Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 05:54 PM JST

PDB ID	:	6LC5
Title	:	Crystal structure of barley exohydrolaseI W434F in complex with 4'-nitrophenyl thiolaminaribioside
Authors	:	Luang, S.; Streltsov, V.A.; Hrmova, M.
Deposited on	:	2019-11-17
Resolution	:	1.76 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:

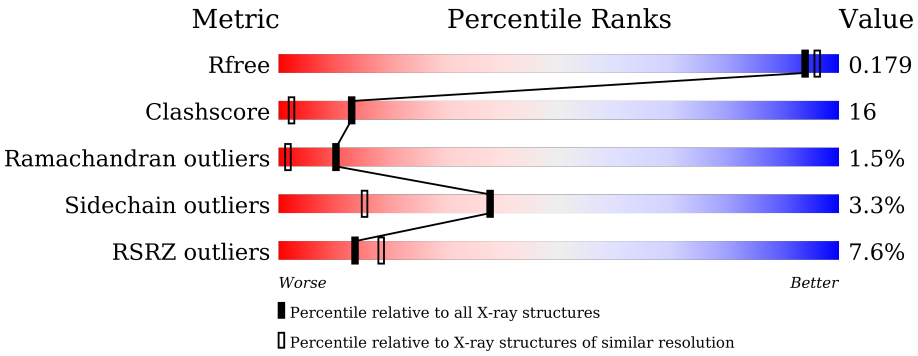
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 <=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	8% 81% 15%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5308 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.

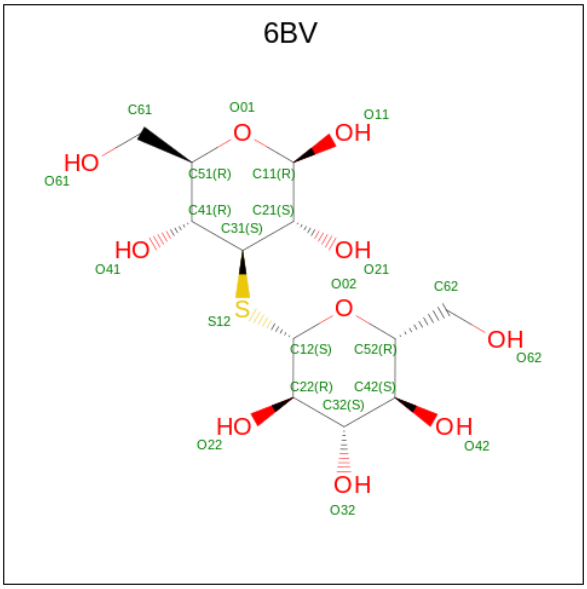
- Molecule 1 is a protein called Beta-D-glucan exohydrolase isoenzyme ExoI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	603	4600	2911	793	869	27	0	19	0

There are 5 discrepancies between the modelled and reference sequences:

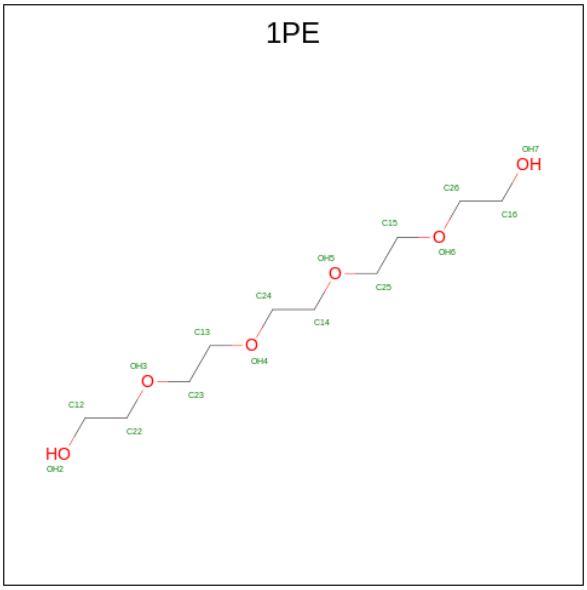
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	HIS	-	expression tag	UNP Q9XEI3
A	-2	HIS	-	expression tag	UNP Q9XEI3
A	-1	ALA	-	expression tag	UNP Q9XEI3
A	320	LYS	ASN	conflict	UNP Q9XEI3
A	434	PHE	TRP	engineered mutation	UNP Q9XEI3

- Molecule 2 is (2 {R},3 {S},4 {S},5 {R},6 {R})-6-(hydroxymethyl)-4-[(2 {S},3 {R},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]sulfanyl-oxane-2,3,5-triol (three-letter code: 6BV) (formula: $C_{12}H_{22}O_{10}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O S 23 12 10 1	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 6 4 2	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 8 5 3	0	1
3	A	1	Total C O 6 4 2	0	0
3	A	1	Total C O 6 4 2	0	0
3	A	1	Total C O 5 3 2	0	0
3	A	1	Total C O 11 7 4	0	1
3	A	1	Total C O 11 7 4	0	1
3	A	1	Total C O 5 3 2	0	0

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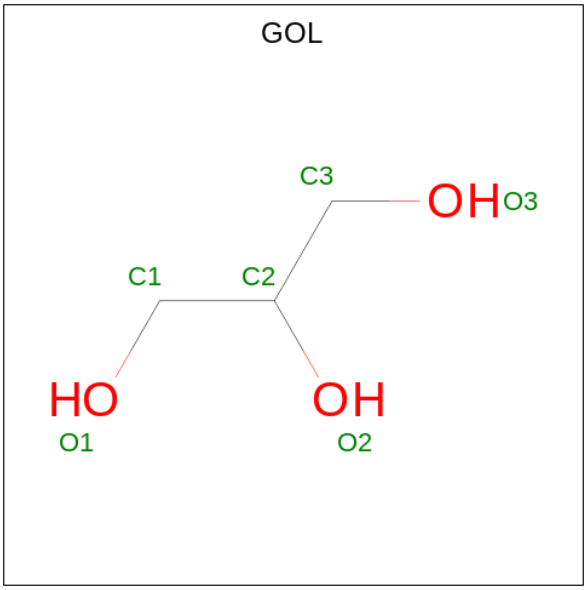
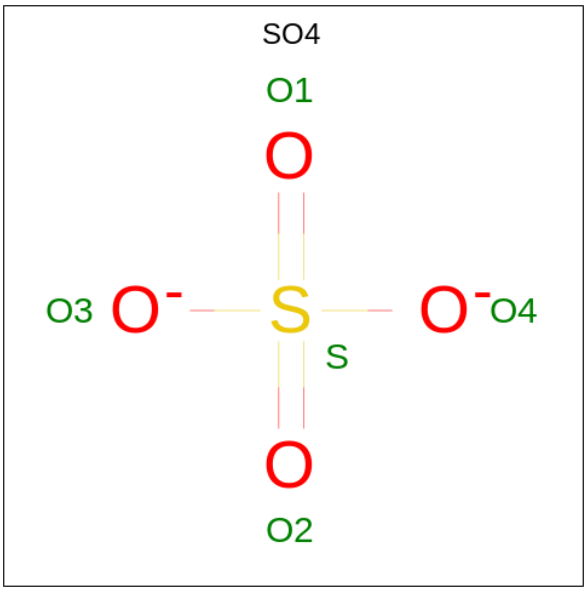
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 19 12 7	0	1

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



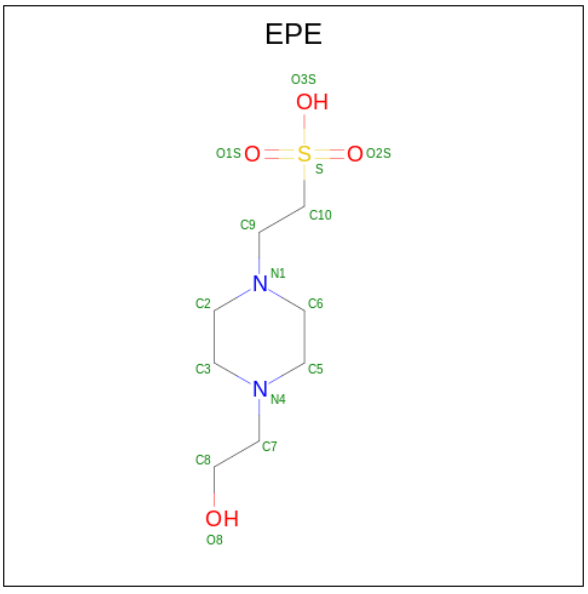
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



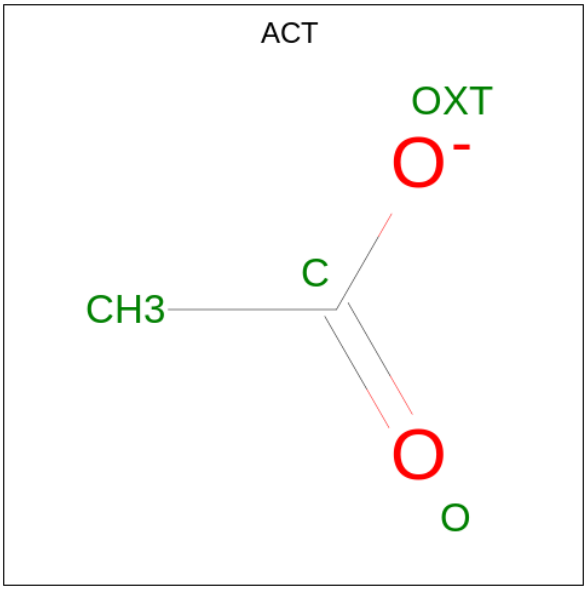
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O S 15 8 2 4 1	0	1
6	A	1	Total C N O S 15 8 2 4 1	0	1
6	A	1	Total C N O S 15 8 2 4 1	0	1

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

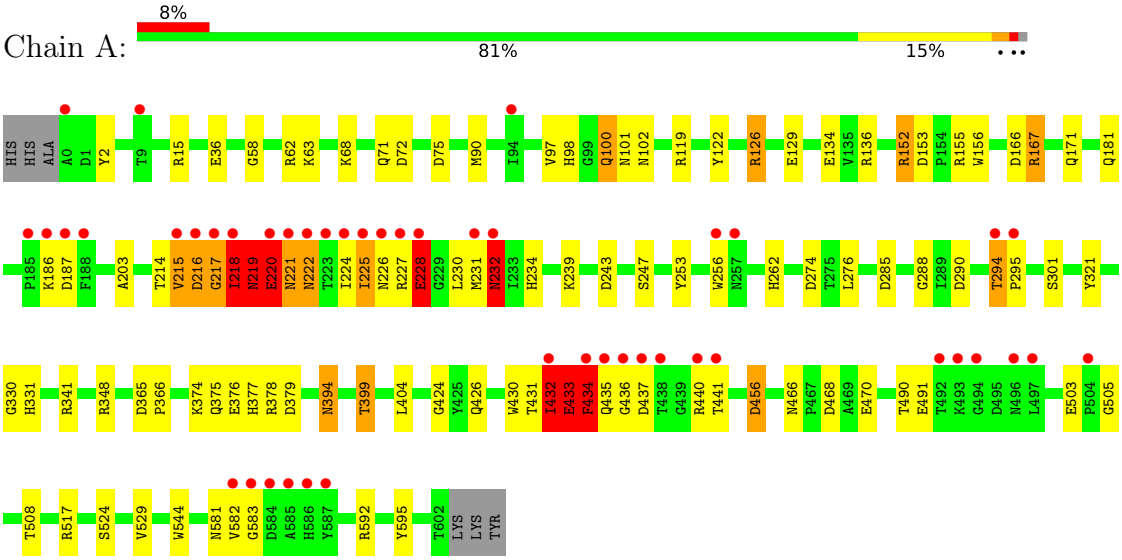
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	502	Total O 502 502	0	0

3 Residue-property plots (i)

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

• Molecule 1: Beta-D-glucan exohydrolase isoenzyme ExoI



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	100.77Å 100.77Å 180.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.96 – 1.76 45.92 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.96-1.76) 99.9 (45.92-1.76)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.63 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.140 , 0.169 0.149 , 0.179	Depositor DCC
R_{free} test set	4631 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 63.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5308	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ACT, SO4, EPE, GOL, 6BV, 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	1.31	24/4754 (0.5%)	1.27	37/6455 (0.6%)

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	7

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	432[A]	ILE	C-O	12.11	1.46	1.23
1	A	432[B]	ILE	C-O	12.11	1.46	1.23
1	A	433	GLU	CD-OE2	-11.64	1.12	1.25
1	A	503	GLU	CD-OE2	9.27	1.35	1.25
1	A	219	ASN	CG-OD1	8.34	1.42	1.24
1	A	126	ARG	CD-NE	-7.54	1.33	1.46
1	A	426	GLN	CB-CG	-7.51	1.32	1.52
1	A	216	ASP	N-CA	7.38	1.61	1.46
1	A	399	THR	CB-CG2	7.15	1.75	1.52
1	A	330	GLY	N-CA	6.80	1.56	1.46
1	A	517[B]	ARG	CZ-NH2	6.65	1.41	1.33
1	A	517[C]	ARG	CZ-NH2	6.65	1.41	1.33
1	A	253	TYR	CG-CD2	-6.57	1.30	1.39
1	A	440	ARG	CZ-NH1	6.50	1.41	1.33
1	A	119	ARG	CZ-NH1	6.43	1.41	1.33
1	A	219	ASN	N-CA	6.28	1.58	1.46
1	A	434[A]	PHE	N-CA	-5.94	1.34	1.46
1	A	433	GLU	C-O	5.87	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	595	TYR	CE2-CZ	-5.50	1.31	1.38
1	A	232	ASN	N-CA	-5.40	1.35	1.46
1	A	433	GLU	N-CA	5.21	1.56	1.46
1	A	321	TYR	CB-CG	-5.14	1.44	1.51
1	A	436	GLY	CA-C	5.05	1.59	1.51
1	A	129	GLU	CG-CD	5.01	1.59	1.51

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	126	ARG	NE-CZ-NH2	-17.79	111.40	120.30
1	A	126	ARG	NE-CZ-NH1	15.14	127.87	120.30
1	A	433	GLU	N-CA-C	13.89	148.50	111.00
1	A	434[A]	PHE	N-CA-CB	-11.51	89.88	110.60
1	A	433	GLU	C-N-CA	10.22	147.25	121.70
1	A	440	ARG	NE-CZ-NH2	-8.91	115.85	120.30
1	A	517[B]	ARG	NE-CZ-NH2	8.20	124.40	120.30
1	A	517[C]	ARG	NE-CZ-NH2	8.20	124.40	120.30
1	A	217	GLY	N-CA-C	-7.57	94.17	113.10
1	A	433	GLU	N-CA-CB	-7.18	97.67	110.60
1	A	126	ARG	CD-NE-CZ	7.16	133.63	123.60
1	A	432[A]	ILE	CB-CA-C	7.12	125.84	111.60
1	A	432[B]	ILE	CB-CA-C	7.12	125.84	111.60
1	A	218[A]	ILE	CA-C-N	6.69	131.91	117.20
1	A	218[B]	ILE	CA-C-N	6.69	131.91	117.20
1	A	119	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	A	517[B]	ARG	CA-CB-CG	6.46	127.61	113.40
1	A	517[C]	ARG	CA-CB-CG	6.46	127.61	113.40
1	A	433	GLU	CA-C-O	6.24	133.21	120.10
1	A	62	ARG	CG-CD-NE	-6.21	98.77	111.80
1	A	152[A]	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	166	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	274	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	243	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	243	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	A	341	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	15	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	216	ASP	N-CA-C	5.63	126.22	111.00
1	A	348	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	75	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	456	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	136	ARG	NE-CZ-NH2	-5.41	117.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	592[A]	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	A	378	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	365	ASP	CB-CG-OD2	-5.16	113.65	118.30
1	A	155	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	A	434[A]	PHE	N-CA-C	5.12	124.81	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	THR	Peptide
1	A	220	GLU	Peptide
1	A	228	GLU	Peptide
1	A	232	ASN	Mainchain
1	A	432[A]	ILE	Peptide
1	A	432[B]	ILE	Peptide
1	A	433	GLU	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	4600	0	4564	121	0
2	A	23	0	0	4	0
3	A	91	0	95	10	0
4	A	24	0	32	5	0
5	A	15	0	0	0	0
6	A	45	0	27	6	0
7	A	8	0	6	1	0
8	A	502	0	0	32	0
All	All	5308	0	4724	145	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 16.

