



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:53 AM UTC

PDB ID : 3ERH / pdb_00003erh
Title : First structural evidence of substrate specificity in mammalian peroxidases: Crystal structures of substrate complexes with lactoperoxidases from two different species
Authors : Sheikh, I.A.; Singh, N.; Singh, A.K.; Sinha, M.; Singh, S.B.; Bhushan, A.; Kaur, P.; Srinivasan, A.; Sharma, S.; Singh, T.P.
Deposited on : 2008-10-02
Resolution : 2.40 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

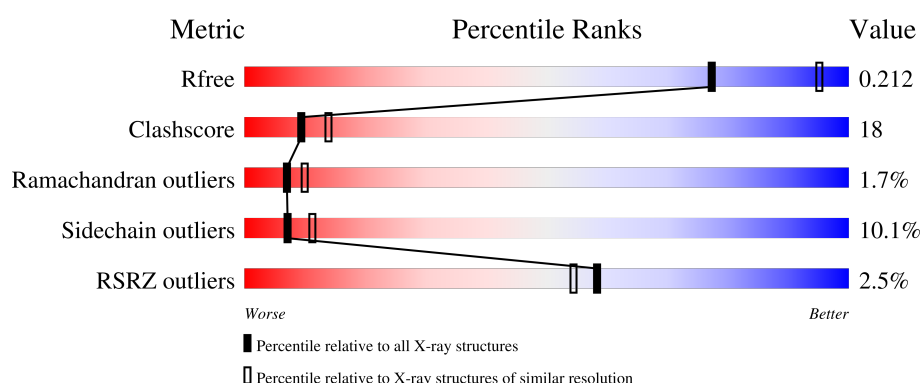
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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% 65% 26% 7% .
2	B	2	50% 50%
2	C	2	50% 50%
3	D	3	33% 67%
4	E	4	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
8	IOD	A	611	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5378 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
			4778	3040	847	864	1	26			

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



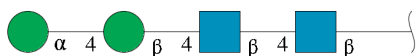
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 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.



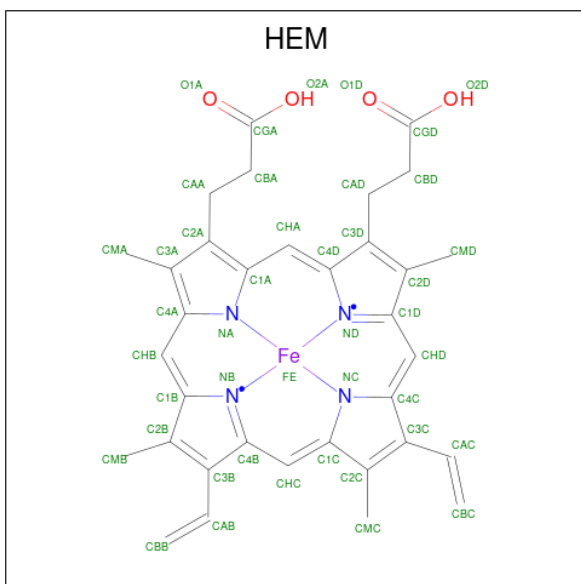
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



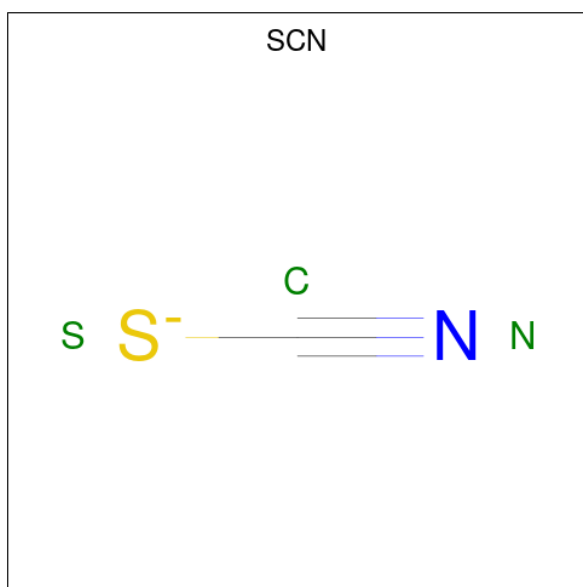
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- 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	C	Fe	N O	0	0
			43	34	1	4 4		

- 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		
6	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 8 is IODIDE ION (CCD ID: IOD) (formula: I).

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

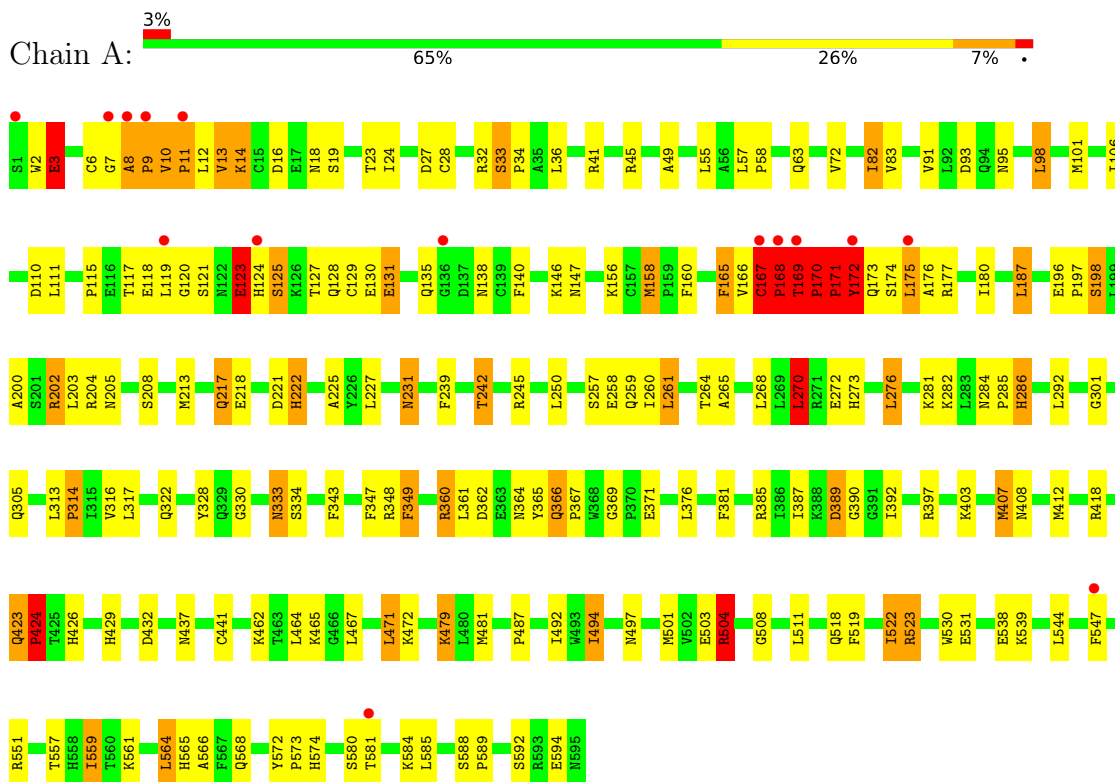
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	398	Total	O	0	0
			398	398		

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



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



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

Chain D:  33% 67%

MAG1
MAG2
MAN3

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

Chain E:  100%

MAG1
MAG2
BMA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.21Å 80.54Å 77.88Å 90.00° 102.64° 90.00°	Depositor
Resolution (Å)	19.46 – 2.40 19.46 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.46-2.40) 98.6 (19.46-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.41Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.180 , 0.195 0.182 , 0.212	Depositor DCC
R_{free} test set	1290 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5378	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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: HEM, SEP, BMA, CA, NAG, SCN, IOD, MAN

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	0.65	9/4896 (0.2%)	1.31	81/6640 (1.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	PRO	N-CA	13.72	1.64	1.47
1	A	367	PRO	CA-C	-8.61	1.42	1.52
1	A	170	PRO	CA-C	7.49	1.59	1.52
1	A	222	HIS	C-N	-6.62	1.23	1.33
1	A	367	PRO	C-N	-5.74	1.25	1.33
1	A	568	GLN	CA-CB	5.53	1.62	1.53
1	A	10	VAL	N-CA	-5.38	1.40	1.47
1	A	424	PRO	CA-C	-5.34	1.44	1.52
1	A	173	GLN	N-CA	5.13	1.52	1.46

