



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 04:09 PM JST

PDB ID : 7DAH
Title : Adenosine triphosphate phosphoribosyltransferase from *Vibrio cholerae* in complex with ATP and PRPP
Authors : Pal, R.K.; Gourinath, S.; Biswal, B.K.
Deposited on : 2020-10-16
Resolution : 2.92 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 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 : 2.23.2
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) : 2.23.2

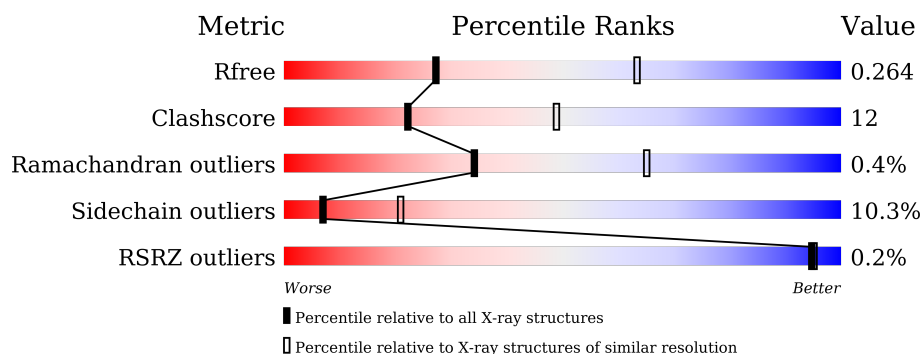
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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	310	 72% 19% • 7%
1	B	310	 69% 22% • 6%
1	C	310	 69% 20% • 7%
1	D	310	 73% 18% • 7%
1	E	310	 75% 17% • 5%
1	F	310	 71% 17% • 7%

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
2	PEG	D	401	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13159 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 ATP phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2149	1362	372	399	16			
1	B	292	Total	C	N	O	S	0	0	0
			2131	1361	358	398	14			
1	C	288	Total	C	N	O	S	0	0	0
			2134	1350	370	398	16			
1	D	287	Total	C	N	O	S	0	0	0
			2142	1353	375	398	16			
1	E	293	Total	C	N	O	S	0	0	0
			2123	1350	365	394	14			
1	F	287	Total	C	N	O	S	0	0	0
			2105	1335	363	393	14			

There are 36 discrepancies between the modelled and reference sequences:

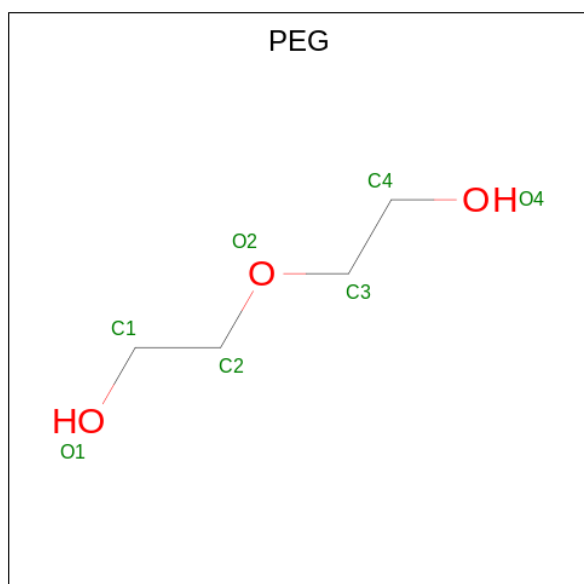
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP C3LU29
A	-4	HIS	-	expression tag	UNP C3LU29
A	-3	HIS	-	expression tag	UNP C3LU29
A	-2	HIS	-	expression tag	UNP C3LU29
A	-1	HIS	-	expression tag	UNP C3LU29
A	0	HIS	-	expression tag	UNP C3LU29
B	-5	HIS	-	expression tag	UNP C3LU29
B	-4	HIS	-	expression tag	UNP C3LU29
B	-3	HIS	-	expression tag	UNP C3LU29
B	-2	HIS	-	expression tag	UNP C3LU29
B	-1	HIS	-	expression tag	UNP C3LU29
B	0	HIS	-	expression tag	UNP C3LU29
C	-5	HIS	-	expression tag	UNP C3LU29
C	-4	HIS	-	expression tag	UNP C3LU29
C	-3	HIS	-	expression tag	UNP C3LU29
C	-2	HIS	-	expression tag	UNP C3LU29
C	-1	HIS	-	expression tag	UNP C3LU29