All (145) 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:399:THR:CB	1:A:399:THR:CG2	1.75	1.63
2:A:701:6BV:S12	8:A:810:HOH:O	2.06	1.11
1:A:432[B]:ILE:CD1	8:A:1043:HOH:O	2.00	1.07
1:A:432[B]:ILE:HG12	1:A:433:GLU:H	1.07	1.07
2:A:701:6BV:C12	8:A:810:HOH:O	2.01	1.05
2:A:701:6BV:O02	8:A:810:HOH:O	1.77	1.03
4:A:713:GOL:O2	8:A:811:HOH:O	1.80	0.97
1:A:432[B]:ILE:HG12	1:A:433:GLU:N	1.83	0.93
1:A:466[A]:ASN:ND2	1:A:508:THR:OG1	2.02	0.93
1:A:432[B]:ILE:HD11	8:A:1043:HOH:O	1.67	0.85
1:A:394:ASN:HD21	1:A:404:LEU:H	1.21	0.85
1:A:432[B]:ILE:HD12	8:A:1043:HOH:O	1.71	0.81
1:A:432[B]:ILE:CG1	1:A:433:GLU:H	1.93	0.79
1:A:100:GLN:HE21	1:A:100:GLN:HA	1.50	0.77
1:A:122:TYR:CE2	1:A:126:ARG:HD2	2.19	0.77
1:A:374[A]:LYS:NZ	8:A:815:HOH:O	2.18	0.76
1:A:262:HIS:HE1	1:A:285:ASP:H	1.33	0.75
4:A:714:GOL:O3	8:A:812:HOH:O	2.04	0.74
2:A:701:6BV:O41	8:A:810:HOH:O	2.05	0.74
1:A:215:VAL:HG12	8:A:1204:HOH:O	1.86	0.73
1:A:219:ASN:O	1:A:219:ASN:ND2	2.22	0.73
1:A:470[B]:GLU:OE1	8:A:813:HOH:O	2.07	0.72
4:A:716:GOL:O2	8:A:814:HOH:O	2.08	0.72
1:A:432[B]:ILE:CG1	1:A:433:GLU:N	2.52	0.72
1:A:219:ASN:O	1:A:220:GLU:OE1	2.08	0.72
1:A:470[A]:GLU:OE2	8:A:803:HOH:O	0.71	0.71
1:A:221:ASN:HA	1:A:222:ASN:HD22	1.57	0.70
1:A:468:ASP:OD1	1:A:470[A]:GLU:HG2	1.91	0.69
1:A:435:GLN:HE22	1:A:490:THR:CG2	2.05	0.69
1:A:230:LEU:HB2	1:A:256:TRP:CZ2	2.27	0.69
1:A:431:THR:O	1:A:432[B]:ILE:HG23	1.93	0.68
1:A:228:GLU:HG2	1:A:232:ASN:HB2	1.75	0.67
1:A:221:ASN:CB	1:A:222:ASN:HB2	2.26	0.66
1:A:181:GLN:HE21	1:A:203:ALA:H	1.42	0.65
1:A:68:LYS:HE3	8:A:841:HOH:O	1.96	0.65
1:A:134:GLU:OE2	1:A:377:HIS:HD2	1.81	0.64
1:A:97:VAL:H	1:A:101:ASN:HD21	1.45	0.64
1:A:215:VAL:N	1:A:221:ASN:OD1	2.25	0.63
1:A:234:HIS:HD2	8:A:1072:HOH:O	1.81	0.63
1:A:100:GLN:HE21	1:A:100:GLN:CA	2.12	0.62
1:A:262:HIS:CE1	1:A:285:ASP:H	2.17	0.62
1:A:432[B]:ILE:HG21	1:A:441:THR:HB	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432[B]:ILE:CG2	8:A:1041:HOH:O	2.49	0.60
1:A:221:ASN:CA	1:A:222:ASN:HB2	2.32	0.59
1:A:331:HIS:HD2	8:A:1220:HOH:O	1.85	0.59
1:A:435:GLN:HE22	1:A:490:THR:HG22	1.67	0.59
1:A:122:TYR:CD2	1:A:126:ARG:HD2	2.38	0.58
1:A:375:GLN:HB3	3:A:712[B]:1PE:H122	1.88	0.56
1:A:399:THR:CG2	1:A:399:THR:CA	2.78	0.55
1:A:432[B]:ILE:HG23	8:A:1041:HOH:O	2.06	0.55
1:A:490:THR:OG1	1:A:491:GLU:N	2.37	0.55
4:A:713:GOL:H2	8:A:821:HOH:O	2.06	0.55
1:A:221:ASN:HA	1:A:222:ASN:ND2	2.22	0.54
1:A:435:GLN:HE22	1:A:490:THR:HG21	1.72	0.54
1:A:470[B]:GLU:HG2	8:A:813:HOH:O	2.07	0.53
1:A:239:LYS:HD3	1:A:276:LEU:HD22	1.91	0.53
1:A:122:TYR:O	1:A:126:ARG:HD3	2.08	0.53
1:A:430:TRP:CZ2	1:A:434[A]:PHE:HE1	2.26	0.53
1:A:68:LYS:HE2	1:A:72:ASP:OD1	2.09	0.53
3:A:703:1PE:H161	3:A:703:1PE:C25	2.38	0.52
1:A:399:THR:CG2	1:A:399:THR:OG1	2.52	0.52
1:A:376:GLU:HB3	6:A:720[B]:EPE:H81	1.91	0.52
1:A:221:ASN:HA	1:A:222:ASN:HB2	1.92	0.52
1:A:181:GLN:HE22	1:A:247:SER:H	1.58	0.52
1:A:228:GLU:HA	1:A:231:MET:H	1.75	0.52
1:A:58:GLY:H	1:A:102:ASN:ND2	2.08	0.51
1:A:97:VAL:H	1:A:101:ASN:ND2	2.09	0.50
1:A:377:HIS:HE1	8:A:1053:HOH:O	1.94	0.49
1:A:187:ASP:OD1	1:A:187:ASP:N	2.38	0.49
1:A:167:ARG:HH21	1:A:171:GLN:HE22	1.60	0.48
1:A:262:HIS:CE1	1:A:288:GLY:HA3	2.48	0.48
3:A:712[A]:1PE:H231	8:A:1111:HOH:O	2.13	0.48
1:A:217:GLY:O	1:A:219:ASN:HB2	2.13	0.47
1:A:431:THR:C	1:A:432[B]:ILE:HG23	2.35	0.47
1:A:134:GLU:OE2	1:A:377:HIS:CD2	2.65	0.47
3:A:702:1PE:H122	8:A:849:HOH:O	2.13	0.47
1:A:167:ARG:HH21	1:A:171:GLN:NE2	2.13	0.46
1:A:100:GLN:HA	1:A:100:GLN:NE2	2.25	0.46
1:A:152[A]:ARG:H	1:A:218[A]:ILE:HD11	1.79	0.46
1:A:379:ASP:OD2	3:A:712[B]:1PE:OH2	2.33	0.46
1:A:221:ASN:OD1	1:A:222:ASN:HB2	2.16	0.46
1:A:181:GLN:NE2	1:A:203:ALA:H	2.13	0.45
1:A:225:ILE:CG2	1:A:256:TRP:CH2	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:SER:O	1:A:331:HIS:HE1	1.99	0.45
1:A:215:VAL:H	1:A:221:ASN:CG	2.16	0.45
3:A:705[B]:1PE:H221	8:A:1215:HOH:O	2.17	0.45
1:A:430:TRP:HE3	1:A:433:GLU:OE1	2.00	0.45
6:A:721[A]:EPE:O1S	8:A:816:HOH:O	2.21	0.45
1:A:456:ASP:HB2	8:A:1114:HOH:O	2.17	0.44
1:A:234:HIS:CD2	8:A:1072:HOH:O	2.64	0.44
1:A:529:VAL:O	4:A:713:GOL:O1	2.18	0.43
1:A:2:TYR:HA	3:A:702:1PE:H221	2.00	0.43
1:A:430:TRP:CZ2	1:A:434[A]:PHE:CE1	3.06	0.43
1:A:153:ASP:HB3	1:A:218[A]:ILE:HG13	2.01	0.43
1:A:220:GLU:O	1:A:221:ASN:O	2.38	0.42
3:A:704:1PE:OH4	3:A:704:1PE:C22	2.67	0.42
1:A:215:VAL:HG11	1:A:224:ILE:HD12	2.01	0.42
1:A:221:ASN:CG	1:A:222:ASN:HB2	2.39	0.42
1:A:466[A]:ASN:ND2	1:A:508:THR:HG1	2.16	0.41
1:A:58:GLY:H	1:A:102:ASN:HD21	1.66	0.41
1:A:432[B]:ILE:HG21	1:A:432[B]:ILE:HD13	1.49	0.41
1:A:215:VAL:HG22	1:A:221:ASN:OD1	2.19	0.41
1:A:225:ILE:HG22	1:A:256:TRP:CH2	2.56	0.41
1:A:376:GLU:HB3	6:A:720[B]:EPE:C8	2.51	0.41
1:A:181:GLN:HE22	1:A:247:SER:N	2.19	0.41
1:A:230:LEU:HB2	1:A:256:TRP:HZ2	1.83	0.41
1:A:226:ASN:O	1:A:227:ARG:C	2.59	0.41
1:A:227:ARG:O	1:A:228:GLU:O	2.39	0.41
1:A:524:SER:O	1:A:544:TRP:HA	2.21	0.41
1:A:71:GLN:HE22	1:A:366:PRO:HA	1.85	0.40
1:A:432[B]:ILE:HD13	1:A:437:ASP:HB3	2.03	0.40
1:A:294:THR:HA	1:A:295:PRO:C	2.42	0.40
1:A:424:GLY:HA3	1:A:437:ASP:O	2.21	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	612/609 (100%)	580 (95%)	22 (4%)	10 (2%)	9 1

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218[A]	ILE
1	A	218[B]	ILE
1	A	219	ASN
1	A	220	GLU
1	A	221	ASN
1	A	228	GLU
1	A	433	GLU
1	A	434[A]	PHE
1	A	222	ASN
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	496/490 (101%)	480 (97%)	16 (3%)	39 16

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

Mol	Chain	Res	Type
1	A	36	GLU
1	A	63	LYS
1	A	90	MET
1	A	98	HIS
1	A	100	GLN
1	A	167	ARG
1	A	186	LYS
1	A	215	VAL
1	A	216	ASP

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Mol	Chain	Res	Type
1	A	219	ASN
1	A	220	GLU
1	A	225	ILE
1	A	290	ASP
1	A	294	THR
1	A	394	ASN
1	A	433	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
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	199	ASN
1	A	222	ASN
1	A	234	HIS
1	A	262	HIS
1	A	331	HIS
1	A	377	HIS
1	A	394	ASN
1	A	435	GLN
1	A	581	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

