-N2-C2
2	B	1662	NAG	C8-C7-N2-C2
2	A	1672	NAG	C8-C7-N2-C2
2	B	672	NAG	C8-C7-N2-C2
2	A	671	NAG	C8-C7-N2-C2
2	A	662	NAG	C8-C7-N2-C2
2	A	681	NAG	C8-C7-N2-C2
2	A	671	NAG	O5-C5-C6-O6
2	B	1671	NAG	O5-C5-C6-O6
2	A	671	NAG	C4-C5-C6-O6
2	B	1671	NAG	C4-C5-C6-O6
2	A	661	NAG	O7-C7-N2-C2
2	B	1661	NAG	O7-C7-N2-C2
2	B	1671	NAG	O7-C7-N2-C2
2	B	1681	NAG	O7-C7-N2-C2
2	B	1662	NAG	O7-C7-N2-C2
2	A	1672	NAG	O7-C7-N2-C2
2	B	672	NAG	O7-C7-N2-C2
2	A	671	NAG	O7-C7-N2-C2

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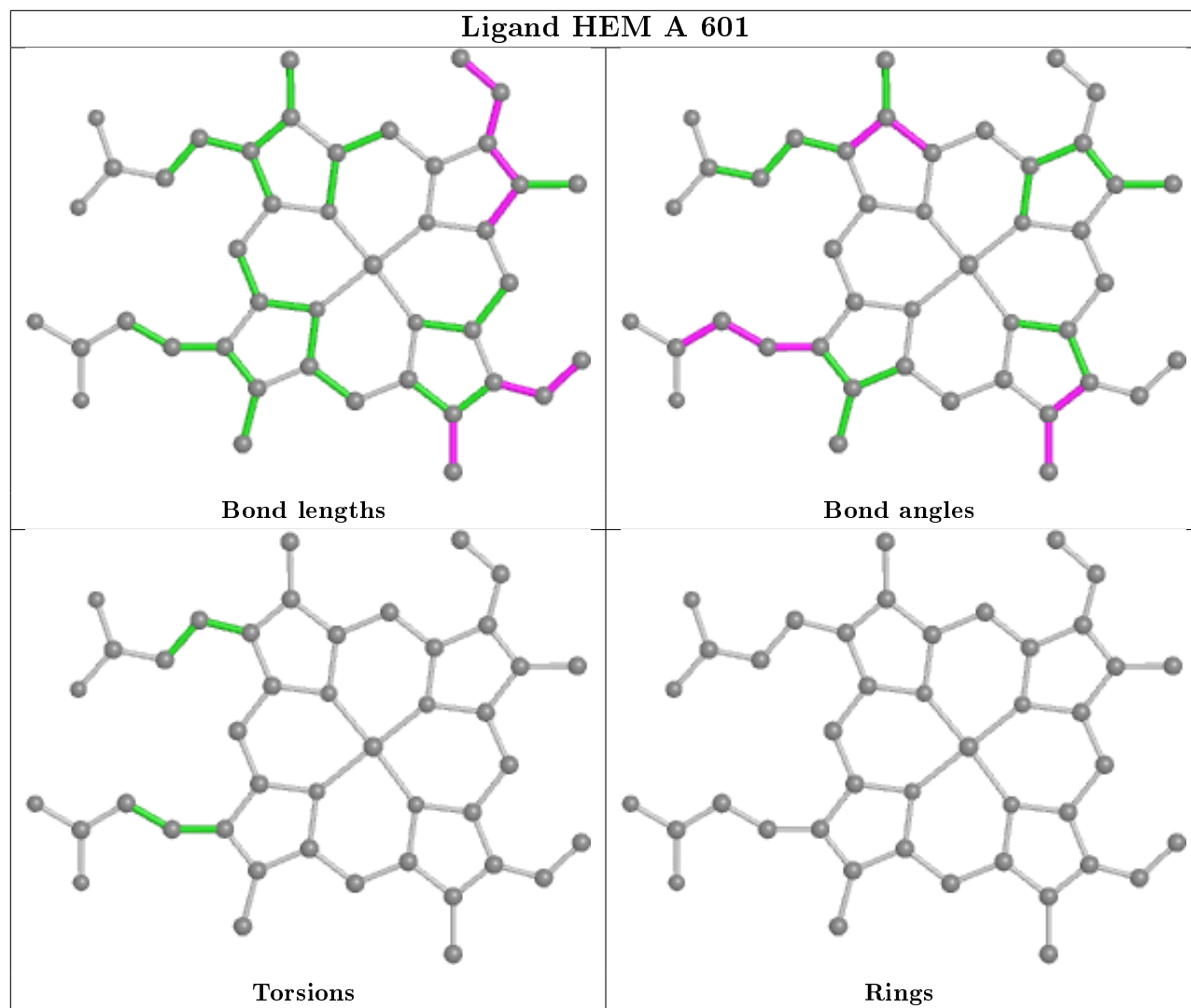
Mol	Chain	Res	Type	Atoms
2	A	662	NAG	O7-C7-N2-C2
2	A	681	NAG	O7-C7-N2-C2
3	B	1802	BOG	C3'-C4'-C5'-C6'
3	A	802	BOG	C3'-C4'-C5'-C6'
3	A	802	BOG	C1'-C2'-C3'-C4'
3	A	802	BOG	O1-C1'-C2'-C3'
3	B	1802	BOG	C1'-C2'-C3'-C4'
3	A	801	BOG	C1'-C2'-C3'-C4'
3	B	1802	BOG	O1-C1'-C2'-C3'
3	A	801	BOG	C3'-C4'-C5'-C6'
3	B	1802	BOG	C4-C5-C6-O6
3	B	1802	BOG	O5-C5-C6-O6
2	B	1681	NAG	C3-C2-N2-C7
2	A	681	NAG	C3-C2-N2-C7
3	B	1802	BOG	C2'-C3'-C4'-C5'
3	A	801	BOG	O1-C1'-C2'-C3'

