



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:34 AM UTC

PDB ID : 1EBV / pdb_00001ebv
Title : OVINE PGHS-1 COMPLEXED WITH SALICYL HYDROXAMIC ACID
Authors : Loll, P.J.; Sharkey, C.T.; O'Connor, S.J.; Fitzgerald, D.J.
Deposited on : 2000-01-24
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) 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

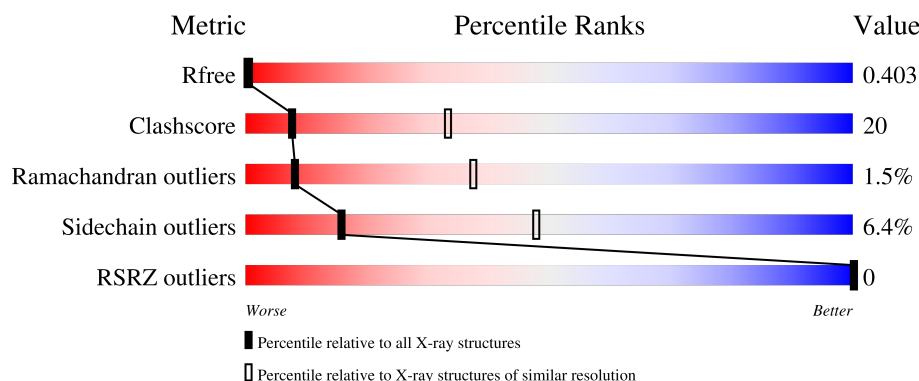
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	551	
2	B	2	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4594 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	0	0
			4481	2905	758	790	28			

There are 2 discrepancies between the modelled and reference sequences:

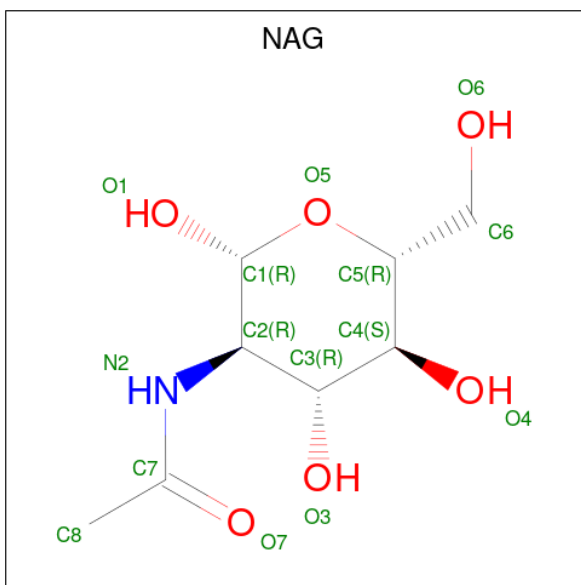
Chain	Residue	Modelled	Actual	Comment	Reference
A	92	LEU	MET	conflict	UNP P05979
A	530	OAS	SER	modified residue	UNP P05979

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



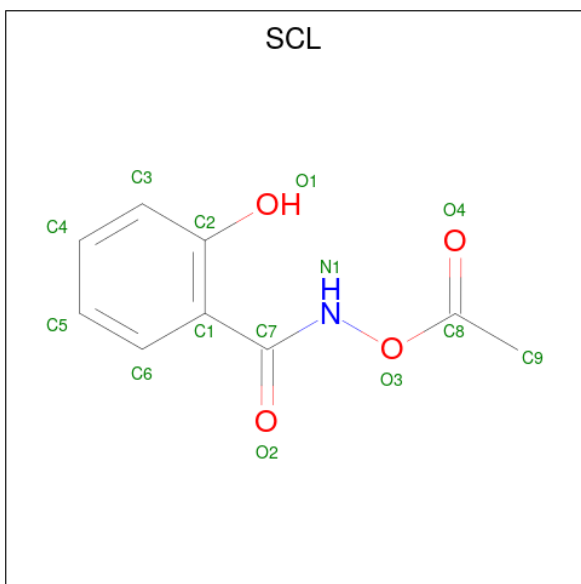
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



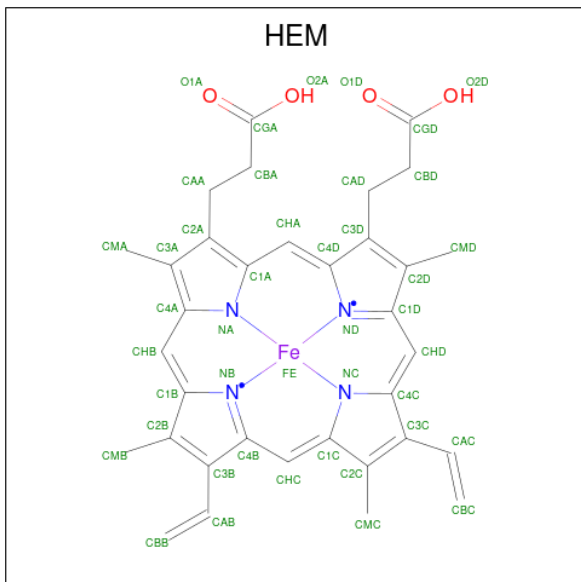
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is ACETIC ACID SALICYLOYL-AMINO-ESTER (CCD ID: SCL) (formula: $C_9H_9NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	9	1	4		