27 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	$\#\|Z\| > 2$
5	SO4	A	718	-	4,4,4	0.46	0	6,6,6	0.57	0
3	1PE	A	703	-	5,5,15	0.66	0	4,4,14	0.87	0
3	1PE	A	707	-	5,5,15	0.63	0	4,4,14	0.78	0
3	1PE	A	704	-	6,6,15	0.37	0	5,5,14	0.83	0
3	1PE	A	706	-	5,5,15	0.68	0	4,4,14	1.26	1 (25%)
4	GOL	A	713	-	5,5,5	0.38	0	5,5,5	1.02	0
3	1PE	A	705[A]	-	5,5,15	0.93	0	4,4,14	1.29	1 (25%)
3	1PE	A	712[A]	-	12,12,15	0.84	0	11,11,14	1.10	1 (9%)
7	ACT	A	723	-	3,3,3	0.96	0	3,3,3	2.69	2 (66%)
3	1PE	A	705[B]	-	5,5,15	1.16	0	4,4,14	2.27	1 (25%)
4	GOL	A	715	-	5,5,5	0.92	0	5,5,5	0.89	0
3	1PE	A	712[B]	-	12,10,15	0.68	0	11,9,14	0.81	0
3	1PE	A	710[A]	-	7,7,15	0.93	0	6,6,14	1.39	1 (16%)
6	EPE	A	721[A]	-	15,15,15	1.65	3 (20%)	18,20,20	4.02	10 (55%)
5	SO4	A	717	-	4,4,4	0.54	0	6,6,6	0.82	0
5	SO4	A	719	-	4,4,4	1.25	1 (25%)	6,6,6	1.79	2 (33%)
3	1PE	A	702	-	6,6,15	0.51	0	5,5,14	0.68	0
3	1PE	A	710[B]	-	7,7,15	0.98	0	6,6,14	1.33	1 (16%)
3	1PE	A	711	-	4,4,15	0.84	0	3,3,14	0.44	0
4	GOL	A	714	-	5,5,5	0.64	0	5,5,5	1.28	0
2	6BV	A	701	-	23,24,24	1.56	5 (21%)	29,35,35	3.27	10 (34%)
3	1PE	A	708	-	4,4,15	0.99	0	3,3,14	1.68	1 (33%)
7	ACT	A	724	-	3,3,3	0.67	0	3,3,3	1.18	0
4	GOL	A	716	-	5,5,5	0.42	0	5,5,5	1.08	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
3	1PE	A	703	-	-	2/3/3/13	-
3	1PE	A	707	-	-	1/3/3/13	-
3	1PE	A	704	-	-	1/4/4/13	-
3	1PE	A	706	-	-	3/3/3/13	-
4	GOL	A	713	-	-	4/4/4/4	-
3	1PE	A	705[A]	-	-	1/3/3/13	-
3	1PE	A	712[A]	-	-	5/10/10/13	-
3	1PE	A	705[B]	-	-	2/3/3/13	-
4	GOL	A	715	-	-	4/4/4/4	-
3	1PE	A	712[B]	-	-	3/10/8/13	-
3	1PE	A	710[A]	-	-	3/5/5/13	-
6	EPE	A	721[A]	-	-	5/9/19/19	0/1/1/1
3	1PE	A	702	-	-	3/4/4/13	-
3	1PE	A	710[B]	-	-	4/5/5/13	-
3	1PE	A	711	-	-	0/2/2/13	-
4	GOL	A	714	-	-	2/4/4/4	-
2	6BV	A	701	-	-	2/8/48/48	0/2/2/2
3	1PE	A	708	-	-	2/2/2/13	-
4	GOL	A	716	-	-	4/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	721[A]	EPE	C10-S	-3.39	1.72	1.77
2	A	701	6BV	C12-C22	3.34	1.59	1.53
6	A	721[A]	EPE	O2S-S	2.84	1.53	1.45
2	A	701	6BV	O02-C52	-2.79	1.37	1.44
2	A	701	6BV	O32-C32	2.72	1.49	1.43
6	A	721[A]	EPE	C3-C2	2.35	1.60	1.51
2	A	701	6BV	C42-C52	2.23	1.57	1.53
5	A	719	SO4	O2-S	2.11	1.57	1.46
2	A	701	6BV	O02-C12	2.10	1.45	1.42

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	6BV	C12-O02-C52	8.80	128.81	112.58
2	A	701	6BV	O02-C12-C22	-8.58	99.52	110.31
6	A	721[A]	EPE	O1S-S-C10	8.19	116.78	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	721[A]	EPE	O3S-S-O1S	-6.74	94.80	111.27
2	A	701	6BV	C22-C12-S12	-6.66	101.03	111.30
6	A	721[A]	EPE	C9-N1-C2	6.63	128.20	111.23
2	A	701	6BV	C12-C22-C32	6.55	123.53	110.59
6	A	721[A]	EPE	C5-N4-C3	5.26	120.68	108.83
6	A	721[A]	EPE	C7-N4-C3	4.96	123.92	111.23
6	A	721[A]	EPE	C6-N1-C2	4.90	119.86	108.83
3	A	705[B]	1PE	OH3-C22-C12	4.23	128.67	110.07
6	A	721[A]	EPE	O3S-S-C10	4.11	112.42	105.77
6	A	721[A]	EPE	C5-C6-N1	-3.95	102.55	110.64
7	A	723	ACT	O-C-CH3	-3.63	108.19	122.33
2	A	701	6BV	C62-C52-C42	-3.49	104.83	113.00
2	A	701	6BV	O42-C42-C52	3.47	117.92	109.30
5	A	719	SO4	O4-S-O3	-2.85	96.91	109.06
2	A	701	6BV	C11-O01-C51	2.82	118.97	113.66
3	A	710[A]	1PE	OH3-C23-C13	2.80	123.02	110.39
3	A	710[B]	1PE	OH3-C23-C13	2.80	123.02	110.39
7	A	723	ACT	OXT-C-CH3	2.80	126.73	115.18
3	A	708	1PE	OH2-C12-C22	-2.79	95.60	111.81
5	A	719	SO4	O4-S-O2	2.77	123.78	109.31
2	A	701	6BV	O02-C52-C62	2.74	113.24	106.44
2	A	701	6BV	C12-S12-C31	2.70	108.51	100.26
6	A	721[A]	EPE	C6-C5-N4	-2.69	105.12	110.64
2	A	701	6BV	O22-C22-C12	-2.52	105.64	110.27
3	A	706	1PE	C23-OH3-C22	2.47	121.74	112.90
6	A	721[A]	EPE	O2S-S-C10	2.34	109.74	106.92
3	A	712[A]	1PE	OH3-C22-C12	-2.32	99.87	110.07
3	A	705[A]	1PE	OH2-C12-C22	2.03	123.58	111.81

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	713	GOL	O1-C1-C2-C3
4	A	714	GOL	O1-C1-C2-C3
4	A	715	GOL	O1-C1-C2-O2
4	A	715	GOL	O1-C1-C2-C3
4	A	716	GOL	O1-C1-C2-C3
6	A	721[A]	EPE	C8-C7-N4-C5
6	A	721[A]	EPE	C9-C10-S-O1S
6	A	721[A]	EPE	C9-C10-S-O3S
3	A	710[A]	1PE	C13-C23-OH3-C22

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Mol	Chain	Res	Type	Atoms
3	A	704	1PE	C13-C23-OH3-C22
3	A	712[A]	1PE	C14-C24-OH4-C13
3	A	703	1PE	C16-C26-OH6-C15
3	A	705[B]	1PE	C12-C22-OH3-C23
3	A	710[A]	1PE	OH4-C13-C23-OH3
3	A	710[B]	1PE	OH4-C13-C23-OH3
3	A	702	1PE	OH2-C12-C22-OH3
3	A	712[B]	1PE	OH2-C12-C22-OH3
2	A	701	6BV	O01-C51-C61-O61
3	A	705[A]	1PE	C12-C22-OH3-C23
4	A	714	GOL	O1-C1-C2-O2
3	A	712[A]	1PE	OH2-C12-C22-OH3
4	A	713	GOL	C1-C2-C3-O3
4	A	713	GOL	O1-C1-C2-O2
4	A	716	GOL	O1-C1-C2-O2
3	A	710[B]	1PE	C13-C23-OH3-C22
3	A	702	1PE	OH4-C13-C23-OH3
3	A	712[A]	1PE	OH4-C13-C23-OH3
4	A	716	GOL	O2-C2-C3-O3
3	A	702	1PE	C13-C23-OH3-C22
3	A	706	1PE	OH2-C12-C22-OH3
4	A	715	GOL	O2-C2-C3-O3
4	A	713	GOL	O2-C2-C3-O3
3	A	708	1PE	OH2-C12-C22-OH3
4	A	715	GOL	C1-C2-C3-O3
3	A	712[B]	1PE	C12-C22-OH3-C23
3	A	710[B]	1PE	OH2-C12-C22-OH3
6	A	721[A]	EPE	C9-C10-S-O2S
2	A	701	6BV	O02-C52-C62-O62
3	A	706	1PE	C13-C23-OH3-C22
3	A	712[A]	1PE	C12-C22-OH3-C23
3	A	705[B]	1PE	OH2-C12-C22-OH3
6	A	721[A]	EPE	C10-C9-N1-C6
3	A	706	1PE	C12-C22-OH3-C23
3	A	708	1PE	C12-C22-OH3-C23
3	A	712[A]	1PE	C13-C23-OH3-C22
3	A	712[B]	1PE	OH4-C13-C23-OH3
3	A	707	1PE	C13-C23-OH3-C22
3	A	703	1PE	C25-C15-OH6-C26
3	A	710[A]	1PE	C12-C22-OH3-C23
4	A	716	GOL	C1-C2-C3-O3
3	A	710[B]	1PE	C12-C22-OH3-C23

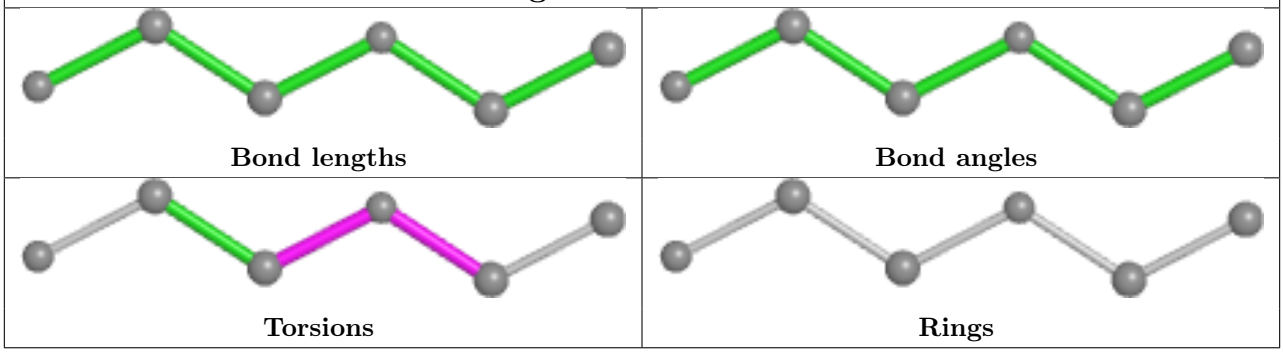
There are no ring outliers.

14 monomers are involved in 21 short contacts:

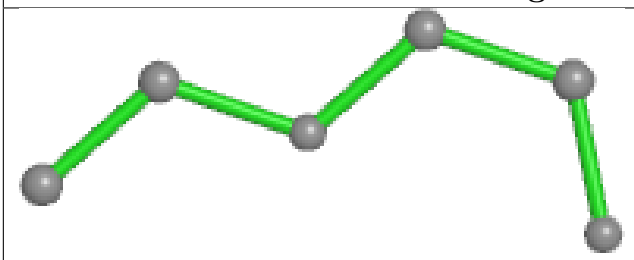
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	1PE	1	0
3	A	704	1PE	1	0
4	A	713	GOL	3	0
3	A	712[A]	1PE	1	0
7	A	723	ACT	1	0
3	A	705[B]	1PE	1	0
3	A	712[B]	1PE	2	0
3	A	710[A]	1PE	1	0
6	A	721[A]	EPE	1	0
3	A	702	1PE	2	0
3	A	710[B]	1PE	1	0
4	A	714	GOL	1	0
2	A	701	6BV	4	0
4	A	716	GOL	1	0

