



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:37 PM UTC

PDB ID : 6JGK / pdb_00006jgk
Title : Crystal structure of barley exohydrolaseI W434F mutant in complex with 4I, 4III,4V-S-trithiocellohexaose
Authors : Luang, S.; Streltsov, V.A.; Hrmova, M.
Deposited on : 2019-02-14
Resolution : 1.66 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

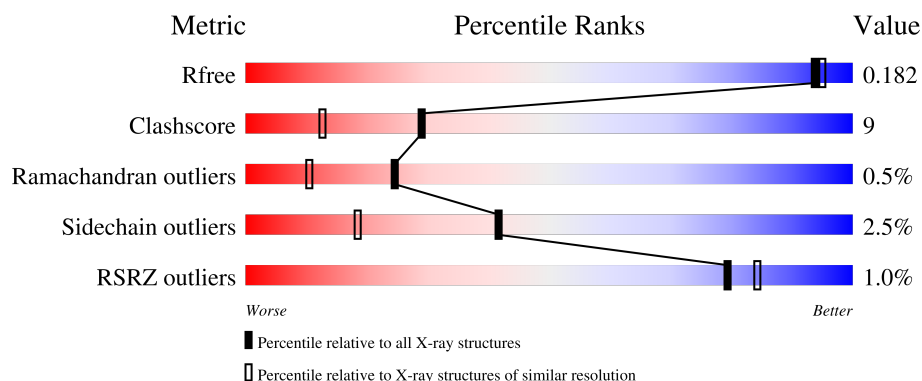
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.66 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	609	% 84% 13% .
2	B	3	33% 33% 33%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5528 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	606	Total	C	N	O	S	20	16	0
			4645	2934	811	873	27			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	HIS	-	expression tag	UNP A0A287SCR5
A	-2	HIS	-	expression tag	UNP A0A287SCR5
A	-1	ALA	-	expression tag	UNP A0A287SCR5
A	0	ALA	-	expression tag	UNP A0A287SCR5
A	320	LYS	ASN	conflict	UNP A0A287SCR5
A	434	PHE	TRP	engineered mutation	UNP A0A287SCR5

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	O	S	0	1	0
			34	18	14	2			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



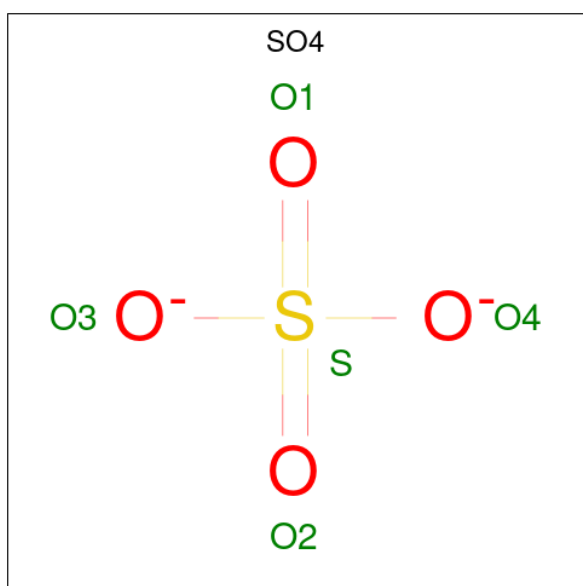
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

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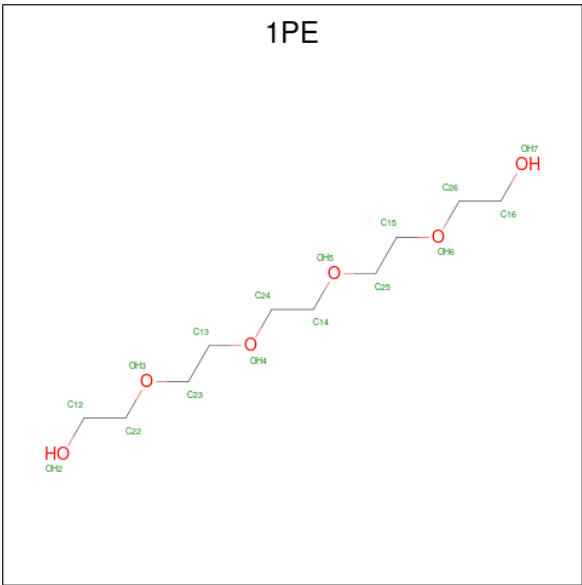
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			5	3	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			5	3	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	1
			13	8	5		
6	A	1	Total	C	O	0	0
			5	3	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			8	5	3		

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

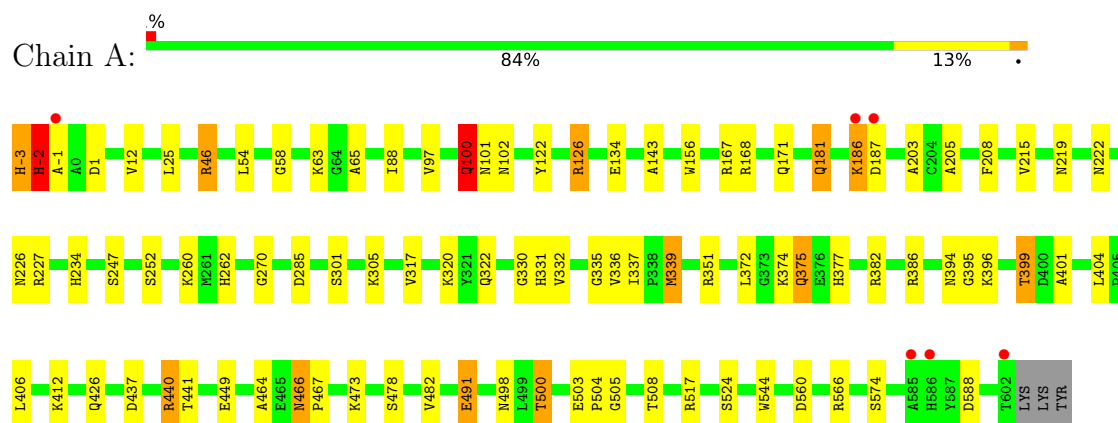
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	672	Total	O	0	0
			672	672		

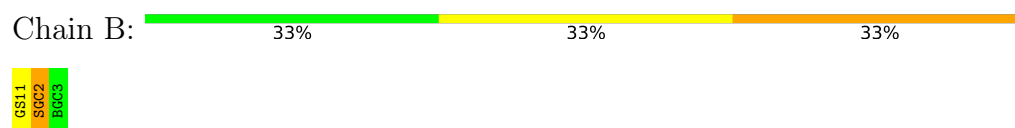
3 Residue-property plots

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: Uncharacterized protein



- Molecule 2: beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-1-thio-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.61Å 100.61Å 181.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.03 – 1.66 44.03 – 1.66	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.03-1.66) 99.7 (44.03-1.66)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.66Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.141 , 0.171 0.154 , 0.182	Depositor DCC
R_{free} test set	5486 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5528	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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: SGC, NAG, BGC, GS1, GOL, SO4, ACT, 1PE

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	1.53	32/4834 (0.7%)	1.30	20/6556 (0.3%)

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 (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	-2	HIS	C-N	14.35	1.53	1.33
1	A	126	ARG	CD-NE	-9.46	1.33	1.46
1	A	503	GLU	CD-OE2	7.38	1.39	1.25
1	A	317	VAL	CA-CB	-6.99	1.50	1.54
1	A	100	GLN	CD-OE1	6.89	1.36	1.23
1	A	466[A]	ASN	N-CA	-6.86	1.39	1.46
1	A	466[B]	ASN	N-CA	-6.86	1.39	1.46
1	A	336	VAL	N-CA	-6.85	1.38	1.46
1	A	399	THR	CB-CG2	-6.75	1.30	1.52
1	A	401	ALA	CA-C	6.29	1.59	1.53
1	A	337	ILE	N-CA	6.11	1.51	1.46
1	A	-2	HIS	N-CA	5.98	1.53	1.46
1	A	88	ILE	CA-C	5.91	1.57	1.53
1	A	330	GLY	N-CA	5.79	1.53	1.45
1	A	260	LYS	N-CA	5.68	1.53	1.46
1	A	500[A]	THR	C-O	5.68	1.30	1.24
1	A	500[B]	THR	C-O	5.68	1.30	1.24
1	A	270	GLY	N-CA	5.64	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	339	MET	SD-CE	-5.61	1.65	1.79
1	A	181	GLN	CD-OE1	5.59	1.34	1.23
1	A	1	ASP	CA-C	5.51	1.61	1.52
1	A	205	ALA	C-O	5.51	1.30	1.24
1	A	504	PRO	C-O	5.50	1.34	1.23
1	A	375	GLN	N-CA	-5.40	1.39	1.46
1	A	426	GLN	CB-CG	-5.34	1.36	1.52
1	A	65	ALA	N-CA	5.23	1.52	1.46
1	A	395	GLY	N-CA	5.18	1.52	1.45
1	A	226	ASN	C-O	5.16	1.30	1.23
1	A	372	LEU	N-CA	-5.12	1.39	1.46
1	A	143	ALA	C-O	5.11	1.30	1.24
1	A	305	LYS	CA-CB	5.10	1.61	1.53
1	A	100	GLN	CD-NE2	-5.07	1.22	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ARG	NE-CZ-NH1	11.64	133.14	121.50
1	A	126	ARG	NE-CZ-NH2	-11.30	109.03	119.20
1	A	-2	HIS	O-C-N	-9.74	109.63	122.59
1	A	126	ARG	CD-NE-CZ	8.23	135.93	124.40
1	A	-2	HIS	CA-C-N	7.22	135.32	121.54
1	A	-2	HIS	C-N-CA	7.22	135.32	121.54
1	A	399	THR	N-CA-CB	-6.43	100.95	110.53
1	A	560	ASP	N-CA-C	-6.00	104.74	111.28
1	A	46	ARG	NE-CZ-NH2	5.75	124.37	119.20
1	A	305	LYS	N-CA-C	5.70	117.16	111.07
1	A	208	PHE	CA-C-N	5.49	131.57	121.70
1	A	208	PHE	C-N-CA	5.49	131.57	121.70
1	A	335	GLY	N-CA-C	5.38	122.52	115.47
1	A	588	ASP	O-C-N	5.35	125.56	121.23
1	A	412	LYS	CB-CG-CD	-5.22	99.29	111.30
1	A	478	SER	N-CA-C	5.16	116.98	111.36
1	A	46	ARG	CA-C-O	5.13	125.98	120.70
1	A	449	GLU	CG-CD-OE1	5.11	130.16	118.40
1	A	-2	HIS	N-CA-C	5.01	121.47	110.80
1	A	351	ARG	NE-CZ-NH1	5.01	126.51	121.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-3	HIS	Peptide
1	A	187	ASP	Peptide

5.2 Too-close contacts [i](#)

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	4645	0	4629	68	0
2	B	34	0	23	3	0
3	A	42	0	39	2	0
4	A	36	0	48	5	0
5	A	20	0	0	1	0
6	A	63	0	66	11	0
7	A	16	0	12	0	0
8	A	672	0	0	35	0
All	All	5528	0	4817	82	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 9.

