



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:51 AM UTC

PDB ID : 3KRQ / pdb_00003krq
Title : Crystal structure of the complex of lactoperoxidase with a potent inhibitor amino-triazole at 2.2a resolution
Authors : Singh, A.K.; Singh, N.; Sinha, M.; Kushwaha, G.S.; Kaur, P.; Srinivasan, A.; Sharma, S.; Singh, T.P.
Deposited on : 2009-11-19
Resolution : 2.25 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

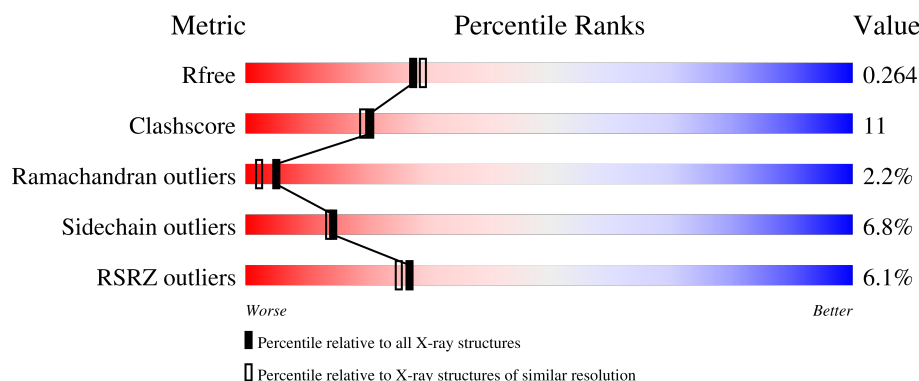
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	6% 66% 25% 7%
2	B	3	100%
2	D	3	33% 67%
3	C	3	100%

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Mol	Chain	Length	Quality of chain
4	E	2	50% 50%

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
7	IOD	A	615	-	-	X	-
8	3TR	A	607	-	-	X	-

2 Entry composition [i](#)

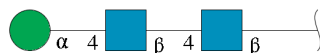
There are 11 unique types of molecules in this entry. The entry contains 5418 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lactoperoxidase.

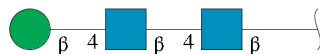
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	P	S	0	0	0
			4774	3037	847	863	1	26			

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



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

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



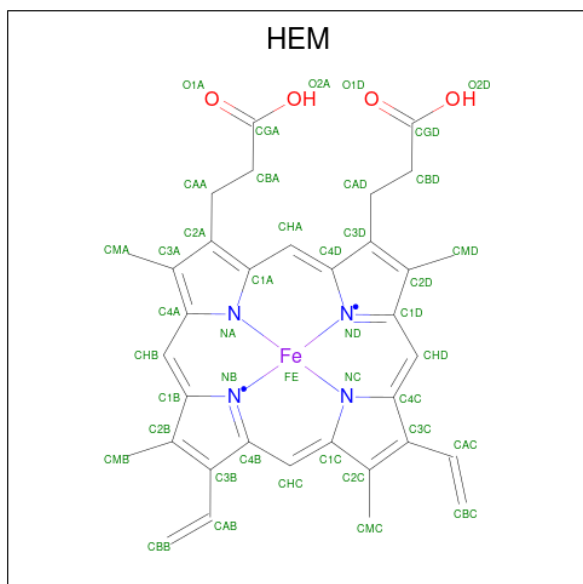
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



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

- 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
			43	34	1	4	4	

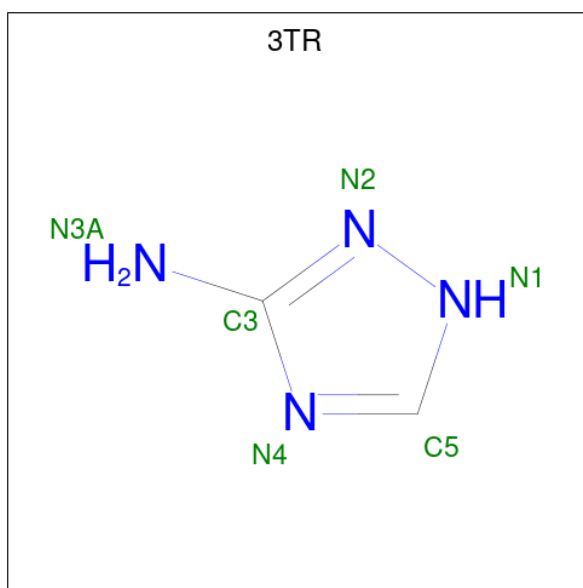
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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

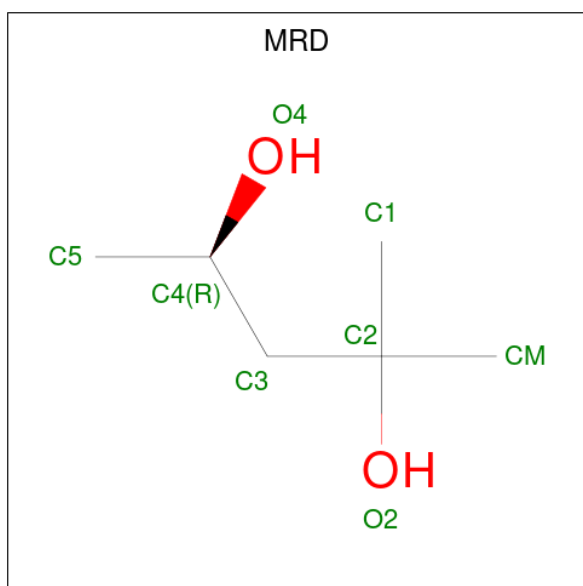
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	7	Total	I	0	0
			7	7		

- Molecule 8 is 3-AMINO-1,2,4-TRIAZOLE (CCD ID: 3TR) (formula: $C_2H_4N_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	N	0	0
			6	2	4		
8	A	1	Total	C	N	0	0
			6	2	4		

- Molecule 9 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			8	6	2		

- 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		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	421	Total	O	0	0
			421	421		

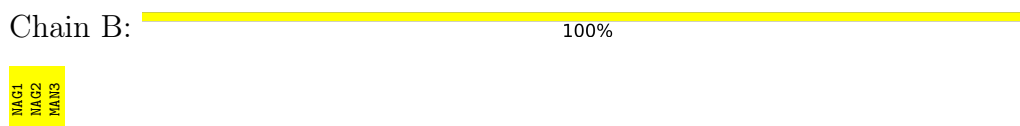
3 Residue-property plots [i](#)

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



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





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

Chain C:  100%



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

Chain E:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.49Å 81.11Å 73.93Å 90.00° 100.82° 90.00°	Depositor
Resolution (Å)	19.91 – 2.25 19.91 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.91-2.25) 99.8 (19.91-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.26Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.226 , 0.249 0.234 , 0.264	Depositor DCC
R_{free} test set	1527 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.1	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	5418	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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: BMA, NDG, MAN, PEG, HEM, IOD, SEP, MRD, NAG, 3TR, CA

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	1.07	40/4891 (0.8%)	1.64	130/6634 (2.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	PRO	C-N	11.85	1.45	1.33
1	A	171	PRO	N-CA	10.75	1.60	1.47
1	A	170	PRO	CA-C	10.59	1.62	1.52
1	A	122	ASN	N-CA	9.92	1.58	1.46
1	A	171	PRO	CA-C	9.75	1.62	1.52
1	A	207	SER	C-N	9.19	1.43	1.33
1	A	504	ARG	NE-CZ	8.44	1.42	1.33
1	A	121	SER	C-N	7.78	1.44	1.33
1	A	208	SER	CA-C	7.53	1.59	1.52
1	A	8	ALA	CA-C	7.51	1.62	1.52
1	A	504	ARG	CD-NE	7.36	1.56	1.46
1	A	169	THR	C-N	7.20	1.41	1.33
1	A	11	PRO	CA-C	7.19	1.62	1.52
1	A	169	THR	N-CA	-7.10	1.36	1.46
1	A	169	THR	CA-C	6.89	1.61	1.52
1	A	18	ASN	CA-C	-6.88	1.44	1.52
1	A	231	ASN	CA-C	6.51	1.61	1.52
1	A	588	SER	CA-C	6.45	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	ALA	N-CA	6.25	1.54	1.46
1	A	232	LYS	N-CA	6.05	1.53	1.45
1	A	11	PRO	C-N	5.83	1.41	1.33
1	A	594	GLU	CA-C	5.82	1.60	1.52
1	A	6	CYS	CA-C	5.81	1.59	1.52
1	A	208	SER	N-CA	5.79	1.53	1.46
1	A	538	GLU	CA-CB	5.76	1.63	1.53
1	A	428	ILE	C-N	-5.76	1.26	1.33
1	A	258	GLU	C-O	-5.62	1.17	1.24
1	A	388	LYS	CA-CB	5.58	1.60	1.53
1	A	589	PRO	N-CA	5.54	1.54	1.47
1	A	504	ARG	CB-CG	5.45	1.68	1.52
1	A	536	PHE	CA-C	5.43	1.59	1.52
1	A	539	LYS	CA-C	5.40	1.60	1.52
1	A	207	SER	CA-C	5.32	1.60	1.52
1	A	245	ARG	CA-CB	5.24	1.61	1.53
1	A	429	HIS	N-CA	-5.18	1.40	1.46
1	A	504	ARG	CA-CB	5.15	1.61	1.53
1	A	7	GLY	C-N	5.12	1.44	1.33
1	A	232	LYS	CA-C	5.11	1.60	1.53
1	A	504	ARG	CG-CD	5.09	1.67	1.52
1	A	170	PRO	N-CA	5.07	1.57	1.46