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP C3LU29
D	-5	HIS	-	expression tag	UNP C3LU29
D	-4	HIS	-	expression tag	UNP C3LU29
D	-3	HIS	-	expression tag	UNP C3LU29
D	-2	HIS	-	expression tag	UNP C3LU29
D	-1	HIS	-	expression tag	UNP C3LU29
D	0	HIS	-	expression tag	UNP C3LU29
E	-5	HIS	-	expression tag	UNP C3LU29
E	-4	HIS	-	expression tag	UNP C3LU29
E	-3	HIS	-	expression tag	UNP C3LU29
E	-2	HIS	-	expression tag	UNP C3LU29
E	-1	HIS	-	expression tag	UNP C3LU29
E	0	HIS	-	expression tag	UNP C3LU29
F	-5	HIS	-	expression tag	UNP C3LU29
F	-4	HIS	-	expression tag	UNP C3LU29
F	-3	HIS	-	expression tag	UNP C3LU29
F	-2	HIS	-	expression tag	UNP C3LU29
F	-1	HIS	-	expression tag	UNP C3LU29
F	0	HIS	-	expression tag	UNP C3LU29

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃) (labeled as "Ligand of Interest" by depositor).



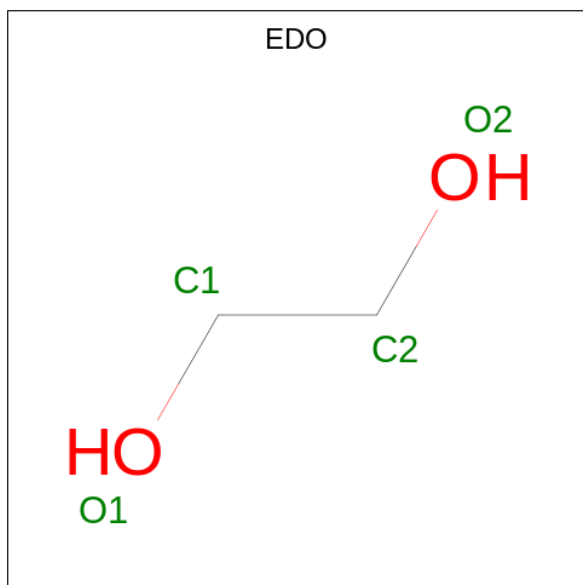
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		

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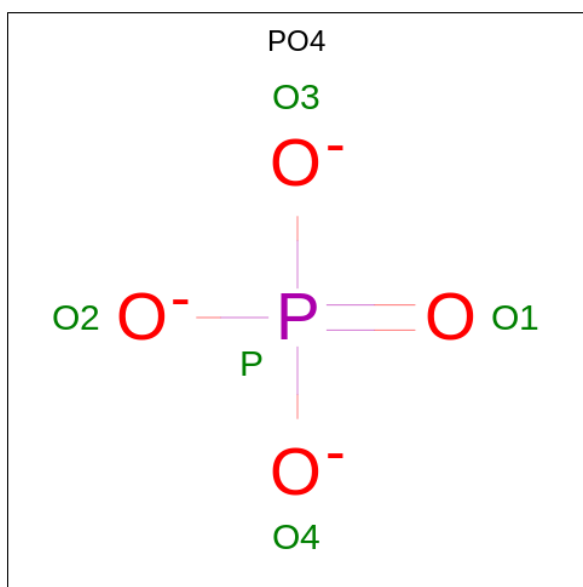
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂) (labeled as "Ligand of Interest" by depositor).



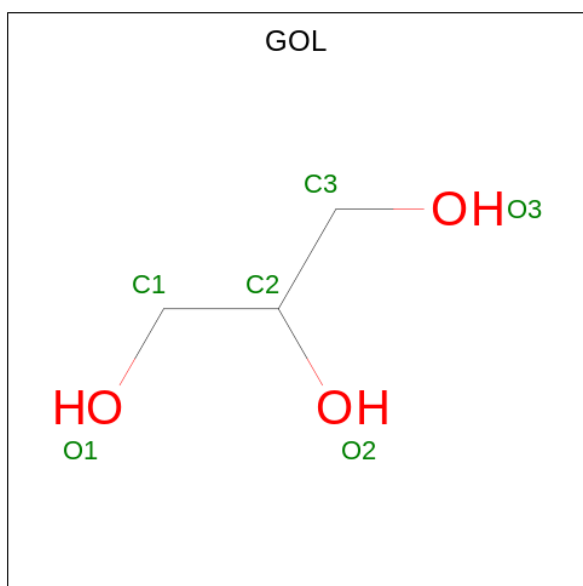
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