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

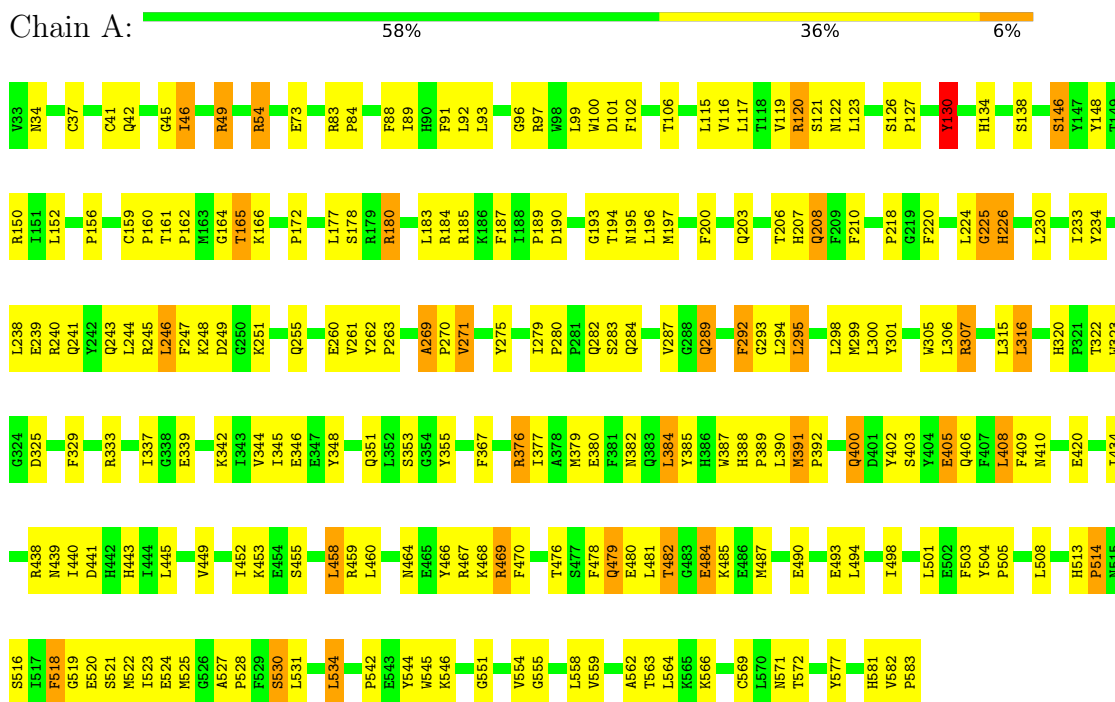


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.87Å 207.46Å 221.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.50 – 3.20 23.50 – 3.20	Depositor EDS
% Data completeness (in resolution range)	81.8 (23.50-3.20) 67.3 (23.50-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.33 (at 3.10Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.218 , 0.248 0.400 , 0.403	Depositor DCC
R_{free} test set	2813 reflections (8.03%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 23.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.57	EDS
Total number of atoms	4594	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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: SCL, HEM, NAG, OAS

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	0.48	0/4609	1.00	24/6253 (0.4%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	TYR	N-CA-C	-6.97	99.23	110.32
1	A	146	SER	N-CA-C	-6.97	104.75	113.18
1	A	480	GLU	N-CA-C	-6.55	104.32	112.90
1	A	41	CYS	N-CA-C	6.46	118.46	109.15
1	A	224	LEU	N-CA-C	-6.17	102.35	110.43
1	A	130	TYR	N-CA-C	6.10	119.43	110.59
1	A	346	GLU	N-CA-C	6.03	120.37	112.89
1	A	279	ILE	CA-C-N	6.00	126.56	120.38
1	A	279	ILE	C-N-CA	6.00	126.56	120.38
1	A	225	GLY	N-CA-C	-5.86	107.30	114.92
1	A	569	CYS	N-CA-C	5.77	119.13	111.75
1	A	208	GLN	N-CA-C	-5.66	106.21	113.23
1	A	46	ILE	N-CA-C	5.66	116.46	108.36
1	A	519	GLY	N-CA-C	5.66	121.82	112.66
1	A	391	MET	CA-C-N	5.43	126.63	119.84
1	A	391	MET	C-N-CA	5.43	126.63	119.84
1	A	408	LEU	N-CA-C	5.17	121.80	110.80
1	A	238	LEU	N-CA-C	5.14	117.29	111.02
1	A	508	LEU	N-CA-C	5.13	119.25	112.89
1	A	269	ALA	CA-C-N	5.11	126.23	119.84
1	A	269	ALA	C-N-CA	5.11	126.23	119.84
1	A	287	VAL	N-CA-C	5.07	119.88	109.34
1	A	503	PHE	N-CA-C	5.06	117.19	111.02
1	A	73	GLU	N-CA-C	-5.00	102.66	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4481	0	4385	181	0
2	B	28	0	25	0	0
3	A	28	0	26	3	0
4	A	14	0	9	5	0
5	A	43	0	30	4	0
All	All	4594	0	4475	182	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 20.

