



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 01:37 PM EDT

PDB ID : 2QQT / pdb_00002qqt
Title : Crystal structure of the complex of bovine lactoperoxidase with acetyl salicylic acid at 2.5 Å resolution
Authors : Singh, A.K.; Singh, N.; Sharma, S.; Kaur, P.; Singh, T.P.
Deposited on : 2007-07-27
Resolution : 2.50 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	:	9.0.015 (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

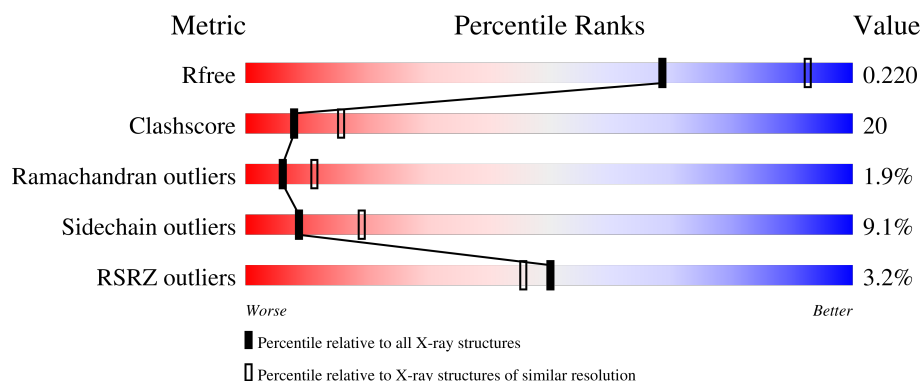
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	3% 60% 31% 8%
2	B	3	33% 67%
2	D	3	33% 67%
3	C	2	50% 50%
3	E	2	100%

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
4	AIN	A	596	-	X	X	-

2 Entry composition [i](#)

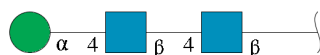
There are 9 unique types of molecules in this entry. The entry contains 5295 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 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 an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



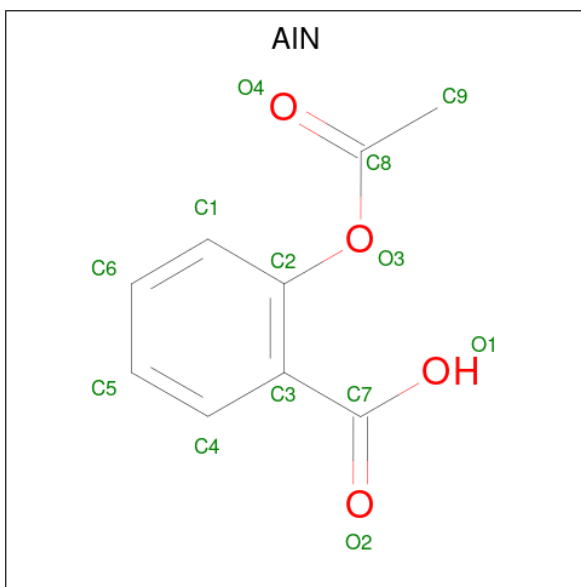
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 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
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-(ACETYLOXY)BENZOIC ACID (CCD ID: AIN) (formula: C₉H₈O₄).

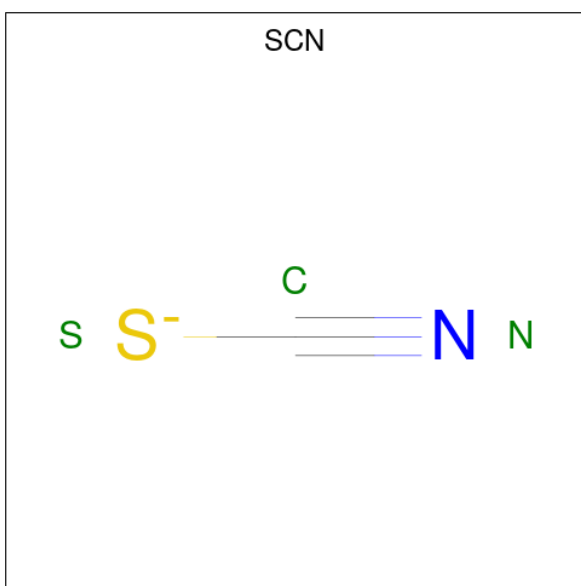


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	9	4		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).

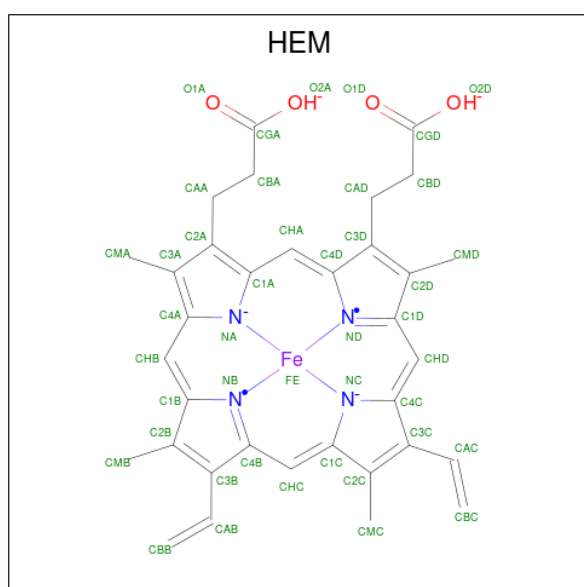


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 7 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	7	Total I 7 7	0	0

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

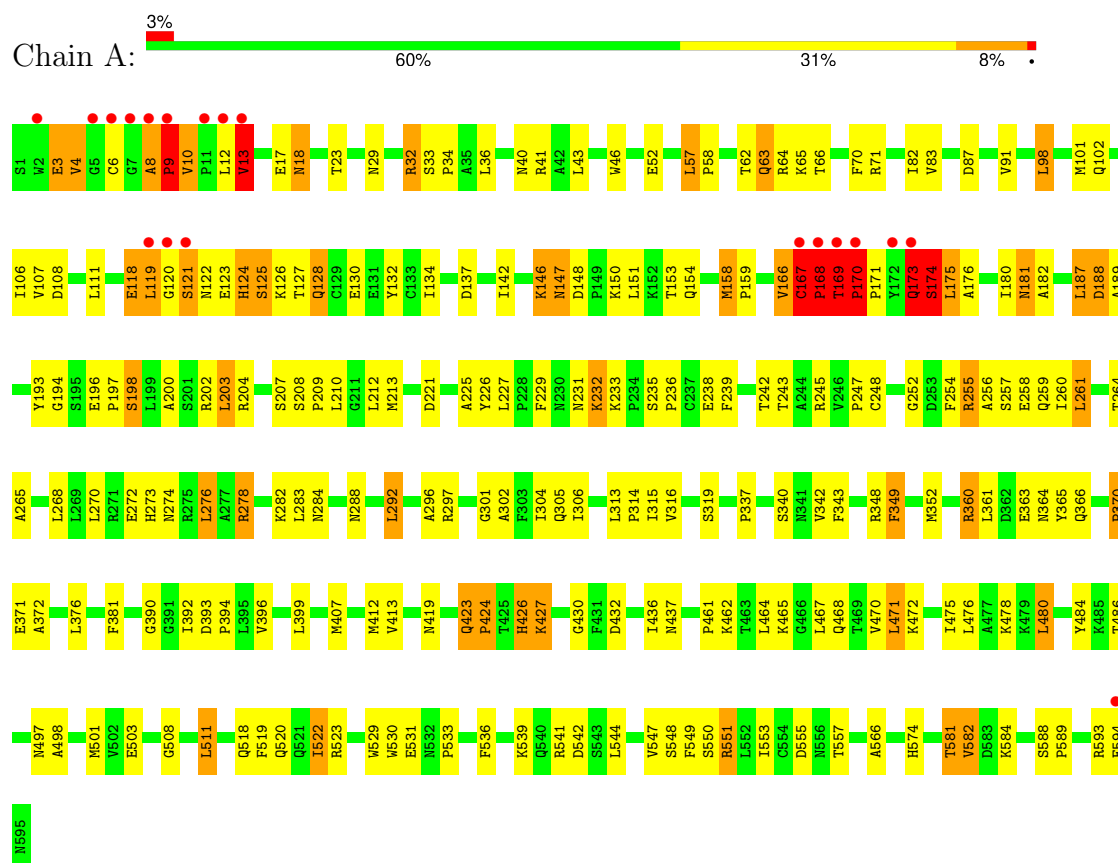
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	320	Total O 320 320	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: Lactoperoxidase



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



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





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 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	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.66Å 80.52Å 77.97Å 90.00° 102.65° 90.00°	Depositor
Resolution (Å)	19.44 – 2.50 19.44 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.44-2.50) 98.6 (19.44-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.49Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.194 , 0.211 0.184 , 0.220	Depositor DCC
R_{free} test set	1161 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 78.1	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	0.93	EDS
Total number of atoms	5295	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.80% 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: SEP, HEM, CA, SCN, MAN, AIN, NAG, IOD