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

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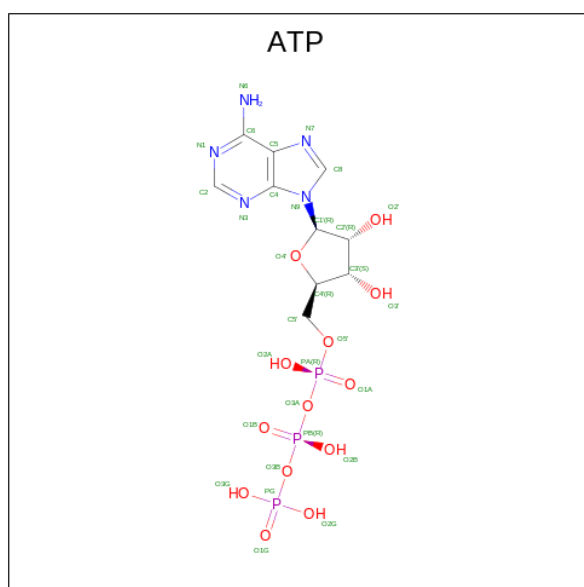
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

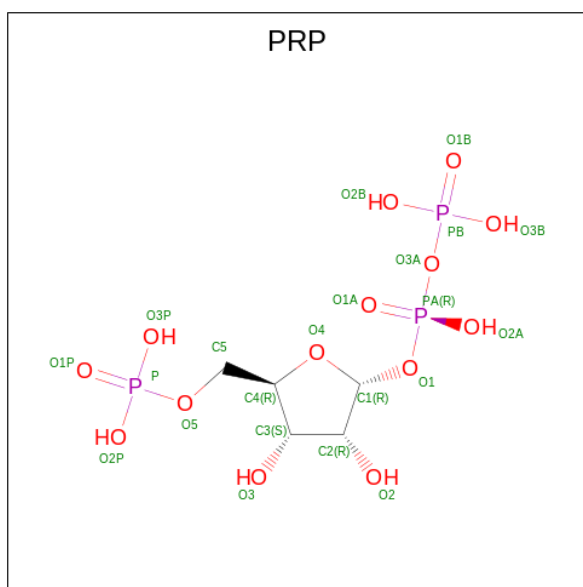
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 8 is 1-O-pyrophosphono-5-O-phosphono-alpha-D-ribofuranose (three-letter code: PRP) (formula: C₅H₁₃O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	O	P	0	0
			22	5	14	3		
8	F	1	Total	C	O	P	0	0
			22	5	14	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	35	Total	O	0	0
			35	35		
9	B	27	Total	O	0	0
			27	27		
9	C	47	Total	O	0	0
			47	47		
9	D	42	Total	O	0	0
			42	42		
9	E	22	Total	O	0	0
			22	22		
9	F	26	Total	O	0	0
			26	26		

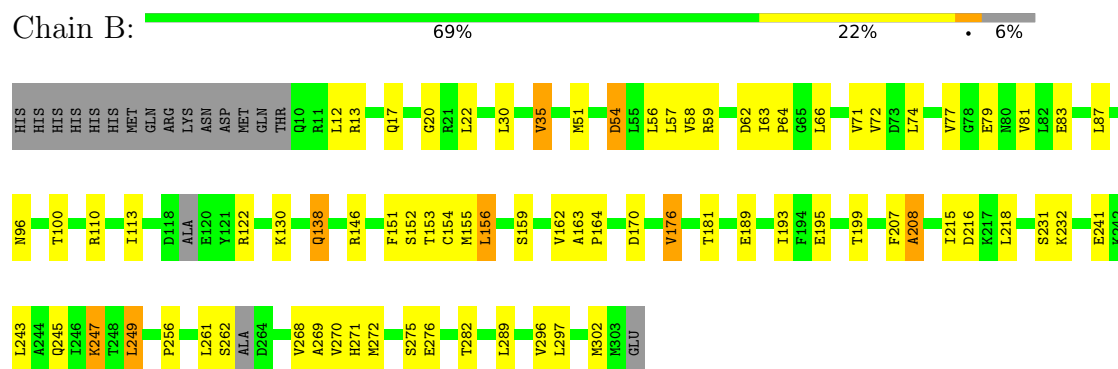
3 Residue-property plots

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.

