



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 05:59 PM JST

PDB ID : 7C73 / pdb_00007c73
Title : Crystal structure of yak lactoperoxidase using data obtained from crystals soaked in MgCl₂ at 2.70 Å resolution
Authors : Singh, P.K.; Pandey, S.N.; Rani, C.; Ahmad, N.; Viswanathan, V.; Sharma, P.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2020-05-22
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 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	:	1.8.5 (274361), CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

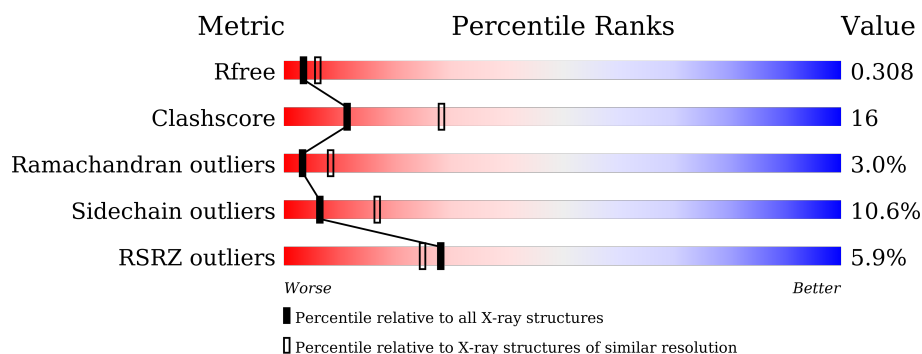
1 Overall quality at a glance

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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.

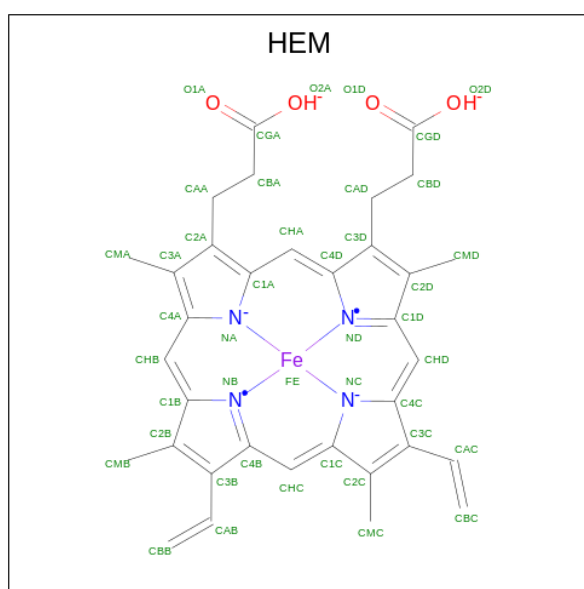
Mol	Chain	Length	Quality of chain
1	A	595	6% 62% 31% 6% .

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 Lactoperoxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	P	S	0	0	0
			4774	3037	847	863	1	26			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

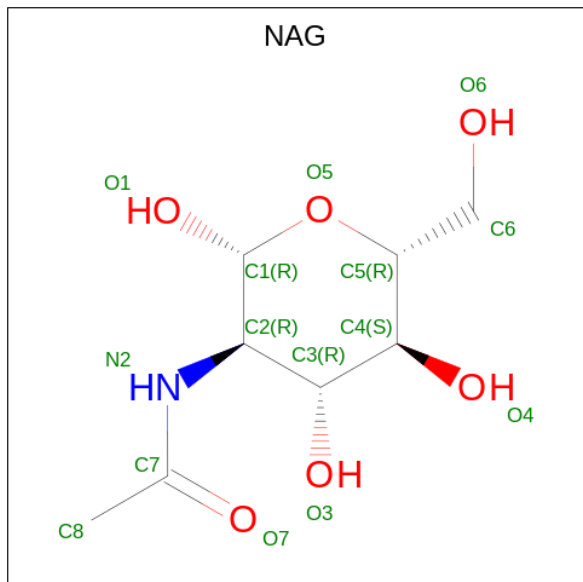


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Ca 2 2	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

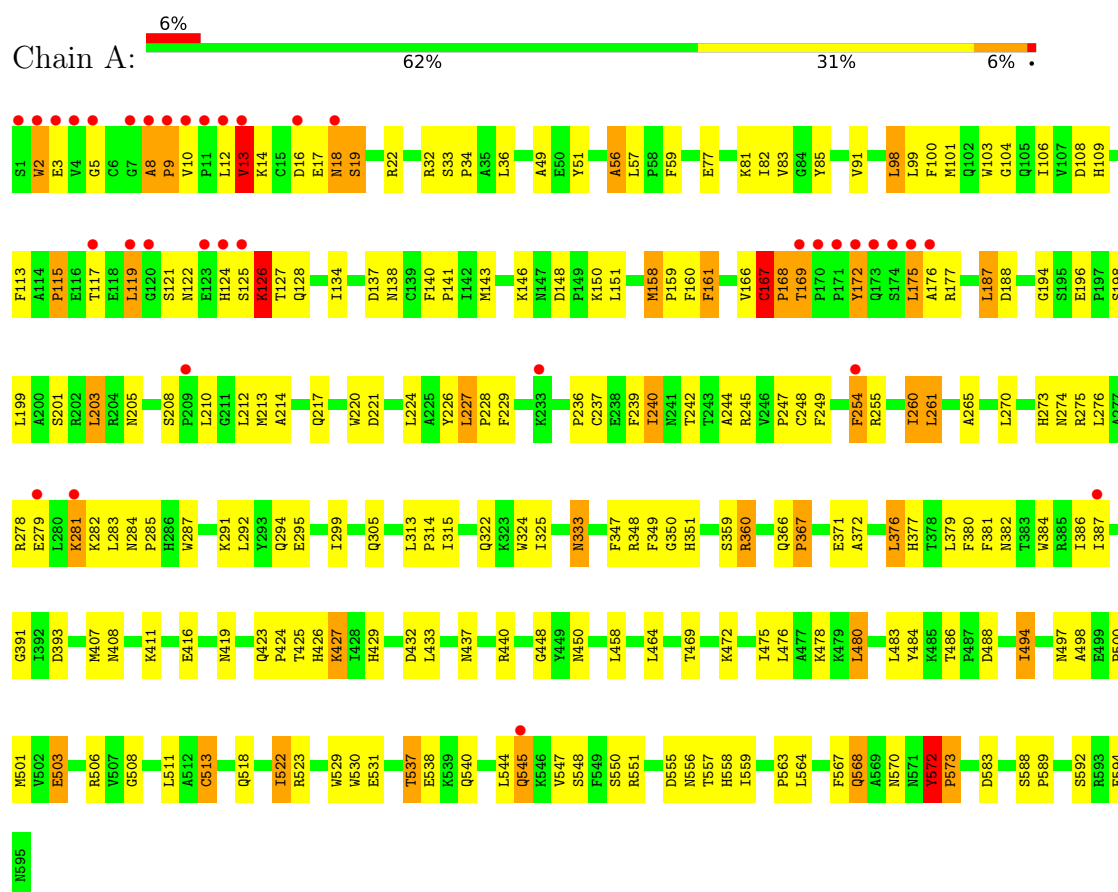
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	242	Total	O	0	0
			242	242		

