



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:01 PM UTC

PDB ID : 3R4X / pdb_00003r4x
Title : Crystal structure of bovine lactoperoxidase complexed with pyrazine-2-carboxamide at 2 Å resolution
Authors : Pandey, N.; Singh, R.P.; Singh, A.K.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2011-03-18
Resolution : 2.01 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

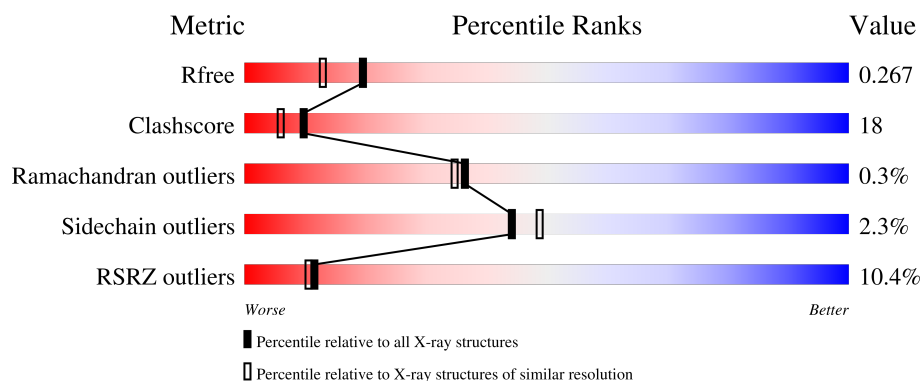
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	10% 71% 26% .
2	B	2	50% 50%
2	C	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
11	GOL	A	622	-	X	X	-
6	IOD	A	610	-	-	X	-
9	PZA	A	618	-	-	X	-
9	PZA	A	619	-	-	X	-

2 Entry composition [i](#)

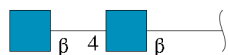
There are 13 unique types of molecules in this entry. The entry contains 5468 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

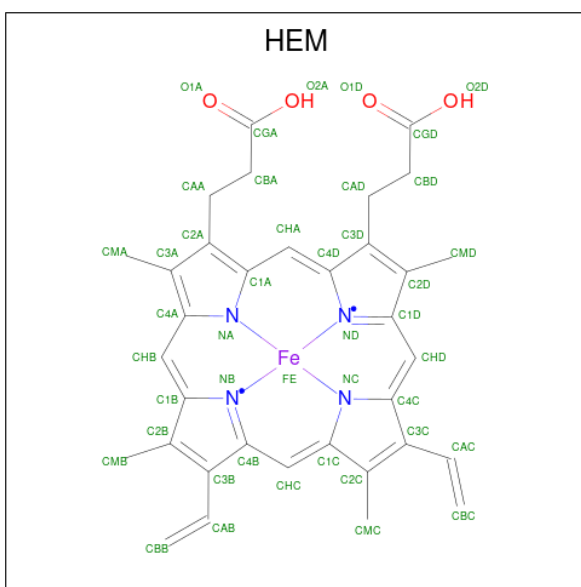


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

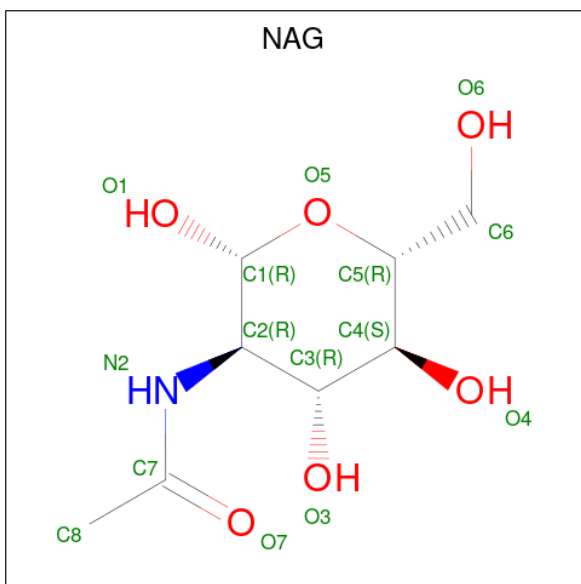
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

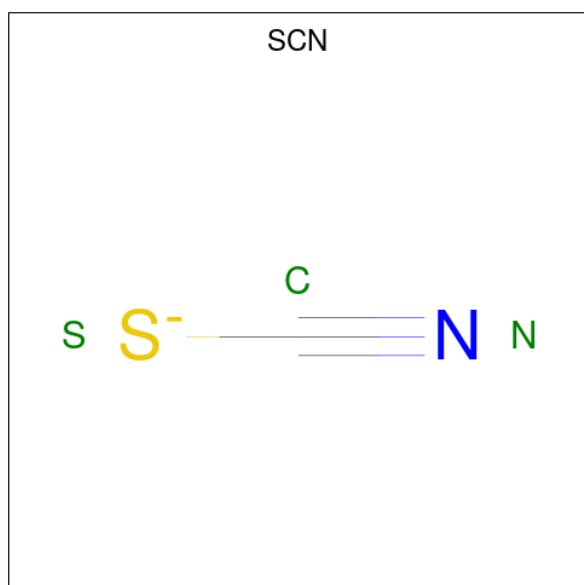
- Molecule 6 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	11	Total	I	0	0
			11	11		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

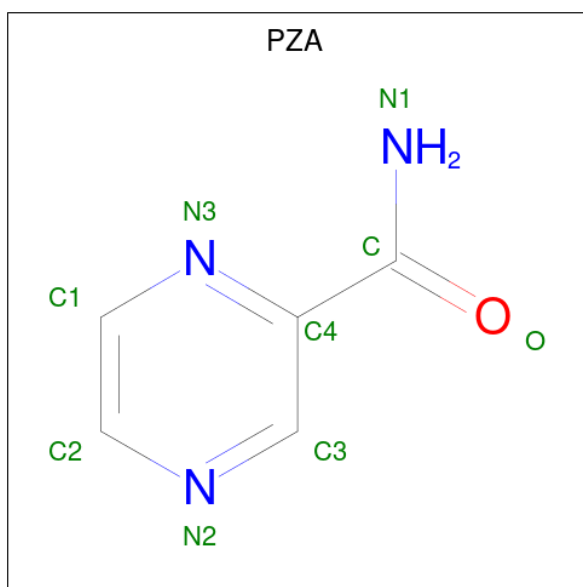
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		

- Molecule 8 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



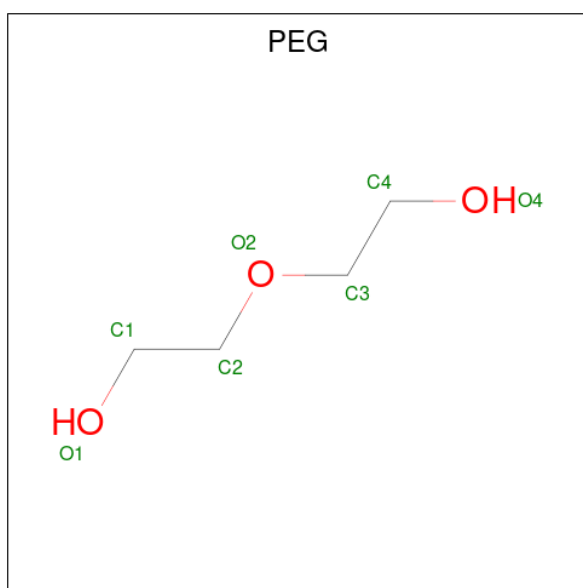
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 9 is PYRAZINE-2-CARBOXAMIDE (CCD ID: PZA) (formula: C₅H₅N₃O).