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

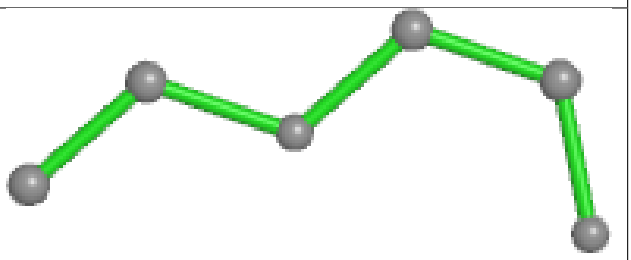
Ligand 1PE A 703



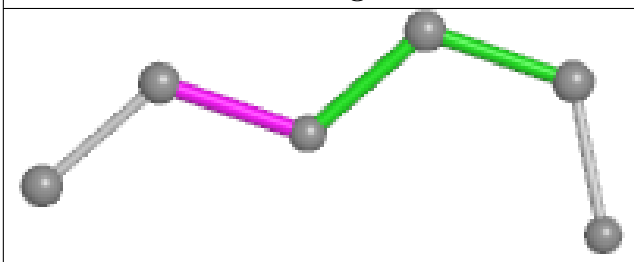
Ligand 1PE A 707



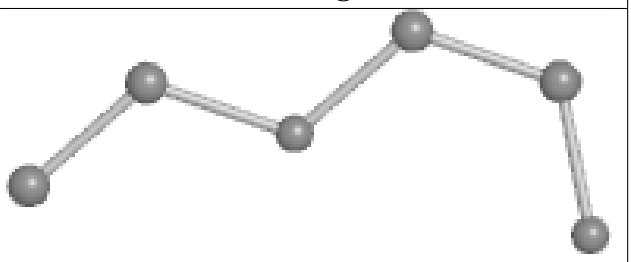
Bond lengths



Bond angles

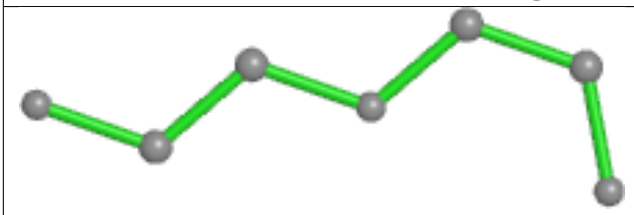


Torsions

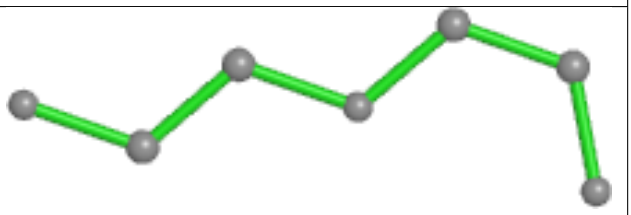


Rings

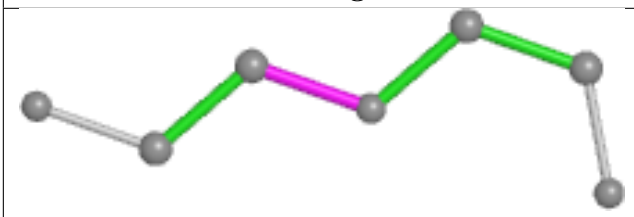
Ligand 1PE A 704



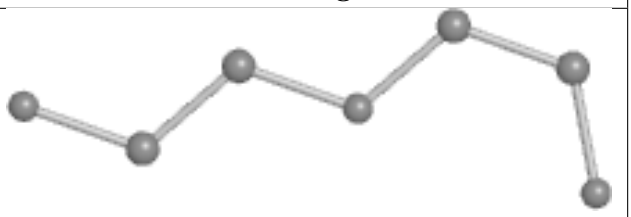
Bond lengths



Bond angles

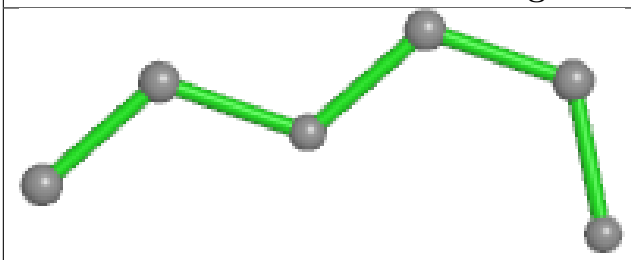


Torsions

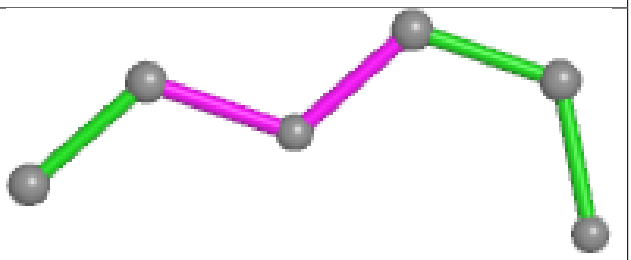


Rings

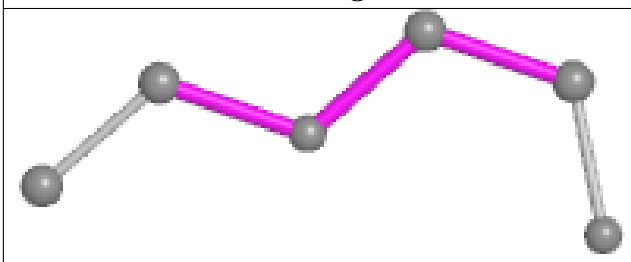
Ligand 1PE A 706



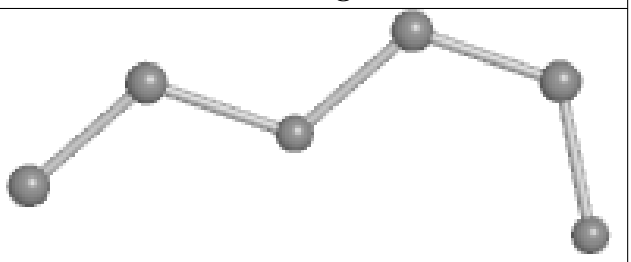
Bond lengths



Bond angles

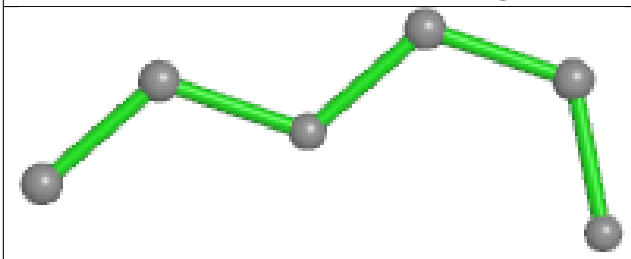


Torsions

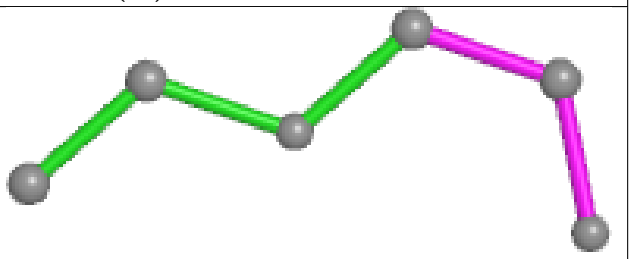


Rings

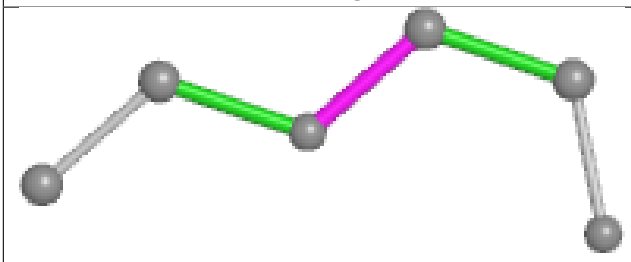
Ligand 1PE A 705 (A)



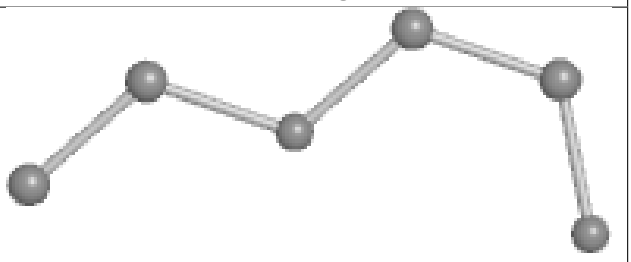
Bond lengths



Bond angles

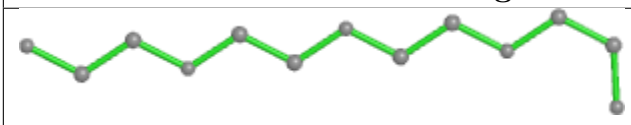


Torsions

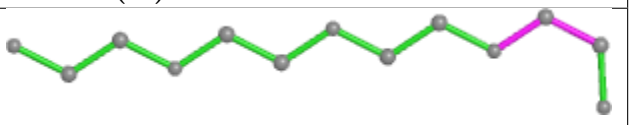


Rings

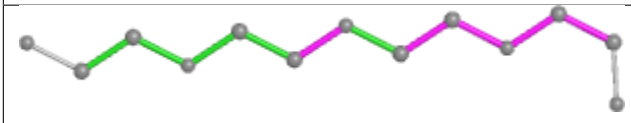
Ligand 1PE A 712 (A)



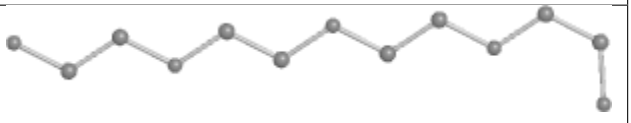
Bond lengths



Bond angles

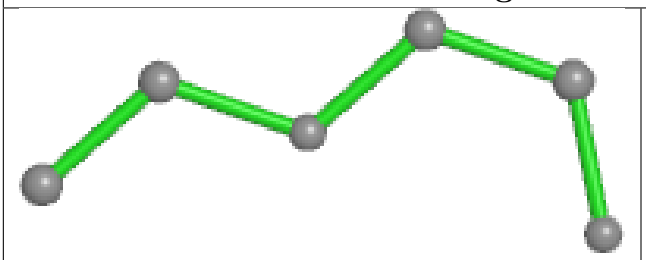


Torsions

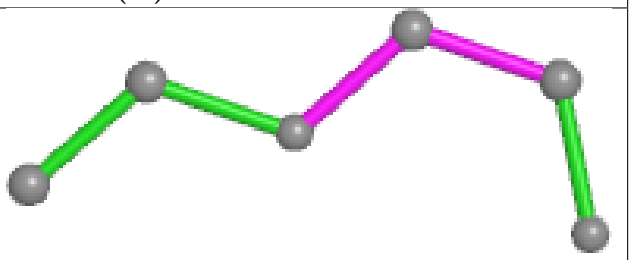


Rings

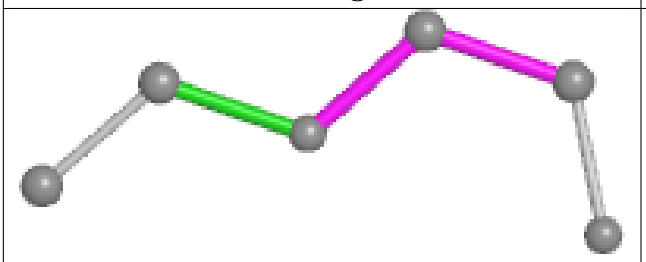
Ligand 1PE A 705 (B)



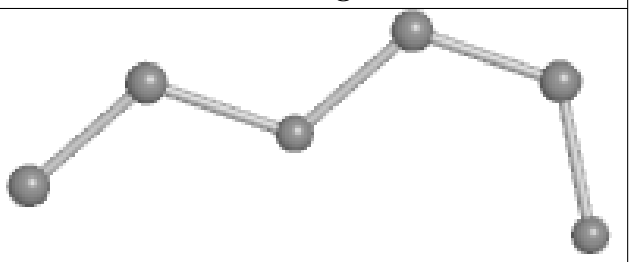
Bond lengths



Bond angles

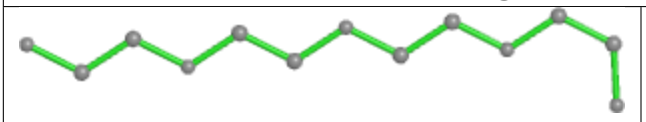


Torsions

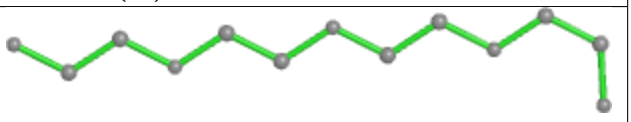


Rings

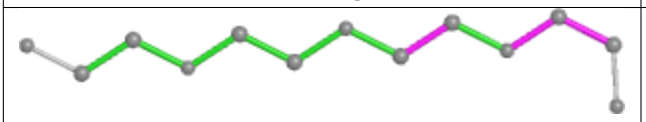
Ligand 1PE A 712 (B)



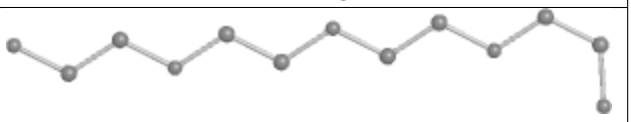
Bond lengths



Bond angles

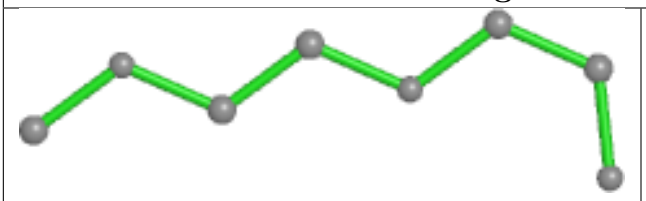


Torsions

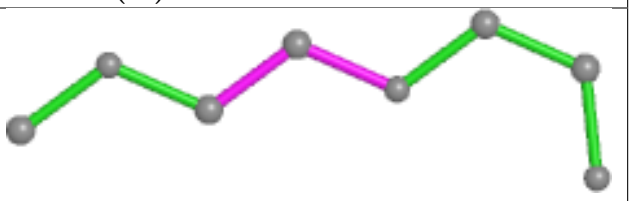


Rings

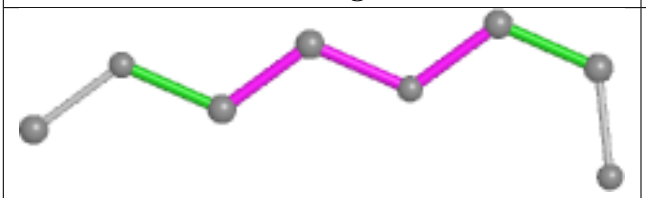
Ligand 1PE A 710 (A)



