



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:10 PM UTC

PDB ID : 3FAQ / pdb_00003faq
Title : Crystal structure of lactoperoxidase complex with cyanide
Authors : Sheikh, I.A.; Singh, N.; Sharma, S.; Kaur, P.; Srinivasan, A.; Singh, T.P.
Deposited on : 2008-11-18
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

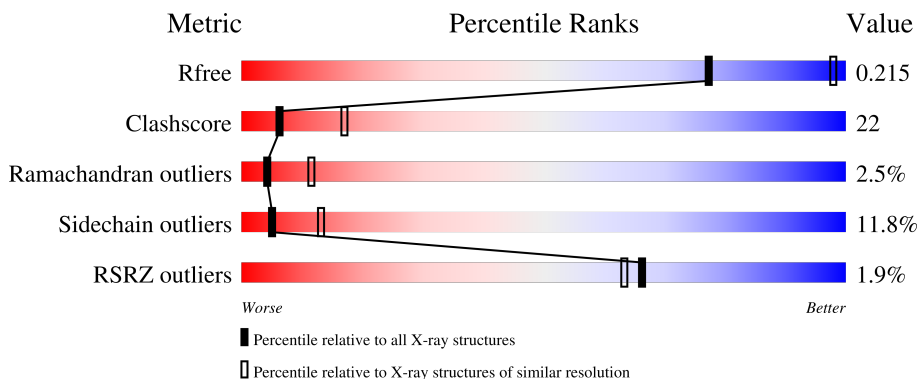
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	595	 2% 54% 35% 10%
2	B	2	 100%
2	C	2	 50% 50%
3	D	3	 33% 67%
4	E	4	 25% 25% 50%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 5256 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.

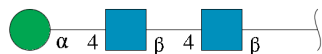
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	595	4778	3040	847	864	1	26	0	0	0

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



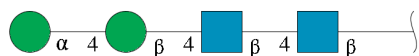
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	28	16	2	10	0	0	0
2	C	2	28	16	2	10	0	0	0

- 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.



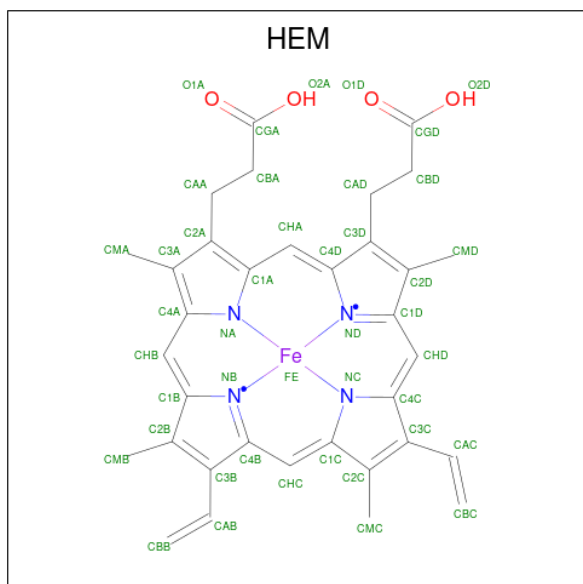
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	3	39	22	2	15	0	0	0

- 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.



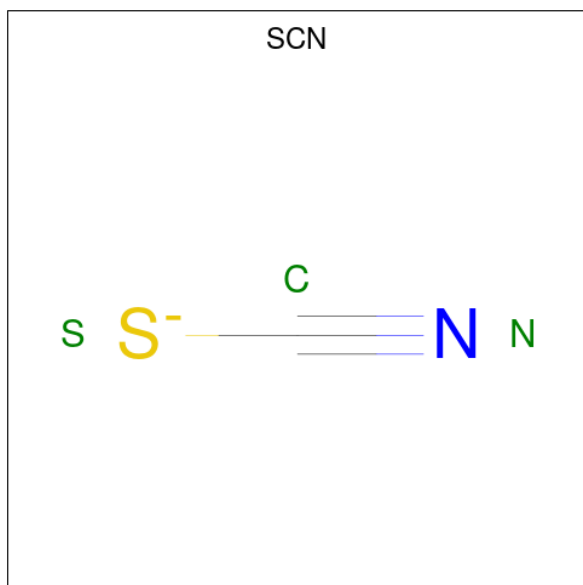
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	4	50	28	2	20	0	0	0

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



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

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

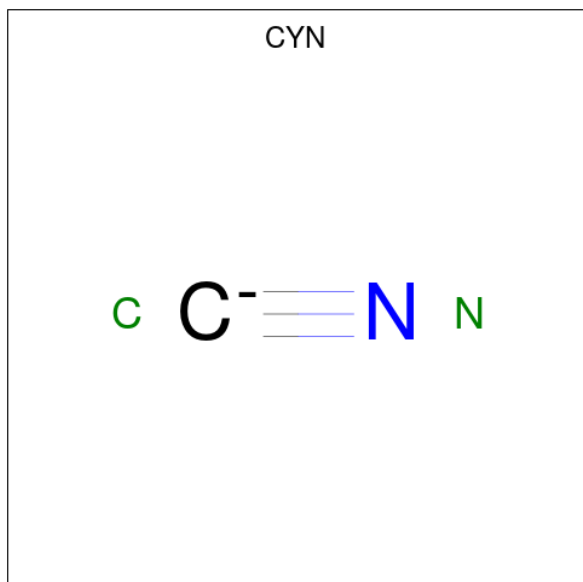


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	S	0	0
			3	1	1	1		
6	A	1	Total	C	N	S	0	0
			3	1	1	1		

- 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 CYANIDE ION (CCD ID: CYN) (formula: CN).



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

- Molecule 9 is IODIDE ION (CCD ID: IOD) (formula: I).

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

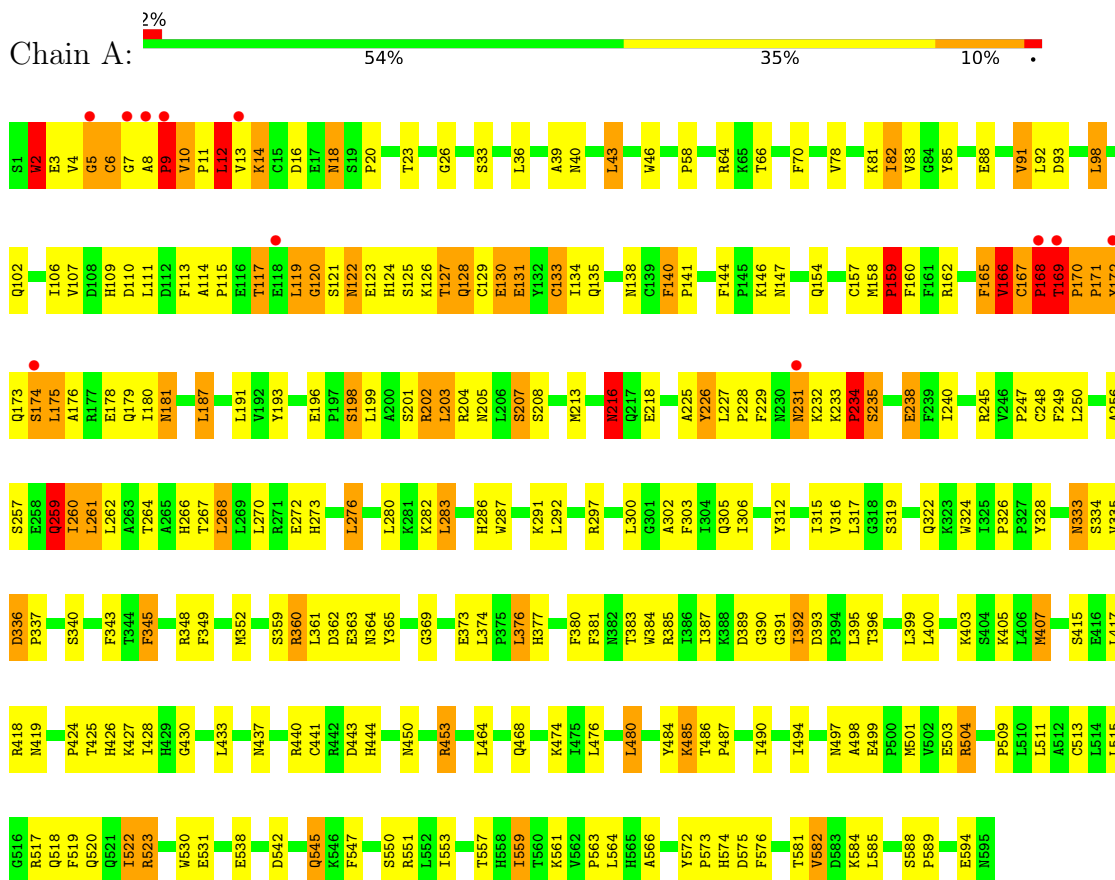
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	274	Total O 274 274	0	0