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	CYS	CA-C-N	22.06	147.42	119.84
1	A	167	CYS	C-N-CA	22.06	147.42	119.84
1	A	233	LYS	N-CA-C	-16.64	87.12	110.08
1	A	234	PRO	CA-N-CD	-15.41	90.42	112.00
1	A	316	VAL	N-CA-C	-13.46	98.93	111.45
1	A	168	PRO	CA-N-CD	-12.99	93.82	112.00
1	A	19	SER	CA-C-N	12.28	132.01	119.24
1	A	19	SER	C-N-CA	12.28	132.01	119.24
1	A	169	THR	CA-C-N	11.93	132.67	120.38
1	A	169	THR	C-N-CA	11.93	132.67	120.38
1	A	233	LYS	CA-C-N	10.58	133.07	119.84
1	A	233	LYS	C-N-CA	10.58	133.07	119.84
1	A	111	LEU	N-CA-C	10.14	124.16	111.69
1	A	82	ILE	CB-CA-C	-10.10	102.06	111.05
1	A	504	ARG	CB-CA-C	10.00	126.89	111.39
1	A	366	GLN	OE1-CD-NE2	-9.79	112.81	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	594	GLU	N-CA-C	9.79	131.65	110.80
1	A	19	SER	N-CA-C	9.73	121.92	109.65
1	A	540	GLN	OE1-CD-NE2	-9.68	112.92	122.60
1	A	217	GLN	OE1-CD-NE2	-9.63	112.97	122.60
1	A	305	GLN	OE1-CD-NE2	-9.62	112.98	122.60
1	A	173	GLN	OE1-CD-NE2	-9.59	113.01	122.60
1	A	428	ILE	N-CA-C	9.57	123.44	108.89
1	A	131	GLU	N-CA-C	9.56	121.47	111.14
1	A	592	SER	CA-C-N	9.35	139.75	122.74
1	A	592	SER	C-N-CA	9.35	139.75	122.74
1	A	121	SER	CA-C-N	9.28	139.26	121.54
1	A	121	SER	C-N-CA	9.28	139.26	121.54
1	A	135	GLN	OE1-CD-NE2	-9.25	113.35	122.60
1	A	171	PRO	N-CA-C	9.21	124.96	110.50
1	A	322	GLN	OE1-CD-NE2	-9.06	113.54	122.60
1	A	336	ASP	CA-CB-CG	9.00	121.60	112.60
1	A	171	PRO	CA-N-CD	-8.95	99.47	112.00
1	A	532	ASN	CA-CB-CG	8.90	121.50	112.60
1	A	521	GLN	OE1-CD-NE2	-8.87	113.73	122.60
1	A	174	SER	N-CA-C	8.85	123.85	112.34
1	A	234	PRO	N-CD-CG	8.74	116.30	103.20
1	A	19	SER	CA-C-O	8.72	127.52	119.76
1	A	591	ALA	N-CA-C	8.64	129.21	110.80
1	A	168	PRO	N-CA-CB	8.51	112.18	103.25
1	A	330	GLY	N-CA-C	8.16	121.43	112.29
1	A	19	SER	O-C-N	8.13	130.04	121.42
1	A	232	LYS	N-CA-C	7.99	121.33	110.55
1	A	168	PRO	N-CD-CG	7.98	115.17	103.20
1	A	169	THR	CB-CA-C	7.95	125.83	110.17
1	A	122	ASN	CA-CB-CG	7.86	120.46	112.60
1	A	18	ASN	N-CA-C	-7.85	101.92	114.09
1	A	234	PRO	N-CA-CB	7.71	111.35	103.25
1	A	58	PRO	N-CA-C	7.66	122.53	110.50
1	A	14	LYS	N-CA-C	-7.57	100.77	110.53
1	A	231	ASN	CA-CB-CG	7.51	120.11	112.60
1	A	207	SER	CA-C-N	7.45	132.54	122.56
1	A	207	SER	C-N-CA	7.45	132.54	122.56
1	A	589	PRO	CA-N-CD	-7.45	101.58	112.00
1	A	87	ASP	N-CA-C	7.20	120.00	108.41
1	A	305	GLN	CG-CD-NE2	7.10	127.05	116.40
1	A	20	PRO	CA-C-N	-7.09	111.46	122.87
1	A	20	PRO	C-N-CA	-7.09	111.46	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	592	SER	N-CA-C	7.09	120.93	110.30
1	A	82	ILE	N-CA-C	7.04	117.19	111.62
1	A	521	GLN	CG-CD-NE2	7.04	126.96	116.40
1	A	167	CYS	C-N-CD	-7.00	96.29	125.00
1	A	170	PRO	CA-C-N	6.98	128.81	120.23
1	A	170	PRO	C-N-CA	6.98	128.81	120.23
1	A	225	ALA	N-CA-C	6.76	120.03	110.50
1	A	135	GLN	CG-CD-NE2	6.65	126.37	116.40
1	A	83	VAL	N-CA-C	6.60	117.38	110.72
1	A	169	THR	C-N-CD	-6.58	98.04	125.00
1	A	453	ARG	N-CA-C	-6.54	104.15	111.28
1	A	234	PRO	CB-CA-C	6.53	122.33	111.56
1	A	217	GLN	CG-CD-NE2	6.51	126.16	116.40
1	A	594	GLU	CB-CG-CD	6.49	123.63	112.60
1	A	540	GLN	CG-CD-NE2	6.48	126.12	116.40
1	A	349	PHE	N-CA-C	-6.40	104.73	112.54
1	A	296	ALA	N-CA-C	-6.29	103.73	111.40
1	A	322	GLN	CG-CD-NE2	6.29	125.83	116.40
1	A	504	ARG	CB-CG-CD	6.28	125.73	111.30
1	A	58	PRO	CA-C-N	-6.21	112.17	121.05
1	A	58	PRO	C-N-CA	-6.21	112.17	121.05
1	A	129	CYS	N-CA-C	-6.17	104.48	111.14
1	A	6	CYS	N-CA-C	6.11	119.20	109.24
1	A	231	ASN	N-CA-C	6.11	121.55	112.94
1	A	173	GLN	CG-CD-NE2	6.06	125.49	116.40
1	A	84	GLY	N-CA-C	6.01	122.53	112.85
1	A	233	LYS	C-N-CD	-5.99	100.46	125.00
1	A	168	PRO	CB-CA-C	5.96	121.39	111.56
1	A	245	ARG	CA-C-N	-5.95	116.83	123.02
1	A	245	ARG	C-N-CA	-5.95	116.83	123.02
1	A	566	ALA	N-CA-C	5.92	119.33	111.75
1	A	366	GLN	CG-CD-NE2	5.90	125.24	116.40
1	A	254	PHE	N-CA-C	5.81	118.36	111.33
1	A	31	ARG	N-CA-C	5.81	117.61	111.28
1	A	153	THR	N-CA-C	5.79	121.92	114.56
1	A	405	LYS	N-CA-C	-5.77	101.94	110.48
1	A	312	TYR	N-CA-C	5.76	118.67	111.24
1	A	10	VAL	CA-C-N	-5.76	112.64	119.84
1	A	10	VAL	C-N-CA	-5.76	112.64	119.84
1	A	233	LYS	CA-C-O	-5.74	114.44	120.70
1	A	166	VAL	N-CA-C	5.73	117.58	108.87
1	A	43	LEU	N-CA-C	-5.66	101.91	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	ILE	N-CA-C	5.65	117.46	108.87
1	A	59	PHE	N-CA-C	-5.64	101.94	110.24
1	A	208	SER	O-C-N	5.64	127.61	121.23
1	A	208	SER	CA-C-O	5.58	123.94	119.59
1	A	159	PRO	CA-N-CD	-5.55	104.23	112.00
1	A	15	CYS	CA-C-N	5.54	127.71	120.28
1	A	15	CYS	C-N-CA	5.54	127.71	120.28
1	A	412	MET	N-CA-C	5.52	118.36	111.24
1	A	23	THR	N-CA-C	-5.51	103.43	110.53
1	A	9	PRO	CA-C-N	5.44	132.19	122.13
1	A	9	PRO	C-N-CA	5.44	132.19	122.13
1	A	386	ILE	CB-CA-C	-5.43	104.80	111.92
1	A	248	CYS	N-CA-C	-5.43	103.73	110.41
1	A	9	PRO	CB-CA-C	5.41	120.48	111.56
1	A	326	PRO	CA-N-CD	-5.41	104.43	112.00
1	A	12	LEU	N-CA-C	5.36	117.64	110.35
1	A	592	SER	CA-C-O	5.36	126.58	120.80
1	A	170	PRO	N-CA-C	5.32	117.18	110.70
1	A	253	ASP	CA-C-N	5.25	127.57	120.38
1	A	253	ASP	C-N-CA	5.25	127.57	120.38
1	A	504	ARG	CG-CD-NE	5.25	123.54	112.00
1	A	213	MET	N-CA-C	-5.22	101.19	109.96
1	A	390	GLY	N-CA-C	5.21	121.89	114.85
1	A	34	PRO	N-CA-C	5.18	122.17	113.78
1	A	113	PHE	CA-CB-CG	5.14	118.94	113.80
1	A	182	ALA	N-CA-C	5.14	119.43	113.20
1	A	582	VAL	N-CA-C	5.14	115.97	108.58
1	A	564	LEU	N-CA-C	-5.12	105.78	112.23
1	A	407	MET	N-CA-C	-5.08	102.86	110.23
1	A	504	ARG	CD-NE-CZ	5.01	131.41	124.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	SEP	Peptide
1	A	423	GLN	Peptide