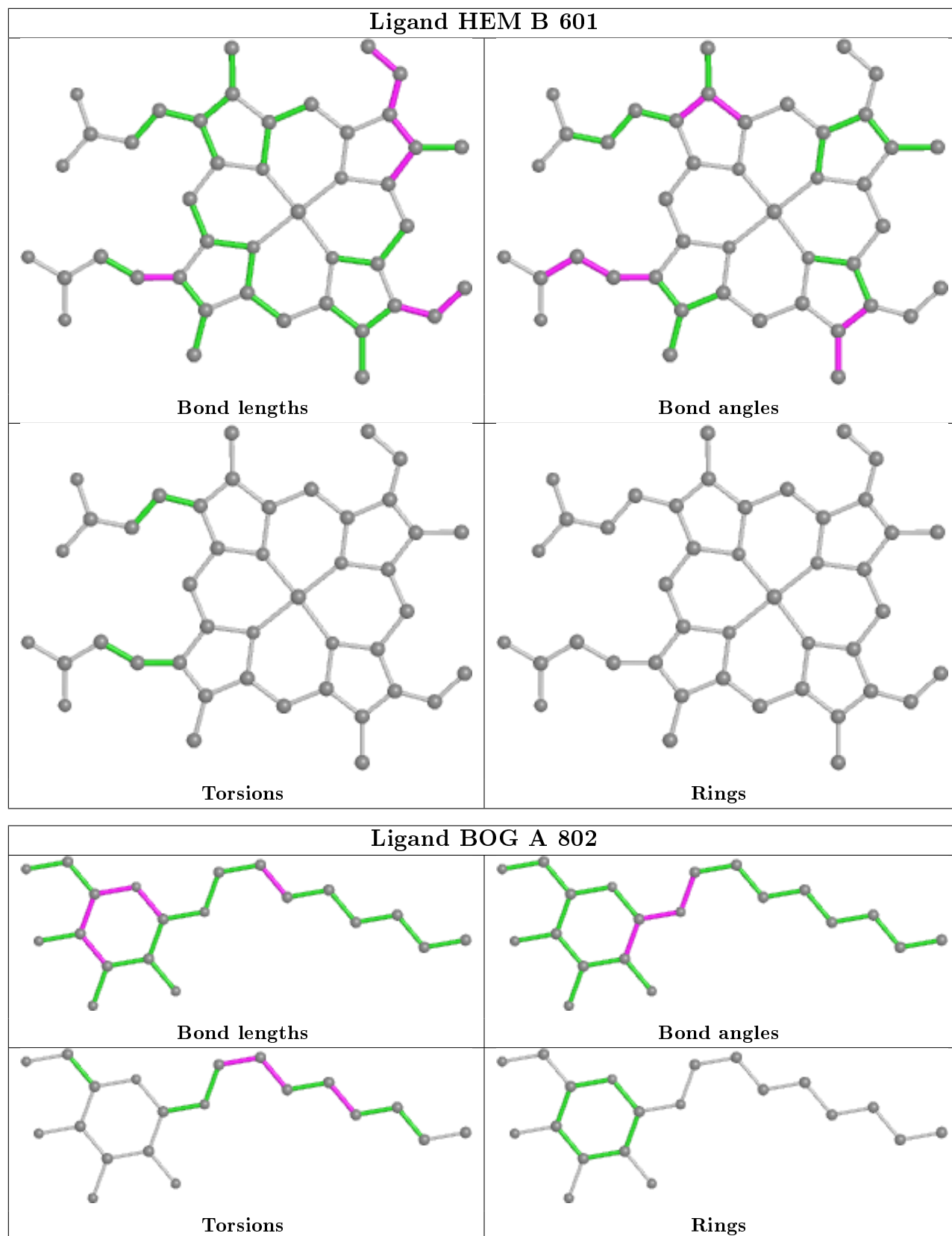
There are no ring outliers.