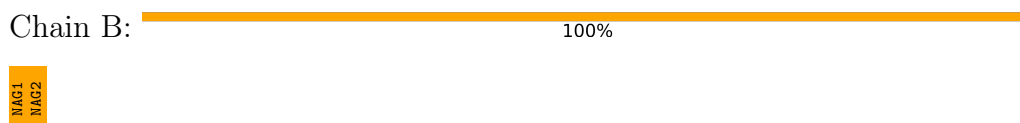
3 Residue-property plots i

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


- Molecule 1: Lactoperoxidase



- 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

Chain C:  50% 50%


MAG1
MAG2

- 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:  25% 25% 50%

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	54.45Å 80.67Å 77.80Å 90.00° 102.87° 90.00°	Depositor
Resolution (Å)	11.94 – 2.70 11.94 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.0 (11.94-2.70) 88.0 (11.94-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.70Å)	Xtrriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.208 , 0.235 0.177 , 0.215	Depositor DCC
R_{free} test set	824 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtrriage
Anisotropy	0.401	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 94.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5256	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, BMA, SCN, CA, HEM, SEP, CYN, 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	0.67	10/4896 (0.2%)	1.61	82/6640 (1.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	PRO	CA-C	-8.48	1.40	1.52
1	A	234	PRO	C-N	-7.07	1.22	1.33
1	A	234	PRO	N-CD	6.78	1.57	1.47
1	A	122	ASN	N-CA	6.61	1.54	1.46
1	A	14	LYS	N-CA	6.26	1.54	1.46
1	A	13	VAL	CA-C	5.88	1.59	1.52
1	A	233	LYS	N-CA	-5.74	1.36	1.46
1	A	12	LEU	C-N	5.27	1.40	1.33
1	A	9	PRO	N-CA	5.04	1.53	1.47
1	A	13	VAL	C-N	5.01	1.40	1.33

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	LYS	CA-C-N	44.07	174.93	119.84
1	A	233	LYS	C-N-CA	44.07	174.93	119.84
1	A	166	VAL	N-CA-C	24.32	134.06	111.45
1	A	234	PRO	CA-N-CD	-23.48	79.14	112.00
1	A	234	PRO	N-CA-CB	19.65	123.88	103.25
1	A	234	PRO	N-CD-CG	15.44	126.36	103.20
1	A	216	ASN	CA-CB-CG	15.20	127.80	112.60
1	A	231	ASN	CA-CB-CG	11.93	124.53	112.60
1	A	594	GLU	N-CA-C	10.72	122.93	111.03
1	A	13	VAL	N-CA-C	10.57	120.36	110.74
1	A	545	GLN	OE1-CD-NE2	-10.35	112.25	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	LYS	CB-CA-C	9.71	121.32	110.15
1	A	173	GLN	N-CA-C	9.18	125.38	113.18
1	A	259	GLN	OE1-CD-NE2	-8.89	113.71	122.60
1	A	7	GLY	N-CA-C	8.87	121.51	110.96
1	A	387	ILE	N-CA-C	8.77	118.78	110.53
1	A	154	GLN	OE1-CD-NE2	-8.73	113.87	122.60
1	A	427	LYS	N-CA-C	8.68	123.86	113.28
1	A	119	LEU	N-CA-C	-8.58	100.64	112.30
1	A	172	TYR	N-CA-C	8.50	122.03	110.55
1	A	9	PRO	CA-N-CD	-8.48	100.13	112.00
1	A	111	LEU	N-CA-C	8.29	121.89	111.69
1	A	140	PHE	CA-C-N	8.13	128.20	119.90
1	A	140	PHE	C-N-CA	8.13	128.20	119.90
1	A	121	SER	N-CA-C	-8.09	95.08	108.34
1	A	82	ILE	N-CA-C	8.07	118.50	111.56
1	A	131	GLU	N-CA-C	8.04	121.61	111.24
1	A	390	GLY	N-CA-C	8.02	125.68	114.85
1	A	233	LYS	O-C-N	7.96	131.17	121.29
1	A	83	VAL	N-CA-C	7.78	121.87	111.44
1	A	316	VAL	N-CA-C	-7.71	104.34	111.67
1	A	234	PRO	CA-C-N	-7.67	100.19	122.21
1	A	234	PRO	C-N-CA	-7.67	100.19	122.21
1	A	170	PRO	CA-C-N	7.65	129.40	119.84
1	A	170	PRO	C-N-CA	7.65	129.40	119.84
1	A	18	ASN	CA-CB-CG	7.28	119.88	112.60
1	A	122	ASN	CA-CB-CG	7.20	119.80	112.60
1	A	10	VAL	CA-C-N	7.14	128.76	119.84
1	A	10	VAL	C-N-CA	7.14	128.76	119.84
1	A	233	LYS	C-N-CD	-7.12	95.82	125.00
1	A	428	ILE	N-CA-C	7.00	120.06	109.20
1	A	259	GLN	CG-CD-NE2	6.97	126.86	116.40
1	A	233	LYS	CA-C-O	6.97	128.32	119.54
1	A	43	LEU	N-CA-C	-6.78	101.58	110.53
1	A	545	GLN	CG-CD-NE2	6.74	126.51	116.40
1	A	33	SER	CA-C-N	6.63	128.13	119.84
1	A	33	SER	C-N-CA	6.63	128.13	119.84
1	A	10	VAL	N-CA-C	-6.48	101.22	107.76
1	A	122	ASN	N-CA-C	-6.44	97.08	110.80
1	A	174	SER	N-CA-C	6.44	124.52	110.80
1	A	154	GLN	CG-CD-NE2	6.33	125.90	116.40
1	A	122	ASN	N-CA-CB	6.32	121.17	110.49
1	A	110	ASP	N-CA-C	-6.23	104.03	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ALA	N-CA-C	6.19	119.64	110.48
1	A	166	VAL	CB-CA-C	-6.00	104.05	111.92
1	A	78	VAL	N-CA-C	-5.99	103.56	111.05
1	A	124	HIS	N-CA-C	-5.98	104.65	113.61
1	A	159	PRO	CB-CA-C	5.90	119.05	111.56
1	A	336	ASP	CA-C-N	5.88	126.39	120.04
1	A	336	ASP	C-N-CA	5.88	126.39	120.04
1	A	216	ASN	CB-CA-C	5.80	119.99	109.83
1	A	453	ARG	N-CA-C	-5.67	105.09	111.28
1	A	345	PHE	N-CA-C	-5.63	106.95	113.88
1	A	33	SER	N-CA-C	-5.63	99.53	108.82
1	A	26	GLY	N-CA-C	-5.58	107.95	115.21
1	A	92	LEU	N-CA-C	5.58	118.37	110.50
1	A	559	ILE	N-CA-C	-5.57	102.40	109.80
1	A	20	PRO	N-CA-C	-5.56	108.30	114.92
1	A	407	MET	N-CA-C	-5.48	102.28	110.23
1	A	256	ALA	N-CA-C	5.42	117.89	111.33
1	A	120	GLY	N-CA-C	5.29	125.71	113.18
1	A	566	ALA	N-CA-C	5.26	118.49	111.75
1	A	114	ALA	CA-C-N	5.24	125.24	119.89
1	A	114	ALA	C-N-CA	5.24	125.24	119.89
1	A	23	THR	N-CA-C	-5.24	102.24	110.36
1	A	181	ASN	N-CA-C	-5.18	100.07	108.52
1	A	2	TRP	N-CA-C	5.13	121.73	110.80
1	A	441	CYS	N-CA-C	-5.09	105.73	111.28
1	A	102	GLN	N-CA-C	5.08	116.82	111.28
1	A	359	SER	N-CA-C	5.01	117.92	109.95
1	A	369	GLY	CA-C-N	5.00	124.69	119.64
1	A	369	GLY	C-N-CA	5.00	124.69	119.64

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	4690	205	0
2	B	28	0	25	1	0
2	C	28	0	25	1	0
3	D	39	0	34	5	0
4	E	50	0	43	4	0
5	A	43	0	30	0	0
6	A	6	0	0	0	0
7	A	1	0	0	0	0
8	A	2	0	0	1	0
9	A	7	0	0	0	0
10	A	274	0	0	15	0
All	All	5256	0	4847	216	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 22.