3 Residue-property plots [i](#)

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

• Molecule 1: Lactoperoxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.88Å 79.93Å 75.05Å 90.00° 101.35° 90.00°	Depositor
Resolution (Å)	47.58 – 2.70 47.58 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.58-2.70) 97.6 (47.58-2.70)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.218 , 0.306 0.220 , 0.308	Depositor DCC
R_{free} test set	843 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.7	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	5103	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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: CA, NAG, HEM, SEP

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	1.01	0/4891	1.48	14/6634 (0.2%)

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	A	0	4

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	115	PRO	CB-CA-C	-6.57	102.98	111.39
1	A	254	PHE	CB-CA-C	6.03	121.30	109.72
1	A	167	CYS	CB-CA-C	5.80	121.60	110.17
1	A	194	GLY	CA-C-O	-5.69	117.68	122.29
1	A	126	LYS	CA-C-N	5.51	128.13	120.63
1	A	126	LYS	C-N-CA	5.51	128.13	120.63
1	A	34	PRO	N-CA-C	5.39	120.84	113.84
1	A	159	PRO	CB-CA-C	-5.39	104.50	111.39
1	A	408	ASN	CB-CA-C	5.37	118.41	110.14
1	A	83	VAL	CA-C-N	5.25	125.33	120.34
1	A	83	VAL	C-N-CA	5.25	125.33	120.34
1	A	503	GLU	CB-CG-CD	5.09	121.25	112.60
1	A	448	GLY	CA-C-N	5.01	128.34	120.82
1	A	448	GLY	C-N-CA	5.01	128.34	120.82

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	VAL	Peptide
1	A	172	TYR	Peptide
1	A	2	TRP	Peptide
1	A	572	TYR	Peptide

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	4774	0	4688	151	0
2	A	43	0	30	5	0
3	A	2	0	0	0	0
4	A	42	0	39	4	0
5	A	242	0	0	17	0
All	All	5103	0	4757	156	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 16.