All (182) 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:185:ARG:HE	1:A:438:ARG:HD3	1.29	0.97
1:A:150:ARG:HB3	1:A:379:MET:HE3	1.58	0.86
1:A:294:LEU:HD22	1:A:409:PHE:CE2	2.13	0.84
1:A:530:OAS:OAC	4:A:700:SCL:H5	1.78	0.83
1:A:563:THR:HG22	1:A:566:LYS:HD3	1.60	0.83
1:A:185:ARG:HH21	1:A:438:ARG:HH11	1.26	0.83
1:A:172:PRO:HB2	1:A:177:LEU:HD22	1.61	0.81
1:A:513:HIS:HB3	1:A:514:PRO:HD2	1.59	0.81
1:A:294:LEU:HD22	1:A:409:PHE:HE2	1.46	0.79
1:A:523:ILE:HA	4:A:700:SCL:O1	1.83	0.79
1:A:150:ARG:HD3	1:A:152:LEU:O	1.91	0.71
1:A:241:GLN:NE2	1:A:245:ARG:HH11	1.87	0.71
1:A:577:TYR:CE2	1:A:583:PRO:HD3	2.26	0.71
1:A:84:PRO:HG2	1:A:89:ILE:HD11	1.74	0.70
1:A:513:HIS:HB3	1:A:514:PRO:CD	2.22	0.70
1:A:185:ARG:HH21	1:A:438:ARG:NH1	1.90	0.69
1:A:563:THR:HG23	1:A:566:LYS:H	1.58	0.67
1:A:367:PHE:CD2	1:A:542:PRO:HG3	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:GLU:HG2	1:A:562:ALA:HB2	1.78	0.65
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.79	0.64
1:A:240:ARG:HG3	1:A:271:VAL:CG2	2.28	0.64
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.37	0.64
1:A:384:LEU:C	1:A:384:LEU:HD23	2.23	0.64
1:A:226:HIS:CE1	1:A:376:ARG:HD2	2.33	0.64
1:A:126:SER:HA	1:A:127:PRO:C	2.22	0.64
1:A:208:GLN:NE2	1:A:230:LEU:H	1.96	0.63
1:A:280:PRO:HG2	1:A:283:SER:OG	1.99	0.63
1:A:241:GLN:HE21	1:A:245:ARG:HH11	1.46	0.62
1:A:582:VAL:HG23	1:A:583:PRO:HD2	1.81	0.62
1:A:130:TYR:HB3	1:A:134:HIS:O	1.99	0.62
1:A:449:VAL:O	1:A:453:LYS:HG3	1.99	0.61
1:A:54:ARG:HH11	1:A:54:ARG:HB2	1.64	0.61
1:A:226:HIS:HB3	1:A:377:ILE:H	1.66	0.61
1:A:93:LEU:HD13	1:A:355:TYR:CE1	2.35	0.61
1:A:115:LEU:O	1:A:119:VAL:HG23	2.01	0.60
1:A:380:GLU:HG3	1:A:460:LEU:HD11	1.83	0.60
1:A:458:LEU:HB3	1:A:460:LEU:HD23	1.83	0.60
1:A:255:GLN:HG2	1:A:263:PRO:O	2.02	0.60
1:A:134:HIS:HD2	1:A:138:SER:OG	1.84	0.60
1:A:234:TYR:CE2	1:A:333:ARG:HG3	2.37	0.59
1:A:294:LEU:O	1:A:295:LEU:HG	2.02	0.59
1:A:208:GLN:HE21	1:A:230:LEU:H	1.50	0.59
1:A:459:ARG:HH21	1:A:459:ARG:HG2	1.67	0.59
1:A:184:ARG:HA	1:A:438:ARG:O	2.02	0.59
1:A:193:GLY:O	1:A:582:VAL:HG12	2.03	0.59
1:A:554:VAL:HG23	1:A:555:GLY:H	1.67	0.58
1:A:88:PHE:O	1:A:91:PHE:HB3	2.03	0.58
1:A:245:ARG:HD2	1:A:329:PHE:CZ	2.39	0.58
1:A:306:LEU:C	1:A:306:LEU:HD23	2.30	0.57
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.87	0.57
1:A:479:GLN:HG3	1:A:485:LYS:HZ1	1.70	0.57
1:A:521:SER:HB3	1:A:525:MET:HE3	1.87	0.57
1:A:207:HIS:HB3	1:A:289:GLN:HE21	1.70	0.56
1:A:581:HIS:ND1	1:A:582:VAL:O	2.36	0.56
1:A:239:GLU:CD	1:A:239:GLU:H	2.14	0.55
1:A:248:LYS:HG2	1:A:249:ASP:OD1	2.05	0.55
1:A:403:SER:OG	1:A:406:GLN:HG3	2.06	0.55
1:A:441:ASP:OD2	1:A:443:HIS:HB2	2.05	0.55
1:A:481:LEU:HD22	1:A:501:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:PHE:CE2	1:A:542:PRO:HG3	2.42	0.54
1:A:582:VAL:CG2	1:A:583:PRO:HD2	2.36	0.54
1:A:195:ASN:OD1	1:A:197:MET:HB3	2.08	0.54
1:A:46:ILE:HD12	1:A:46:ILE:N	2.23	0.53
1:A:200:PHE:CE1	1:A:391:MET:HE1	2.43	0.53
1:A:152:LEU:HD21	1:A:469:ARG:CG	2.39	0.53
1:A:389:PRO:HG3	1:A:440:ILE:HG12	1.91	0.53
1:A:577:TYR:HE2	1:A:583:PRO:HD3	1.73	0.53
1:A:342:LYS:HD2	1:A:559:VAL:O	2.08	0.53
1:A:513:HIS:O	1:A:514:PRO:C	2.52	0.53
1:A:391:MET:HE2	5:A:601:HEM:HBB1	1.90	0.52
1:A:260:GLU:HB2	1:A:262:TYR:HE1	1.73	0.52
1:A:479:GLN:CG	1:A:485:LYS:HZ1	2.23	0.52
1:A:282:GLN:H	1:A:282:GLN:CD	2.15	0.52
1:A:282:GLN:OE1	1:A:282:GLN:N	2.40	0.52
1:A:420:GLU:HG3	1:A:572:THR:HB	1.92	0.51
1:A:159:CYS:HB3	1:A:164:GLY:O	2.10	0.51
1:A:307:ARG:HG2	1:A:571:ASN:HB3	1.91	0.51
1:A:513:HIS:HB2	1:A:516:SER:OG	2.11	0.51
1:A:45:GLY:C	1:A:46:ILE:HD12	2.36	0.50
1:A:246:LEU:O	1:A:247:PHE:HB2	2.10	0.50
1:A:233:ILE:HD13	1:A:305:TRP:HB3	1.92	0.50
1:A:261:VAL:O	1:A:307:ARG:NH1	2.44	0.50
1:A:410:ASN:ND2	3:A:681:NAG:H82	2.26	0.50
1:A:464:ASN:O	1:A:467:ARG:HB2	2.11	0.50
1:A:527:ALA:HB1	4:A:700:SCL:O4	2.11	0.50
1:A:180:ARG:HD3	1:A:490:GLU:OE2	2.12	0.50
1:A:230:LEU:HD13	1:A:337:ILE:HG12	1.94	0.50
1:A:390:LEU:HD21	1:A:434:ILE:HD11	1.93	0.50
1:A:165:THR:HG22	1:A:166:LYS:HG2	1.93	0.50
1:A:459:ARG:HG2	1:A:459:ARG:NH2	2.25	0.49
1:A:156:PRO:HB2	1:A:159:CYS:SG	2.52	0.49
1:A:185:ARG:NH2	1:A:438:ARG:NH1	2.59	0.49
1:A:460:LEU:HD13	1:A:466:TYR:OH	2.12	0.49