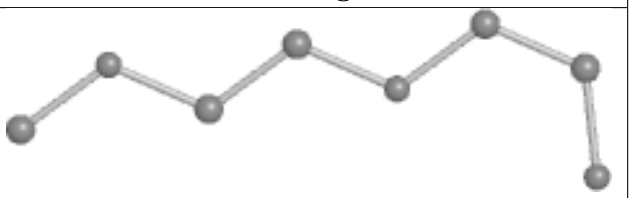
Bond lengths



Bond angles

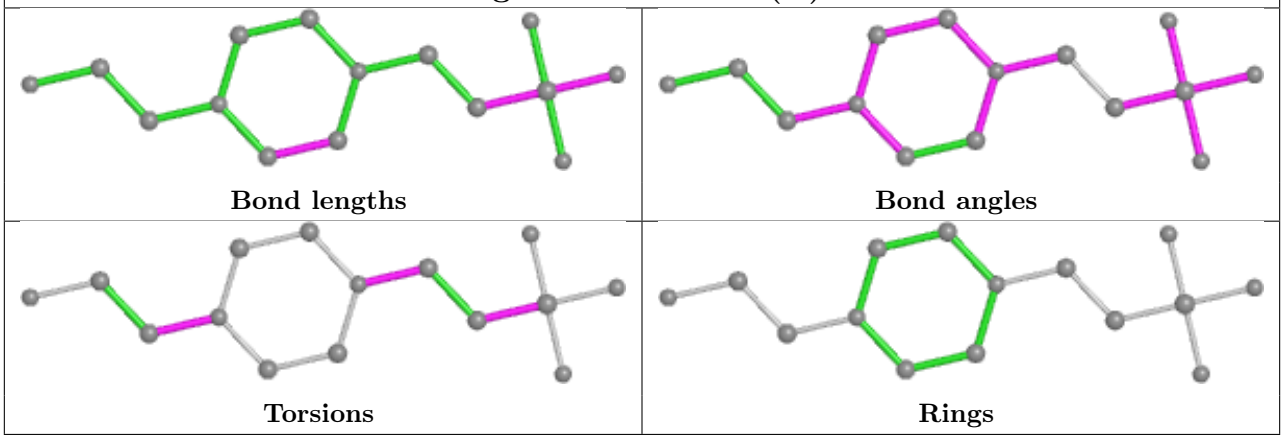


Torsions

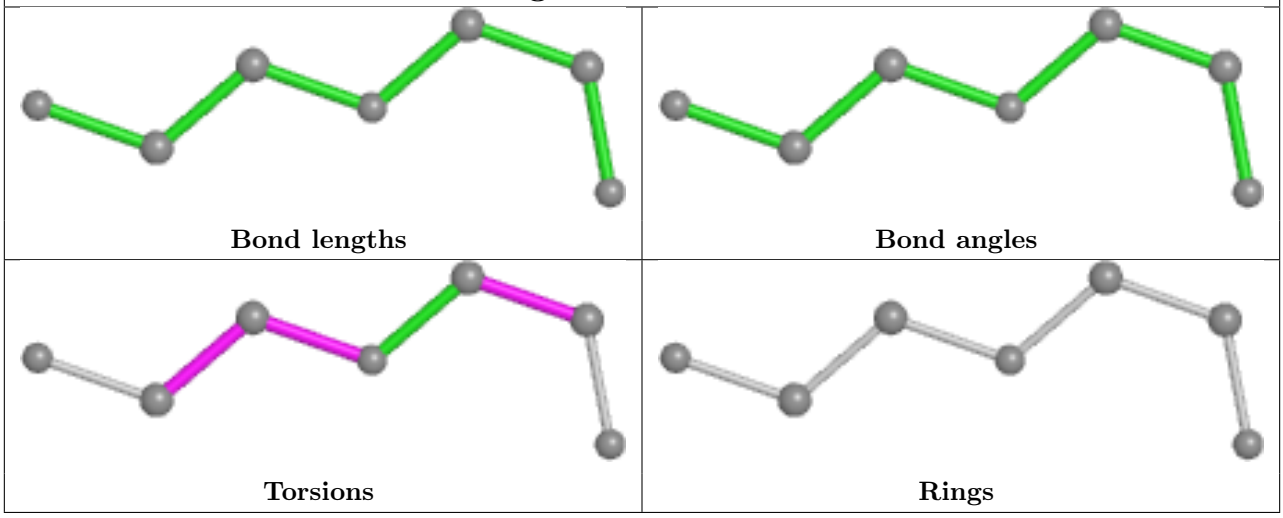


Rings

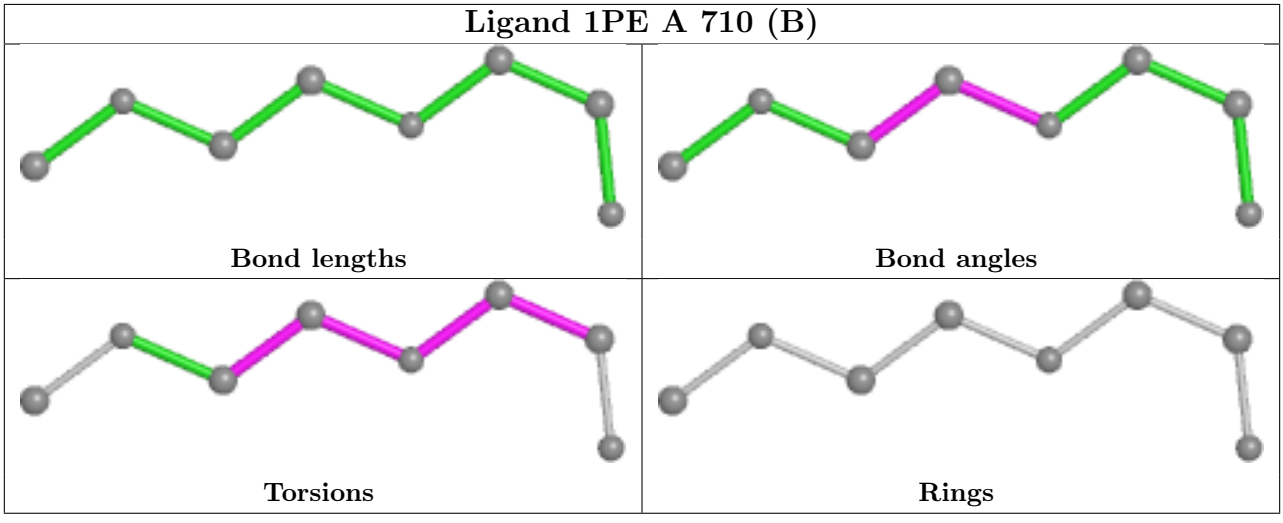
Ligand EPE A 721 (A)



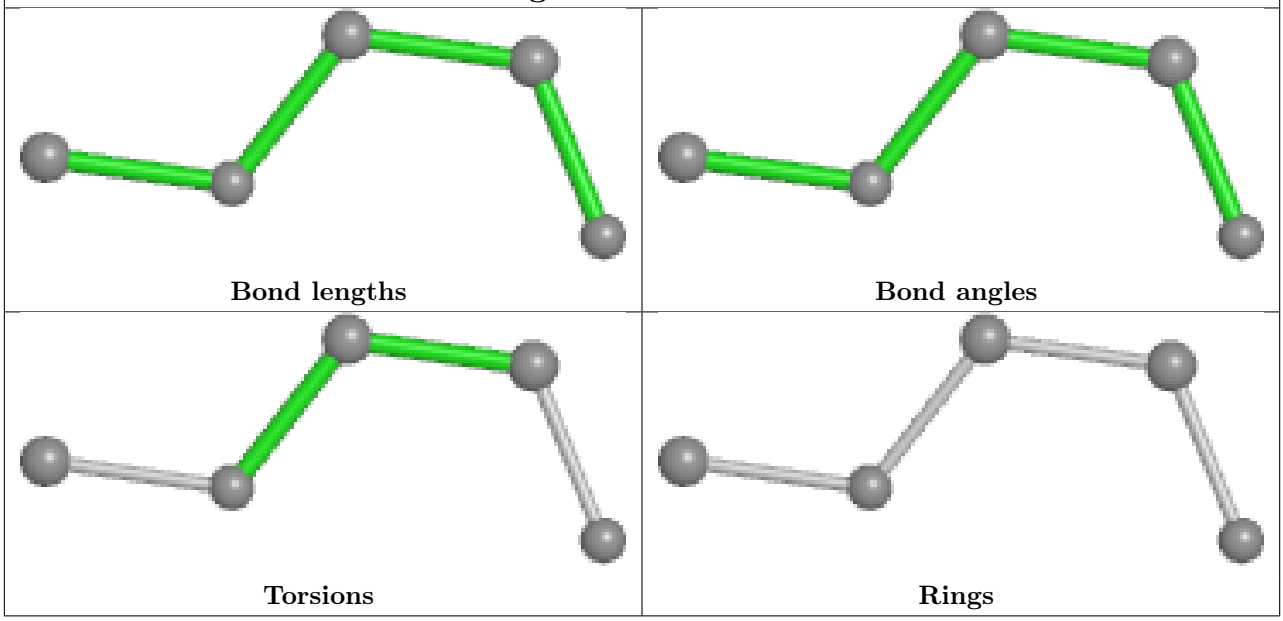
Ligand 1PE A 702



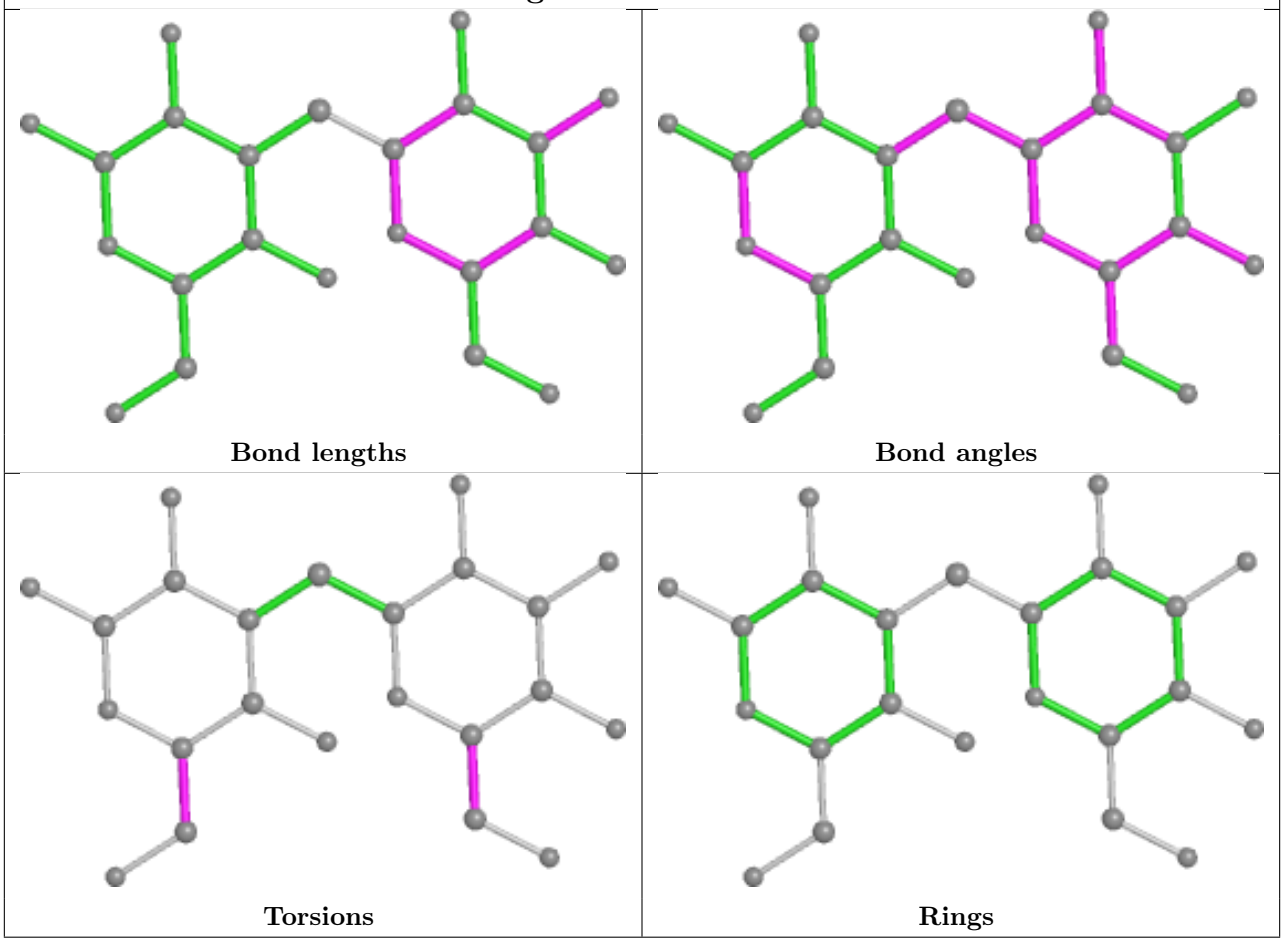
Ligand 1PE A 710 (B)



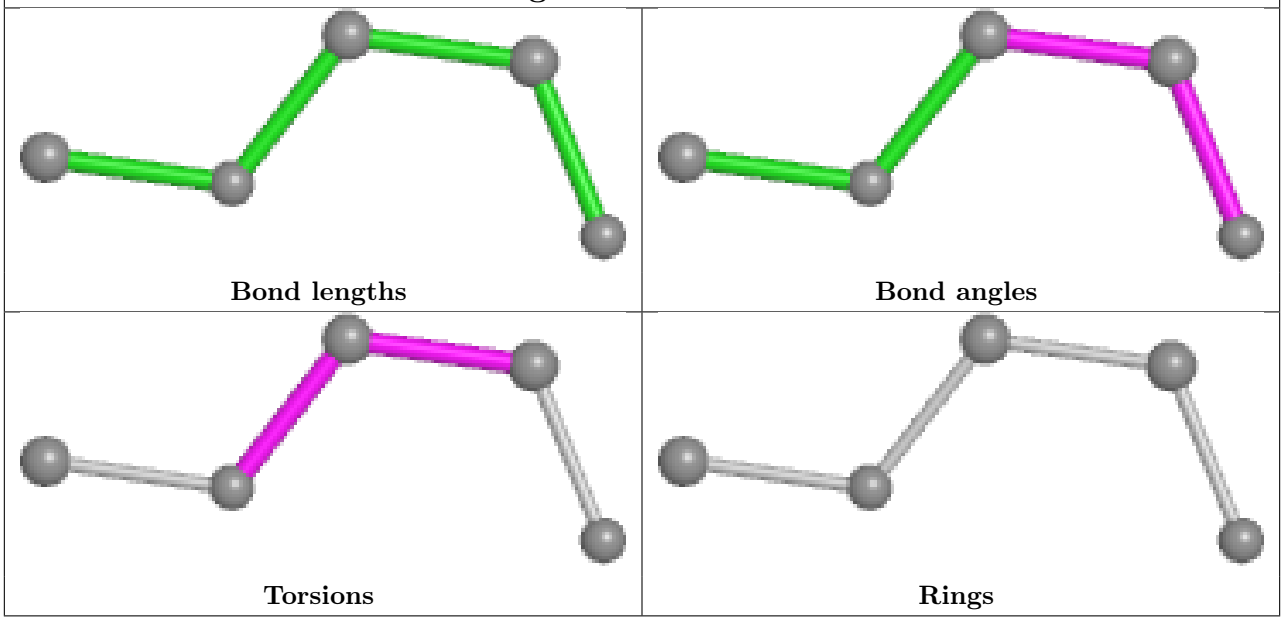
Ligand 1PE A 711



Ligand 6BV A 701



Ligand 1PE A 708



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, 95^{th} 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	603/609 (99%)	0.30	46 (7%)	13	18	13, 20, 46, 115	7 (1%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	224	ILE	16.1
1	A	225	ILE	11.8
1	A	215	VAL	9.9
1	A	223	THR	9.6
1	A	226	ASN	7.0
1	A	216	ASP	6.1
1	A	585	ALA	6.0
1	A	221	ASN	5.8
1	A	586	HIS	5.8
1	A	231	MET	5.8
1	A	220	GLU	5.7
1	A	228	GLU	5.6
1	A	432[A]	ILE	5.6
1	A	434[A]	PHE	4.9
1	A	187	ASP	4.9
1	A	438	THR	4.7
1	A	496	ASN	4.5
1	A	218[A]	ILE	4.3
1	A	584[B]	ASP	3.9
1	A	257	ASN	3.7
1	A	227	ARG	3.7
1	A	440	ARG	3.7
1	A	186	LYS	3.6
1	A	217	GLY	3.6
1	A	188	PHE	3.5
1	A	232	ASN	3.5
1	A	256	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	222	ASN	3.5
1	A	437	ASP	3.5
1	A	0	ALA	3.2
1	A	494	GLY	3.1
1	A	294	THR	3.0
1	A	582	VAL	3.0
1	A	497	LEU	2.9
1	A	504	PRO	2.8
1	A	185	PRO	2.6
1	A	435	GLN	2.4
1	A	587	TYR	2.3
1	A	436	GLY	2.3
1	A	295	PRO	2.3
1	A	492	THR	2.2
1	A	583	GLY	2.2
1	A	493	LYS	2.1
1	A	94	ILE	2.1
1	A	9	THR	2.0
1	A	441	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EPE	A	722[B]	15/15	0.58	0.32	36,46,70,70	15
6	EPE	A	721[A]	15/15	0.62	0.32	26,49,65,68	15
3	1PE	A	709[A]	11/16	0.64	0.30	53,59,65,73	0
7	ACT	A	723	4/4	0.66	0.18	47,48,53,54	0