All (156) 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:196:GLU:HB3	1:A:198:SEP:O1P	1.67	0.94
1:A:294:GLN:NE2	5:A:701:HOH:O	2.13	0.82
1:A:8:ALA:O	1:A:10:VAL:N	2.20	0.74
1:A:260:ILE:HD11	1:A:386:ILE:HG13	1.71	0.71
1:A:158:MET:HE1	1:A:432:ASP:H	1.55	0.70
2:A:601:HEM:HMB1	2:A:601:HEM:HBB2	1.73	0.70
1:A:196:GLU:CB	1:A:198:SEP:O1P	2.41	0.69
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.75	0.69
4:A:604:NAG:H3	5:A:712:HOH:O	1.91	0.68
1:A:18:ASN:O	1:A:19:SER:C	2.39	0.66
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.30	0.66
1:A:8:ALA:CB	1:A:9:PRO:HD3	2.27	0.65
1:A:205:ASN:HD22	1:A:212:LEU:HD12	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:PHE:HD1	5:A:829:HOH:O	1.80	0.65
1:A:167:CYS:HB2	1:A:168:PRO:CD	2.26	0.65
1:A:229:PHE:CD1	1:A:247:PRO:HG2	2.30	0.65
4:A:604:NAG:C3	5:A:712:HOH:O	2.44	0.65
1:A:572:TYR:CD2	1:A:573:PRO:HD3	2.32	0.65
1:A:167:CYS:HB2	1:A:168:PRO:HD3	1.79	0.64
1:A:137:ASP:O	5:A:702:HOH:O	2.15	0.64
1:A:167:CYS:CB	1:A:168:PRO:HD3	2.27	0.64
1:A:325:ILE:HG22	5:A:704:HOH:O	1.97	0.64
1:A:140:PHE:O	1:A:160:PHE:HB3	1.98	0.63
1:A:199:LEU:HD22	1:A:254:PHE:CZ	2.33	0.62
1:A:227:LEU:HD22	1:A:270:LEU:HD22	1.81	0.62
1:A:220:TRP:HD1	5:A:870:HOH:O	1.81	0.61
1:A:450:ASN:ND2	1:A:488:ASP:OD1	2.26	0.60
1:A:124:HIS:O	1:A:127:THR:N	2.35	0.60
1:A:226:TYR:OH	1:A:391:GLY:HA2	2.02	0.59
1:A:550:SER:OG	1:A:563:PRO:O	2.13	0.59
1:A:429:HIS:NE2	5:A:707:HOH:O	2.32	0.59
1:A:9:PRO:HG2	1:A:167:CYS:O	2.04	0.58
1:A:351:HIS:CE1	1:A:433:LEU:HD21	2.39	0.58
1:A:393:ASP:OD1	5:A:703:HOH:O	2.17	0.58
1:A:8:ALA:HB3	1:A:9:PRO:CD	2.34	0.58
1:A:281:LYS:HD3	1:A:285:PRO:HA	1.85	0.57
1:A:426:HIS:O	1:A:427:LYS:HG2	2.04	0.57
1:A:3:GLU:HG2	1:A:175:LEU:HD13	1.86	0.57
1:A:544:LEU:O	1:A:547:VAL:HG22	2.04	0.57
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.87	0.57
1:A:494:ILE:C	1:A:494:ILE:HD13	2.30	0.57
1:A:518:GLN:O	1:A:522:ILE:HG23	2.05	0.56
1:A:217:GLN:HB2	5:A:897:HOH:O	2.05	0.55
1:A:237:CYS:HA	1:A:381:PHE:O	2.06	0.55
1:A:476:LEU:HD21	1:A:498:ALA:HB1	1.88	0.55
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.41	0.55
1:A:9:PRO:CD	1:A:167:CYS:O	2.55	0.55
1:A:423:GLN:HE21	1:A:423:GLN:HA	1.72	0.55
1:A:260:ILE:HG23	1:A:261:LEU:HD13	1.88	0.54
1:A:167:CYS:CB	1:A:168:PRO:CD	2.86	0.54
1:A:545:GLN:HE21	1:A:545:GLN:H	1.55	0.54
1:A:260:ILE:HG13	1:A:386:ILE:HD11	1.90	0.54
1:A:333:ASN:C	1:A:333:ASN:ND2	2.65	0.54
1:A:12:LEU:O	1:A:13:VAL:O	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:HB2	1:A:249:PHE:CD1	2.43	0.54
1:A:8:ALA:CB	1:A:9:PRO:CD	2.86	0.53
1:A:113:PHE:CE2	1:A:115:PRO:HG3	2.42	0.53
1:A:551:ARG:HD3	1:A:583:ASP:O	2.08	0.53
1:A:333:ASN:ND2	1:A:333:ASN:O	2.39	0.53
1:A:175:LEU:HG	1:A:176:ALA:N	2.24	0.53
1:A:295:GLU:O	1:A:299:ILE:HG13	2.08	0.53
1:A:548:SER:OG	1:A:551:ARG:HB2	2.09	0.52
1:A:82:ILE:HD11	1:A:483:LEU:HD12	1.92	0.52
1:A:472:LYS:HD2	1:A:500:PRO:HG2	1.90	0.52
1:A:124:HIS:O	1:A:126:LYS:N	2.42	0.52
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.08	0.52
1:A:572:TYR:HD2	1:A:573:PRO:HD3	1.73	0.52
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.45	0.51
1:A:522:ILE:HD12	1:A:522:ILE:C	2.35	0.51
1:A:9:PRO:CG	1:A:167:CYS:O	2.59	0.51
1:A:203:LEU:HB3	1:A:213:MET:HE1	1.91	0.51
1:A:158:MET:HE1	1:A:432:ASP:N	2.24	0.51
1:A:494:ILE:HD13	1:A:494:ILE:O	2.10	0.51
1:A:221:ASP:HB2	1:A:226:TYR:CE1	2.47	0.50
1:A:384:TRP:CZ2	4:A:605:NAG:O7	2.64	0.50
1:A:287:TRP:HA	5:A:802:HOH:O	2.11	0.50
1:A:242:THR:O	1:A:245:ARG:HG2	2.12	0.49
1:A:588:SER:N	1:A:589:PRO:HD2	2.28	0.49
1:A:376:LEU:HG	5:A:864:HOH:O	2.11	0.49
1:A:187:LEU:O	1:A:305:GLN:NE2	2.45	0.49
1:A:220:TRP:CD1	5:A:870:HOH:O	2.61	0.49
1:A:349:PHE:CB	1:A:497:ASN:HD21	2.25	0.49
1:A:360:ARG:NH1	1:A:371:GLU:O	2.46	0.49
1:A:150:LYS:NZ	1:A:419:ASN:O	2.46	0.48
1:A:161:PHE:CD1	1:A:161:PHE:N	2.81	0.48
1:A:376:LEU:HB3	1:A:416:GLU:HB3	1.96	0.48
1:A:366:GLN:O	1:A:367:PRO:C	2.56	0.48
1:A:168:PRO:HB2	1:A:169:THR:H	1.51	0.48
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.49	0.48
1:A:99:LEU:HG	1:A:567:PHE:CE1	2.49	0.47
1:A:484:TYR:C	1:A:486:THR:H	2.22	0.47
1:A:508:GLY:HA3	5:A:777:HOH:O	2.14	0.47
1:A:359:SER:HA	1:A:372:ALA:O	2.13	0.47
1:A:98:LEU:HD22	1:A:101:MET:HE3	1.96	0.47
1:A:108:ASP:HA	1:A:347:PHE:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ILE:HD13	1:A:480:LEU:HD13	1.96	0.47
1:A:275:ARG:HD2	1:A:555:ASP:HB3	1.97	0.47
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.51	0.46
2:A:601:HEM:HBC2	2:A:601:HEM:CMC	2.45	0.46
1:A:224:LEU:HD11	1:A:558:HIS:CE1	2.49	0.46
1:A:325:ILE:O	5:A:704:HOH:O	2.20	0.46
1:A:537:THR:HG23	1:A:540:GLN:OE1	2.16	0.46
1:A:122:ASN:O	1:A:122:ASN:ND2	2.48	0.46
1:A:273:HIS:HD2	1:A:274:ASN:OD1	1.99	0.46
1:A:568:GLN:O	1:A:570:ASN:ND2	2.48	0.45
1:A:101:MET:C	1:A:101:MET:SD	3.00	0.45
1:A:141:PRO:HG2	1:A:143:MET:HE3	1.99	0.45
1:A:203:LEU:HB3	1:A:213:MET:CE	2.47	0.45
1:A:324:TRP:CE2	1:A:513:CYS:HA	2.52	0.45
1:A:188:ASP:N	1:A:188:ASP:OD1	2.49	0.45
1:A:239:PHE:CZ	1:A:427:LYS:HB2	2.52	0.44
1:A:347:PHE:HB3	2:A:601:HEM:HMD3	2.00	0.44
1:A:450:ASN:HB2	5:A:830:HOH:O	2.18	0.44
1:A:348:ARG:C	1:A:350:GLY:N	2.74	0.44
1:A:349:PHE:CD1	1:A:349:PHE:C	2.96	0.44
1:A:160:PHE:CZ	1:A:440:ARG:NH1	2.85	0.44
1:A:187:LEU:HD23	1:A:187:LEU:HA	1.81	0.43
1:A:260:ILE:CD1	1:A:386:ILE:HG13	2.44	0.43
1:A:494:ILE:C	1:A:494:ILE:CD1	2.90	0.43
1:A:106:ILE:HD11	1:A:265:ALA:HB3	1.99	0.43
1:A:117:THR:OG1	1:A:138:ASN:ND2	2.52	0.43
1:A:214:ALA:O	1:A:228:PRO:CG	2.66	0.43
1:A:8:ALA:O	1:A:9:PRO:C	2.61	0.43
1:A:106:ILE:HD11	1:A:265:ALA:CB	2.48	0.43
1:A:501:MET:SD	1:A:506:ARG:HA	2.59	0.43
1:A:237:CYS:O	1:A:240:ILE:HD13	2.19	0.43
1:A:347:PHE:HB3	2:A:601:HEM:CMD	2.49	0.42
1:A:458:LEU:HD23	5:A:815:HOH:O	2.19	0.42
1:A:556:ASN:O	1:A:557:THR:HG23	2.19	0.42
1:A:407:MET:HB3	1:A:501:MET:CE	2.49	0.42
1:A:244:ALA:HB2	4:A:605:NAG:O5	2.20	0.42
1:A:313:LEU:N	1:A:314:PRO:CD	2.82	0.42
1:A:12:LEU:O	1:A:13:VAL:C	2.62	0.42
1:A:236:PRO:HD2	1:A:248:CYS:SG	2.59	0.42
1:A:32:ARG:HD2	1:A:333:ASN:HD21	1.83	0.42
1:A:109:HIS:HA	1:A:255:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:MET:HE3	1:A:101:MET:HB3	1.93	0.41
1:A:119:LEU:HD23	1:A:119:LEU:O	2.20	0.41
1:A:100:PHE:HE1	1:A:315:ILE:HG13	1.85	0.41
1:A:379:LEU:HA	1:A:382:ASN:CB	2.50	0.41
1:A:592:SER:OG	1:A:594:GLU:OE2	2.39	0.41
1:A:229:PHE:CE1	1:A:247:PRO:HD2	2.55	0.41
1:A:148:ASP:O	1:A:151:LEU:HB2	2.21	0.41
1:A:126:LYS:H	1:A:126:LYS:HG3	1.71	0.41
1:A:77:GLU:HG2	1:A:81:LYS:HD2	2.03	0.41
1:A:199:LEU:HD22	1:A:254:PHE:HZ	1.85	0.41
1:A:284:ASN:N	1:A:285:PRO:HD3	2.35	0.41
1:A:291:LYS:O	1:A:295:GLU:HB2	2.21	0.41
1:A:103:TRP:O	1:A:104:GLY:C	2.64	0.41
1:A:49:ALA:HB1	1:A:51:TYR:CE2	2.56	0.40
1:A:56:ALA:HB1	1:A:177:ARG:HD3	2.02	0.40
1:A:138:ASN:O	1:A:161:PHE:HA	2.21	0.40
1:A:351:HIS:CD2	1:A:433:LEU:HD21	2.56	0.40
1:A:480:LEU:HD12	1:A:480:LEU:HA	1.90	0.40
1:A:85:TYR:CD1	1:A:411:LYS:HA	2.57	0.40
1:A:210:LEU:O	1:A:292:LEU:HD23	2.21	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	592/595 (100%)	518 (88%)	56 (10%)	18 (3%)	3 8