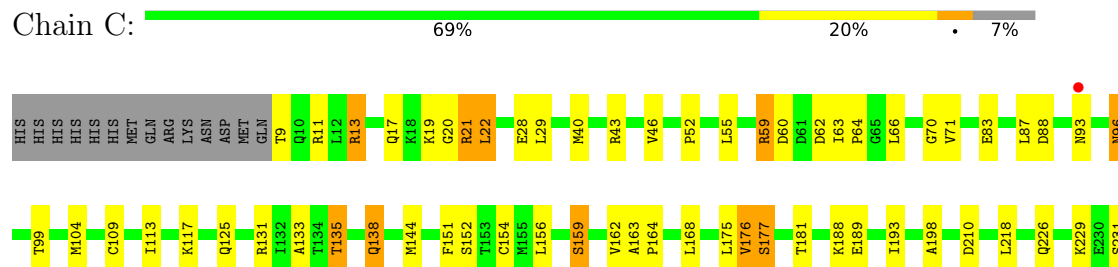
• Molecule 1: ATP phosphoribosyltransferase

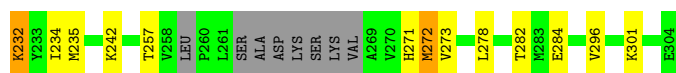


• Molecule 1: ATP phosphoribosyltransferase



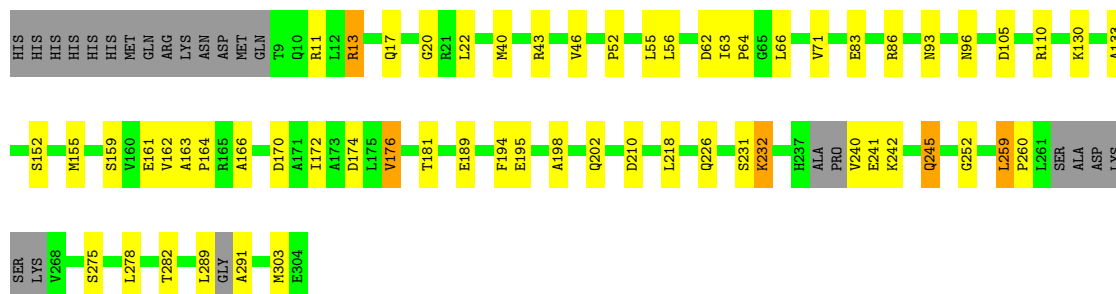
• Molecule 1: ATP phosphoribosyltransferase





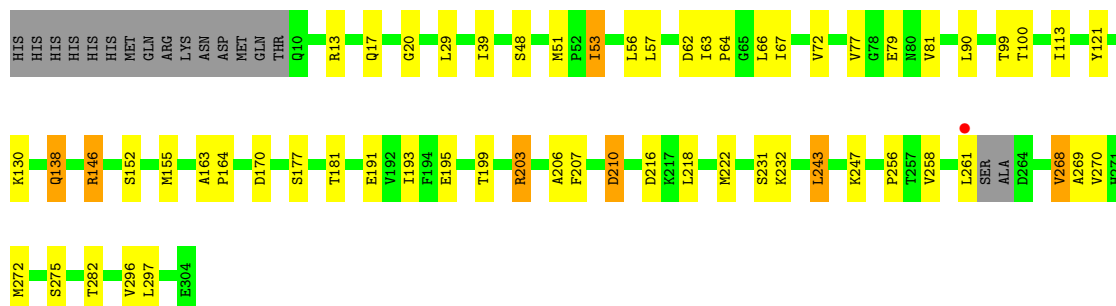
- Molecule 1: ATP phosphoribosyltransferase

Chain D: 73% 18% 7%



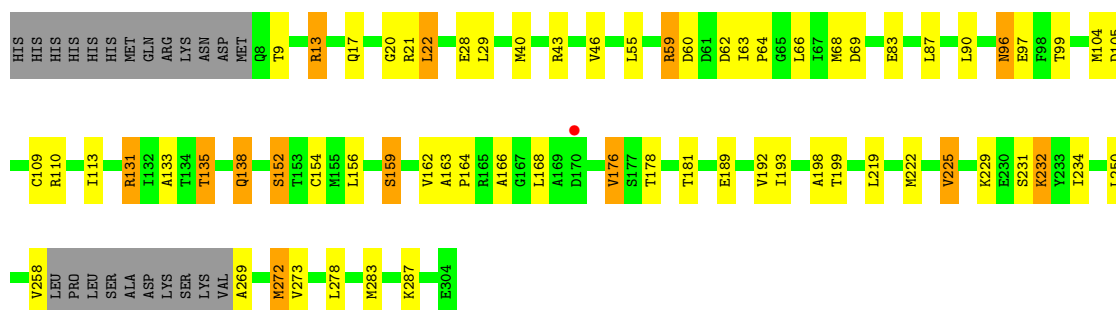
- Molecule 1: ATP phosphoribosyltransferase

