



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2022 – 12:16 PM JST

PDB ID : 6JGB
Title : Crystal structure of barley exohydrolaseI W286F mutant in complex with methyl 6-thio-beta-gentiobioside
Authors : Luang, S.; Streltsov, V.A.; Hrmova, M.
Deposited on : 2019-02-13
Resolution : 1.47 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

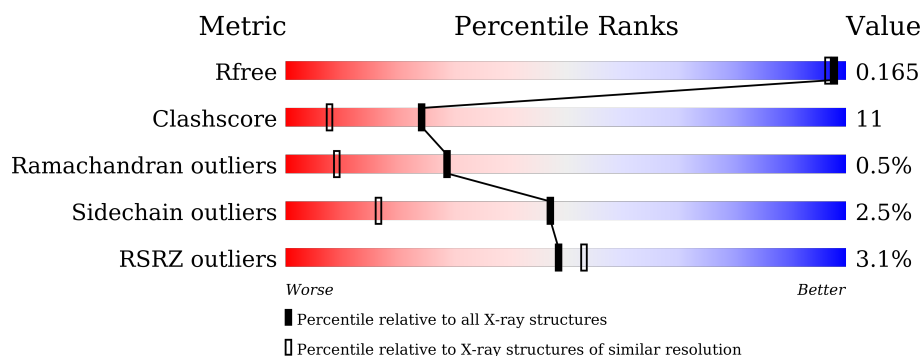
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.47 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}	130704	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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	<div> <div>3%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
2	B	2	<div>100%</div>

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
6	1PE	A	720	-	X	-	-
6	1PE	A	722	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5481 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 BETA-D-GLUCAN GLUCOHYDROLASE ISOENZYME EXO1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	606	Total	C	N	O	S	0	19	0
			4621	2921	801	871	28			

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	286	PHE	TRP	engineered mutation	UNP A0A287SCR5
A	320	LYS	ASN	conflict	UNP A0A287SCR5

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-6)-methyl 6-thio-beta-D-glucopyranoside.

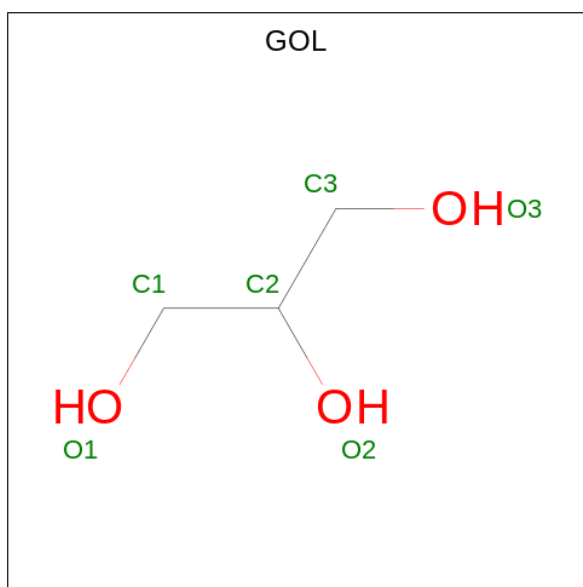
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	O	S	0	0	0
			24	13	10	1			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: 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 (three-letter code: GOL) (formula: $C_3H_8O_3$).



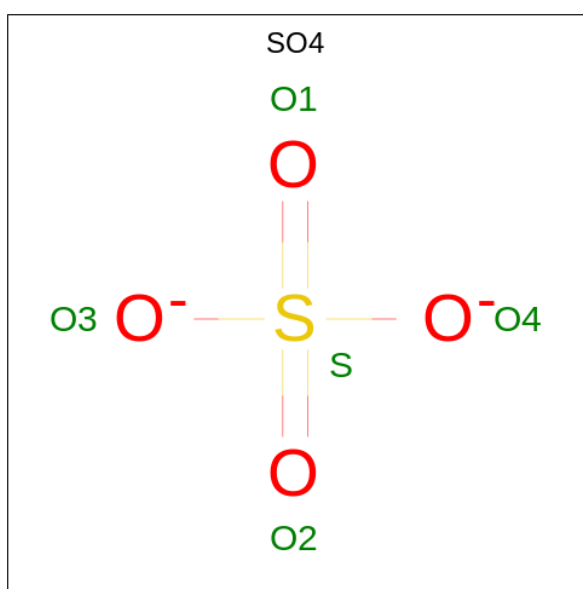
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

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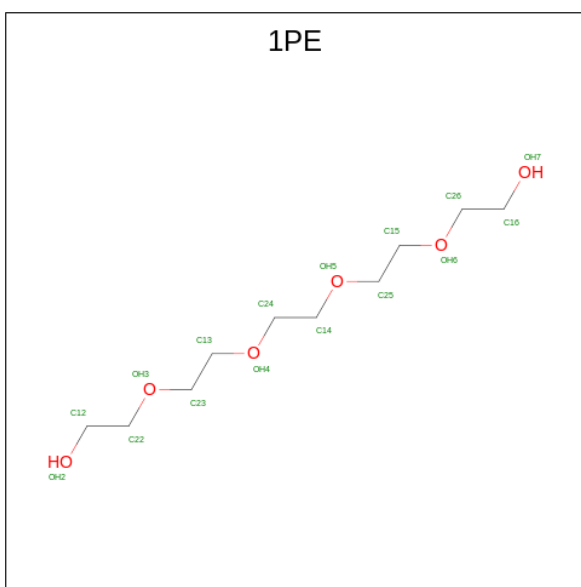
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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



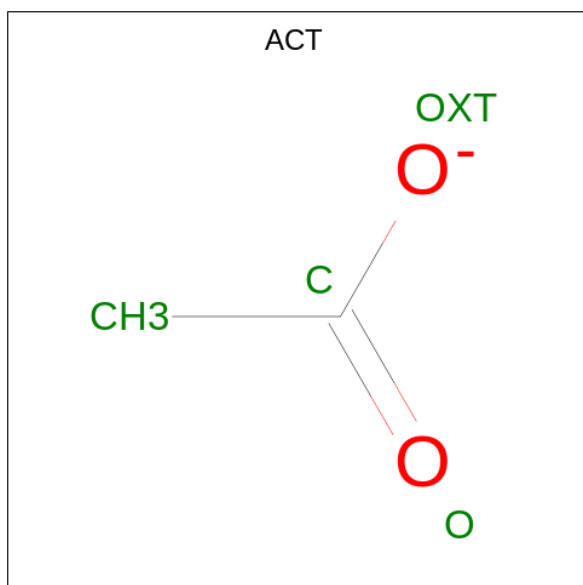
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 5 3 2	0	0
6	A	1	Total C O 5 3 2	0	0
6	A	1	Total C O 10 6 4	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 5 3 2	0	0
6	A	1	Total C O 8 5 3	0	0
6	A	1	Total C O 8 5 3	0	0
6	A	1	Total C O 5 3 2	0	0
6	A	1	Total C O 6 4 2	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 5 3 2	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 5 3 2	0	0

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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		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



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		
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		

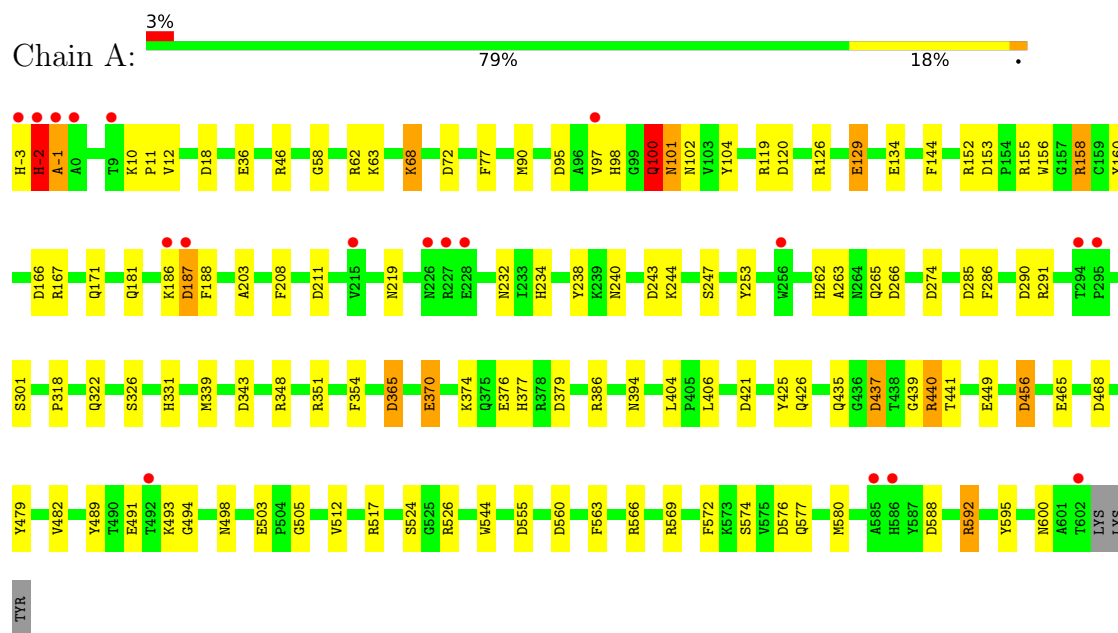
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	631	Total 631	O 631	0	0

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: BETA-D-GLUCAN GLUCOHYDROLASE ISOENZYME EXO1



• Molecule 2: beta-D-glucopyranose-(1-6)-methyl 6-thio-beta-D-glucopyranoside



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.83Å 100.83Å 181.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.40 – 1.47 40.36 – 1.47	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.40-1.47) 99.5 (40.36-1.47)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.47Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.146 , 0.163 0.149 , 0.165	Depositor DCC
R_{free} test set	7903 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	5481	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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: U1Y, 1PE, ACT, SO4, BGC, NAG, GOL

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	1.33	20/4784 (0.4%)	1.46	78/6491 (1.2%)

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	1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	503	GLU	CD-OE2	13.92	1.41	1.25
1	A	517[A]	ARG	CZ-NH1	11.15	1.47	1.33
1	A	129[A]	GLU	CD-OE1	9.12	1.35	1.25
1	A	595	TYR	CE2-CZ	-8.11	1.28	1.38
1	A	370[A]	GLU	CG-CD	7.46	1.63	1.51
1	A	370[B]	GLU	CG-CD	7.46	1.63	1.51
1	A	440[A]	ARG	CZ-NH1	7.06	1.42	1.33
1	A	426	GLN	CB-CG	-6.96	1.33	1.52
1	A	100	GLN	CD-OE1	6.10	1.37	1.24
1	A	326	SER	CB-OG	5.92	1.50	1.42
1	A	101	ASN	CG-OD1	5.70	1.36	1.24
1	A	440[A]	ARG	CZ-NH2	5.52	1.40	1.33
1	A	376	GLU	CD-OE2	5.51	1.31	1.25
1	A	62	ARG	CA-CB	-5.40	1.42	1.53
1	A	104	TYR	CE1-CZ	-5.37	1.31	1.38
1	A	160	TYR	CE1-CZ	-5.31	1.31	1.38
1	A	479	TYR	CB-CG	-5.29	1.43	1.51
1	A	449	GLU	CD-OE2	5.22	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	569	ARG	CB-CG	-5.17	1.38	1.52
1	A	253	TYR	CG-CD1	-5.13	1.32	1.39