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA

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Mol	Chain	Res	Type
1	A	13	VAL
1	A	18	ASN
1	A	125	SER
1	A	167	CYS
1	A	168	PRO
1	A	169	THR
1	A	572	TYR
1	A	2	TRP
1	A	9	PRO
1	A	573	PRO
1	A	17	GLU
1	A	424	PRO
1	A	19	SER
1	A	56	ALA
1	A	14	LYS
1	A	367	PRO
1	A	5	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	517/517 (100%)	462 (89%)	55 (11%)	6 17

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	16	ASP
1	A	22	ARG
1	A	33	SER
1	A	36	LEU
1	A	57	LEU
1	A	91	VAL
1	A	98	LEU
1	A	119	LEU

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Mol	Chain	Res	Type
1	A	121	SER
1	A	126	LYS
1	A	128	GLN
1	A	134	ILE
1	A	146	LYS
1	A	158	MET
1	A	161	PHE
1	A	172	TYR
1	A	175	LEU
1	A	187	LEU
1	A	201	SER
1	A	203	LEU
1	A	208	SER
1	A	227	LEU
1	A	240	ILE
1	A	260	ILE
1	A	261	LEU
1	A	276	LEU
1	A	278	ARG
1	A	279	GLU
1	A	281	LYS
1	A	282	LYS
1	A	283	LEU
1	A	322	GLN
1	A	333	ASN
1	A	360	ARG
1	A	376	LEU
1	A	387	ILE
1	A	425	THR
1	A	427	LYS
1	A	464	LEU
1	A	469	THR
1	A	475	ILE
1	A	478	LYS
1	A	480	LEU
1	A	494	ILE
1	A	503	GLU
1	A	511	LEU
1	A	513	CYS
1	A	522	ILE
1	A	537	THR
1	A	538	GLU

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Mol	Chain	Res	Type
1	A	545	GLN
1	A	559	ILE
1	A	564	LEU
1	A	568	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	122	ASN
1	A	138	ASN
1	A	154	GLN
1	A	273	HIS
1	A	322	GLN
1	A	329	GLN
1	A	333	ASN
1	A	408	ASN
1	A	423	GLN
1	A	497	ASN
1	A	545	GLN
1	A	568	GLN
1	A	570	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	SEP	A	198	1	8,9,10	0.69	0	8,12,14	0.96	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
1	SEP	A	198	1	-	2/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	198	SEP	N-CA-CB-OG
1	A	198	SEP	CA-CB-OG-P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
4	NAG	A	603	-	14,14,15	0.73	0	17,19,21	2.03	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	601	5,1	50,50,50	1.77	10 (20%)	66,82,82	1.66	14 (21%)
4	NAG	A	604	1	14,14,15	0.33	0	17,19,21	0.69	0
4	NAG	A	605	1	14,14,15	0.44	0	17,19,21	1.03	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
4	NAG	A	603	-	-	1/6/23/26	0/1/1/1
2	HEM	A	601	5,1	-	4/14/54/54	-
4	NAG	A	604	1	-	2/6/23/26	0/1/1/1
4	NAG	A	605	1	-	2/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	FE-NB	5.84	2.13	1.94
2	A	601	HEM	FE-NC	4.25	2.09	1.95
2	A	601	HEM	C1B-NB	-3.98	1.33	1.40
2	A	601	HEM	C4D-ND	-3.33	1.34	1.40
2	A	601	HEM	FE-ND	-2.56	1.86	1.94
2	A	601	HEM	CMB-C2B	2.28	1.55	1.50
2	A	601	HEM	C1D-ND	-2.25	1.34	1.38
2	A	601	HEM	C1D-C2D	2.18	1.48	1.44
2	A	601	HEM	CMD-C2D	2.04	1.55	1.50
2	A	601	HEM	C3C-C4C	-2.03	1.42	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	CHA-C4D-ND	4.52	129.94	124.37
2	A	601	HEM	CBA-CAA-C2A	-4.36	100.50	112.63
4	A	603	NAG	O5-C1-C2	-4.30	104.49	111.29
4	A	603	NAG	C1-C2-N2	3.98	117.28	110.49
2	A	601	HEM	CHD-C1D-ND	3.69	128.43	124.42
2	A	601	HEM	C1B-NB-C4B	3.47	108.66	105.07
2	A	601	HEM	CHA-C4D-C3D	-3.11	119.49	125.33
4	A	603	NAG	O3-C3-C2	-2.93	103.40	109.47
4	A	603	NAG	O5-C5-C6	-2.87	102.71	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	CHC-C4B-NB	2.71	127.36	124.42
2	A	601	HEM	CHB-C1B-NB	2.70	127.70	124.37
2	A	601	HEM	CBD-CAD-C3D	-2.67	105.20	112.63
2	A	601	HEM	C4D-ND-C1D	2.58	107.74	105.07
2	A	601	HEM	CHD-C1D-C2D	-2.56	120.98	124.98
2	A	601	HEM	C4C-NC-C1C	2.45	107.75	105.35
2	A	601	HEM	C1D-C2D-C3D	-2.26	104.58	106.96
2	A	601	HEM	CAD-CBD-CGD	-2.21	108.85	113.60
4	A	603	NAG	C1-O5-C5	-2.12	109.31	112.19
2	A	601	HEM	CHB-C1B-C2B	-2.09	120.94	126.73