All (216) 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:547:PHE:HE2	1:A:585:LEU:HD22	1.33	0.93
1:A:175:LEU:CD2	1:A:176:ALA:H	1.88	0.86
1:A:196:GLU:HB3	1:A:198:SEP:O1P	1.74	0.85
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.57	0.85
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.15	0.82
1:A:169:THR:H	1:A:170:PRO:CD	1.95	0.80
1:A:425:THR:HB	1:A:426:HIS:CD2	2.19	0.78
1:A:123:GLU:HG3	1:A:125:SER:H	1.50	0.77
1:A:91:VAL:HG13	1:A:405:LYS:HG3	1.68	0.75
1:A:581:THR:O	1:A:581:THR:HG22	1.86	0.75
1:A:229:PHE:CD1	1:A:247:PRO:HG2	2.22	0.75
1:A:127:THR:HG23	1:A:131:GLU:HG3	1.68	0.74
1:A:302:ALA:O	1:A:306:ILE:HG13	1.90	0.72
1:A:123:GLU:HB3	1:A:126:LYS:NZ	2.05	0.71
1:A:588:SER:OG	1:A:589:PRO:HD3	1.91	0.70
1:A:10:VAL:HB	10:A:717:HOH:O	1.91	0.70
1:A:227:LEU:HD23	1:A:270:LEU:HD22	1.72	0.70
1:A:476:LEU:HD21	1:A:498:ALA:HB1	1.72	0.69
1:A:106:ILE:HG23	1:A:191:LEU:HD11	1.75	0.69
1:A:175:LEU:HD22	1:A:176:ALA:H	1.56	0.69
10:A:966:HOH:O	2:C:1:NAG:H61	1.92	0.69
1:A:503:GLU:O	1:A:504:ARG:HB2	1.90	0.68
1:A:175:LEU:HD23	1:A:176:ALA:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:GLU:HB3	1:A:126:LYS:CE	2.25	0.67
1:A:123:GLU:HB3	1:A:126:LYS:HE3	1.77	0.67
1:A:260:ILE:HD11	1:A:385:ARG:CB	2.25	0.67
1:A:187:LEU:HD13	1:A:305:GLN:HA	1.75	0.67
1:A:260:ILE:HD11	1:A:385:ARG:HB2	1.76	0.66
1:A:204:ARG:HD3	10:A:826:HOH:O	1.96	0.66
10:A:972:HOH:O	4:E:2:NAG:H2	1.94	0.66
1:A:146:LYS:O	1:A:147:ASN:HB2	1.94	0.66
1:A:130:GLU:HA	1:A:159:PRO:HG3	1.76	0.66
1:A:168:PRO:HB2	1:A:170:PRO:HD2	1.77	0.66
1:A:328:TYR:CD1	1:A:523:ARG:HD3	2.31	0.65
1:A:400:LEU:HD11	1:A:553:ILE:HD13	1.79	0.65
1:A:328:TYR:HD1	1:A:523:ARG:HD3	1.60	0.65
1:A:169:THR:N	1:A:170:PRO:CD	2.58	0.65
1:A:235:SER:HB3	1:A:238:GLU:HB2	1.80	0.64
1:A:547:PHE:CE2	1:A:585:LEU:HD22	2.24	0.63
1:A:126:LYS:NZ	1:A:126:LYS:HB2	2.13	0.63
1:A:165:PHE:CE2	1:A:172:TYR:HB2	2.34	0.63
1:A:179:GLN:HG2	1:A:444:HIS:CE1	2.33	0.63
1:A:81:LYS:HD2	10:A:941:HOH:O	1.98	0.62
1:A:226:TYR:OH	1:A:391:GLY:HA2	2.00	0.62
1:A:487:PRO:HA	1:A:490:ILE:HG13	1.80	0.62
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.47	0.61
1:A:168:PRO:HG3	1:A:172:TYR:CD1	2.36	0.61
4:E:1:NAG:H61	4:E:2:NAG:C7	2.31	0.60
1:A:287:TRP:CE2	1:A:291:LYS:HE3	2.36	0.60
3:D:2:NAG:H2	3:D:2:NAG:H61	1.84	0.60
1:A:381:PHE:CZ	1:A:424:PRO:HB3	2.36	0.60
1:A:130:GLU:CD	1:A:426:HIS:HD1	2.10	0.60
1:A:324:TRP:O	1:A:326:PRO:HD2	2.03	0.59
1:A:165:PHE:HE2	1:A:172:TYR:HB2	1.65	0.59
1:A:393:ASP:HB2	10:A:753:HOH:O	2.03	0.59
1:A:574:HIS:HD2	1:A:575:ASP:OD1	1.86	0.59
1:A:205:ASN:OD1	1:A:207:SER:HB2	2.02	0.59
1:A:58:PRO:HD3	1:A:162:ARG:CZ	2.33	0.59
1:A:348:ARG:HD3	1:A:437:ASN:ND2	2.17	0.59
1:A:123:GLU:HB3	1:A:126:LYS:HZ2	1.67	0.59
1:A:166:VAL:CG2	1:A:178:GLU:HB2	2.32	0.58
1:A:109:HIS:NE2	8:A:605:CYN:N	2.50	0.58
1:A:168:PRO:HG2	1:A:169:THR:N	2.18	0.58
1:A:106:ILE:HG23	1:A:191:LEU:CD1	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:THR:HB	1:A:426:HIS:HD2	1.67	0.58
1:A:82:ILE:HD13	1:A:480:LEU:HD13	1.86	0.58
1:A:557:THR:OG1	1:A:559:ILE:HG12	2.04	0.58
1:A:126:LYS:HB2	1:A:126:LYS:HZ2	1.70	0.57
1:A:123:GLU:CB	1:A:126:LYS:HE3	2.34	0.57
1:A:333:ASN:HD22	1:A:333:ASN:N	2.03	0.57
1:A:417:LEU:HD22	1:A:433:LEU:HD22	1.86	0.57
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.04	0.56
1:A:169:THR:N	1:A:170:PRO:HD3	2.20	0.56
1:A:561:LYS:HE2	10:A:915:HOH:O	2.05	0.56
1:A:335:VAL:O	1:A:337:PRO:HD3	2.06	0.56
1:A:376:LEU:HD22	1:A:376:LEU:O	2.06	0.56
4:E:1:NAG:H61	4:E:2:NAG:O7	2.06	0.56
1:A:257:SER:O	1:A:381:PHE:HA	2.06	0.56
1:A:550:SER:HB2	1:A:582:VAL:HG11	1.86	0.56
1:A:117:THR:HG21	1:A:138:ASN:CG	2.31	0.55
1:A:129:CYS:HB2	10:A:733:HOH:O	2.07	0.55
1:A:175:LEU:HD22	1:A:176:ALA:N	2.21	0.55
1:A:407:MET:HB3	1:A:501:MET:CE	2.37	0.55
4:E:2:NAG:O4	4:E:3:BMA:H61	2.06	0.55
1:A:3:GLU:HG2	1:A:5:GLY:H	1.72	0.54
1:A:165:PHE:O	1:A:180:ILE:HD11	2.06	0.54
1:A:513:CYS:O	1:A:517:ARG:HG3	2.07	0.54
1:A:2:TRP:CG	1:A:3:GLU:N	2.75	0.53
1:A:166:VAL:HG22	1:A:178:GLU:O	2.09	0.53
1:A:216:ASN:HB2	1:A:228:PRO:HA	1.89	0.53
1:A:123:GLU:HG3	1:A:125:SER:N	2.21	0.52
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.44	0.52
1:A:98:LEU:HD11	1:A:261:LEU:HD21	1.92	0.52
1:A:202:ARG:HD2	1:A:250:LEU:HD21	1.90	0.52
1:A:165:PHE:CD1	1:A:165:PHE:N	2.78	0.52
1:A:260:ILE:CD1	1:A:385:ARG:HB2	2.39	0.52
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.45	0.51
1:A:175:LEU:CD2	1:A:176:ALA:N	2.66	0.51
1:A:426:HIS:CD2	1:A:426:HIS:N	2.78	0.51
1:A:324:TRP:HZ3	10:A:724:HOH:O	1.93	0.50
1:A:362:ASP:C	1:A:362:ASP:OD1	2.55	0.50
1:A:504:ARG:HG3	10:A:909:HOH:O	2.11	0.50
1:A:519:PHE:CD1	1:A:522:ILE:HD11	2.47	0.50
1:A:484:TYR:C	1:A:486:THR:H	2.18	0.50
1:A:563:PRO:HD3	1:A:576:PHE:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:CYS:HB3	1:A:167:CYS:SG	2.53	0.49
1:A:8:ALA:N	1:A:9:PRO:CD	2.76	0.49
1:A:349:PHE:HB2	1:A:497:ASN:HD21	1.77	0.49
1:A:98:LEU:CD1	1:A:261:LEU:HD21	2.43	0.49
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.47	0.49
1:A:499:GLU:OE1	1:A:509:PRO:HD2	2.13	0.49
1:A:43:LEU:CD2	1:A:181:ASN:HB2	2.43	0.49
1:A:46:TRP:CE2	1:A:340:SER:HB3	2.48	0.48
1:A:144:PHE:HE2	1:A:158:MET:HE3	1.78	0.48
1:A:199:LEU:C	1:A:201:SER:H	2.21	0.48
1:A:572:TYR:CE2	1:A:573:PRO:HB3	2.48	0.48
1:A:260:ILE:HD11	1:A:385:ARG:HB3	1.93	0.48
1:A:484:TYR:O	1:A:486:THR:N	2.44	0.48
1:A:126:LYS:HB3	10:A:911:HOH:O	2.14	0.48
1:A:581:THR:O	1:A:581:THR:CG2	2.56	0.47
1:A:187:LEU:CD1	1:A:305:GLN:HA	2.44	0.47
1:A:240:ILE:HD11	1:A:384:TRP:HD1	1.79	0.47
1:A:286:HIS:HB2	10:A:901:HOH:O	2.13	0.47
1:A:453:ARG:NH1	1:A:499:GLU:OE2	2.45	0.47
1:A:16:ASP:OD1	1:A:16:ASP:O	2.32	0.47
1:A:272:GLU:HG3	1:A:276:LEU:HD22	1.94	0.47
1:A:360:ARG:NH2	1:A:389:ASP:OD2	2.47	0.47
1:A:245:ARG:HH21	1:A:245:ARG:HG3	1.79	0.47
1:A:503:GLU:O	1:A:504:ARG:CB	2.57	0.47
1:A:272:GLU:O	1:A:276:LEU:HD22	2.15	0.46
1:A:240:ILE:HD12	1:A:240:ILE:C	2.40	0.46
1:A:166:VAL:HG21	1:A:178:GLU:HB2	1.96	0.46
1:A:144:PHE:HE2	1:A:158:MET:CE	2.29	0.46
1:A:187:LEU:HB3	1:A:305:GLN:HG2	1.96	0.46
1:A:162:ARG:HA	1:A:443:ASP:OD2	2.15	0.46
1:A:160:PHE:CD1	1:A:160:PHE:C	2.94	0.46
1:A:407:MET:HE2	10:A:920:HOH:O	2.16	0.45
1:A:407:MET:HB3	1:A:501:MET:HE2	1.97	0.45
1:A:287:TRP:NE1	1:A:291:LYS:HE3	2.32	0.45
1:A:106:ILE:O	1:A:107:VAL:C	2.59	0.45
1:A:262:LEU:O	1:A:266:HIS:HD2	2.00	0.45
1:A:166:VAL:CG2	1:A:178:GLU:O	2.64	0.45
3:D:2:NAG:H61	3:D:2:NAG:C2	2.46	0.45
1:A:127:THR:HG23	1:A:131:GLU:CG	2.42	0.45
1:A:259:GLN:O	1:A:260:ILE:C	2.60	0.45
1:A:70:PHE:CD1	1:A:485:LYS:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LEU:HD11	1:A:553:ILE:CD1	2.44	0.45
3:D:2:NAG:H2	3:D:2:NAG:C6	2.46	0.45
3:D:2:NAG:H4	3:D:3:MAN:H2	1.71	0.45
1:A:120:GLY:HA2	1:A:123:GLU:OE1	2.17	0.45
1:A:349:PHE:CB	1:A:497:ASN:HD21	2.30	0.45
1:A:419:ASN:O	1:A:430:GLY:HA2	2.16	0.44
1:A:199:LEU:C	1:A:201:SER:N	2.73	0.44
1:A:333:ASN:N	1:A:333:ASN:ND2	2.65	0.44
1:A:450:ASN:HD21	1:A:487:PRO:HB2	1.81	0.44
1:A:333:ASN:ND2	1:A:333:ASN:H	2.15	0.44
1:A:82:ILE:HG21	1:A:494:ILE:HD11	1.99	0.44
1:A:133:CYS:SG	1:A:157:CYS:CB	3.06	0.44
1:A:193:TYR:CE2	1:A:297:ARG:HG3	2.52	0.44
1:A:227:LEU:HD22	10:A:758:HOH:O	2.16	0.44
1:A:319:SER:OG	1:A:503:GLU:HB3	2.18	0.44
1:A:572:TYR:HA	1:A:573:PRO:HA	1.70	0.44
1:A:300:LEU:O	1:A:303:PHE:HB3	2.18	0.44
1:A:547:PHE:CE2	1:A:585:LEU:HD13	2.52	0.44
1:A:58:PRO:HD3	1:A:162:ARG:NH1	2.32	0.44
1:A:268:LEU:HD11	1:A:392:ILE:CD1	2.48	0.44
1:A:324:TRP:C	1:A:326:PRO:HD2	2.43	0.44
1:A:2:TRP:CG	1:A:3:GLU:H	2.36	0.43
1:A:345:PHE:HZ	1:A:440:ARG:HG3	1.83	0.43
1:A:135:GLN:HB2	1:A:141:PRO:HD2	2.00	0.43
1:A:249:PHE:CE2	1:A:383:THR:HG22	2.52	0.43
1:A:312:TYR:O	1:A:315:ILE:HG12	2.19	0.43
1:A:203:LEU:HB3	1:A:213:MET:HE1	2.01	0.43
1:A:282:LYS:HB2	1:A:282:LYS:HE3	1.67	0.43
1:A:8:ALA:N	1:A:9:PRO:HD2	2.33	0.43
1:A:264:THR:O	1:A:267:THR:HB	2.19	0.43
1:A:168:PRO:CG	1:A:169:THR:N	2.75	0.43
1:A:268:LEU:HD11	1:A:392:ILE:HD11	2.01	0.43
3:D:2:NAG:C2	3:D:2:NAG:C6	2.96	0.43
1:A:4:VAL:O	1:A:4:VAL:HG23	2.18	0.43
1:A:264:THR:HG23	1:A:392:ILE:HB	2.01	0.42
1:A:364:ASN:O	1:A:365:TYR:HB2	2.19	0.42
1:A:36:LEU:HA	1:A:36:LEU:HD12	1.71	0.42
1:A:93:ASP:O	1:A:403:LYS:HD3	2.19	0.42
2:B:1:NAG:C6	2:B:2:NAG:C1	2.97	0.42
1:A:202:ARG:HD3	10:A:872:HOH:O	2.19	0.42
1:A:85:TYR:OH	1:A:88:GLU:OE1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:HD22	1:A:283:LEU:O	2.19	0.42
1:A:333:ASN:HD22	1:A:334:SER:N	2.16	0.42
1:A:3:GLU:OE1	1:A:6:CYS:SG	2.76	0.41
1:A:130:GLU:HG2	1:A:426:HIS:CE1	2.55	0.41
1:A:202:ARG:CD	1:A:250:LEU:HD21	2.49	0.41
1:A:248:CYS:HA	1:A:383:THR:HG21	2.02	0.41
1:A:360:ARG:O	1:A:361:LEU:HD23	2.20	0.41
1:A:113:PHE:O	1:A:115:PRO:HD3	2.20	0.41
1:A:376:LEU:HD13	1:A:380:PHE:CZ	2.55	0.41
1:A:396:THR:O	1:A:399:LEU:HB2	2.19	0.41
1:A:345:PHE:CZ	1:A:440:ARG:HG3	2.55	0.41
1:A:468:GLN:CD	1:A:474:LYS:HG2	2.45	0.41
1:A:276:LEU:O	1:A:280:LEU:HG	2.21	0.41
1:A:336:ASP:HA	1:A:337:PRO:HD2	1.96	0.41
1:A:373:GLU:O	1:A:374:LEU:HD23	2.20	0.41
1:A:395:LEU:HD23	1:A:395:LEU:HA	1.93	0.41
1:A:240:ILE:HD11	1:A:384:TRP:CD1	2.56	0.41
1:A:125:SER:HA	1:A:128:GLN:HB3	2.02	0.41
1:A:39:ALA:O	1:A:40:ASN:HB2	2.21	0.41
1:A:168:PRO:C	1:A:169:THR:OG1	2.64	0.41
1:A:235:SER:CB	1:A:238:GLU:HB2	2.50	0.41
1:A:66:THR:HB	1:A:70:PHE:N	2.36	0.41
1:A:324:TRP:CZ2	1:A:513:CYS:HB2	2.56	0.40
1:A:12:LEU:H	1:A:12:LEU:HG	1.57	0.40
1:A:343:PHE:CG	1:A:518:GLN:HG2	2.56	0.40
1:A:345:PHE:HE2	1:A:440:ARG:HB3	1.86	0.40
1:A:515:LEU:HD23	1:A:515:LEU:HA	1.92	0.40
1:A:140:PHE:O	1:A:160:PHE:HB3	2.22	0.40
1:A:324:TRP:C	1:A:326:PRO:CD	2.94	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%)	537 (91%)	40 (7%)	15 (2%)	4 11