All (82) 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:498:ASN:HD21	3:A:704:NAG:C1	1.32	1.39
1:A:517[B]:ARG:CD	8:A:807:HOH:O	1.67	1.31
1:A:498:ASN:HB3	8:A:843:HOH:O	1.25	1.31
8:A:811:HOH:O	2:B:2:SGC:H61	1.41	1.19
1:A:517[B]:ARG:HD3	8:A:807:HOH:O	1.27	1.13
8:A:811:HOH:O	2:B:2:SGC:S4	2.07	1.11
1:A:498:ASN:ND2	3:A:704:NAG:C1	2.16	1.08
1:A:466[A]:ASN:ND2	1:A:508:THR:OG1	1.95	0.99
1:A:491[A]:GLU:OE1	8:A:811:HOH:O	1.81	0.98
6:A:722:1PE:H261	8:A:1321:HOH:O	1.69	0.91
1:A:322:GLN:CD	8:A:844:HOH:O	2.14	0.90
1:A:46:ARG:HD3	8:A:1023:HOH:O	1.72	0.89
1:A:394:ASN:HD21	1:A:404:LEU:H	1.22	0.87
1:A:374[B]:LYS:NZ	8:A:809:HOH:O	1.59	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:709:GOL:O1	8:A:813:HOH:O	1.97	0.81
1:A:122:TYR:CE2	1:A:126:ARG:HD2	2.16	0.79
1:A:156:TRP:HE1	1:A:219:ASN:HD22	1.32	0.76
1:A:227[A]:ARG:NH1	8:A:812:HOH:O	1.93	0.75
1:A:440[A]:ARG:HD2	8:A:1293:HOH:O	1.86	0.75
1:A:262:HIS:HE1	1:A:285:ASP:H	1.38	0.71
1:A:100:GLN:HE21	1:A:100:GLN:HA	1.56	0.70
1:A:500[B]:THR:HG22	8:A:1002:HOH:O	1.91	0.69
4:A:709:GOL:H11	8:A:989:HOH:O	1.95	0.66
1:A:181:GLN:HE21	1:A:203:ALA:H	1.44	0.65
1:A:491[A]:GLU:CD	8:A:811:HOH:O	2.33	0.64
1:A:134:GLU:OE2	1:A:377:HIS:HD2	1.81	0.63
1:A:517[B]:ARG:NH2	8:A:820:HOH:O	2.30	0.63
1:A:97:VAL:H	1:A:101:ASN:HD21	1.45	0.62
1:A:339:MET:HA	1:A:339:MET:HE2	1.81	0.61
1:A:12:VAL:HB	6:A:719:1PE:H251	1.83	0.60
1:A:100:GLN:HE21	1:A:100:GLN:CA	2.15	0.59
6:A:719:1PE:OH7	6:A:719:1PE:C15	2.51	0.59
6:A:724:1PE:H222	8:A:1302:HOH:O	2.02	0.58
1:A:331:HIS:HD2	8:A:1334:HOH:O	1.86	0.58
1:A:262:HIS:CE1	1:A:285:ASP:H	2.22	0.57
1:A:122:TYR:O	1:A:126:ARG:HD3	2.05	0.56
1:A:181:GLN:HE22	1:A:247:SER:H	1.54	0.55
1:A:234:HIS:HE1	8:A:1348:HOH:O	1.90	0.55
1:A:58:GLY:H	1:A:102:ASN:ND2	2.06	0.54
1:A:167:ARG:HH21	1:A:171:GLN:HE22	1.57	0.53
1:A:396:LYS:O	6:A:725:1PE:H261	2.06	0.53
1:A:517[B]:ARG:CD	8:A:1239:HOH:O	2.57	0.53
1:A:168:ARG:NH2	5:A:712:SO4:O2	2.42	0.53
1:A:234:HIS:HD2	8:A:1162:HOH:O	1.92	0.53
1:A:386:ARG:HH22	6:A:726:1PE:C26	2.21	0.52
1:A:186:LYS:H	1:A:186:LYS:CD	2.22	0.52
6:A:719:1PE:OH7	6:A:719:1PE:H152	2.10	0.52
1:A:25:LEU:HD13	1:A:339:MET:HE1	1.93	0.51
1:A:374[A]:LYS:CE	8:A:814:HOH:O	2.55	0.50
1:A:122:TYR:CZ	1:A:126:ARG:HD2	2.47	0.48
1:A:186:LYS:H	1:A:186:LYS:CE	2.27	0.48
1:A:252:SER:OG	4:A:707:GOL:H31	2.14	0.48
1:A:322:GLN:CG	8:A:844:HOH:O	2.58	0.48
1:A:374[A]:LYS:NZ	8:A:814:HOH:O	2.02	0.47
1:A:97:VAL:H	1:A:101:ASN:ND2	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ARG:HH22	6:A:726:1PE:H262	1.79	0.47
4:A:710:GOL:C1	8:A:1350:HOH:O	2.63	0.47
1:A:517[B]:ARG:NH1	8:A:810:HOH:O	1.79	0.47
1:A:122:TYR:CD2	1:A:126:ARG:HD2	2.50	0.46
1:A:215:VAL:HG23	1:A:222:ASN:O	2.16	0.45
4:A:710:GOL:H12	8:A:1350:HOH:O	2.17	0.45
1:A:134:GLU:OE2	1:A:377:HIS:CD2	2.66	0.44
1:A:382:ARG:HH12	6:A:724:1PE:C12	2.30	0.44
1:A:524:SER:O	1:A:544:TRP:HA	2.18	0.43
8:A:811:HOH:O	2:B:2:SGC:C6	2.26	0.43
1:A:404:LEU:HD23	1:A:406:LEU:HG	2.01	0.42
1:A:473[B]:LYS:NZ	8:A:837:HOH:O	2.52	0.42
1:A:167:ARG:NH2	1:A:171:GLN:HE22	2.17	0.42
1:A:167:ARG:HH21	1:A:171:GLN:NE2	2.16	0.42
1:A:375:GLN:OE1	8:A:815:HOH:O	2.22	0.42
1:A:156:TRP:HE1	1:A:219:ASN:ND2	2.09	0.42
1:A:437:ASP:HB3	1:A:441:THR:HG21	2.02	0.42
1:A:466[A]:ASN:ND2	1:A:508:THR:HG1	2.13	0.42
1:A:301:SER:O	1:A:331:HIS:HE1	2.02	0.42
1:A:332:VAL:HG11	1:A:339:MET:HE1	2.03	0.41
1:A:566:ARG:HD2	8:A:1303:HOH:O	2.21	0.41
6:A:716:1PE:H262	8:A:959:HOH:O	2.21	0.41
6:A:723[A]:1PE:OH4	8:A:816:HOH:O	2.22	0.41
1:A:186:LYS:H	1:A:186:LYS:HD2	1.85	0.41

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	620/609 (102%)	595 (96%)	22 (4%)	3 (0%)	24 10

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-2	HIS
1	A	-1	ALA
1	A	505	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	503/490 (103%)	487 (97%)	16 (3%)	34	12

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	HIS
1	A	-2	HIS
1	A	54	LEU
1	A	63	LYS
1	A	100	GLN
1	A	186	LYS
1	A	320	LYS
1	A	399	THR
1	A	440[A]	ARG
1	A	440[B]	ARG
1	A	482[A]	VAL
1	A	482[B]	VAL
1	A	491[A]	GLU
1	A	491[B]	GLU
1	A	574[A]	SER
1	A	574[B]	SER

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	71	GLN

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Mol	Chain	Res	Type
1	A	100	GLN
1	A	101	ASN
1	A	102	ASN
1	A	112	ASN
1	A	171	GLN
1	A	181	GLN
1	A	219	ASN
1	A	234	HIS
1	A	262	HIS
1	A	331	HIS
1	A	377	HIS
1	A	394	ASN
1	A	498	ASN
1	A	581	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	$\# Z > 2$
3	NAG	A	703	1	14,14,15	1.05	2 (14%)	17,19,21	2.23	7 (41%)

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
3	NAG	A	703	1	-	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)
3	A	703	NAG	C2-N2	2.30	1.50	1.46
3	A	703	NAG	C1-C2	2.01	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	703	NAG	O7-C7-C8	-5.59	112.11	122.05
3	A	703	NAG	O7-C7-N2	3.08	127.43	121.98
3	A	703	NAG	C1-C2-N2	2.96	115.10	110.43
3	A	703	NAG	O4-C4-C3	2.84	117.06	110.38
3	A	703	NAG	C8-C7-N2	2.61	120.45	116.12
3	A	703	NAG	C2-N2-C7	2.45	126.18	122.90
3	A	703	NAG	O3-C3-C2	-2.20	104.84	109.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

3 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	GS1	B	1	2	11,12,12	0.70	0	15,17,17	2.83	6 (40%)
2	SGC	B	2	2	10,11,12	1.87	3 (30%)	12,15,17	1.39	2 (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
2	GS1	B	1	2	-	2/2/22/22	0/1/1/1
2	SGC	B	2	2	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	SGC	C5-C4	4.13	1.56	1.53
2	B	2	SGC	C3-C4	-2.41	1.51	1.53
2	B	2	SGC	O5-C5	2.04	1.47	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GS1	C1-O5-C5	5.68	122.72	112.55
2	B	1	GS1	O5-C5-C4	5.17	119.02	109.70
2	B	1	GS1	O6-C6-C5	-5.08	94.03	111.33
2	B	1	GS1	C6-C5-C4	-3.65	104.06	113.02
2	B	2	SGC	C1-C2-C3	-2.92	105.40	109.64
2	B	2	SGC	C1-O5-C5	-2.78	108.45	112.19
2	B	1	GS1	O5-C1-C2	-2.66	106.65	110.32
2	B	1	GS1	C3-C4-C5	2.03	113.92	110.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