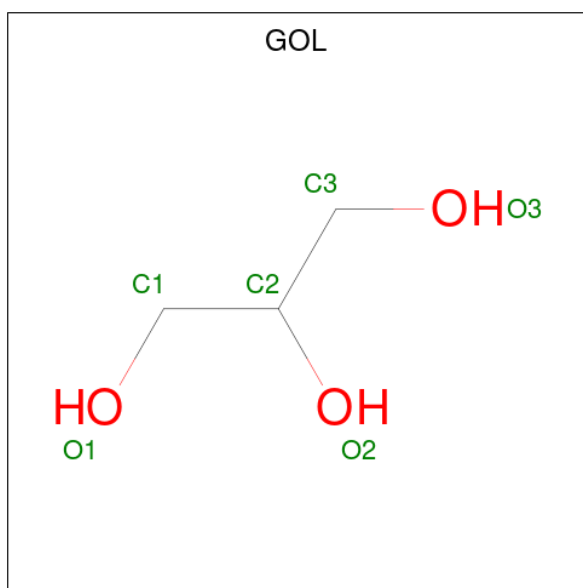
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			9	5	3	1		
9	A	1	Total	C	N	O	0	0
			9	5	3	1		

- Molecule 10 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



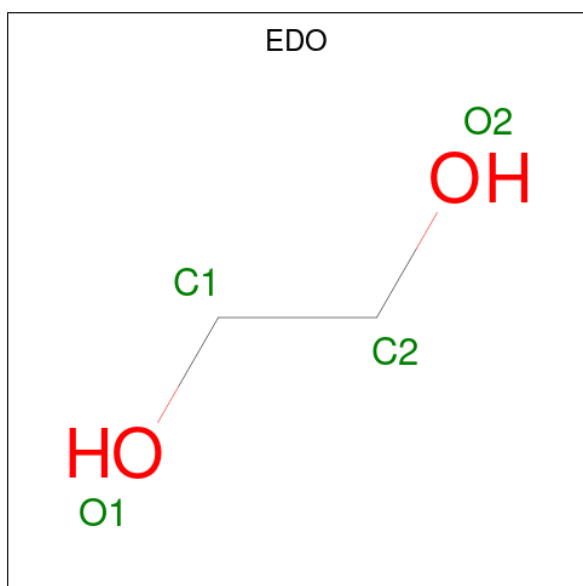
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			7	4	3		
10	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 11 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			6	3	3		
11	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 12 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			4	2	2		

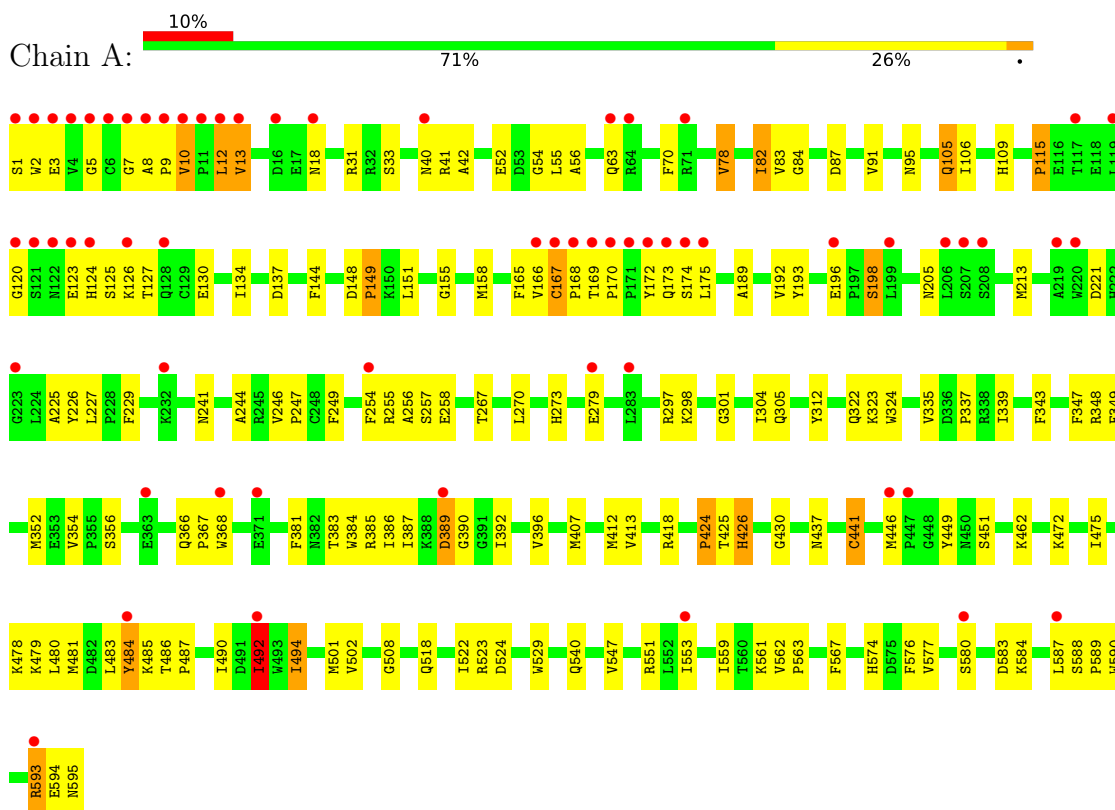
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	499	Total	O	0	0
			499	499		

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



MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.92Å 79.72Å 77.00Å 90.00° 102.22° 90.00°	Depositor
Resolution (Å)	75.26 – 2.01 75.26 – 2.01	Depositor EDS
% Data completeness (in resolution range)	97.8 (75.26-2.01) 97.8 (75.26-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.89 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.210 , 0.256 0.228 , 0.267	Depositor DCC
R_{free} test set	2120 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.908	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 39.5	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	0.94	EDS
Total number of atoms	5468	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 5.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, ZN, SCN, GOL, EDO, PEG, NAG, HEM, CA, PZA, SEP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.02	13/4891 (0.3%)	1.22	41/6634 (0.6%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	547	VAL	CA-CB	10.72	1.64	1.54
1	A	413	VAL	CA-CB	8.02	1.64	1.54
1	A	562	VAL	CA-CB	6.99	1.64	1.54
1	A	481	MET	C-O	-6.96	1.15	1.24
1	A	83	VAL	CA-CB	6.47	1.63	1.54
1	A	492	ILE	CA-CB	6.36	1.62	1.54
1	A	106	ILE	CG1-CD1	-5.41	1.30	1.51
1	A	424	PRO	C-O	-5.41	1.17	1.23
1	A	502	VAL	CA-CB	5.36	1.60	1.54
1	A	392	ILE	CA-CB	5.33	1.61	1.54
1	A	483	LEU	C-O	-5.06	1.18	1.24
1	A	105	GLN	C-O	-5.05	1.18	1.24
1	A	56	ALA	CA-CB	5.01	1.61	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	GLN	N-CA-C	9.45	124.37	111.71
1	A	82	ILE	N-CA-C	7.98	118.83	112.12
1	A	5	GLY	N-CA-C	7.87	119.42	111.95
1	A	426	HIS	N-CA-C	-7.58	97.90	109.95
1	A	256	ALA	N-CA-C	7.16	120.92	111.75
1	A	386	ILE	CB-CA-C	-7.00	102.87	112.04
1	A	115	PRO	N-CA-C	6.96	121.99	111.14
1	A	13	VAL	N-CA-C	6.28	116.90	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	VAL	N-CA-C	6.25	114.84	109.02
1	A	354	VAL	CA-C-O	6.20	122.81	119.15
1	A	225	ALA	N-CA-C	6.15	119.91	110.20
1	A	483	LEU	N-CA-C	6.11	117.81	111.03
1	A	562	VAL	N-CA-C	6.10	115.90	109.01
1	A	412	MET	N-CA-C	6.00	118.98	111.24
1	A	389	ASP	N-CA-C	5.96	117.44	110.41
1	A	55	LEU	N-CA-C	5.93	120.31	112.72
1	A	78	VAL	N-CA-C	-5.91	104.59	110.62
1	A	508	GLY	CA-C-N	5.87	125.08	118.97
1	A	508	GLY	C-N-CA	5.87	125.08	118.97
1	A	82	ILE	CB-CA-C	-5.82	105.20	110.91
1	A	426	HIS	CB-CA-C	5.79	119.97	109.37
1	A	312	TYR	N-CA-C	5.78	118.45	111.40
1	A	390	GLY	N-CA-C	5.73	123.03	114.95
1	A	524	ASP	N-CA-C	5.73	118.30	111.71
1	A	40	ASN	N-CA-C	5.72	119.57	112.24
1	A	31	ARG	N-CA-C	5.70	117.58	111.36
1	A	484	TYR	N-CA-C	-5.69	99.97	109.24
1	A	356	SER	N-CA-C	5.65	119.89	112.89
1	A	244	ALA	N-CA-C	-5.62	105.15	112.23
1	A	484	TYR	CA-C-N	-5.60	111.64	122.06
1	A	484	TYR	C-N-CA	-5.60	111.64	122.06
1	A	33	SER	CA-C-N	5.59	125.26	119.56
1	A	33	SER	C-N-CA	5.59	125.26	119.56
1	A	87	ASP	N-CA-C	5.40	117.04	108.67
1	A	574	HIS	N-CA-C	5.32	116.77	111.07
1	A	134	ILE	CB-CA-C	-5.28	103.75	110.98
1	A	192	VAL	CB-CA-C	-5.25	105.33	111.94
1	A	84	GLY	N-CA-C	5.24	120.05	112.82
1	A	148	ASP	N-CA-C	5.20	116.22	109.72
1	A	441	CYS	N-CA-C	-5.18	104.90	111.11
1	A	449	TYR	N-CA-C	5.08	117.48	111.33