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	CYS	O-C-N	-18.29	100.29	121.32
1	A	172	TYR	N-CA-C	15.99	131.89	109.18
1	A	168	PRO	N-CA-C	12.93	139.11	112.47
1	A	121	SER	N-CA-C	-10.79	98.82	113.18
1	A	123	GLU	N-CA-C	10.41	124.92	110.24
1	A	316	VAL	N-CA-C	-9.87	102.29	111.67
1	A	124	HIS	N-CA-C	-9.82	100.95	113.72
1	A	217	GLN	OE1-CD-NE2	-9.75	112.85	122.60
1	A	568	GLN	OE1-CD-NE2	-9.66	112.94	122.60
1	A	173	GLN	OE1-CD-NE2	-9.52	113.08	122.60
1	A	366	GLN	OE1-CD-NE2	-9.37	113.23	122.60
1	A	135	GLN	OE1-CD-NE2	-9.18	113.42	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	PRO	CA-C-N	8.54	142.63	121.80
1	A	168	PRO	C-N-CA	8.54	142.63	121.80
1	A	172	TYR	CA-C-N	8.28	137.35	121.54
1	A	172	TYR	C-N-CA	8.28	137.35	121.54
1	A	171	PRO	N-CA-C	8.20	129.36	112.47
1	A	222	HIS	CB-CA-C	-8.16	100.14	111.73
1	A	173	GLN	N-CA-C	8.03	127.89	110.80
1	A	330	GLY	N-CA-C	7.62	119.19	111.95
1	A	140	PHE	CA-C-N	7.54	127.58	119.89
1	A	140	PHE	C-N-CA	7.54	127.58	119.89
1	A	568	GLN	CG-CD-NE2	7.25	127.27	116.40
1	A	423	GLN	CA-C-N	7.08	126.60	119.24
1	A	423	GLN	C-N-CA	7.08	126.60	119.24
1	A	508	GLY	CA-C-N	6.96	126.21	118.97
1	A	508	GLY	C-N-CA	6.96	126.21	118.97
1	A	173	GLN	CG-CD-NE2	6.95	126.82	116.40
1	A	566	ALA	N-CA-C	6.86	120.75	112.38
1	A	135	GLN	CG-CD-NE2	6.79	126.59	116.40
1	A	82	ILE	N-CA-C	6.78	117.39	111.56
1	A	158	MET	N-CA-C	-6.78	100.08	110.32
1	A	170	PRO	N-CA-C	6.74	118.93	110.70
1	A	426	HIS	CA-CB-CG	-6.67	107.13	113.80
1	A	366	GLN	CG-CD-NE2	6.57	126.25	116.40
1	A	217	GLN	CG-CD-NE2	6.51	126.17	116.40
1	A	225	ALA	N-CA-C	6.48	119.08	110.53
1	A	169	THR	CA-C-N	6.43	127.00	120.38
1	A	169	THR	C-N-CA	6.43	127.00	120.38
1	A	504	ARG	CD-NE-CZ	6.37	133.32	124.40
1	A	559	ILE	N-CA-C	-6.30	100.64	109.21
1	A	125	SER	N-CA-C	-6.21	104.61	111.82
1	A	131	GLU	N-CA-C	6.16	118.08	111.36
1	A	10	VAL	N-CA-C	-6.15	102.92	108.95
1	A	222	HIS	CA-CB-CG	6.07	119.87	113.80
1	A	349	PHE	N-CA-C	-5.91	104.97	111.82
1	A	172	TYR	N-CA-CB	-5.90	101.90	111.22
1	A	412	MET	N-CA-C	5.87	120.54	111.56
1	A	111	LEU	N-CA-C	5.87	120.61	112.45
1	A	169	THR	N-CA-CB	5.83	120.74	110.37
1	A	429	HIS	N-CA-C	-5.76	101.59	109.71
1	A	110	ASP	N-CA-C	-5.71	105.03	112.23
1	A	95	ASN	N-CA-C	5.71	117.74	110.61
1	A	222	HIS	CB-CG-ND1	-5.64	114.24	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	PRO	CA-N-CD	-5.63	104.11	112.00
1	A	369	GLY	CA-C-N	5.63	126.88	119.84
1	A	369	GLY	C-N-CA	5.63	126.88	119.84
1	A	167	CYS	N-CA-C	-5.62	97.38	109.81
1	A	128	GLN	N-CA-C	-5.59	105.71	112.54
1	A	33	SER	CA-C-N	5.57	126.81	119.84
1	A	33	SER	C-N-CA	5.57	126.81	119.84
1	A	23	THR	N-CA-C	-5.50	103.43	110.53
1	A	170	PRO	CB-CA-C	5.47	117.60	110.92
1	A	260	ILE	N-CA-C	5.46	116.85	110.62
1	A	83	VAL	N-CA-C	5.46	120.09	112.50
1	A	138	ASN	N-CA-C	5.44	119.63	113.15
1	A	270	LEU	N-CA-C	-5.37	105.43	111.28
1	A	239	PHE	N-CA-C	5.36	117.81	111.33
1	A	387	ILE	N-CA-C	5.29	115.50	110.42
1	A	389	ASP	N-CA-C	5.29	116.65	110.41
1	A	168	PRO	CA-N-CD	-5.28	104.60	112.00
1	A	407	MET	N-CA-C	-5.25	102.61	110.23
1	A	390	GLY	N-CA-C	5.24	121.98	114.64
1	A	72	VAL	CA-C-N	5.15	125.08	119.78
1	A	72	VAL	C-N-CA	5.15	125.08	119.78
1	A	208	SER	CA-C-N	5.12	126.24	119.84
1	A	208	SER	C-N-CA	5.12	126.24	119.84
1	A	568	GLN	CB-CG-CD	5.04	121.16	112.60
1	A	367	PRO	CB-CA-C	5.03	117.97	111.64
1	A	492	ILE	N-CA-C	5.01	115.62	110.36
1	A	441	CYS	N-CA-C	-5.01	105.73	111.14

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	4778	0	4685	159	0
2	B	28	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	28	0	25	2	0
3	D	39	0	34	3	0
4	E	50	0	43	9	0
5	A	43	0	30	5	0
6	A	6	0	0	1	0
7	A	1	0	0	0	0
8	A	7	0	0	3	0
9	A	398	0	0	46	0
All	All	5378	0	4842	177	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 18.