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	A	12	LEU
1	A	168	PRO
1	A	169	THR
1	A	171	PRO
1	A	174	SER
1	A	234	PRO
1	A	14	LYS
1	A	485	LYS
1	A	2	TRP
1	A	122	ASN
1	A	9	PRO
1	A	18	ASN
1	A	133	CYS
1	A	5	GLY

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%)	456 (88%)	61 (12%)	5 13

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

Mol	Chain	Res	Type
1	A	6	CYS
1	A	9	PRO
1	A	64	ARG
1	A	91	VAL
1	A	98	LEU
1	A	117	THR

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Mol	Chain	Res	Type
1	A	119	LEU
1	A	127	THR
1	A	128	GLN
1	A	130	GLU
1	A	134	ILE
1	A	159	PRO
1	A	165	PHE
1	A	166	VAL
1	A	167	CYS
1	A	168	PRO
1	A	169	THR
1	A	171	PRO
1	A	175	LEU
1	A	187	LEU
1	A	202	ARG
1	A	203	LEU
1	A	207	SER
1	A	208	SER
1	A	216	ASN
1	A	218	GLU
1	A	226	TYR
1	A	231	ASN
1	A	232	LYS
1	A	234	PRO
1	A	235	SER
1	A	238	GLU
1	A	259	GLN
1	A	260	ILE
1	A	261	LEU
1	A	268	LEU
1	A	276	LEU
1	A	283	LEU
1	A	292	LEU
1	A	317	LEU
1	A	322	GLN
1	A	333	ASN
1	A	352	MET
1	A	360	ARG
1	A	363	GLU
1	A	376	LEU
1	A	392	ILE
1	A	415	SER

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Mol	Chain	Res	Type
1	A	418	ARG
1	A	464	LEU
1	A	480	LEU
1	A	504	ARG
1	A	511	LEU
1	A	520	GLN
1	A	522	ILE
1	A	523	ARG
1	A	538	GLU
1	A	542	ASP
1	A	545	GLN
1	A	564	LEU
1	A	582	VAL

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	68	ASN
1	A	128	GLN
1	A	147	ASN
1	A	284	ASN
1	A	333	ASN
1	A	408	ASN
1	A	437	ASN
1	A	497	ASN
1	A	520	GLN
1	A	574	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	1.44	1 (12%)	7,12,14	3.50	3 (42%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-O1P	3.06	1.60	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	OG-CB-CA	7.58	115.52	108.14
1	A	198	SEP	O2P-P-OG	3.96	116.99	106.67
1	A	198	SEP	O3P-P-O1P	-2.69	100.36	110.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	198	SEP	CA-CB-OG-P
1	A	198	SEP	CB-OG-P-O2P
1	A	198	SEP	CB-OG-P-O3P
1	A	198	SEP	CB-OG-P-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates i