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	158	0
2	B	28	0	25	0	0
2	C	28	0	25	1	0
3	A	1	0	0	0	0
4	A	43	0	30	7	0
5	A	28	0	26	4	0
6	A	11	0	0	4	0
7	A	1	0	0	0	0
8	A	3	0	0	0	0
9	A	18	0	10	18	0
10	A	14	0	20	4	0
11	A	12	0	14	6	0
12	A	8	0	12	1	0
13	A	499	0	0	22	0
All	All	5468	0	4849	173	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 (173) 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:12:LEU:HD23	1:A:13:VAL:N	1.40	1.36
1:A:10:VAL:HG11	1:A:41:ARG:CZ	1.65	1.26
5:A:603:NAG:O7	11:A:622:GOL:H11	1.39	1.20
1:A:424:PRO:O	1:A:425:THR:HG22	1.37	1.19
1:A:593:ARG:HH11	1:A:593:ARG:HG2	0.96	1.11
1:A:123:GLU:HG3	1:A:125:SER:H	1.00	1.08
1:A:167:CYS:CB	1:A:168:PRO:CD	2.31	1.08
1:A:167:CYS:HB2	1:A:168:PRO:HD2	1.28	1.07
1:A:105:GLN:HE21	9:A:618:PZA:H2	1.02	1.02
1:A:167:CYS:HB3	1:A:168:PRO:CD	1.91	1.00
1:A:167:CYS:HB3	1:A:168:PRO:HD3	1.46	0.97
1:A:167:CYS:CB	1:A:168:PRO:HD2	1.92	0.96
1:A:169:THR:HB	1:A:170:PRO:HD3	1.48	0.95
1:A:593:ARG:HG2	1:A:593:ARG:NH1	1.71	0.93
1:A:123:GLU:HG3	1:A:125:SER:N	1.83	0.93
1:A:196:GLU:HB3	1:A:198:SEP:O3P	1.70	0.90
9:A:618:PZA:H5	9:A:619:PZA:C	2.02	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:VAL:CG1	1:A:41:ARG:CZ	2.52	0.87
1:A:593:ARG:HH11	1:A:593:ARG:CG	1.85	0.87
1:A:168:PRO:HG3	1:A:172:TYR:HD1	1.38	0.86
1:A:12:LEU:HD23	1:A:12:LEU:C	2.00	0.86
1:A:54:GLY:HA2	13:A:905:HOH:O	1.74	0.85
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.57	0.85
1:A:12:LEU:HD23	1:A:13:VAL:H	1.41	0.85
1:A:279:GLU:HG2	1:A:587:LEU:HD12	1.57	0.85
1:A:12:LEU:CD2	1:A:13:VAL:N	2.34	0.84
1:A:255:ARG:HA	9:A:619:PZA:N2	1.94	0.82
1:A:9:PRO:CD	1:A:167:CYS:HA	2.10	0.81
1:A:424:PRO:O	1:A:425:THR:CG2	2.28	0.79
1:A:462:LYS:HD2	13:A:802:HOH:O	1.83	0.78
1:A:10:VAL:HG11	1:A:41:ARG:NH2	2.00	0.77
1:A:105:GLN:NE2	9:A:618:PZA:H2	1.82	0.75
1:A:124:HIS:HB2	1:A:127:THR:HB	1.68	0.75
1:A:10:VAL:CG1	1:A:41:ARG:NH2	2.50	0.74
1:A:168:PRO:HG3	1:A:172:TYR:CD1	2.21	0.74
1:A:339:ILE:HD13	1:A:522:ILE:HD11	1.71	0.72
1:A:9:PRO:HG2	1:A:167:CYS:O	1.92	0.70
1:A:95:ASN:HD22	11:A:622:GOL:H12	1.57	0.69
1:A:109:HIS:NE2	9:A:618:PZA:C	2.56	0.69
1:A:396:VAL:HG11	1:A:553:ILE:HD12	1.74	0.69
1:A:105:GLN:HG3	9:A:618:PZA:N1	2.08	0.68
1:A:12:LEU:HD23	1:A:13:VAL:CA	2.23	0.68
1:A:9:PRO:HG2	1:A:167:CYS:CA	2.24	0.68
1:A:10:VAL:HG11	1:A:41:ARG:NH1	2.08	0.67
1:A:494:ILE:HD13	1:A:494:ILE:O	1.94	0.67
1:A:127:THR:HA	13:A:933:HOH:O	1.95	0.67
1:A:227:LEU:HD22	1:A:270:LEU:HD22	1.75	0.67
1:A:12:LEU:C	1:A:12:LEU:CD2	2.66	0.66
1:A:105:GLN:HG3	9:A:618:PZA:H1	1.62	0.65
1:A:258:GLU:HB2	9:A:619:PZA:H4	1.77	0.65
6:A:612:IOD:I	13:A:891:HOH:O	2.85	0.64
1:A:418:ARG:HH22	10:A:620:PEG:C4	2.11	0.64
1:A:63:GLN:H	1:A:63:GLN:CD	2.06	0.63
1:A:105:GLN:NE2	9:A:618:PZA:H4	2.13	0.63
1:A:475:ILE:HG22	1:A:479:LYS:HE3	1.81	0.62
1:A:9:PRO:HD2	1:A:167:CYS:HA	1.81	0.62
1:A:78:VAL:HG21	1:A:484:TYR:OH	2.00	0.61
1:A:82:ILE:HD13	1:A:480:LEU:HD23	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:THR:N	1:A:170:PRO:CD	2.63	0.61
9:A:618:PZA:H5	9:A:619:PZA:N1	2.16	0.60
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.36	0.60
1:A:165:PHE:CZ	1:A:169:THR:O	2.54	0.60
1:A:424:PRO:C	1:A:425:THR:HG22	2.22	0.60
1:A:559:ILE:HG23	6:A:605:IOD:I	2.73	0.59
1:A:492:ILE:C	1:A:492:ILE:HD13	2.28	0.58
1:A:105:GLN:HE21	9:A:618:PZA:H4	1.69	0.58
1:A:492:ILE:HD13	1:A:492:ILE:O	2.05	0.57
1:A:168:PRO:HB2	1:A:170:PRO:O	2.06	0.56
1:A:407:MET:HB3	1:A:501:MET:HE3	1.88	0.56
1:A:18:ASN:ND2	13:A:709:HOH:O	2.37	0.56
1:A:594:GLU:O	1:A:595:ASN:HB2	2.06	0.56
1:A:229:PHE:CG	1:A:247:PRO:HG2	2.41	0.55
1:A:9:PRO:HG2	1:A:167:CYS:C	2.32	0.55
1:A:10:VAL:HG12	1:A:41:ARG:NH2	2.21	0.55
1:A:105:GLN:CG	9:A:618:PZA:N1	2.70	0.55
1:A:580:SER:HA	11:A:623:GOL:O2	2.07	0.55
1:A:339:ILE:CD1	1:A:522:ILE:HD11	2.35	0.54
1:A:9:PRO:CG	1:A:167:CYS:HA	2.36	0.54
1:A:82:ILE:HD13	1:A:480:LEU:CD2	2.38	0.54
1:A:229:PHE:CD1	1:A:247:PRO:HG2	2.43	0.54
1:A:472:LYS:HE3	12:A:625:EDO:H21	1.89	0.53
5:A:603:NAG:O7	11:A:622:GOL:C1	2.33	0.53
1:A:63:GLN:CD	1:A:63:GLN:N	2.66	0.53
1:A:169:THR:HB	1:A:170:PRO:CD	2.31	0.53
4:A:602:HEM:HMC2	4:A:602:HEM:HBC2	1.91	0.53
1:A:551:ARG:HD3	1:A:583:ASP:O	2.09	0.53