Chain E: 75% 17% 5%



- Molecule 1: ATP phosphoribosyltransferase

Chain F: 71% 17% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	136.60Å 136.60Å 121.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.32 – 2.92 28.30 – 2.92	Depositor EDS
% Data completeness (in resolution range)	99.6 (28.32-2.92) 99.7 (28.30-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.216 , 0.268 0.215 , 0.264	Depositor DCC
R_{free} test set	2553 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 23.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l 0.470 for h,-h-k,-l 0.010 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13159	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, MG, PRP, ATP, PEG, PO4, 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	0.80	0/2170	0.95	0/2924
1	B	0.80	1/2155 (0.0%)	0.97	0/2916
1	C	0.78	1/2157 (0.0%)	0.94	0/2911
1	D	0.82	0/2164	0.97	0/2917
1	E	0.80	0/2150	0.95	1/2912 (0.0%)
1	F	0.79	1/2129 (0.0%)	0.94	0/2876
All	All	0.80	3/12925 (0.0%)	0.95	1/17456 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	28	GLU	CD-OE1	5.36	1.31	1.25
1	B	276	GLU	CD-OE1	5.30	1.31	1.25
1	C	28	GLU	CD-OE1	5.12	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	146	ARG	CB-CA-C	5.08	120.57	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	257	THR	Peptide
1	D	259	LEU	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	2149	0	2130	50	0
1	B	2131	0	2087	65	0
1	C	2134	0	2101	64	0
1	D	2142	0	2124	43	0
1	E	2123	0	2056	44	0
1	F	2105	0	2057	58	0
2	A	7	0	10	0	0
2	D	7	0	10	4	0
3	A	8	0	12	0	0
3	C	4	0	6	0	0
3	D	12	0	18	1	0
3	E	4	0	6	0	0
3	F	4	0	6	0	0
4	A	5	0	0	0	0
4	D	5	0	0	0	0
5	A	6	0	8	0	0
5	D	6	0	8	1	0
6	C	1	0	0	0	0
6	F	1	0	0	0	0
7	C	31	0	12	2	0
7	F	31	0	12	2	0
8	C	22	0	8	2	0
8	F	22	0	8	2	0
9	A	35	0	0	2	0
9	B	27	0	0	4	0
9	C	47	0	0	6	0
9	D	42	0	0	1	0
9	E	22	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	26	0	0	0	0
All	All	13159	0	12679	301	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 12.