All (177) 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:504:ARG:NH2	8:A:611:IOD:I	2.64	1.01
1:A:584:LYS:HD2	9:A:819:HOH:O	1.59	1.00
1:A:197:PRO:HD2	1:A:198:SEP:O3P	1.62	1.00
1:A:156:LYS:HD2	9:A:750:HOH:O	1.64	0.95
9:A:986:HOH:O	4:E:1:NAG:H3	1.64	0.95
1:A:127:THR:HG23	1:A:131:GLU:HG3	1.51	0.92
1:A:481:MET:SD	1:A:487:PRO:HD3	2.10	0.89
1:A:2:TRP:HB3	1:A:175:LEU:HG	1.57	0.86
1:A:196:GLU:HB3	1:A:198:SEP:O3P	1.75	0.85
1:A:115:PRO:HD2	9:A:965:HOH:O	1.77	0.84
1:A:106:ILE:HD11	1:A:265:ALA:HB1	1.60	0.84
1:A:175:LEU:HD22	1:A:176:ALA:H	1.44	0.83
1:A:82:ILE:HD11	1:A:479:LYS:HB2	1.60	0.83
1:A:63:GLN:HB3	9:A:941:HOH:O	1.79	0.82
9:A:943:HOH:O	4:E:2:NAG:H61	1.79	0.81
1:A:9:PRO:HG2	1:A:41:ARG:CZ	2.11	0.80
1:A:407:MET:HB3	1:A:501:MET:HE3	1.61	0.80
1:A:175:LEU:CD2	1:A:176:ALA:H	1.94	0.80
1:A:547:PHE:HE2	1:A:585:LEU:HD22	1.47	0.79
1:A:9:PRO:O	1:A:11:PRO:HD3	1.81	0.79
5:A:605:HEM:HMC2	5:A:605:HEM:HBC2	1.65	0.79
1:A:580:SER:HB2	9:A:921:HOH:O	1.84	0.76
1:A:169:THR:HB	1:A:170:PRO:HD3	1.68	0.76
4:E:2:NAG:H62	4:E:3:BMA:O5	1.85	0.76
9:A:1001:HOH:O	4:E:4:MAN:H2	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:LYS:HE3	9:A:985:HOH:O	1.91	0.71
1:A:127:THR:HG23	1:A:131:GLU:CG	2.20	0.71
1:A:565:HIS:CE1	2:B:2:NAG:H81	2.25	0.71
1:A:170:PRO:HB3	1:A:171:PRO:HD2	1.73	0.70
1:A:166:VAL:HG12	1:A:180:ILE:HG12	1.74	0.69
1:A:503:GLU:HG3	9:A:794:HOH:O	1.93	0.68
1:A:172:TYR:HB3	9:A:827:HOH:O	1.93	0.68
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.29	0.68
1:A:174:SER:HA	9:A:936:HOH:O	1.93	0.67
9:A:806:HOH:O	4:E:2:NAG:H2	1.95	0.67
1:A:504:ARG:NE	8:A:611:IOD:I	2.97	0.66
1:A:175:LEU:HD22	1:A:176:ALA:N	2.08	0.66
1:A:227:LEU:HD23	1:A:270:LEU:HD22	1.78	0.66
1:A:565:HIS:ND1	2:B:2:NAG:H81	2.11	0.65
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.62	0.64
1:A:8:ALA:N	1:A:9:PRO:HD2	2.13	0.64
1:A:588:SER:OG	1:A:589:PRO:HD3	1.99	0.63
1:A:504:ARG:CZ	8:A:611:IOD:I	3.16	0.63
9:A:808:HOH:O	2:C:2:NAG:H4	1.98	0.63
1:A:123:GLU:HG3	1:A:125:SER:HB3	1.81	0.63
1:A:465:LYS:HD2	9:A:748:HOH:O	1.99	0.63
1:A:127:THR:CG2	1:A:131:GLU:HG3	2.28	0.62
1:A:8:ALA:N	1:A:9:PRO:CD	2.62	0.62
1:A:242:THR:HG21	9:A:928:HOH:O	1.99	0.62
1:A:13:VAL:HA	9:A:754:HOH:O	2.01	0.61
1:A:407:MET:HB3	1:A:501:MET:CE	2.29	0.61
1:A:106:ILE:HD11	1:A:265:ALA:CB	2.30	0.60
1:A:257:SER:O	1:A:381:PHE:HA	2.02	0.60
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.84	0.60
1:A:564:LEU:HB3	1:A:565:HIS:HD2	1.66	0.59
1:A:282:LYS:HD3	9:A:927:HOH:O	2.02	0.59
9:A:699:HOH:O	4:E:3:BMA:H3	2.02	0.59
1:A:284:ASN:HA	1:A:286:HIS:CE1	2.38	0.59
1:A:360:ARG:NH2	1:A:389:ASP:OD2	2.36	0.58
1:A:93:ASP:O	1:A:403:LYS:HD3	2.04	0.58
1:A:328:TYR:CD1	1:A:523:ARG:HD3	2.39	0.58
1:A:504:ARG:HD2	9:A:803:HOH:O	2.05	0.57
1:A:561:LYS:HG3	9:A:813:HOH:O	2.05	0.57
1:A:129:CYS:HB2	9:A:698:HOH:O	2.04	0.57
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.39	0.57
1:A:9:PRO:CG	1:A:41:ARG:NE	2.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LYS:O	1:A:147:ASN:HB2	2.05	0.56
1:A:120:GLY:HA3	9:A:786:HOH:O	2.06	0.56
1:A:169:THR:CB	1:A:170:PRO:CD	2.82	0.56
1:A:169:THR:HB	1:A:170:PRO:CD	2.36	0.56
1:A:538:GLU:HB3	9:A:981:HOH:O	2.05	0.55
1:A:197:PRO:CD	1:A:198:SEP:O3P	2.48	0.55
1:A:165:PHE:CE1	1:A:177:ARG:NH2	2.75	0.55
1:A:9:PRO:HG3	1:A:41:ARG:HD3	1.89	0.55
1:A:11:PRO:O	1:A:13:VAL:HG22	2.06	0.55
1:A:200:ALA:O	1:A:204:ARG:HG3	2.07	0.55
5:A:605:HEM:HBC2	5:A:605:HEM:CMC	2.36	0.55
1:A:165:PHE:O	1:A:180:ILE:HD11	2.07	0.54
1:A:322:GLN:HG3	9:A:755:HOH:O	2.06	0.54
1:A:360:ARG:O	1:A:361:LEU:HD23	2.07	0.54
1:A:362:ASP:O	1:A:365:TYR:N	2.35	0.54
1:A:175:LEU:CD2	1:A:176:ALA:N	2.67	0.54
1:A:16:ASP:HB3	1:A:19:SER:HB2	1.90	0.53
1:A:408:ASN:HB2	9:A:768:HOH:O	2.08	0.53
1:A:572:TYR:CZ	1:A:573:PRO:HB3	2.43	0.53
1:A:205:ASN:OD1	1:A:205:ASN:C	2.52	0.52
1:A:10:VAL:HG12	9:A:817:HOH:O	2.10	0.52
1:A:481:MET:SD	1:A:487:PRO:CD	2.94	0.52
1:A:272:GLU:HG3	1:A:276:LEU:HD22	1.92	0.51
1:A:8:ALA:HB3	9:A:798:HOH:O	2.10	0.51
1:A:172:TYR:CD2	1:A:172:TYR:N	2.72	0.51
1:A:301:GLY:O	1:A:305:GLN:HG3	2.10	0.51
1:A:349:PHE:CB	1:A:497:ASN:HD21	2.22	0.51
1:A:98:LEU:HD22	1:A:101:MET:HE3	1.93	0.51
1:A:557:THR:OG1	1:A:559:ILE:HG12	2.11	0.51
1:A:588:SER:N	1:A:589:PRO:CD	2.75	0.50
1:A:221:ASP:O	1:A:222:HIS:HB2	2.11	0.50
1:A:281:LYS:HD2	1:A:285:PRO:HA	1.94	0.50
1:A:362:ASP:OD1	1:A:362:ASP:C	2.55	0.50
1:A:381:PHE:CZ	1:A:424:PRO:HG3	2.47	0.50
1:A:187:LEU:HD13	1:A:305:GLN:HA	1.93	0.50
1:A:360:ARG:NH1	1:A:371:GLU:O	2.44	0.50
9:A:840:HOH:O	3:D:2:NAG:H3	2.12	0.50
1:A:9:PRO:HG2	1:A:41:ARG:NE	2.26	0.49
1:A:286:HIS:ND1	1:A:286:HIS:N	2.46	0.49
1:A:397:ARG:HG2	1:A:559:ILE:HD12	1.94	0.49
1:A:242:THR:O	1:A:245:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:GLY:C	1:A:9:PRO:HD2	2.37	0.49
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.48	0.48
9:A:942:HOH:O	4:E:4:MAN:H5	2.13	0.48
1:A:9:PRO:HG3	1:A:41:ARG:CD	2.43	0.48
1:A:572:TYR:CE2	1:A:573:PRO:HB3	2.49	0.48
1:A:467:LEU:HG	1:A:471:LEU:HD22	1.94	0.47
1:A:118:GLU:CB	9:A:834:HOH:O	2.61	0.47
1:A:118:GLU:HG3	9:A:770:HOH:O	2.14	0.47
1:A:165:PHE:CZ	1:A:169:THR:O	2.67	0.47
1:A:349:PHE:CA	1:A:497:ASN:HD21	2.26	0.47
1:A:175:LEU:HD13	9:A:708:HOH:O	2.14	0.47
1:A:503:GLU:HB2	9:A:742:HOH:O	2.15	0.47
1:A:385:ARG:O	1:A:389:ASP:HB3	2.15	0.47
1:A:313:LEU:HB2	1:A:314:PRO:CD	2.45	0.46
1:A:462:LYS:HG3	9:A:790:HOH:O	2.14	0.46
1:A:333:ASN:HD22	1:A:334:SER:N	2.13	0.46
1:A:82:ILE:HG21	1:A:494:ILE:HD11	1.96	0.46
1:A:123:GLU:OE1	1:A:123:GLU:N	2.48	0.46
1:A:347:PHE:HB3	5:A:605:HEM:HMD3	1.98	0.46
1:A:57:LEU:HA	1:A:58:PRO:HD3	1.83	0.46
1:A:175:LEU:HA	9:A:883:HOH:O	2.15	0.46
1:A:27:ASP:O	1:A:28:CYS:HB2	2.16	0.46
1:A:175:LEU:HD23	1:A:176:ALA:H	1.77	0.45
1:A:349:PHE:HA	1:A:497:ASN:ND2	2.29	0.45
3:D:2:NAG:H4	3:D:3:MAN:H2	1.32	0.45
1:A:574:HIS:HB3	9:A:886:HOH:O	2.15	0.45
1:A:2:TRP:CB	1:A:175:LEU:HG	2.39	0.45
1:A:581:THR:O	1:A:581:THR:HG22	2.17	0.45
5:A:605:HEM:HMC2	5:A:605:HEM:CBC	2.42	0.45
1:A:544:LEU:HD23	1:A:547:PHE:CZ	2.52	0.45
1:A:63:GLN:HG3	9:A:917:HOH:O	2.16	0.44
1:A:259:GLN:OE1	1:A:261:LEU:HB2	2.16	0.44
1:A:202:ARG:HD2	1:A:250:LEU:HD21	1.98	0.44
1:A:165:PHE:N	1:A:165:PHE:CD1	2.85	0.44
1:A:264:THR:HG23	1:A:392:ILE:HB	1.99	0.44
9:A:910:HOH:O	3:D:3:MAN:H4	2.17	0.44
1:A:2:TRP:O	1:A:3:GLU:C	2.61	0.44
4:E:2:NAG:H62	4:E:3:BMA:C5	2.48	0.44
5:A:605:HEM:CMB	5:A:605:HEM:HBB2	2.48	0.43
9:A:829:HOH:O	2:C:2:NAG:H3	2.19	0.43
1:A:45:ARG:CZ	1:A:49:ALA:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ASN:HA	9:A:686:HOH:O	2.18	0.43
1:A:572:TYR:HA	1:A:573:PRO:HA	1.82	0.43
1:A:118:GLU:HB2	9:A:834:HOH:O	2.18	0.42
1:A:55:LEU:HD21	9:A:1005:HOH:O	2.19	0.42
1:A:165:PHE:HZ	9:A:939:HOH:O	2.02	0.42
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.17	0.42
1:A:565:HIS:HD1	2:B:2:NAG:H81	1.82	0.42
1:A:313:LEU:HB2	1:A:314:PRO:HD3	2.00	0.42
1:A:24:ILE:HD13	1:A:24:ILE:HA	1.92	0.42
1:A:258:GLU:OE1	1:A:259:GLN:HG2	2.20	0.42
1:A:362:ASP:N	1:A:366:GLN:O	2.43	0.42
1:A:519:PHE:CD1	1:A:522:ILE:HD11	2.55	0.42
1:A:258:GLU:HG3	6:A:608:SCN:S	2.59	0.42
1:A:125:SER:C	1:A:127:THR:N	2.76	0.41
1:A:261:LEU:HD12	1:A:261:LEU:HA	1.89	0.41
1:A:14:LYS:HE2	1:A:14:LYS:HB3	1.86	0.41
1:A:364:ASN:O	1:A:365:TYR:HB2	2.21	0.41
4:E:2:NAG:H62	4:E:3:BMA:C6	2.51	0.41
1:A:32:ARG:NH1	9:A:1014:HOH:O	2.53	0.41
1:A:63:GLN:HB2	9:A:773:HOH:O	2.20	0.41
1:A:381:PHE:CE2	1:A:424:PRO:HD3	2.55	0.41
1:A:432:ASP:OD1	1:A:432:ASP:C	2.63	0.40
1:A:564:LEU:HD12	1:A:564:LEU:HA	1.93	0.40
1:A:33:SER:HA	1:A:34:PRO:HD2	1.89	0.40
1:A:158:MET:HE1	1:A:432:ASP:HB2	2.04	0.40
1:A:160:PHE:CD1	1:A:160:PHE:C	2.99	0.40
1:A:82:ILE:CD1	1:A:479:LYS:HB2	2.42	0.40
1:A:196:GLU:HA	1:A:197:PRO:HD3	1.85	0.40
1:A:361:LEU:HA	1:A:366:GLN:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	552 (93%)	30 (5%)	10 (2%)	7 10