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	ARG	NE-CZ-NH2	18.15	129.38	120.30
1	A	152	ARG	NE-CZ-NH2	14.45	127.52	120.30
1	A	440[A]	ARG	NE-CZ-NH2	-12.56	114.02	120.30
1	A	152	ARG	NE-CZ-NH1	-11.93	114.34	120.30
1	A	351	ARG	NE-CZ-NH1	11.52	126.06	120.30
1	A	243	ASP	CB-CG-OD2	-11.08	108.33	118.30
1	A	517[A]	ARG	NE-CZ-NH2	-10.40	115.10	120.30
1	A	46	ARG	NE-CZ-NH1	-10.39	115.11	120.30
1	A	243	ASP	CB-CG-OD1	10.32	127.58	118.30
1	A	440[A]	ARG	NE-CZ-NH1	9.96	125.28	120.30
1	A	120	ASP	CB-CG-OD2	-9.83	109.45	118.30
1	A	166	ASP	CB-CG-OD2	-9.44	109.81	118.30
1	A	211	ASP	CB-CG-OD1	9.20	126.58	118.30
1	A	153	ASP	CB-CG-OD1	9.13	126.52	118.30
1	A	129[A]	GLU	OE1-CD-OE2	8.87	133.94	123.30
1	A	526	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	A	208	PHE	CB-CG-CD2	-8.38	114.94	120.80
1	A	456	ASP	CB-CG-OD1	-8.35	110.78	118.30
1	A	437	ASP	CB-CG-OD2	-8.23	110.89	118.30
1	A	379	ASP	CB-CG-OD2	-8.18	110.94	118.30
1	A	503	GLU	OE1-CD-OE2	8.14	133.07	123.30
1	A	46	ARG	CD-NE-CZ	8.12	134.97	123.60
1	A	592[A]	ARG	CG-CD-NE	-7.90	95.22	111.80
1	A	517[A]	ARG	NE-CZ-NH1	-7.76	116.42	120.30
1	A	449	GLU	OE1-CD-OE2	-7.74	114.01	123.30
1	A	386	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	A	449	GLU	CG-CD-OE1	7.29	132.88	118.30
1	A	517[A]	ARG	NH1-CZ-NH2	7.24	127.36	119.40
1	A	77	PHE	CB-CG-CD2	-7.07	115.85	120.80
1	A	322	GLN	O-C-N	7.00	133.90	122.70
1	A	158	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	A	440[A]	ARG	CG-CD-NE	-6.95	97.21	111.80
1	A	555	ASP	CB-CG-OD2	-6.95	112.05	118.30
1	A	440[A]	ARG	CD-NE-CZ	6.93	133.30	123.60
1	A	563	PHE	CB-CG-CD1	6.76	125.53	120.80
1	A	592[A]	ARG	NE-CZ-NH2	6.69	123.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	TYR	CB-CG-CD1	-6.65	117.01	121.00
1	A	468	ASP	CB-CG-OD1	6.63	124.27	118.30
1	A	376	GLU	OE1-CD-OE2	-6.45	115.56	123.30
1	A	365	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	465	GLU	OE1-CD-OE2	6.33	130.90	123.30
1	A	126	ARG	NE-CZ-NH1	-6.31	117.14	120.30
1	A	274	ASP	CB-CG-OD1	6.25	123.93	118.30
1	A	370[A]	GLU	OE1-CD-OE2	-6.21	115.85	123.30
1	A	370[B]	GLU	OE1-CD-OE2	-6.21	115.85	123.30
1	A	588	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	119	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	A	376	GLU	CG-CD-OE1	6.10	130.50	118.30
1	A	566[A]	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	A	566[B]	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	A	188	PHE	CB-CG-CD1	-5.89	116.67	120.80
1	A	592[A]	ARG	NE-CZ-NH1	-5.87	117.37	120.30
1	A	343	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	A	456	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	208	PHE	CB-CG-CD1	5.77	124.84	120.80
1	A	120	ASP	OD1-CG-OD2	5.74	134.21	123.30
1	A	104	TYR	CZ-CE2-CD2	-5.72	114.66	119.80
1	A	10	LYS	CD-CE-NZ	-5.65	98.71	111.70
1	A	437	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	238	TYR	CB-CG-CD2	5.55	124.33	121.00
1	A	569	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	95	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	A	425	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	A	119	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	566[A]	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	566[B]	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	479	TYR	CB-CG-CD2	5.38	124.23	121.00
1	A	72	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	A	18	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	A	348	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	365	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	144	PHE	CB-CG-CD2	-5.18	117.17	120.80
1	A	572	PHE	CB-CG-CD2	-5.17	117.18	120.80
1	A	158	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	155	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	A	576	ASP	CB-CG-OD2	-5.12	113.70	118.30
1	A	595	TYR	CB-CG-CD1	5.09	124.05	121.00
1	A	354	PHE	CB-CG-CD2	5.06	124.34	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	ASP	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	4621	0	4557	82	0
2	B	24	0	8	0	0
3	A	42	0	39	6	0
4	A	30	0	40	3	0
5	A	5	0	0	0	0
6	A	96	0	110	44	0
7	A	32	0	24	0	0
8	A	631	0	0	33	0
All	All	5481	0	4778	106	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 (106) 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:703:NAG:C1	0.92	1.53
1:A:600:ASN:HD21	3:A:702:NAG:C1	1.27	1.45
1:A:498:ASN:ND2	3:A:703:NAG:C1	1.76	1.39
1:A:370[B]:GLU:CD	8:A:801:HOH:O	1.73	1.25
1:A:600:ASN:ND2	3:A:702:NAG:C1	2.00	1.21
1:A:370[B]:GLU:OE2	8:A:801:HOH:O	1.53	1.18
6:A:725:1PE:C26	8:A:1043:HOH:O	1.92	1.16
6:A:725:1PE:H261	8:A:1043:HOH:O	1.47	1.08
4:A:709:GOL:H11	8:A:1282:HOH:O	1.55	1.05
1:A:577:GLN:HB3	1:A:580[B]:MET:CE	1.95	0.96
6:A:717:1PE:C24	8:A:1279:HOH:O	2.16	0.94
1:A:435[B]:GLN:OE1	8:A:802:HOH:O	1.91	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ASN:HD21	1:A:404:LEU:H	1.21	0.88
1:A:156:TRP:HE1	1:A:219:ASN:HD22	1.26	0.83
6:A:725:1PE:H262	8:A:1043:HOH:O	1.67	0.82
1:A:377:HIS:HE1	6:A:715:1PE:C23	1.94	0.81
4:A:709:GOL:C1	8:A:1282:HOH:O	2.22	0.81
1:A:262:HIS:HE1	1:A:285:ASP:H	1.34	0.76
1:A:291:ARG:HH22	6:A:711:1PE:C23	1.99	0.75
1:A:435[B]:GLN:NE2	1:A:493:LYS:HG3	2.05	0.72
6:A:720:1PE:C22	8:A:1010:HOH:O	2.37	0.71
1:A:12:VAL:HB	6:A:717:1PE:H121	1.71	0.71
1:A:100:GLN:HE21	1:A:100:GLN:HA	1.55	0.71
1:A:181:GLN:HE21	1:A:203:ALA:H	1.37	0.70
1:A:266:ASP:HA	6:A:726:1PE:H161	1.74	0.69
6:A:720:1PE:H232	8:A:1010:HOH:O	1.91	0.69
1:A:577:GLN:HB3	1:A:580[B]:MET:HE2	1.75	0.69
6:A:716:1PE:H151	8:A:984:HOH:O	1.94	0.66
6:A:720:1PE:H222	8:A:1010:HOH:O	1.94	0.66
1:A:377:HIS:CE1	6:A:715:1PE:C23	2.78	0.66
1:A:97:VAL:H	1:A:101:ASN:HD21	1.42	0.66
1:A:498:ASN:OD1	8:A:804:HOH:O	2.12	0.66
1:A:265:GLN:HE21	6:A:726:1PE:C26	2.09	0.66
6:A:715:1PE:OH3	8:A:805:HOH:O	2.13	0.66
1:A:232[B]:ASN:OD1	8:A:806:HOH:O	2.14	0.65
1:A:240:ASN:HD21	6:A:716:1PE:C25	2.08	0.65
1:A:134:GLU:OE2	1:A:377:HIS:HD2	1.80	0.65
1:A:600:ASN:ND2	3:A:702:NAG:C2	2.62	0.63
1:A:265:GLN:HE21	6:A:726:1PE:H262	1.64	0.63
1:A:240:ASN:HD21	6:A:716:1PE:H252	1.64	0.62
1:A:262:HIS:CE1	1:A:285:ASP:H	2.18	0.62
1:A:167:ARG:HH21	1:A:171:GLN:HE22	1.50	0.60
1:A:265:GLN:HB3	6:A:719:1PE:H231	1.83	0.59
6:A:716:1PE:C14	8:A:1343:HOH:O	2.50	0.58
1:A:374[A]:LYS:NZ	6:A:715:1PE:C23	2.68	0.57
1:A:58:GLY:H	1:A:102:ASN:ND2	2.03	0.56
1:A:365:ASP:HB2	6:A:720:1PE:H121	1.87	0.56
1:A:435[B]:GLN:HE22	1:A:493:LYS:HG3	1.69	0.56
1:A:100:GLN:HE21	1:A:100:GLN:CA	2.18	0.56
1:A:234:HIS:HE1	8:A:1330:HOH:O	1.88	0.56
1:A:97:VAL:H	1:A:101:ASN:ND2	2.03	0.56
1:A:600:ASN:HD21	3:A:702:NAG:C2	2.09	0.55
6:A:722:1PE:H222	8:A:1174:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:GLN:CB	6:A:719:1PE:H231	2.38	0.54
6:A:718:1PE:C23	8:A:831:HOH:O	2.55	0.54
1:A:265:GLN:NE2	6:A:726:1PE:H262	2.23	0.53
1:A:167:ARG:HH21	1:A:171:GLN:NE2	2.06	0.53
1:A:156:TRP:HE1	1:A:219:ASN:ND2	2.00	0.53
1:A:331:HIS:HD2	8:A:1322:HOH:O	1.92	0.52
6:A:720:1PE:C23	8:A:1010:HOH:O	2.54	0.52
1:A:234:HIS:HD2	8:A:1192:HOH:O	1.93	0.52
1:A:181:GLN:HE22	1:A:247:SER:H	1.59	0.50
1:A:482[B]:VAL:CG2	1:A:512:VAL:HG11	2.42	0.50
1:A:265:GLN:H	6:A:719:1PE:H231	1.78	0.48
1:A:68[A]:LYS:CE	8:A:1100:HOH:O	2.61	0.48
1:A:11:PRO:HB3	6:A:717:1PE:H222	1.95	0.48
1:A:240:ASN:HD21	6:A:716:1PE:H251	1.79	0.48
1:A:524:SER:O	1:A:544:TRP:HA	2.14	0.48
1:A:286:PHE:CE2	1:A:318:PRO:HG3	2.49	0.47
6:A:721:1PE:C23	8:A:1082:HOH:O	2.62	0.47
1:A:68[A]:LYS:HE3	8:A:1365:HOH:O	2.15	0.47
1:A:577:GLN:HB3	1:A:580[B]:MET:HE3	1.91	0.46
1:A:577:GLN:CB	1:A:580[B]:MET:CE	2.81	0.46
1:A:167:ARG:NH2	1:A:171:GLN:HE22	2.14	0.45
6:A:721:1PE:H222	8:A:1115:HOH:O	2.15	0.45
1:A:301:SER:O	1:A:331:HIS:HE1	2.00	0.44
1:A:439:GLY:HA2	6:A:722:1PE:H122	1.99	0.44
1:A:-3:HIS:HB3	8:A:939:HOH:O	2.18	0.44
1:A:437:ASP:HB3	1:A:441:THR:HG21	2.00	0.44
1:A:134:GLU:OE2	1:A:377:HIS:CD2	2.67	0.43
1:A:263:ALA:O	6:A:719:1PE:C13	2.66	0.43
1:A:489:TYR:CD1	1:A:494:GLY:HA3	2.54	0.42
1:A:421:ASP:O	6:A:722:1PE:H121	2.20	0.42
1:A:491:GLU:OE1	6:A:711:1PE:H122	2.19	0.42
6:A:717:1PE:H222	6:A:717:1PE:H132	1.78	0.42
1:A:158:ARG:HD2	1:A:491:GLU:HG2	2.02	0.42
1:A:339:MET:HE3	1:A:339:MET:HB2	1.69	0.42
1:A:374[A]:LYS:HZ1	6:A:715:1PE:C23	2.33	0.42
1:A:129[A]:GLU:HB3	8:A:1029:HOH:O	2.20	0.41
4:A:709:GOL:H31	8:A:1258:HOH:O	2.18	0.41
1:A:-2:HIS:O	1:A:-1:ALA:HB3	2.19	0.41
1:A:592[A]:ARG:NE	8:A:815:HOH:O	2.43	0.41
1:A:244:LYS:HZ1	6:A:716:1PE:C16	2.34	0.41
1:A:560:ASP:CG	8:A:851:HOH:O	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLN:HE22	1:A:247:SER:N	2.19	0.41
1:A:404:LEU:HD23	1:A:406:LEU:HG	2.03	0.40
1:A:456:ASP:HB2	8:A:1137:HOH:O	2.20	0.40
1:A:577:GLN:HB3	1:A:580[B]:MET:HE1	1.93	0.40
1:A:339:MET:CE	1:A:339:MET:HA	2.50	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	615/609 (101%)	594 (97%)	18 (3%)	3 (0%)	29 9

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	505	GLY
1	A	-1	ALA
1	A	-2	HIS

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	498/490 (102%)	484 (97%)	14 (3%)	43 13

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	HIS
1	A	36	GLU
1	A	63	LYS
1	A	68[A]	LYS
1	A	68[B]	LYS
1	A	90	MET
1	A	98	HIS
1	A	100	GLN
1	A	186	LYS
1	A	187	ASP
1	A	290	ASP
1	A	440[A]	ARG
1	A	574[A]	SER
1	A	574[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-2	HIS
1	A	71	GLN
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	265	GLN
1	A	331	HIS
1	A	377	HIS
1	A	394	ASN
1	A	498	ASN
1	A	600	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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
3	NAG	A	703	-	14,14,15	1.07	2 (14%)	17,19,21	2.61	9 (52%)
3	NAG	A	701	-	14,14,15	0.80	0	17,19,21	1.77	4 (23%)
3	NAG	A	702	-	14,14,15	1.02	1 (7%)	17,19,21	2.03	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
3	NAG	A	703	-	-	2/6/23/26	0/1/1/1
3	NAG	A	701	-	-	0/6/23/26	0/1/1/1
3	NAG	A	702	-	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	NAG	C2-N2	2.50	1.50	1.46
3	A	703	NAG	C4-C3	2.27	1.58	1.52
3	A	703	NAG	C2-N2	2.05	1.49	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	703	NAG	O5-C1-C2	4.79	118.86	111.29
3	A	703	NAG	C3-C4-C5	4.55	118.35	110.24
3	A	703	NAG	C4-C3-C2	4.07	116.98	111.02
3	A	702	NAG	C1-O5-C5	-4.04	106.72	112.19
3	A	701	NAG	C2-N2-C7	3.81	128.33	122.90
3	A	702	NAG	O7-C7-C8	-3.62	115.33	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	703	NAG	C1-O5-C5	-3.33	107.67	112.19
3	A	702	NAG	C8-C7-N2	3.31	121.69	116.10
3	A	703	NAG	C8-C7-N2	3.07	121.29	116.10
3	A	701	NAG	O7-C7-C8	-3.03	116.44	122.06
3	A	701	NAG	C1-C2-N2	2.95	115.53	110.49
3	A	703	NAG	O4-C4-C5	-2.84	102.26	109.30
3	A	703	NAG	O7-C7-C8	-2.71	117.02	122.06
3	A	703	NAG	C1-C2-N2	-2.56	106.11	110.49
3	A	701	NAG	C8-C7-N2	2.50	120.33	116.10
3	A	703	NAG	O5-C5-C6	2.15	110.58	107.20
3	A	702	NAG	C3-C4-C5	2.09	113.97	110.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	703	NAG	C4-C5-C6-O6
3	A	703	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	NAG	2	0
3	A	702	NAG	4	0

5.5 Carbohydrates ⓘ

2 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	UIY	B	1	2	13,13,13	0.88	1 (7%)	18,18,18	1.60	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	B	2	2	11,11,12	3.93	3 (27%)	15,15,17	3.24	8 (53%)

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	U1Y	B	1	2	-	0/4/24/24	0/1/1/1
2	BGC	B	2	2	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	BGC	C2-C3	-11.91	1.35	1.52
2	B	2	BGC	C4-C5	3.18	1.59	1.53
2	B	2	BGC	O5-C1	2.91	1.48	1.43
2	B	1	U1Y	O5-C5	2.01	1.49	1.44

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	BGC	C1-C2-C3	8.97	120.69	109.67
2	B	1	U1Y	O1-C1-C2	-5.15	102.12	108.15
2	B	2	BGC	O3-C3-C2	4.53	118.68	109.99
2	B	2	BGC	C2-C3-C4	3.68	117.27	110.89
2	B	2	BGC	C3-C4-C5	-3.51	103.98	110.24
2	B	2	BGC	O2-C2-C3	2.58	115.31	110.14
2	B	2	BGC	O4-C4-C3	2.49	116.10	110.35
2	B	1	U1Y	O2-C2-C3	-2.30	105.03	110.35
2	B	2	BGC	O5-C1-C2	-2.20	107.37	110.77
2	B	2	BGC	O4-C4-C5	2.18	114.71	109.30