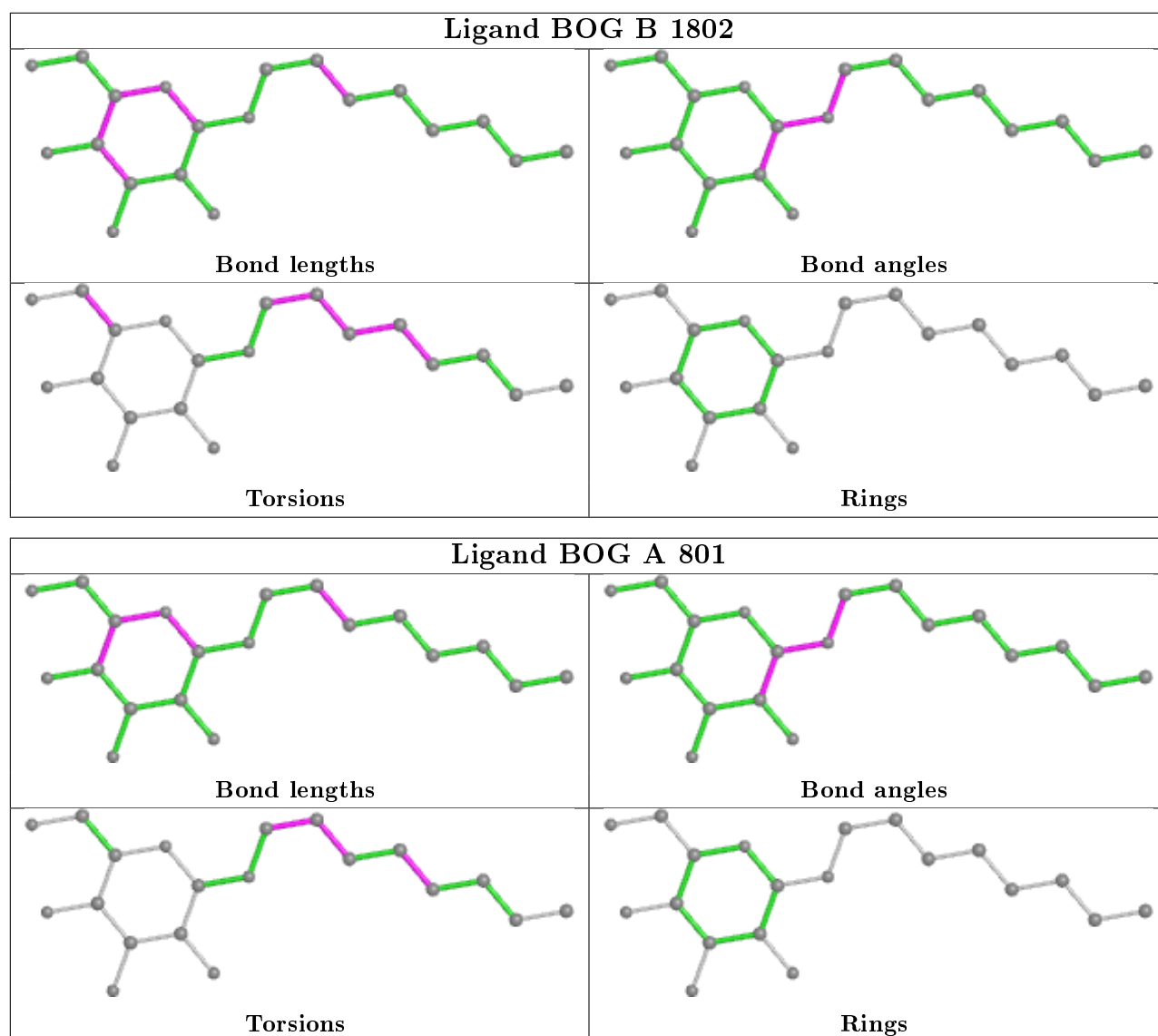
8 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	HEM	4	0
2	B	1681	NAG	2	0
2	B	1671	NAG	3	0
4	B	601	HEM	4	0
3	A	802	BOG	5	0
3	B	1802	BOG	11	0
2	A	671	NAG	3	0
2	A	681	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	551/580 (95%)	-0.49	3 (0%)	91 92	9, 20, 43, 68	0
1	B	551/580 (95%)	-0.53	4 (0%)	87 89	9, 20, 43, 68	0
All	All	1102/1160 (95%)	-0.51	7 (0%)	89 91	9, 20, 43, 68	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	107	PHE	3.0
1	B	281	PRO	2.6
1	B	282	GLN	2.4
1	B	409	PHE	2.2
1	B	399	PRO	2.1
1	A	98	TRP	2.1
1	A	215	LYS	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](#)