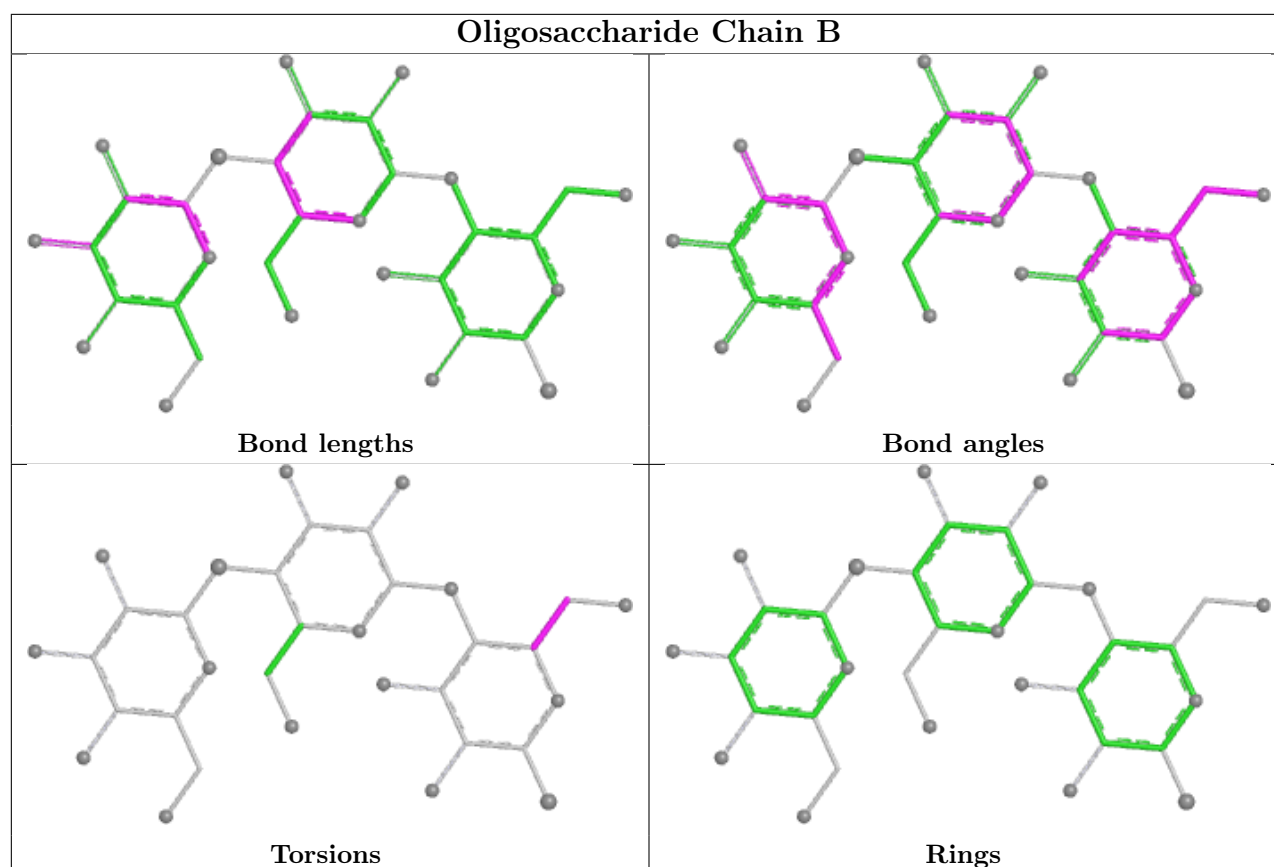
Mol	Chain	Res	Type	Atoms
2	B	1	GS1	C4-C5-C6-O6
2	B	1	GS1	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	SGC	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 oligosaccharide.



5.6 Ligand geometry [i](#)

29 ligands 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	$\# Z > 2$
6	1PE	A	721	-	3,3,15	0.40	0	2,2,14	0.91	0
4	GOL	A	709	-	5,5,5	1.40	1 (20%)	5,5,5	0.86	0
4	GOL	A	711	-	5,5,5	0.74	0	5,5,5	0.98	0
7	ACT	A	730	-	3,3,3	0.75	0	3,3,3	1.06	0
4	GOL	A	707	-	5,5,5	0.22	0	5,5,5	0.86	0
7	ACT	A	727	-	3,3,3	0.68	0	3,3,3	1.69	2 (66%)
7	ACT	A	729	-	3,3,3	1.27	0	3,3,3	1.03	0
3	NAG	A	705	1	14,14,15	1.19	3 (21%)	17,19,21	1.82	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	A	715	-	4,4,4	0.58	0	6,6,6	0.36	0
6	1PE	A	723[B]	-	9,9,15	0.87	0	8,8,14	1.58	2 (25%)
5	SO4	A	712	-	4,4,4	0.48	0	6,6,6	0.24	0
4	GOL	A	706	-	5,5,5	0.79	0	5,5,5	0.52	0
4	GOL	A	708	-	5,5,5	0.71	0	5,5,5	1.34	1 (20%)
6	1PE	A	725	-	3,3,15	0.68	0	2,2,14	1.01	0
6	1PE	A	716	-	3,3,15	0.66	0	2,2,14	1.07	0
6	1PE	A	726	-	7,7,15	0.71	0	6,6,14	0.96	0
7	ACT	A	728	-	3,3,3	1.35	0	3,3,3	2.30	2 (66%)
6	1PE	A	724	-	4,4,15	1.40	1 (25%)	3,3,14	1.20	0
6	1PE	A	723[A]	-	9,9,15	0.85	0	8,8,14	1.60	2 (25%)
6	1PE	A	722	-	3,3,15	0.45	0	2,2,14	0.74	0
6	1PE	A	720	-	4,4,15	0.38	0	3,3,14	0.60	0
3	NAG	A	703	1	14,14,15	1.05	2 (14%)	17,19,21	2.23	7 (41%)
3	NAG	A	704	-	14,14,15	0.96	0	17,19,21	1.38	3 (17%)
6	1PE	A	719	-	6,6,15	0.58	0	5,5,14	0.77	0
6	1PE	A	717	-	4,4,15	0.60	0	3,3,14	0.16	0
6	1PE	A	718	-	3,3,15	0.38	0	2,2,14	0.77	0
5	SO4	A	714	-	4,4,4	0.64	0	6,6,6	1.42	1 (16%)
5	SO4	A	713	-	4,4,4	0.55	0	6,6,6	0.42	0
4	GOL	A	710	-	5,5,5	0.42	0	5,5,5	1.11	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	A	721	-	-	1/1/1/13	-
4	GOL	A	709	-	-	2/4/4/4	-
4	GOL	A	711	-	-	4/4/4/4	-
4	GOL	A	707	-	-	4/4/4/4	-
3	NAG	A	705	1	-	0/6/23/26	0/1/1/1
6	1PE	A	723[B]	-	-	6/7/7/13	-
4	GOL	A	706	-	-	2/4/4/4	-
4	GOL	A	708	-	-	0/4/4/4	-
6	1PE	A	725	-	-	1/1/1/13	-
6	1PE	A	716	-	-	0/1/1/13	-
6	1PE	A	726	-	-	2/5/5/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	A	724	-	-	1/2/2/13	-
6	1PE	A	723[A]	-	-	5/7/7/13	-
6	1PE	A	722	-	-	1/1/1/13	-
6	1PE	A	720	-	-	1/2/2/13	-
3	NAG	A	703	1	-	0/6/23/26	0/1/1/1
3	NAG	A	704	-	-	1/6/23/26	0/1/1/1
6	1PE	A	719	-	-	2/4/4/13	-
6	1PE	A	717	-	-	1/2/2/13	-
6	1PE	A	718	-	-	0/1/1/13	-
4	GOL	A	710	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	NAG	C2-N2	2.30	1.50	1.46
6	A	724	1PE	OH3-C23	2.28	1.53	1.42
3	A	705	NAG	C1-C2	2.22	1.55	1.52
3	A	705	NAG	C3-C2	2.22	1.57	1.52
3	A	705	NAG	C4-C5	2.09	1.57	1.53
4	A	709	GOL	O2-C2	2.06	1.49	1.43
3	A	703	NAG	C1-C2	2.01	1.55	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	703	NAG	O7-C7-C8	-5.59	112.11	122.05
6	A	723[A]	1PE	OH6-C15-C25	3.09	124.44	110.35
6	A	723[B]	1PE	OH6-C15-C25	3.09	124.44	110.35
3	A	703	NAG	O7-C7-N2	3.08	127.43	121.98
3	A	705	NAG	O7-C7-C8	-3.03	116.66	122.05
3	A	705	NAG	C6-C5-C4	2.98	120.34	113.02
3	A	703	NAG	C1-C2-N2	2.96	115.10	110.43
3	A	704	NAG	C1-C2-N2	-2.96	105.77	110.43
3	A	705	NAG	O5-C1-C2	-2.96	106.71	111.29
6	A	723[A]	1PE	C26-OH6-C15	2.88	125.88	113.26
6	A	723[B]	1PE	C26-OH6-C15	2.88	125.88	113.26
7	A	728	ACT	OXT-C-CH3	2.85	127.02	115.05
3	A	703	NAG	O4-C4-C3	2.84	117.06	110.38
7	A	728	ACT	O-C-CH3	-2.79	111.11	122.53
5	A	714	SO4	O4-S-O2	2.65	123.40	109.56
3	A	703	NAG	C8-C7-N2	2.61	120.45	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	705	NAG	C1-O5-C5	-2.58	108.73	112.19
3	A	704	NAG	C3-C4-C5	2.54	114.83	110.23
3	A	703	NAG	C2-N2-C7	2.45	126.18	122.90
3	A	705	NAG	C2-N2-C7	2.30	125.98	122.90
3	A	703	NAG	O3-C3-C2	-2.20	104.84	109.40
3	A	704	NAG	O5-C1-C2	2.16	114.64	111.29
3	A	705	NAG	O5-C5-C4	-2.13	105.64	110.83
4	A	708	GOL	O1-C1-C2	-2.12	100.85	110.38
7	A	727	ACT	OXT-C-O	-2.07	114.34	122.03
3	A	705	NAG	O4-C4-C5	2.06	114.40	109.32
7	A	727	ACT	OXT-C-CH3	2.05	123.66	115.05

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	707	GOL	O1-C1-C2-C3
4	A	709	GOL	O1-C1-C2-C3
4	A	711	GOL	O1-C1-C2-C3
4	A	711	GOL	C1-C2-C3-O3
6	A	723[A]	1PE	C16-C26-OH6-C15
6	A	723[B]	1PE	C16-C26-OH6-C15
6	A	723[A]	1PE	OH5-C14-C24-OH4
4	A	707	GOL	O1-C1-C2-O2
6	A	723[A]	1PE	OH6-C15-C25-OH5
6	A	723[B]	1PE	OH6-C15-C25-OH5
6	A	719	1PE	OH6-C15-C25-OH5
4	A	707	GOL	C1-C2-C3-O3
4	A	710	GOL	O1-C1-C2-C3
6	A	717	1PE	OH2-C12-C22-OH3
4	A	707	GOL	O2-C2-C3-O3
4	A	709	GOL	O1-C1-C2-O2
4	A	711	GOL	O2-C2-C3-O3
6	A	719	1PE	C16-C26-OH6-C15
3	A	704	NAG	O5-C5-C6-O6
4	A	711	GOL	O1-C1-C2-O2
4	A	706	GOL	O1-C1-C2-C3
6	A	723[B]	1PE	OH5-C14-C24-OH4
6	A	723[A]	1PE	C24-C14-OH5-C25
6	A	721	1PE	OH7-C16-C26-OH6
6	A	725	1PE	OH7-C16-C26-OH6
6	A	720	1PE	OH7-C16-C26-OH6