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	0.69	10/4891 (0.2%)	1.29	77/6634 (1.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	ARG	CD-NE	-13.72	1.27	1.46
1	A	9	PRO	C-N	-11.47	1.25	1.33
1	A	169	THR	CA-C	7.45	1.62	1.52
1	A	9	PRO	CA-C	-7.33	1.42	1.52
1	A	3	GLU	CA-C	-7.12	1.45	1.53
1	A	108	ASP	N-CA	6.46	1.53	1.46
1	A	423	GLN	CA-C	6.35	1.61	1.52
1	A	107	VAL	C-N	6.27	1.41	1.33
1	A	167	CYS	N-CA	-6.04	1.37	1.46
1	A	121	SER	CA-C	-5.39	1.46	1.52

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	VAL	N-CA-C	-13.30	98.98	111.48
1	A	9	PRO	CA-C-N	-12.68	112.30	123.33
1	A	9	PRO	C-N-CA	-12.68	112.30	123.33
1	A	17	GLU	N-CA-C	11.55	126.89	113.38
1	A	169	THR	CA-C-N	11.28	132.00	120.38
1	A	169	THR	C-N-CA	11.28	132.00	120.38
1	A	125	SER	N-CA-C	-10.86	99.53	111.36
1	A	412	MET	N-CA-C	9.96	122.08	111.03
1	A	423	GLN	CB-CA-C	9.56	123.24	108.61
1	A	147	ASN	CA-CB-CG	9.47	122.07	112.60
1	A	423	GLN	OE1-CD-NE2	-9.37	113.23	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	GLN	CA-C-N	8.93	128.25	118.97
1	A	423	GLN	C-N-CA	8.93	128.25	118.97
1	A	167	CYS	N-CA-C	-8.36	91.34	109.81
1	A	424	PRO	O-C-N	8.23	131.47	122.17
1	A	33	SER	CA-C-N	7.97	129.81	119.84
1	A	33	SER	C-N-CA	7.97	129.81	119.84
1	A	508	GLY	CA-C-N	7.80	127.35	119.24
1	A	508	GLY	C-N-CA	7.80	127.35	119.24
1	A	208	SER	CA-C-N	7.47	129.18	119.84
1	A	208	SER	C-N-CA	7.47	129.18	119.84
1	A	119	LEU	N-CA-C	-7.41	101.17	111.39
1	A	424	PRO	CA-C-O	7.37	130.72	120.03
1	A	233	LYS	N-CA-C	-7.33	99.25	110.32
1	A	225	ALA	N-CA-C	7.23	120.07	110.53
1	A	232	LYS	N-CA-C	7.10	125.91	110.80
1	A	29	ASN	N-CA-C	-6.98	103.60	111.14
1	A	390	GLY	N-CA-C	6.97	125.04	115.00
1	A	111	LEU	N-CA-C	6.85	121.97	112.45
1	A	254	PHE	N-CA-C	6.82	120.86	112.54
1	A	9	PRO	CA-N-CD	-6.68	102.65	112.00
1	A	167	CYS	CB-CA-C	6.60	123.18	110.17
1	A	174	SER	N-CA-C	6.57	124.80	110.80
1	A	43	LEU	N-CA-C	-6.40	101.00	110.48
1	A	475	ILE	N-CA-C	6.39	116.55	110.42
1	A	121	SER	CA-C-N	-6.32	113.53	122.63
1	A	121	SER	C-N-CA	-6.32	113.53	122.63
1	A	260	ILE	N-CA-C	6.29	118.91	111.05
1	A	424	PRO	CA-C-N	6.28	131.33	120.58
1	A	424	PRO	C-N-CA	6.28	131.33	120.58
1	A	128	GLN	N-CA-C	-6.17	105.01	112.54
1	A	582	VAL	N-CA-C	6.16	117.17	108.36
1	A	423	GLN	CG-CD-NE2	6.09	125.53	116.40
1	A	87	ASP	N-CA-C	6.02	118.11	108.41
1	A	363	GLU	N-CA-C	5.96	120.16	113.01
1	A	284	ASN	CA-C-N	5.92	125.79	119.28
1	A	284	ASN	C-N-CA	5.92	125.79	119.28
1	A	566	ALA	N-CA-C	5.88	119.93	112.87
1	A	108	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	426	HIS	CA-CB-CG	-5.80	108.00	113.80
1	A	137	ASP	CB-CA-C	-5.79	109.88	116.54
1	A	166	VAL	O-C-N	5.76	129.77	122.57
1	A	10	VAL	CB-CA-C	5.71	115.67	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	SER	N-CA-C	-5.70	106.19	113.02
1	A	23	THR	N-CA-C	-5.64	103.25	110.53
1	A	170	PRO	CA-C-N	5.62	126.87	119.84
1	A	170	PRO	C-N-CA	5.62	126.87	119.84
1	A	83	VAL	N-CA-C	5.42	118.70	111.44
1	A	542	ASP	CA-CB-CG	5.41	118.01	112.60
1	A	423	GLN	N-CA-C	-5.40	103.36	110.39
1	A	102	GLN	N-CA-C	5.39	117.15	111.28
1	A	168	PRO	N-CA-C	5.38	123.56	112.47
1	A	173	GLN	N-CA-C	5.31	122.11	110.80
1	A	256	ALA	N-CA-C	5.24	118.46	111.75
1	A	181	ASN	N-CA-C	-5.23	98.87	108.02
1	A	193	TYR	N-CA-C	5.21	119.68	113.23
1	A	188	ASP	N-CA-C	5.17	120.72	113.02
1	A	243	THR	N-CA-C	-5.16	107.12	113.41
1	A	10	VAL	CA-C-N	-5.13	112.92	120.46
1	A	10	VAL	C-N-CA	-5.13	112.92	120.46
1	A	296	ALA	N-CA-C	-5.10	105.61	111.07
1	A	349	PHE	N-CA-C	-5.07	106.20	112.38
1	A	71	ARG	CA-C-N	-5.05	118.39	123.04
1	A	71	ARG	C-N-CA	-5.05	118.39	123.04
1	A	34	PRO	N-CA-C	5.05	122.86	112.47
1	A	121	SER	N-CA-C	-5.03	100.71	108.90
1	A	427	LYS	N-CA-C	5.01	119.34	112.88