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	107	0
2	B	39	0	34	0	0
2	D	39	0	34	0	0
3	C	39	0	34	0	0
4	E	28	0	24	0	0
5	A	43	0	30	2	0
6	A	1	0	0	0	0
7	A	7	0	0	2	0
8	A	12	0	8	5	0
9	A	8	0	14	0	0
10	A	7	0	10	0	0
11	A	421	0	0	5	0
All	All	5418	0	4875	111	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 11.

All (111) 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)
8:A:607:3TR:H5	8:A:608:3TR:H5	1.44	0.99
1:A:18:ASN:O	1:A:20:PRO:HD3	1.66	0.94
1:A:424:PRO:O	7:A:615:IOD:I	2.65	0.85
1:A:432:ASP:O	1:A:436:ILE:HD13	1.77	0.84
1:A:208:SER:HB2	1:A:210:LEU:HD12	1.60	0.82
1:A:175:LEU:HD22	1:A:176:ALA:H	1.48	0.78
1:A:284:ASN:HD22	1:A:286:HIS:CE1	2.02	0.77
1:A:72:VAL:O	1:A:72:VAL:HG13	1.83	0.75
1:A:400:LEU:HD11	1:A:553:ILE:HD13	1.70	0.73
1:A:158:MET:SD	1:A:431:PHE:HA	2.30	0.72
1:A:392:ILE:O	1:A:396:VAL:HG23	1.89	0.71
1:A:172:TYR:C	1:A:173:GLN:HG3	2.14	0.70
1:A:208:SER:CB	1:A:210:LEU:HD12	2.22	0.70
8:A:607:3TR:C5	8:A:608:3TR:H5	2.21	0.68
1:A:234:PRO:O	1:A:236:PRO:HD3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:PRO:HB3	7:A:615:IOD:I	2.65	0.67
1:A:18:ASN:O	1:A:20:PRO:CD	2.40	0.67
1:A:197:PRO:O	1:A:198:SEP:C	2.43	0.66
1:A:202:ARG:O	1:A:202:ARG:HG2	1.96	0.66
1:A:105:GLN:HE22	1:A:259:GLN:HE21	1.44	0.65
1:A:51:TYR:HB3	1:A:57:LEU:O	1.95	0.65
1:A:170:PRO:CB	1:A:171:PRO:HD2	2.27	0.65
1:A:113:PHE:CE2	1:A:115:PRO:HG3	2.33	0.64
1:A:58:PRO:HB2	1:A:61:TRP:HB2	1.82	0.62
1:A:232:LYS:HB3	1:A:233:LYS:O	2.01	0.60
1:A:72:VAL:O	1:A:72:VAL:CG1	2.49	0.60
1:A:58:PRO:O	1:A:59:PHE:C	2.44	0.59
1:A:481:MET:SD	1:A:487:PRO:HD3	2.41	0.59
1:A:284:ASN:HD22	1:A:286:HIS:HE1	1.50	0.58
1:A:10:VAL:HG13	1:A:10:VAL:O	2.04	0.57
1:A:257:SER:O	1:A:381:PHE:HA	2.05	0.56
1:A:10:VAL:O	1:A:10:VAL:HG22	2.06	0.56
1:A:227:LEU:CD1	1:A:267:THR:HA	2.36	0.56
1:A:210:LEU:HA	1:A:292:LEU:CD1	2.37	0.54
1:A:517:ARG:O	1:A:521:GLN:HG3	2.07	0.54
1:A:208:SER:C	1:A:210:LEU:H	2.16	0.54
1:A:310:ARG:O	1:A:314:PRO:HG2	2.08	0.54
1:A:117:THR:HG21	1:A:138:ASN:CG	2.34	0.53
1:A:258:GLU:HG3	8:A:607:3TR:C5	2.39	0.52
1:A:210:LEU:HA	1:A:292:LEU:HD12	1.90	0.52
1:A:486:THR:C	1:A:488:ASP:N	2.65	0.52
1:A:313:LEU:N	1:A:314:PRO:CD	2.72	0.52
1:A:175:LEU:HD22	1:A:176:ALA:N	2.20	0.52
1:A:544:LEU:O	1:A:547:VAL:HG22	2.09	0.52
1:A:170:PRO:HB3	1:A:171:PRO:HD2	1.92	0.51
1:A:170:PRO:CB	1:A:171:PRO:CD	2.89	0.50
1:A:227:LEU:HD13	1:A:267:THR:HA	1.93	0.50
1:A:33:SER:N	1:A:34:PRO:CD	2.75	0.49
1:A:402:LYS:NZ	11:A:680:HOH:O	2.45	0.49
1:A:8:ALA:HB1	1:A:9:PRO:CD	2.43	0.49
1:A:471:LEU:HD21	1:A:480:LEU:HD23	1.95	0.49
1:A:210:LEU:HB3	11:A:962:HOH:O	2.13	0.48
1:A:237:CYS:HA	1:A:381:PHE:O	2.13	0.48
1:A:170:PRO:HB2	1:A:171:PRO:HD2	1.95	0.48
1:A:286:HIS:CD2	1:A:594:GLU:OE1	2.67	0.48
1:A:33:SER:N	1:A:34:PRO:HD3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:PHE:CG	1:A:115:PRO:HD3	2.49	0.47
1:A:260:ILE:HD11	1:A:386:ILE:HG13	1.95	0.47
1:A:56:ALA:O	1:A:58:PRO:HD3	2.15	0.47
1:A:441:CYS:SG	1:A:492:ILE:HG22	2.54	0.47
1:A:213:MET:HB3	1:A:270:LEU:HD11	1.97	0.46
1:A:393:ASP:N	1:A:394:PRO:CD	2.77	0.46
1:A:164:GLY:HA2	11:A:708:HOH:O	2.15	0.46
1:A:539:LYS:HB3	1:A:589:PRO:HG3	1.97	0.46
1:A:560:THR:HA	1:A:579:CYS:SG	2.55	0.46
1:A:150:LYS:HD3	1:A:158:MET:HE2	1.98	0.46
1:A:362:ASP:OD1	1:A:362:ASP:C	2.57	0.46
1:A:8:ALA:HB1	1:A:9:PRO:HD2	1.98	0.46
1:A:464:LEU:HD21	1:A:478:LYS:HE2	1.98	0.46
1:A:450:ASN:HD21	1:A:487:PRO:HB2	1.82	0.45
1:A:57:LEU:HA	1:A:58:PRO:HD2	1.72	0.45
1:A:486:THR:C	1:A:488:ASP:H	2.23	0.45
1:A:99:LEU:HD23	1:A:566:ALA:HB1	1.99	0.45
1:A:169:THR:H	1:A:170:PRO:HD2	1.82	0.45
1:A:175:LEU:HD23	1:A:175:LEU:HA	1.79	0.45
1:A:362:ASP:O	1:A:365:TYR:N	2.46	0.45
1:A:24:ILE:HD12	1:A:200:ALA:HB2	1.98	0.44
1:A:19:SER:HA	1:A:20:PRO:HD2	1.22	0.44
1:A:196:GLU:HG3	1:A:197:PRO:N	2.29	0.44
1:A:108:ASP:OD1	1:A:108:ASP:C	2.61	0.44
1:A:452:TRP:CD1	1:A:492:ILE:HD13	2.53	0.44
1:A:393:ASP:O	1:A:397:ARG:HG3	2.17	0.44
1:A:486:THR:O	1:A:488:ASP:N	2.51	0.43
1:A:218:GLU:O	1:A:219:ALA:HB2	2.17	0.43
1:A:375:PRO:O	1:A:376:LEU:C	2.60	0.43
1:A:432:ASP:OD1	1:A:432:ASP:C	2.61	0.43
1:A:474:LYS:NZ	11:A:966:HOH:O	2.51	0.43
1:A:187:LEU:HD23	1:A:305:GLN:HA	2.00	0.43
1:A:255:ARG:HA	8:A:608:3TR:N4	2.34	0.43
1:A:499:GLU:HA	1:A:500:PRO:HD3	1.89	0.43
1:A:213:MET:CB	1:A:270:LEU:HD11	2.48	0.42
1:A:208:SER:HA	1:A:209:PRO:HD2	1.64	0.42
1:A:423:GLN:HA	1:A:424:PRO:HD3	1.67	0.42
1:A:468:GLN:HG2	1:A:474:LYS:HA	2.01	0.42
1:A:8:ALA:O	1:A:9:PRO:C	2.62	0.42
1:A:246:VAL:CG1	1:A:387:ILE:HD12	2.49	0.42
1:A:109:HIS:NE2	8:A:607:3TR:N3A	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:PRO:O	1:A:236:PRO:CD	2.63	0.42
5:A:655:HEM:HBC2	5:A:655:HEM:HMC1	2.02	0.42
1:A:8:ALA:CB	1:A:9:PRO:CD	2.98	0.41
1:A:82:ILE:HD12	1:A:480:LEU:HD13	2.03	0.41
1:A:124:HIS:O	1:A:127:THR:N	2.54	0.41
1:A:91:VAL:HG12	1:A:411:LYS:HD3	2.02	0.41
1:A:114:ALA:HB3	11:A:624:HOH:O	2.21	0.41
1:A:351:HIS:CE1	1:A:437:ASN:HD21	2.37	0.41
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.56	0.41
5:A:655:HEM:HBB2	5:A:655:HEM:CMB	2.50	0.41
1:A:208:SER:CB	1:A:210:LEU:CD1	2.98	0.40
1:A:446:MET:HA	1:A:446:MET:HE2	2.04	0.40
1:A:142:ILE:HB	1:A:158:MET:HB2	2.03	0.40
1:A:102:GLN:HE22	1:A:105:GLN:HE21	1.68	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%)	541 (91%)	38 (6%)	13 (2%)	5 2