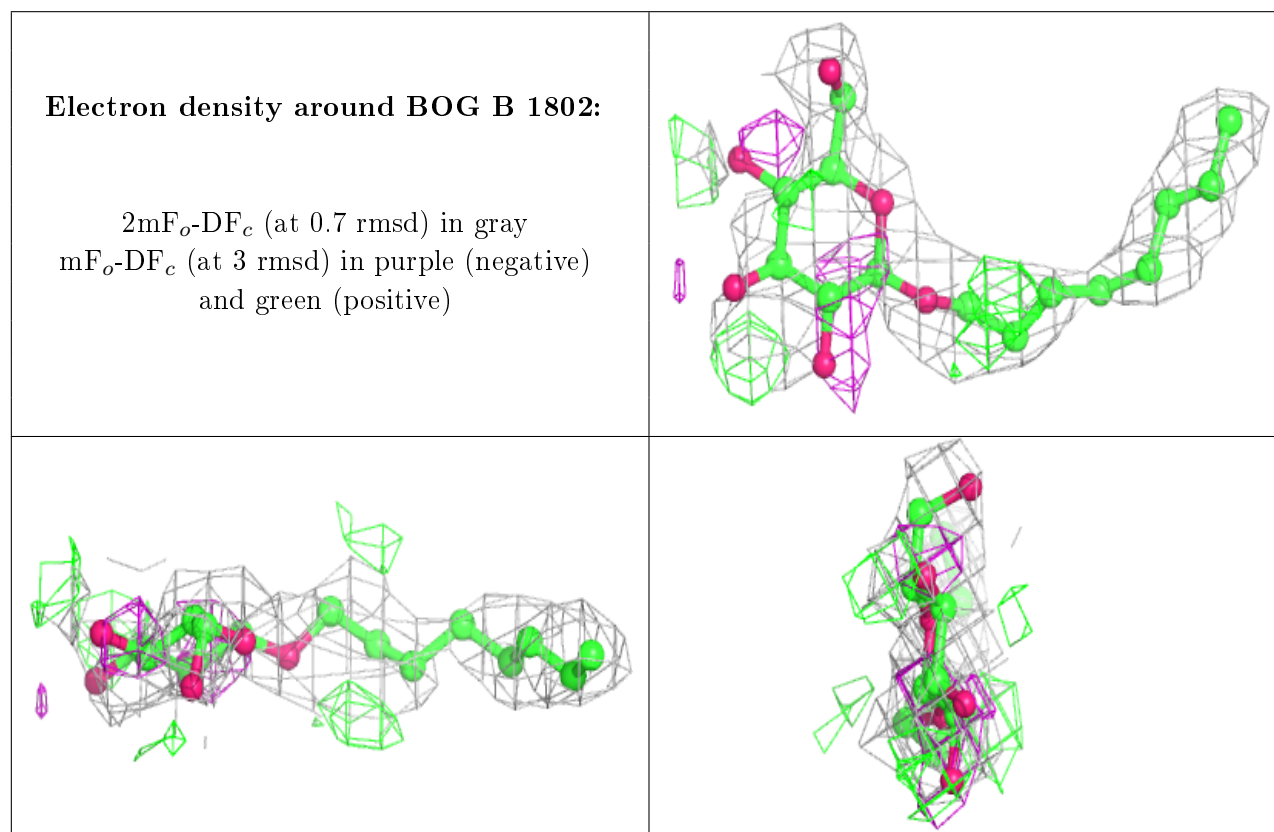
There are no monosaccharides in this entry.