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	0.59	0	17,19,21	1.52	4 (23%)
2	NAG	B	2	2	14,14,15	0.71	0	17,19,21	1.35	2 (11%)
2	NAG	C	1	1,2	14,14,15	0.66	0	17,19,21	0.92	1 (5%)
2	NAG	C	2	2	14,14,15	0.76	0	17,19,21	2.33	5 (29%)
3	NAG	D	1	1,3	14,14,15	0.78	0	17,19,21	0.94	1 (5%)
3	NAG	D	2	3	14,14,15	1.10	1 (7%)	17,19,21	0.88	1 (5%)
3	MAN	D	3	3	11,11,12	0.73	0	15,15,17	1.81	2 (13%)
4	NAG	E	1	1,4	14,14,15	0.94	1 (7%)	17,19,21	1.48	1 (5%)
4	NAG	E	2	4	14,14,15	1.48	3 (21%)	17,19,21	1.58	2 (11%)
4	BMA	E	3	4	11,11,12	0.84	0	15,15,17	0.60	0
4	MAN	E	4	4	11,11,12	0.58	0	15,15,17	0.51	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. ^{1,2} 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	-	2/6/23/26	0/1/1/1
2	NAG	C	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1
3	MAN	D	3	3	-	0/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	1/1/1/1
4	MAN	E	4	4	-	2/2/19/22	1/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	NAG	C1-C2	2.77	1.56	1.52
4	E	2	NAG	C1-C2	2.70	1.56	1.52
4	E	2	NAG	O5-C5	2.33	1.48	1.43
4	E	2	NAG	O5-C1	2.17	1.47	1.43
4	E	1	NAG	C3-C2	2.08	1.56	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	5.83	119.99	112.19
3	D	3	MAN	C1-C2-C3	5.80	118.09	109.64
2	C	2	NAG	O5-C1-C2	4.90	118.87	111.29
4	E	1	NAG	C4-C3-C2	4.70	117.91	111.02
4	E	2	NAG	C1-O5-C5	4.18	117.78	112.19
2	B	2	NAG	C4-C3-C2	4.07	116.99	111.02
2	B	1	NAG	C4-C3-C2	-3.80	105.44	111.02
2	C	2	NAG	C6-C5-C4	3.08	120.57	113.02
2	C	2	NAG	C2-N2-C7	-2.99	118.89	122.90
2	B	1	NAG	C2-N2-C7	-2.85	119.09	122.90
3	D	3	MAN	C2-C3-C4	2.64	115.50	110.86
2	C	2	NAG	C3-C4-C5	2.45	114.67	110.23
2	B	2	NAG	C2-N2-C7	-2.43	119.64	122.90
2	B	1	NAG	C3-C4-C5	-2.30	106.07	110.23
3	D	2	NAG	C1-O5-C5	2.28	115.24	112.19
3	D	1	NAG	C2-N2-C7	-2.25	119.89	122.90
2	B	1	NAG	C1-C2-N2	2.20	113.90	110.43
4	E	2	NAG	O7-C7-N2	2.11	125.71	121.98
2	C	1	NAG	C2-N2-C7	-2.00	120.22	122.90

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	4	MAN	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
4	E	4	MAN	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C1-C2-N2-C7

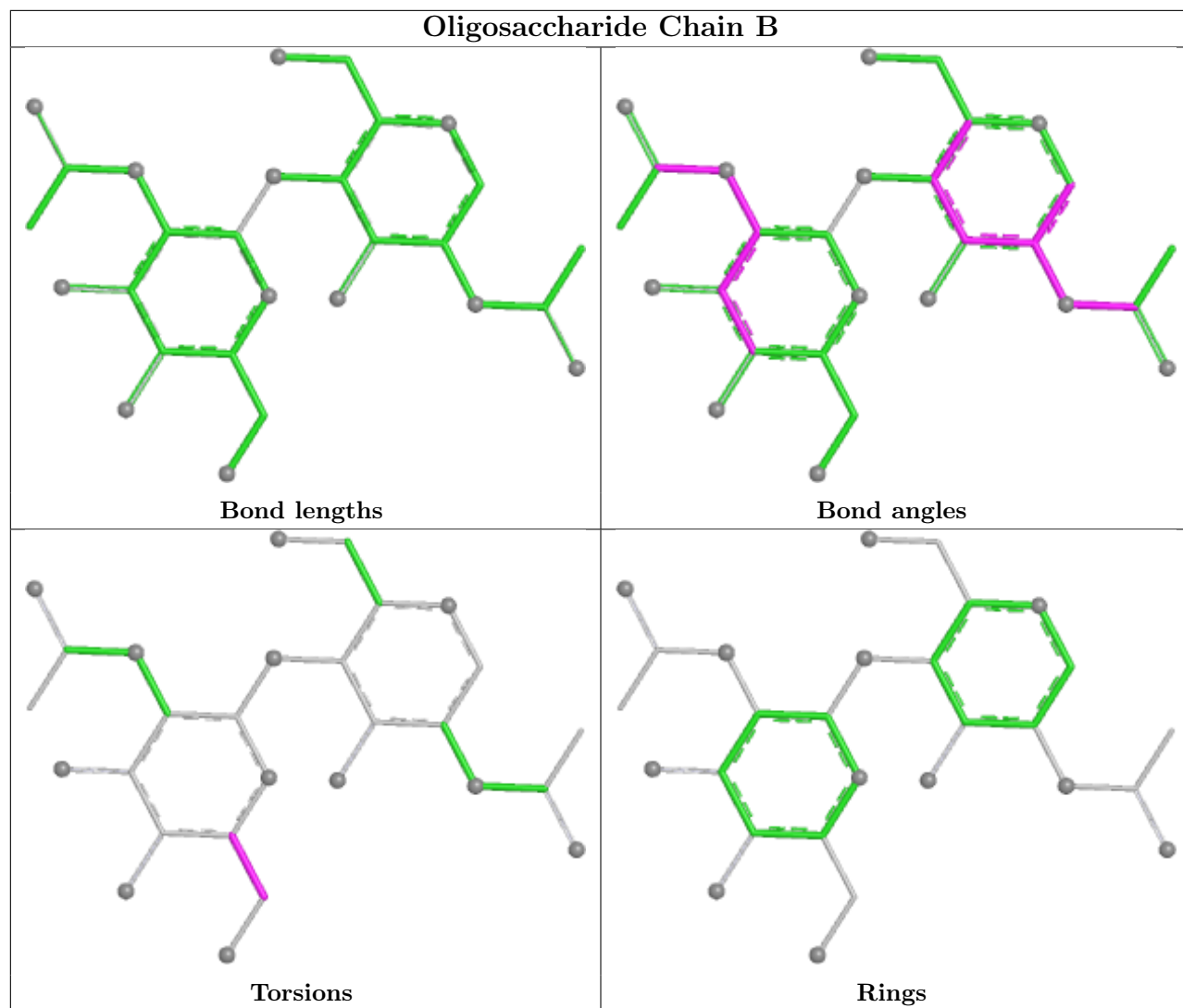
All (2) ring outliers are listed below:

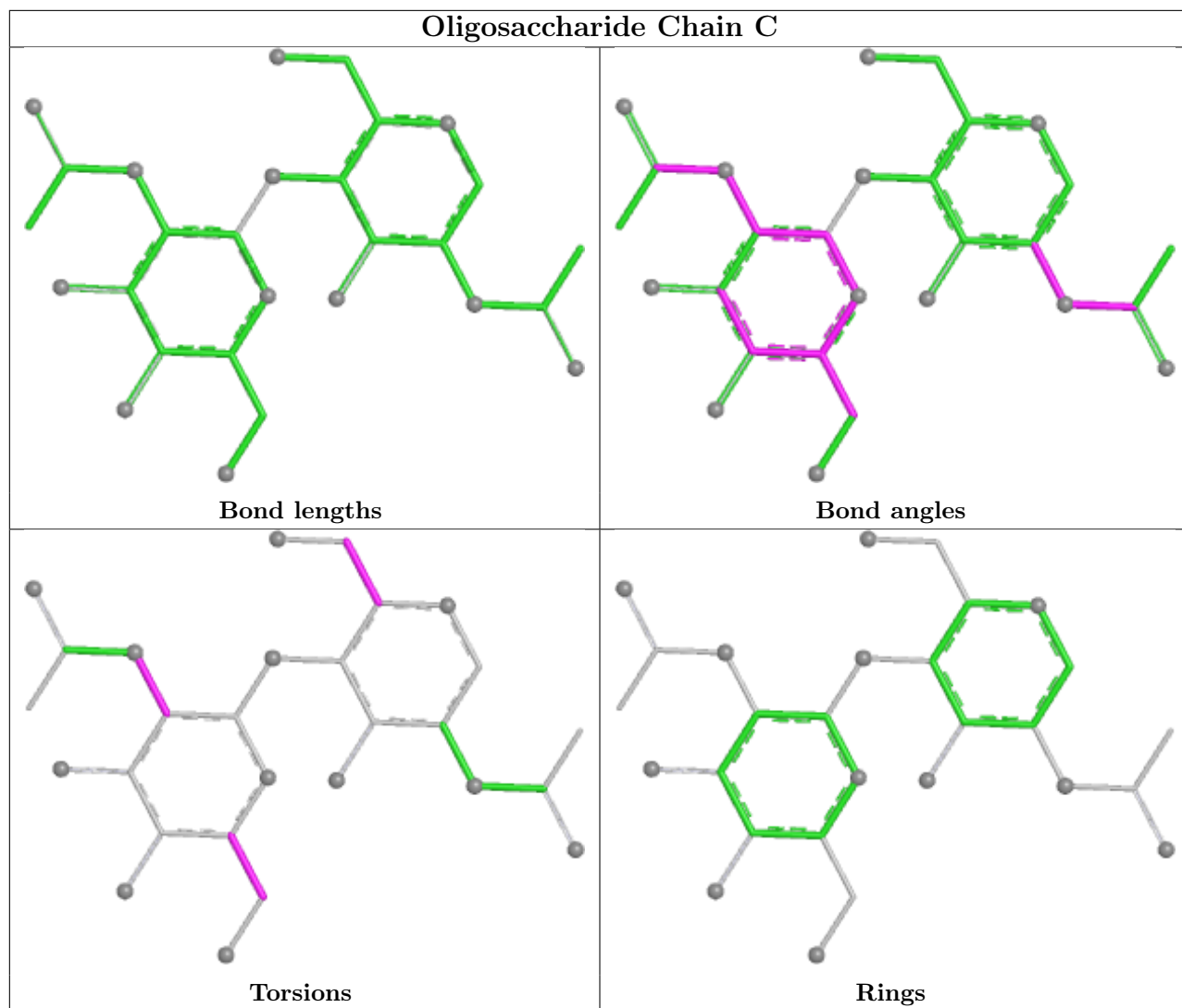
Mol	Chain	Res	Type	Atoms
4	E	4	MAN	C1-C2-C3-C4-C5-O5
4	E	3	BMA	C1-C2-C3-C4-C5-O5