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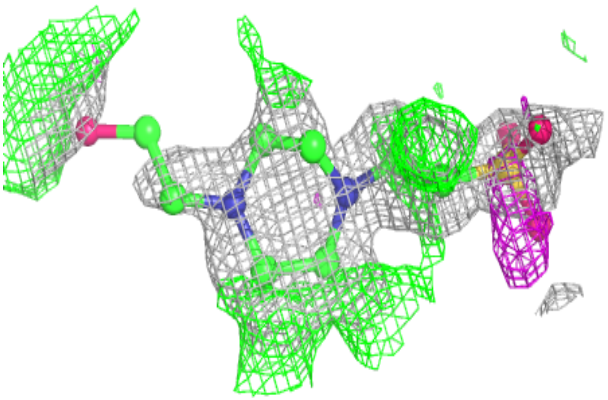
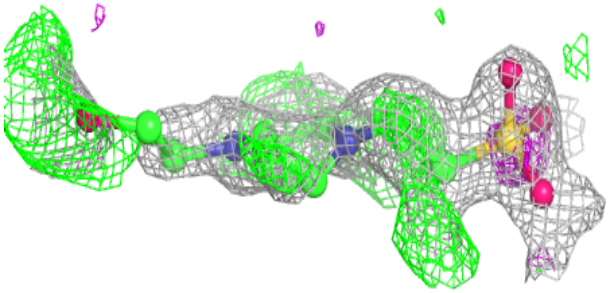
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	1PE	A	705[A]	6/16	0.76	0.23	13,27,39,46	2
3	1PE	A	705[B]	6/16	0.76	0.23	26,30,39,46	2
3	1PE	A	710[B]	8/16	0.77	0.26	39,49,64,72	3
3	1PE	A	710[A]	8/16	0.77	0.26	39,49,64,72	3
6	EPE	A	720[B]	15/15	0.79	0.23	22,38,85,91	15
3	1PE	A	707	6/16	0.80	0.20	56,61,68,69	0
3	1PE	A	703	6/16	0.80	0.17	57,62,66,69	0
7	ACT	A	724	4/4	0.82	0.47	54,59,60,63	0
3	1PE	A	711	5/16	0.83	0.18	47,58,60,65	0
3	1PE	A	706	6/16	0.83	0.17	53,53,65,70	0
4	GOL	A	714	6/6	0.85	0.17	43,51,54,72	0
3	1PE	A	702	7/16	0.89	0.29	48,57,62,65	0
3	1PE	A	712[B]	11/16	0.90	0.20	20,24,58,59	6
3	1PE	A	708	5/16	0.90	0.14	32,32,47,49	0
5	SO4	A	719	5/5	0.90	0.30	30,38,56,57	0
3	1PE	A	712[A]	13/16	0.90	0.20	18,35,58,59	8
5	SO4	A	717	5/5	0.91	0.20	37,38,42,42	5
5	SO4	A	718	5/5	0.91	0.17	34,49,52,53	5
3	1PE	A	704	7/16	0.92	0.32	34,49,57,61	0
2	6BV	A	701	23/23	0.94	0.18	12,19,44,51	23
4	GOL	A	715	6/6	0.94	0.12	20,27,30,30	0
4	GOL	A	716	6/6	0.96	0.12	20,34,41,47	0
4	GOL	A	713	6/6	0.97	0.16	30,33,34,41	6

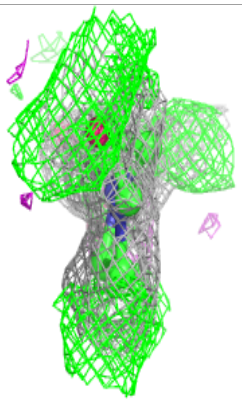
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EPE A 721 (A):

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

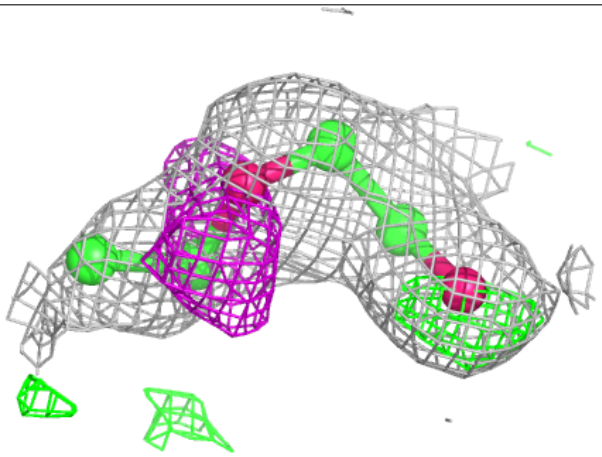


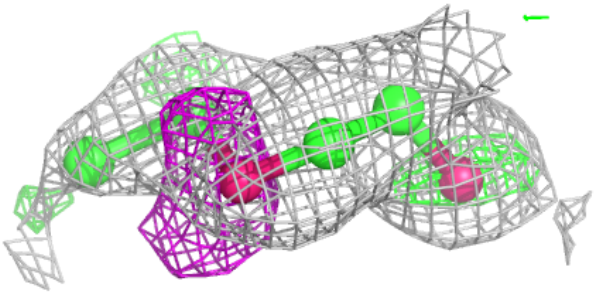


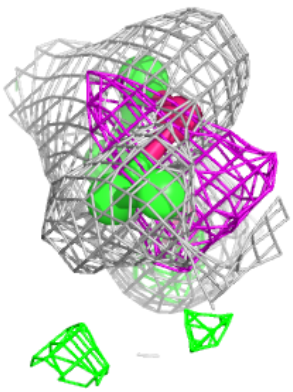


Electron density around 1PE A 705 (A):

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

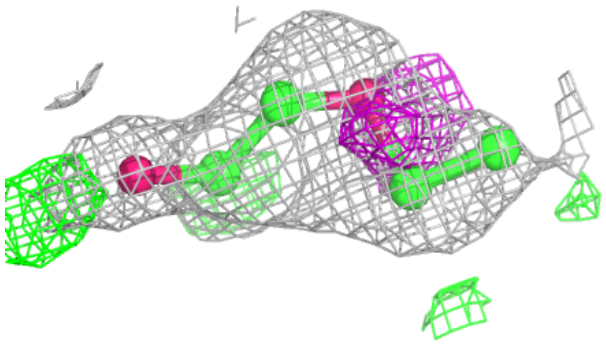


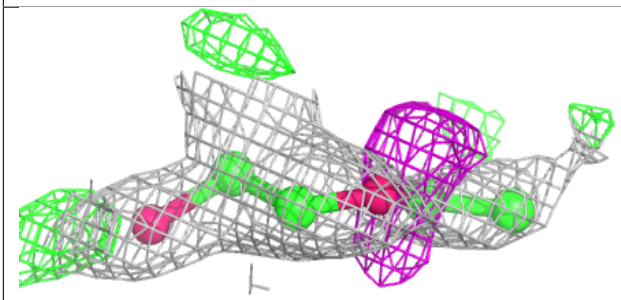


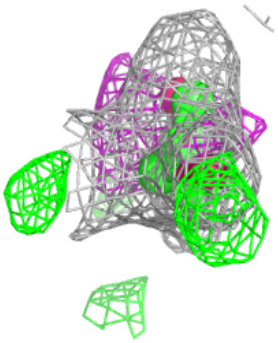


Electron density around 1PE A 705 (B):

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

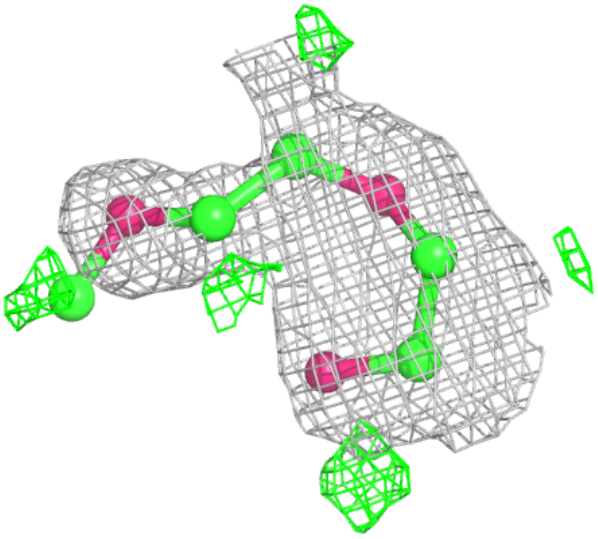


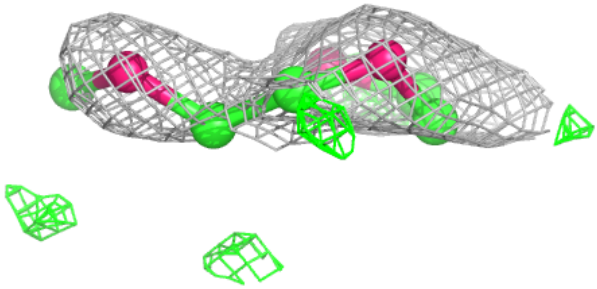


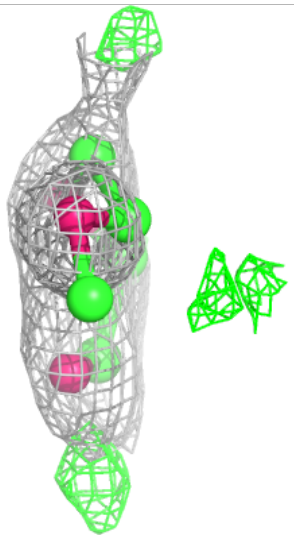


Electron density around 1PE A 710 (B):

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

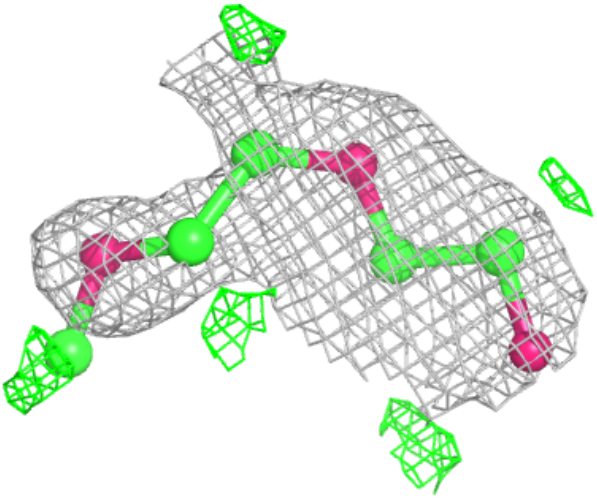


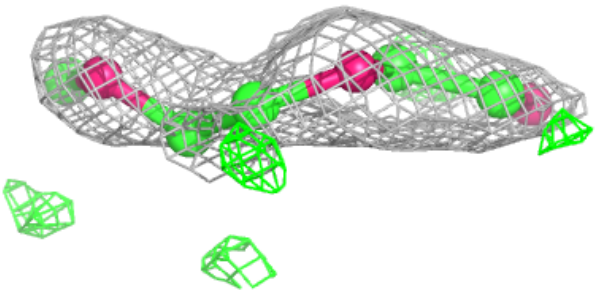


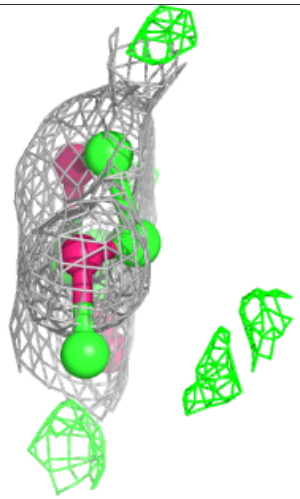


Electron density around 1PE A 710 (A):