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	4774	0	4687	179	0
2	B	39	0	34	1	0
2	D	39	0	34	4	0
3	C	28	0	25	0	0
3	E	28	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	13	0	7	19	0
5	A	1	0	0	0	0
6	A	3	0	0	0	0
7	A	7	0	0	1	0
8	A	43	0	30	9	0
9	A	320	0	0	23	0
All	All	5295	0	4842	192	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 (192) 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:O2P	1.54	1.07
1:A:175:LEU:HD22	1:A:176:ALA:H	1.18	1.03
1:A:424:PRO:HG3	4:A:596:AIN:H4	1.42	1.01
1:A:235:SER:HB3	1:A:238:GLU:HG2	1.44	0.99
1:A:424:PRO:HD3	4:A:596:AIN:H5	1.45	0.97
1:A:8:ALA:C	1:A:10:VAL:H	1.74	0.95
1:A:4:VAL:HG13	1:A:4:VAL:O	1.65	0.94
1:A:173:GLN:HG2	1:A:174:SER:H	1.33	0.92
1:A:169:THR:HG22	1:A:170:PRO:HD3	1.50	0.92
1:A:146:LYS:HE2	9:A:1256:HOH:O	1.71	0.91
1:A:106:ILE:HD11	1:A:265:ALA:HB1	1.55	0.89
1:A:175:LEU:CD2	1:A:176:ALA:H	1.86	0.87
1:A:424:PRO:CD	4:A:596:AIN:H5	2.04	0.87
1:A:32:ARG:HB3	1:A:32:ARG:HH11	1.38	0.86
1:A:424:PRO:CG	4:A:596:AIN:H4	2.06	0.84
1:A:282:LYS:HD3	9:A:1234:HOH:O	1.78	0.83
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.59	0.82
1:A:8:ALA:HB3	1:A:9:PRO:CD	2.10	0.82
1:A:169:THR:CG2	1:A:170:PRO:HD3	2.11	0.79
1:A:227:LEU:HD23	1:A:270:LEU:HD22	1.65	0.78
1:A:106:ILE:HD11	1:A:265:ALA:CB	2.18	0.73
1:A:239:PHE:CZ	1:A:427:LYS:HG2	2.24	0.73
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.71	0.71
1:A:258:GLU:OE1	1:A:259:GLN:HG2	1.90	0.71
1:A:4:VAL:O	1:A:4:VAL:CG1	2.36	0.71
8:A:605:HEM:HMB1	8:A:605:HEM:HBB2	1.71	0.71
1:A:319:SER:HB3	9:A:1301:HOH:O	1.91	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLU:HG2	1:A:65:LYS:HE3	1.72	0.70
1:A:519:PHE:CD1	1:A:522:ILE:HD11	2.28	0.69
4:A:596:AIN:H1	8:A:605:HEM:CMA	2.22	0.69
1:A:119:LEU:HD21	1:A:170:PRO:HG3	1.75	0.69
4:A:596:AIN:H1	8:A:605:HEM:HMA2	1.74	0.69
1:A:173:GLN:CG	1:A:174:SER:H	2.04	0.68
1:A:123:GLU:HG3	1:A:125:SER:H	1.58	0.68
1:A:10:VAL:HG12	1:A:40:ASN:O	1.93	0.67
1:A:130:GLU:HG3	1:A:159:PRO:HG3	1.75	0.67
1:A:173:GLN:HG2	1:A:174:SER:N	2.09	0.67
1:A:302:ALA:O	1:A:306:ILE:HG13	1.95	0.66
1:A:255:ARG:CD	4:A:596:AIN:H92	2.26	0.65
1:A:170:PRO:CB	1:A:171:PRO:CD	2.75	0.64
1:A:381:PHE:HZ	4:A:596:AIN:C4	2.11	0.64
1:A:381:PHE:HZ	4:A:596:AIN:H4	1.61	0.63
1:A:274:ASN:O	1:A:278:ARG:HG2	2.00	0.62
1:A:392:ILE:O	1:A:396:VAL:HG23	2.00	0.62
1:A:173:GLN:CG	1:A:174:SER:N	2.63	0.62
1:A:197:PRO:HB2	1:A:198:SEP:O3P	2.00	0.62
1:A:348:ARG:HH11	1:A:437:ASN:ND2	1.98	0.62
1:A:12:LEU:HB2	9:A:1305:HOH:O	2.00	0.61
1:A:122:ASN:N	9:A:1196:HOH:O	2.33	0.61
1:A:533:PRO:HB3	9:A:1186:HOH:O	2.00	0.61
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.35	0.61
1:A:8:ALA:C	1:A:10:VAL:N	2.43	0.61
1:A:62:THR:HG22	1:A:64:ARG:HG2	1.80	0.61
1:A:301:GLY:O	1:A:305:GLN:HG3	1.99	0.60
1:A:424:PRO:CG	4:A:596:AIN:C4	2.78	0.60
1:A:12:LEU:O	1:A:13:VAL:HG13	2.02	0.60
1:A:32:ARG:HB3	1:A:32:ARG:NH1	2.13	0.60
1:A:255:ARG:HD2	4:A:596:AIN:H92	1.83	0.60
1:A:544:LEU:O	1:A:547:VAL:HG13	2.03	0.59
1:A:282:LYS:HG2	9:A:1171:HOH:O	2.03	0.59
1:A:121:SER:O	1:A:122:ASN:HB3	2.02	0.59
1:A:10:VAL:HG23	9:A:1305:HOH:O	2.02	0.58
1:A:407:MET:HB3	1:A:501:MET:CE	2.34	0.58
1:A:255:ARG:HG2	4:A:596:AIN:O2	2.03	0.58
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.38	0.58
1:A:426:HIS:HB3	9:A:1167:HOH:O	2.03	0.57
1:A:393:ASP:OD1	1:A:557:THR:HB	2.04	0.57
2:D:1:NAG:H62	2:D:2:NAG:C1	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:PRO:CD	4:A:596:AIN:C5	2.80	0.57
1:A:8:ALA:O	1:A:10:VAL:N	2.36	0.56
1:A:550:SER:O	1:A:553:ILE:HB	2.06	0.56
1:A:8:ALA:HB3	1:A:9:PRO:HD2	1.84	0.56
9:A:1324:HOH:O	2:D:3:MAN:H61	2.06	0.56
1:A:175:LEU:HD22	1:A:176:ALA:N	2.03	0.55
1:A:146:LYS:HE3	9:A:1052:HOH:O	2.05	0.55
1:A:582:VAL:HA	9:A:1308:HOH:O	2.07	0.55
1:A:360:ARG:NH1	1:A:372:ALA:HA	2.22	0.55
1:A:170:PRO:HB3	1:A:171:PRO:HD2	1.89	0.55
1:A:407:MET:HB3	1:A:501:MET:HE3	1.88	0.54
1:A:258:GLU:OE1	1:A:259:GLN:CG	2.54	0.54
1:A:66:THR:HB	1:A:70:PHE:O	2.07	0.54
1:A:170:PRO:HB3	1:A:171:PRO:CD	2.38	0.54
1:A:200:ALA:O	1:A:204:ARG:HG3	2.08	0.54
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.43	0.54
1:A:10:VAL:HG21	1:A:41:ARG:NH2	2.23	0.53
1:A:272:GLU:HG3	1:A:276:LEU:HD22	1.90	0.53
1:A:462:LYS:HD2	9:A:1085:HOH:O	2.09	0.53
1:A:549:PHE:O	1:A:553:ILE:HG12	2.09	0.53
1:A:360:ARG:C	1:A:361:LEU:HD23	2.34	0.53
1:A:188:ASP:O	1:A:189:ALA:HB3	2.10	0.52
1:A:364:ASN:O	1:A:365:TYR:HB2	2.09	0.52
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.45	0.52
1:A:8:ALA:HB1	9:A:1226:HOH:O	2.09	0.51
1:A:467:LEU:HG	1:A:471:LEU:HD22	1.91	0.51
1:A:476:LEU:HD21	1:A:498:ALA:HB1	1.92	0.51
1:A:381:PHE:CZ	4:A:596:AIN:C4	2.92	0.51
1:A:239:PHE:CE1	1:A:427:LYS:HG2	2.46	0.51
1:A:158:MET:HE2	1:A:430:GLY:O	2.11	0.51
1:A:170:PRO:CB	1:A:171:PRO:HD2	2.40	0.51
1:A:120:GLY:HA2	1:A:123:GLU:HB2	1.93	0.50
1:A:370:PRO:HG2	1:A:371:GLU:HG3	1.93	0.50
1:A:62:THR:HG21	1:A:64:ARG:NH1	2.27	0.50
1:A:393:ASP:HB2	1:A:394:PRO:HD3	1.93	0.50
1:A:236:PRO:HD2	1:A:248:CYS:SG	2.52	0.50
1:A:519:PHE:HD1	1:A:522:ILE:HD11	1.73	0.50
1:A:62:THR:HG21	1:A:64:ARG:HH11	1.77	0.49
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.76	0.49
1:A:146:LYS:HG3	1:A:147:ASN:ND2	2.28	0.49
1:A:187:LEU:HD13	1:A:305:GLN:HA	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:ARG:NH2	1:A:555:ASP:OD1	2.36	0.48
1:A:142:ILE:CD1	1:A:436:ILE:HD13	2.44	0.48
1:A:370:PRO:HG2	1:A:371:GLU:H	1.78	0.48
1:A:132:TYR:HB3	9:A:1243:HOH:O	2.13	0.48
1:A:257:SER:O	1:A:381:PHE:HA	2.14	0.47
1:A:259:GLN:OE1	1:A:261:LEU:HB2	2.14	0.47
4:A:596:AIN:C1	8:A:605:HEM:HMA2	2.43	0.47
1:A:130:GLU:CD	1:A:426:HIS:HD1	2.22	0.47
1:A:203:LEU:HD21	1:A:252:GLY:HA2	1.96	0.47
1:A:588:SER:N	1:A:589:PRO:CD	2.76	0.47
8:A:605:HEM:HMC2	8:A:605:HEM:HBC2	1.96	0.47
1:A:36:LEU:HG	1:A:337:PRO:HD2	1.97	0.47
1:A:134:ILE:HD11	9:A:1243:HOH:O	2.14	0.47
1:A:272:GLU:O	1:A:276:LEU:HB2	2.14	0.47
1:A:313:LEU:N	1:A:314:PRO:CD	2.78	0.47
1:A:549:PHE:CE2	1:A:553:ILE:HD11	2.50	0.47
1:A:168:PRO:HB3	1:A:170:PRO:HD2	1.97	0.46
1:A:478:LYS:HE3	1:A:478:LYS:HB2	1.82	0.46
1:A:8:ALA:CB	1:A:9:PRO:CD	2.78	0.46
1:A:187:LEU:HD21	1:A:304:ILE:HG22	1.98	0.46
1:A:46:TRP:CE2	1:A:340:SER:HB3	2.50	0.46
1:A:242:THR:O	1:A:245:ARG:NH2	2.48	0.46
1:A:231:ASN:HB3	9:A:1099:HOH:O	2.15	0.46
1:A:166:VAL:HB	1:A:167:CYS:H	1.48	0.46
1:A:381:PHE:CZ	4:A:596:AIN:H4	2.46	0.46
1:A:106:ILE:CD1	1:A:265:ALA:HB1	2.35	0.45
1:A:182:ALA:HB1	9:A:1064:HOH:O	2.16	0.45
1:A:32:ARG:HH11	1:A:32:ARG:CB	2.20	0.45
1:A:541:ARG:NH2	9:A:1102:HOH:O	2.49	0.45
1:A:9:PRO:HG2	1:A:167:CYS:O	2.17	0.45
1:A:342:VAL:HG12	7:A:608:IOD:I	2.87	0.45
1:A:352:MET:HG2	1:A:413:VAL:HG23	1.99	0.45
1:A:574:HIS:HB2	9:A:1228:HOH:O	2.17	0.45
1:A:461:PRO:HG3	1:A:470:VAL:HG21	1.97	0.45
1:A:118:GLU:HB3	1:A:119:LEU:H	1.56	0.44
1:A:484:TYR:C	1:A:486:THR:H	2.26	0.44
1:A:581:THR:HG23	1:A:581:THR:O	2.18	0.44
1:A:98:LEU:HD13	1:A:399:LEU:HD23	1.99	0.43
1:A:10:VAL:HG21	1:A:41:ARG:CZ	2.48	0.43
1:A:424:PRO:HD3	4:A:596:AIN:C5	2.32	0.43
1:A:581:THR:O	1:A:581:THR:CG2	2.65	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:596:AIN:C1	8:A:605:HEM:CMA	2.94	0.43
1:A:8:ALA:CB	1:A:9:PRO:HD3	2.46	0.43
1:A:57:LEU:HA	1:A:58:PRO:HD3	1.78	0.43
1:A:194:GLY:HA2	1:A:252:GLY:O	2.18	0.43
2:D:1:NAG:C6	2:D:2:NAG:C1	2.97	0.43
1:A:361:LEU:HB3	1:A:365:TYR:HA	2.00	0.43
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.54	0.42
1:A:229:PHE:CD1	1:A:247:PRO:HG2	2.55	0.42
1:A:432:ASP:O	1:A:436:ILE:HG12	2.19	0.42
1:A:588:SER:OG	1:A:589:PRO:HD3	2.18	0.42
1:A:148:ASP:O	1:A:151:LEU:HB2	2.19	0.42
1:A:150:LYS:O	1:A:154:GLN:N	2.48	0.42
1:A:32:ARG:NH1	1:A:32:ARG:CB	2.82	0.42
1:A:150:LYS:HZ2	1:A:154:GLN:HE22	1.68	0.42
1:A:202:ARG:O	1:A:202:ARG:HG2	2.19	0.42
1:A:288:ASN:O	1:A:292:LEU:CD2	2.68	0.42
1:A:503:GLU:HG3	9:A:1268:HOH:O	2.19	0.42
1:A:175:LEU:CD2	1:A:176:ALA:N	2.68	0.42
1:A:364:ASN:O	1:A:366:GLN:NE2	2.47	0.41
1:A:468:GLN:O	1:A:472:LYS:N	2.53	0.41
4:A:596:AIN:H1	8:A:605:HEM:C3A	2.54	0.41
1:A:423:GLN:HA	1:A:424:PRO:HD2	1.68	0.41
2:B:1:NAG:H61	2:B:2:NAG:C1	2.49	0.41
2:D:2:NAG:H4	2:D:3:MAN:H2	1.55	0.41
1:A:98:LEU:HD22	1:A:101:MET:HE3	2.01	0.41
1:A:124:HIS:O	1:A:128:GLN:N	2.42	0.41
1:A:343:PHE:CG	1:A:518:GLN:HG2	2.55	0.41
1:A:419:ASN:O	1:A:430:GLY:HA2	2.20	0.41
1:A:297:ARG:HG2	9:A:1192:HOH:O	2.21	0.41
1:A:511:LEU:HD12	1:A:511:LEU:HA	1.79	0.41
1:A:63:GLN:N	1:A:63:GLN:NE2	2.68	0.41
1:A:66:THR:HB	1:A:70:PHE:C	2.46	0.41
1:A:146:LYS:HG3	1:A:147:ASN:N	2.35	0.41
1:A:264:THR:HG23	1:A:392:ILE:HB	2.02	0.41
1:A:210:LEU:HB2	1:A:212:LEU:HG	2.04	0.40
8:A:605:HEM:HBB2	8:A:605:HEM:CMB	2.46	0.40
1:A:146:LYS:CG	1:A:147:ASN:ND2	2.85	0.40
1:A:348:ARG:NH1	8:A:605:HEM:HBA2	2.35	0.40
1:A:480:LEU:HD12	1:A:480:LEU:HA	1.93	0.40
1:A:180:ILE:HG22	1:A:181:ASN:N	2.36	0.40
1:A:381:PHE:CZ	1:A:424:PRO:HG3	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:PHE:HB2	9:A:1208:HOH:O	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%)	542 (92%)	39 (7%)	11 (2%)	6 11