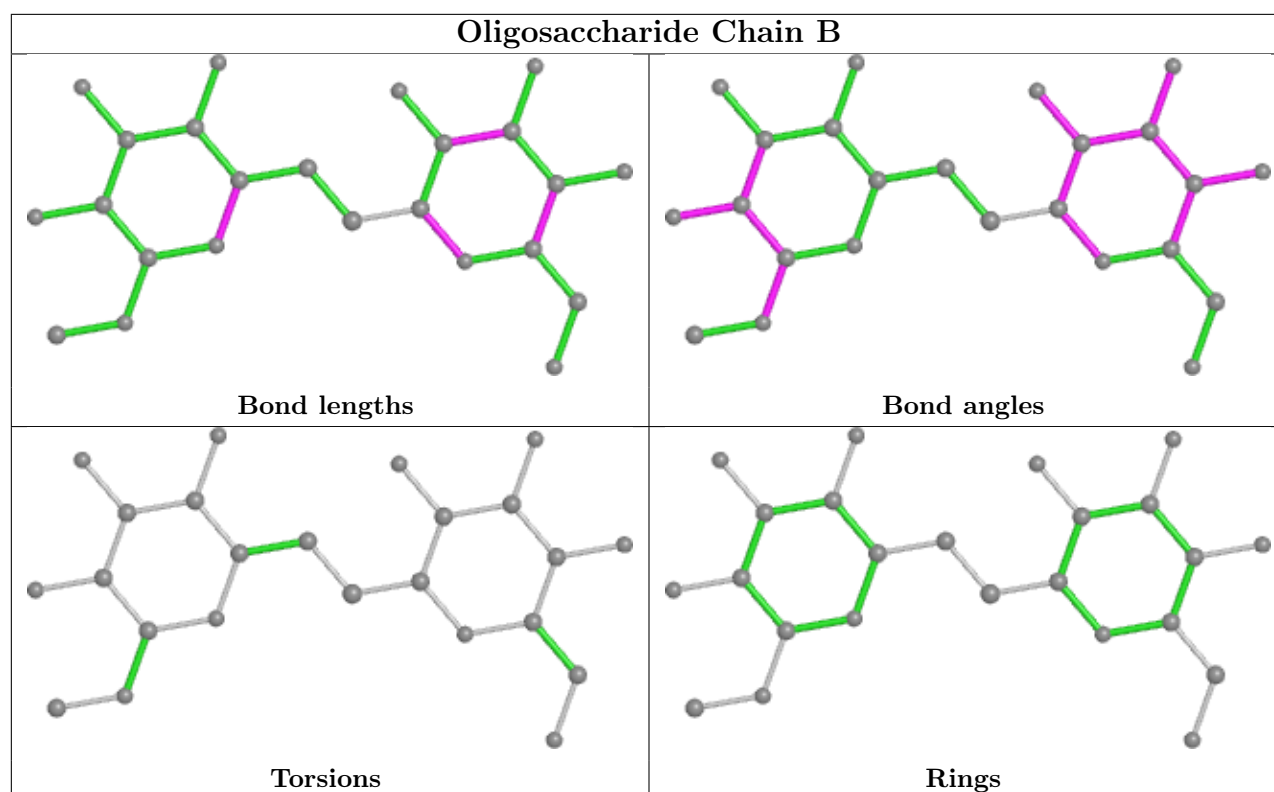
There are no chirality outliers.

There are no torsion outliers.

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](#)

33 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	$\# Z > 2$
7	ACT	A	729	-	3,3,3	0.93	0	3,3,3	0.85	0
7	ACT	A	733	-	3,3,3	1.09	0	3,3,3	0.31	0
4	GOL	A	706	-	5,5,5	0.55	0	5,5,5	1.72	1 (20%)
6	1PE	A	723	-	3,3,15	1.27	0	2,2,14	0.85	0
6	1PE	A	726	-	4,4,15	1.11	0	3,3,14	1.05	0
4	GOL	A	708	-	5,5,5	0.76	0	5,5,5	0.73	0
6	1PE	A	715	-	4,4,15	0.65	0	3,3,14	1.34	1 (33%)
3	NAG	A	701	-	14,14,15	0.80	0	17,19,21	1.77	4 (23%)
6	1PE	A	716	-	7,7,15	1.02	0	6,6,14	1.53	1 (16%)
4	GOL	A	705	-	5,5,5	0.58	0	5,5,5	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	1PE	A	712	-	4,4,15	1.34	0	3,3,14	0.70	0
6	1PE	A	713	-	9,9,15	1.06	0	8,8,14	1.32	0
6	1PE	A	722	-	6,6,15	1.58	1 (16%)	5,5,14	2.47	3 (60%)
7	ACT	A	732	-	3,3,3	0.80	0	3,3,3	0.98	0
7	ACT	A	731	-	3,3,3	0.87	0	3,3,3	0.51	0
3	NAG	A	702	-	14,14,15	1.02	1 (7%)	17,19,21	2.03	4 (23%)
6	1PE	A	714	-	6,6,15	0.61	0	5,5,14	0.59	0
6	1PE	A	724	-	4,4,15	0.79	0	3,3,14	0.70	0
6	1PE	A	718	-	4,4,15	0.50	0	3,3,14	0.66	0
6	1PE	A	717	-	7,7,15	0.96	0	6,6,14	1.23	0
6	1PE	A	721	-	4,4,15	0.86	0	3,3,14	0.31	0
7	ACT	A	728	-	3,3,3	0.83	0	3,3,3	1.30	0
6	1PE	A	711	-	4,4,15	0.60	0	3,3,14	0.54	0
3	NAG	A	703	-	14,14,15	1.07	2 (14%)	17,19,21	2.61	9 (52%)
7	ACT	A	730	-	3,3,3	0.85	0	3,3,3	1.50	1 (33%)
6	1PE	A	725	-	3,3,15	1.02	0	2,2,14	0.81	0
7	ACT	A	727	-	3,3,3	0.76	0	3,3,3	1.29	0
4	GOL	A	709	-	5,5,5	1.27	1 (20%)	5,5,5	2.12	2 (40%)
5	SO4	A	710	-	4,4,4	0.66	0	6,6,6	2.02	2 (33%)
6	1PE	A	720	-	6,6,15	1.47	1 (16%)	5,5,14	1.69	2 (40%)
6	1PE	A	719	-	5,5,15	0.70	0	4,4,14	1.40	1 (25%)
4	GOL	A	707	-	5,5,5	0.75	0	5,5,5	1.37	1 (20%)
7	ACT	A	734	-	3,3,3	1.01	0	3,3,3	0.59	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
4	GOL	A	706	-	-	2/4/4/4	-
6	1PE	A	723	-	-	1/1/1/13	-
6	1PE	A	726	-	-	2/2/2/13	-
4	GOL	A	708	-	-	4/4/4/4	-
6	1PE	A	715	-	-	0/2/2/13	-
3	NAG	A	701	-	-	0/6/23/26	0/1/1/1
6	1PE	A	716	-	-	3/5/5/13	-
4	GOL	A	705	-	-	2/4/4/4	-
6	1PE	A	712	-	-	1/2/2/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	A	713	-	-	5/7/7/13	-
6	1PE	A	722	-	-	3/4/4/13	-
3	NAG	A	702	-	-	0/6/23/26	0/1/1/1
6	1PE	A	714	-	-	2/4/4/13	-
6	1PE	A	724	-	-	2/2/2/13	-
6	1PE	A	718	-	-	0/2/2/13	-
6	1PE	A	717	-	-	4/5/5/13	-
6	1PE	A	721	-	-	2/2/2/13	-
6	1PE	A	711	-	-	2/2/2/13	-
3	NAG	A	703	-	-	2/6/23/26	0/1/1/1
6	1PE	A	725	-	-	1/1/1/13	-
4	GOL	A	709	-	-	2/4/4/4	-
6	1PE	A	720	-	-	3/4/4/13	-
6	1PE	A	719	-	-	2/3/3/13	-
4	GOL	A	707	-	-	4/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	722	1PE	OH3-C23	2.76	1.54	1.42
6	A	720	1PE	OH3-C22	2.53	1.53	1.42
3	A	702	NAG	C2-N2	2.50	1.50	1.46
3	A	703	NAG	C4-C3	2.27	1.58	1.52
4	A	709	GOL	C1-C2	-2.14	1.42	1.51
3	A	703	NAG	C2-N2	2.05	1.49	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	703	NAG	O5-C1-C2	4.79	118.86	111.29
3	A	703	NAG	C3-C4-C5	4.55	118.35	110.24
3	A	703	NAG	C4-C3-C2	4.07	116.98	111.02
3	A	702	NAG	C1-O5-C5	-4.04	106.72	112.19
3	A	701	NAG	C2-N2-C7	3.81	128.33	122.90
6	A	722	1PE	OH3-C22-C12	3.75	126.54	110.07
3	A	702	NAG	O7-C7-C8	-3.62	115.33	122.06
3	A	703	NAG	C1-O5-C5	-3.33	107.67	112.19
3	A	702	NAG	C8-C7-N2	3.31	121.69	116.10
5	A	710	SO4	O4-S-O2	3.22	126.14	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	709	GOL	O1-C1-C2	3.18	125.44	110.20
6	A	716	1PE	OH6-C26-C16	3.12	123.78	110.07
4	A	706	GOL	C3-C2-C1	-3.08	99.72	111.70
3	A	703	NAG	C8-C7-N2	3.07	121.29	116.10
6	A	722	1PE	C23-OH3-C22	3.06	126.53	113.29
3	A	701	NAG	O7-C7-C8	-3.03	116.44	122.06
3	A	701	NAG	C1-C2-N2	2.95	115.53	110.49
4	A	709	GOL	O3-C3-C2	2.94	124.28	110.20
3	A	703	NAG	O4-C4-C5	-2.84	102.26	109.30
5	A	710	SO4	O4-S-O3	-2.74	97.35	109.06
3	A	703	NAG	O7-C7-C8	-2.71	117.02	122.06
3	A	703	NAG	C1-C2-N2	-2.56	106.11	110.49
3	A	701	NAG	C8-C7-N2	2.50	120.33	116.10
6	A	719	1PE	C23-OH3-C22	-2.48	104.00	112.90
6	A	720	1PE	C23-OH3-C22	2.47	123.98	113.29
6	A	722	1PE	OH4-C13-C23	2.46	126.09	111.81
4	A	707	GOL	O1-C1-C2	2.35	121.47	110.20
3	A	703	NAG	O5-C5-C6	2.15	110.58	107.20
6	A	715	1PE	C23-OH3-C22	2.11	126.07	112.96
7	A	730	ACT	OXT-C-CH3	2.09	123.82	115.18
3	A	702	NAG	C3-C4-C5	2.09	113.97	110.24
6	A	720	1PE	OH2-C12-C22	-2.00	100.21	111.81

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	706	GOL	C1-C2-C3-O3
4	A	707	GOL	O1-C1-C2-C3
4	A	707	GOL	C1-C2-C3-O3
4	A	708	GOL	O1-C1-C2-C3
4	A	708	GOL	C1-C2-C3-O3
4	A	709	GOL	C1-C2-C3-O3
6	A	713	1PE	C12-C22-OH3-C23
6	A	717	1PE	C13-C23-OH3-C22
6	A	717	1PE	OH4-C13-C23-OH3
6	A	713	1PE	C14-C24-OH4-C13
6	A	717	1PE	OH2-C12-C22-OH3
4	A	709	GOL	O2-C2-C3-O3
6	A	714	1PE	OH7-C16-C26-OH6
6	A	719	1PE	OH2-C12-C22-OH3
6	A	722	1PE	C12-C22-OH3-C23

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Mol	Chain	Res	Type	Atoms
6	A	711	1PE	OH2-C12-C22-OH3
6	A	721	1PE	OH2-C12-C22-OH3
6	A	726	1PE	OH7-C16-C26-OH6
6	A	719	1PE	C13-C23-OH3-C22
4	A	705	GOL	O1-C1-C2-C3
4	A	707	GOL	O2-C2-C3-O3
4	A	708	GOL	O1-C1-C2-O2
4	A	708	GOL	O2-C2-C3-O3
6	A	725	1PE	OH7-C16-C26-OH6
6	A	717	1PE	C23-C13-OH4-C24
3	A	703	NAG	C4-C5-C6-O6
6	A	713	1PE	C23-C13-OH4-C24
6	A	724	1PE	OH2-C12-C22-OH3
6	A	722	1PE	OH4-C13-C23-OH3
4	A	705	GOL	O1-C1-C2-O2
4	A	706	GOL	O2-C2-C3-O3
4	A	707	GOL	O1-C1-C2-O2
6	A	720	1PE	OH2-C12-C22-OH3
6	A	711	1PE	C12-C22-OH3-C23
6	A	716	1PE	OH6-C15-C25-OH5
6	A	713	1PE	C13-C23-OH3-C22
6	A	721	1PE	C12-C22-OH3-C23
6	A	716	1PE	C16-C26-OH6-C15
6	A	724	1PE	C12-C22-OH3-C23
6	A	720	1PE	OH4-C13-C23-OH3
6	A	714	1PE	C16-C26-OH6-C15
3	A	703	NAG	O5-C5-C6-O6
6	A	726	1PE	C16-C26-OH6-C15
6	A	722	1PE	C13-C23-OH3-C22
6	A	720	1PE	C13-C23-OH3-C22
6	A	713	1PE	OH4-C13-C23-OH3
6	A	723	1PE	OH2-C12-C22-OH3
6	A	712	1PE	C12-C22-OH3-C23
6	A	716	1PE	OH7-C16-C26-OH6

There are no ring outliers.

15 monomers are involved in 53 short contacts:

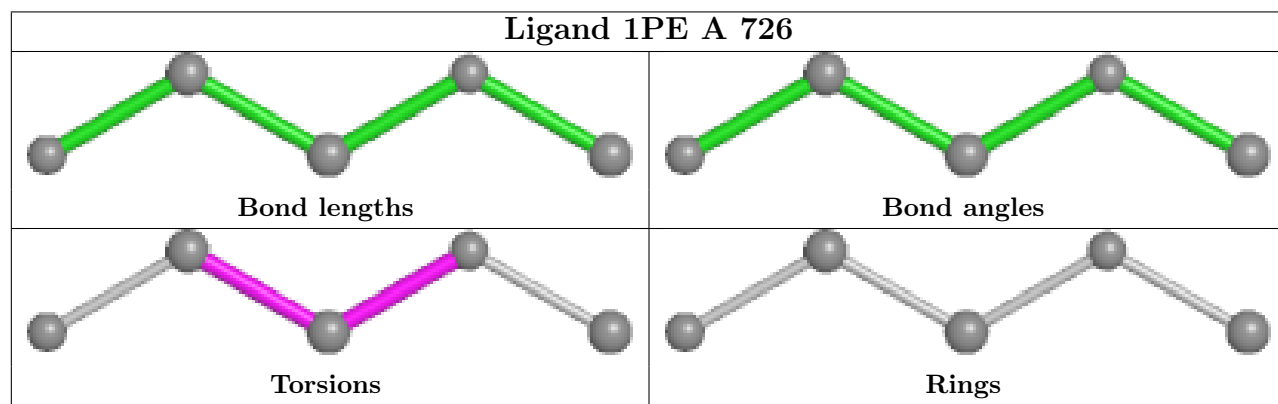
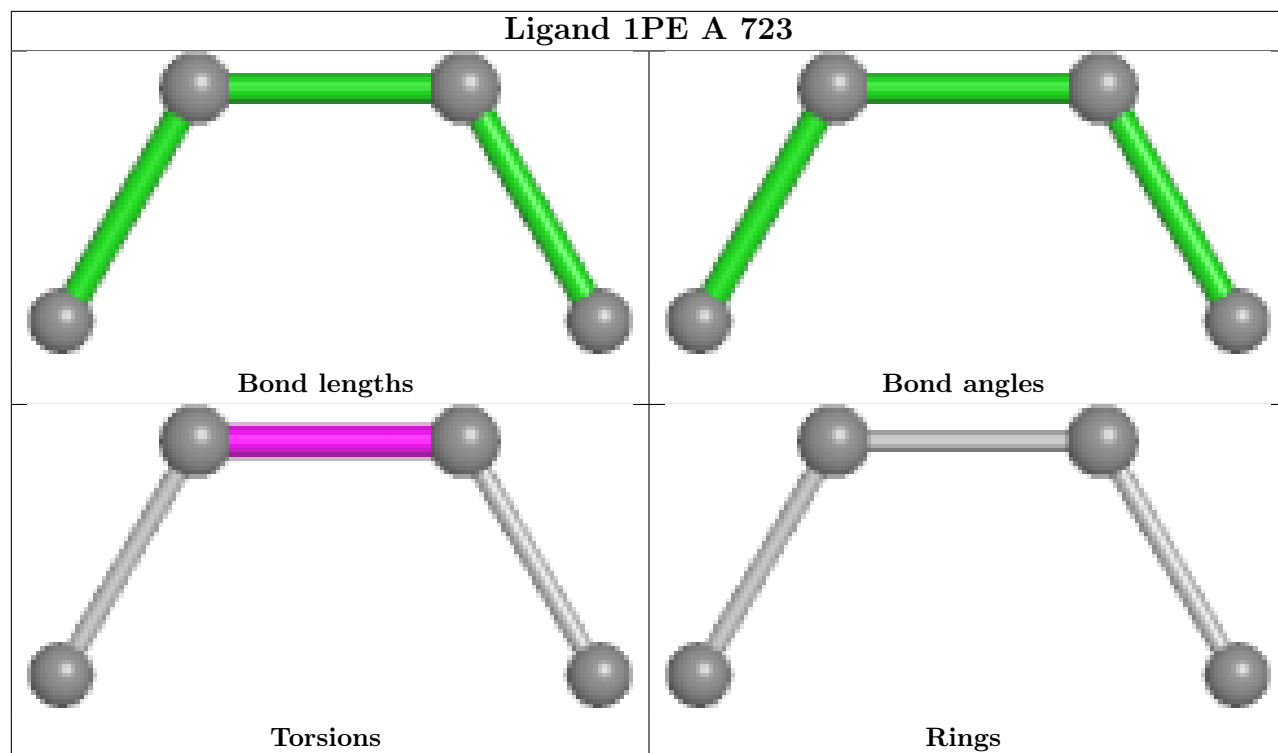
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	726	1PE	4	0
6	A	715	1PE	5	0
6	A	716	1PE	6	0

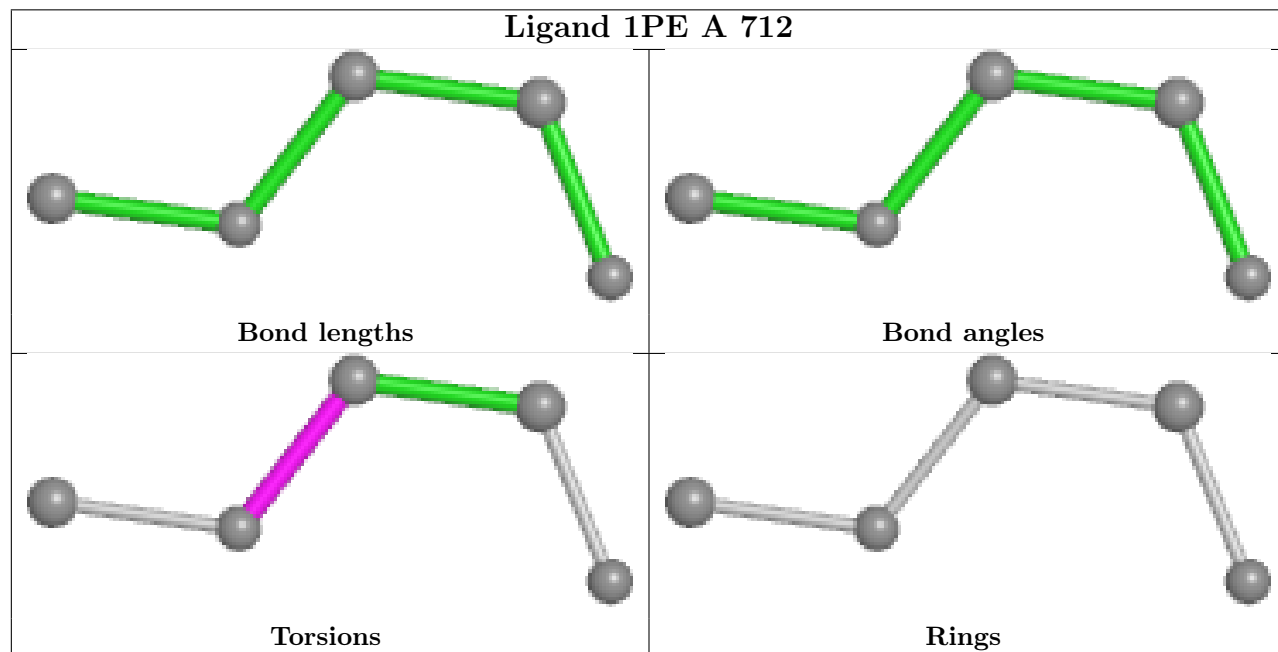
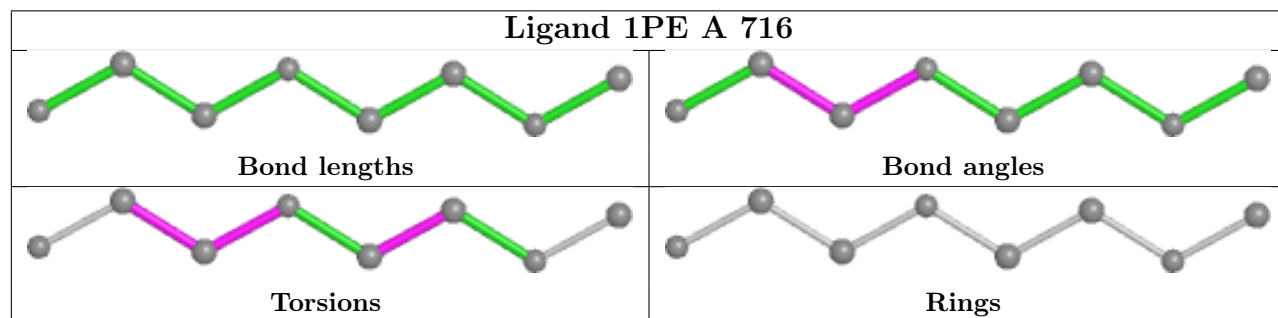
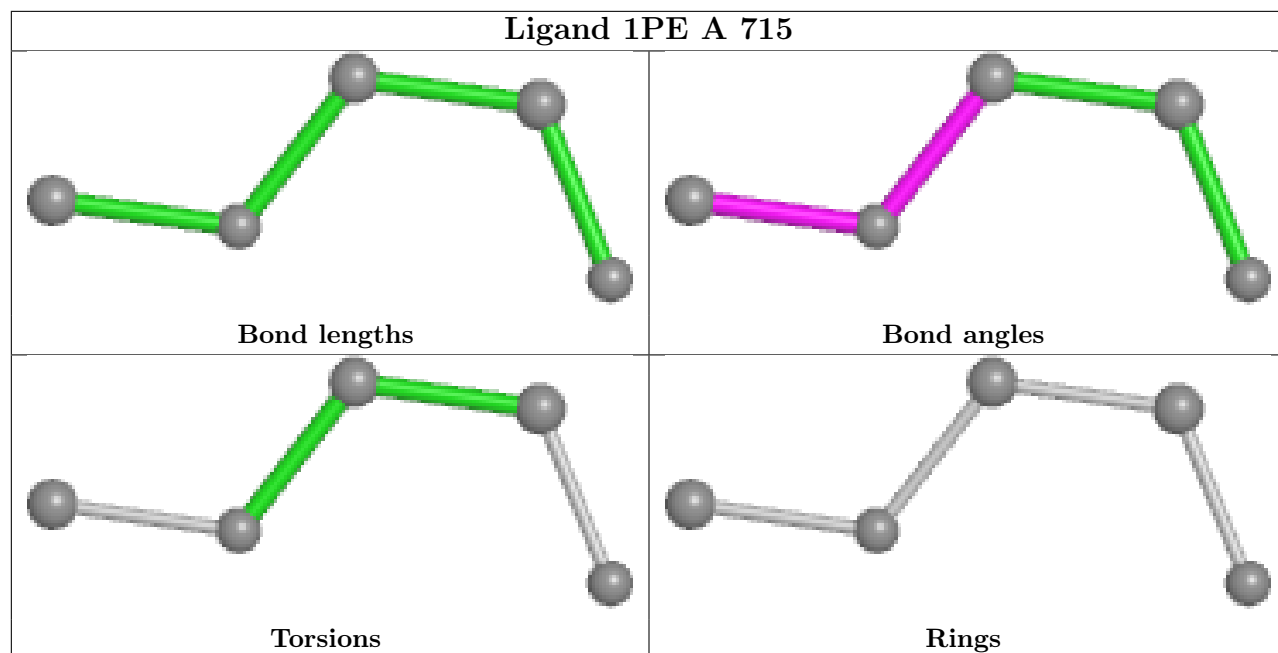
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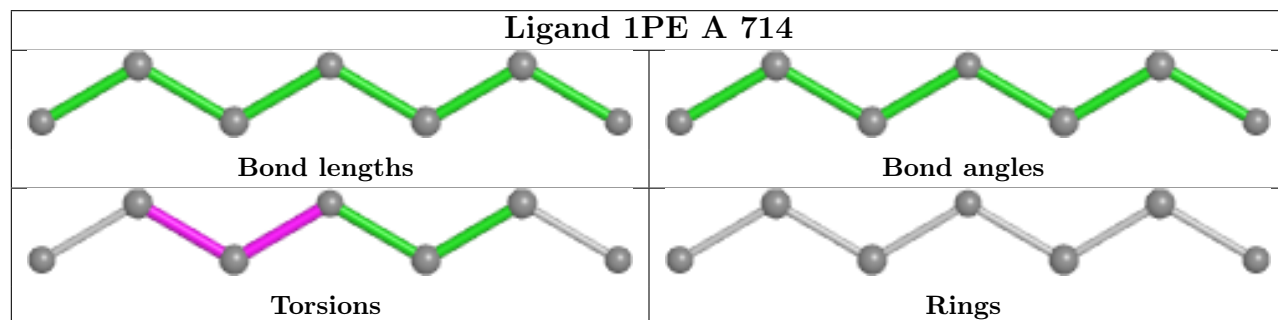
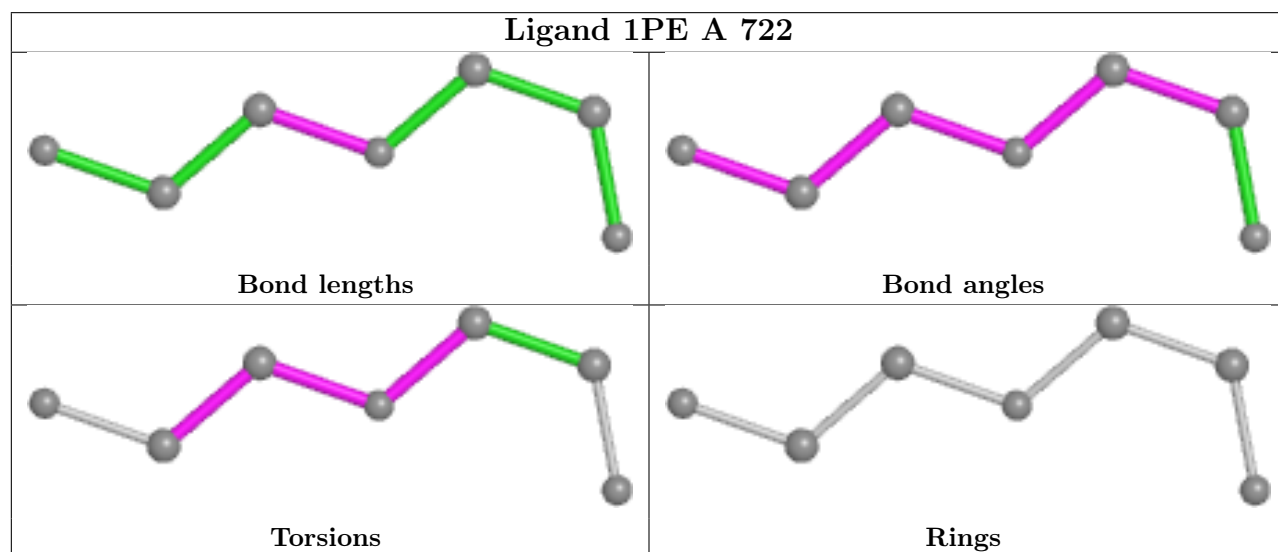
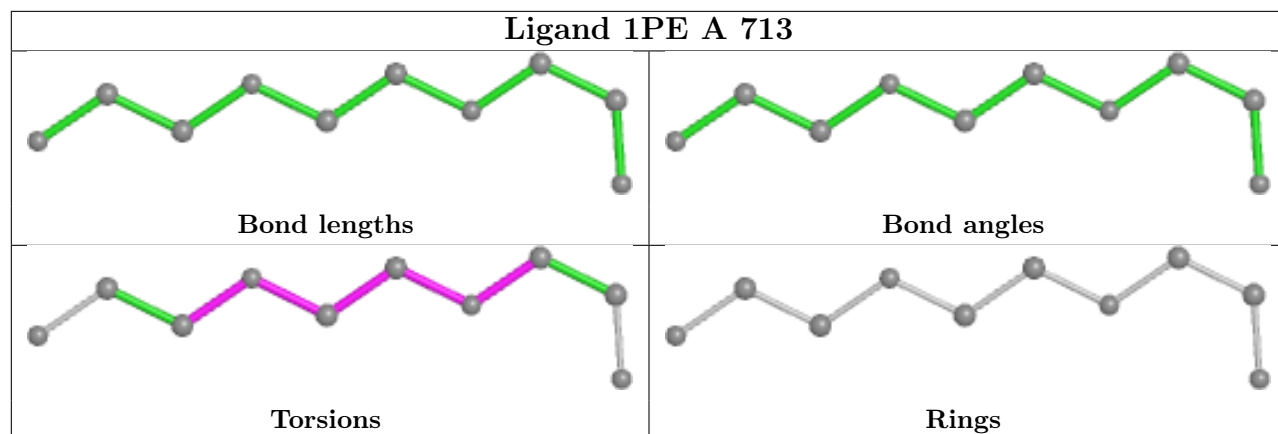
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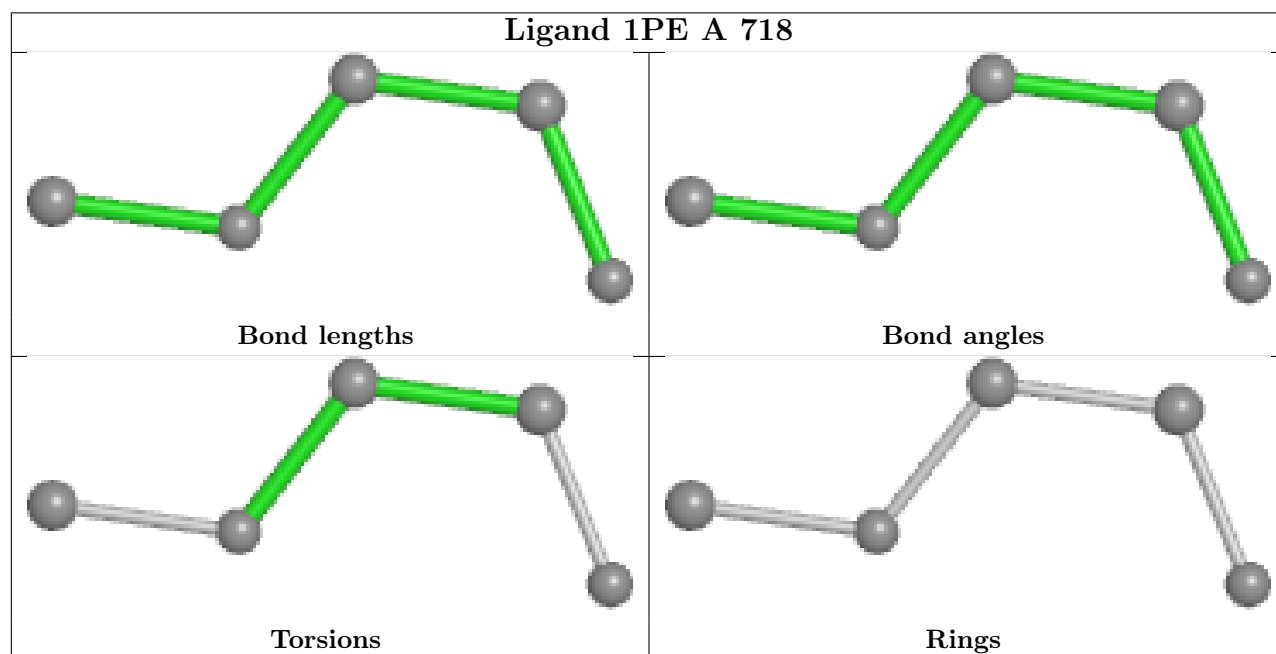
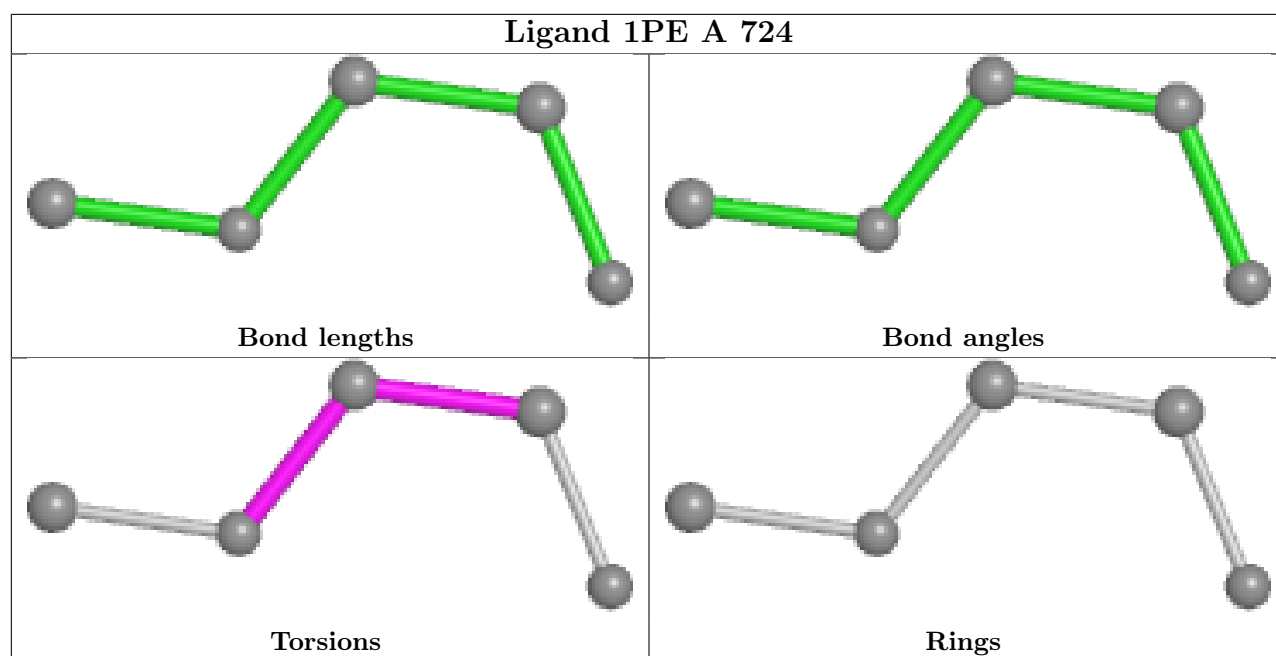
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	713	1PE	2	0
6	A	722	1PE	6	0
3	A	702	NAG	4	0
6	A	718	1PE	1	0
6	A	717	1PE	4	0
6	A	721	1PE	2	0
6	A	711	1PE	2	0
3	A	703	NAG	2	0
6	A	725	1PE	3	0
4	A	709	GOL	3	0
6	A	720	1PE	5	0
6	A	719	1PE	4	0