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	604	NAG	C4-C5-C6-O6
4	A	603	NAG	C8-C7-N2-C2
4	A	605	NAG	O5-C5-C6-O6
4	A	604	NAG	O5-C5-C6-O6
2	A	601	HEM	CAD-CBD-CGD-O2D
2	A	601	HEM	CAD-CBD-CGD-O1D
2	A	601	HEM	CAA-CBA-CGA-O2A
2	A	601	HEM	CAA-CBA-CGA-O1A
4	A	605	NAG	C4-C5-C6-O6

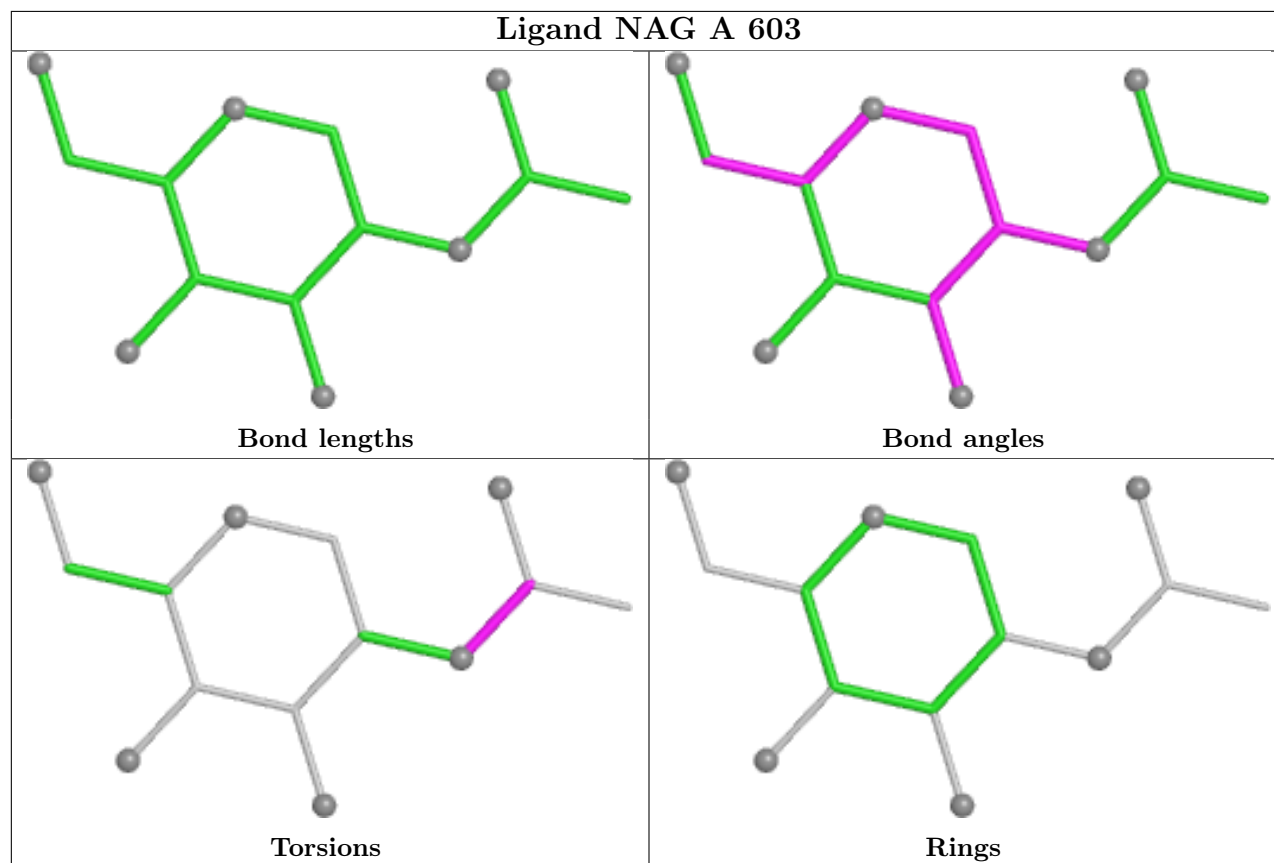
There are no ring outliers.