1:A:149:PRO:HB2	10:A:620:PEG:H22	1.91	0.52
1:A:518:GLN:O	1:A:522:ILE:HG12	2.10	0.52
1:A:383:THR:HG22	1:A:387:ILE:HD12	1.91	0.52
1:A:169:THR:N	1:A:170:PRO:HD2	2.24	0.52
1:A:258:GLU:HG3	9:A:619:PZA:N1	2.25	0.52
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.45	0.52
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.57	0.51
4:A:602:HEM:NC	9:A:618:PZA:N1	2.58	0.51
1:A:451:SER:HA	13:A:1081:HOH:O	2.08	0.51
1:A:426:HIS:HE1	13:A:751:HOH:O	1.92	0.51
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.07	0.51
1:A:323:LYS:HD3	1:A:324:TRP:CE2	2.46	0.51
1:A:227:LEU:HD21	1:A:267:THR:HA	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:610:IOD:I	13:A:864:HOH:O	2.88	0.51
1:A:494:ILE:HD13	1:A:494:ILE:C	2.36	0.50
1:A:109:HIS:NE2	9:A:618:PZA:C4	2.74	0.50
4:A:602:HEM:HBD2	13:A:803:HOH:O	2.10	0.50
1:A:42:ALA:HB2	1:A:166:VAL:HG11	1.93	0.50
1:A:384:TRP:CZ2	2:C:1:NAG:H2	2.45	0.50
1:A:584:LYS:HE3	11:A:623:GOL:H11	1.93	0.49
1:A:407:MET:HB3	1:A:501:MET:CE	2.42	0.49
1:A:70:PHE:CG	1:A:485:LYS:HB2	2.48	0.49
1:A:82:ILE:CD1	1:A:480:LEU:HD23	2.42	0.48
1:A:588:SER:HB2	1:A:589:PRO:HD3	1.94	0.48
1:A:249:PHE:CE1	1:A:383:THR:HG23	2.49	0.48
1:A:301:GLY:O	1:A:305:GLN:HG3	2.14	0.48
1:A:52:GLU:HG2	13:A:872:HOH:O	2.14	0.47
1:A:487:PRO:HA	1:A:490:ILE:HD12	1.96	0.47
10:A:621:PEG:H41	13:A:1047:HOH:O	2.14	0.47
1:A:123:GLU:HG2	1:A:125:SER:HB3	1.97	0.47
5:A:603:NAG:H4	13:A:955:HOH:O	2.15	0.46
1:A:63:GLN:NE2	13:A:727:HOH:O	2.47	0.46
1:A:368:TRP:O	1:A:368:TRP:CE3	2.69	0.46
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.51	0.46
1:A:385:ARG:O	1:A:389:ASP:HB3	2.15	0.46
5:A:603:NAG:H2	11:A:622:GOL:H31	1.97	0.46
1:A:9:PRO:CG	1:A:167:CYS:O	2.61	0.45
1:A:446:MET:HA	1:A:446:MET:HE2	1.99	0.45
1:A:205:ASN:HA	13:A:1088:HOH:O	2.16	0.45
1:A:540:GLN:HG2	1:A:590:TRP:CE2	2.51	0.45
1:A:561:LYS:HA	1:A:577:VAL:O	2.17	0.44
1:A:246:VAL:HG11	1:A:387:ILE:HD12	1.99	0.44
1:A:249:PHE:CZ	1:A:383:THR:HG23	2.52	0.44
1:A:8:ALA:N	1:A:9:PRO:CD	2.80	0.44
1:A:257:SER:O	1:A:381:PHE:HA	2.18	0.44
1:A:123:GLU:HG2	1:A:125:SER:CB	2.48	0.44
1:A:279:GLU:CG	1:A:587:LEU:HD12	2.38	0.44
1:A:418:ARG:HH22	10:A:620:PEG:H42	1.82	0.44
4:A:602:HEM:CMB	4:A:602:HEM:HBB2	2.48	0.43
1:A:298:LYS:HG3	13:A:1128:HOH:O	2.18	0.43
4:A:602:HEM:C1A	9:A:618:PZA:N3	2.87	0.43
1:A:123:GLU:CG	1:A:125:SER:CB	2.96	0.43
1:A:175:LEU:HD12	13:A:729:HOH:O	2.18	0.43
1:A:227:LEU:CD2	1:A:270:LEU:HD22	2.45	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:PHE:CE2	9:A:619:PZA:C1	3.02	0.43
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.54	0.43
1:A:563:PRO:HD3	1:A:576:PHE:CE2	2.54	0.43
1:A:567:PHE:HB2	6:A:610:IOD:I	2.89	0.43
1:A:335:VAL:O	1:A:337:PRO:HD3	2.19	0.42
1:A:396:VAL:CG1	1:A:553:ILE:HD12	2.46	0.42
1:A:349:PHE:CD1	1:A:349:PHE:C	2.97	0.42
1:A:9:PRO:CG	1:A:167:CYS:CA	2.94	0.42
1:A:193:TYR:OH	1:A:297:ARG:HA	2.20	0.42
1:A:366:GLN:O	1:A:367:PRO:C	2.62	0.42
1:A:540:GLN:HG2	1:A:590:TRP:CZ2	2.54	0.42
1:A:595:ASN:C	1:A:595:ASN:HD22	2.26	0.42
1:A:1:SER:N	13:A:722:HOH:O	2.44	0.42
1:A:120:GLY:HA3	1:A:126:LYS:HG3	2.02	0.42
4:A:602:HEM:ND	9:A:618:PZA:O	2.53	0.42
1:A:368:TRP:O	1:A:368:TRP:HE3	2.02	0.42
1:A:241:ASN:HD22	1:A:384:TRP:NE1	2.18	0.41
1:A:123:GLU:CG	1:A:125:SER:HB3	2.50	0.41
1:A:2:TRP:HA	13:A:1056:HOH:O	2.20	0.41
1:A:478:LYS:HE2	13:A:1094:HOH:O	2.21	0.41
1:A:130:GLU:OE1	1:A:426:HIS:ND1	2.51	0.41
1:A:144:PHE:HE2	1:A:158:MET:HE3	1.86	0.41
1:A:151:LEU:HD12	1:A:155:GLY:O	2.21	0.41
1:A:189:ALA:HB2	1:A:304:ILE:HD12	2.02	0.41
1:A:322:GLN:HG2	13:A:1090:HOH:O	2.20	0.41
1:A:352:MET:CB	1:A:407:MET:HG2	2.51	0.41
1:A:487:PRO:HA	1:A:490:ILE:CD1	2.50	0.41
1:A:158:MET:HE2	1:A:430:GLY:O	2.21	0.41
1:A:78:VAL:HG13	1:A:82:ILE:HD12	2.03	0.40
1:A:229:PHE:HZ	1:A:387:ILE:HD13	1.86	0.40
1:A:115:PRO:HG2	13:A:1144:HOH:O	2.21	0.40
1:A:105:GLN:HG3	4:A:602:HEM:C1C	2.56	0.40
1:A:130:GLU:HB2	13:A:751:HOH:O	2.22	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%)	569 (96%)	21 (4%)	2 (0%)	36	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	CYS
1	A	7	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	517/517 (100%)	505 (98%)	12 (2%)	44	49