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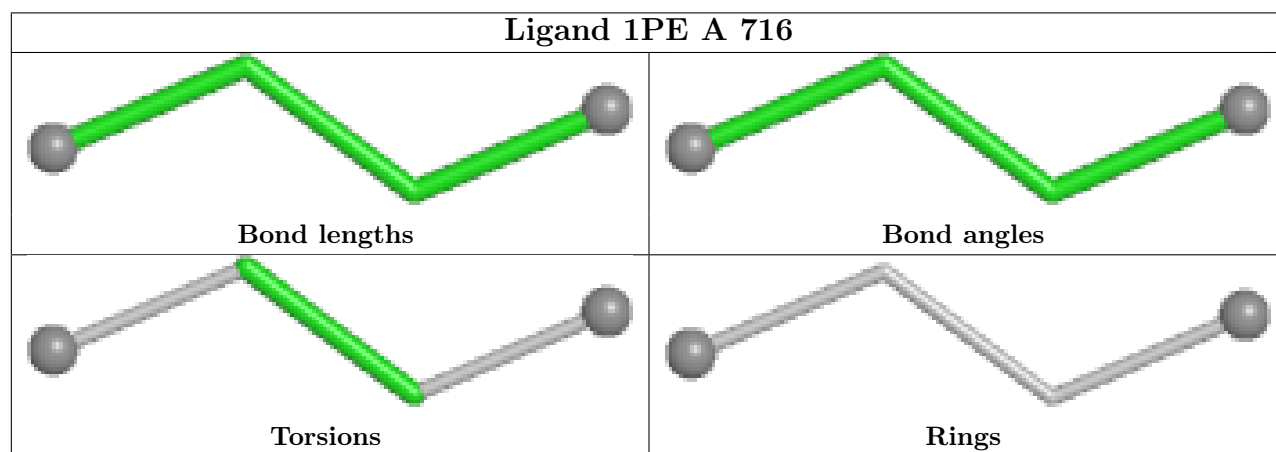
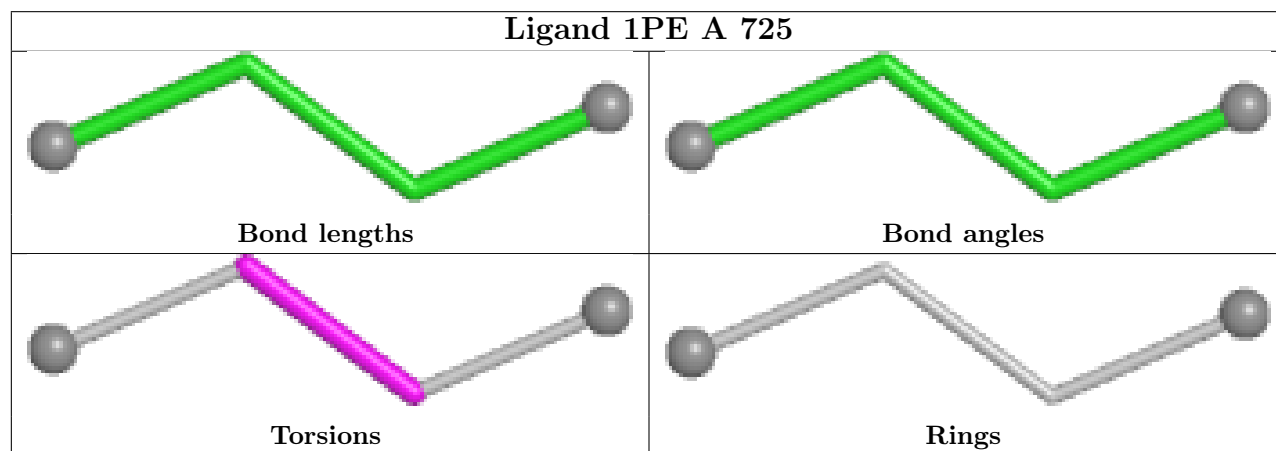
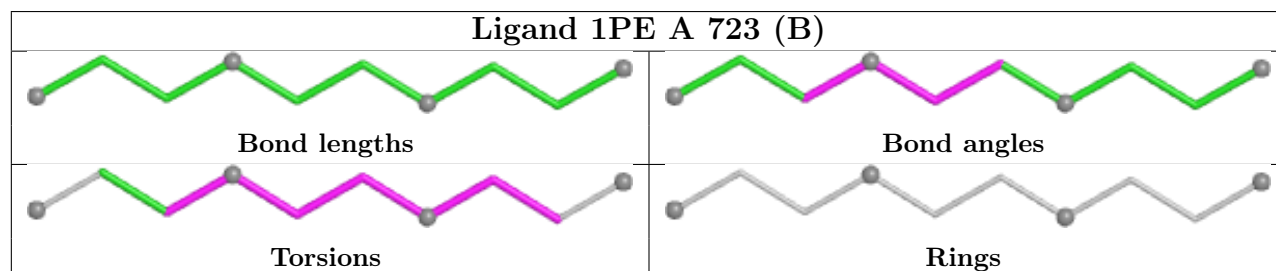
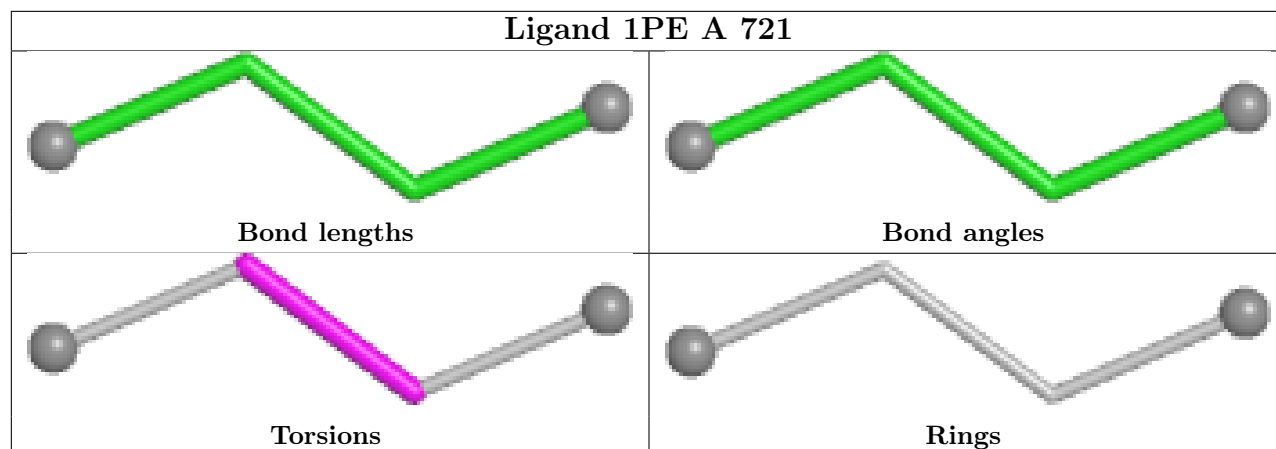
Mol	Chain	Res	Type	Atoms
6	A	723[A]	1PE	C25-C15-OH6-C26
6	A	723[B]	1PE	C25-C15-OH6-C26
6	A	726	1PE	C15-C25-OH5-C14
4	A	706	GOL	O1-C1-C2-O2
6	A	723[B]	1PE	C15-C25-OH5-C14
6	A	722	1PE	OH7-C16-C26-OH6
4	A	710	GOL	O1-C1-C2-O2
6	A	723[B]	1PE	C24-C14-OH5-C25
6	A	726	1PE	OH6-C15-C25-OH5
6	A	724	1PE	C12-C22-OH3-C23