1:A:478:PHE:CZ	1:A:498:ILE:HA	2.48	0.49
1:A:183:LEU:HD23	1:A:184:ARG:N	2.27	0.48
1:A:293:GLY:HA2	1:A:299:MET:CE	2.43	0.48
1:A:518:PHE:CD1	1:A:522:MET:HG2	2.47	0.48
1:A:523:ILE:HA	4:A:700:SCL:HO1	1.77	0.48
1:A:387:TRP:HB2	5:A:601:HEM:HAC	1.96	0.48
1:A:185:ARG:NH2	1:A:438:ARG:HH11	2.03	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:LEU:HD23	1:A:306:LEU:O	2.14	0.48
1:A:152:LEU:HD21	1:A:469:ARG:HG2	1.96	0.47
1:A:344:VAL:HA	1:A:348:TYR:HB3	1.96	0.47
1:A:180:ARG:O	1:A:438:ARG:NH1	2.48	0.47
1:A:203:GLN:HA	5:A:601:HEM:HBC2	1.96	0.47
1:A:388:HIS:N	1:A:389:PRO:CD	2.77	0.47
1:A:389:PRO:HG3	1:A:440:ILE:CG1	2.44	0.47
1:A:121:SER:O	1:A:123:LEU:N	2.48	0.47
1:A:353:SER:HB2	1:A:355:TYR:CD2	2.50	0.47
1:A:544:TYR:O	1:A:546:LYS:N	2.46	0.47
1:A:320:HIS:HE1	1:A:551:GLY:O	1.98	0.46
1:A:120:ARG:NH2	1:A:524:GLU:OE1	2.46	0.46
1:A:420:GLU:CG	1:A:572:THR:HB	2.45	0.46
1:A:208:GLN:HE22	1:A:230:LEU:HD12	1.81	0.46
1:A:478:PHE:O	1:A:482:THR:HG23	2.16	0.46
1:A:197:MET:HE3	1:A:301:TYR:OH	2.16	0.46
1:A:102:PHE:O	1:A:106:THR:HG23	2.15	0.46
1:A:206:THR:HB	1:A:210:PHE:HD2	1.80	0.46
1:A:333:ARG:O	1:A:337:ILE:HG13	2.16	0.46
1:A:403:SER:OG	1:A:405:GLU:HG2	2.16	0.46
1:A:405:GLU:H	1:A:405:GLU:CD	2.24	0.46
1:A:555:GLY:O	1:A:558:LEU:HB2	2.15	0.46
1:A:247:PHE:HA	1:A:325:ASP:OD2	2.16	0.45
1:A:315:LEU:HD23	1:A:315:LEU:HA	1.80	0.45
1:A:42:GLN:HE22	1:A:468:LYS:NZ	2.15	0.45
1:A:384:LEU:HD23	1:A:384:LEU:O	2.16	0.45
1:A:484:GLU:OE2	1:A:487:MET:HB2	2.17	0.45
1:A:123:LEU:O	1:A:469:ARG:NH2	2.49	0.45
1:A:269:ALA:O	1:A:271:VAL:N	2.50	0.45
1:A:121:SER:C	1:A:123:LEU:H	2.25	0.45
1:A:355:TYR:CE1	4:A:700:SCL:H92	2.51	0.45
1:A:534:LEU:HD12	1:A:534:LEU:HA	1.86	0.45
1:A:563:THR:HG22	1:A:566:LYS:HB2	1.98	0.45
1:A:402:TYR:OH	3:A:681:NAG:H61	2.16	0.44
1:A:91:PHE:HD2	1:A:92:LEU:HD12	1.82	0.44
1:A:184:ARG:HB2	1:A:439:ASN:C	2.42	0.44
1:A:190:ASP:OD2	1:A:194:THR:OG1	2.28	0.44
1:A:196:LEU:HD11	1:A:392:PRO:HG3	1.99	0.44
1:A:563:THR:HG22	1:A:566:LYS:CD	2.39	0.44
1:A:54:ARG:HH11	1:A:54:ARG:CB	2.29	0.44
1:A:116:VAL:O	1:A:120:ARG:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ILE:N	1:A:46:ILE:CD1	2.80	0.44
1:A:470:PHE:CD2	1:A:525:MET:HG2	2.52	0.43
1:A:177:LEU:HD12	1:A:177:LEU:HA	1.82	0.43
1:A:410:ASN:HD22	3:A:681:NAG:H82	1.82	0.43
1:A:83:ARG:HA	1:A:84:PRO:HD2	1.90	0.43
1:A:160:PRO:HD2	1:A:164:GLY:O	2.18	0.43
1:A:345:ILE:CD1	1:A:534:LEU:HD23	2.48	0.43
1:A:88:PHE:CZ	1:A:92:LEU:HD11	2.53	0.43
1:A:100:TRP:O	1:A:101:ASP:C	2.61	0.43
1:A:292:PHE:HA	1:A:298:LEU:HD23	2.01	0.43
1:A:452:ILE:O	1:A:455:SER:HB3	2.18	0.43
1:A:225:GLY:O	1:A:226:HIS:C	2.62	0.43
1:A:554:VAL:HG23	1:A:555:GLY:N	2.31	0.43
1:A:49:ARG:CG	1:A:49:ARG:HH11	2.32	0.43
1:A:96:GLY:O	1:A:97:ARG:C	2.62	0.42
1:A:210:PHE:CE1	1:A:382:ASN:HA	2.54	0.42
1:A:531:LEU:HD23	1:A:531:LEU:HA	1.84	0.42
1:A:185:ARG:NE	1:A:438:ARG:HD3	2.12	0.42
1:A:187:PHE:C	1:A:187:PHE:CD1	2.97	0.42
1:A:218:PRO:HB2	1:A:458:LEU:CD1	2.49	0.42
1:A:513:HIS:HE1	1:A:520:GLU:HA	1.85	0.41
1:A:493:GLU:HG3	1:A:494:LEU:N	2.34	0.41
1:A:146:SER:O	1:A:220:PHE:HA	2.19	0.41
1:A:481:LEU:HD22	1:A:501:LEU:CD2	2.50	0.41
1:A:178:SER:HB3	1:A:445:LEU:HD11	2.01	0.41
1:A:260:GLU:HB2	1:A:262:TYR:CE1	2.53	0.41
1:A:400:GLN:CA	1:A:400:GLN:HE21	2.32	0.41
5:A:601:HEM:HMB1	5:A:601:HEM:HBB2	2.02	0.41
1:A:206:THR:HB	1:A:210:PHE:CD2	2.56	0.41
1:A:479:GLN:CB	1:A:485:LYS:NZ	2.84	0.41
1:A:187:PHE:HE1	1:A:189:PRO:HB3	1.86	0.41
1:A:49:ARG:HH11	1:A:49:ARG:HG3	1.86	0.41
1:A:96:GLY:O	1:A:99:LEU:HB3	2.21	0.41
1:A:240:ARG:HG3	1:A:271:VAL:HG22	2.02	0.41
1:A:316:LEU:HD12	1:A:316:LEU:HA	1.91	0.41
1:A:161:THR:HB	1:A:162:PRO:CD	2.51	0.41
1:A:348:TYR:O	1:A:351:GLN:HB3	2.21	0.40
1:A:294:LEU:HD22	1:A:409:PHE:CD2	2.55	0.40
1:A:275:TYR:CE2	1:A:284:GLN:HB3	2.57	0.40
1:A:320:HIS:HB3	1:A:323:TRP:CD1	2.57	0.40
1:A:92:LEU:HD12	1:A:92:LEU:N	2.36	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	548/551 (100%)	485 (88%)	55 (10%)	8 (2%)	8 37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	HIS
1	A	408	LEU
1	A	122	ASN
1	A	292	PHE
1	A	545	TRP
1	A	270	PRO
1	A	295	LEU
1	A	514	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	485/485 (100%)	454 (94%)	31 (6%)	16 48