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	167	CYS
1	A	168	PRO
1	A	169	THR
1	A	174	SER
1	A	593	ARG
1	A	170	PRO
1	A	18	ASN
1	A	9	PRO
1	A	13	VAL
1	A	370	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	517/517 (100%)	470 (91%)	47 (9%)	9 19

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	4	VAL
1	A	6	CYS
1	A	9	PRO
1	A	13	VAL
1	A	18	ASN
1	A	32	ARG
1	A	57	LEU
1	A	63	GLN
1	A	82	ILE
1	A	91	VAL
1	A	98	LEU
1	A	118	GLU
1	A	124	HIS
1	A	126	LYS
1	A	127	THR
1	A	146	LYS
1	A	153	THR
1	A	158	MET
1	A	168	PRO
1	A	173	GLN
1	A	175	LEU
1	A	187	LEU
1	A	203	LEU
1	A	209	PRO
1	A	232	LYS
1	A	261	LEU
1	A	268	LEU
1	A	276	LEU
1	A	278	ARG
1	A	283	LEU
1	A	292	LEU
1	A	315	ILE
1	A	360	ARG
1	A	376	LEU
1	A	464	LEU
1	A	465	LYS
1	A	471	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	480	LEU
1	A	511	LEU
1	A	520	GLN
1	A	522	ILE
1	A	539	LYS
1	A	548	SER
1	A	551	ARG
1	A	581	THR
1	A	594	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	147	ASN
1	A	154	GLN
1	A	217	GLN
1	A	333	ASN
1	A	364	ASN
1	A	437	ASN
1	A	460	GLN
1	A	497	ASN
1	A	520	GLN

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	1.75	2 (25%)	7,12,14	3.56	2 (28%)

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	-	4/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-OG	3.31	1.70	1.60
1	A	198	SEP	OG-CB	2.40	1.53	1.44

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	OG-CB-CA	8.50	116.42	108.14
1	A	198	SEP	OG-P-O1P	3.18	115.03	106.44

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	198	SEP	CB-OG-P-O2P
1	A	198	SEP	CB-OG-P-O1P
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 ⓘ

10 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	0.71	0	17,19,21	1.13	1 (5%)
2	NAG	B	2	2	14,14,15	0.91	1 (7%)	17,19,21	0.72	0
2	MAN	B	3	2	11,11,12	0.83	1 (9%)	15,15,17	0.81	0
3	NAG	C	1	3,1	14,14,15	0.54	0	17,19,21	0.76	0
3	NAG	C	2	3	14,14,15	0.58	0	17,19,21	1.12	1 (5%)
2	NAG	D	1	2,1	14,14,15	0.52	0	17,19,21	0.85	0
2	NAG	D	2	2	14,14,15	0.81	0	17,19,21	1.38	3 (17%)
2	MAN	D	3	2	11,11,12	0.70	0	15,15,17	1.15	1 (6%)
3	NAG	E	1	3,1	14,14,15	1.53	2 (14%)	17,19,21	0.77	1 (5%)
3	NAG	E	2	3	14,14,15	1.48	1 (7%)	17,19,21	1.30	2 (11%)

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	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1
2	MAN	B	3	2	-	0/2/19/22	1/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	MAN	D	3	2	-	2/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	NAG	C1-C2	5.02	1.59	1.52
3	E	1	NAG	C1-C2	3.97	1.57	1.52
3	E	1	NAG	C3-C2	2.80	1.58	1.52
2	B	3	MAN	O5-C5	2.18	1.47	1.43
2	B	2	NAG	C1-C2	2.13	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	MAN	C1-C2-C3	3.70	115.03	109.64
2	D	2	NAG	C4-C3-C2	-3.66	105.66	111.02
3	E	2	NAG	C1-O5-C5	3.41	116.75	112.19
2	D	2	NAG	C1-O5-C5	2.78	115.91	112.19
2	B	1	NAG	C2-N2-C7	-2.44	119.64	122.90
2	D	2	NAG	C2-N2-C7	-2.37	119.72	122.90
3	E	2	NAG	O5-C1-C2	2.29	114.83	111.29
3	C	2	NAG	C2-N2-C7	-2.25	119.88	122.90
3	E	1	NAG	C4-C3-C2	2.16	114.18	111.02

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	MAN	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
2	D	3	MAN	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 5 short contacts:

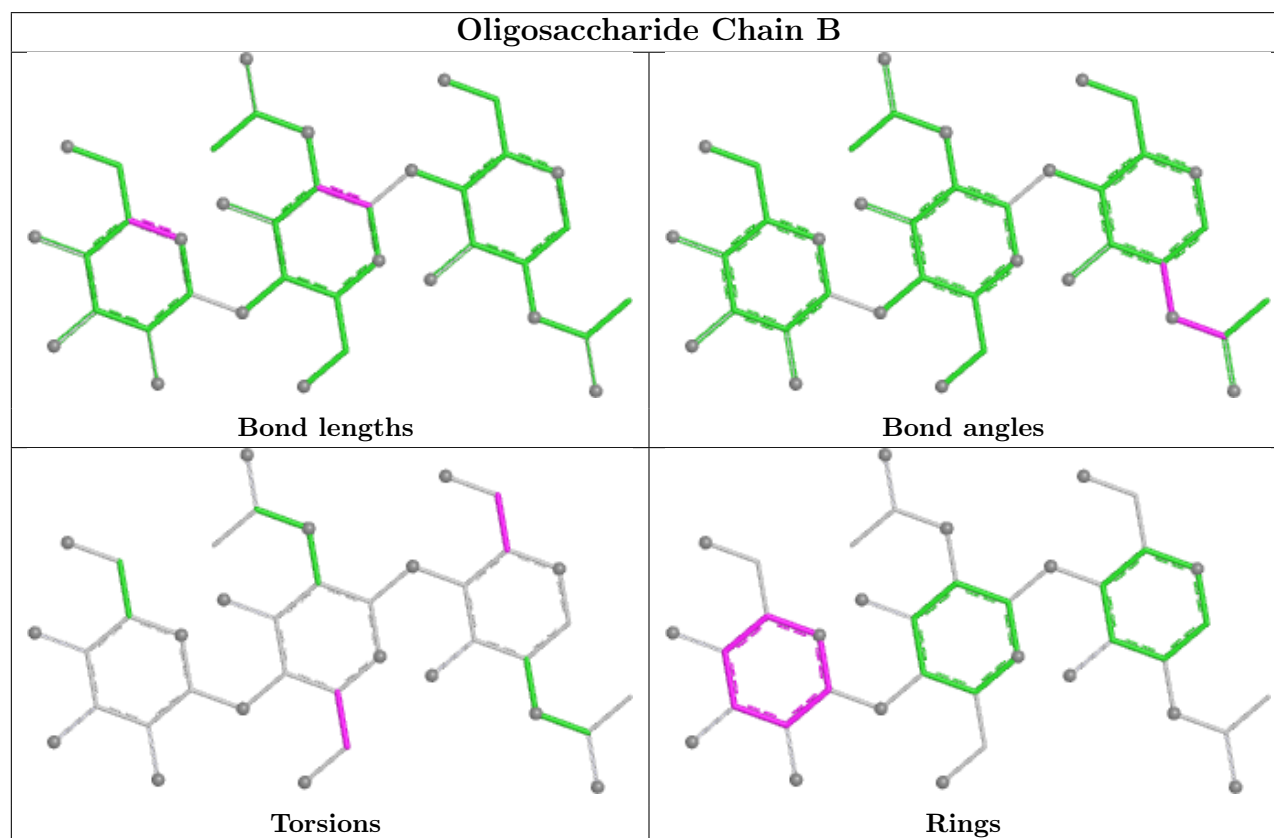
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	2	0
2	B	1	NAG	1	0

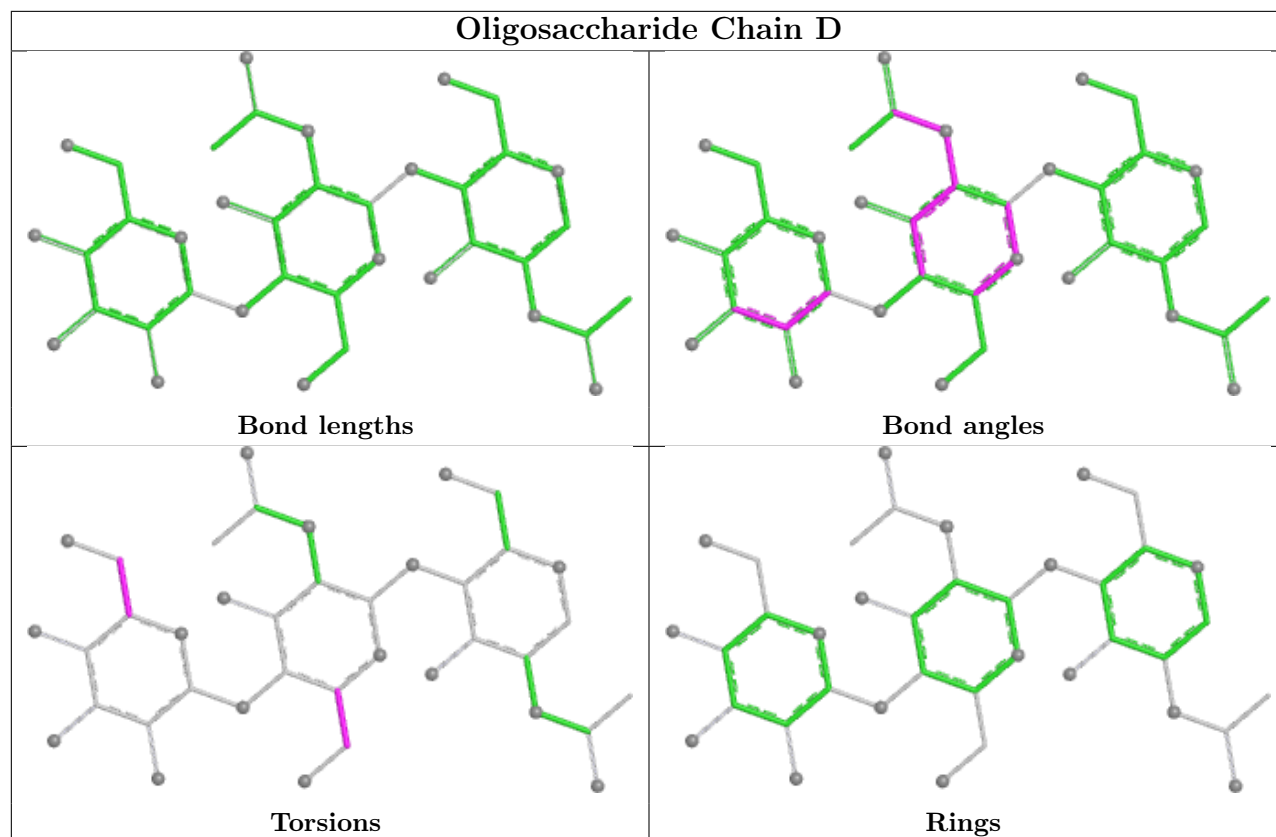
Continued on next page...

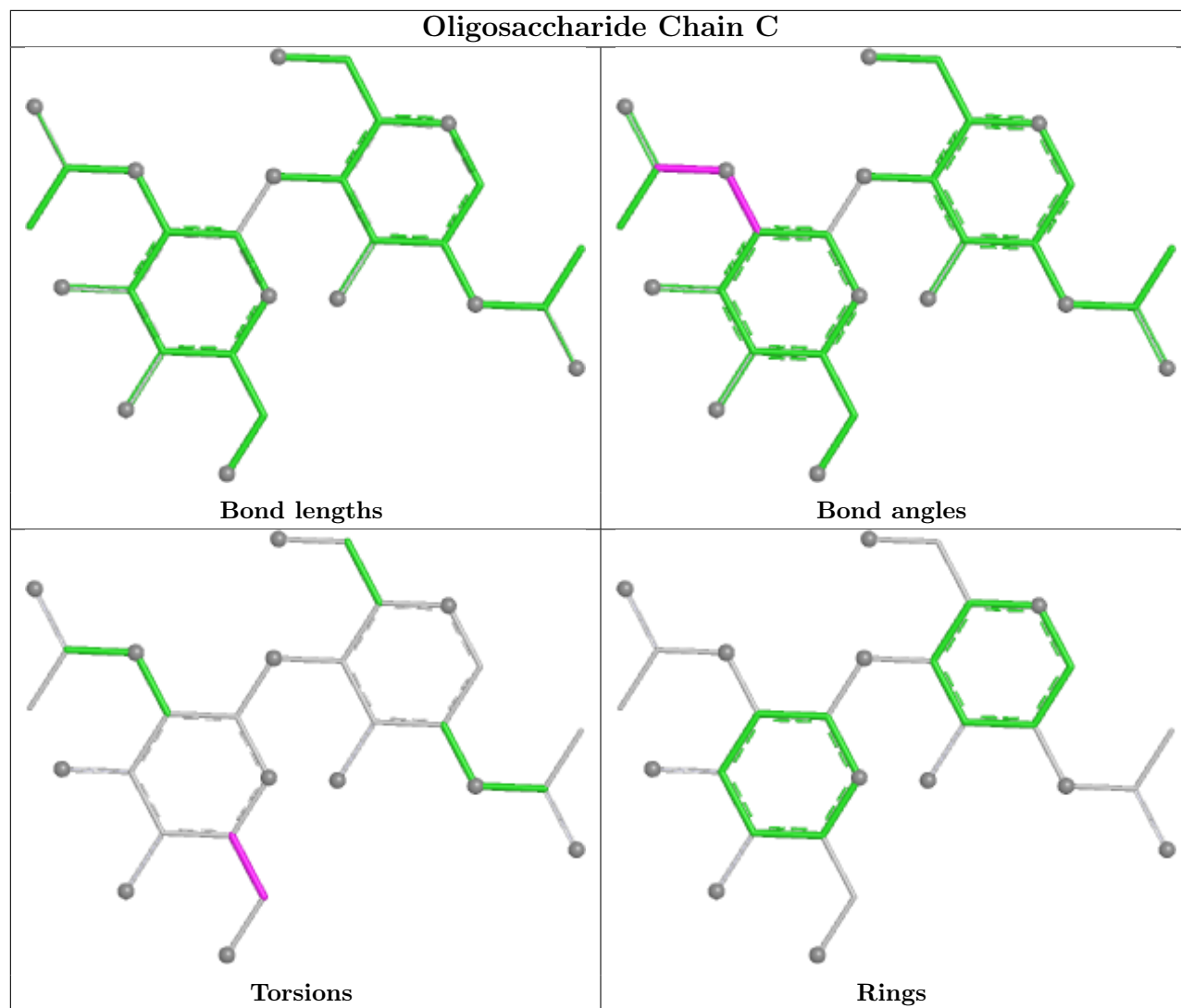
Continued from previous page...