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	A	167	CYS
1	A	169	THR
1	A	18	ASN
1	A	168	PRO
1	A	170	PRO
1	A	171	PRO
1	A	3	GLU
1	A	9	PRO
1	A	8	ALA

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%)	465 (90%)	52 (10%)	7 11

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	6	CYS
1	A	12	LEU
1	A	13	VAL
1	A	14	LYS
1	A	36	LEU
1	A	91	VAL
1	A	98	LEU
1	A	117	THR
1	A	119	LEU
1	A	123	GLU

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Mol	Chain	Res	Type
1	A	130	GLU
1	A	165	PHE
1	A	167	CYS
1	A	168	PRO
1	A	169	THR
1	A	171	PRO
1	A	172	TYR
1	A	175	LEU
1	A	187	LEU
1	A	202	ARG
1	A	203	LEU
1	A	217	GLN
1	A	218	GLU
1	A	231	ASN
1	A	242	THR
1	A	261	LEU
1	A	268	LEU
1	A	270	LEU
1	A	276	LEU
1	A	286	HIS
1	A	292	LEU
1	A	314	PRO
1	A	317	LEU
1	A	333	ASN
1	A	360	ARG
1	A	376	LEU
1	A	418	ARG
1	A	423	GLN
1	A	424	PRO
1	A	464	LEU
1	A	471	LEU
1	A	479	LYS
1	A	494	ILE
1	A	504	ARG
1	A	511	LEU
1	A	522	ILE
1	A	523	ARG
1	A	539	LYS
1	A	564	LEU
1	A	592	SER
1	A	594	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	94	GLN
1	A	135	GLN
1	A	147	ASN
1	A	217	GLN
1	A	322	GLN
1	A	329	GLN
1	A	333	ASN
1	A	364	ASN
1	A	423	GLN
1	A	437	ASN
1	A	460	GLN
1	A	497	ASN
1	A	520	GLN
1	A	545	GLN
1	A	565	HIS
1	A	570	ASN
1	A	574	HIS

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	1.54	1 (12%)	7,12,14	3.80	4 (57%)

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	-	0/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	OG-CB	3.27	1.57	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	OG-P-O1P	7.52	126.77	106.44
1	A	198	SEP	O3P-P-OG	-4.48	94.98	106.67
1	A	198	SEP	O3P-P-O2P	3.30	120.18	107.80
1	A	198	SEP	OG-CB-CA	2.83	110.90	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	3	0

5.5 Carbohydrates ⓘ

11 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	1,2	14,14,15	1.00	1 (7%)	17,19,21	2.45	6 (35%)
2	NAG	B	2	2	14,14,15	0.65	0	17,19,21	2.85	10 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	1,2	14,14,15	0.98	1 (7%)	17,19,21	1.54	3 (17%)
2	NAG	C	2	2	14,14,15	1.30	1 (7%)	17,19,21	2.41	6 (35%)
3	NAG	D	1	1,3	14,14,15	1.30	2 (14%)	17,19,21	2.07	3 (17%)
3	NAG	D	2	3	14,14,15	1.14	1 (7%)	17,19,21	2.15	3 (17%)
3	MAN	D	3	3	11,11,12	0.74	0	15,15,17	2.32	3 (20%)
4	NAG	E	1	1,4	14,14,15	0.87	0	17,19,21	2.41	8 (47%)
4	NAG	E	2	4	14,14,15	0.85	1 (7%)	17,19,21	1.76	5 (29%)
4	BMA	E	3	4	11,11,12	0.60	0	15,15,17	1.63	2 (13%)
4	MAN	E	4	4	11,11,12	0.55	0	15,15,17	1.20	1 (6%)

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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1
2	NAG	C	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	MAN	D	3	3	-	2/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	1/1/1/1
4	MAN	E	4	4	-	0/2/19/22	1/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	NAG	O5-C1	-3.87	1.37	1.43
2	C	2	NAG	O5-C1	-3.46	1.37	1.43
3	D	1	NAG	O5-C1	-3.30	1.38	1.43
2	C	1	NAG	O5-C1	-2.63	1.39	1.43
3	D	1	NAG	C2-N2	-2.57	1.42	1.46
2	B	1	NAG	O5-C1	-2.42	1.39	1.43
4	E	2	NAG	C1-C2	2.21	1.55	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	C1-O5-C5	8.02	122.94	112.19
3	D	1	NAG	O5-C1-C2	-6.83	100.73	111.29
3	D	3	MAN	C1-C2-C3	6.68	119.37	109.64
2	C	2	NAG	C2-N2-C7	-5.97	114.90	122.90
2	B	2	NAG	C2-N2-C7	-5.45	115.59	122.90
2	B	1	NAG	C2-N2-C7	-5.41	115.65	122.90
2	B	2	NAG	O5-C1-C2	-5.12	103.38	111.29
4	E	1	NAG	C2-N2-C7	-5.10	116.06	122.90
4	E	1	NAG	C4-C3-C2	4.93	118.24	111.02
2	B	1	NAG	O5-C1-C2	-4.84	103.80	111.29
4	E	3	BMA	C1-O5-C5	4.72	118.52	112.19
2	C	1	NAG	O5-C1-C2	-4.28	104.66	111.29
3	D	3	MAN	O5-C5-C6	4.27	115.97	107.66
2	B	2	NAG	C4-C3-C2	4.15	117.10	111.02
2	C	2	NAG	O5-C1-C2	-4.10	104.95	111.29
2	B	1	NAG	C1-O5-C5	-4.05	106.76	112.19
4	E	2	NAG	C4-C3-C2	3.97	116.84	111.02
4	E	1	NAG	O5-C1-C2	-3.70	105.57	111.29
4	E	4	MAN	C1-O5-C5	-3.56	107.41	112.19
2	B	2	NAG	C1-C2-N2	3.53	116.00	110.43
2	C	2	NAG	O4-C4-C5	3.44	117.79	109.32
2	B	2	NAG	C8-C7-N2	3.25	121.51	116.12
2	B	2	NAG	C6-C5-C4	-3.25	105.05	113.02
4	E	2	NAG	C3-C4-C5	3.21	116.05	110.23
2	B	1	NAG	O6-C6-C5	-3.20	100.42	111.33
3	D	3	MAN	C2-C3-C4	3.10	116.31	110.86
2	B	1	NAG	C3-C4-C5	-2.83	105.09	110.23
2	C	2	NAG	O7-C7-C8	2.78	127.01	122.05
4	E	1	NAG	O6-C6-C5	-2.78	101.88	111.33
4	E	3	BMA	O5-C5-C6	2.59	112.71	107.66
3	D	1	NAG	C1-O5-C5	-2.52	108.81	112.19
4	E	1	NAG	C6-C5-C4	-2.51	106.85	113.02
2	C	2	NAG	O4-C4-C3	-2.50	104.49	110.38
2	C	2	NAG	C4-C3-C2	2.49	114.67	111.02
2	B	2	NAG	O5-C5-C6	2.43	112.39	107.66
2	B	2	NAG	O7-C7-C8	-2.42	117.74	122.05
3	D	1	NAG	O6-C6-C5	-2.38	103.23	111.33
2	B	1	NAG	C8-C7-N2	-2.31	112.28	116.12
4	E	2	NAG	C1-O5-C5	2.25	115.20	112.19
2	B	2	NAG	O5-C5-C4	2.25	116.29	110.83
2	C	1	NAG	O3-C3-C4	2.23	115.64	110.38
4	E	1	NAG	O3-C3-C4	-2.23	105.13	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2	NAG	C6-C5-C4	-2.21	107.58	113.02
4	E	1	NAG	O5-C5-C6	2.20	111.94	107.66
3	D	2	NAG	O5-C5-C4	2.15	116.06	110.83
4	E	2	NAG	C1-C2-N2	2.11	113.76	110.43
2	B	2	NAG	O3-C3-C2	-2.07	105.09	109.40
3	D	2	NAG	O4-C4-C5	2.04	114.36	109.32
4	E	1	NAG	C8-C7-N2	2.04	119.50	116.12
2	C	1	NAG	O7-C7-C8	-2.02	118.46	122.05