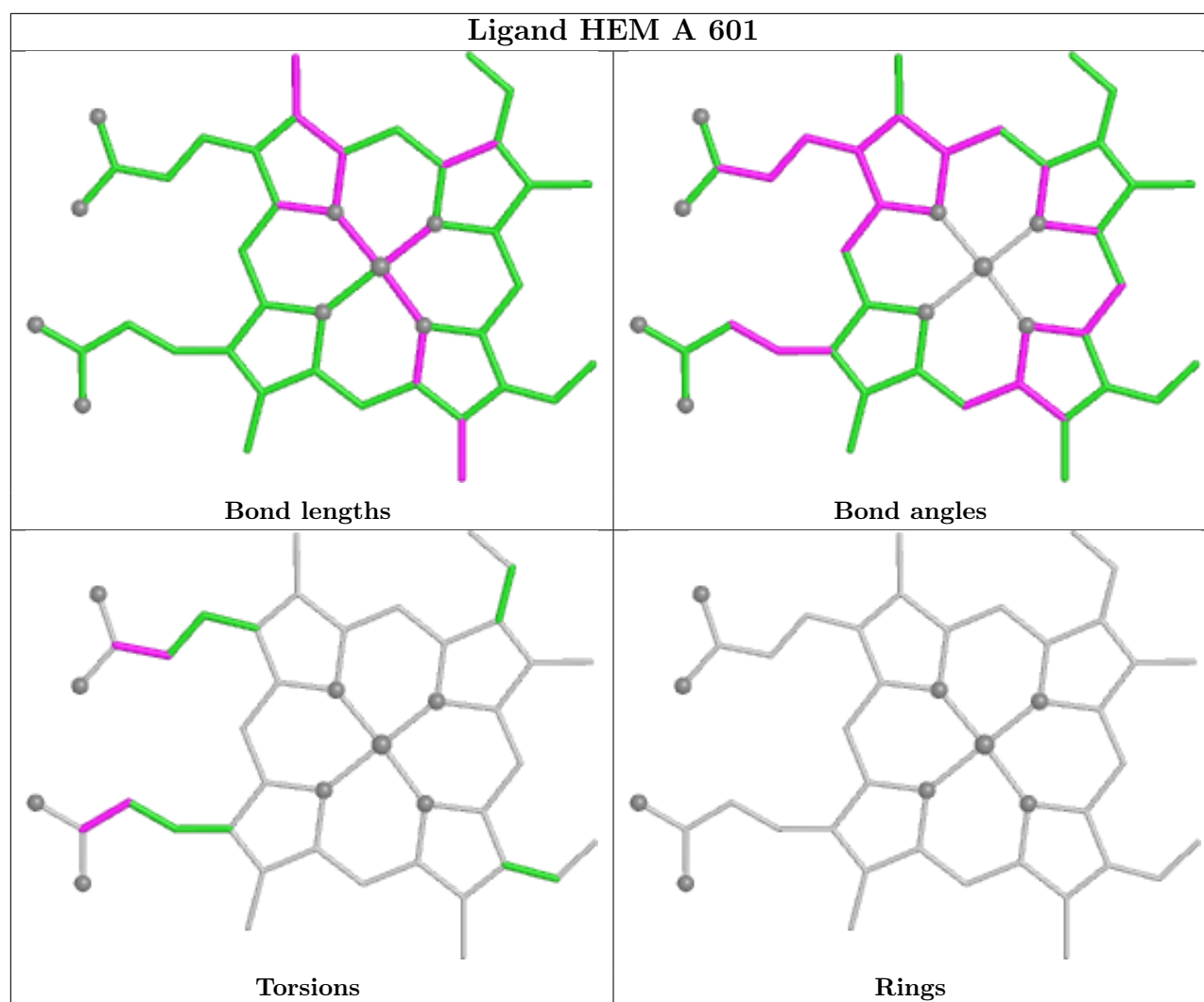
3 monomers are involved in 9 short contacts:

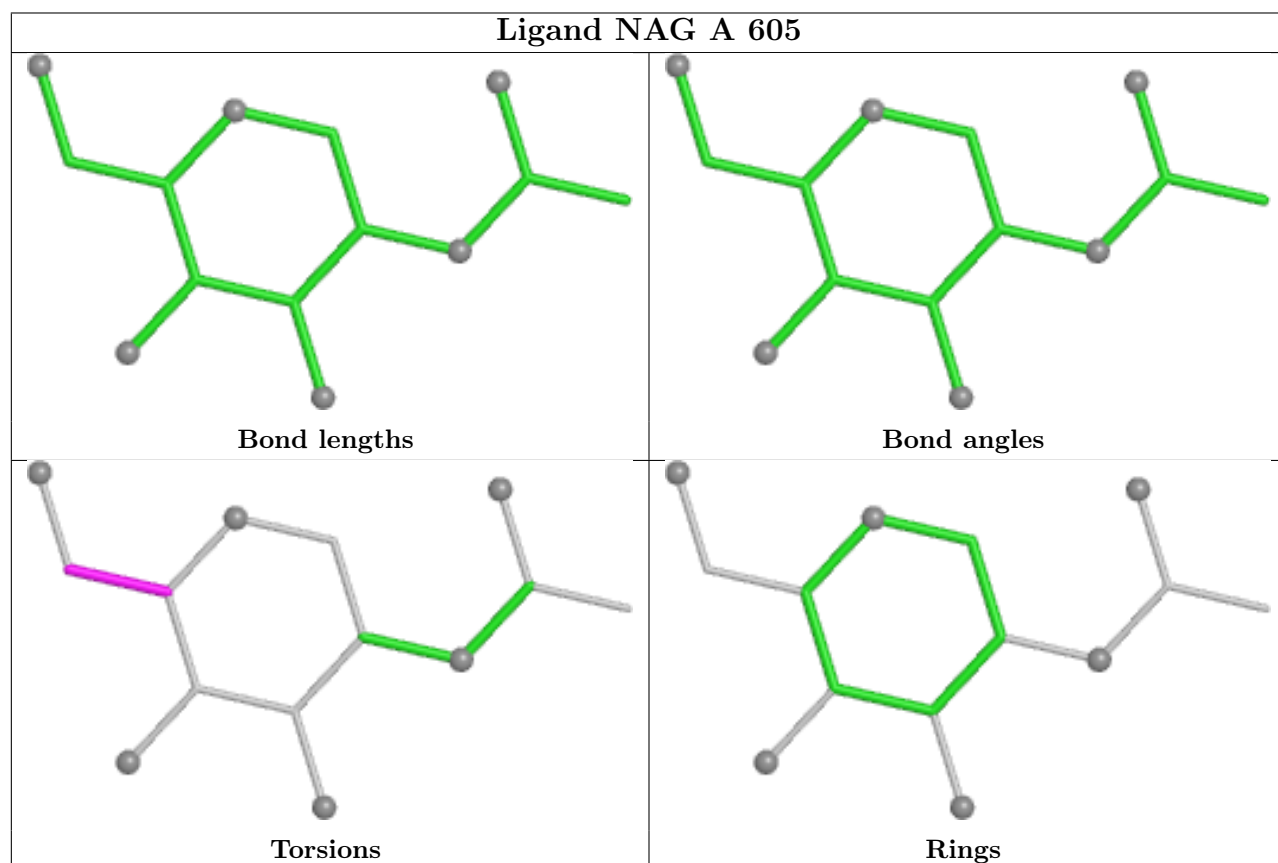
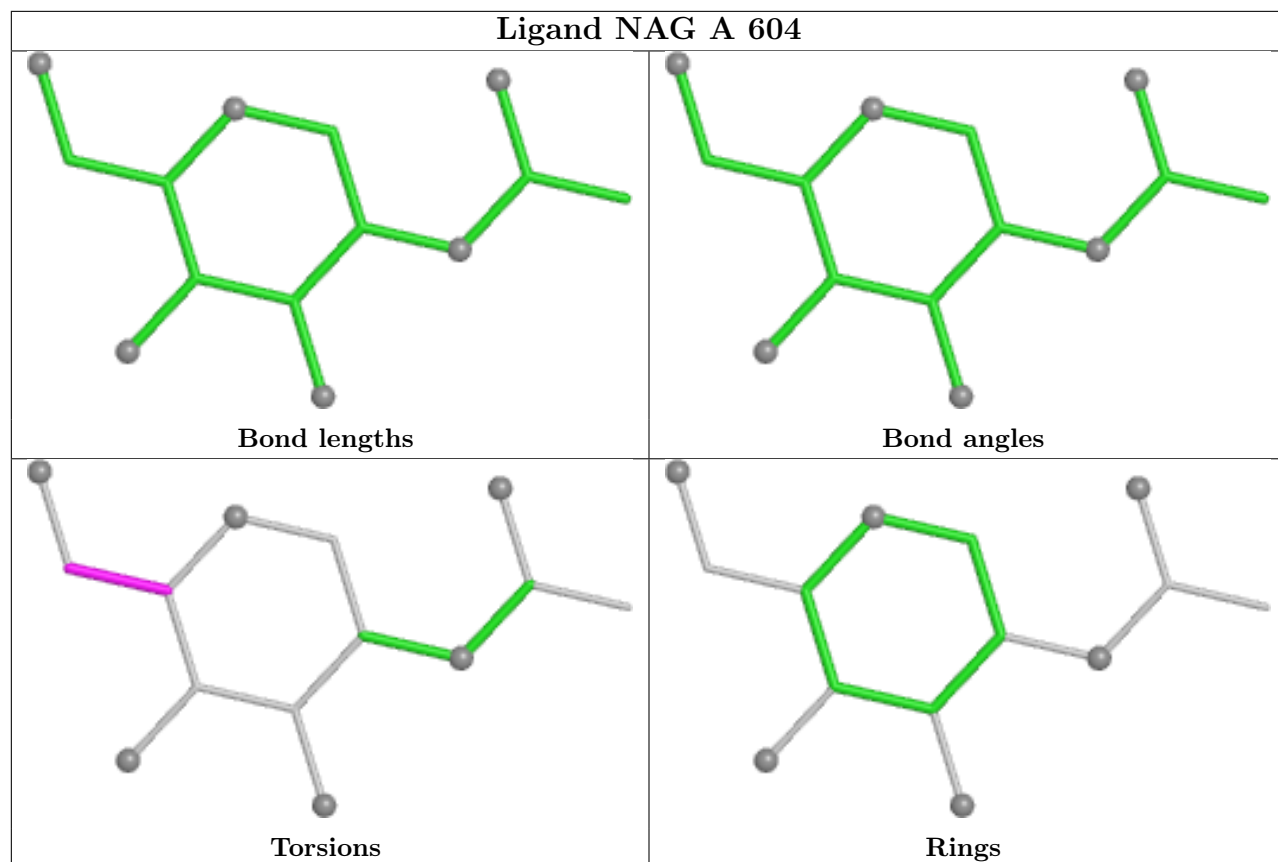
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	5	0
4	A	604	NAG	2	0
4	A	605	NAG	2	0