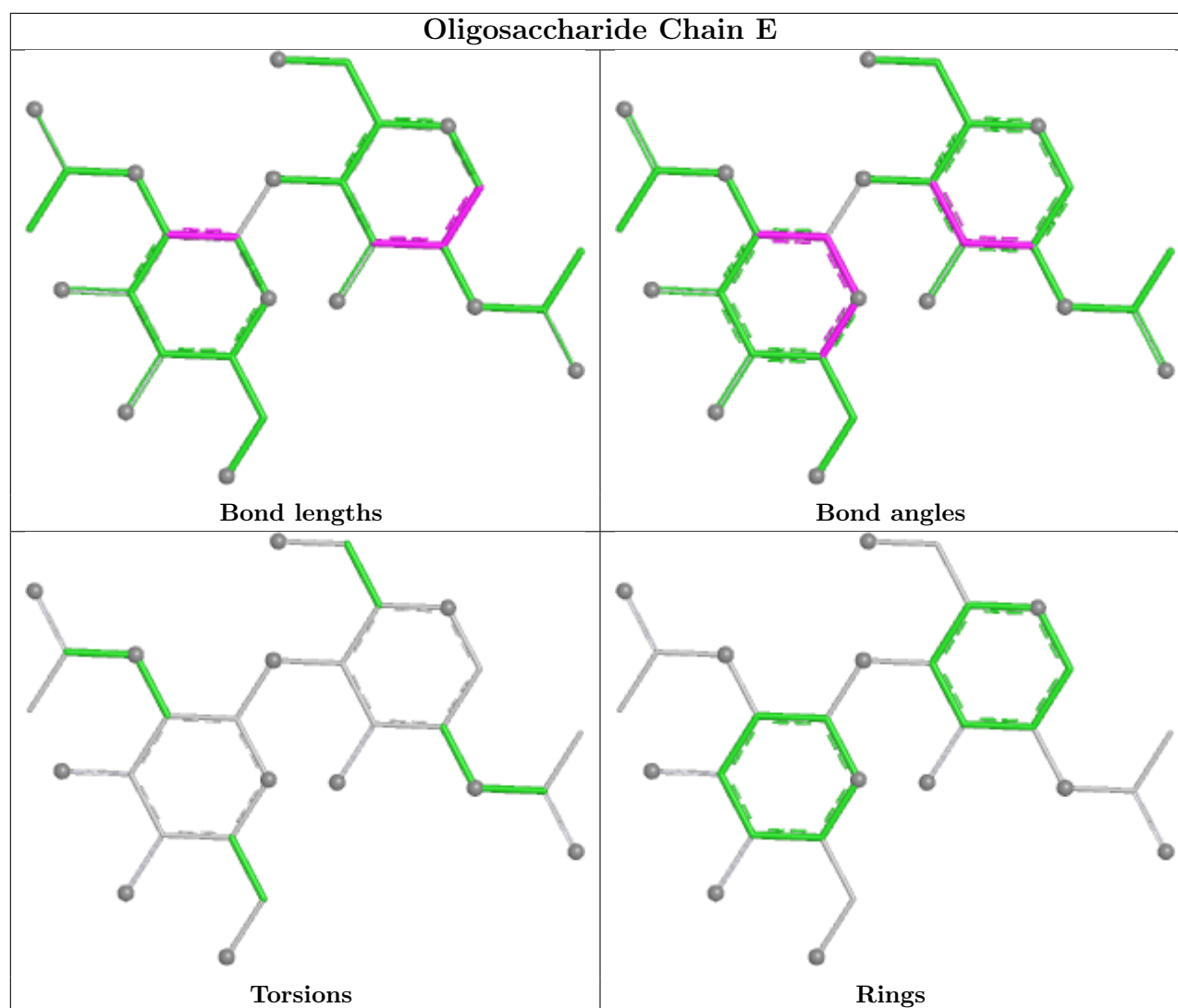
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	3	0
2	D	3	MAN	2	0
2	B	2	NAG	1	0

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









5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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$
6	SCN	A	607	-	1,2,2	1.58	0	0,1,1	-	-
8	HEM	A	605	9,1	50,50,50	2.30	18 (36%)	67,82,82	1.42	8 (11%)
4	AIN	A	596	-	13,13,13	3.87	5 (38%)	17,17,17	4.07	9 (52%)

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
8	HEM	A	605	9,1	-	4/14/54/54	-
4	AIN	A	596	-	-	4/8/8/8	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	596	AIN	C4-C3	7.33	1.51	1.39
8	A	605	HEM	C3D-C2D	6.65	1.51	1.36
4	A	596	AIN	C1-C2	6.23	1.52	1.39
4	A	596	AIN	C6-C1	6.07	1.49	1.38
4	A	596	AIN	C3-C2	5.63	1.51	1.40
8	A	605	HEM	CBA-CGA	-5.45	1.38	1.50
8	A	605	HEM	CMC-C2C	4.45	1.59	1.50
4	A	596	AIN	O3-C8	4.38	1.51	1.36
8	A	605	HEM	CAB-C3B	4.01	1.58	1.47
8	A	605	HEM	CAC-C3C	3.89	1.57	1.47
8	A	605	HEM	FE-NC	3.75	2.07	1.95
8	A	605	HEM	C4D-C3D	3.02	1.50	1.45
8	A	605	HEM	C1B-C2B	2.87	1.50	1.44
8	A	605	HEM	FE-NA	2.81	2.04	1.95
8	A	605	HEM	CAD-C3D	2.69	1.58	1.51
8	A	605	HEM	C4A-C3A	2.51	1.49	1.43
8	A	605	HEM	FE-ND	2.47	2.02	1.94
8	A	605	HEM	C3C-C2C	2.46	1.42	1.37
8	A	605	HEM	CHA-C1A	-2.41	1.34	1.39
8	A	605	HEM	C1D-C2D	2.41	1.49	1.44
8	A	605	HEM	C2A-C3A	-2.35	1.32	1.38
8	A	605	HEM	C4A-NA	-2.15	1.35	1.39
8	A	605	HEM	O2A-CGA	-2.05	1.24	1.30

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	596	AIN	C2-O3-C8	10.34	139.46	117.66
4	A	596	AIN	O3-C8-O4	8.91	141.63	122.43
4	A	596	AIN	O3-C8-C9	-5.83	98.33	110.97
4	A	596	AIN	C5-C6-C1	-3.72	115.65	120.24
8	A	605	HEM	O2D-CGD-CBD	3.42	124.82	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	605	HEM	CHD-C1D-ND	3.36	128.04	124.42
8	A	605	HEM	O1D-CGD-CBD	-3.31	112.60	123.09
8	A	605	HEM	C3B-C4B-NB	3.10	111.70	109.47
8	A	605	HEM	C4D-ND-C1D	3.03	108.79	105.21
4	A	596	AIN	O1-C7-O2	-2.91	117.09	123.35
8	A	605	HEM	CAD-C3D-C4D	2.87	129.69	124.70
4	A	596	AIN	C6-C5-C4	2.77	123.65	120.24
8	A	605	HEM	CMA-C3A-C4A	2.66	129.47	125.42
4	A	596	AIN	C6-C1-C2	2.60	124.32	119.60
8	A	605	HEM	CBD-CAD-C3D	-2.43	105.81	112.53
4	A	596	AIN	O3-C2-C1	2.14	124.04	118.89
4	A	596	AIN	C2-C3-C7	2.09	127.50	123.73

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	596	AIN	C9-C8-O3-C2
4	A	596	AIN	O4-C8-O3-C2
4	A	596	AIN	C1-C2-O3-C8
4	A	596	AIN	C3-C2-O3-C8
8	A	605	HEM	CAD-CBD-CGD-O1D
8	A	605	HEM	CAD-CBD-CGD-O2D
8	A	605	HEM	CAA-CBA-CGA-O2A
8	A	605	HEM	CAA-CBA-CGA-O1A