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
3	D	3	MAN	O5-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
3	D	3	MAN	C4-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	4	MAN	C1-C2-C3-C4-C5-O5
4	E	3	BMA	C1-C2-C3-C4-C5-O5

8 monomers are involved in 17 short contacts:

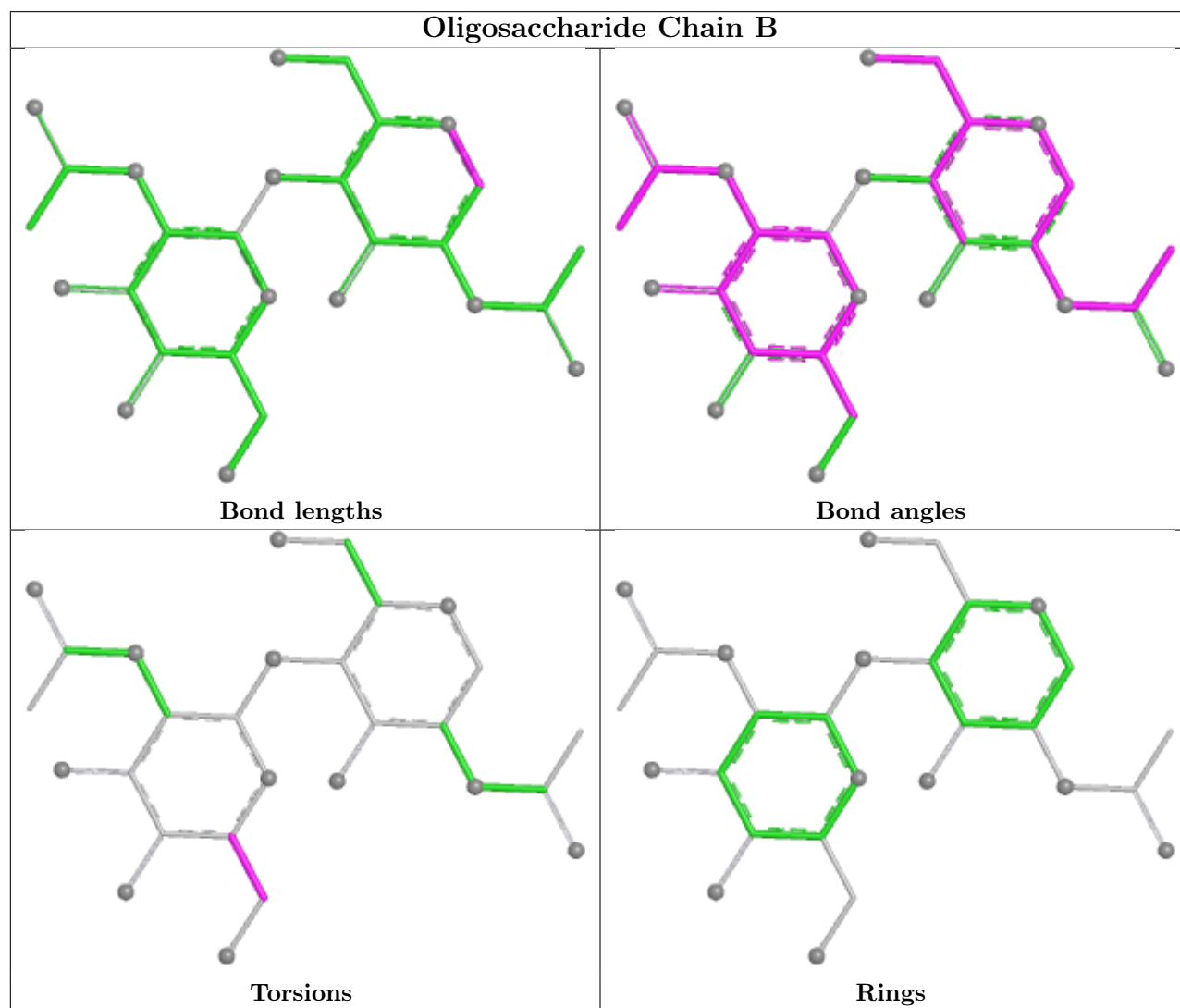
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	1	0
4	E	4	MAN	2	0
4	E	3	BMA	4	0
2	C	2	NAG	2	0
2	B	2	NAG	3	0