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	12	LEU
1	A	91	VAL
1	A	137	ASP
1	A	149	PRO
1	A	174	SER
1	A	347	PHE
1	A	441	CYS
1	A	486	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	492	ILE
1	A	494	ILE
1	A	593	ARG

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

Mol	Chain	Res	Type
1	A	102	GLN
1	A	105	GLN
1	A	147	ASN
1	A	259	GLN
1	A	322	GLN
1	A	329	GLN
1	A	366	GLN
1	A	468	GLN
1	A	497	ASN
1	A	545	GLN
1	A	556	ASN
1	A	570	ASN
1	A	571	ASN
1	A	574	HIS
1	A	595	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SEP	A	198	1	8,9,10	1.67	1 (12%)	7,12,14	1.34	1 (14%)

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	3.56	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	OG-CB-CA	2.36	110.44	108.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

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](#)

4 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	0.49	0	17,19,21	0.83	0
2	NAG	B	2	2	14,14,15	1.09	2 (14%)	17,19,21	1.44	3 (17%)
2	NAG	C	1	1,2	14,14,15	0.66	0	17,19,21	0.73	0
2	NAG	C	2	2	14,14,15	0.44	0	17,19,21	2.20	4 (23%)

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	-	2/6/23/26	0/1/1/1
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	C8-C7	2.56	1.55	1.50
2	B	2	NAG	C1-C2	2.05	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	6.95	121.50	112.19
2	B	2	NAG	C4-C3-C2	3.27	115.81	111.02
2	C	2	NAG	C4-C3-C2	-2.89	106.79	111.02
2	B	2	NAG	C1-O5-C5	-2.64	108.65	112.19
2	C	2	NAG	C1-C2-N2	2.54	114.44	110.43
2	C	2	NAG	O5-C5-C4	2.52	116.96	110.83
2	B	2	NAG	C2-N2-C7	2.19	125.84	122.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

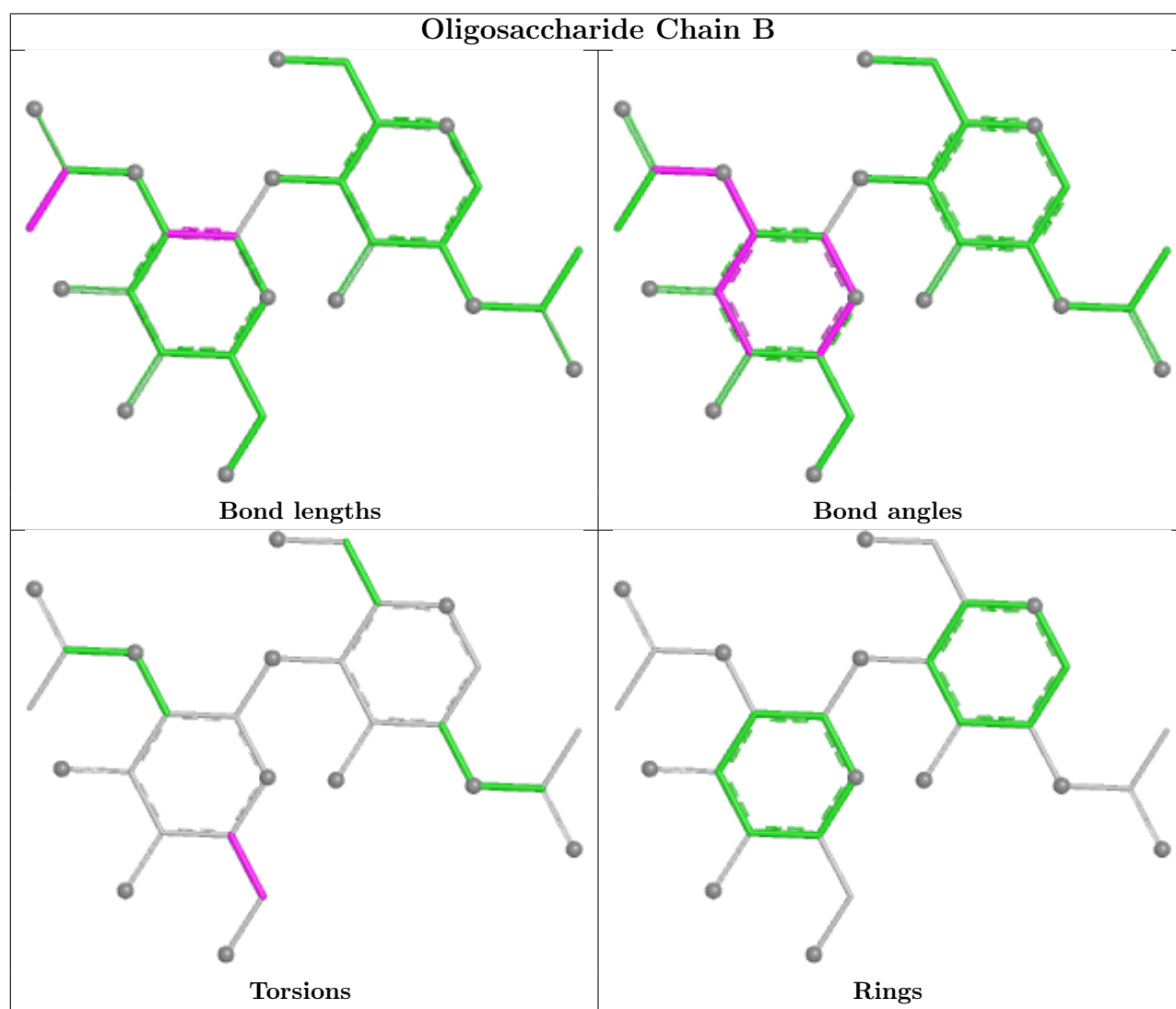
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6

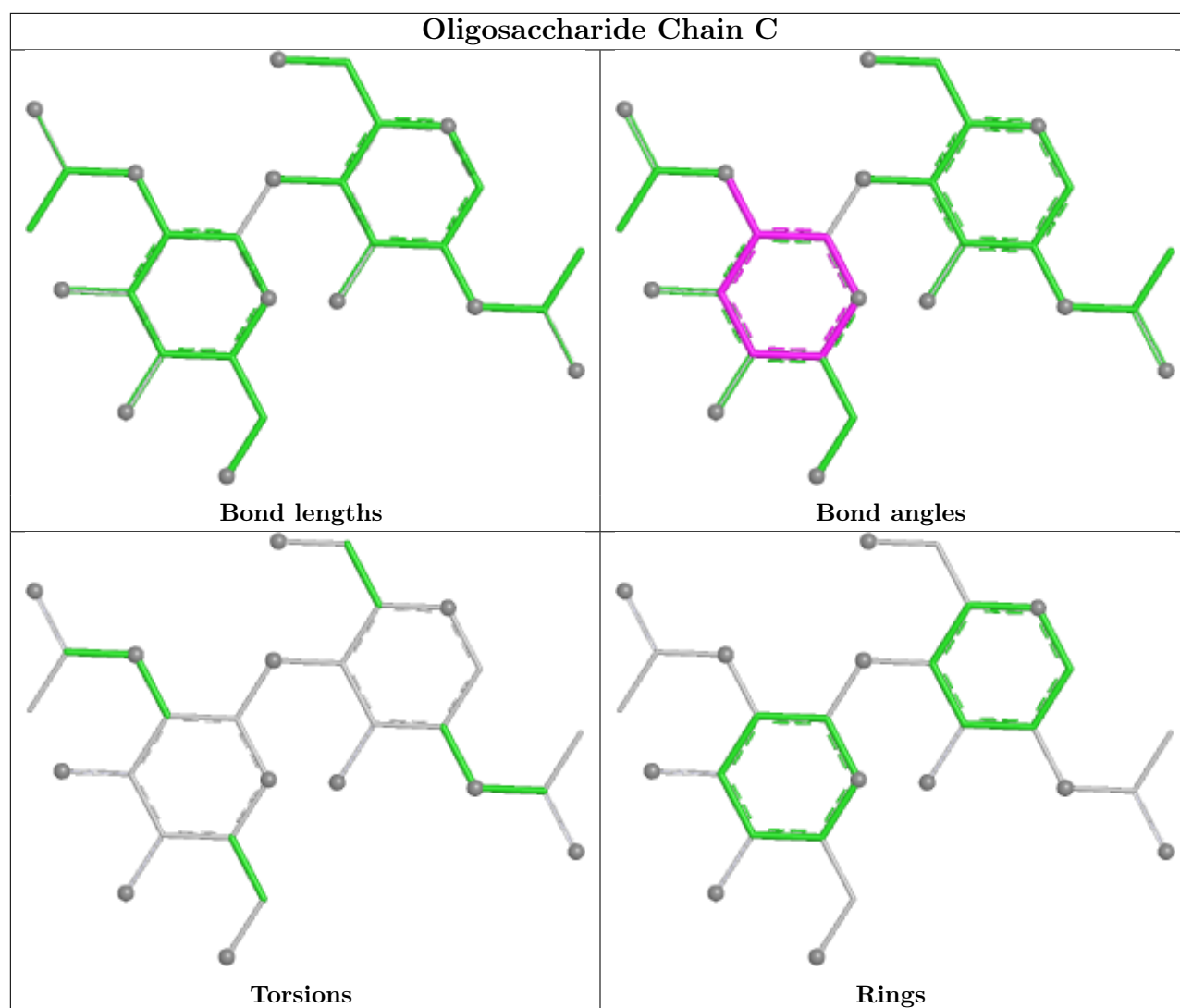
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	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 25 ligands modelled in this entry, 13 are monoatomic - leaving 12 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	$\# Z > 2$
5	NAG	A	604	1	14,14,15	0.44	0	17,19,21	0.80	0
4	HEM	A	602	9,1	50,50,50	2.36	17 (34%)	67,82,82	1.94	16 (23%)
12	EDO	A	624	-	3,3,3	0.87	0	2,2,2	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	603	1	14,14,15	0.77	1 (7%)	17,19,21	1.71	3 (17%)
11	GOL	A	622	-	5,5,5	3.46	2 (40%)	5,5,5	2.65	4 (80%)
10	PEG	A	621	-	6,6,6	1.45	1 (16%)	5,5,5	0.93	0
9	PZA	A	619	-	9,9,9	0.40	0	11,11,11	1.86	3 (27%)
12	EDO	A	625	-	3,3,3	0.41	0	2,2,2	0.46	0
9	PZA	A	618	4	9,9,9	0.54	0	11,11,11	1.89	5 (45%)
11	GOL	A	623	-	5,5,5	1.07	0	5,5,5	1.23	1 (20%)
10	PEG	A	620	-	6,6,6	1.60	1 (16%)	5,5,5	0.98	0
8	SCN	A	617	-	1,2,2	1.21	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	NAG	A	604	1	-	0/6/23/26	0/1/1/1
4	HEM	A	602	9,1	-	4/14/54/54	-
12	EDO	A	624	-	-	0/1/1/1	-
5	NAG	A	603	1	-	0/6/23/26	0/1/1/1
11	GOL	A	622	-	-	2/4/4/4	-
10	PEG	A	621	-	-	4/4/4/4	-
9	PZA	A	619	-	-	4/4/4/4	0/1/1/1
12	EDO	A	625	-	-	0/1/1/1	-
9	PZA	A	618	4	-	4/4/4/4	0/1/1/1
11	GOL	A	623	-	-	2/4/4/4	-
10	PEG	A	620	-	-	1/4/4/4	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	622	GOL	O2-C2	-7.16	1.22	1.43
4	A	602	HEM	C3D-C2D	6.89	1.51	1.36
4	A	602	HEM	FE-NB	5.50	2.11	1.94
4	A	602	HEM	C4D-ND	-5.34	1.31	1.40
4	A	602	HEM	CAB-C3B	4.28	1.58	1.47
4	A	602	HEM	FE-ND	4.05	2.07	1.94
4	A	602	HEM	C1A-C2A	3.87	1.52	1.44
4	A	602	HEM	CMC-C2C	3.82	1.58	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	HEM	CHD-C4C	3.35	1.44	1.38
10	A	620	PEG	C2-C1	-3.23	1.32	1.49
4	A	602	HEM	C1B-NB	-3.20	1.34	1.40
4	A	602	HEM	CAC-C3C	2.97	1.55	1.47
4	A	602	HEM	C1C-C2C	-2.82	1.39	1.45
4	A	602	HEM	CHD-C1D	2.81	1.45	1.39
10	A	621	PEG	C2-C1	-2.69	1.35	1.49
11	A	622	GOL	O1-C1	2.46	1.52	1.42
4	A	602	HEM	C2A-C3A	-2.36	1.32	1.38
5	A	603	NAG	C8-C7	2.31	1.55	1.50
4	A	602	HEM	CBD-CGD	-2.12	1.45	1.50
4	A	602	HEM	C1D-ND	-2.12	1.34	1.38
4	A	602	HEM	CHA-C1A	-2.11	1.34	1.39
4	A	602	HEM	CHC-C4B	-2.01	1.34	1.39