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

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	594/595 (99%)	0.28	35 (5%) 28 25	14, 33, 90, 138	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	VAL	4.6
1	A	172	TYR	4.0
1	A	170	PRO	3.5
1	A	2	TRP	3.4
1	A	1	SER	3.3
1	A	16	ASP	3.3
1	A	9	PRO	3.2
1	A	119	LEU	3.2
1	A	7	GLY	3.2
1	A	173	GLN	3.1
1	A	171	PRO	3.1
1	A	8	ALA	3.1
1	A	4	VAL	2.8
1	A	174	SER	2.7
1	A	175	LEU	2.7
1	A	11	PRO	2.7
1	A	117	THR	2.6
1	A	169	THR	2.6
1	A	125	SER	2.4
1	A	123	GLU	2.3
1	A	176	ALA	2.3
1	A	18	ASN	2.3
1	A	387	ILE	2.3
1	A	124	HIS	2.3
1	A	279	GLU	2.3
1	A	209	PRO	2.3
1	A	545	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	281	LYS	2.2
1	A	254	PHE	2.2
1	A	5	GLY	2.2
1	A	233	LYS	2.2
1	A	12	LEU	2.2
1	A	10	VAL	2.2
1	A	120	GLY	2.2
1	A	3	GLU	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	A	198	10/11	0.81	0.15	40,52,81,82	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

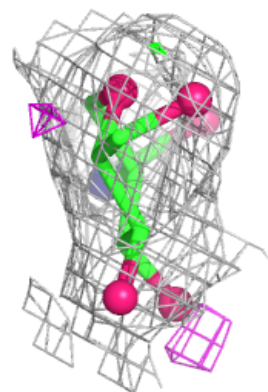
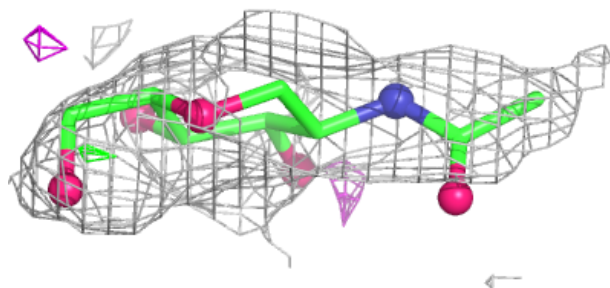
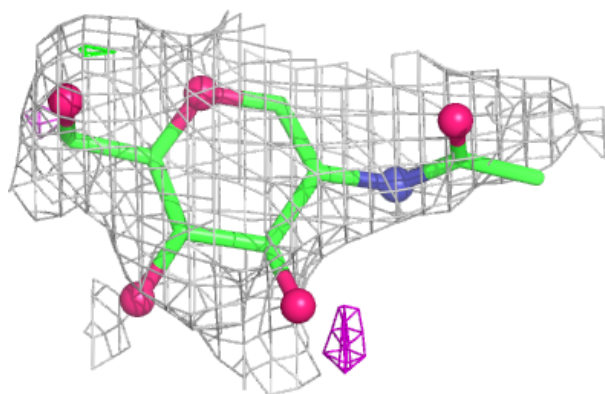
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	604	14/15	0.64	0.18	67,72,75,79	0
4	NAG	A	605	14/15	0.68	0.20	55,61,74,80	0
4	NAG	A	603	14/15	0.79	0.13	48,50,53,56	0
3	CA	A	602	1/1	0.92	0.06	20,20,20,20	0
2	HEM	A	601	43/43	0.96	0.08	20,25,26,27	0
3	CA	A	606	1/1	0.99	0.10	23,23,23,23	0

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.