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	10	VAL
1	A	168	PRO
1	A	170	PRO
1	A	234	PRO
1	A	338	ARG
1	A	209	PRO

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Mol	Chain	Res	Type
1	A	115	PRO
1	A	118	GLU
1	A	173	GLN
1	A	174	SER
1	A	169	THR
1	A	167	CYS

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%)	482 (93%)	35 (7%)	14 14

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	17	GLU
1	A	24	ILE
1	A	33	SER
1	A	41	ARG
1	A	63	GLN
1	A	122	ASN
1	A	125	SER
1	A	126	LYS
1	A	158	MET
1	A	169	THR
1	A	171	PRO
1	A	173	GLN
1	A	175	LEU
1	A	177	ARG
1	A	196	GLU
1	A	207	SER
1	A	208	SER
1	A	210	LEU
1	A	235	SER

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Mol	Chain	Res	Type
1	A	236	PRO
1	A	317	LEU
1	A	322	GLN
1	A	326	PRO
1	A	425	THR
1	A	427	LYS
1	A	441	CYS
1	A	480	LEU
1	A	487	PRO
1	A	504	ARG
1	A	538	GLU
1	A	581	THR
1	A	582	VAL
1	A	593	ARG
1	A	595	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	105	GLN
1	A	231	ASN
1	A	284	ASN
1	A	341	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	1.13	1 (12%)	7,12,14	3.90	5 (71%)

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-OG	2.01	1.66	1.60

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	OG-CB-CA	7.01	114.96	108.14
1	A	198	SEP	O3P-P-OG	6.08	122.52	106.67
1	A	198	SEP	O3P-P-O1P	-2.65	100.53	110.83
1	A	198	SEP	O2P-P-O1P	-2.30	101.88	110.83
1	A	198	SEP	OG-P-O1P	2.28	112.61	106.44

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	1	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	2,1	14,14,15	1.11	1 (7%)	17,19,21	1.09	1 (5%)
2	NAG	B	2	2	14,14,15	1.41	4 (28%)	17,19,21	1.56	3 (17%)
2	MAN	B	3	2	11,11,12	1.11	1 (9%)	15,15,17	0.74	0
3	NAG	C	1	3,1	14,14,15	0.74	0	17,19,21	0.79	1 (5%)
3	NAG	C	2	3	14,14,15	0.80	0	17,19,21	1.55	2 (11%)
3	BMA	C	3	3	11,11,12	1.06	1 (9%)	15,15,17	1.57	4 (26%)
2	NAG	D	1	2,1	14,14,15	0.53	0	17,19,21	0.81	1 (5%)
2	NAG	D	2	2	14,14,15	0.71	0	17,19,21	1.05	1 (5%)
2	MAN	D	3	2	11,11,12	0.60	0	15,15,17	0.83	0
4	NAG	E	1	4,1	14,14,15	0.51	0	17,19,21	0.91	0
4	NDG	E	2	4	14,14,15	0.66	0	17,19,21	1.09	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	MAN	B	3	2	-	2/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	MAN	D	3	2	-	1/2/19/22	0/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NDG	E	2	4	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	C3-C2	2.92	1.58	1.52
3	C	3	BMA	C2-C3	2.73	1.56	1.52
2	B	3	MAN	C2-C3	2.66	1.56	1.52
2	B	2	NAG	C4-C3	2.32	1.58	1.52
2	B	2	NAG	C1-C2	2.13	1.55	1.52
2	B	1	NAG	C3-C2	2.13	1.57	1.52
2	B	2	NAG	O4-C4	2.09	1.48	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C4-C3-C2	4.88	118.17	111.02
2	B	2	NAG	C4-C3-C2	4.86	118.14	111.02
3	C	3	BMA	C2-C3-C4	3.35	116.76	110.86
2	B	1	NAG	C4-C3-C2	3.09	115.55	111.02
2	D	2	NAG	C4-C3-C2	2.94	115.33	111.02
3	C	2	NAG	C2-N2-C7	-2.87	119.06	122.90
3	C	3	BMA	C3-C4-C5	2.81	115.33	110.23
3	C	3	BMA	C1-C2-C3	2.73	113.62	109.64
4	E	2	NDG	C1-O5-C5	2.71	115.82	112.19
4	E	2	NDG	C2-N2-C7	-2.47	119.58	122.90
3	C	3	BMA	C1-O5-C5	-2.44	108.92	112.19
2	D	1	NAG	C2-N2-C7	-2.18	119.97	122.90
3	C	1	NAG	C2-N2-C7	-2.11	120.07	122.90
2	B	2	NAG	C3-C4-C5	2.11	114.05	110.23
2	B	2	NAG	O5-C1-C2	-2.06	108.11	111.29

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	3	BMA	O5-C5-C6-O6
4	E	2	NDG	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
4	E	2	NDG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6