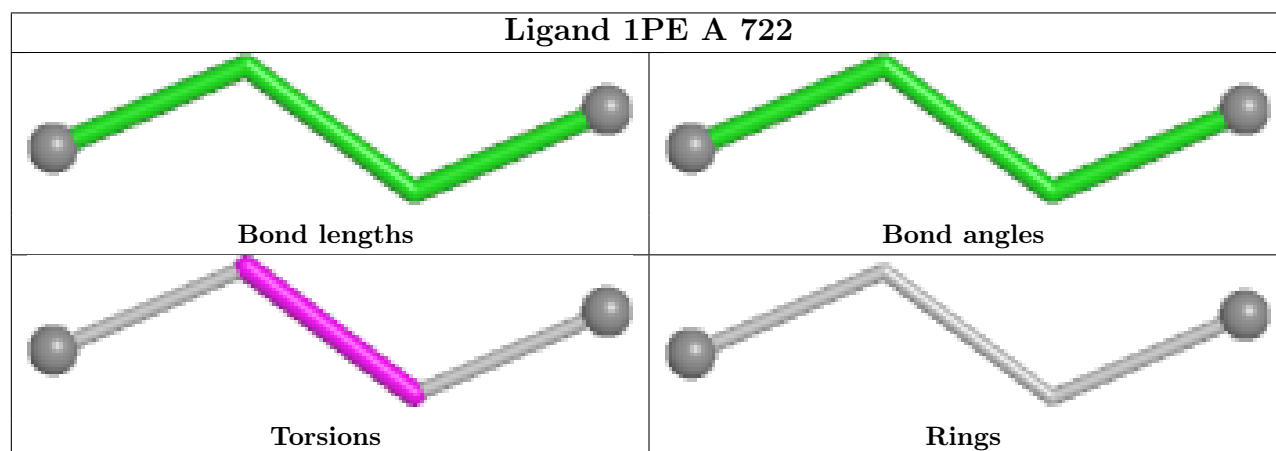
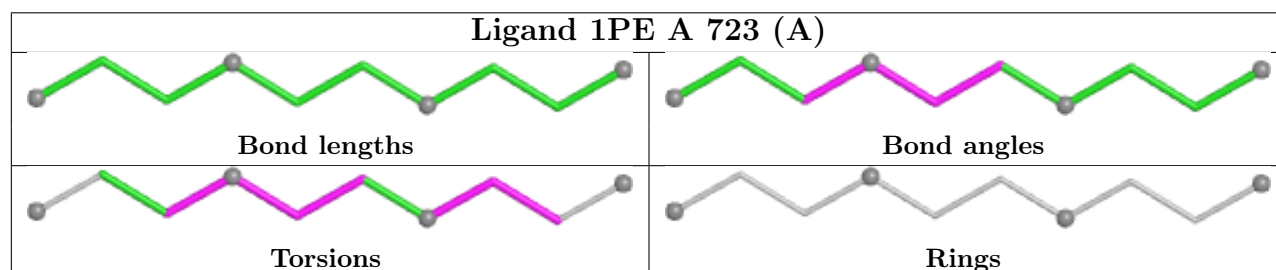
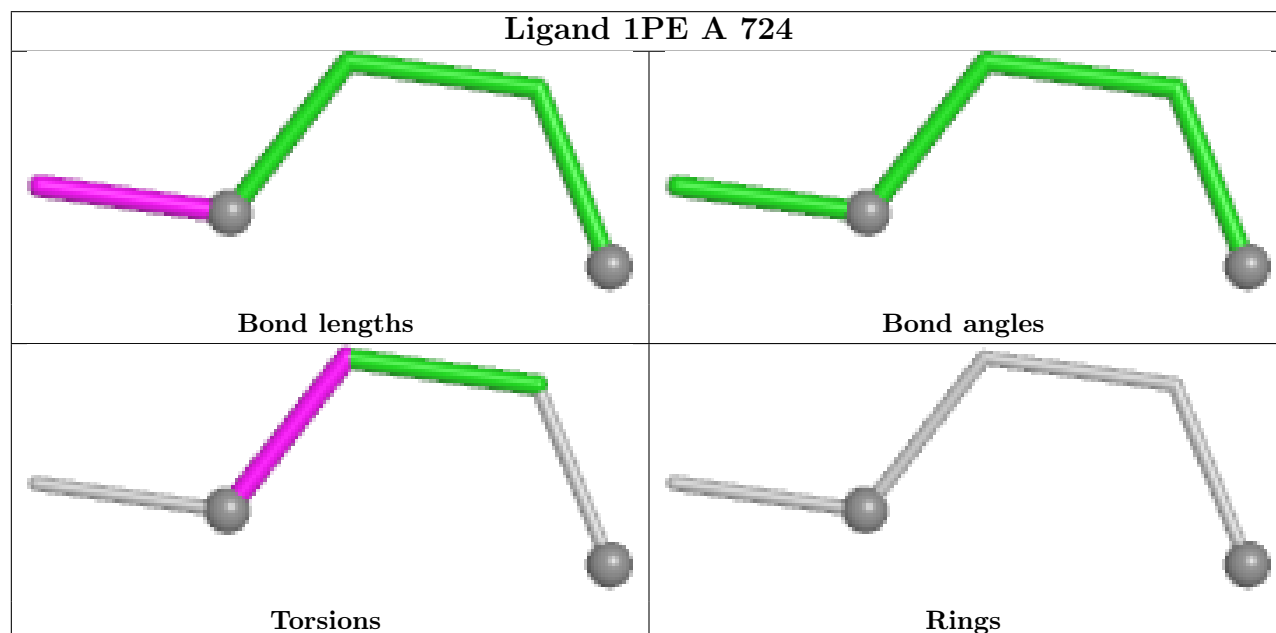
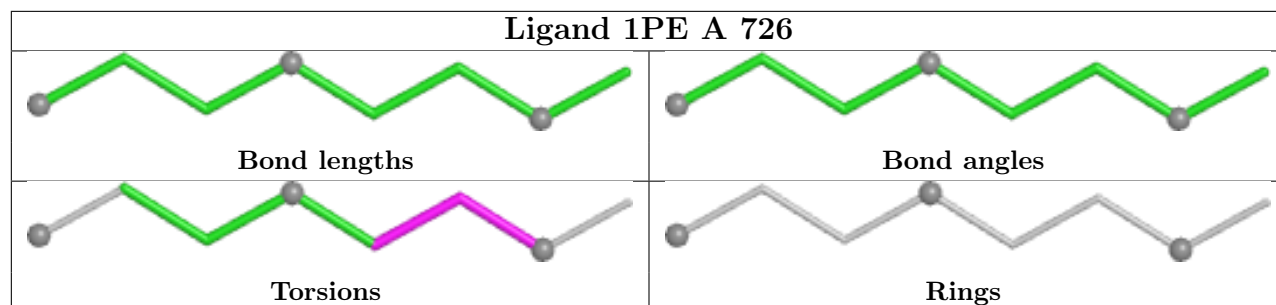
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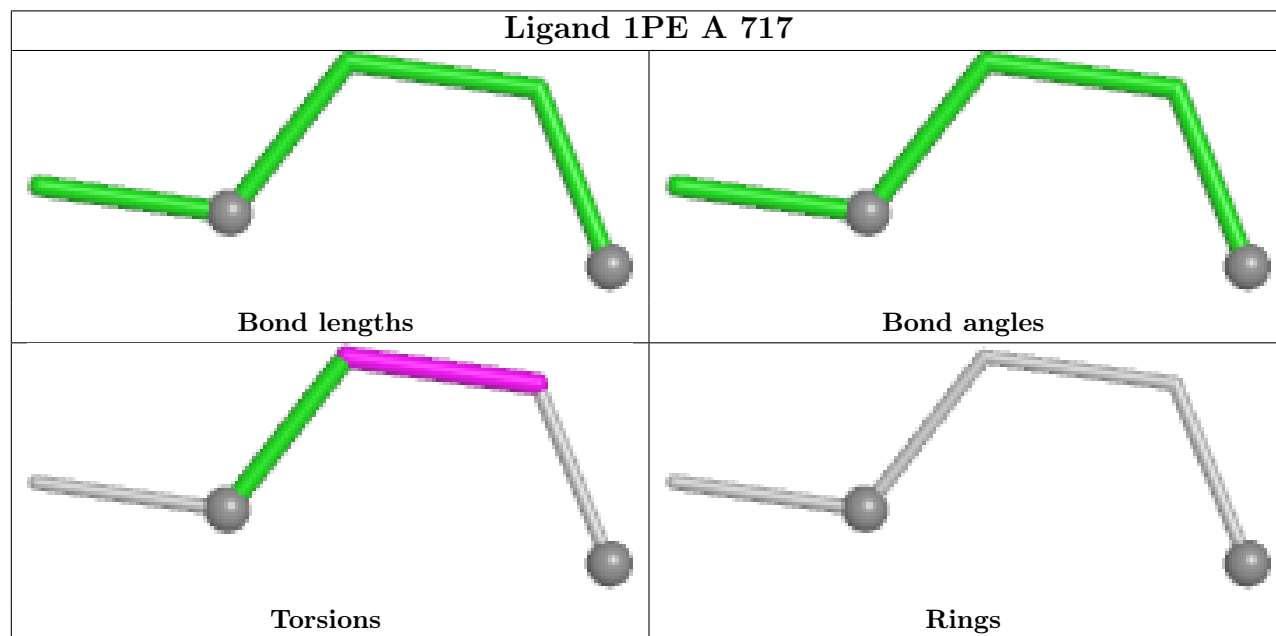
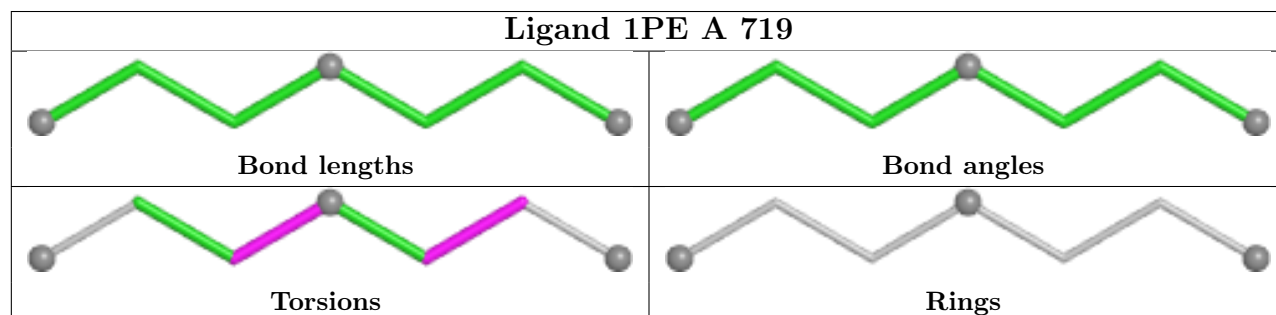
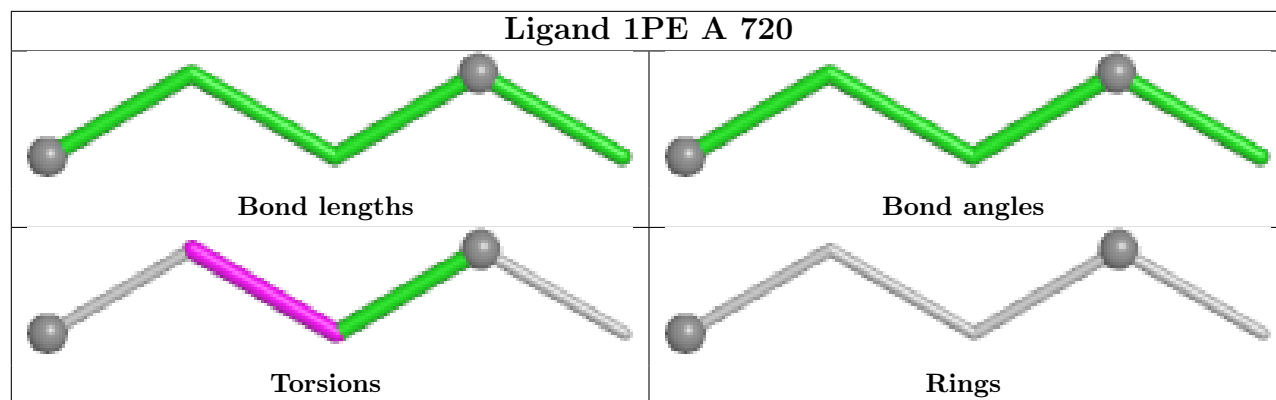
12 monomers are involved in 19 short contacts:

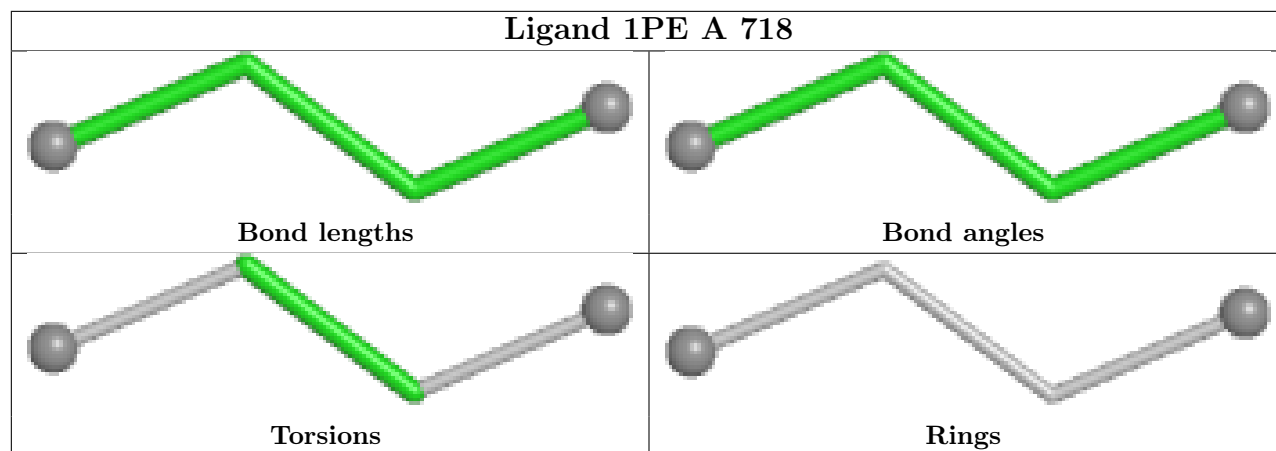
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	709	GOL	2	0
4	A	707	GOL	1	0
5	A	712	SO4	1	0
6	A	725	1PE	1	0
6	A	716	1PE	1	0
6	A	726	1PE	2	0
6	A	724	1PE	2	0
6	A	723[A]	1PE	1	0
6	A	722	1PE	1	0
3	A	704	NAG	2	0
6	A	719	1PE	3	0
4	A	710	GOL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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	604/609 (99%)	-0.31	6 (0%) 79 84	15, 23, 37, 78	15 (2%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-1	ALA	4.6
1	A	586	HIS	3.9
1	A	186	LYS	3.1
1	A	187	ASP	2.9
1	A	602	THR	2.6
1	A	585	ALA	2.3

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.