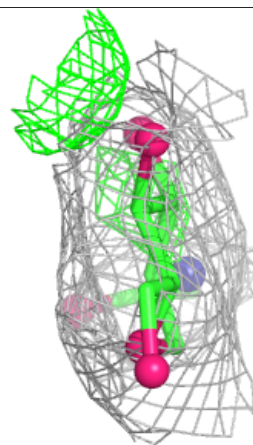
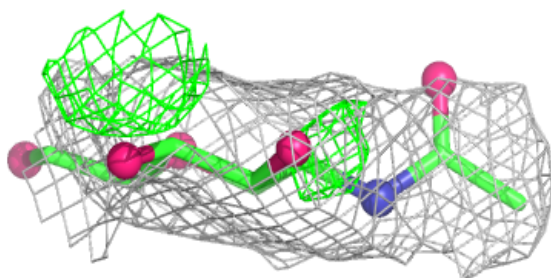
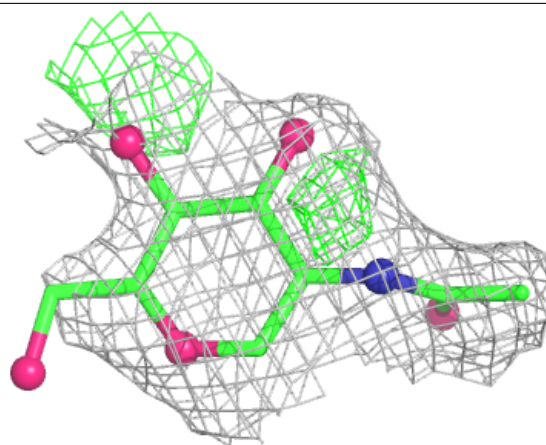
Electron density around NAG A 604:

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



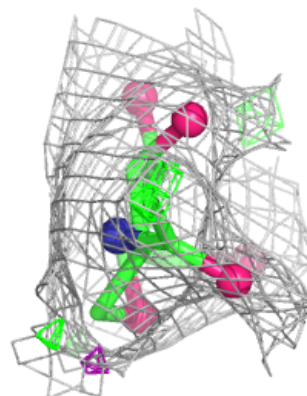
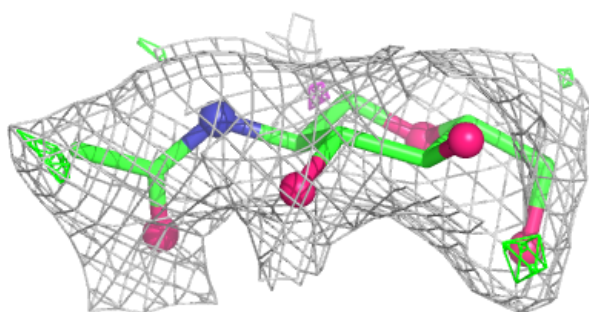
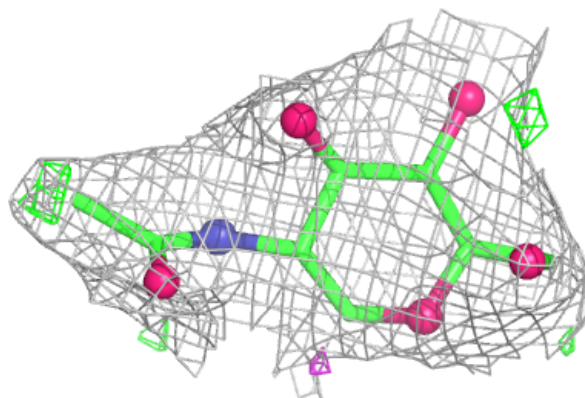
Electron density around NAG A 605:

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



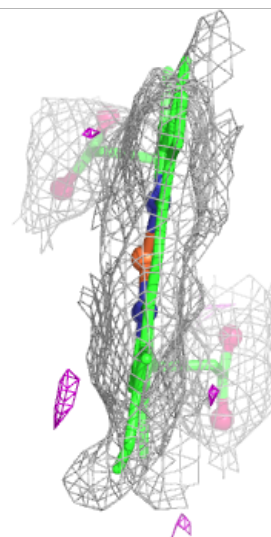
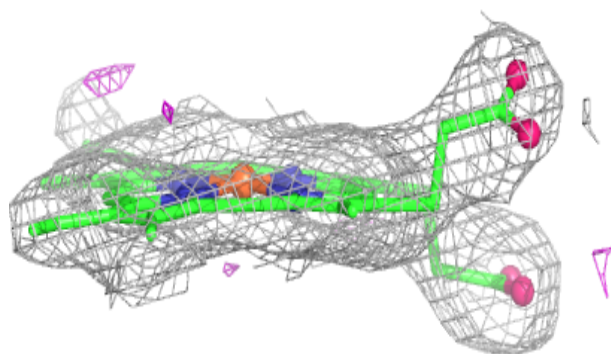
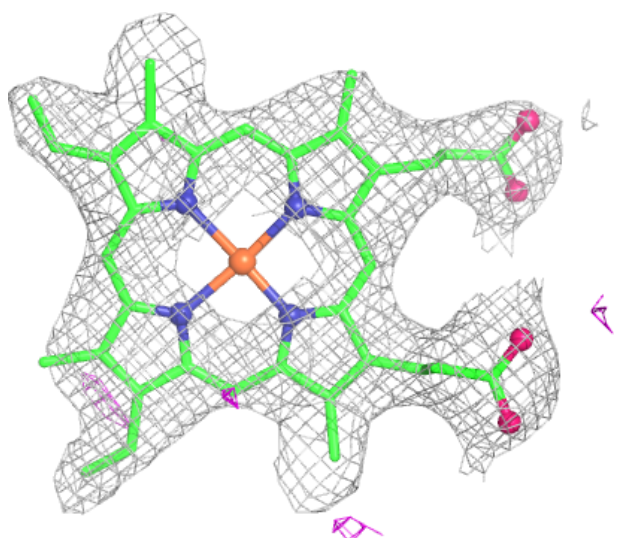
Electron density around NAG A 603:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.