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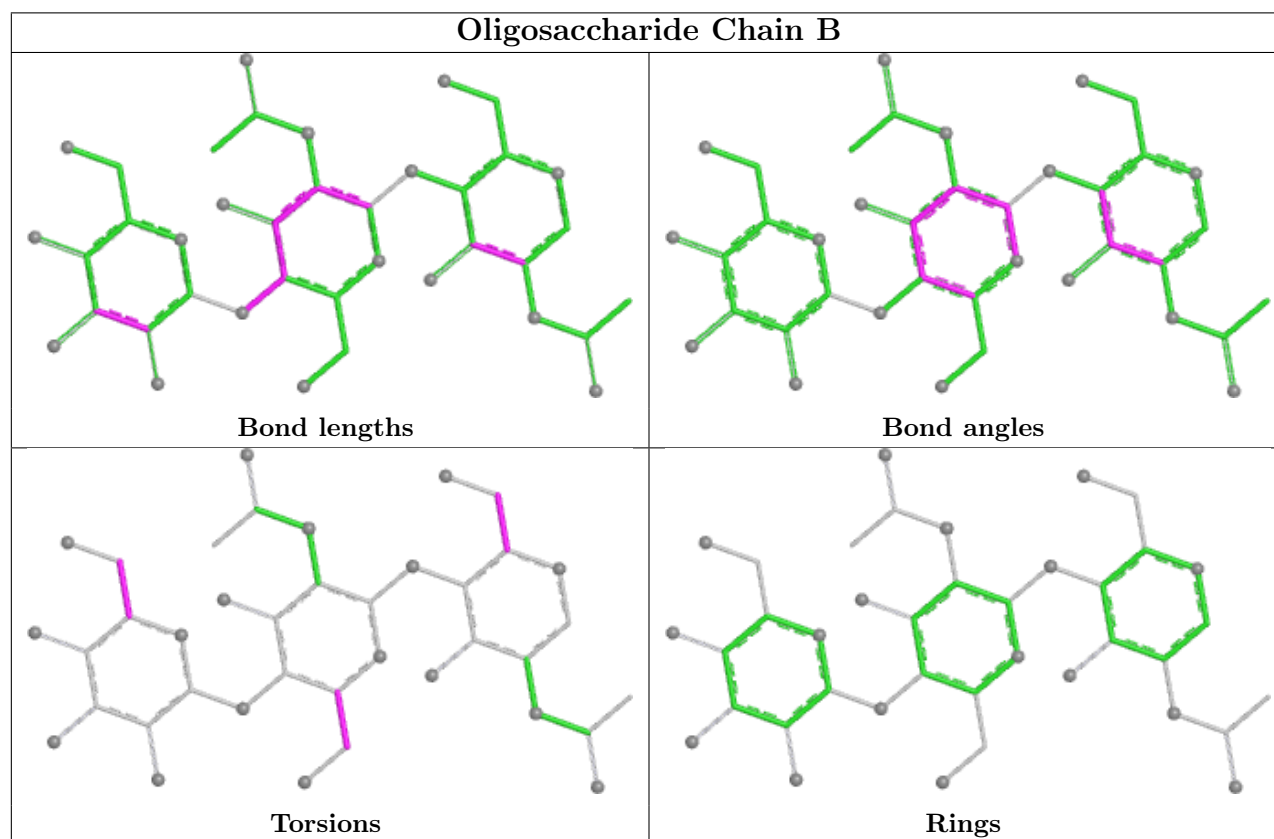
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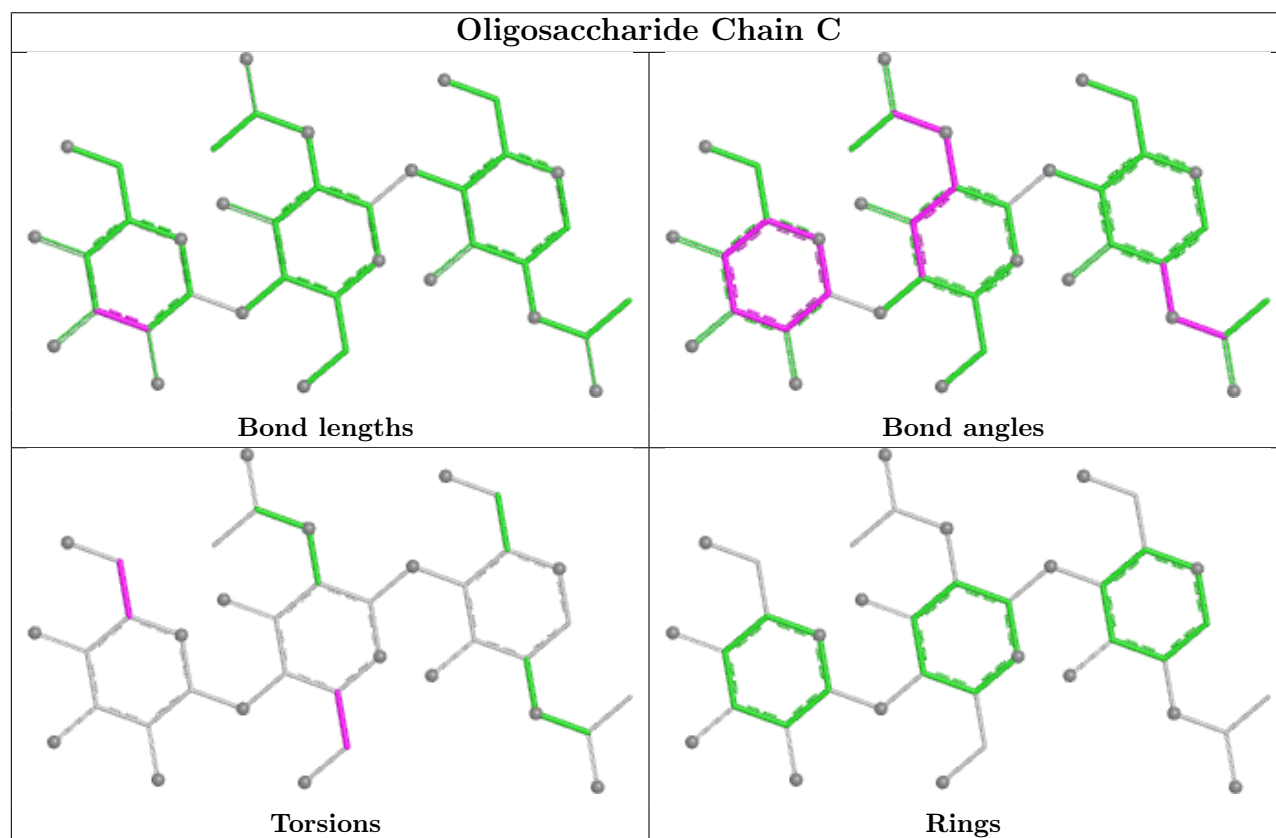
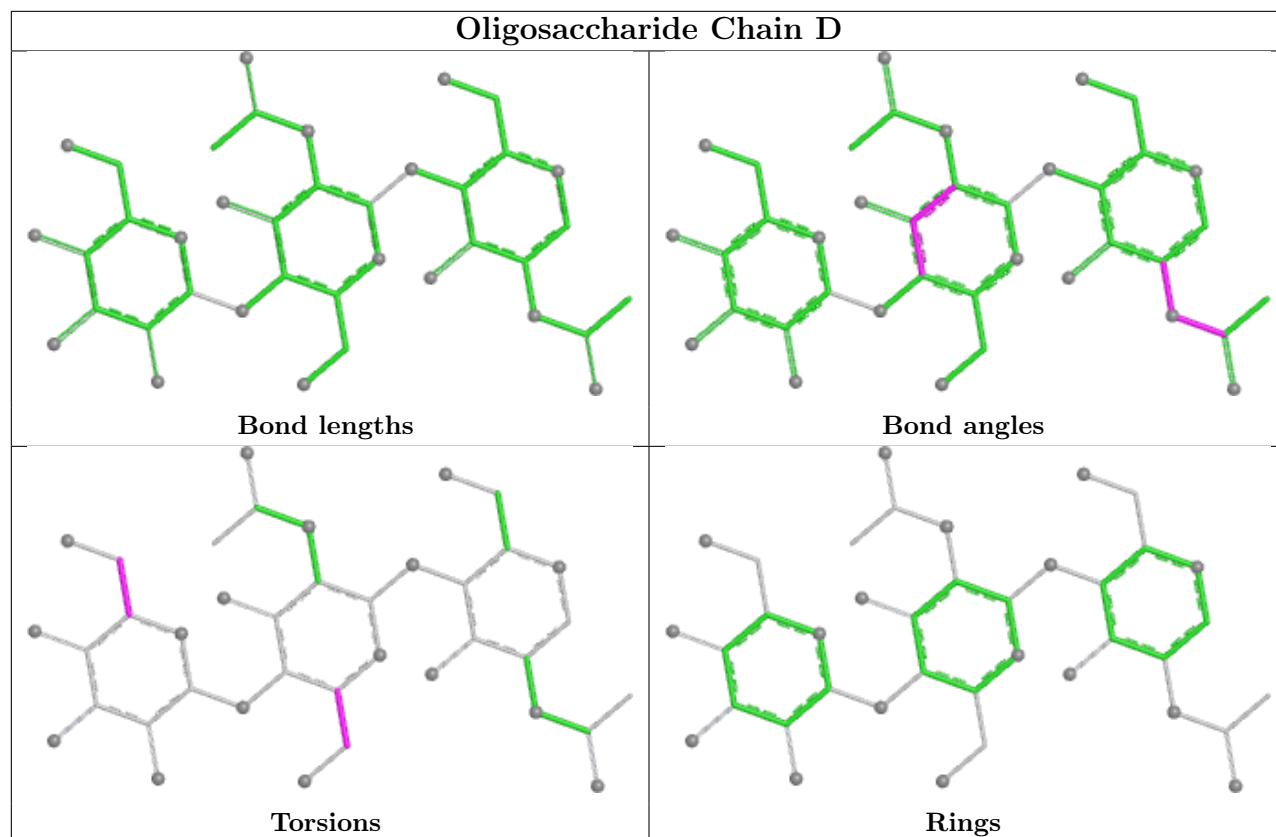
Mol	Chain	Res	Type	Atoms
3	C	3	BMA	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
2	D	3	MAN	O5-C5-C6-O6
2	B	3	MAN	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	B	3	MAN	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6