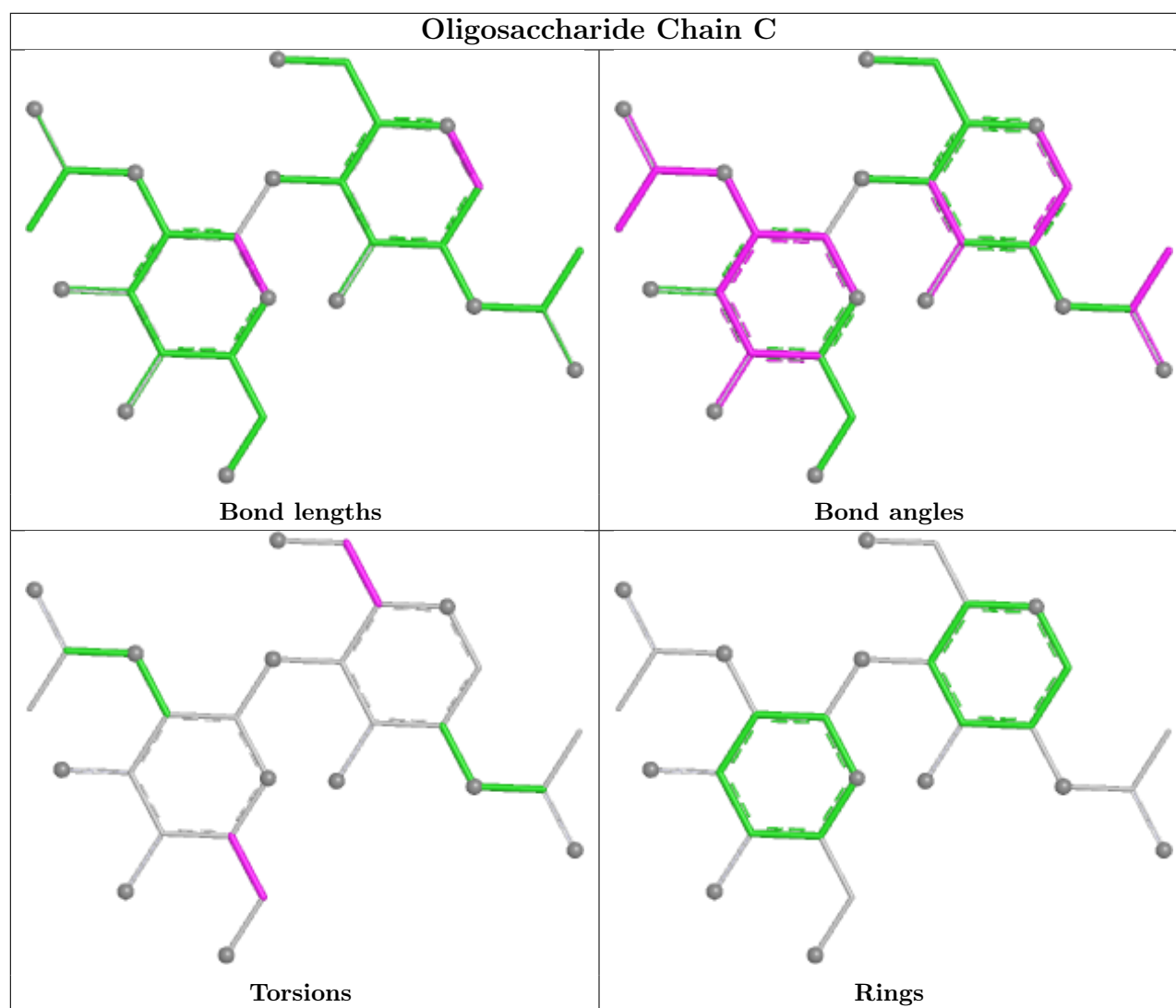
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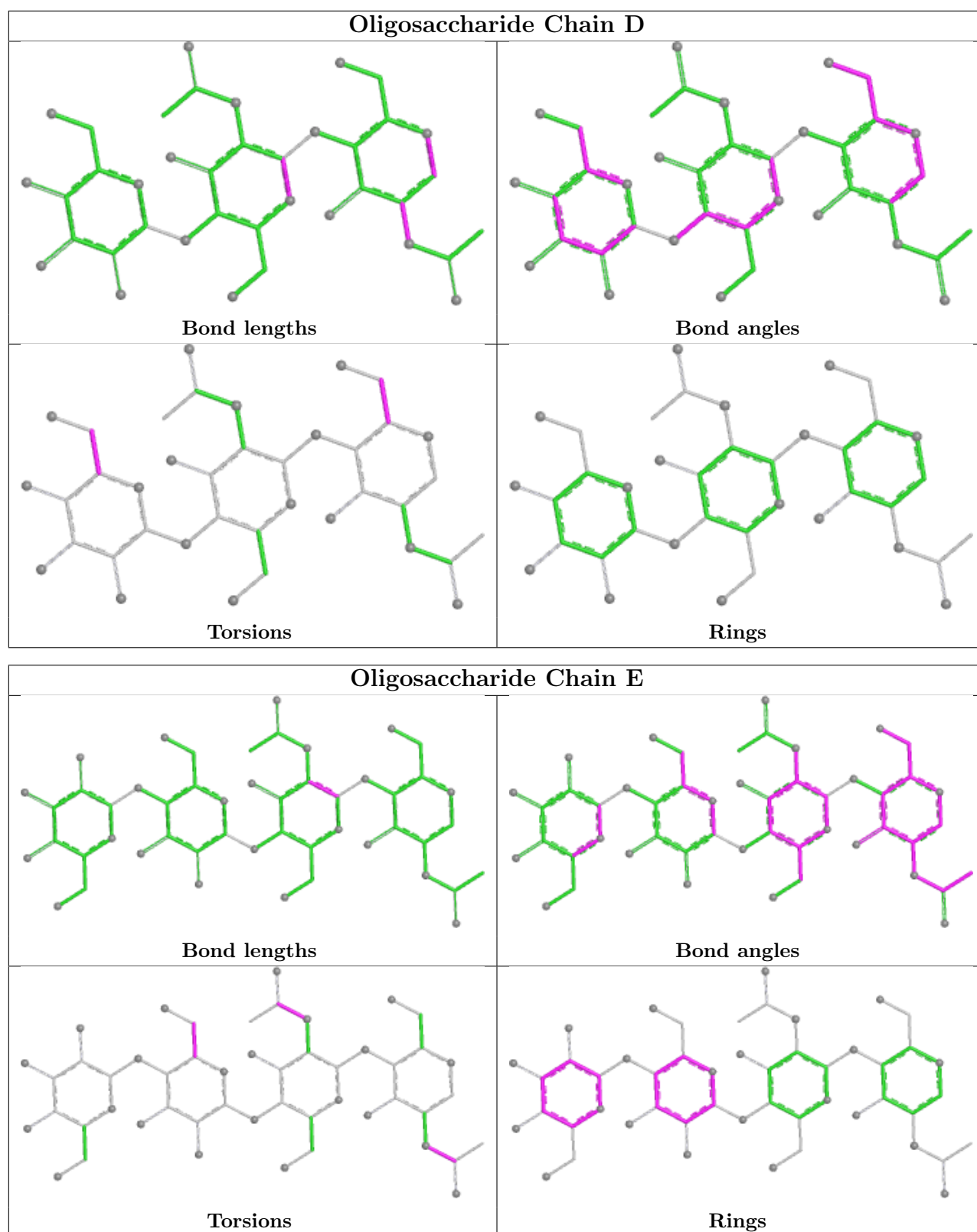
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	NAG	5	0
3	D	3	MAN	2	0
3	D	2	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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	0.50	0	0,1,1	-	-
5	HEM	A	605	1,9	50,50,50	1.88	13 (26%)	67,82,82	1.52	13 (19%)
6	SCN	A	608	-	1,2,2	0.15	0	0,1,1	-	-

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
5	HEM	A	605	1,9	-	2/14/54/54	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	605	HEM	C3D-C2D	6.40	1.50	1.36
5	A	605	HEM	C4D-C3D	4.24	1.52	1.45
5	A	605	HEM	CAB-C3B	3.56	1.56	1.47
5	A	605	HEM	CMA-C3A	3.25	1.57	1.50
5	A	605	HEM	CAC-C3C	3.21	1.56	1.47
5	A	605	HEM	FE-NC	3.20	2.05	1.95
5	A	605	HEM	CHC-C1C	-2.80	1.32	1.38
5	A	605	HEM	CMC-C2C	2.67	1.56	1.50
5	A	605	HEM	C4A-C3A	2.23	1.48	1.43
5	A	605	HEM	C3B-C4B	-2.22	1.40	1.44
5	A	605	HEM	CAA-C2A	2.15	1.56	1.51
5	A	605	HEM	C2A-C3A	-2.14	1.33	1.38
5	A	605	HEM	O2A-CGA	-2.04	1.24	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	605	HEM	CHC-C4B-NB	4.17	128.91	124.42
5	A	605	HEM	C3B-C2B-C1B	4.07	109.47	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	605	HEM	C2B-C1B-NB	-3.10	106.27	109.84
5	A	605	HEM	O2A-CGA-CBA	3.03	123.57	114.00
5	A	605	HEM	CHD-C1D-C2D	-2.76	120.67	125.03
5	A	605	HEM	C4D-ND-C1D	2.48	108.14	105.21
5	A	605	HEM	CAD-C3D-C4D	2.38	128.85	124.70
5	A	605	HEM	CHD-C1D-ND	2.30	126.90	124.42
5	A	605	HEM	O1D-CGD-CBD	-2.18	116.19	123.09
5	A	605	HEM	CMD-C2D-C1D	2.12	128.35	125.03
5	A	605	HEM	C1B-NB-C4B	2.11	107.70	105.21
5	A	605	HEM	O2A-CGA-O1A	-2.02	118.13	123.33
5	A	605	HEM	CBB-CAB-C3B	-2.01	117.49	127.53

There are no chirality outliers.

All (2) torsion outliers are listed below:

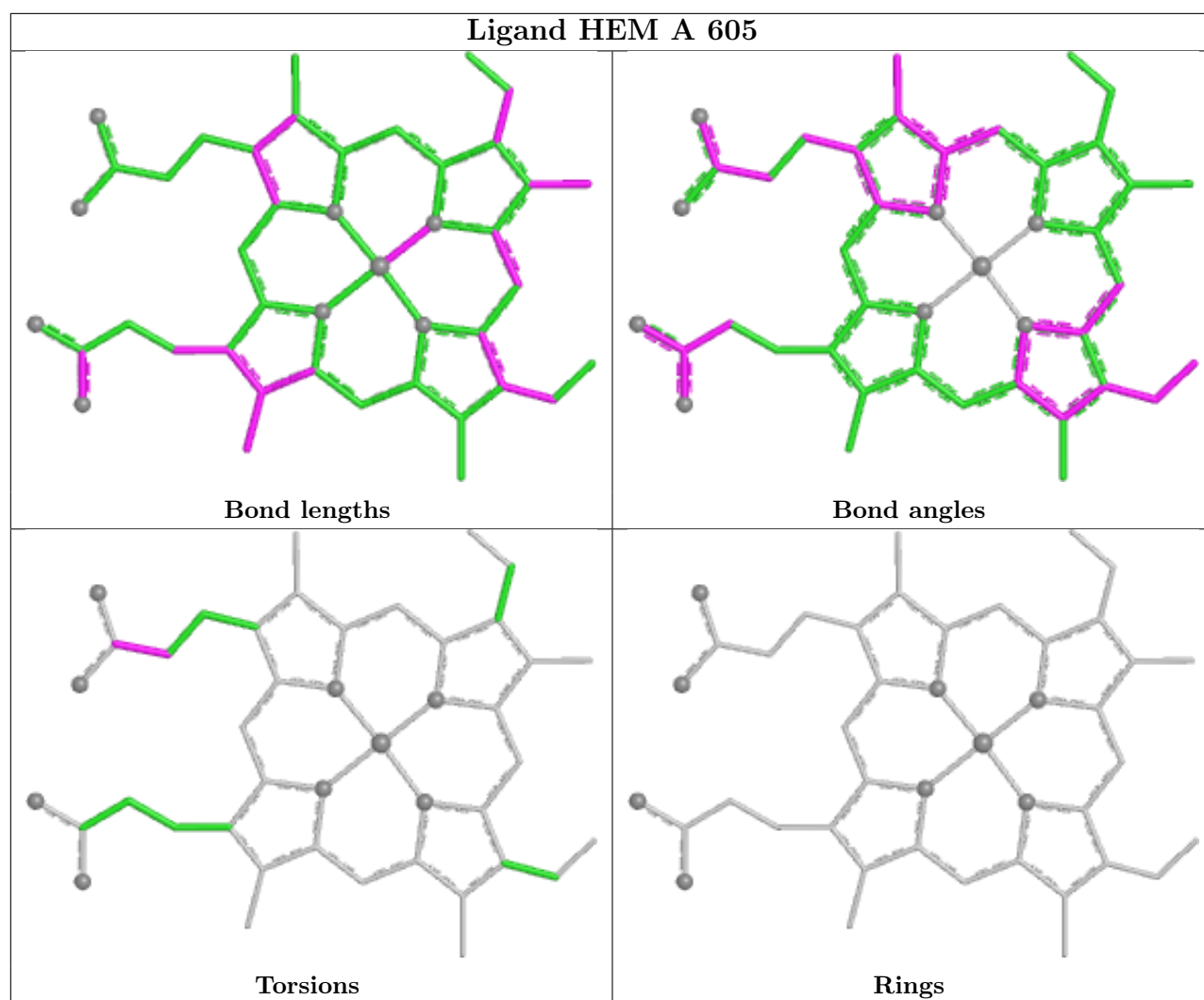
Mol	Chain	Res	Type	Atoms
5	A	605	HEM	CAD-CBD-CGD-O2D
5	A	605	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	605	HEM	5	0
6	A	608	SCN	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 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%)	-0.31	15 (2%) 58 54	19, 34, 76, 100	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	PRO	4.1
1	A	8	ALA	4.0
1	A	169	THR	3.6
1	A	136	GLY	3.3
1	A	167	CYS	3.3
1	A	175	LEU	3.3
1	A	1	SER	3.1
1	A	172	TYR	2.9
1	A	7	GLY	2.9
1	A	547	PHE	2.4
1	A	581	THR	2.2
1	A	11	PRO	2.2
1	A	124	HIS	2.2
1	A	9	PRO	2.2
1	A	119	LEU	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	0.94	0.09	21,32,37,39	0

6.3 Carbohydrates

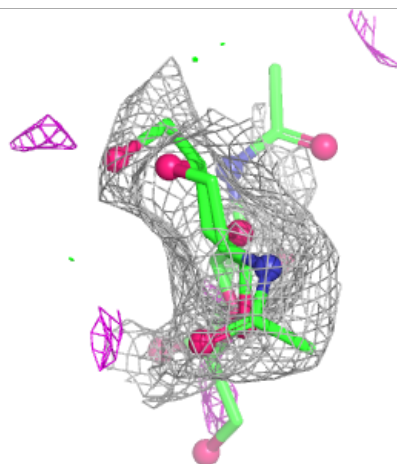
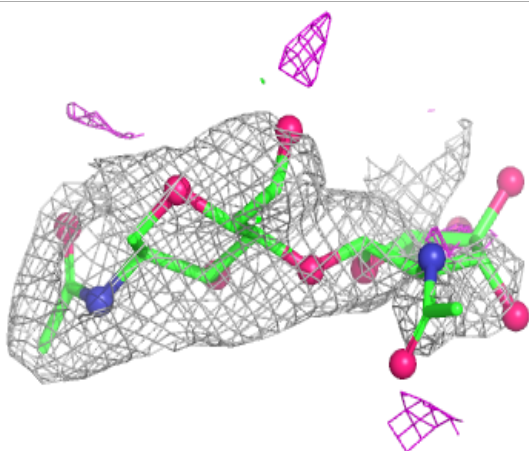
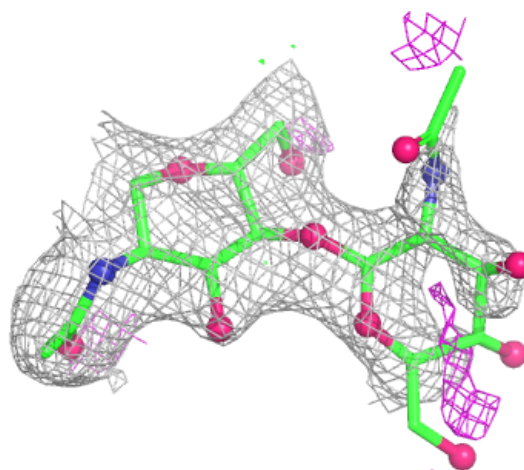
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	E	4	11/12	0.14	0.13	111,113,114,114	0
4	NAG	E	2	14/15	0.46	0.12	92,97,101,105	0
4	BMA	E	3	11/12	0.47	0.12	109,111,112,113	0
3	MAN	D	3	11/12	0.61	0.10	87,89,91,92	0
4	NAG	E	1	14/15	0.63	0.10	58,66,74,84	0
2	NAG	B	2	14/15	0.64	0.14	77,84,90,91	0
2	NAG	C	2	14/15	0.72	0.11	64,71,73,73	0
3	NAG	D	2	14/15	0.80	0.11	61,73,76,81	0
2	NAG	B	1	14/15	0.80	0.10	52,59,71,72	0
3	NAG	D	1	14/15	0.92	0.08	35,44,48,55	0
2	NAG	C	1	14/15	0.93	0.07	38,42,55,57	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.

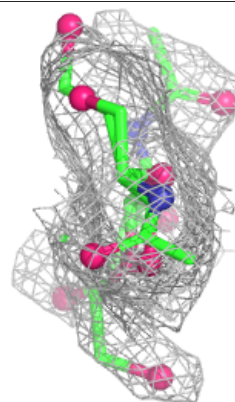
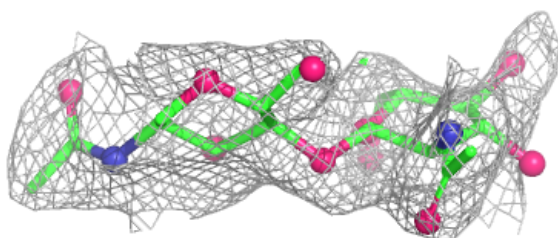
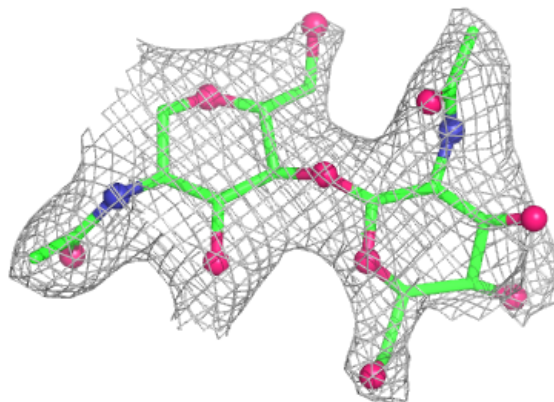
Electron density around Chain B:

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

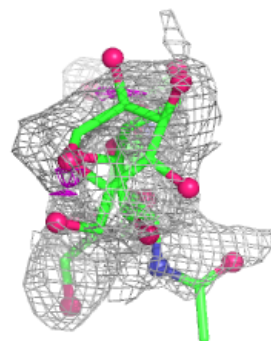
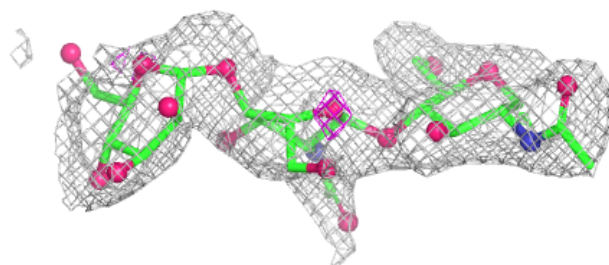
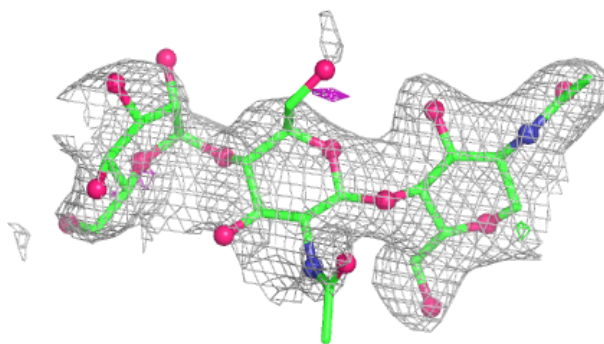