All (301) 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:D:17:GLN:NE2	1:D:20:GLY:HA3	1.77	0.99
1:A:17:GLN:NE2	1:A:20:GLY:HA3	1.75	0.99
1:B:17:GLN:NE2	1:B:20:GLY:HA3	1.78	0.99
1:E:17:GLN:NE2	1:E:20:GLY:HA3	1.79	0.97
1:C:17:GLN:NE2	1:C:20:GLY:HA3	1.78	0.97
1:F:17:GLN:NE2	1:F:20:GLY:HA3	1.79	0.95
1:A:259:LEU:CB	1:A:268:VAL:CB	2.49	0.90
1:B:155:MET:O	1:B:156:LEU:HD13	1.76	0.83
1:B:87:LEU:CB	1:B:138:GLN:HG2	2.09	0.83
1:B:155:MET:C	1:B:156:LEU:HD13	2.00	0.82
1:A:159:SER:O	1:A:162:VAL:HG12	1.80	0.81
1:D:17:GLN:HE21	1:D:20:GLY:HA3	1.45	0.81
1:A:17:GLN:HE21	1:A:20:GLY:HA3	1.44	0.80
1:C:159:SER:O	1:C:162:VAL:HG12	1.83	0.79
1:B:17:GLN:HE21	1:B:20:GLY:HA3	1.46	0.79
1:C:17:GLN:HE21	1:C:20:GLY:HA3	1.47	0.78
1:E:17:GLN:HE21	1:E:20:GLY:HA3	1.47	0.77
1:F:159:SER:O	1:F:162:VAL:HG12	1.84	0.77
1:F:17:GLN:HE21	1:F:20:GLY:HA3	1.46	0.76
1:F:21:ARG:HG2	1:F:22:LEU:H	1.49	0.76
1:B:35:VAL:HA	1:B:51:MET:CE	2.16	0.75
1:E:138:GLN:HE21	1:E:138:GLN:HA	1.50	0.74
1:B:153:THR:HB	9:B:419:HOH:O	1.87	0.74
1:B:74:LEU:HD11	1:B:215:ILE:CD1	2.18	0.73
1:B:87:LEU:HB2	1:B:138:GLN:HG2	1.69	0.73
1:D:252:GLY:HA2	1:D:275:SER:OG	1.89	0.72
1:C:21:ARG:HG2	1:C:22:LEU:H	1.54	0.72
1:A:93:ASN:HD21	1:B:79:GLU:HG2	1.57	0.70
1:B:87:LEU:HB3	1:B:138:GLN:HG2	1.73	0.70
1:B:155:MET:O	1:B:156:LEU:CD1	2.39	0.69
1:E:48:SER:CB	1:E:53:ILE:HG23	2.22	0.69
1:B:74:LEU:HD11	1:B:215:ILE:HD12	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:PRO:O	1:E:67:ILE:HG22	1.94	0.68
1:C:40:MET:O	1:C:40:MET:HG3	1.94	0.67
1:A:289:LEU:O	1:A:291:ALA:N	2.27	0.67
1:E:177:SER:HA	9:E:512:HOH:O	1.93	0.67
1:D:289:LEU:O	1:D:291:ALA:N	2.28	0.67
1:D:202:GLN:HE22	3:D:402:EDO:H21	1.59	0.67
1:B:151:PHE:HE1	9:B:416:HOH:O	1.78	0.67
1:F:29:LEU:CD2	1:F:104:MET:HE1	2.27	0.65
1:B:35:VAL:HA	1:B:51:MET:HE3	1.77	0.65
1:F:231:SER:O	1:F:232:LYS:HD2	1.97	0.65
1:B:12:LEU:HD11	1:B:215:ILE:HD11	1.79	0.64
1:F:96:ASN:C	1:F:96:ASN:HD22	2.00	0.64
1:F:131:ARG:HD2	1:F:152:SER:HB2	1.79	0.63
1:C:231:SER:O	1:C:232:LYS:HD2	1.98	0.63
1:E:261:LEU:C	9:E:508:HOH:O	2.38	0.63
1:F:176:VAL:HG11	1:F:189:GLU:OE1	1.98	0.62
1:D:11:ARG:HH11	1:D:52:PRO:HA	1.64	0.62
1:D:13:ARG:NH2	1:F:166:ALA:O	2.32	0.62
1:B:30:LEU:O	1:B:35:VAL:HG13	1.99	0.62
1:D:231:SER:O	1:D:232:LYS:HD2	1.99	0.62
1:D:17:GLN:HE21	1:D:20:GLY:CA	2.13	0.62
1:C:210:ASP:HB2	9:C:527:HOH:O	1.99	0.62
1:F:17:GLN:HE21	1:F:20:GLY:CA	2.12	0.61
1:D:159:SER:O	1:D:162:VAL:HG12	1.98	0.61