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.

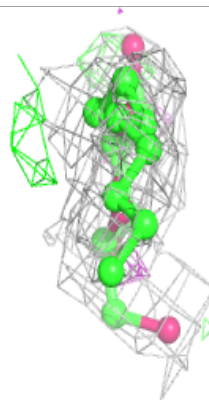
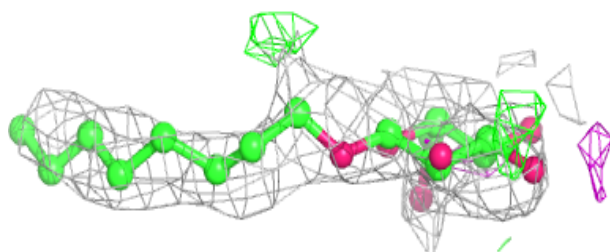
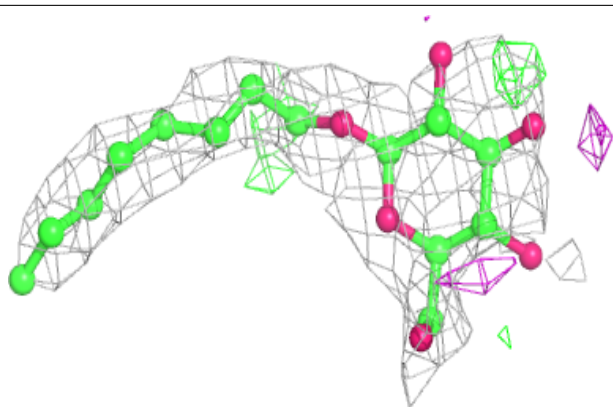
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	B	1662	14/15	0.38	0.74	63,84,96,96	0
2	NAG	A	662	14/15	0.48	0.47	63,84,96,96	0
2	NAG	A	661	14/15	0.67	0.31	50,59,64,78	0
2	NAG	B	672	14/15	0.69	0.29	32,38,65,76	0
3	BOG	B	1802	20/20	0.71	0.36	37,54,64,68	0
2	NAG	B	1661	14/15	0.73	0.28	50,59,64,78	0
2	NAG	A	681	14/15	0.77	0.27	31,36,42,42	0
3	BOG	A	802	20/20	0.78	0.29	37,54,64,68	0
2	NAG	A	1672	14/15	0.80	0.31	32,38,65,76	0
2	NAG	B	1681	14/15	0.80	0.23	31,36,42,42	0
3	BOG	A	801	20/20	0.83	0.35	37,63,68,68	0
2	NAG	B	1671	14/15	0.90	0.14	5,16,23,24	0
5	FLP	B	1701	18/18	0.92	0.19	17,22,33,47	0
2	NAG	A	671	14/15	0.92	0.16	5,16,23,24	0
5	FLP	A	701	18/18	0.94	0.20	17,22,33,47	0
4	HEM	A	601	43/43	0.94	0.16	15,22,49,65	0
4	HEM	B	601	43/43	0.95	0.15	15,22,49,65	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.

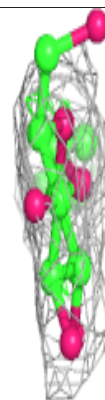
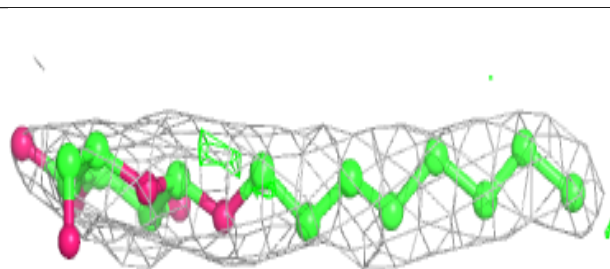
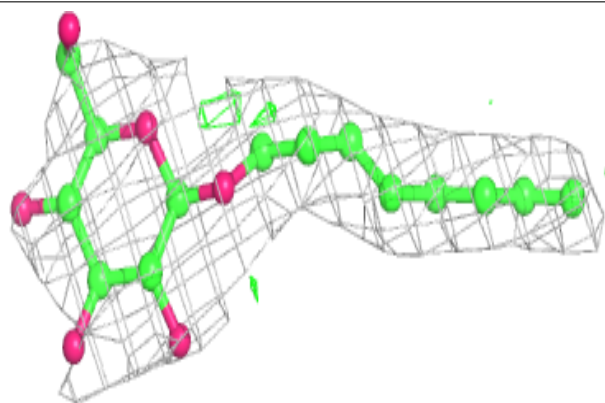