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	54	ARG
1	A	117	LEU
1	A	120	ARG
1	A	130	TYR
1	A	165	THR
1	A	180	ARG
1	A	243	GLN
1	A	244	LEU
1	A	246	LEU
1	A	251	LYS
1	A	271	VAL
1	A	289	GLN
1	A	300	LEU
1	A	307	ARG
1	A	316	LEU
1	A	322	THR
1	A	376	ARG
1	A	384	LEU
1	A	385	TYR
1	A	400	GLN
1	A	405	GLU
1	A	458	LEU
1	A	469	ARG
1	A	476	THR
1	A	479	GLN
1	A	482	THR
1	A	484	GLU
1	A	518	PHE
1	A	534	LEU
1	A	564	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	56	GLN
1	A	90	HIS
1	A	95	HIS
1	A	134	HIS
1	A	170	GLN
1	A	207	HIS
1	A	208	GLN

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Mol	Chain	Res	Type
1	A	237	ASN
1	A	241	GLN
1	A	375	ASN
1	A	400	GLN
1	A	443	HIS
1	A	513	HIS
1	A	515	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	OAS	A	530	1	7,8,9	0.68	0	4,9,11	1.38	1 (25%)

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	OAS	A	530	1	-	2/5/7/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	530	OAS	CB-OG-C1A	2.36	122.90	117.08

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	530	OAS	C-CA-CB-OG
1	A	530	OAS	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	530	OAS	1	0

5.5 Carbohydrates

2 monosaccharides 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	B	1	2,1	14,14,15	0.53	0	17,19,21	0.83	1 (5%)
2	NAG	B	2	2	14,14,15	0.47	0	17,19,21	0.83	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	B	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	1	NAG	C2-N2-C7	-2.13	120.05	122.90

There are no chirality outliers.