1:C:17:GLN:HE21	1:C:20:GLY:CA	2.13	0.61
1:C:29:LEU:CD2	1:C:104:MET:HE1	2.31	0.61
1:A:71:VAL:HG13	1:C:168:LEU:CD2	2.31	0.61
1:E:203:ARG:NH2	1:E:207:PHE:CZ	2.68	0.60
1:B:17:GLN:HE21	1:B:20:GLY:CA	2.13	0.60
1:E:203:ARG:NH2	1:E:207:PHE:CE2	2.69	0.60
1:D:17:GLN:HE22	1:D:20:GLY:HA3	1.63	0.60
1:E:48:SER:HB3	1:E:53:ILE:HG23	1.82	0.60
1:A:11:ARG:HH11	1:A:52:PRO:HA	1.66	0.60
1:C:96:ASN:C	1:C:96:ASN:HD22	2.04	0.60
1:F:109:CYS:SG	7:F:404:ATP:H2'	2.41	0.60
1:C:17:GLN:HE22	1:C:20:GLY:HA3	1.64	0.59
1:F:110:ARG:CZ	1:F:176:VAL:HG12	2.33	0.59
1:E:17:GLN:HE21	1:E:20:GLY:CA	2.15	0.58
1:E:256:PRO:HB2	1:E:270:VAL:HG13	1.85	0.58
1:B:207:PHE:O	1:B:208:ALA:HB3	2.03	0.58
1:B:138:GLN:HE21	1:B:138:GLN:HA	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:GLN:HE21	1:A:20:GLY:CA	2.12	0.58
1:C:87:LEU:HB3	1:C:138:GLN:HG3	1.85	0.58
1:B:249:LEU:HD22	1:B:249:LEU:O	2.03	0.58
1:D:13:ARG:NH1	1:D:71:VAL:O	2.37	0.58
1:F:113:ILE:HD12	1:F:193:ILE:HG21	1.84	0.58
1:F:87:LEU:HB3	1:F:138:GLN:CG	2.34	0.58
1:B:17:GLN:NE2	1:B:20:GLY:CA	2.63	0.58
1:F:87:LEU:HB3	1:F:138:GLN:HG3	1.84	0.57
1:C:125:GLN:HG2	9:C:524:HOH:O	2.03	0.57
1:E:297:LEU:N	1:E:297:LEU:HD12	2.18	0.57
1:B:17:GLN:HE22	1:B:20:GLY:HA3	1.65	0.57
1:D:71:VAL:HG13	1:F:168:LEU:CD2	2.34	0.57
1:F:234:ILE:HD11	1:F:278:LEU:HD13	1.87	0.57
1:A:17:GLN:HE22	1:A:20:GLY:HA3	1.62	0.57
1:D:93:ASN:HB2	1:E:100:THR:HG21	1.87	0.56
1:A:176:VAL:HG11	1:A:189:GLU:OE1	2.04	0.56
1:C:234:ILE:HD12	1:C:296:VAL:HG22	1.87	0.56
1:B:297:LEU:N	1:B:297:LEU:HD12	2.21	0.56
1:C:87:LEU:HB3	1:C:138:GLN:CG	2.35	0.56
1:C:272:MET:HG2	1:C:273:VAL:N	2.19	0.56
1:C:17:GLN:NE2	1:C:20:GLY:CA	2.62	0.55
1:D:17:GLN:NE2	1:D:20:GLY:CA	2.63	0.55
1:B:87:LEU:HB3	1:B:138:GLN:CG	2.36	0.55
1:D:195:GLU:H	2:D:401:PEG:C2	2.20	0.55
1:D:176:VAL:HG11	1:D:189:GLU:OE1	2.06	0.55
1:B:176:VAL:HG11	1:B:189:GLU:OE1	2.07	0.55
1:E:17:GLN:HE22	1:E:20:GLY:HA3	1.66	0.55
1:F:159:SER:N	8:F:403:PRP:O2B	2.29	0.55
1:F:21:ARG:HG2	1:F:22:LEU:N	2.20	0.55
1:D:161:GLU:OE2	1:D:174:ASP:OD2	2.25	0.55
1:E:261:LEU:HD21	1:E:269:ALA:HB2	1.89	0.54
1:A:43:ARG:HD2	1:A:45:VAL:O	2.07	0.54
1:B:159:SER:O	1:B:162:VAL:HG23	2.07	0.54
1:E:17:GLN:NE2	1:E:20:GLY:CA	2.64	0.54
1:A:71:VAL:CG1	1:C:168:LEU:CD2	2.85	0.54
1:A:135:THR:HG22	1:A:160:VAL:CG2	2.38	0.54
1:D:240:VAL:CB	1:D:241:GLU:OE1	2.55	0.54
1:A:17:GLN:NE2	1:A:20:GLY:CA	2.62	0.54
1:C:40:MET:O	1:C:40:MET:CG	2.54	0.54
1:D:93:ASN:HD21	1:E:79:GLU:HG2	1.73	0.54