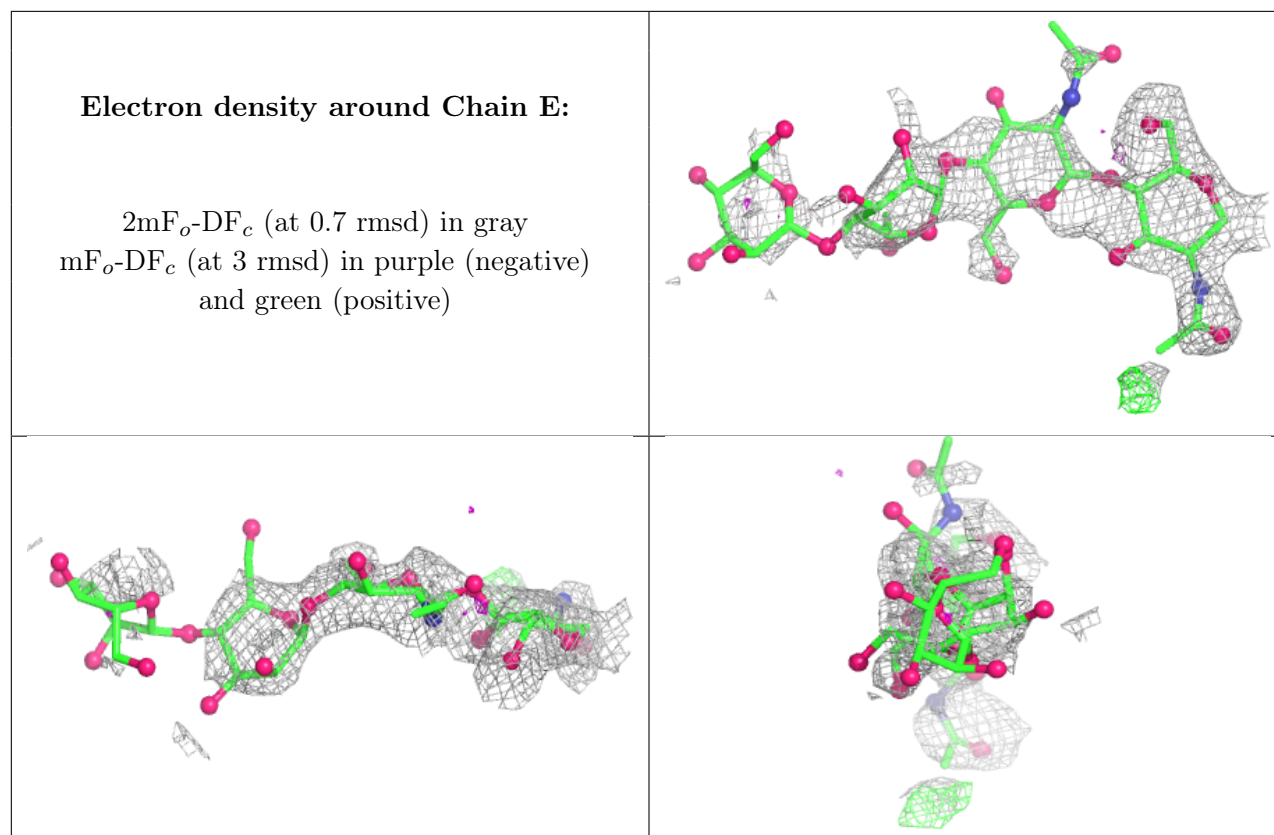
Electron density around Chain C:

$2mF_o-DF_c$ (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)





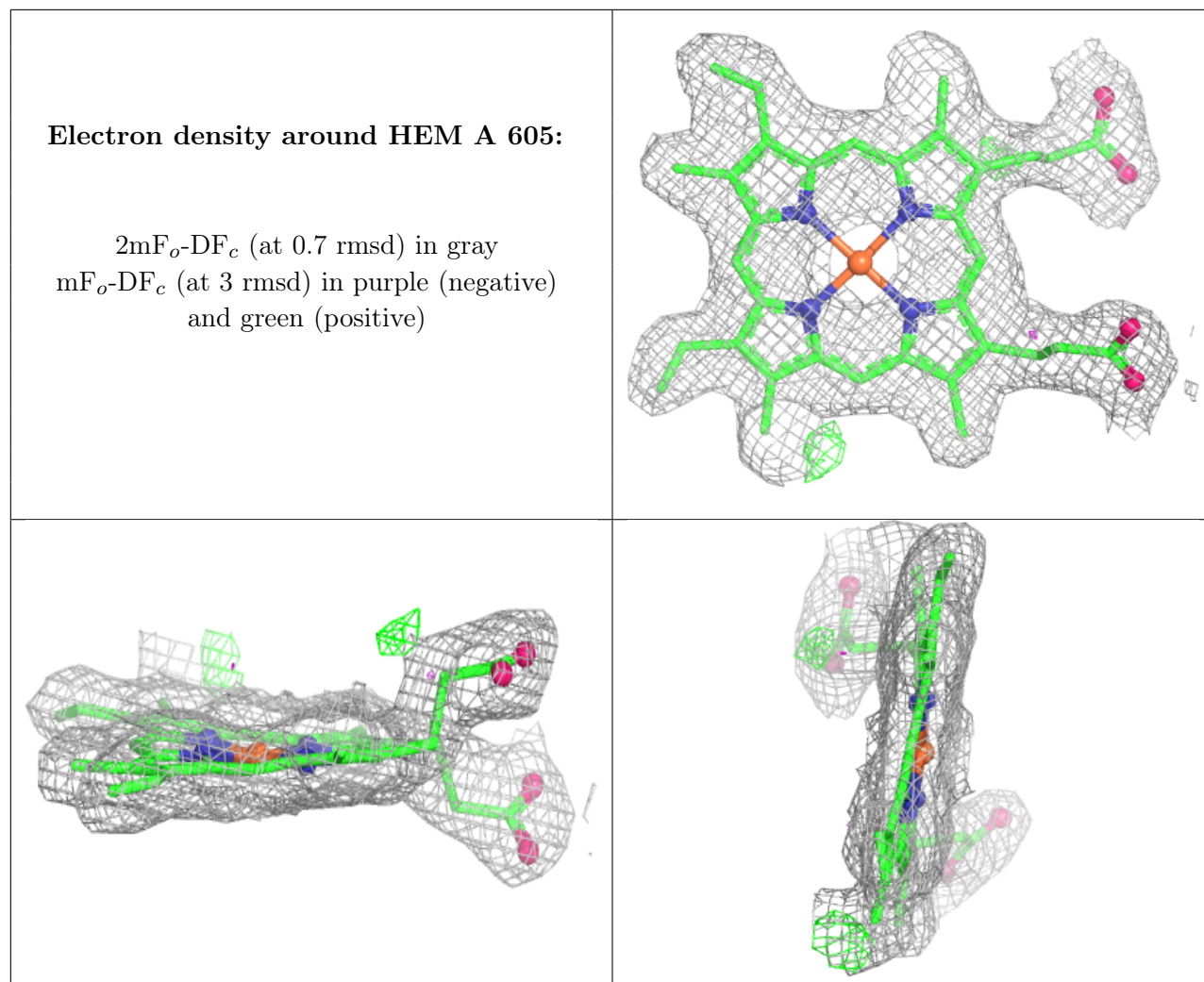
6.4 Ligands ⓘ

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
8	IOD	A	611	1/1	0.94	0.11	100,100,100,100	0
8	IOD	A	613	1/1	0.94	0.08	88,88,88,88	0
6	SCN	A	607	3/3	0.96	0.09	20,20,20,26	0
6	SCN	A	608	3/3	0.97	0.10	21,21,26,34	0
8	IOD	A	610	1/1	0.97	0.12	85,85,85,85	0
7	CA	A	609	1/1	0.98	0.04	25,25,25,25	0
5	HEM	A	605	43/43	0.98	0.05	7,20,26,27	0
8	IOD	A	614	1/1	0.98	0.07	69,69,69,69	0
8	IOD	A	612	1/1	0.99	0.07	75,75,75,75	0
8	IOD	A	615	1/1	1.00	0.02	28,28,28,28	0
8	IOD	A	616	1/1	1.00	0.09	54,54,54,54	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 ⓘ

There are no such residues in this entry.