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	HEM	CMD-C2D-C1D	7.75	137.15	125.03
4	A	602	HEM	CAD-C3D-C4D	5.80	134.80	124.70
5	A	603	NAG	C1-O5-C5	4.21	117.83	112.19
4	A	602	HEM	C4C-C3C-C2C	-3.96	103.38	106.81
5	A	603	NAG	O5-C1-C2	-3.56	105.78	111.29
9	A	619	PZA	C4-C-N1	3.42	119.58	116.22
9	A	618	PZA	C4-C-N1	3.28	119.45	116.22
4	A	602	HEM	C3D-C4D-ND	3.28	113.77	110.17
4	A	602	HEM	C4D-C3D-C2D	-3.28	102.12	106.89
4	A	602	HEM	C1D-C2D-C3D	-3.25	103.56	106.98
11	A	622	GOL	O2-C2-C1	3.17	122.30	109.18
5	A	603	NAG	C1-C2-N2	3.15	115.39	110.43
11	A	622	GOL	O2-C2-C3	3.03	121.70	109.18
11	A	622	GOL	C3-C2-C1	-2.87	101.28	111.80
4	A	602	HEM	CAD-C3D-C2D	-2.70	122.81	127.87
4	A	602	HEM	CMB-C2B-C1B	2.63	129.15	125.03
9	A	619	PZA	C1-N3-C4	2.63	120.32	116.93
9	A	618	PZA	C4-C3-N2	-2.63	118.53	121.97
4	A	602	HEM	C4D-ND-C1D	2.60	108.28	105.21
9	A	618	PZA	C1-N3-C4	2.57	120.25	116.93
4	A	602	HEM	CMD-C2D-C3D	-2.53	119.30	126.15
11	A	623	GOL	O2-C2-C3	-2.50	98.81	109.18
9	A	618	PZA	C2-N2-C3	2.40	121.05	116.85
11	A	622	GOL	O1-C1-C2	-2.35	99.81	110.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	618	PZA	C2-C1-N3	-2.31	118.94	122.19
4	A	602	HEM	CHD-C1D-C2D	-2.30	121.40	125.03
9	A	619	PZA	C2-N2-C3	2.19	120.68	116.85
4	A	602	HEM	C3B-C4B-NB	2.15	111.01	109.47
4	A	602	HEM	C4C-NC-C1C	-2.07	102.45	105.82
4	A	602	HEM	C4A-CHB-C1B	2.07	131.11	126.25
4	A	602	HEM	O1D-CGD-CBD	-2.06	116.56	123.09
4	A	602	HEM	CAA-C2A-C3A	2.00	131.56	127.07

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	618	PZA	O-C-C4-N3
9	A	619	PZA	N1-C-C4-C3
9	A	619	PZA	N1-C-C4-N3
9	A	619	PZA	O-C-C4-C3
9	A	619	PZA	O-C-C4-N3
9	A	618	PZA	N1-C-C4-N3
11	A	623	GOL	C1-C2-C3-O3
9	A	618	PZA	N1-C-C4-C3
9	A	618	PZA	O-C-C4-C3
10	A	621	PEG	O1-C1-C2-O2
10	A	620	PEG	O2-C3-C4-O4
11	A	623	GOL	O2-C2-C3-O3
11	A	622	GOL	O1-C1-C2-O2
11	A	622	GOL	O2-C2-C3-O3
10	A	621	PEG	O2-C3-C4-O4
10	A	621	PEG	C4-C3-O2-C2
4	A	602	HEM	CAD-CBD-CGD-O2D
4	A	602	HEM	CAA-CBA-CGA-O1A
4	A	602	HEM	CAA-CBA-CGA-O2A
4	A	602	HEM	CAD-CBD-CGD-O1D
10	A	621	PEG	C1-C2-O2-C3

There are no ring outliers.

9 monomers are involved in 34 short contacts:

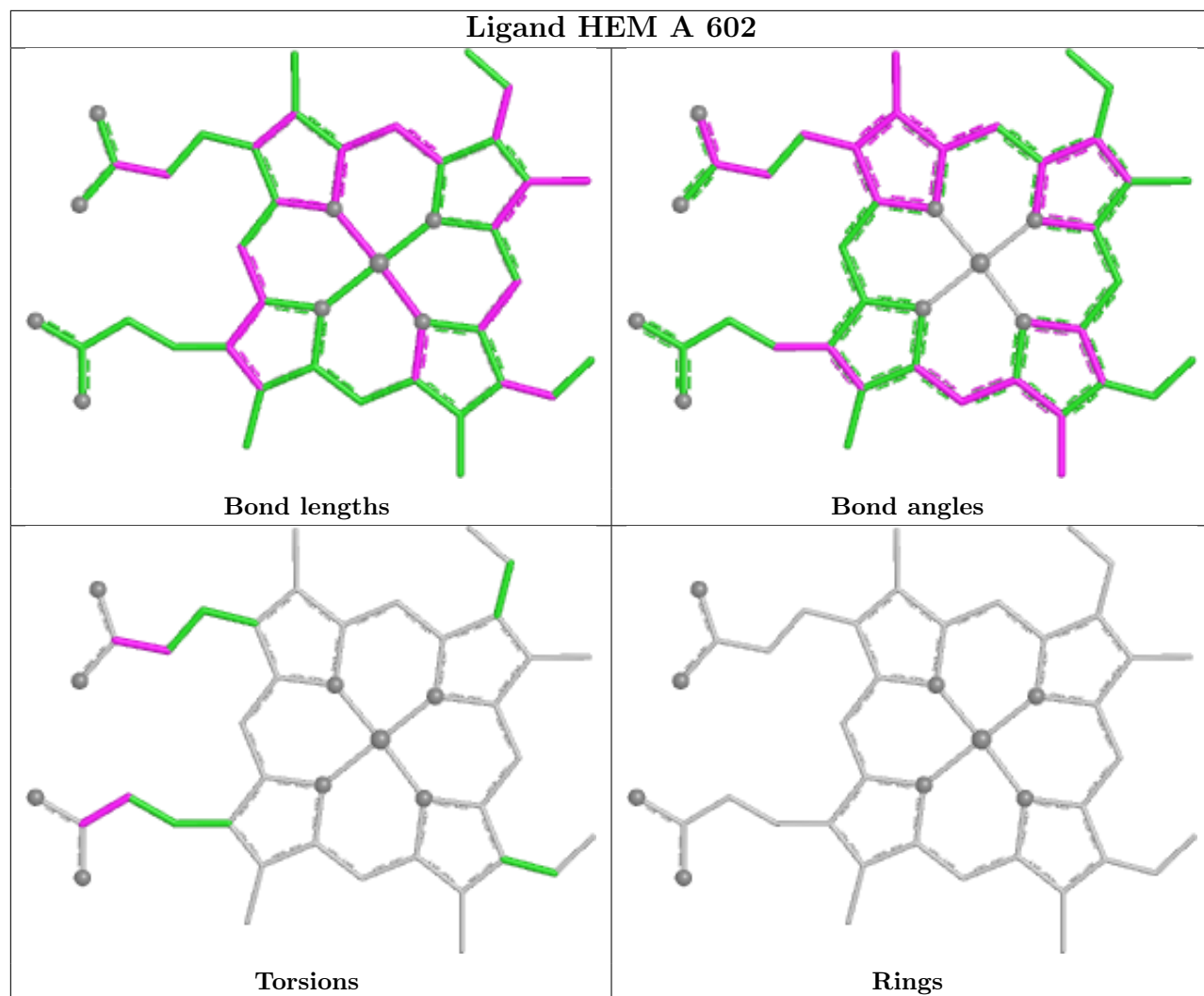
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	HEM	7	0
5	A	603	NAG	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	622	GOL	4	0
10	A	621	PEG	1	0
9	A	619	PZA	6	0
12	A	625	EDO	1	0
9	A	618	PZA	14	0
11	A	623	GOL	2	0
10	A	620	PEG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	594/595 (99%)	0.72	62 (10%)	11 10	15, 31, 57, 94	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	TYR	8.1
1	A	2	TRP	7.1
1	A	11	PRO	6.3
1	A	12	LEU	6.0
1	A	171	PRO	5.6
1	A	10	VAL	5.3
1	A	173	GLN	5.2
1	A	4	VAL	5.0
1	A	170	PRO	4.9
1	A	119	LEU	4.8
1	A	13	VAL	4.4
1	A	174	SER	4.3
1	A	117	THR	4.1
1	A	169	THR	3.9
1	A	123	GLU	3.9
1	A	8	ALA	3.7
1	A	283	LEU	3.6
1	A	199	LEU	3.5
1	A	484	TYR	3.4
1	A	120	GLY	3.4
1	A	7	GLY	3.3
1	A	175	LEU	3.3
1	A	254	PHE	3.2
1	A	9	PRO	3.2
1	A	6	CYS	3.1
1	A	124	HIS	3.0
1	A	220	TRP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	279	GLU	3.0
1	A	168	PRO	3.0
1	A	5	GLY	2.9
1	A	167	CYS	2.8
1	A	368	TRP	2.6
1	A	121	SER	2.6
1	A	219	ALA	2.5
1	A	63	GLN	2.5
1	A	1	SER	2.5
1	A	128	GLN	2.4
1	A	207	SER	2.4
1	A	208	SER	2.4
1	A	122	ASN	2.4
1	A	206	LEU	2.4
1	A	16	ASP	2.4
1	A	64	ARG	2.4
1	A	580	SER	2.4
1	A	71	ARG	2.3
1	A	553	ILE	2.3
1	A	223	GLY	2.3
1	A	447	PRO	2.2
1	A	593	ARG	2.1
1	A	363	GLU	2.1
1	A	3	GLU	2.1
1	A	18	ASN	2.1
1	A	232	LYS	2.1
1	A	196	GLU	2.1
1	A	371	GLU	2.0
1	A	446	MET	2.0
1	A	389	ASP	2.0
1	A	492	ILE	2.0
1	A	166	VAL	2.0
1	A	40	ASN	2.0
1	A	587	LEU	2.0
1	A	126	LYS	2.0

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

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.

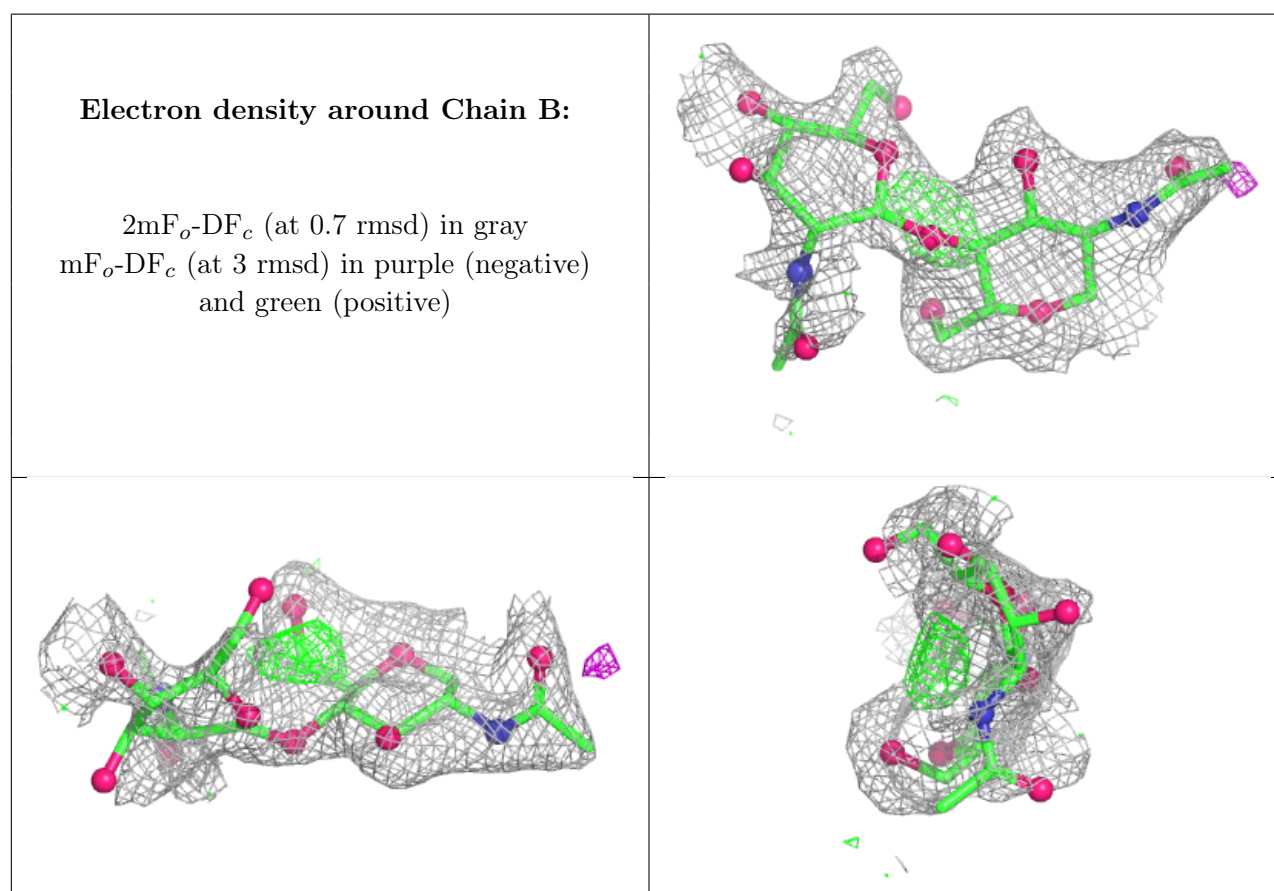
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	SEP	A	198	10/11	0.80	0.19	39,40,41,41	0