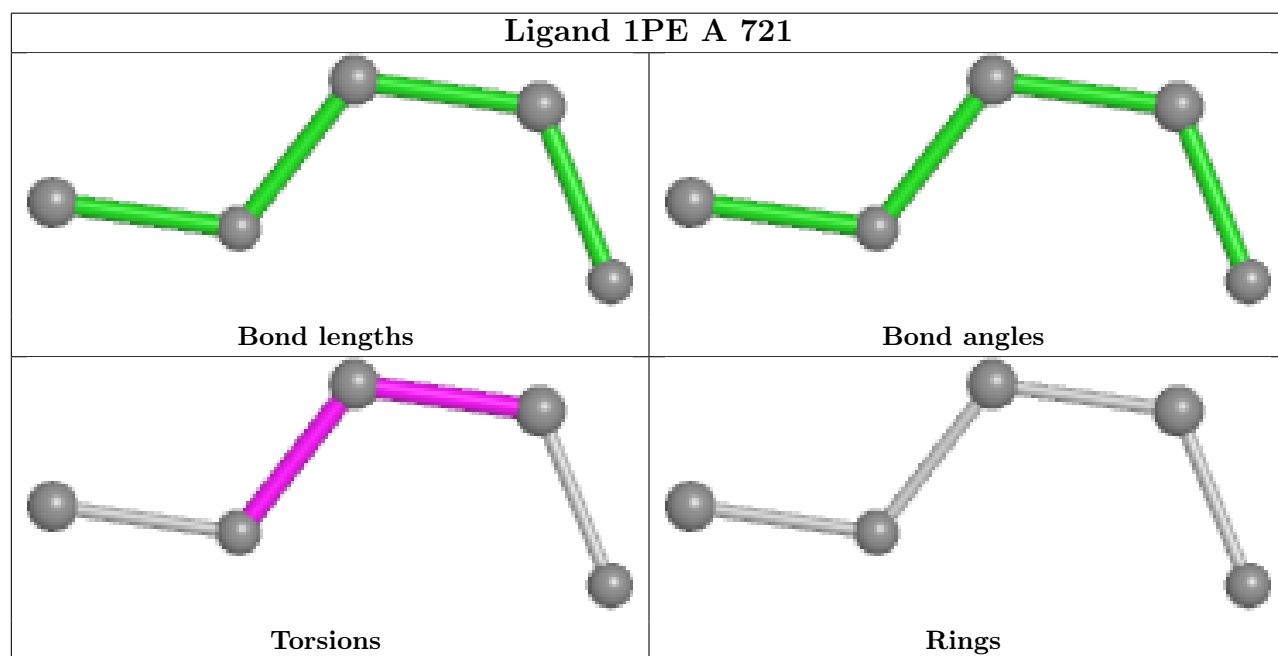
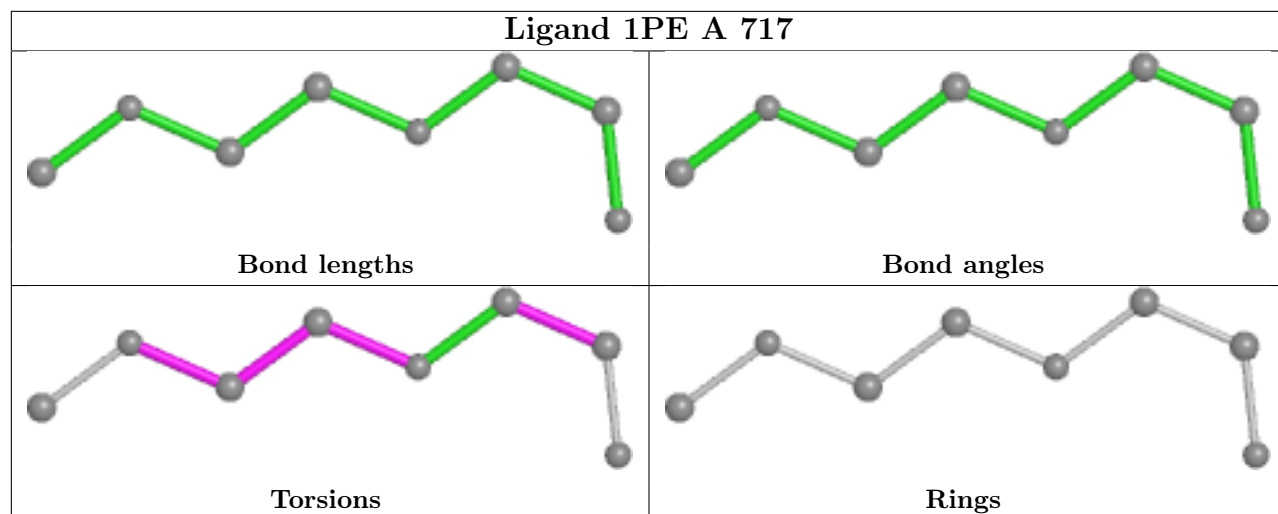
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

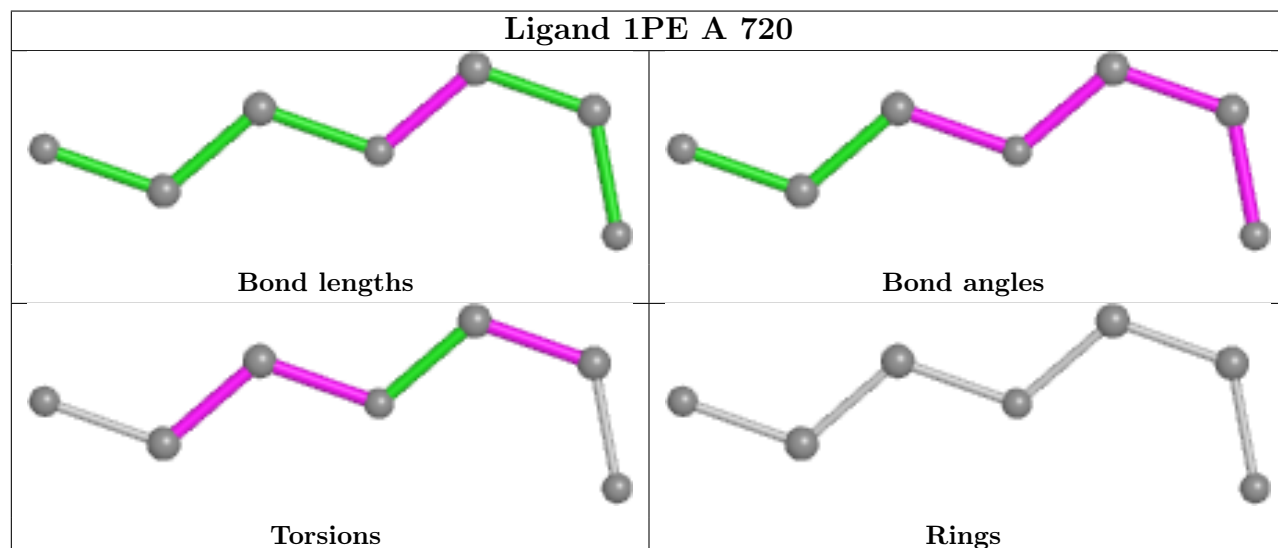
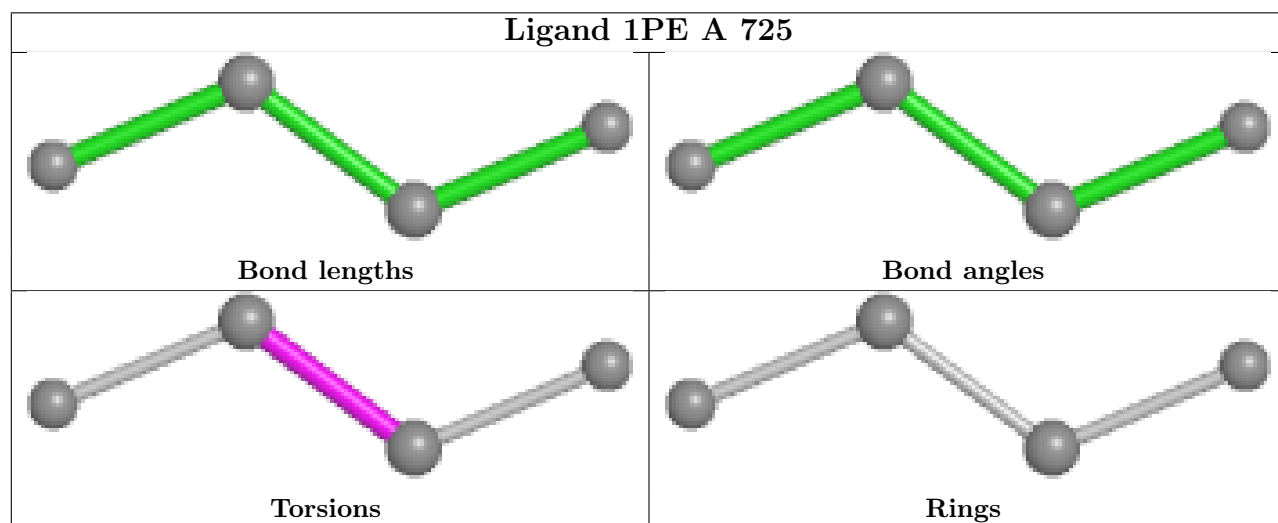
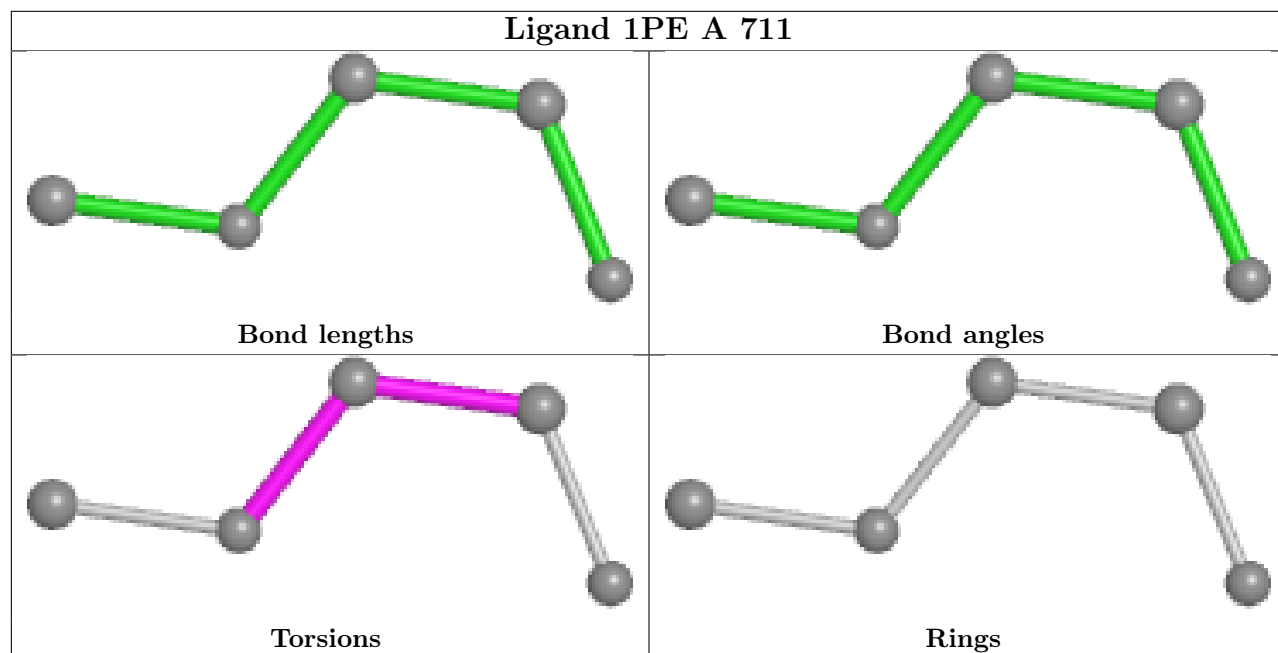