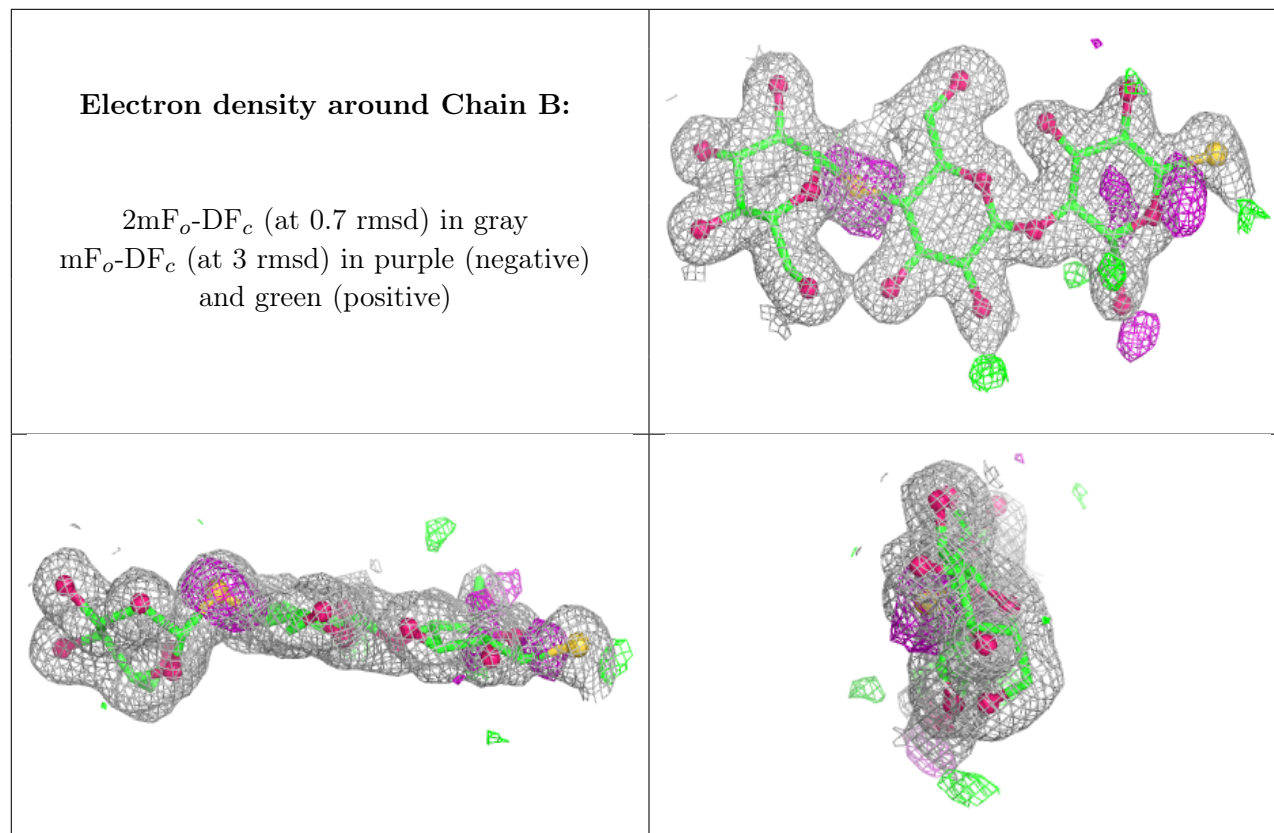
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	703	14/15	0.78	0.14	51,67,82,83	0

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	GS1	B	1	12/12	0.82	0.14	36,51,62,64	0
2	SGC	B	2	11/12	0.96	0.08	24,29,34,34	0
2	BGC	B	3[B]	11/12	0.97	0.05	20,22,27,27	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($\text{\AA}^2$)	Q<0.9
5	SO4	A	712	5/5	0.65	0.11	85,95,112,123	0
5	SO4	A	715	5/5	0.66	0.12	81,99,103,105	0
7	ACT	A	728	4/4	0.68	0.25	48,50,55,64	0
6	1PE	A	718	4/16	0.69	0.17	58,61,62,69	0
3	NAG	A	704	14/15	0.71	0.15	57,75,82,82	0
6	1PE	A	725	4/16	0.74	0.20	46,50,53,56	0

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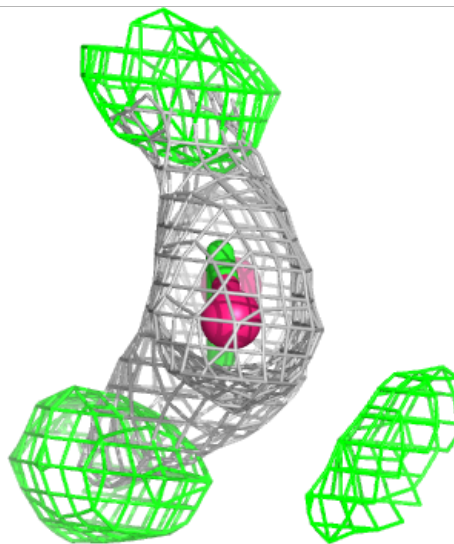
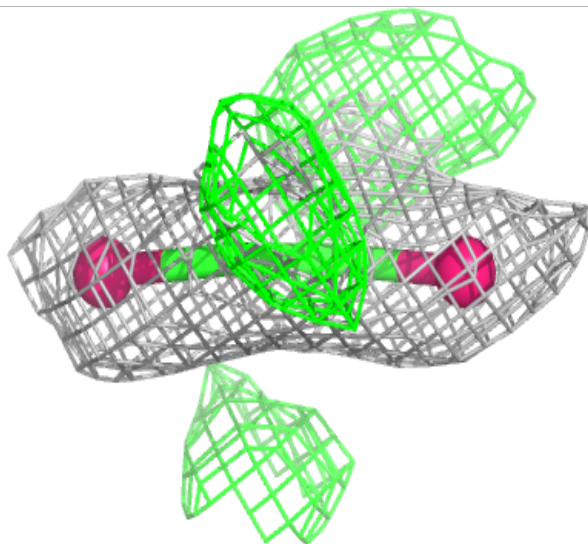
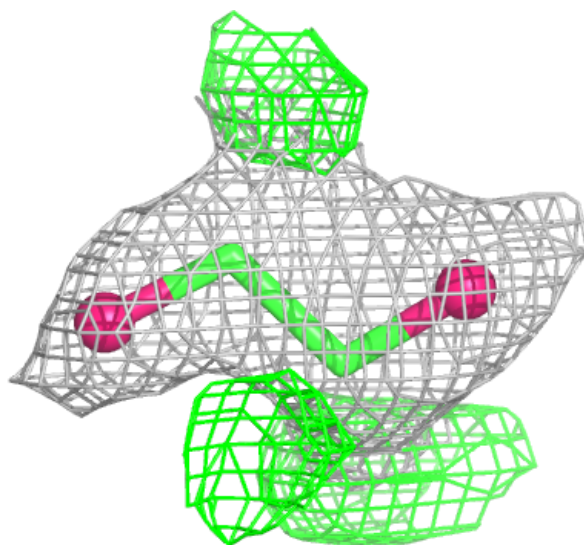
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	706	6/6	0.76	0.20	43,62,62,68	0
7	ACT	A	729	4/4	0.77	0.19	52,67,67,69	0
3	NAG	A	703	14/15	0.78	0.14	51,67,82,83	0
6	1PE	A	716	4/16	0.79	0.21	53,53,54,62	0
6	1PE	A	726	8/16	0.79	0.22	47,61,79,85	0
4	GOL	A	709	6/6	0.80	0.19	36,49,55,60	0
6	1PE	A	717	5/16	0.82	0.17	55,58,61,62	0
4	GOL	A	708	6/6	0.85	0.18	50,57,70,72	0
6	1PE	A	720	5/16	0.85	0.16	49,55,61,65	0
7	ACT	A	727	4/4	0.87	0.14	41,50,58,68	0
6	1PE	A	723[A]	10/16	0.87	0.19	36,56,67,71	3
6	1PE	A	723[B]	10/16	0.87	0.19	36,53,67,71	3
7	ACT	A	730	4/4	0.87	0.15	56,58,62,63	0
3	NAG	A	705	14/15	0.88	0.12	39,46,67,68	0
6	1PE	A	724	5/16	0.88	0.14	26,27,36,36	5
6	1PE	A	721	4/16	0.89	0.17	37,50,59,61	0
5	SO4	A	713	5/5	0.89	0.12	38,45,48,48	5
4	GOL	A	710	6/6	0.90	0.12	31,46,50,54	0
6	1PE	A	719	7/16	0.91	0.12	32,46,56,57	0
6	1PE	A	722	4/16	0.92	0.13	31,33,48,50	0
5	SO4	A	714	5/5	0.95	0.07	23,27,32,33	5
4	GOL	A	707	6/6	0.95	0.17	32,32,35,36	6
4	GOL	A	711	6/6	0.95	0.10	24,42,43,45	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.

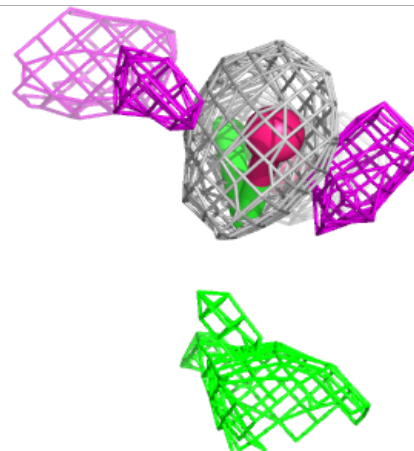
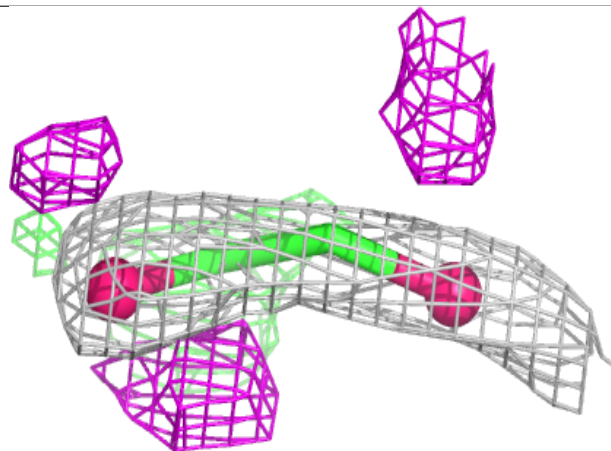
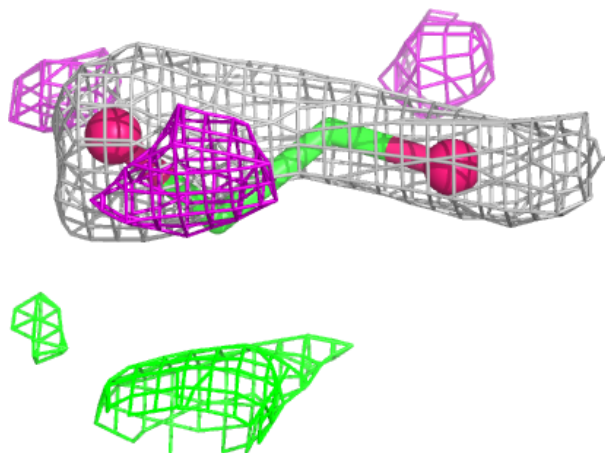
Electron density around 1PE A 718:

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



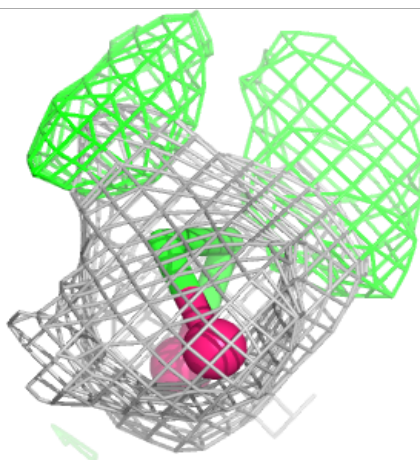
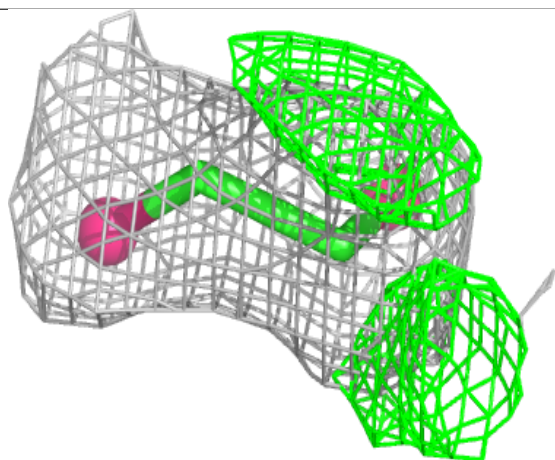
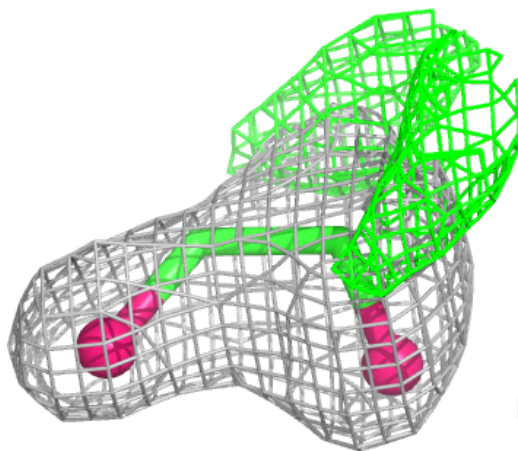
Electron density around 1PE A 725:

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



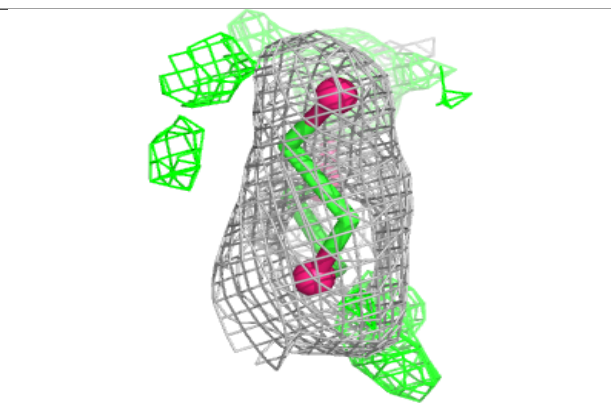
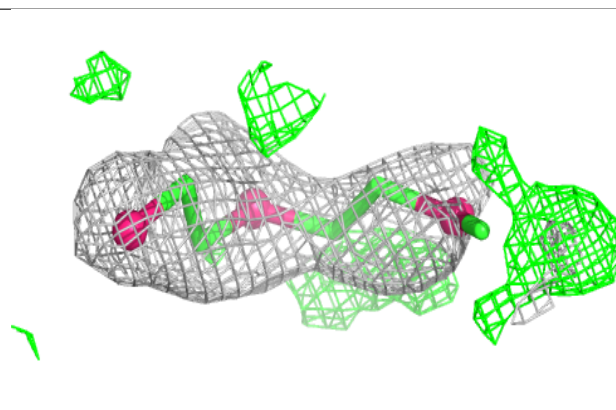
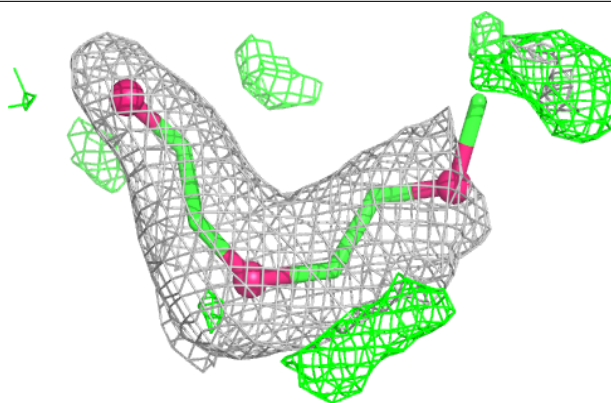
Electron density around 1PE A 716:

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

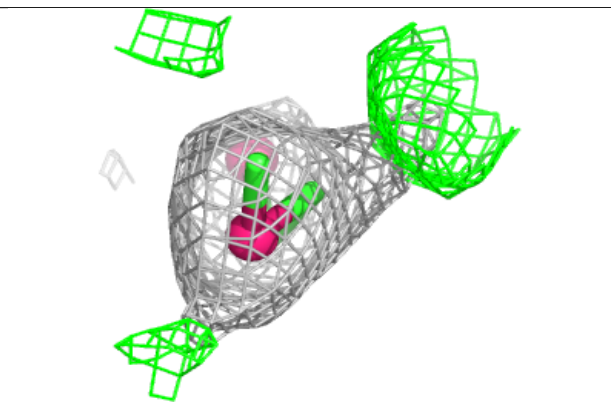
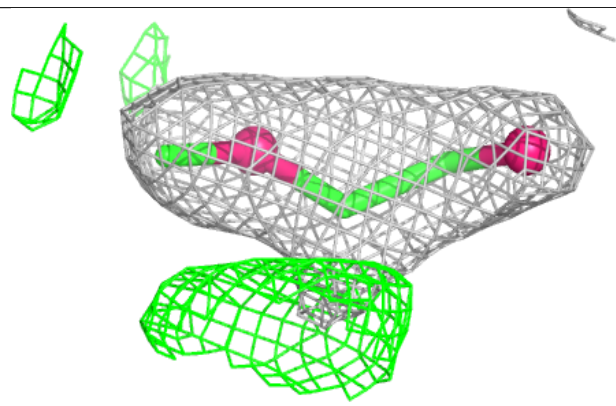
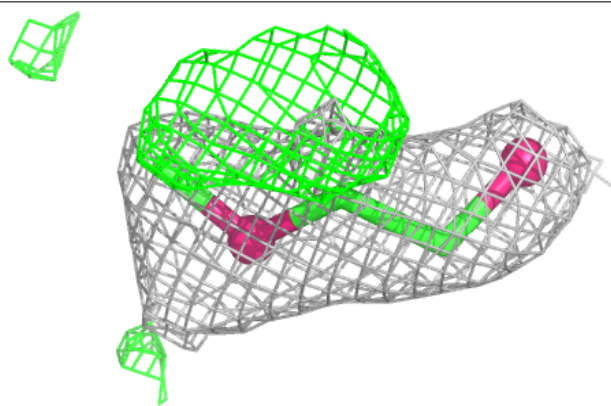


Electron density around 1PE A 726:

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

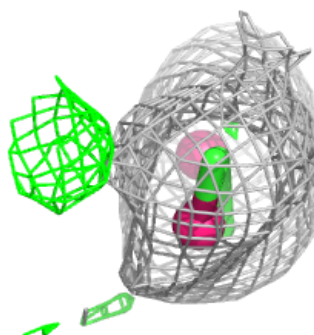
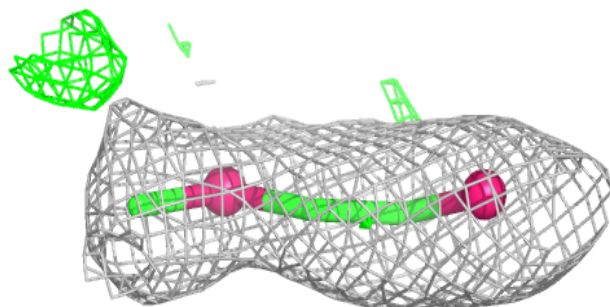
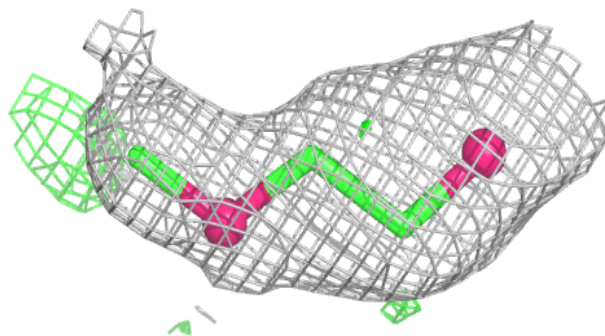
**Electron density around 1PE A 717:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

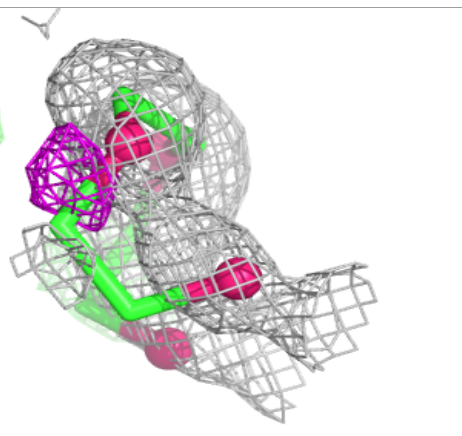
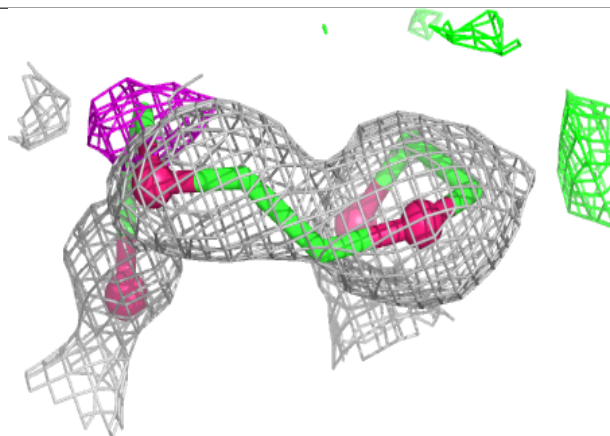
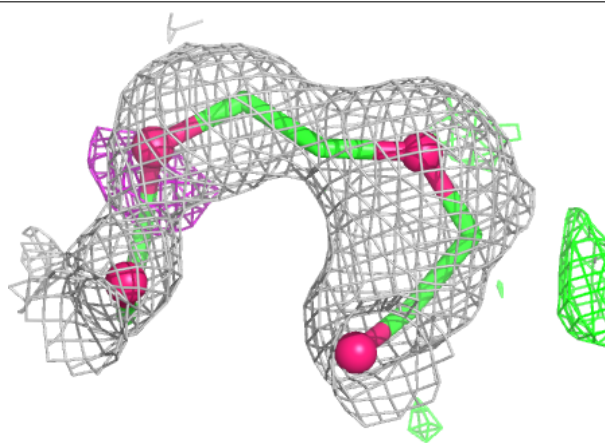


Electron density around 1PE A 720:

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and green (positive)