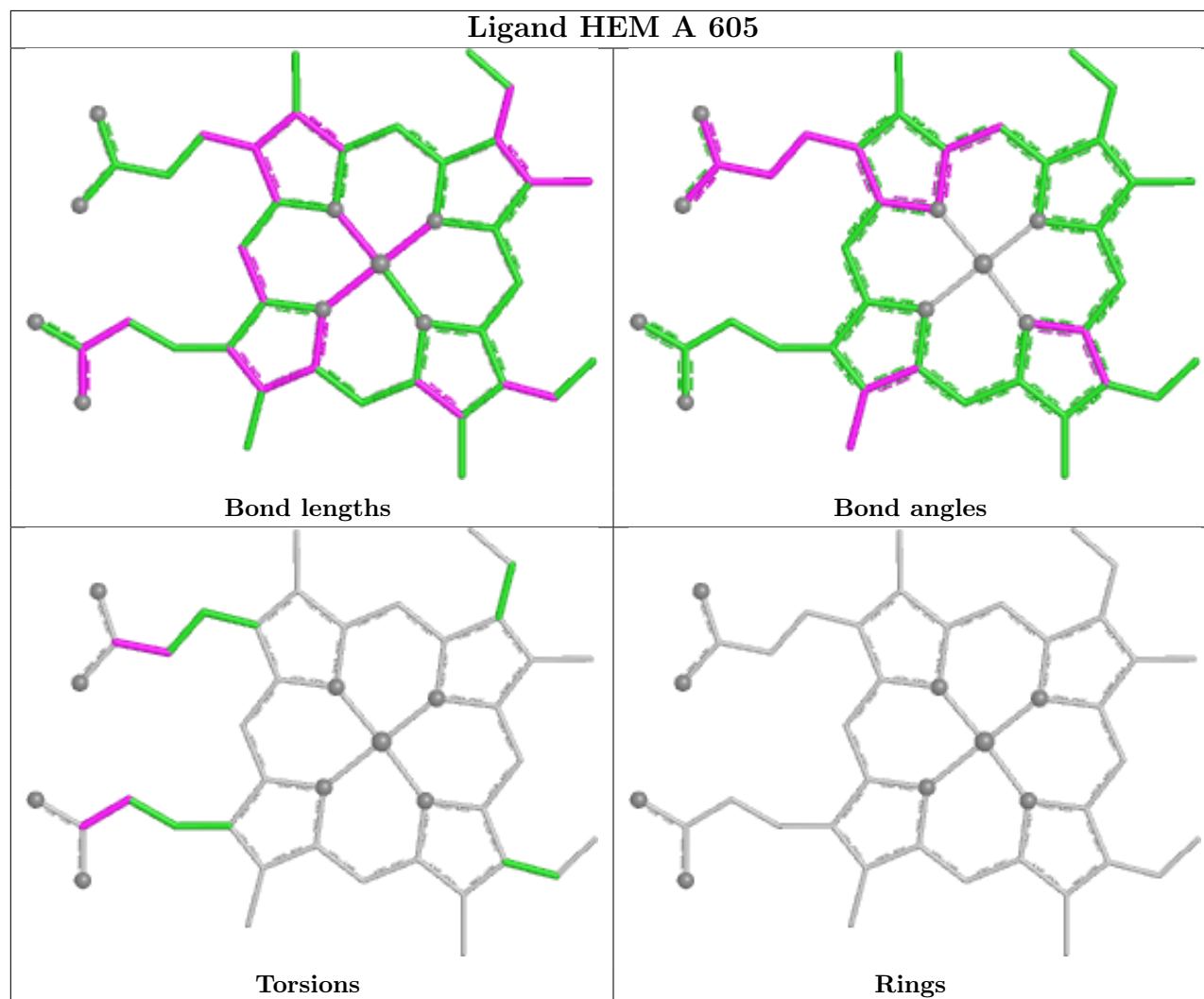
There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	605	HEM	9	0
4	A	596	AIN	19	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	594/595 (99%)	-0.12	19 (3%) 50 46	12, 30, 75, 100	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	ALA	3.7
1	A	5	GLY	3.4
1	A	119	LEU	3.4
1	A	11	PRO	3.3
1	A	169	THR	3.1
1	A	2	TRP	3.1
1	A	7	GLY	2.9
1	A	9	PRO	2.8
1	A	168	PRO	2.8
1	A	120	GLY	2.8
1	A	170	PRO	2.8
1	A	594	GLU	2.8
1	A	167	CYS	2.7
1	A	12	LEU	2.4
1	A	172	TYR	2.4
1	A	121	SER	2.4
1	A	173	GLN	2.4
1	A	13	VAL	2.3
1	A	6	CYS	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($\text{\AA}^2$)	Q<0.9
1	SEP	A	198	10/11	0.91	0.12	28,32,44,48	0

6.3 Carbohydrates

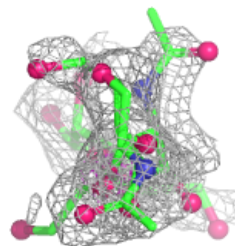
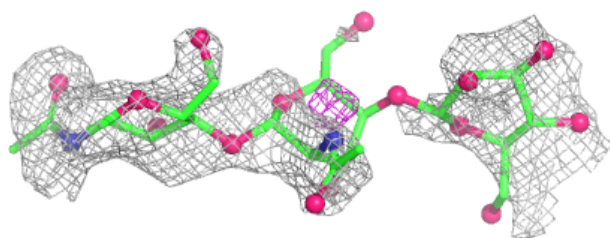
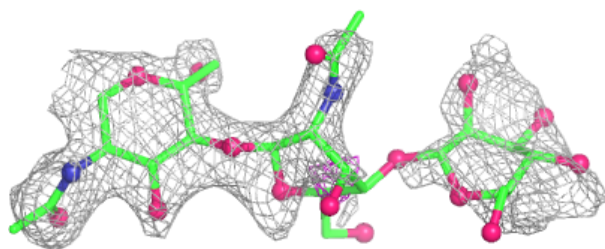
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	B	3	11/12	0.51	0.14	90,91,93,93	0
3	NAG	E	2	14/15	0.52	0.17	79,83,86,86	0
2	MAN	D	3	11/12	0.56	0.15	80,80,81,82	0
3	NAG	E	1	14/15	0.62	0.17	58,64,67,74	0
2	NAG	B	2	14/15	0.66	0.15	78,83,85,88	0
2	NAG	D	2	14/15	0.71	0.13	67,69,73,77	0
3	NAG	C	2	14/15	0.71	0.13	61,65,67,67	0
2	NAG	B	1	14/15	0.79	0.11	55,58,64,71	0
3	NAG	C	1	14/15	0.86	0.10	42,49,52,56	0
2	NAG	D	1	14/15	0.89	0.11	52,55,57,62	0

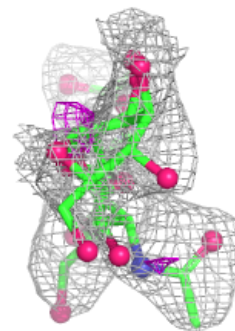
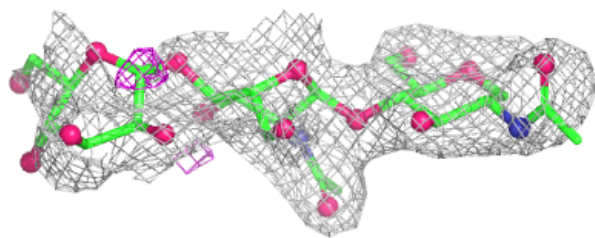
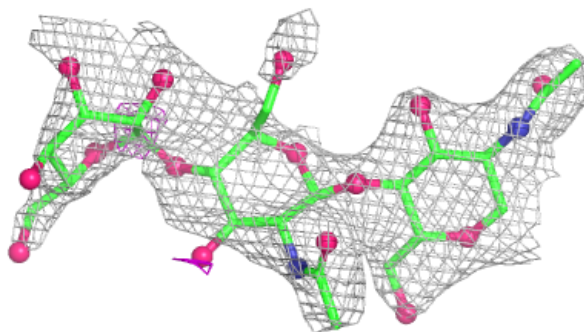
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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

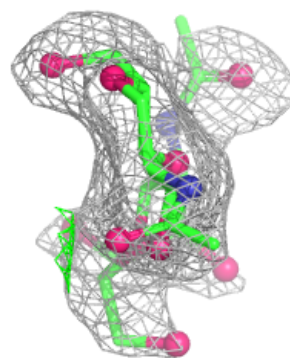
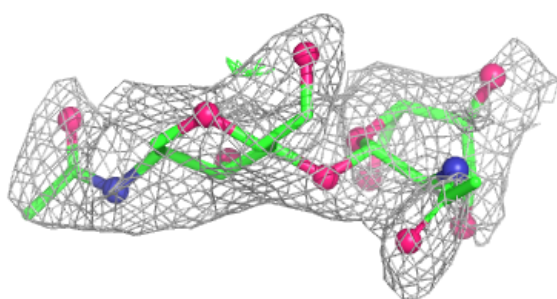
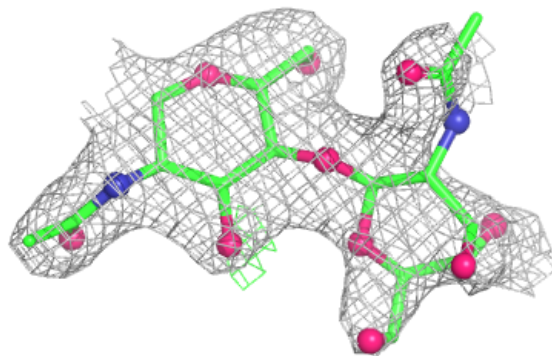
**Electron density around Chain D:**