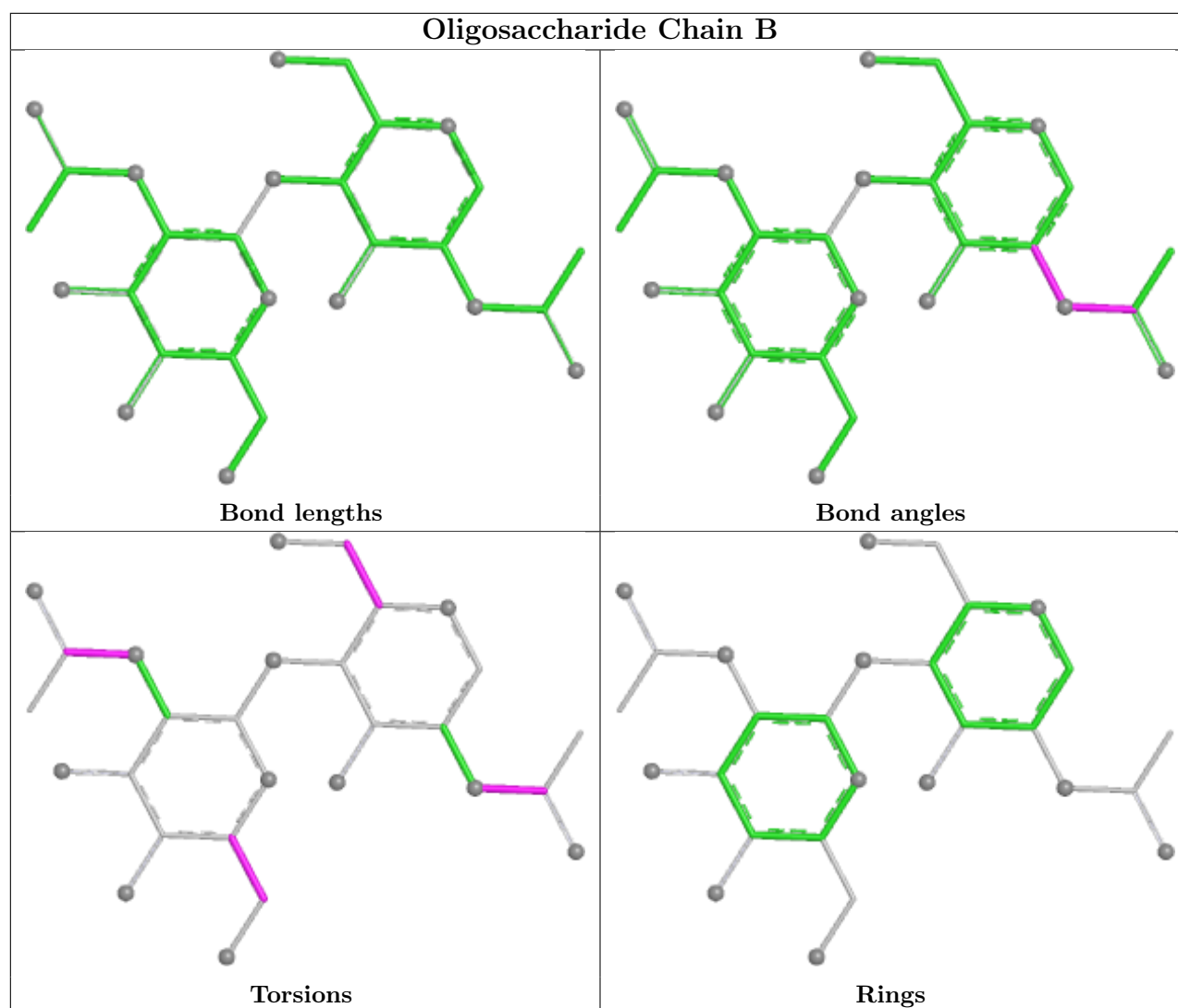
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	1	NAG	O7-C7-N2-C2
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	681	1	14,14,15	0.49	0	17,19,21	0.98	1 (5%)
3	NAG	A	661	1	14,14,15	0.56	0	17,19,21	0.78	1 (5%)
4	SCL	A	700	-	14,14,14	1.50	4 (28%)	16,18,18	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	HEM	A	601	1	50,50,50	1.41	6 (12%)	67,82,82	1.40	12 (17%)

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
3	NAG	A	681	1	-	3/6/23/26	0/1/1/1
3	NAG	A	661	1	-	0/6/23/26	0/1/1/1
4	SCL	A	700	-	-	3/9/9/9	0/1/1/1
5	HEM	A	601	1	-	6/14/54/54	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	HEM	CBB-CAB	3.33	1.46	1.30
5	A	601	HEM	CBC-CAC	3.16	1.45	1.30
4	A	700	SCL	C5-C6	2.80	1.43	1.38
5	A	601	HEM	C3B-C4B	2.64	1.50	1.44
5	A	601	HEM	CAB-C3B	-2.60	1.40	1.47
5	A	601	HEM	C2A-C3A	-2.51	1.32	1.38
4	A	700	SCL	C6-C1	2.36	1.43	1.39
5	A	601	HEM	CAC-C3C	-2.19	1.41	1.47
4	A	700	SCL	O3-N1	2.19	1.44	1.40
4	A	700	SCL	C3-C2	2.10	1.43	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	HEM	CAA-C2A-C1A	3.74	132.24	124.94
5	A	601	HEM	C3B-C4B-NB	3.67	112.10	109.47
5	A	601	HEM	C2D-C1D-ND	2.99	113.36	109.90
5	A	601	HEM	CBA-CAA-C2A	2.67	119.92	112.53
5	A	601	HEM	C4B-C3B-C2B	-2.60	104.89	107.28
5	A	601	HEM	C4C-C3C-C2C	-2.56	104.59	106.81
3	A	681	NAG	C2-N2-C7	-2.55	119.49	122.90
5	A	601	HEM	C2A-C1A-NA	2.53	112.96	110.15
5	A	601	HEM	C1D-C2D-C3D	-2.45	104.40	106.98
5	A	601	HEM	C4A-C3A-C2A	2.35	109.50	106.82
5	A	601	HEM	C1A-C2A-C3A	-2.28	103.34	106.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	HEM	C2B-C1B-NB	2.23	112.40	109.84
3	A	661	NAG	C2-N2-C7	-2.17	119.99	122.90
5	A	601	HEM	CAC-C3C-C4C	2.01	129.62	124.82

There are no chirality outliers.