Electron density around BOG A 802:

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

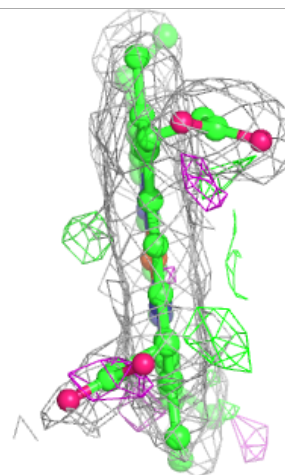
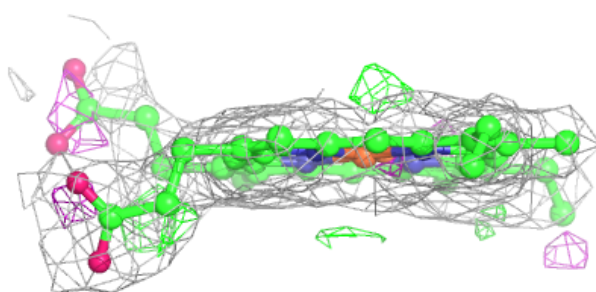
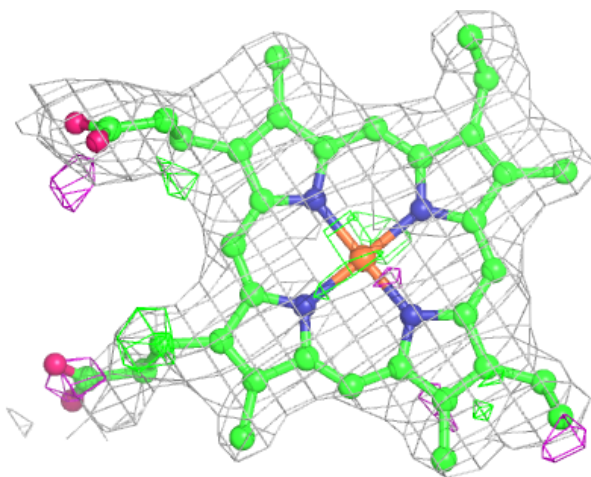
**Electron density around BOG A 801:**

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



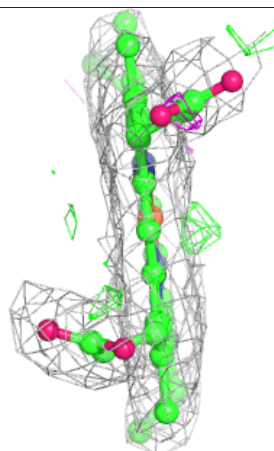
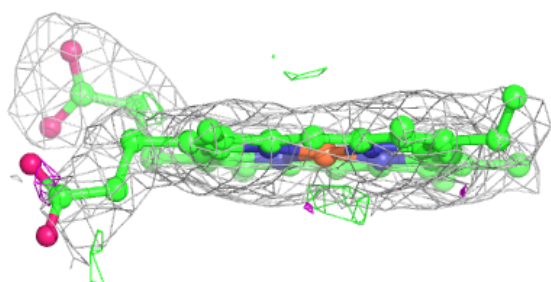
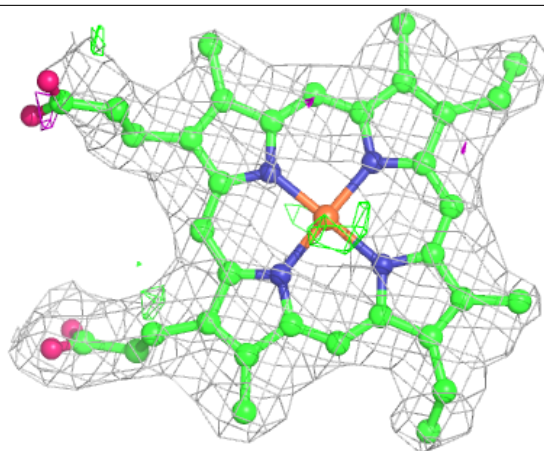
Electron density around HEM A 601:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.