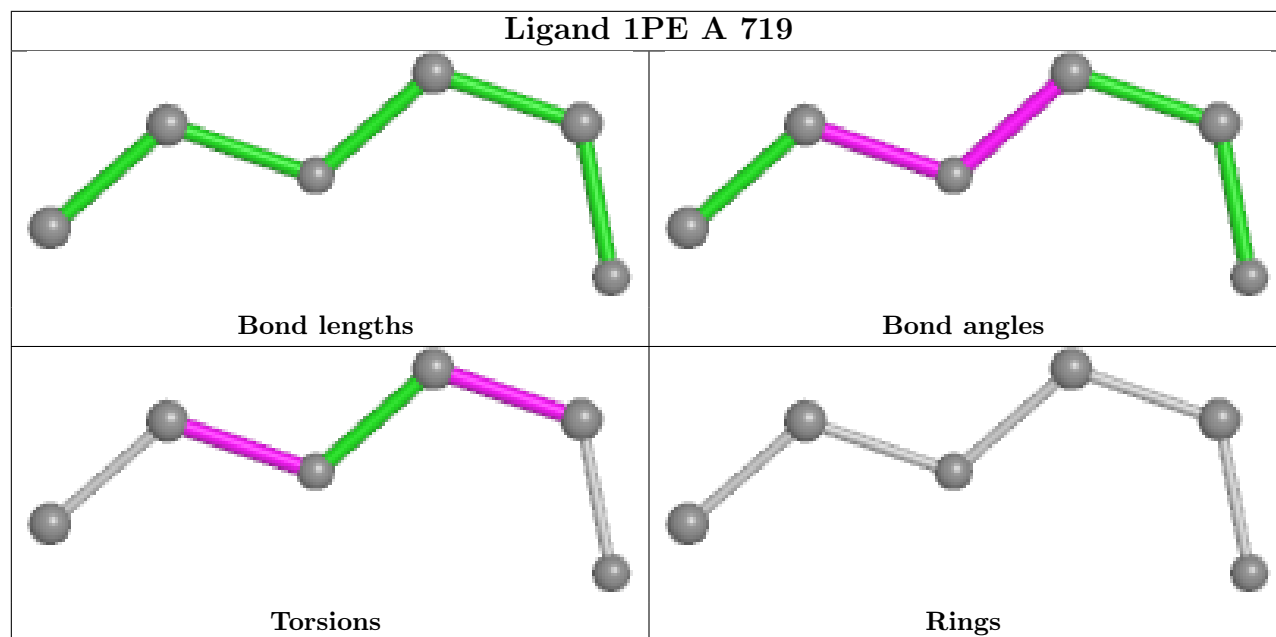












5.7 Other polymers [i](#)

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	606/609 (99%)	-0.14	19 (3%)	49 53	13, 19, 33, 80	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	586	HIS	6.7
1	A	585	ALA	5.3
1	A	-2	HIS	5.2
1	A	294	THR	4.7
1	A	187	ASP	4.6
1	A	228	GLU	3.8
1	A	186	LYS	3.8
1	A	-3	HIS	3.6
1	A	215	VAL	3.5
1	A	226	ASN	3.4
1	A	-1	ALA	3.2
1	A	256	TRP	2.8
1	A	295	PRO	2.8
1	A	227[B]	ARG	2.4
1	A	602	THR	2.3
1	A	97	VAL	2.3
1	A	9	THR	2.2
1	A	0	ALA	2.1
1	A	492	THR	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.

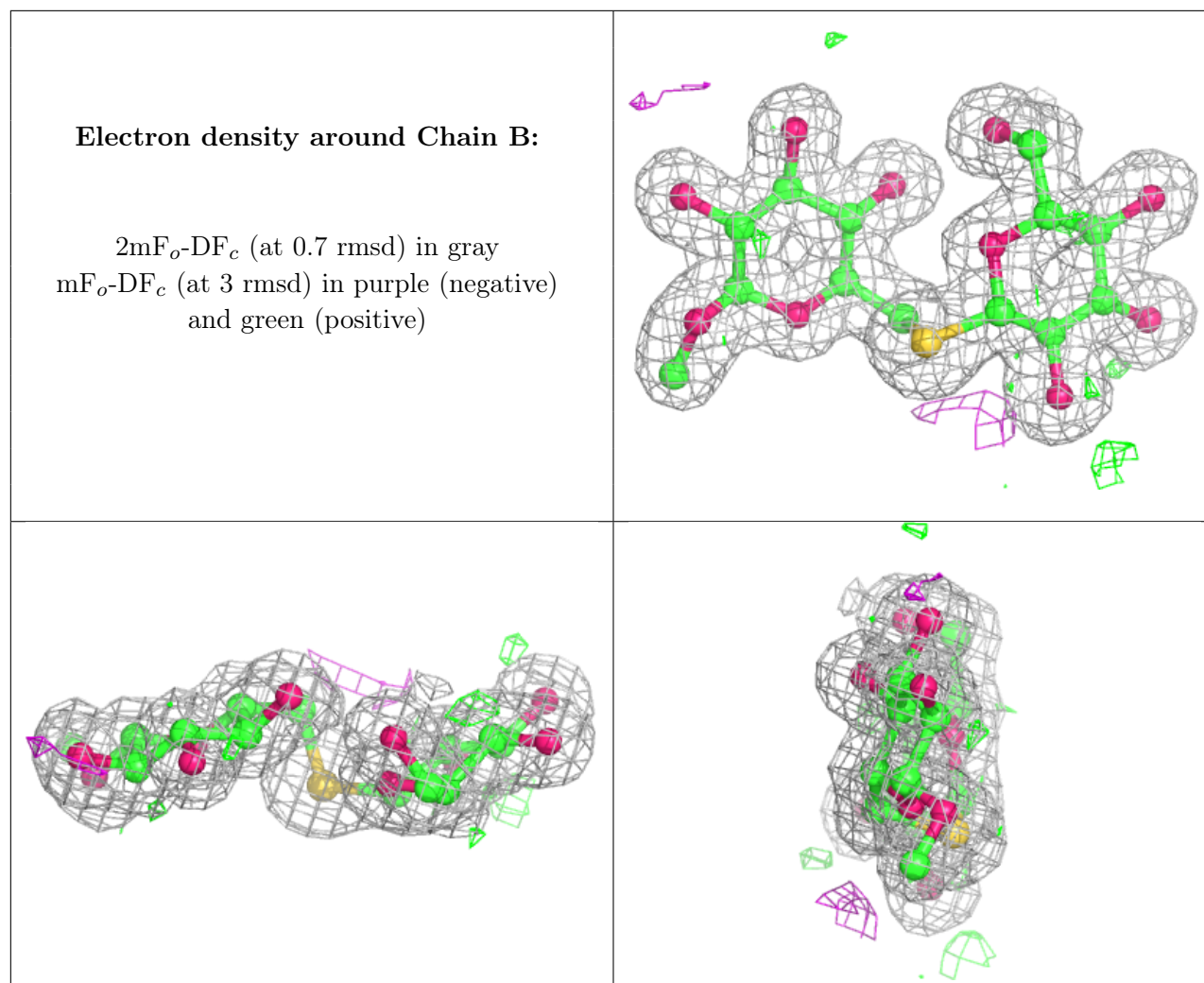
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	A	703	14/15	0.68	0.36	63,86,94,103	0
3	NAG	A	702	14/15	0.69	0.32	51,78,85,87	0
3	NAG	A	701	14/15	0.84	0.29	41,52,69,79	0

6.3 Carbohydrates

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BGC	B	2	11/12	0.96	0.10	13,14,16,17	0
2	U1Y	B	1	13/13	0.98	0.06	15,17,23,28	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 [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(\AA^2)	Q<0.9
7	ACT	A	730	4/4	0.51	0.18	65,67,68,72	0
3	NAG	A	703	14/15	0.68	0.36	63,86,94,103	0
3	NAG	A	702	14/15	0.69	0.32	51,78,85,87	0
7	ACT	A	729	4/4	0.73	0.16	55,56,61,62	0
6	1PE	A	724	5/16	0.76	0.14	50,50,55,64	0
6	1PE	A	723	4/16	0.77	0.23	35,49,55,59	0
6	1PE	A	712	5/16	0.79	0.14	36,44,51,57	0
6	1PE	A	722	7/16	0.79	0.21	25,33,39,51	0
7	ACT	A	734	4/4	0.79	0.31	49,64,65,71	0

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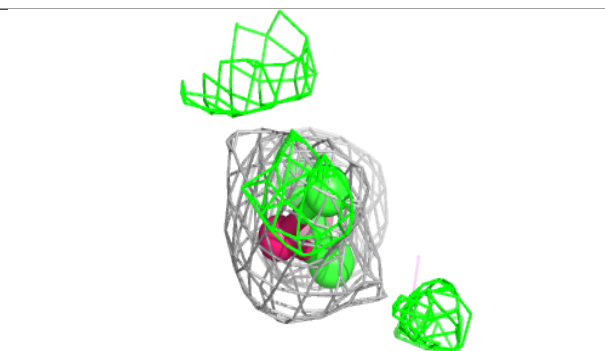
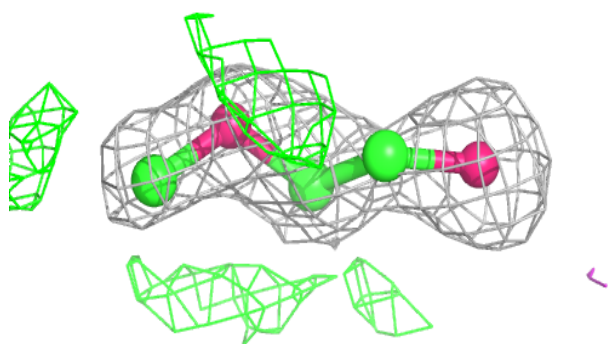
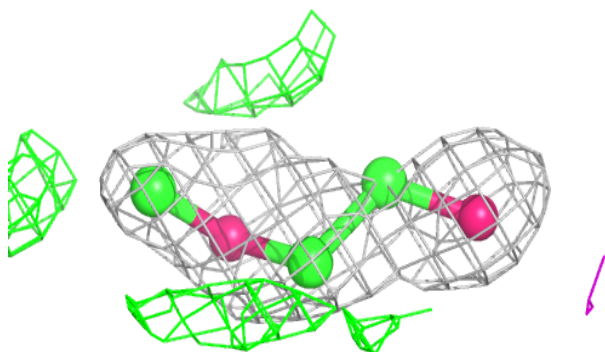
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	1PE	A	716	8/16	0.80	0.25	43,50,59,63	0
7	ACT	A	732	4/4	0.80	0.30	70,71,72,72	0
6	1PE	A	720	7/16	0.80	0.17	31,43,51,64	0
6	1PE	A	714	7/16	0.82	0.12	46,59,79,82	0
7	ACT	A	733	4/4	0.83	0.14	48,57,57,60	0
6	1PE	A	718	5/16	0.83	0.24	48,55,66,68	0
6	1PE	A	726	5/16	0.84	0.32	49,56,65,66	0
3	NAG	A	701	14/15	0.84	0.29	41,52,69,79	0
6	1PE	A	725	4/16	0.84	0.23	33,40,40,43	0
7	ACT	A	731	4/4	0.86	0.16	65,65,66,78	0
6	1PE	A	711	5/16	0.86	0.24	33,33,56,67	0
7	ACT	A	727	4/4	0.87	0.22	57,57,66,67	0
6	1PE	A	713	10/16	0.88	0.21	28,48,57,64	0
6	1PE	A	717	8/16	0.88	0.29	30,45,51,69	0
6	1PE	A	721	5/16	0.88	0.36	31,35,55,59	0
6	1PE	A	719	6/16	0.89	0.26	37,44,51,66	0
4	GOL	A	708	6/6	0.89	0.23	34,55,57,58	0
4	GOL	A	705	6/6	0.89	0.15	41,50,58,64	0
7	ACT	A	728	4/4	0.91	0.17	63,67,70,74	0
5	SO4	A	710	5/5	0.92	0.12	23,26,34,37	5
6	1PE	A	715	5/16	0.92	0.17	20,40,54,60	0
4	GOL	A	709	6/6	0.92	0.18	20,37,40,41	0
4	GOL	A	707	6/6	0.95	0.12	20,34,37,39	0
4	GOL	A	706	6/6	0.95	0.22	24,40,42,48	0