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

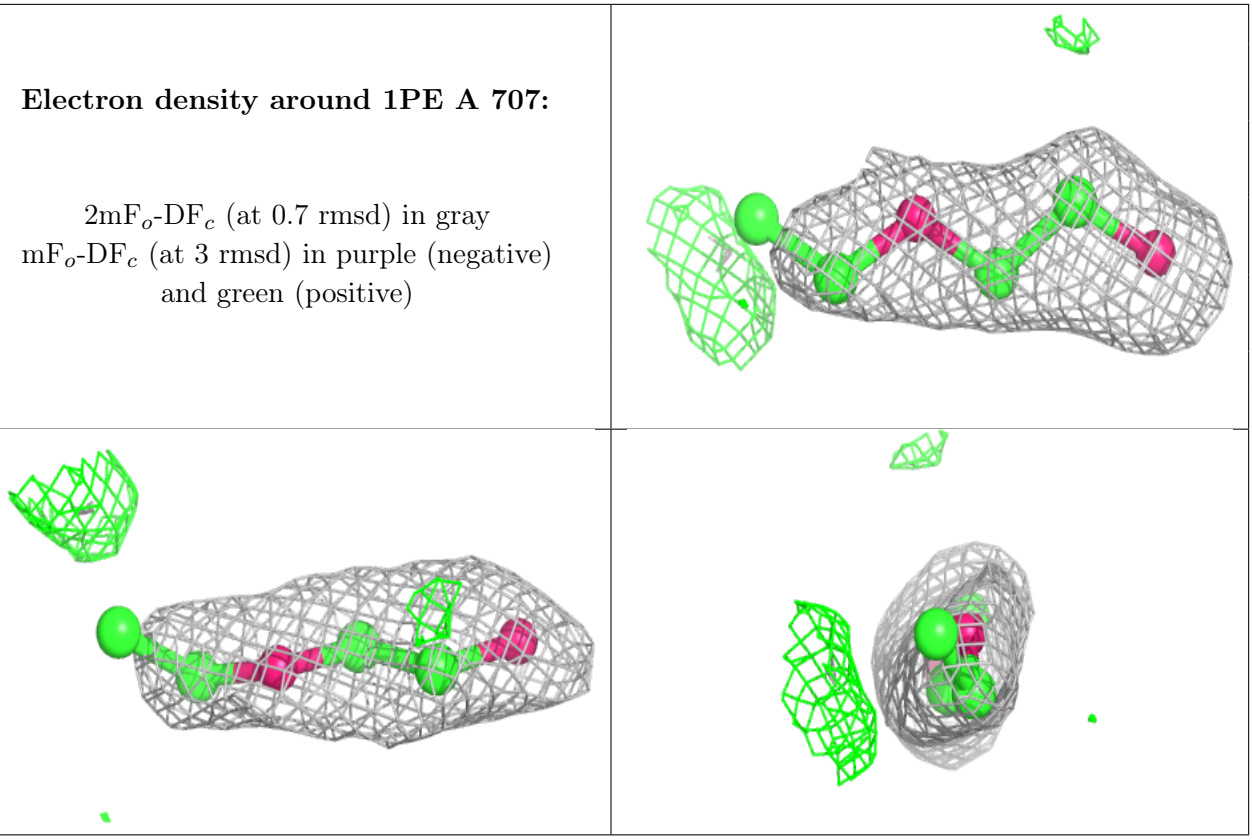






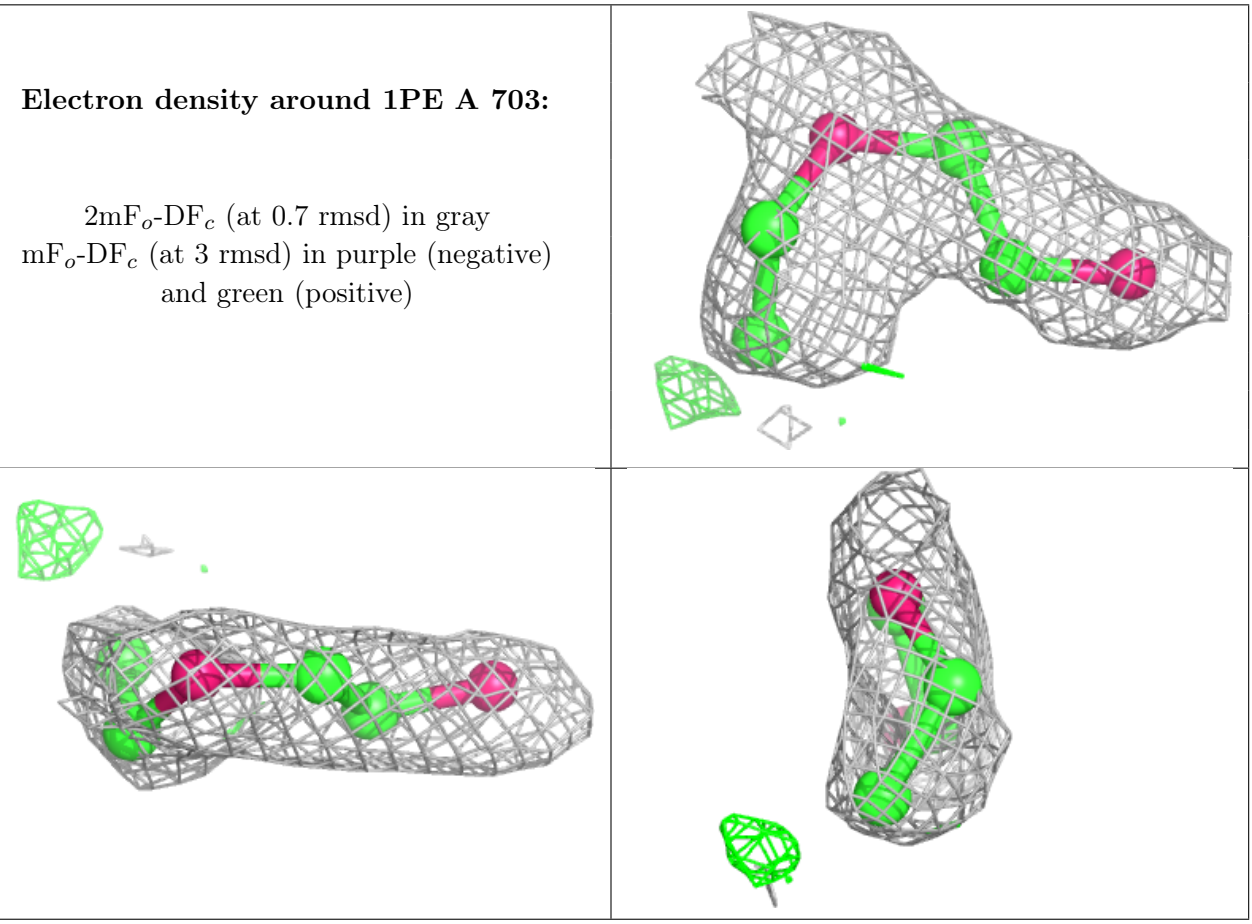
Electron density around 1PE A 707:

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



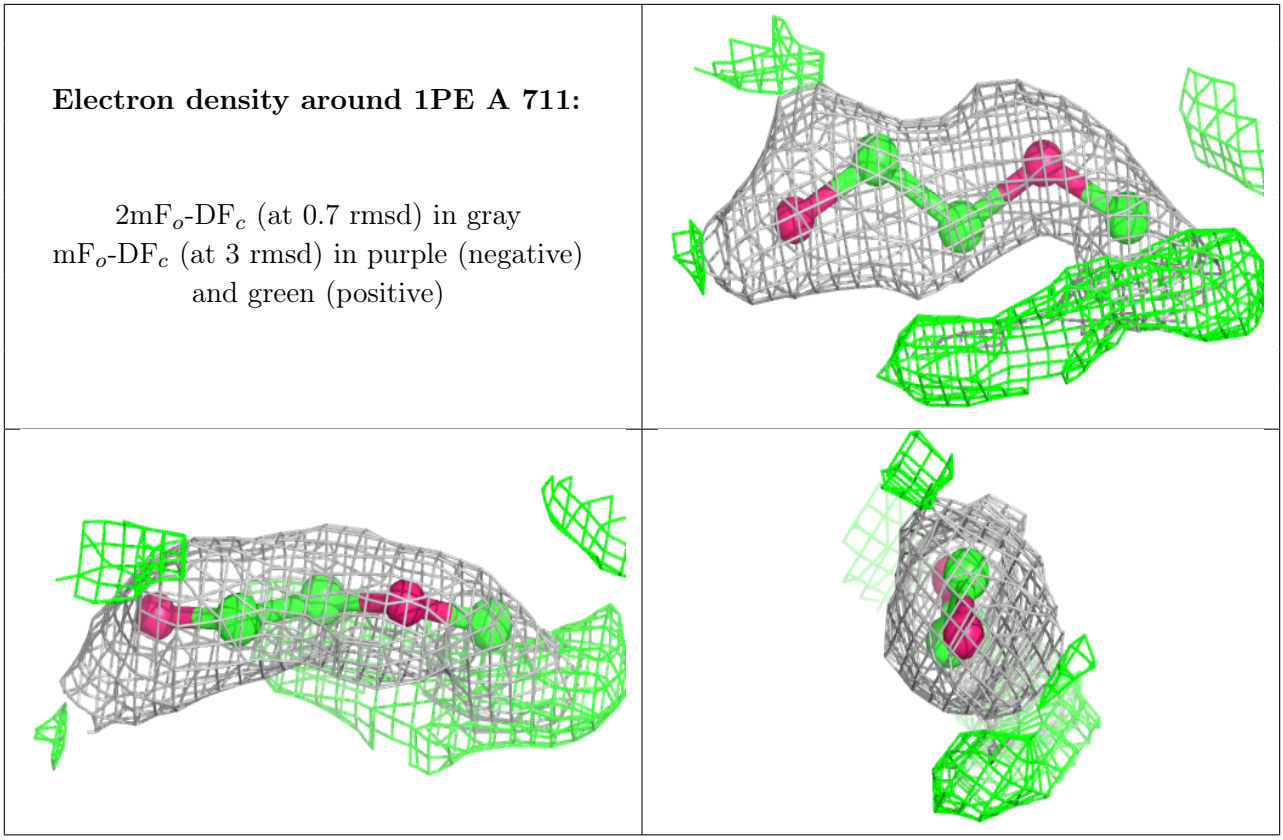
Electron density around 1PE A 703:

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



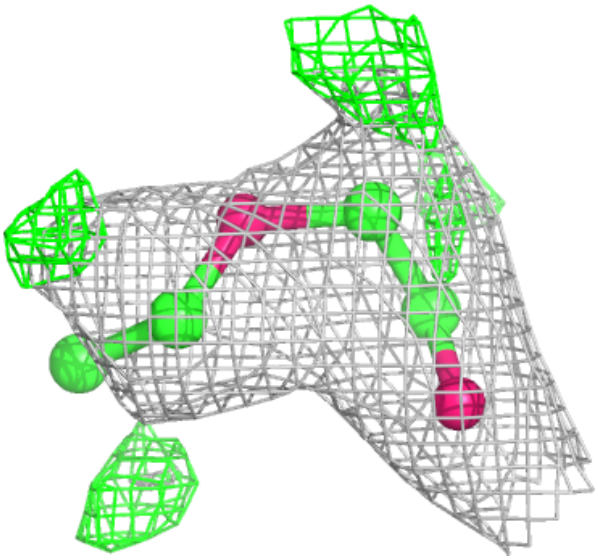
Electron density around 1PE A 711:

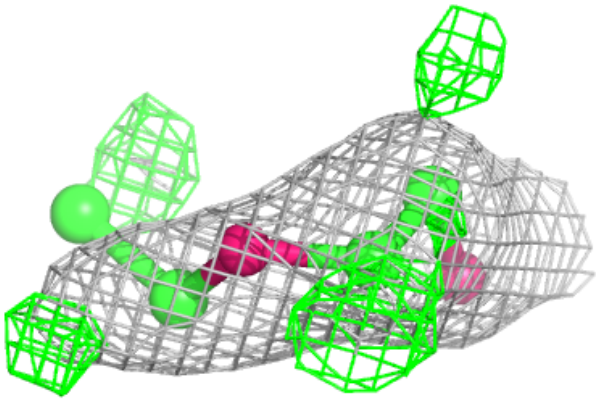
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

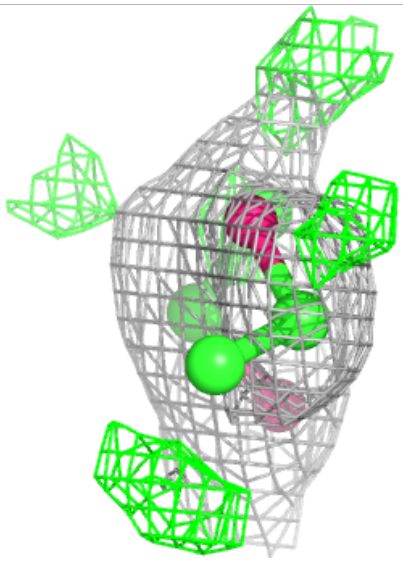


Electron density around 1PE A 706:

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

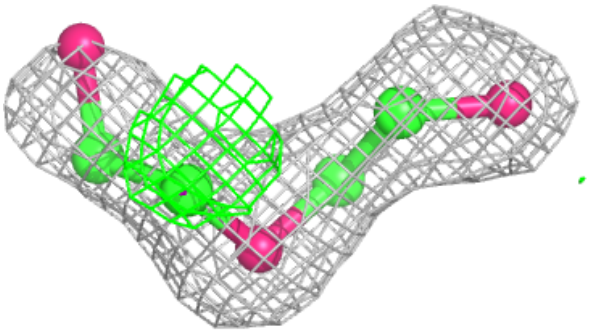


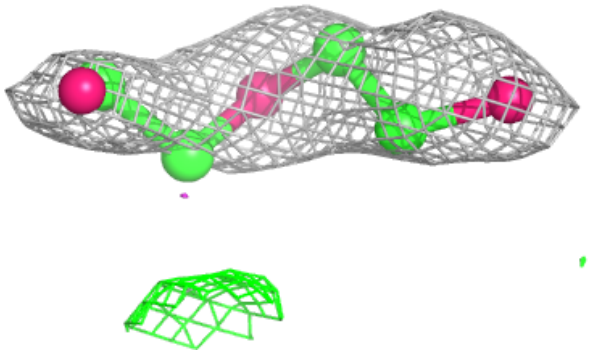


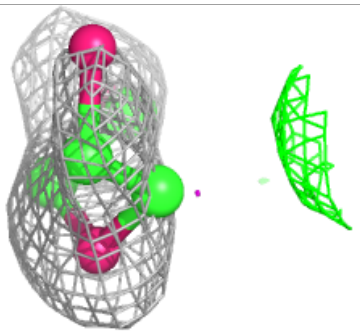


Electron density around 1PE A 702:

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

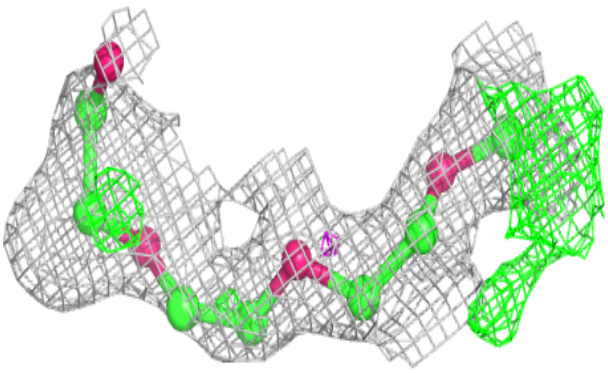


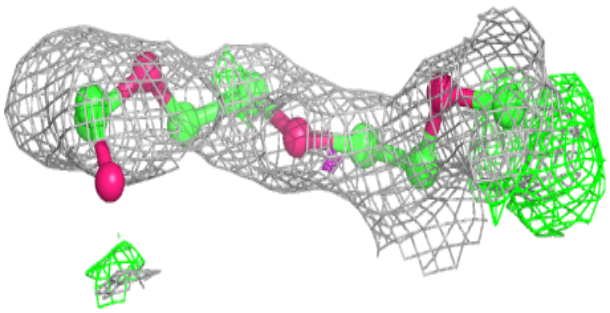


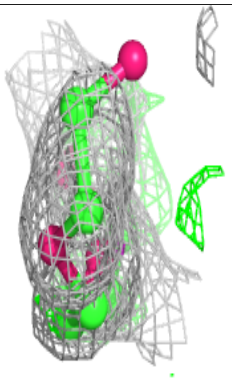


Electron density around 1PE A 712 (B):