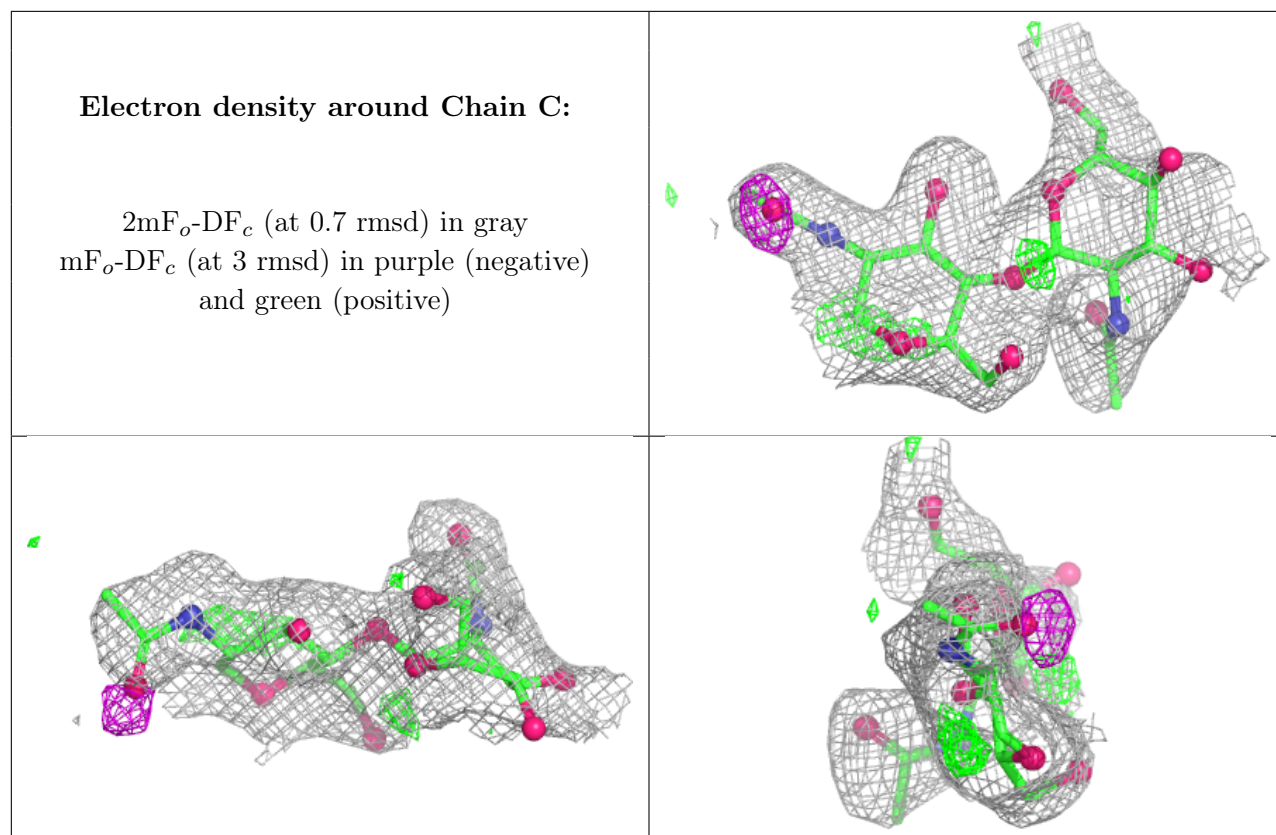
6.3 Carbohydrates [i](#)

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($\text{\AA}^2$)	Q<0.9
2	NAG	B	2	14/15	0.49	0.17	54,57,58,58	0
2	NAG	C	2	14/15	0.59	0.14	51,55,56,56	0
2	NAG	C	1	14/15	0.73	0.15	38,40,43,47	0
2	NAG	B	1	14/15	0.76	0.13	39,44,46,50	0

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





6.4 Ligands ⓘ

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
5	NAG	A	604	14/15	0.54	0.17	39,39,40,40	0
9	PZA	A	618	9/9	0.57	0.31	28,29,30,31	0
9	PZA	A	619	9/9	0.63	0.27	27,27,27,28	9
5	NAG	A	603	14/15	0.64	0.15	47,50,52,52	0
11	GOL	A	623	6/6	0.73	0.16	58,58,59,60	0
11	GOL	A	622	6/6	0.79	0.20	45,46,47,49	0
8	SCN	A	617	3/3	0.81	0.17	30,30,30,30	0
10	PEG	A	620	7/7	0.82	0.13	33,35,36,37	0
10	PEG	A	621	7/7	0.83	0.14	50,51,51,51	0
12	EDO	A	624	4/4	0.89	0.18	41,42,42,43	0
6	IOD	A	610	1/1	0.92	0.09	52,52,52,52	1
12	EDO	A	625	4/4	0.92	0.11	30,31,32,34	0
6	IOD	A	612	1/1	0.93	0.10	55,55,55,55	1
6	IOD	A	605	1/1	0.94	0.09	51,51,51,51	0

Continued on next page...

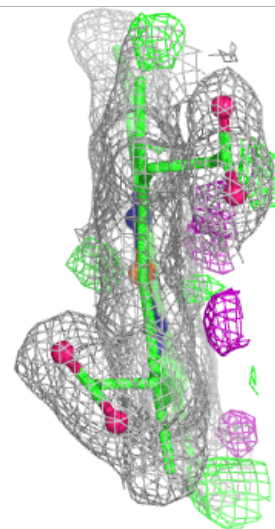
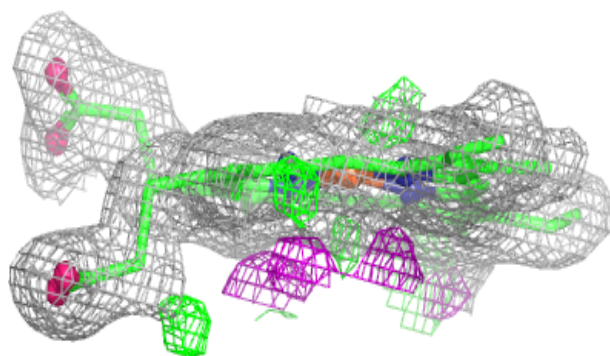
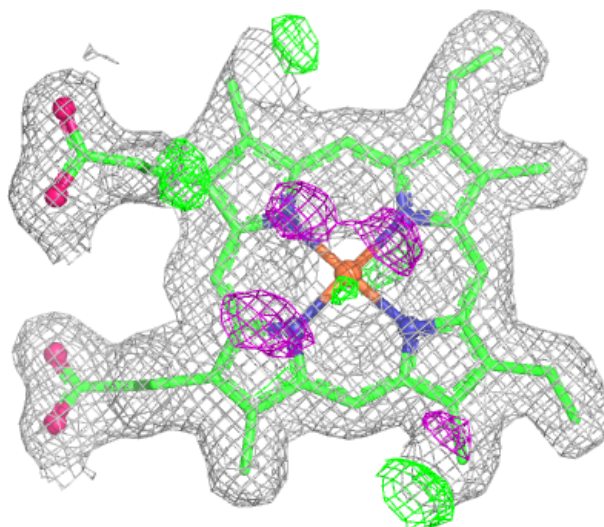
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	IOD	A	615	1/1	0.95	0.14	53,53,53,53	0
6	IOD	A	611	1/1	0.96	0.12	64,64,64,64	1
7	ZN	A	616	1/1	0.97	0.06	44,44,44,44	0
4	HEM	A	602	43/43	0.97	0.08	14,18,22,24	0
6	IOD	A	607	1/1	0.97	0.06	57,57,57,57	0
6	IOD	A	608	1/1	0.97	0.09	58,58,58,58	0
6	IOD	A	609	1/1	0.97	0.14	63,63,63,63	0
6	IOD	A	614	1/1	0.98	0.05	36,36,36,36	0
6	IOD	A	606	1/1	0.98	0.06	40,40,40,40	0
3	CA	A	601	1/1	0.99	0.04	22,22,22,22	0
6	IOD	A	613	1/1	1.00	0.02	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.

Electron density around HEM A 602:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.