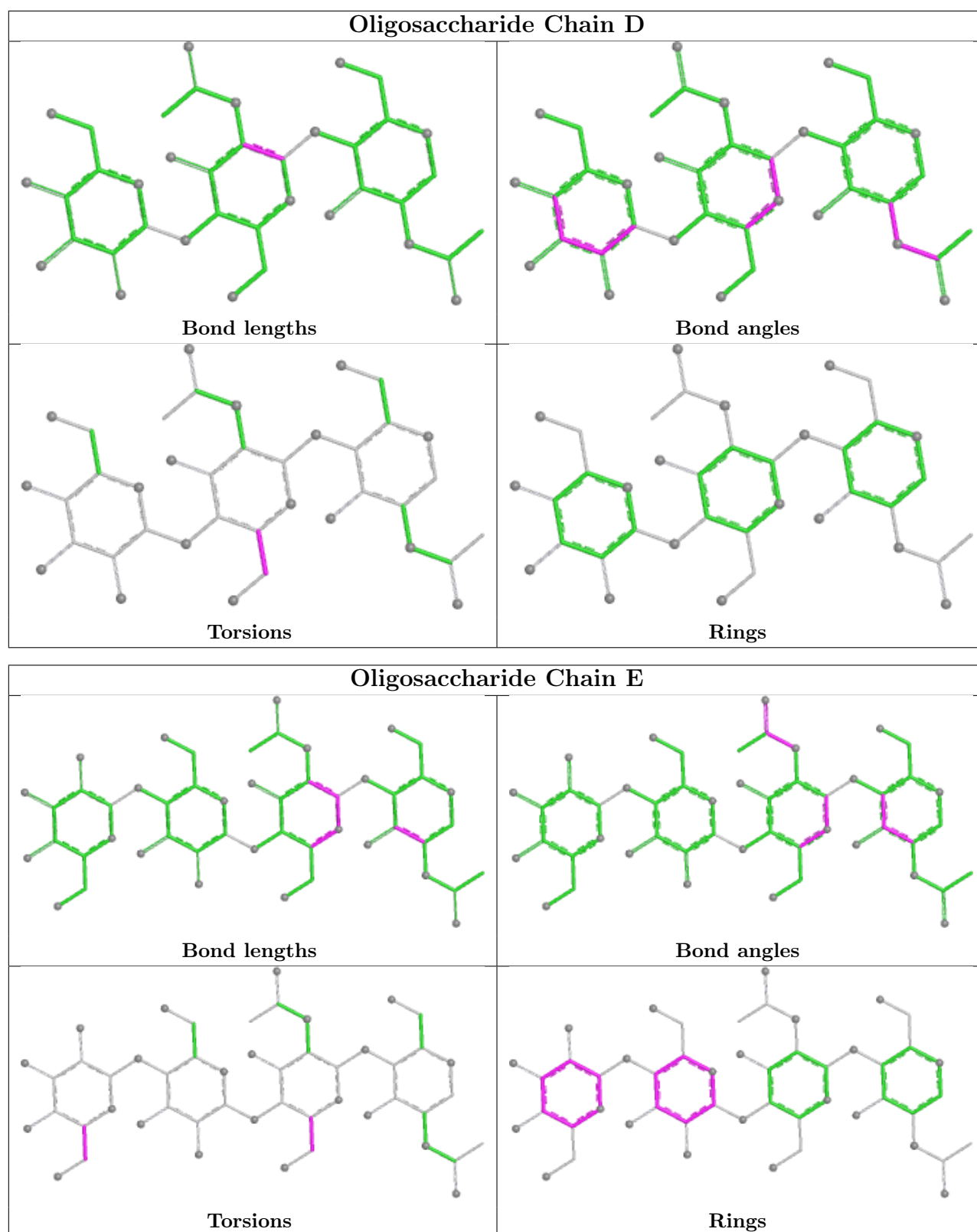
8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	1	0
3	D	2	NAG	5	0
4	E	2	NAG	4	0
2	B	1	NAG	1	0
2	C	1	NAG	1	0
4	E	3	BMA	1	0
4	E	1	NAG	2	0
3	D	3	MAN	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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	SCN	A	603	-	1,2,2	0.37	0	0,1,1	-	-
5	HEM	A	601	1	50,50,50	1.75	9 (18%)	67,82,82	1.61	13 (19%)
8	CYN	A	605	-	1,1,1	0.15	0	-	-	-
6	SCN	A	602	-	1,2,2	0.28	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	601	1	-	4/14/54/54	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	HEM	C3D-C2D	6.60	1.51	1.36
5	A	601	HEM	FE-NC	4.02	2.08	1.95
5	A	601	HEM	FE-ND	3.19	2.04	1.94
5	A	601	HEM	CAD-C3D	2.43	1.57	1.51
5	A	601	HEM	CAB-C3B	2.32	1.53	1.47
5	A	601	HEM	CHD-C4C	-2.21	1.34	1.38
5	A	601	HEM	CMC-C2C	2.19	1.55	1.50
5	A	601	HEM	CAC-C3C	2.18	1.53	1.47
5	A	601	HEM	O2A-CGA	-2.08	1.23	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	HEM	CMB-C2B-C1B	4.21	131.61	125.03
5	A	601	HEM	CHC-C4B-NB	4.07	128.80	124.42
5	A	601	HEM	C4D-ND-C1D	3.71	109.60	105.21
5	A	601	HEM	CAD-C3D-C4D	3.40	130.61	124.70
5	A	601	HEM	CBB-CAB-C3B	-2.98	112.61	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	HEM	C4B-C3B-C2B	2.84	109.89	107.28
5	A	601	HEM	CMB-C2B-C3B	-2.63	122.06	128.43
5	A	601	HEM	CAA-C2A-C1A	2.58	129.98	124.94
5	A	601	HEM	C4A-C3A-C2A	2.56	109.75	106.82
5	A	601	HEM	C3B-C4B-NB	-2.51	107.67	109.47
5	A	601	HEM	CHD-C1D-ND	2.19	126.78	124.42
5	A	601	HEM	CHD-C1D-C2D	-2.15	121.63	125.03
5	A	601	HEM	CHB-C1B-NB	-2.14	121.72	124.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