All (12) torsion outliers are listed below:

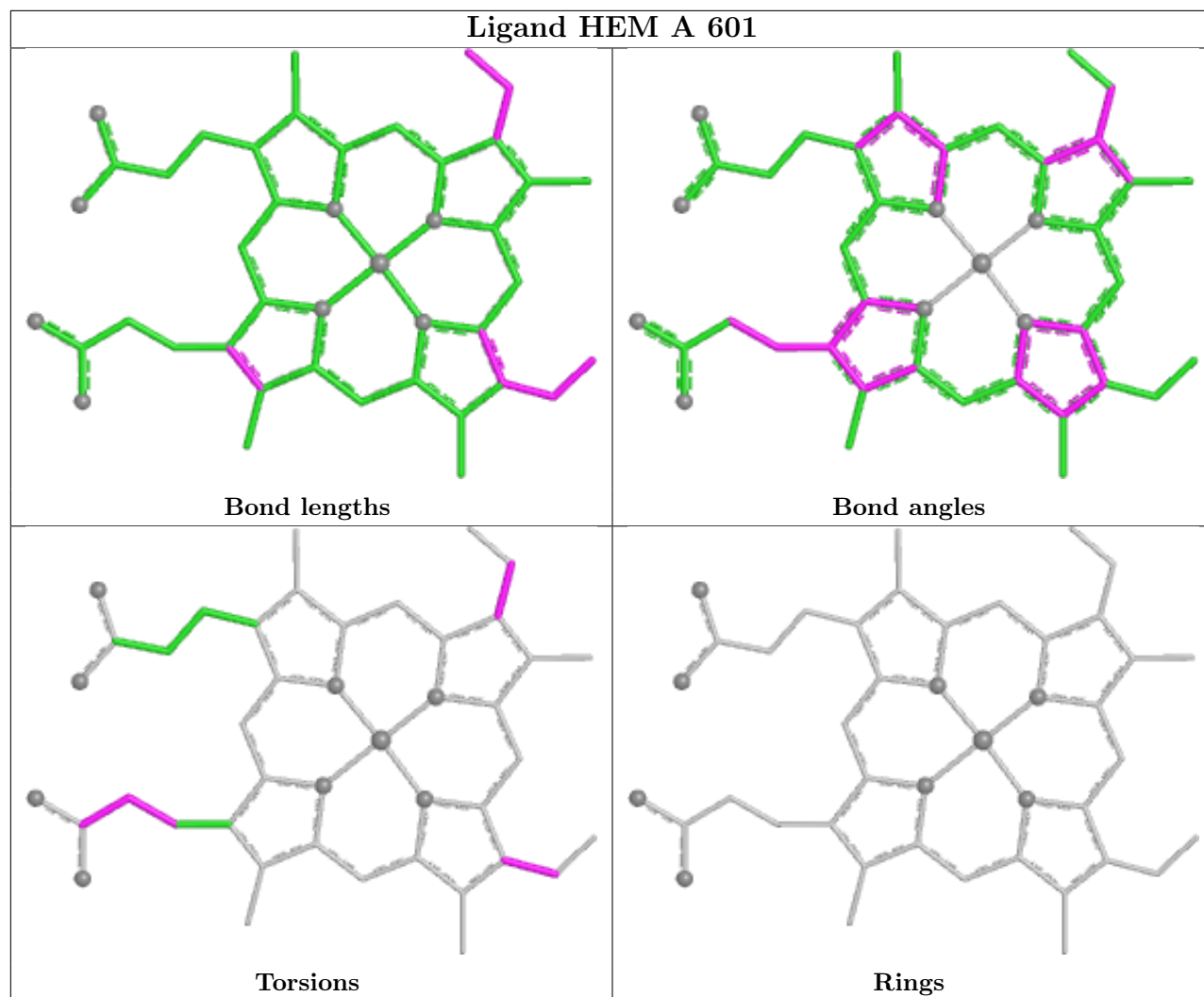
Mol	Chain	Res	Type	Atoms
3	A	681	NAG	C8-C7-N2-C2
3	A	681	NAG	O7-C7-N2-C2
4	A	700	SCL	C7-N1-O3-C8
5	A	601	HEM	C2C-C3C-CAC-CBC
5	A	601	HEM	C2A-CAA-CBA-CGA
4	A	700	SCL	C2-C1-C7-N1
4	A	700	SCL	C2-C1-C7-O2
5	A	601	HEM	C4C-C3C-CAC-CBC
3	A	681	NAG	O5-C5-C6-O6
5	A	601	HEM	CAA-CBA-CGA-O2A
5	A	601	HEM	CAA-CBA-CGA-O1A
5	A	601	HEM	C2B-C3B-CAB-CBB

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	681	NAG	3	0
4	A	700	SCL	5	0
5	A	601	HEM	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 [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	550/551 (99%)	-0.91	0 100 100	1, 11, 32, 53	0

There are no RSRZ outliers to report.

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.