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

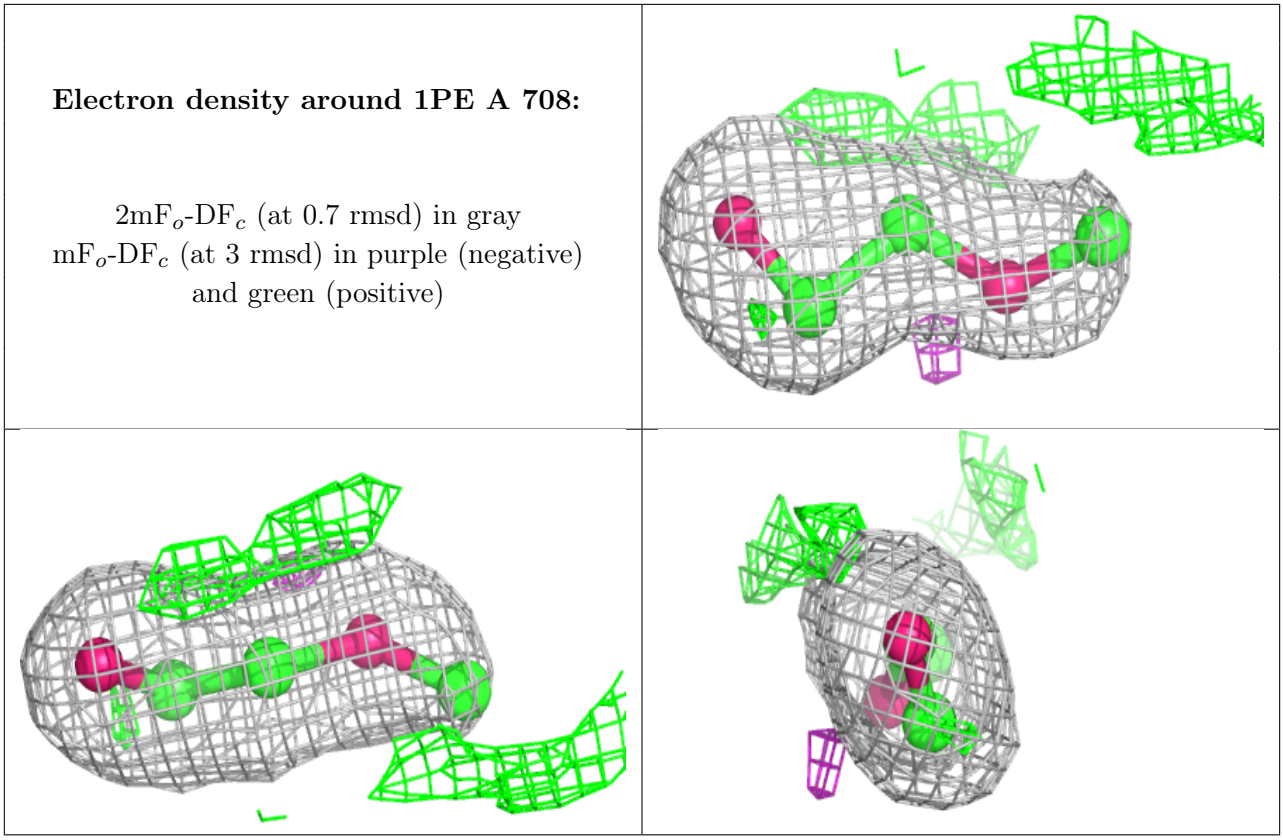






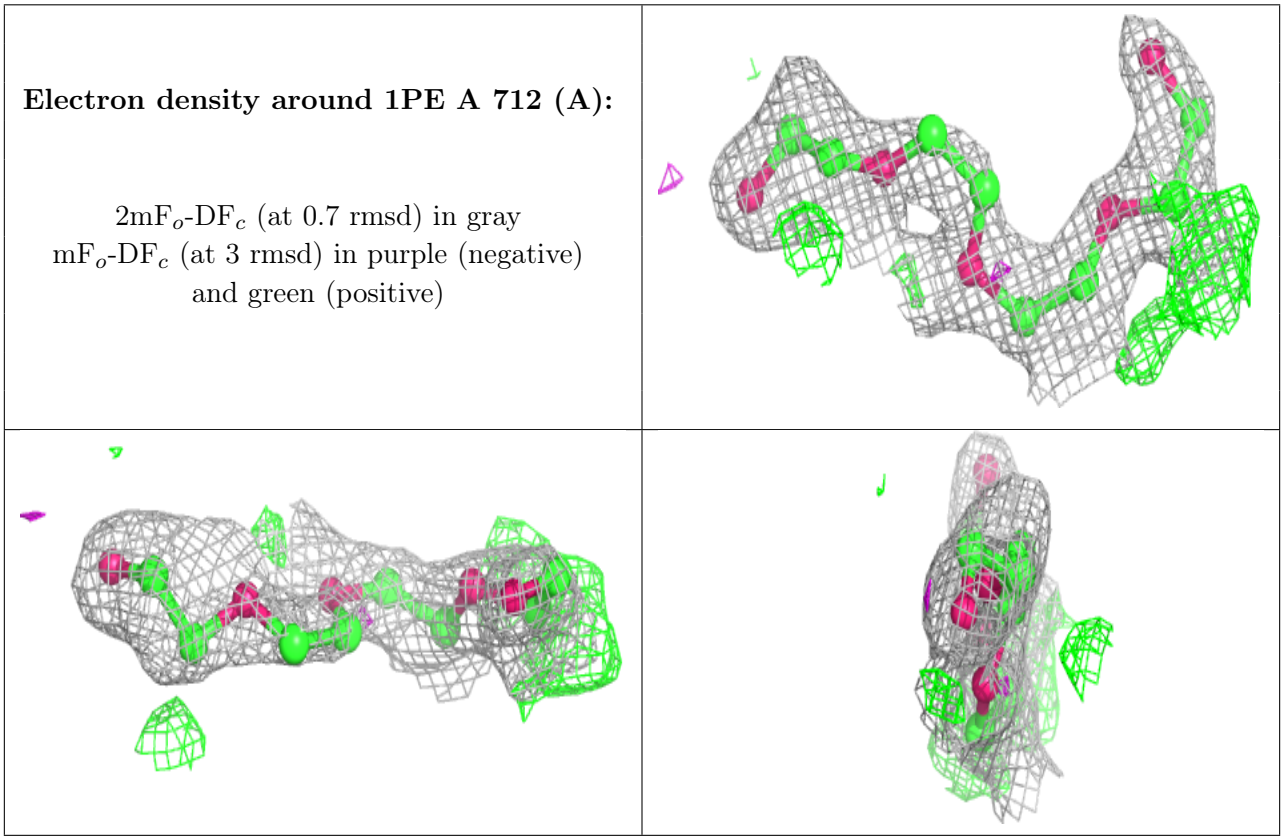
Electron density around 1PE A 708:

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



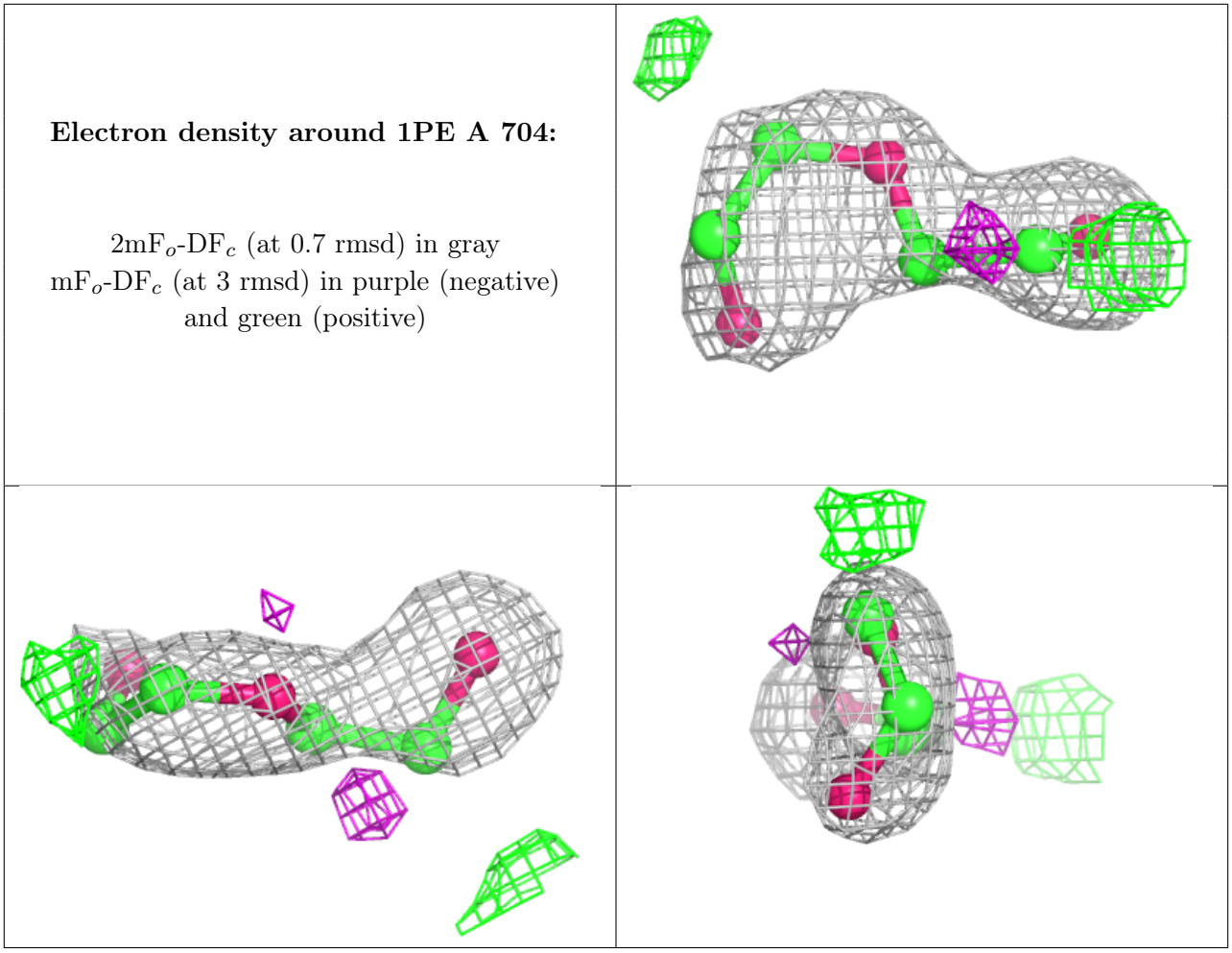
Electron density around 1PE A 712 (A):

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



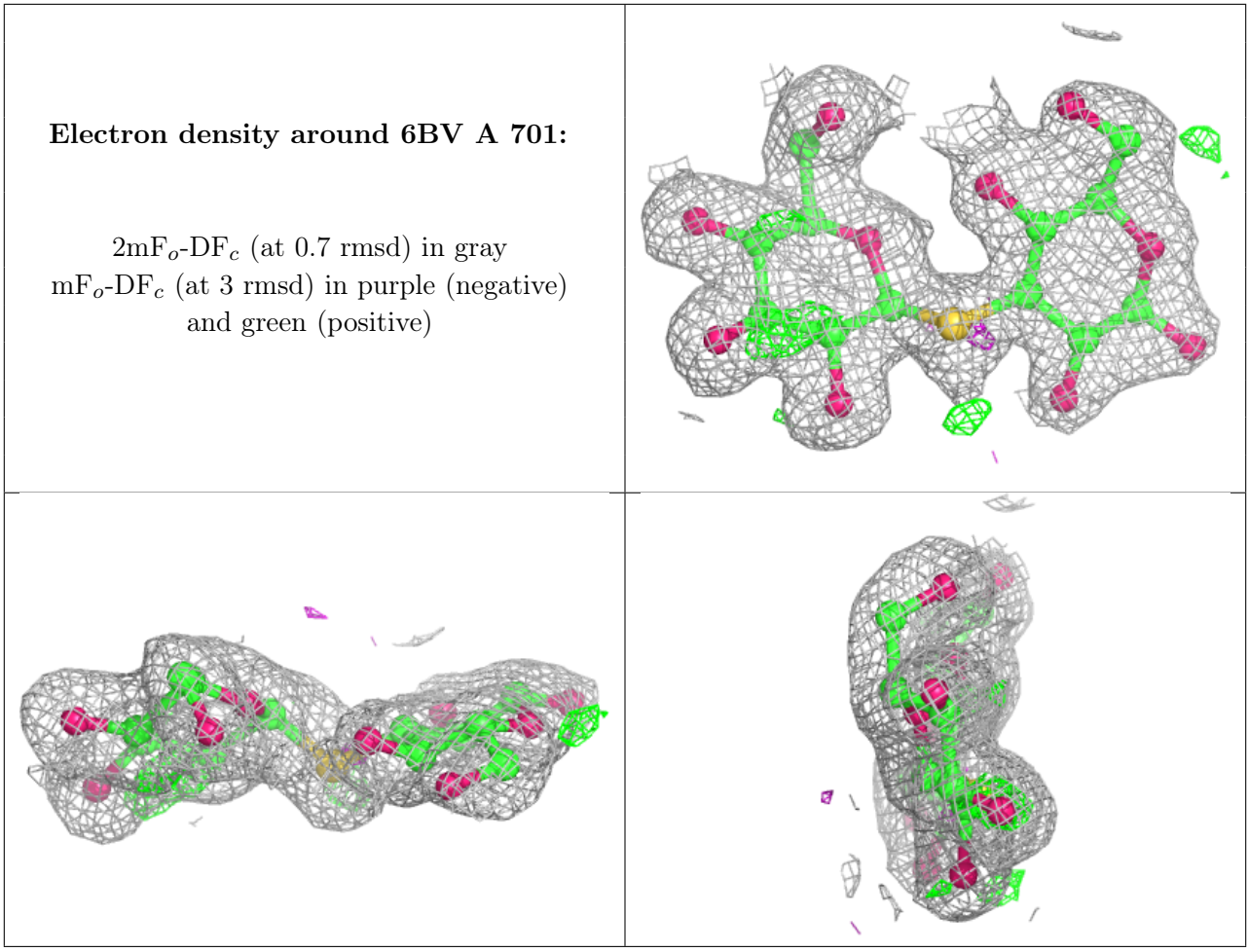
Electron density around 1PE A 704:

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



Electron density around 6BV A 701:

$2mF_o$-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.