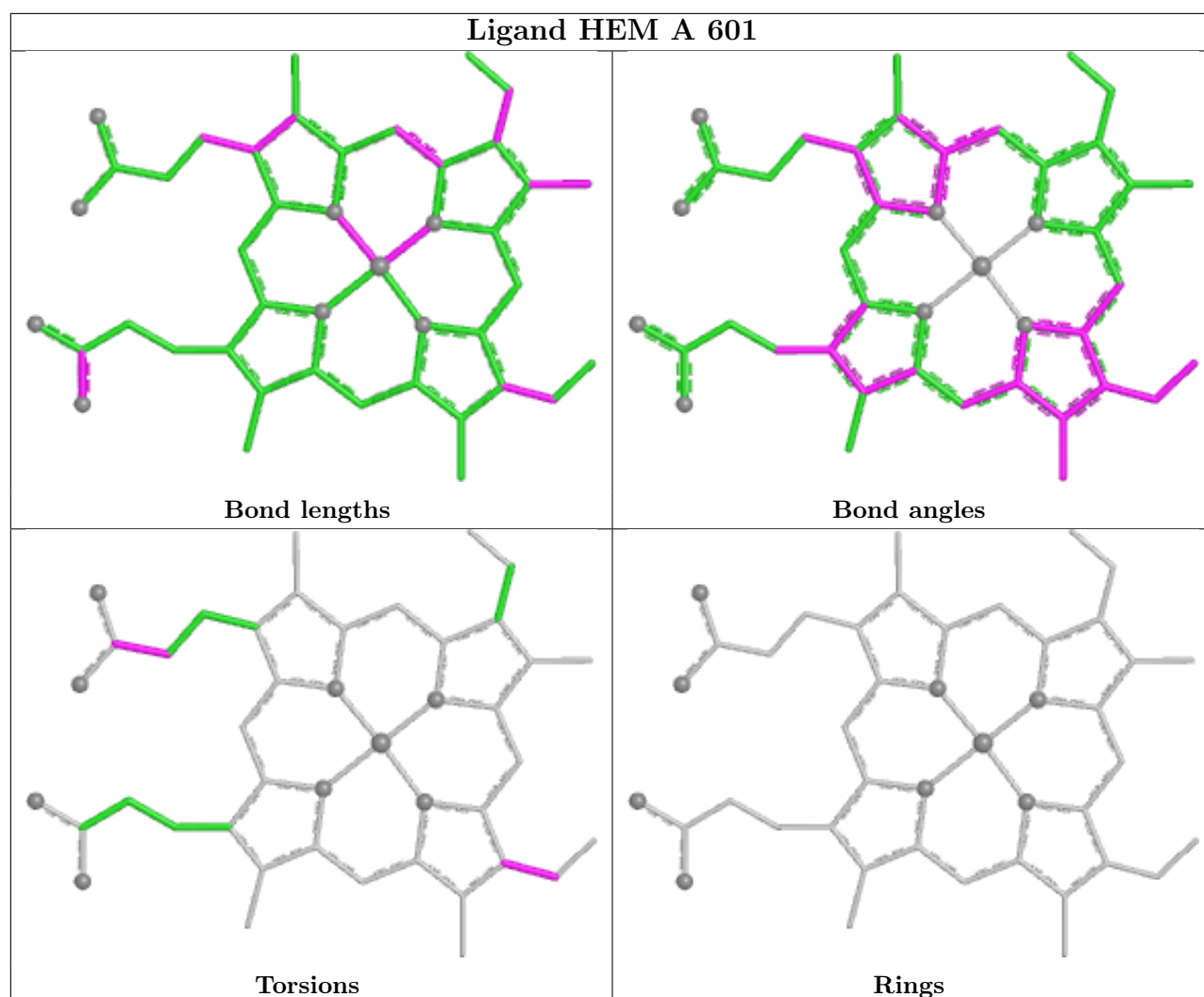
Mol	Chain	Res	Type	Atoms
5	A	601	HEM	C2B-C3B-CAB-CBB
5	A	601	HEM	C4B-C3B-CAB-CBB
5	A	601	HEM	CAD-CBD-CGD-O2D
5	A	601	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	605	CYN	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%)	-0.34	11 (1%) 66 63	10, 28, 72, 100	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	GLY	3.9
1	A	174	SER	3.4
1	A	7	GLY	3.1
1	A	13	VAL	2.7
1	A	172	TYR	2.6
1	A	168	PRO	2.5
1	A	8	ALA	2.5
1	A	9	PRO	2.3
1	A	169	THR	2.1
1	A	118	GLU	2.1
1	A	231	ASN	2.0

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	0.12	31,40,42,43	0

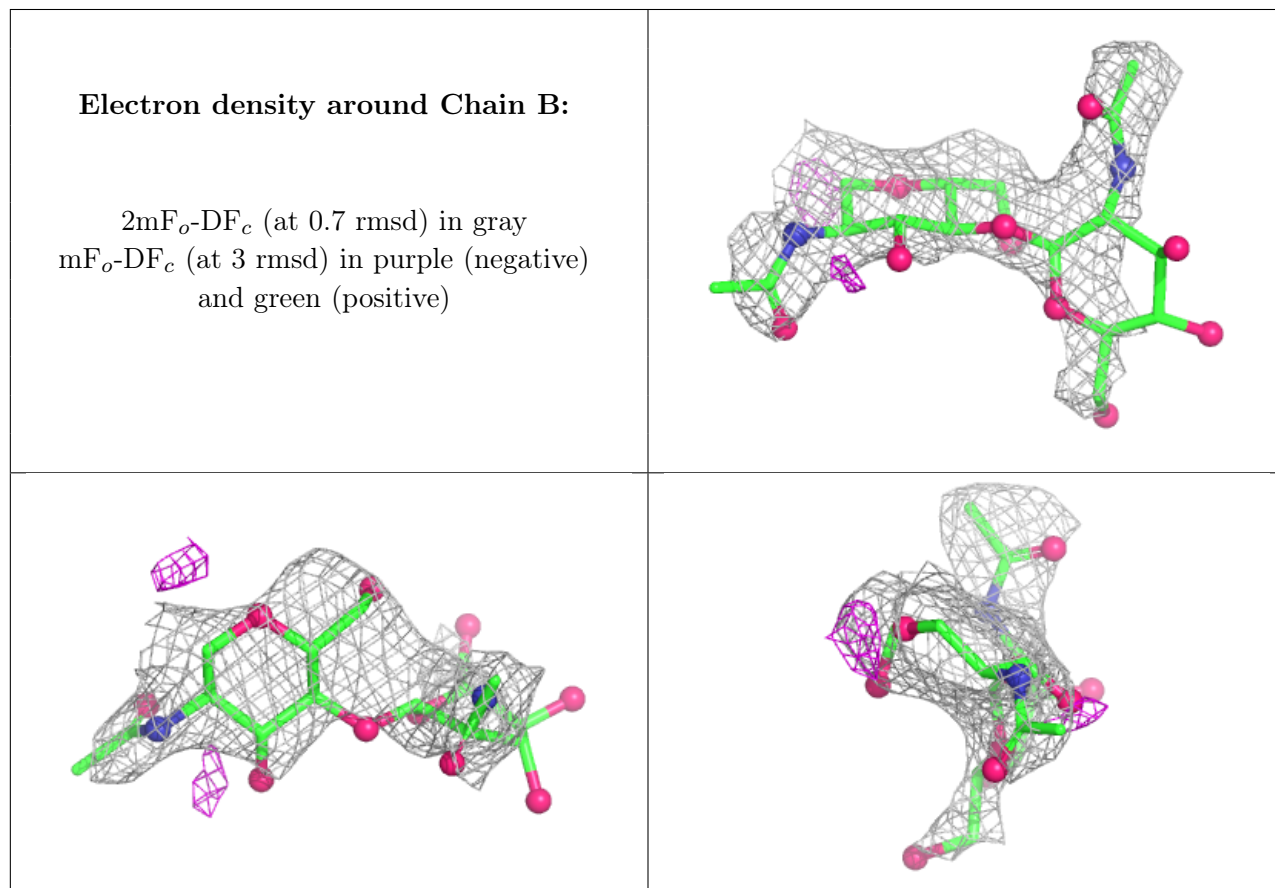
6.3 Carbohydrates [i](#)

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.

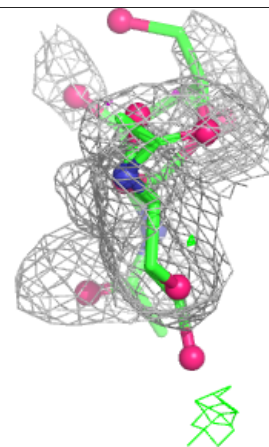
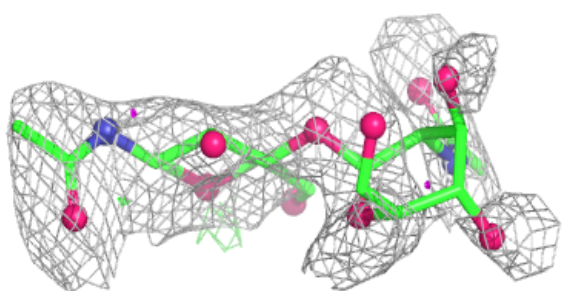
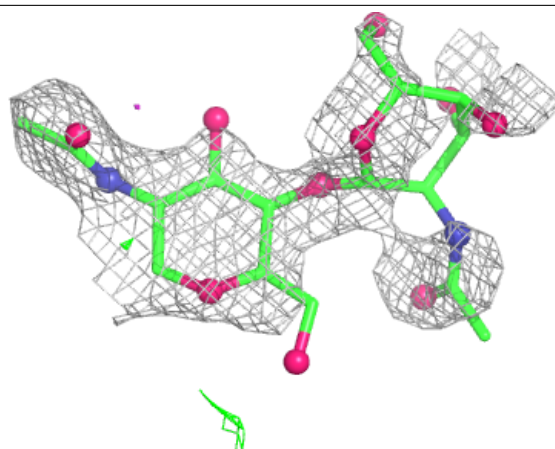
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	E	3	11/12	0.51	0.14	79,80,80,80	0
4	NAG	E	2	14/15	0.52	0.18	74,77,79,80	0
4	MAN	E	4	11/12	0.52	0.13	77,79,79,79	0
3	MAN	D	3	11/12	0.62	0.13	79,81,81,81	0
2	NAG	C	2	14/15	0.66	0.15	59,62,63,63	0
4	NAG	E	1	14/15	0.70	0.13	58,64,67,69	0
2	NAG	B	1	14/15	0.77	0.12	57,63,66,70	0
2	NAG	B	2	14/15	0.78	0.09	73,75,77,77	0
3	NAG	D	2	14/15	0.80	0.11	68,72,75,76	0
2	NAG	C	1	14/15	0.80	0.12	48,50,55,57	0
3	NAG	D	1	14/15	0.93	0.09	51,53,55,61	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.