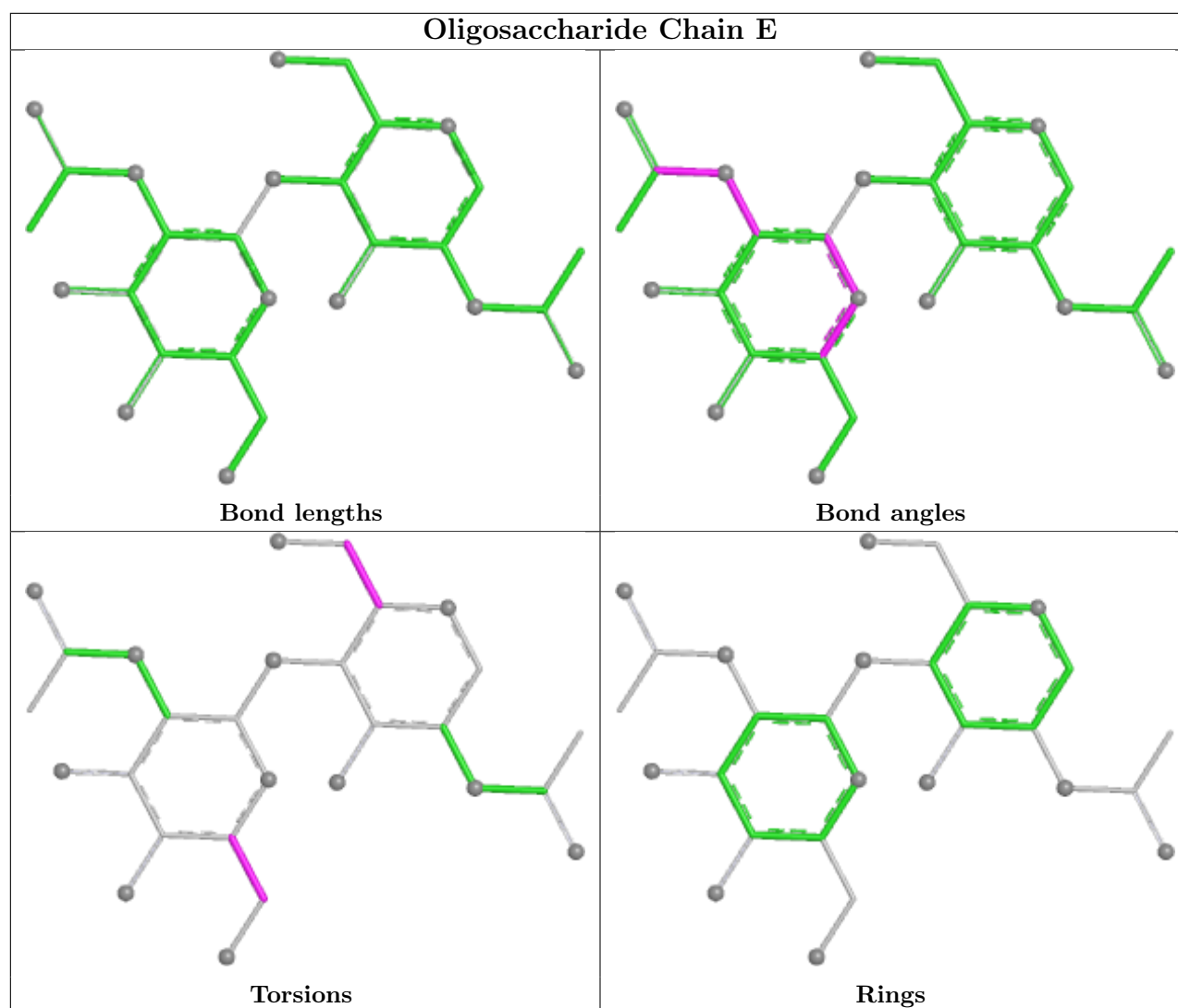
There are no ring outliers.

No monomer is involved in short contacts.

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







5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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	$\# Z > 2$
8	3TR	A	608	-	6,6,6	2.88	2 (33%)	6,7,7	1.50	1 (16%)
9	MRD	A	609	-	7,7,7	0.36	0	9,10,10	0.38	0
10	PEG	A	6071	-	6,6,6	1.56	1 (16%)	5,5,5	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	HEM	A	655	1	50,50,50	2.20	17 (34%)	67,82,82	1.48	11 (16%)
8	3TR	A	607	-	6,6,6	2.86	2 (33%)	6,7,7	1.50	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	3TR	A	608	-	-	-	0/1/1/1
9	MRD	A	609	-	-	5/5/5/5	-
10	PEG	A	6071	-	-	2/4/4/4	-
5	HEM	A	655	1	-	4/14/54/54	-
8	3TR	A	607	-	-	-	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	608	3TR	N1-N2	-6.14	1.23	1.36
8	A	607	3TR	N1-N2	-6.08	1.23	1.36
5	A	655	HEM	FE-ND	5.43	2.11	1.94
5	A	655	HEM	C3D-C2D	5.06	1.47	1.36
5	A	655	HEM	C4D-ND	-4.52	1.32	1.40
5	A	655	HEM	CAC-C3C	4.34	1.59	1.47
5	A	655	HEM	FE-NB	4.21	2.07	1.94
5	A	655	HEM	CAB-C3B	3.74	1.57	1.47
5	A	655	HEM	CMC-C2C	3.52	1.58	1.50
8	A	607	3TR	C3-N4	-3.41	1.32	1.37
8	A	608	3TR	C3-N4	-3.38	1.32	1.37
5	A	655	HEM	CMB-C2B	2.77	1.56	1.50
5	A	655	HEM	CMA-C3A	2.66	1.56	1.50
5	A	655	HEM	C3B-C2B	-2.59	1.31	1.37
5	A	655	HEM	C3C-C2C	-2.49	1.32	1.37
5	A	655	HEM	CBD-CGD	2.42	1.56	1.50
5	A	655	HEM	CBD-CAD	2.38	1.60	1.51
5	A	655	HEM	CAA-C2A	2.27	1.57	1.51
10	A	6071	PEG	O2-C3	2.22	1.51	1.42
5	A	655	HEM	O1D-CGD	2.19	1.29	1.22
5	A	655	HEM	CHC-C4B	-2.18	1.34	1.39
5	A	655	HEM	CAD-C3D	2.16	1.56	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	655	HEM	C4D-ND-C1D	4.36	110.37	105.21
5	A	655	HEM	CAD-CBD-CGD	-4.08	102.85	113.67
5	A	655	HEM	CBD-CAD-C3D	-3.89	101.78	112.53
5	A	655	HEM	C3B-C2B-C1B	2.96	108.63	106.41
5	A	655	HEM	CHA-C1A-NA	2.48	128.36	123.86
5	A	655	HEM	CAD-C3D-C4D	2.44	128.95	124.70
5	A	655	HEM	C4D-C3D-C2D	-2.38	103.42	106.89
5	A	655	HEM	CHD-C1D-ND	2.33	126.93	124.42
8	A	607	3TR	N3A-C3-N4	2.26	125.15	121.53
8	A	608	3TR	N3A-C3-N4	2.24	125.11	121.53
5	A	655	HEM	CHA-C4D-ND	-2.06	121.82	124.37
5	A	655	HEM	CBA-CAA-C2A	-2.03	106.92	112.53
5	A	655	HEM	C1A-CHA-C4D	-2.01	121.52	126.25

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	609	MRD	O2-C2-C3-C4
9	A	609	MRD	CM-C2-C3-C4
9	A	609	MRD	C2-C3-C4-O4
9	A	609	MRD	C2-C3-C4-C5
10	A	6071	PEG	O2-C3-C4-O4
10	A	6071	PEG	C4-C3-O2-C2
5	A	655	HEM	CAA-CBA-CGA-O1A
5	A	655	HEM	CAD-CBD-CGD-O2D
5	A	655	HEM	CAD-CBD-CGD-O1D
5	A	655	HEM	CAA-CBA-CGA-O2A
9	A	609	MRD	C1-C2-C3-C4