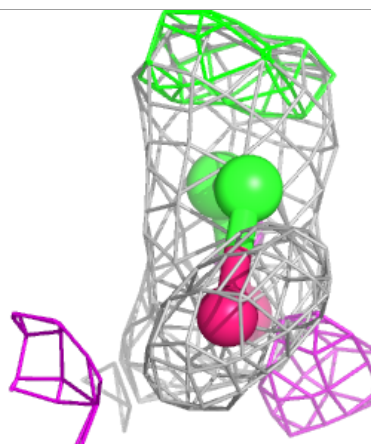
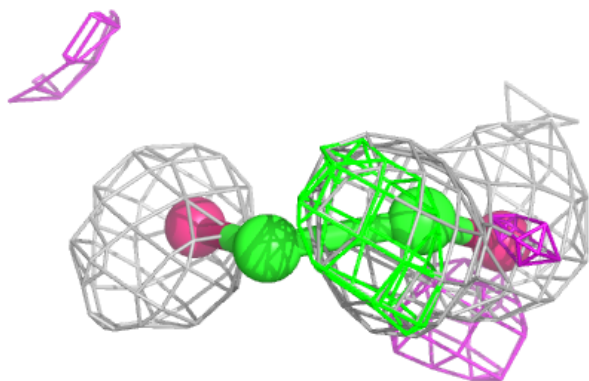
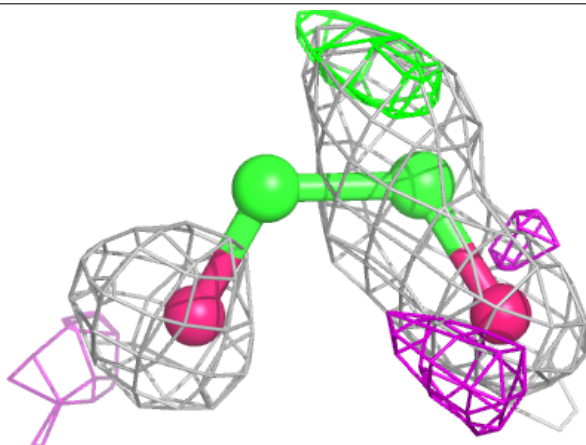
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 1PE A 724:

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

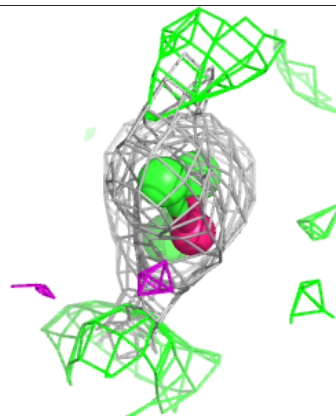
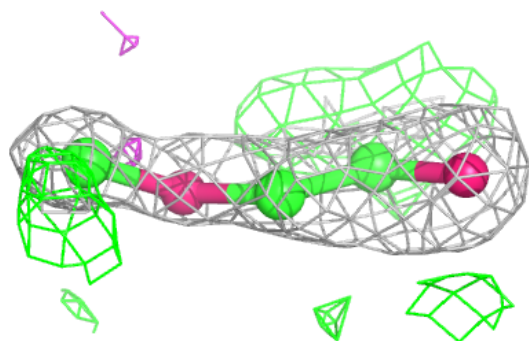
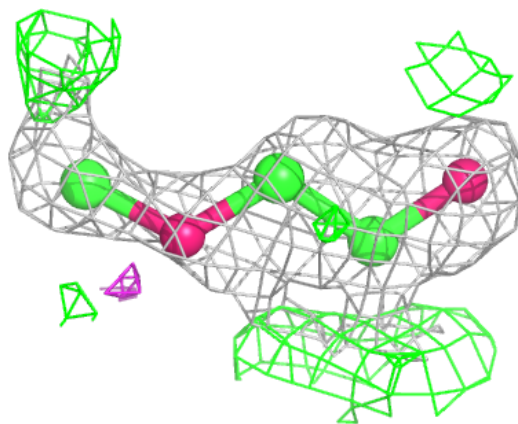
**Electron density around 1PE A 723:**

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



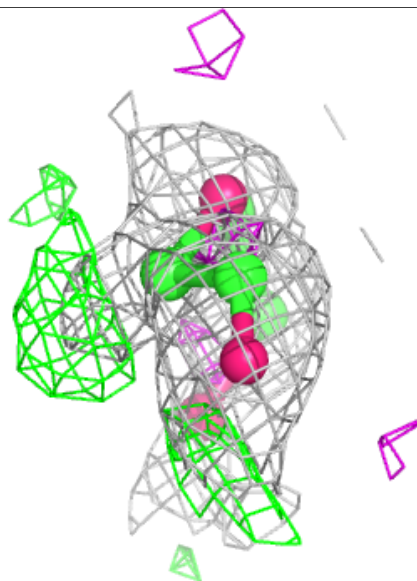
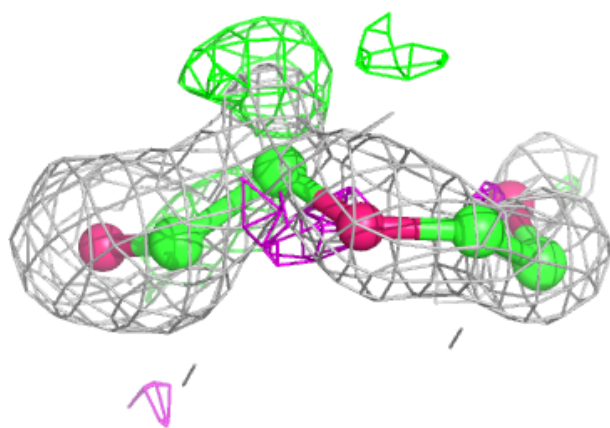
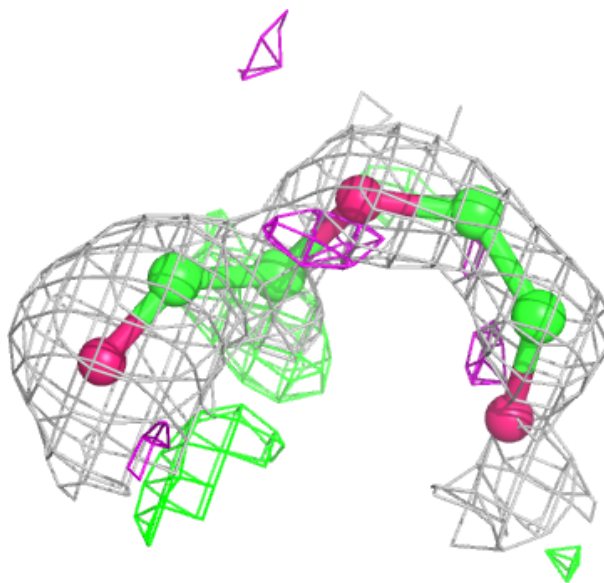
Electron density around 1PE A 712:

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



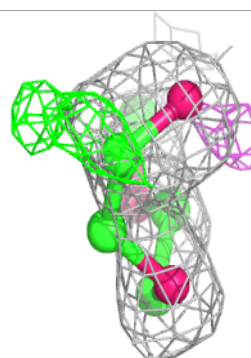
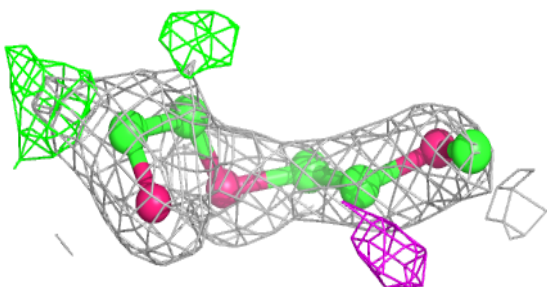
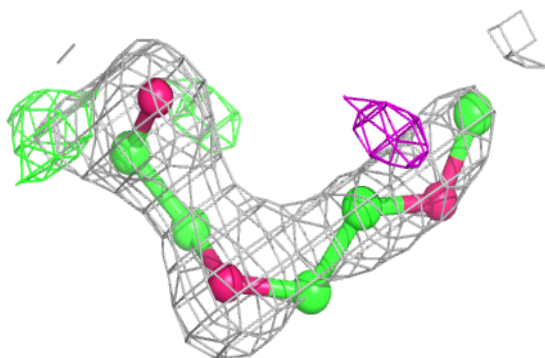
Electron density around 1PE A 722:

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

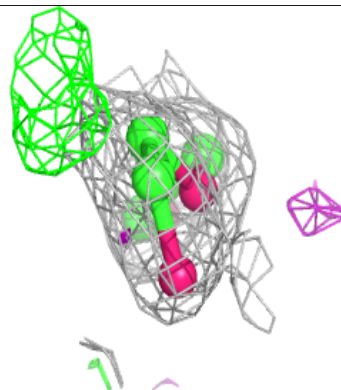
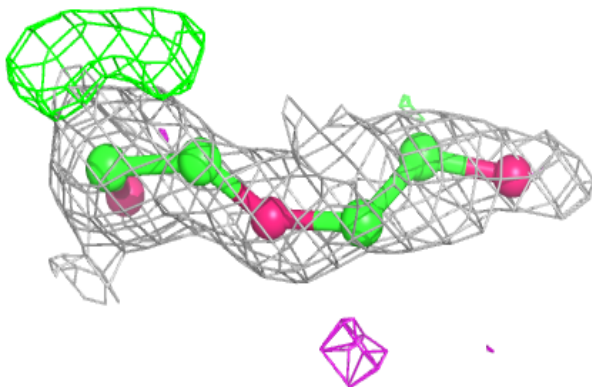
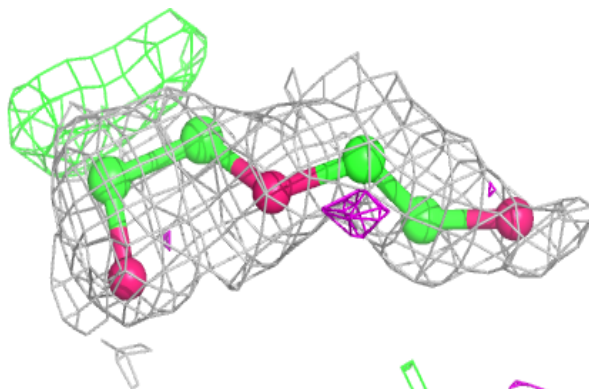


Electron density around 1PE A 716:

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

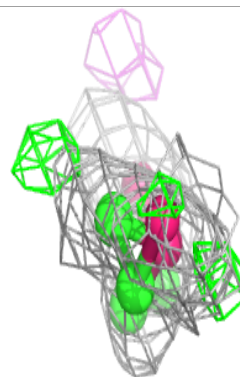
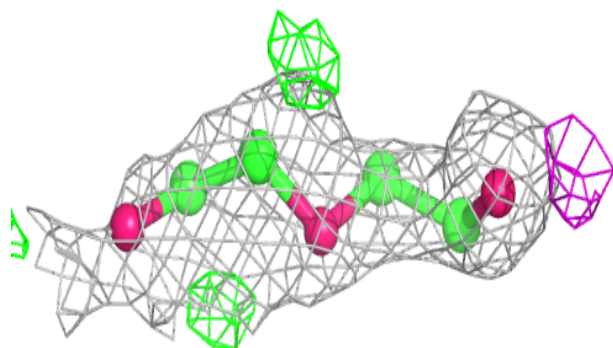
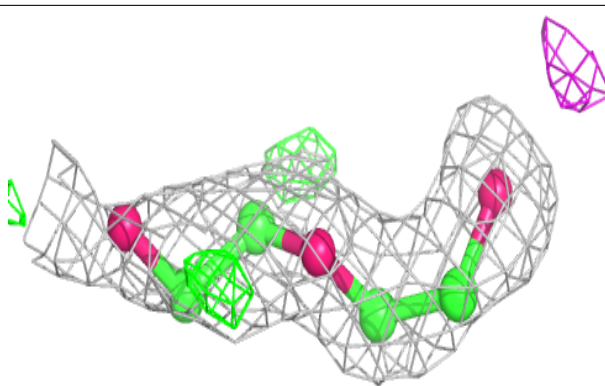
**Electron density around 1PE A 720:**

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

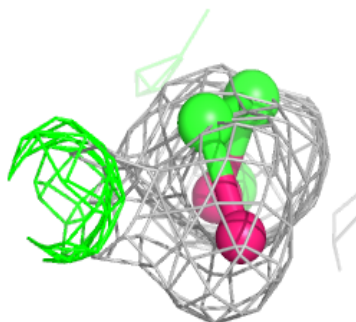
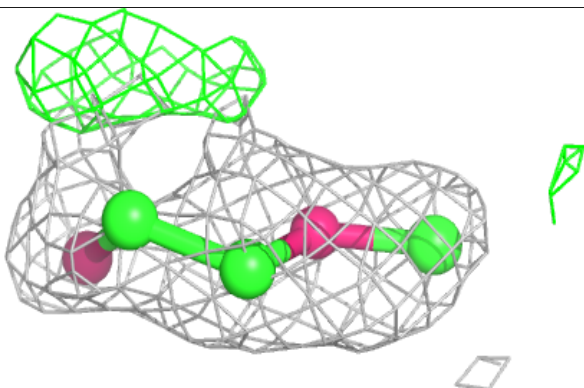
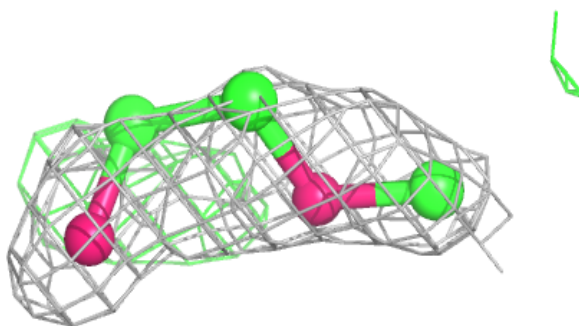


Electron density around 1PE A 714:

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

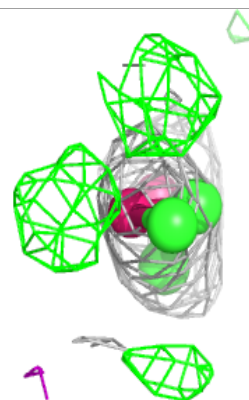
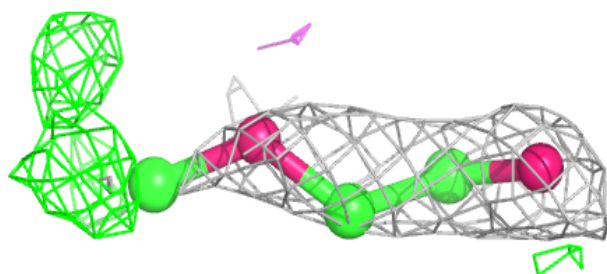
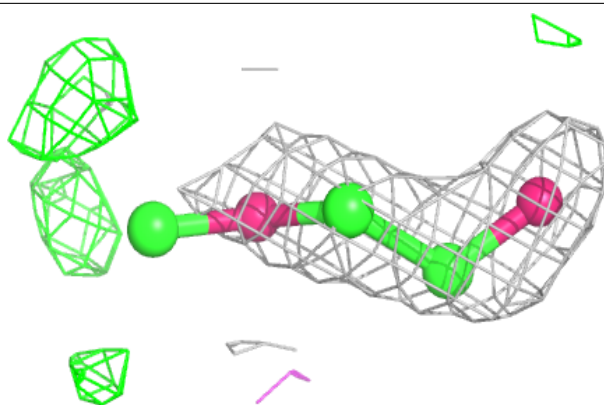
**Electron density around 1PE A 718:**