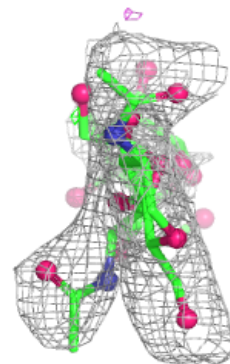
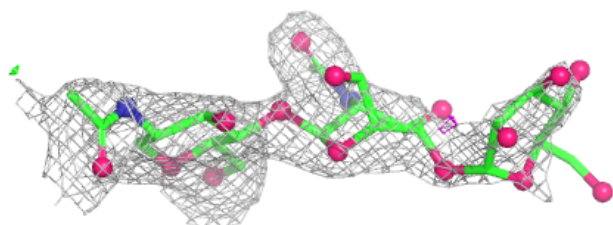
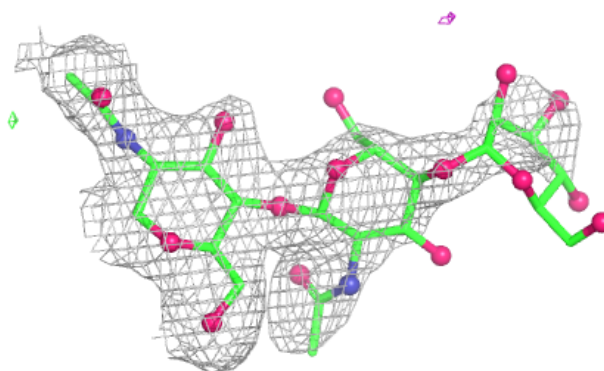


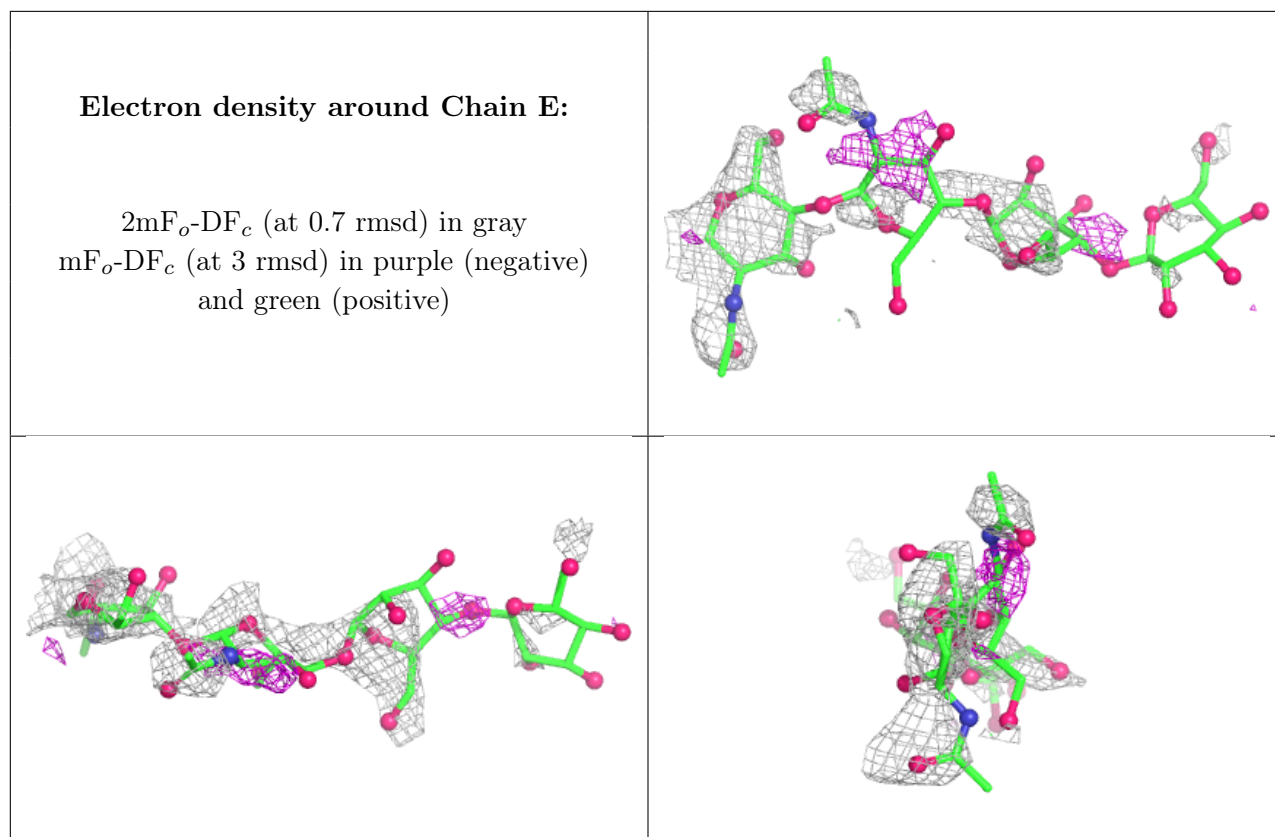
Electron density around Chain C:

$2mF_o-DF_c$ (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)





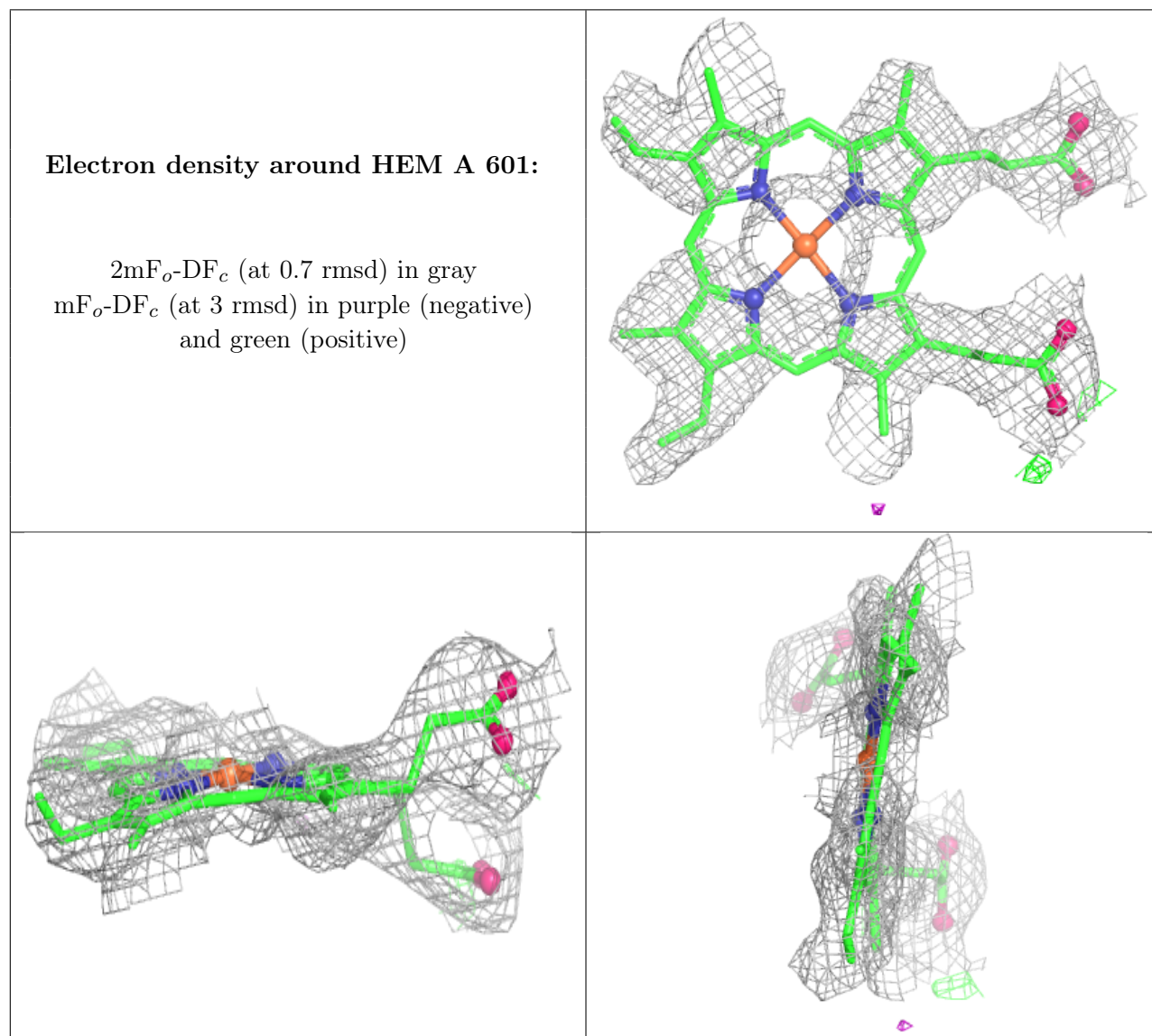
6.4 Ligands [i](#)

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
6	SCN	A	603	3/3	0.94	0.08	32,32,36,37	0
8	CYN	A	605	2/2	0.95	0.10	35,35,35,38	0
5	HEM	A	601	43/43	0.96	0.08	18,26,30,35	0
9	IOD	A	606	1/1	0.96	0.07	52,52,52,52	1
6	SCN	A	602	3/3	0.97	0.07	16,16,16,19	0
7	CA	A	604	1/1	0.97	0.03	17,17,17,17	0
9	IOD	A	609	1/1	0.97	0.05	90,90,90,90	0
9	IOD	A	608	1/1	0.98	0.04	79,79,79,79	0
9	IOD	A	607	1/1	0.98	0.07	56,56,56,56	1
9	IOD	A	610	1/1	0.98	0.05	66,66,66,66	0
9	IOD	A	612	1/1	0.98	0.05	61,61,61,61	0
9	IOD	A	611	1/1	1.00	0.02	21,21,21,21	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.