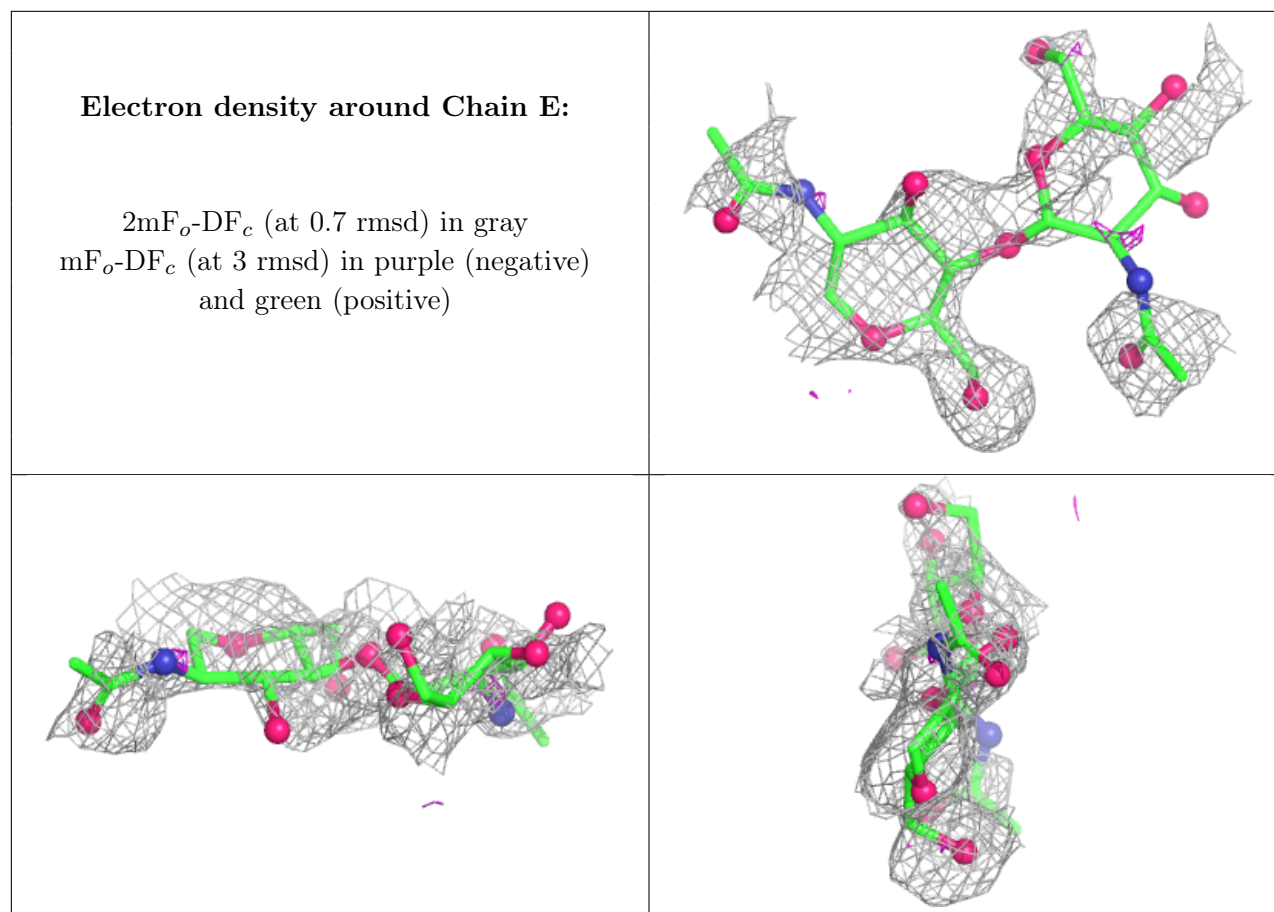
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain C:

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





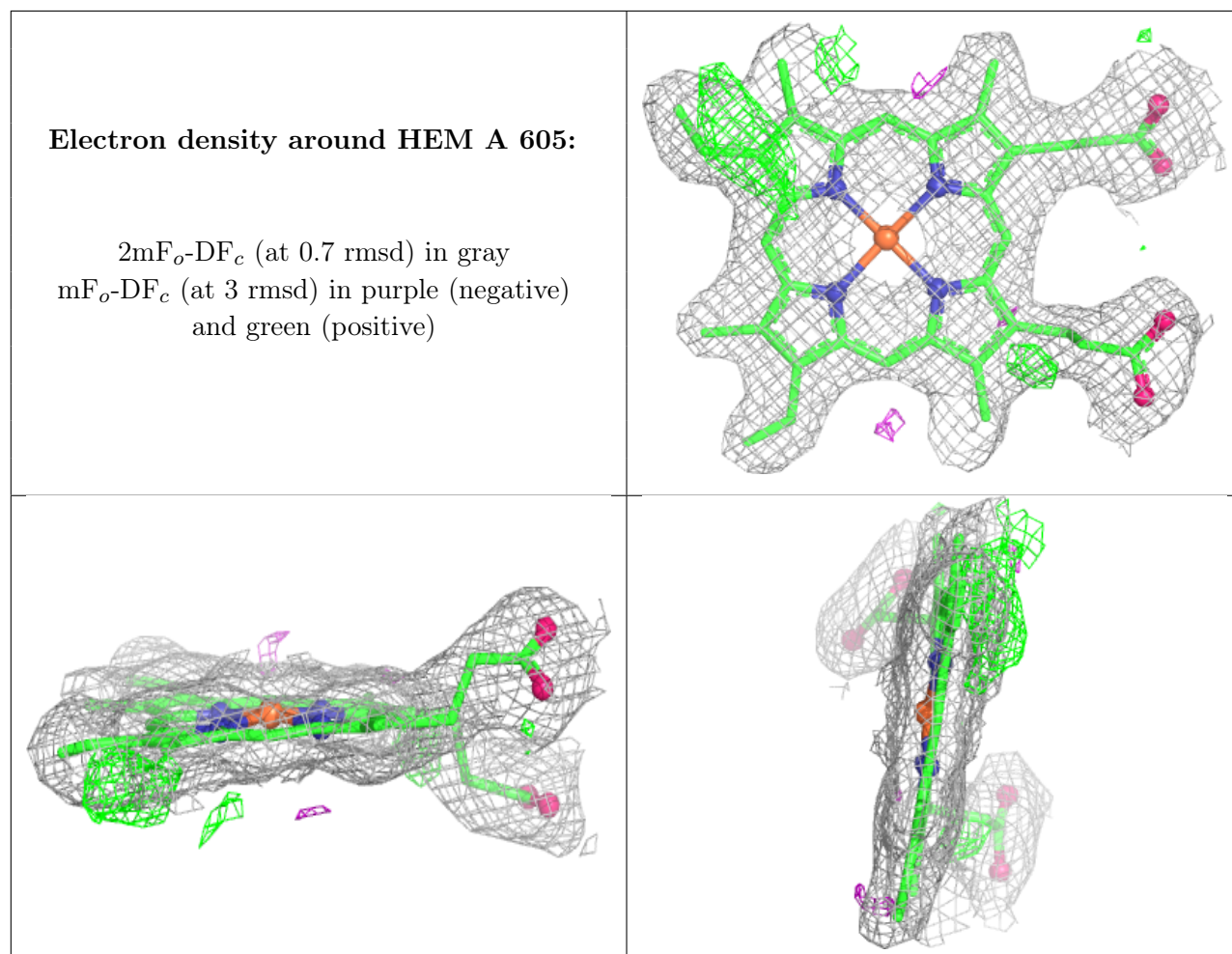
6.4 Ligands [i](#)

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	AIN	A	596	13/13	0.77	0.21	63,67,73,74	0
6	SCN	A	607	3/3	0.89	0.13	32,32,35,41	0
5	CA	A	606	1/1	0.95	0.04	16,16,16,16	0
7	IOD	A	610	1/1	0.95	0.10	100,100,100,100	0
7	IOD	A	612	1/1	0.96	0.15	95,95,95,95	0
8	HEM	A	605	43/43	0.96	0.08	8,16,21,23	0
7	IOD	A	613	1/1	0.98	0.07	70,70,70,70	0
7	IOD	A	614	1/1	0.98	0.12	75,75,75,75	0
7	IOD	A	609	1/1	0.98	0.10	90,90,90,90	0
7	IOD	A	611	1/1	0.99	0.09	79,79,79,79	0
7	IOD	A	608	1/1	1.00	0.01	26,26,26,26	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.