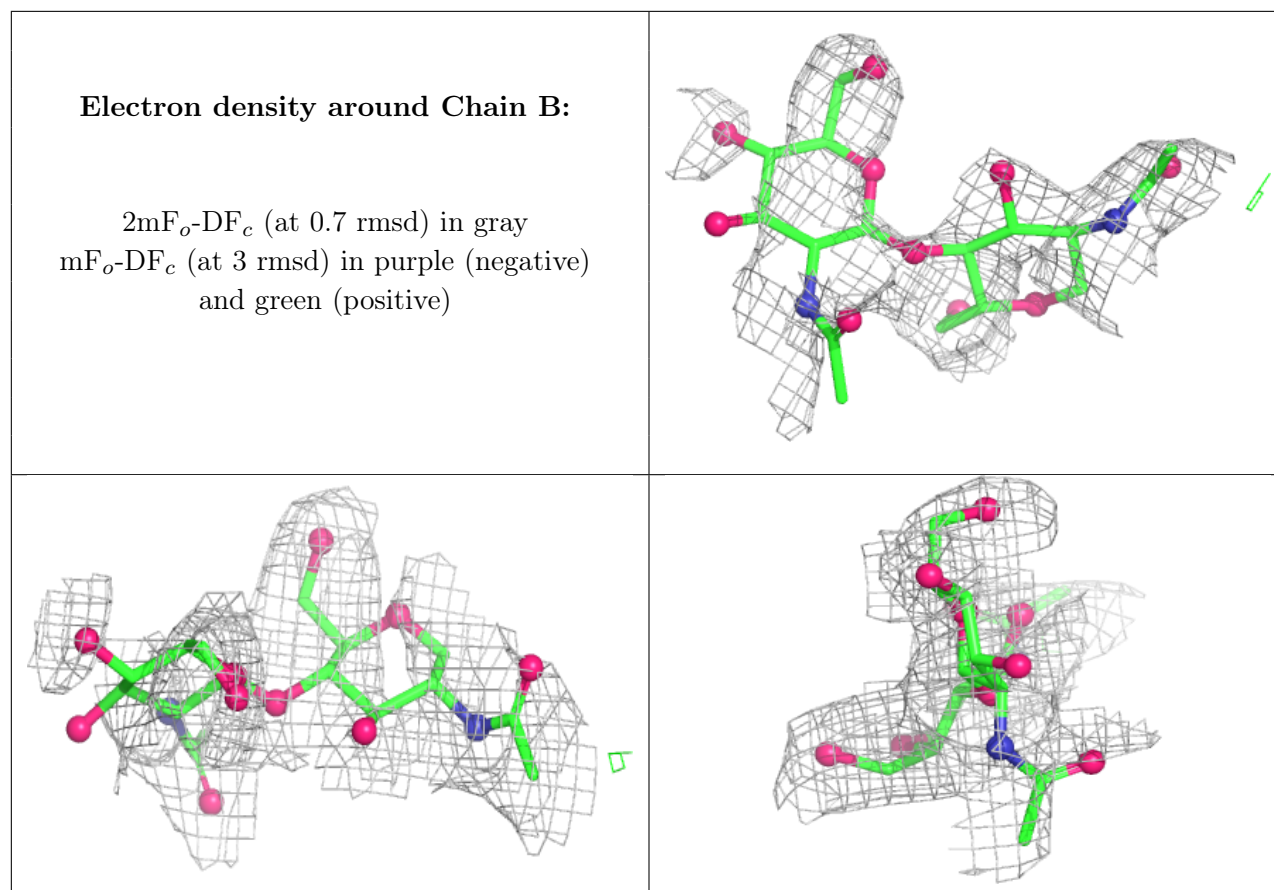
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	OAS	A	530	9/10	0.99	0.06	2,6,14,15	0

6.3 Carbohydrates [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
2	NAG	B	1	14/15	0.98	0.06	5,6,10,13	0
2	NAG	B	2	14/15	0.98	0.09	16,18,20,21	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

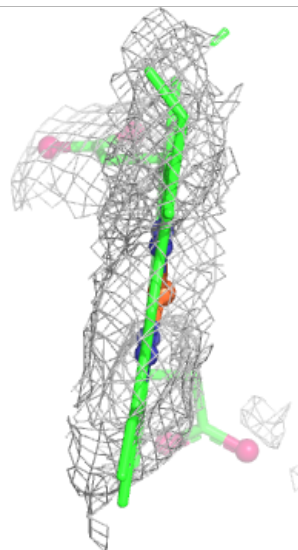
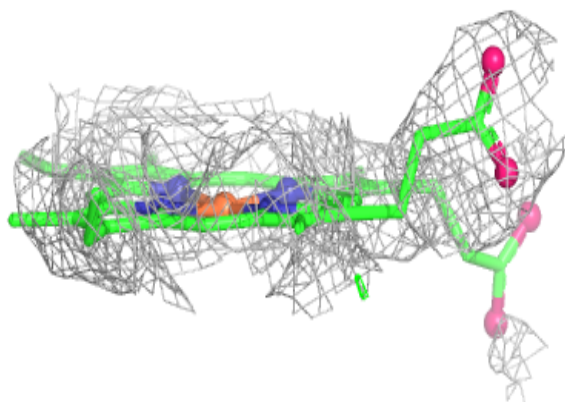
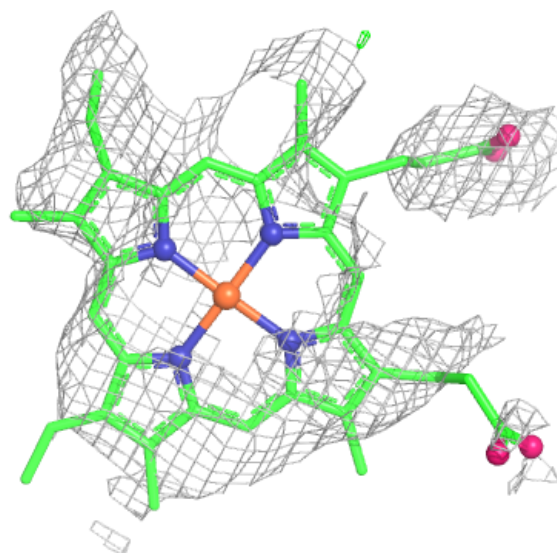
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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	SCL	A	700	14/14	0.97	0.12	51,53,56,57	0
3	NAG	A	681	14/15	0.99	0.07	18,22,24,24	0
3	NAG	A	661	14/15	0.99	0.07	34,36,38,39	0
5	HEM	A	601	43/43	0.99	0.07	13,19,35,41	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 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.