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

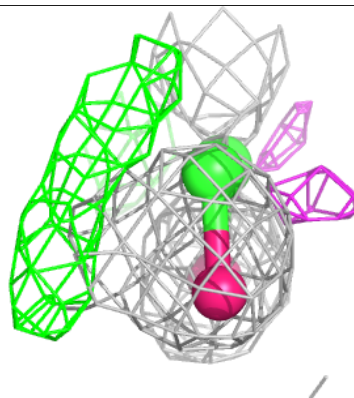
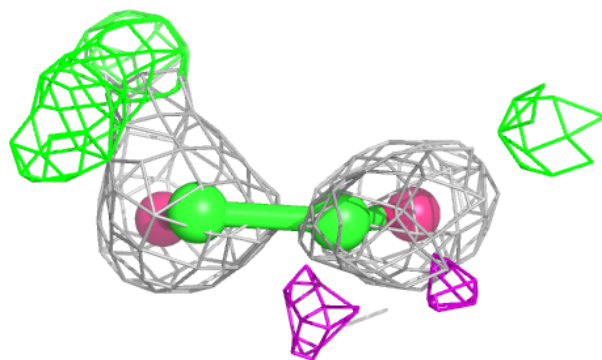
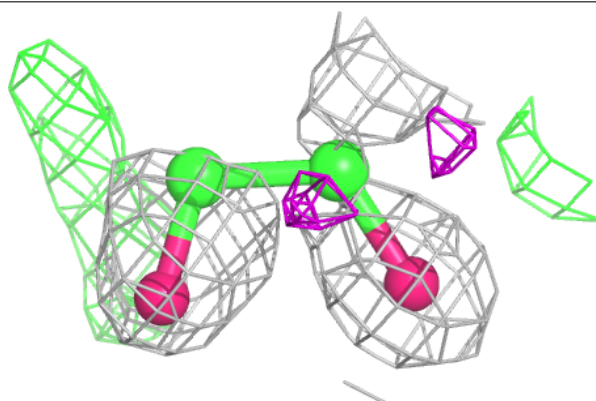


Electron density around 1PE A 726:

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

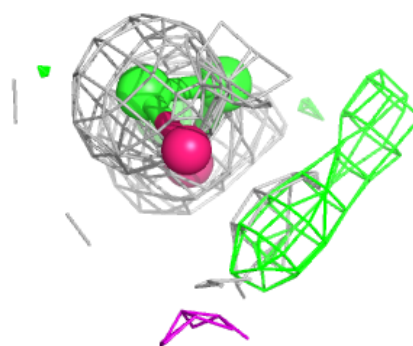
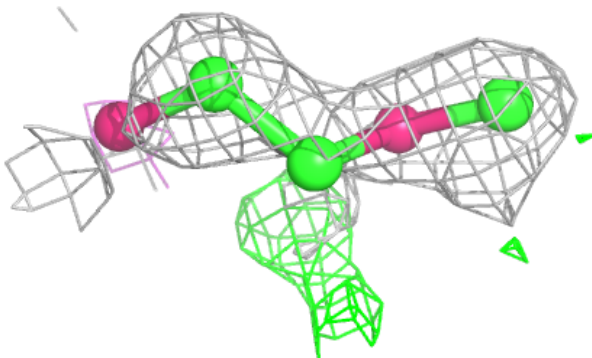
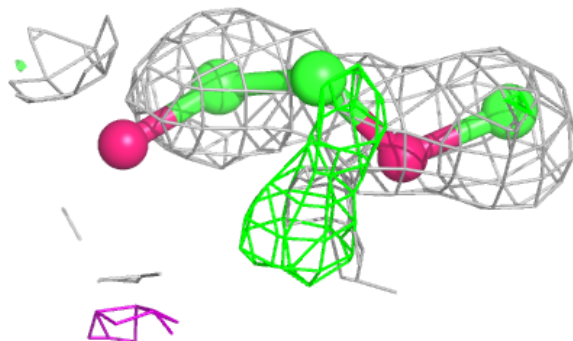
**Electron density around 1PE A 725:**

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



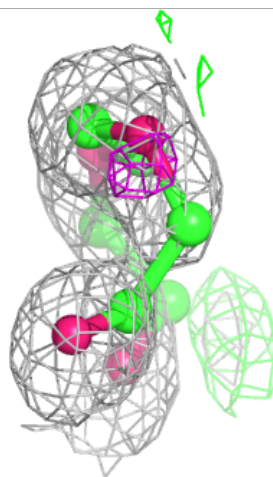
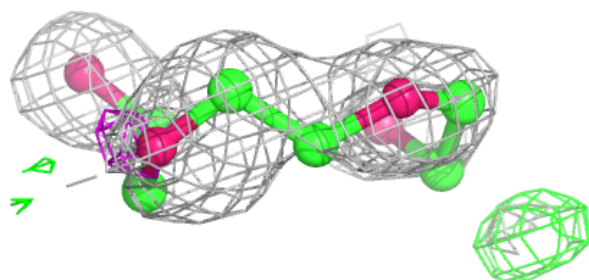
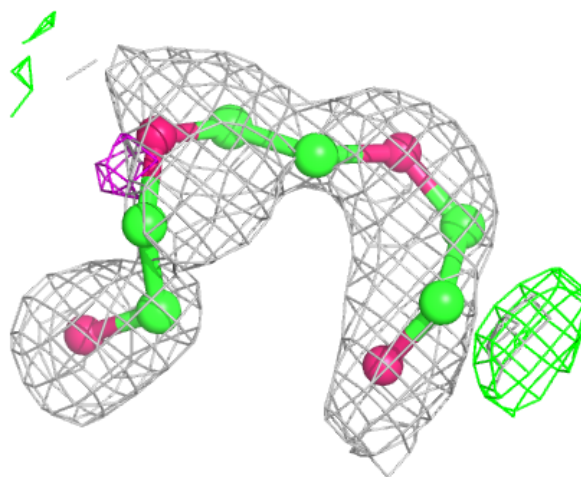
Electron density around 1PE A 711:

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



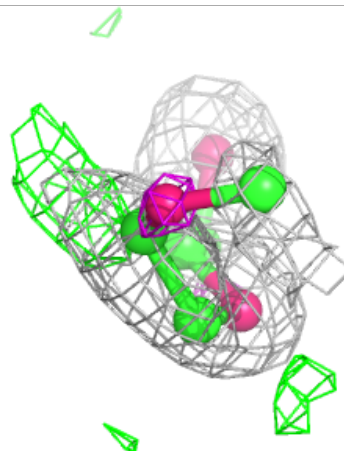
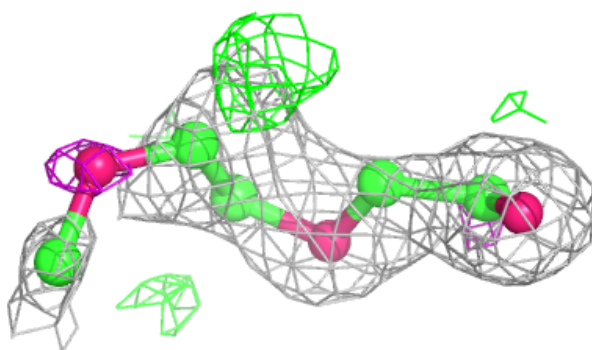
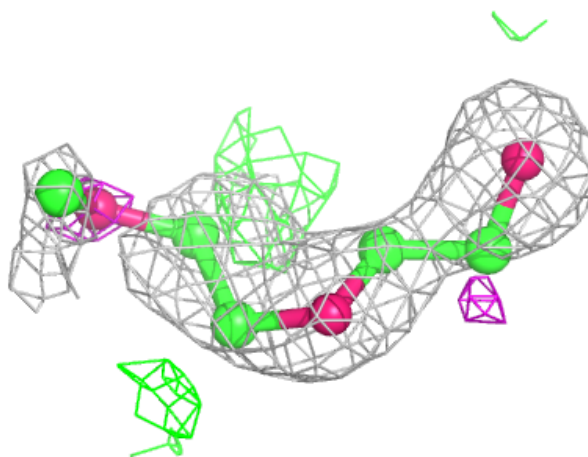
Electron density around 1PE A 713:

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



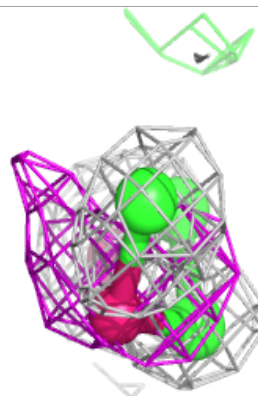
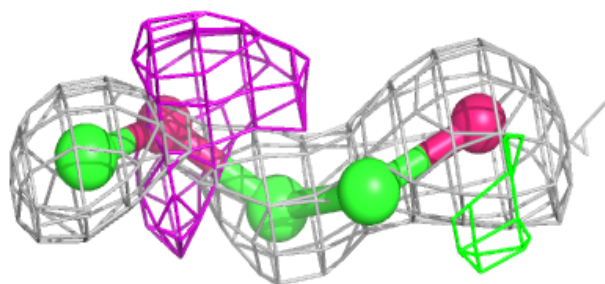
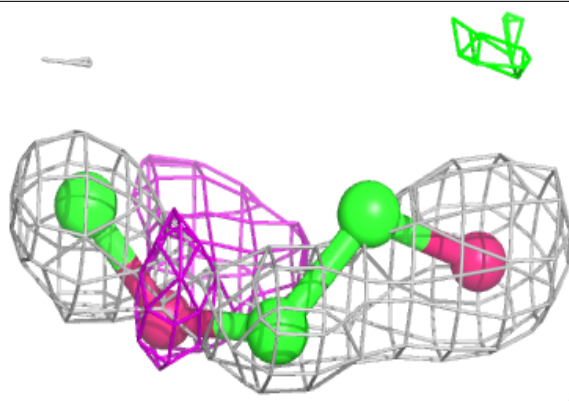
Electron density around 1PE A 717:

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



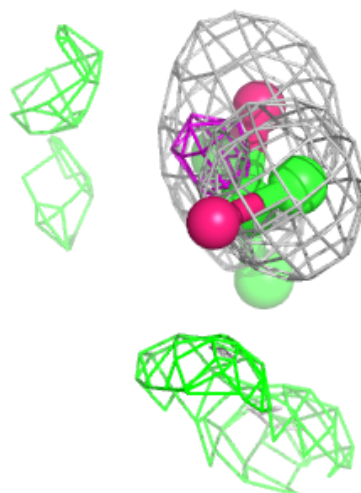
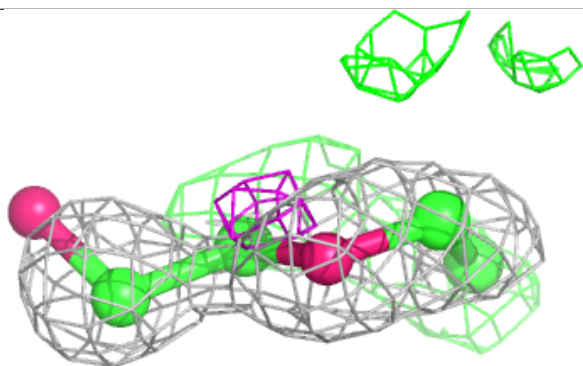
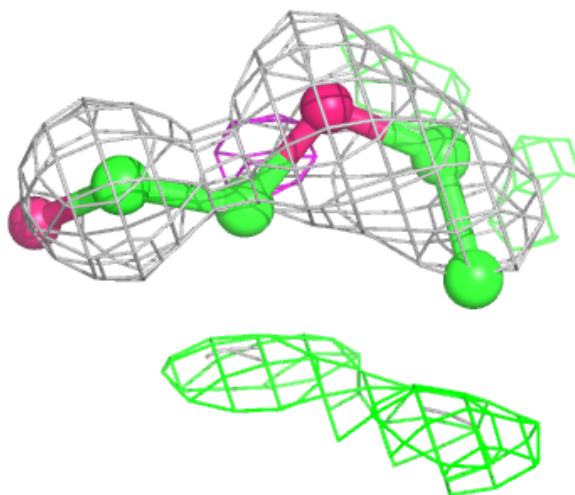
Electron density around 1PE A 721:

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



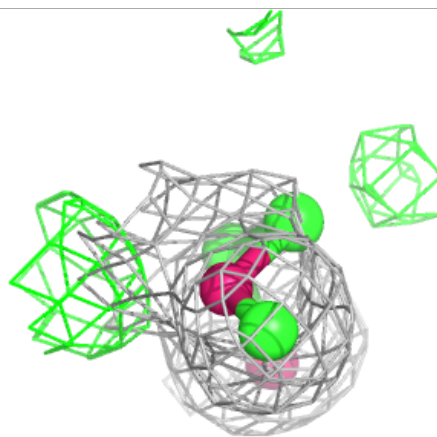
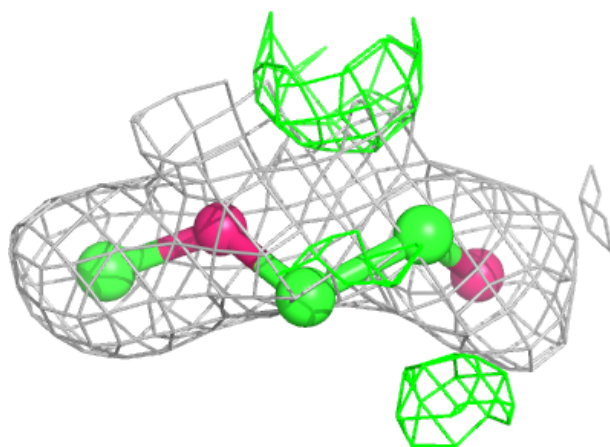
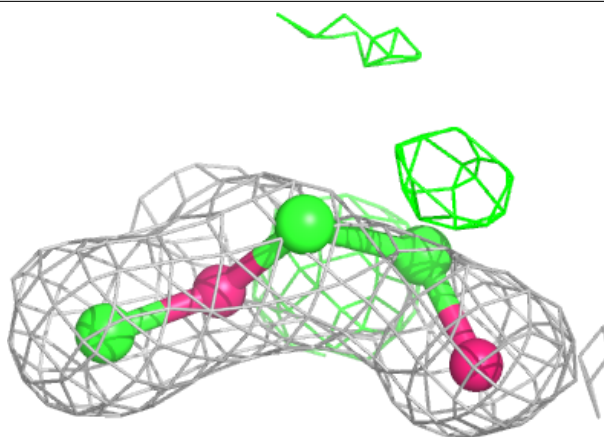
Electron density around 1PE A 719:

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



Electron density around 1PE A 715:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.