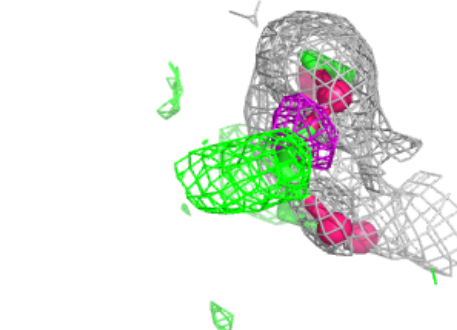
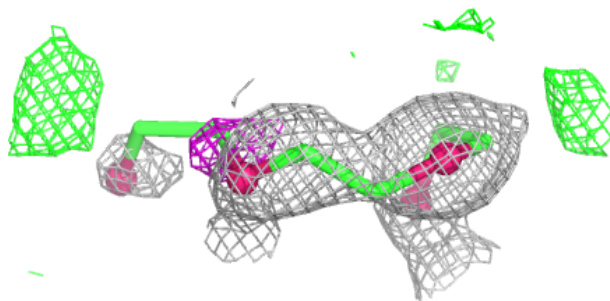
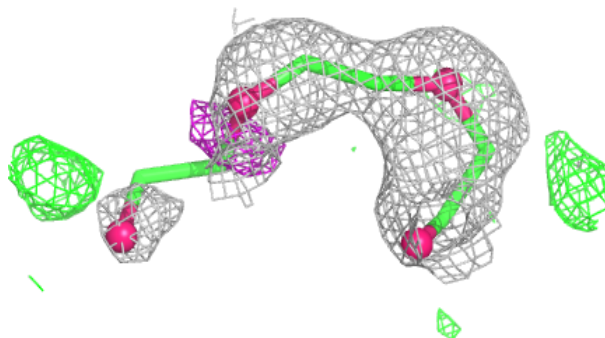
**Electron density around 1PE A 723 (A):**

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and green (positive)

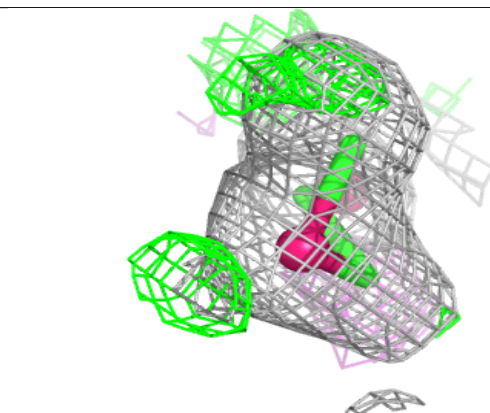
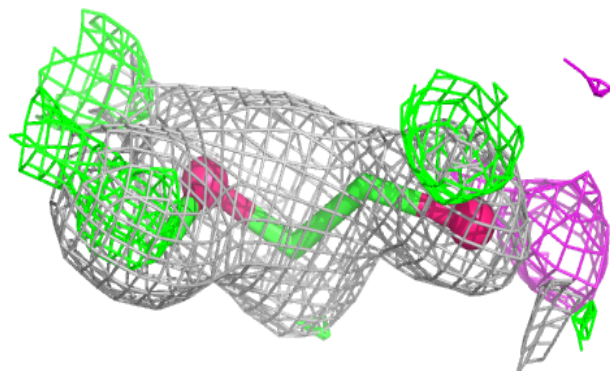
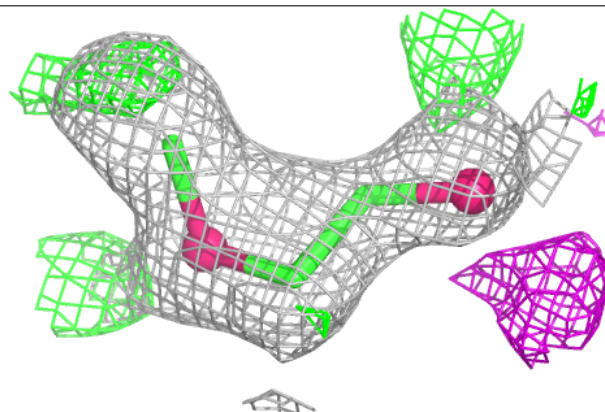


Electron density around 1PE A 723 (B):

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and green (positive)

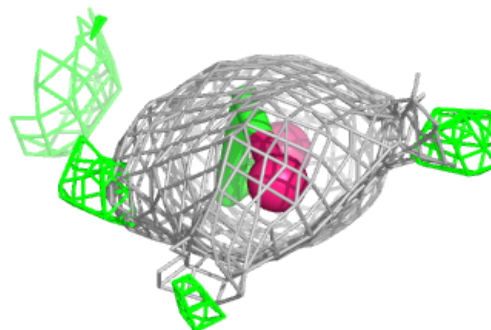
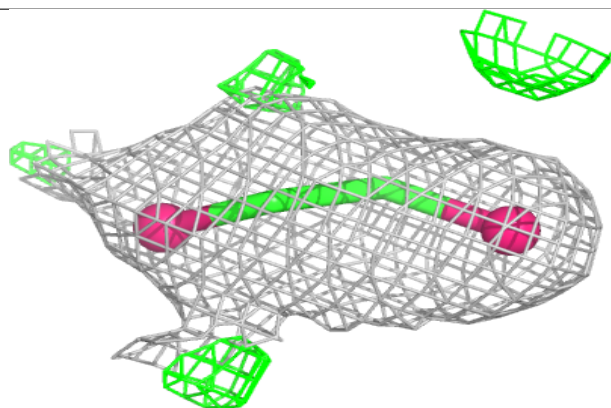
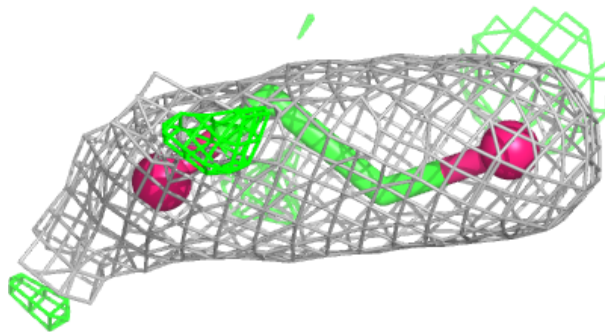
**Electron density around 1PE A 724:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



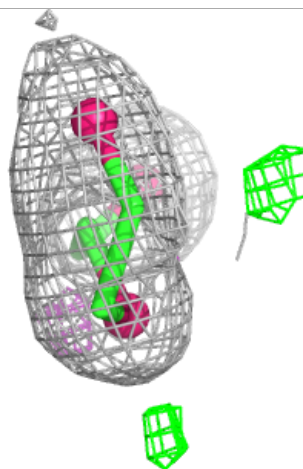
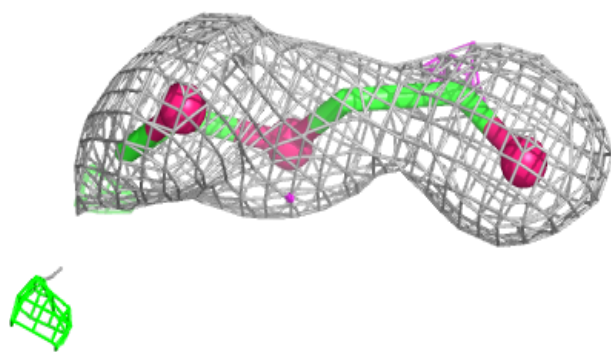
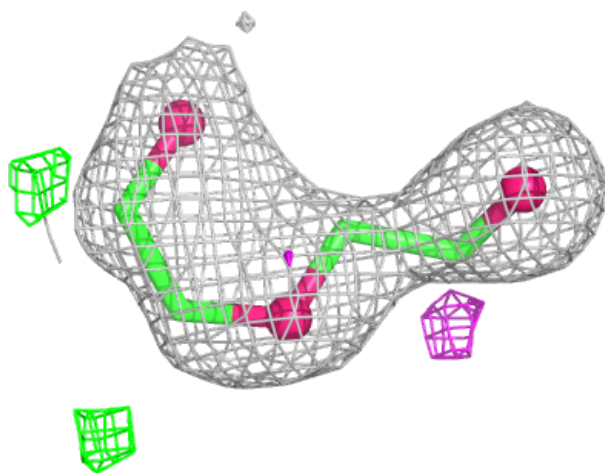
Electron density around 1PE A 721:

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and green (positive)



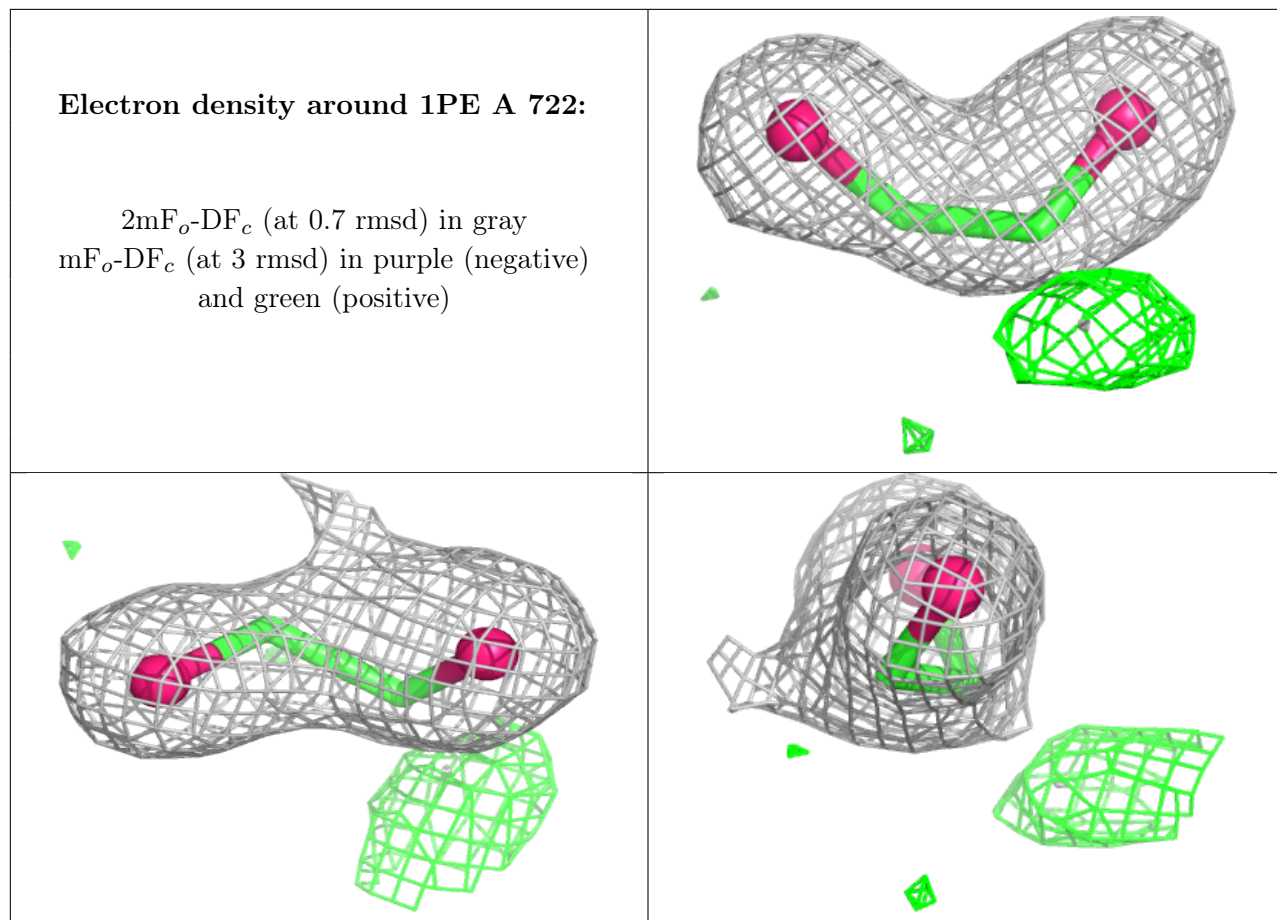
Electron density around 1PE A 719:

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and green (positive)



Electron density around 1PE A 722:

$2mF_o - DF_c$ (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.