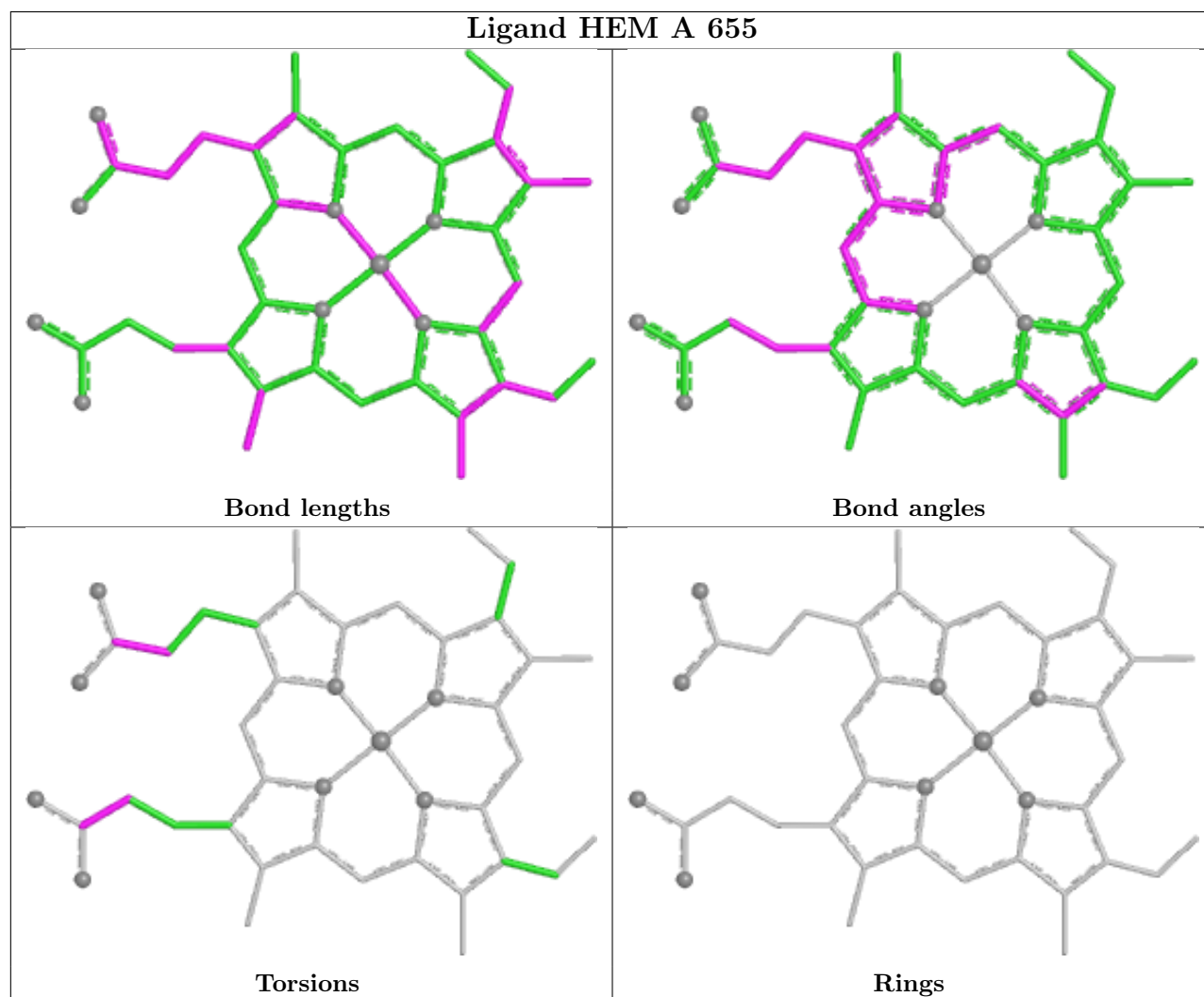
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	608	3TR	3	0
5	A	655	HEM	2	0
8	A	607	3TR	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	0.55	36 (6%) 27 25	30, 51, 94, 100	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	591	ALA	4.1
1	A	2	TRP	3.9
1	A	8	ALA	3.7
1	A	4	VAL	3.5
1	A	175	LEU	3.5
1	A	1	SER	3.3
1	A	538	GLU	3.2
1	A	172	TYR	3.2
1	A	283	LEU	3.1
1	A	13	VAL	2.9
1	A	168	PRO	2.9
1	A	169	THR	2.8
1	A	11	PRO	2.7
1	A	589	PRO	2.7
1	A	167	CYS	2.7
1	A	20	PRO	2.6
1	A	158	MET	2.6
1	A	12	LEU	2.6
1	A	235	SER	2.6
1	A	19	SER	2.5
1	A	436	ILE	2.5
1	A	124	HIS	2.4
1	A	16	ASP	2.4
1	A	121	SER	2.4
1	A	245	ARG	2.4
1	A	51	TYR	2.3
1	A	125	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	10	VAL	2.3
1	A	211	GLY	2.2
1	A	128	GLN	2.2
1	A	127	THR	2.2
1	A	166	VAL	2.1
1	A	171	PRO	2.1
1	A	284	ASN	2.1
1	A	173	GLN	2.0
1	A	210	LEU	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	0.83	0.15	49,55,64,64	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.

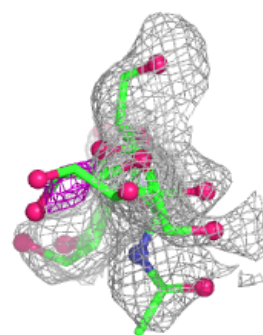
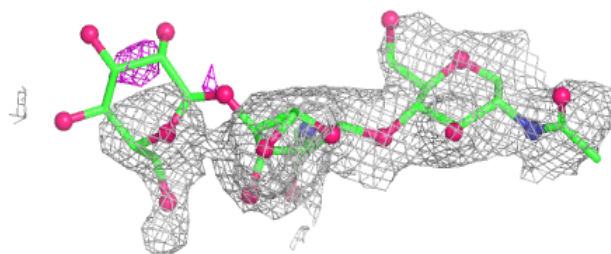
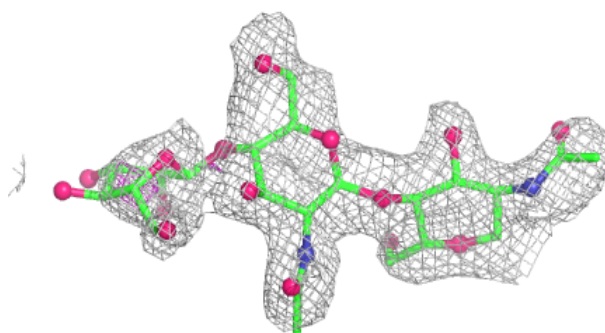
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NDG	E	2	14/15	0.36	0.15	96,99,99,99	0
2	NAG	B	2	14/15	0.42	0.14	95,99,99,99	0
4	NAG	E	1	14/15	0.49	0.13	82,88,92,93	0
2	MAN	B	3	11/12	0.52	0.13	100,100,100,100	0
3	BMA	C	3	11/12	0.52	0.13	96,98,99,99	0
2	MAN	D	3	11/12	0.65	0.10	96,98,98,99	0
2	NAG	B	1	14/15	0.75	0.11	75,81,83,89	0
2	NAG	D	2	14/15	0.75	0.10	83,88,89,93	0
3	NAG	C	2	14/15	0.76	0.11	86,87,90,93	0
3	NAG	C	1	14/15	0.80	0.11	74,77,80,83	0
2	NAG	D	1	14/15	0.85	0.11	62,67,71,77	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

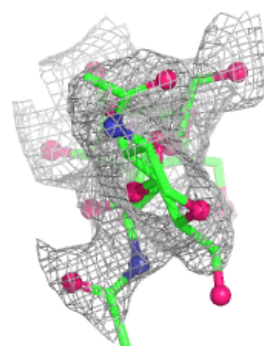
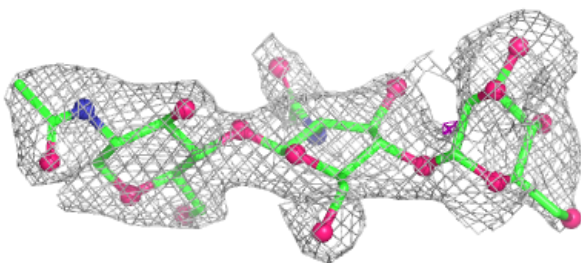
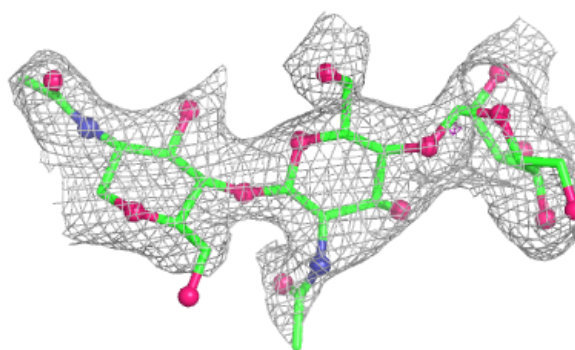
Electron density around Chain B:

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



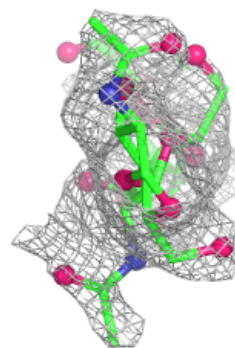
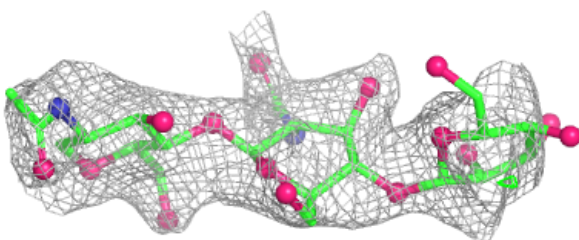
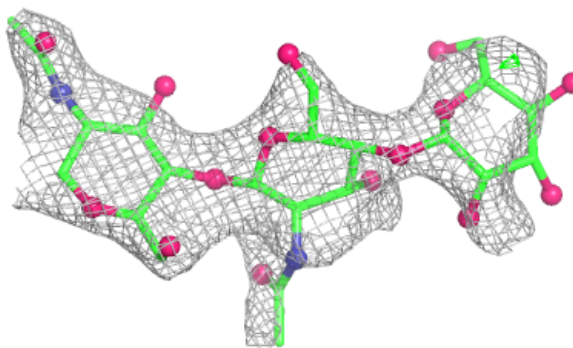
Electron density around Chain D:

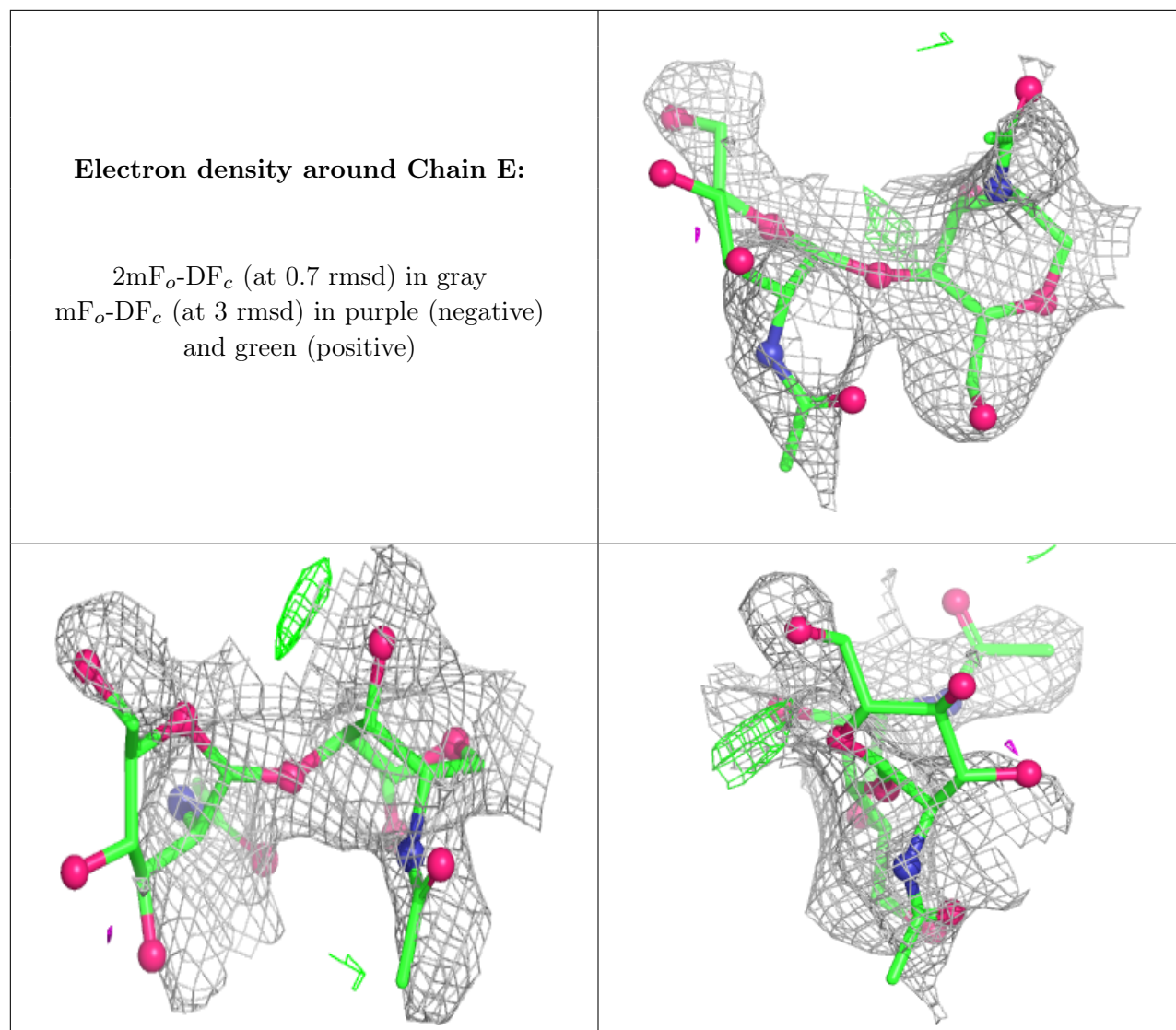
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain C:

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





6.4 Ligands [i](#)

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

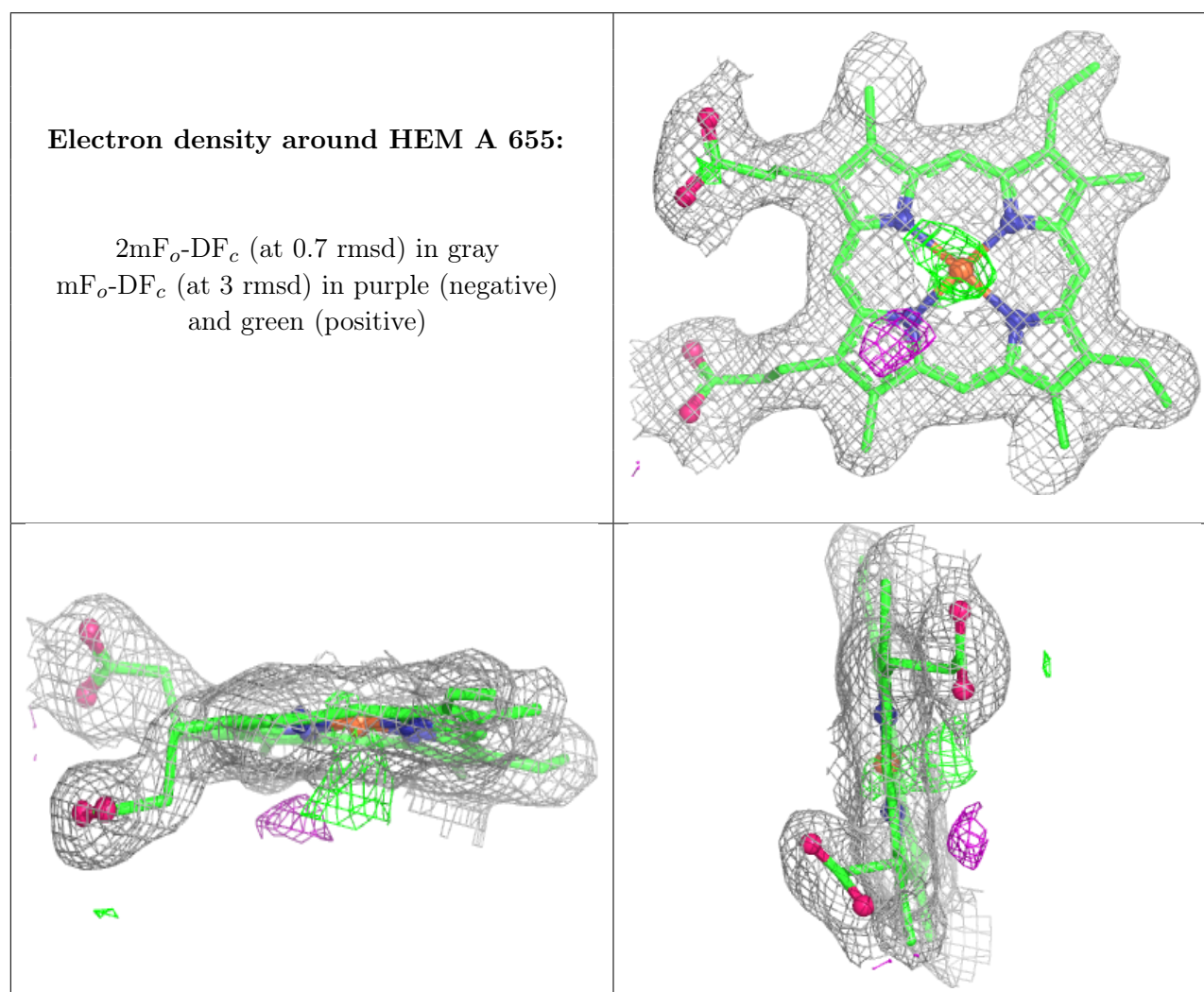
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	PEG	A	6071	7/7	0.62	0.15	43,46,49,49	0
9	MRD	A	609	8/8	0.73	0.14	38,44,46,46	0
8	3TR	A	607	6/6	0.81	0.19	22,30,33,36	0
8	3TR	A	608	6/6	0.84	0.15	45,47,49,50	0
7	IOD	A	616	1/1	0.85	0.08	87,87,87,87	1
7	IOD	A	615	1/1	0.94	0.08	70,70,70,70	0
6	CA	A	656	1/1	0.95	0.29	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	IOD	A	611	1/1	0.96	0.11	93,93,93,93	0
7	IOD	A	614	1/1	0.96	0.10	82,82,82,82	0
5	HEM	A	655	43/43	0.97	0.06	24,31,38,46	0
7	IOD	A	613	1/1	0.98	0.05	62,62,62,62	0
7	IOD	A	612	1/1	0.98	0.09	84,84,84,84	0
7	IOD	A	610	1/1	0.99	0.04	39,39,39,39	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.