1:F:17:GLN:HE22	1:F:20:GLY:HA3	1.66	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:87:LEU:CB	1:F:138:GLN:HG2	2.37	0.54
1:A:86:ARG:HD2	1:B:146:ARG:HD2	1.90	0.53
1:E:203:ARG:NH1	1:E:206:ALA:O	2.41	0.53
1:C:87:LEU:CB	1:C:138:GLN:HG2	2.38	0.53
1:C:113:ILE:HD12	1:C:193:ILE:HG21	1.89	0.53
1:F:87:LEU:CB	1:F:138:GLN:CG	2.87	0.53
1:C:22:LEU:HD21	1:C:198:ALA:HB2	1.90	0.53
1:A:16:ILE:CD1	1:A:76:PHE:CD2	2.92	0.53
1:F:22:LEU:HD21	1:F:198:ALA:HB2	1.90	0.53
1:C:87:LEU:CB	1:C:138:GLN:CG	2.87	0.53
1:F:29:LEU:CD2	1:F:104:MET:CE	2.86	0.52
1:F:178:THR:N	8:F:403:PRP:O3P	2.35	0.52
1:F:17:GLN:NE2	1:F:20:GLY:CA	2.63	0.52
1:A:58:VAL:HG22	1:A:59:ARG:N	2.24	0.52
1:B:256:PRO:HB2	1:B:270:VAL:HG13	1.90	0.52
1:C:131:ARG:HH11	1:C:154:CYS:HB2	1.75	0.52
1:D:194:PHE:HA	2:D:401:PEG:H21	1.92	0.52
1:A:93:ASN:HB2	1:B:100:THR:HG21	1.92	0.52
1:C:11:ARG:CD	9:C:503:HOH:O	2.58	0.52
1:A:71:VAL:HG13	1:C:168:LEU:HD21	1.92	0.51
1:C:87:LEU:HB2	1:C:138:GLN:HG2	1.92	0.51
1:A:36:LYS:HD3	1:A:50:ASN:ND2	2.25	0.51
1:C:29:LEU:CD2	1:C:104:MET:CE	2.88	0.51
1:E:231:SER:O	1:E:232:LYS:HD3	2.11	0.51
1:D:210:ASP:OD1	1:D:210:ASP:N	2.43	0.51
1:A:16:ILE:CD1	1:A:76:PHE:HD2	2.24	0.51
1:E:67:ILE:HD12	1:E:72:VAL:HG23	1.92	0.51
1:E:210:ASP:OD1	1:E:210:ASP:N	2.44	0.50
1:F:96:ASN:C	1:F:96:ASN:ND2	2.64	0.50
1:A:166:ALA:O	1:C:13:ARG:CZ	2.59	0.50
1:B:138:GLN:HE21	1:B:138:GLN:CA	2.25	0.50
1:D:71:VAL:HG13	1:F:168:LEU:HD21	1.93	0.50
1:A:71:VAL:CG1	1:C:168:LEU:HD22	2.42	0.50
1:A:231:SER:O	1:A:232:LYS:HD3	2.11	0.50
1:B:35:VAL:CA	1:B:51:MET:CE	2.90	0.50
1:C:131:ARG:NH1	1:C:154:CYS:HB2	2.26	0.50
1:A:210:ASP:OD1	1:A:210:ASP:N	2.43	0.50
1:F:87:LEU:HB2	1:F:138:GLN:HG2	1.92	0.50
1:B:231:SER:O	1:B:232:LYS:HD3	2.11	0.50
1:D:22:LEU:HD11	1:D:198:ALA:HB2	1.94	0.49
1:F:68:MET:SD	1:F:96:ASN:HA	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:LEU:N	1:B:56:LEU:HD12	2.27	0.49
1:C:96:ASN:C	1:C:96:ASN:ND2	2.66	0.49
1:D:166:ALA:O	1:F:13:ARG:CZ	2.60	0.49
1:C:43:ARG:HD3	9:C:506:HOH:O	2.12	0.49
1:B:207:PHE:O	1:B:208:ALA:CB	2.60	0.49
1:B:245:GLN:HG2	1:B:289:LEU:HD13	1.95	0.49
1:D:56:LEU:HD12	1:D:56:LEU:N	2.27	0.49
5:D:403:GOL:H12	1:F:69:ASP:OD2	2.13	0.49
1:A:56:LEU:HD12	1:A:56:LEU:N	2.27	0.49
1:C:60:ASP:OD1	7:C:402:ATP:O1G	2.31	0.49
1:E:56:LEU:N	1:E:56:LEU:HD12	2.27	0.49
1:C:109:CYS:SG	7:C:402:ATP:H2'	2.53	0.48
1:F:105:ASP:CG	1:F:105:ASP:O	2.51	0.48
1:A:249:LEU:HD11	1:A:285:GLN:HB3	1.95	0.48
1:F:131:ARG:HG2	1:F:152:SER:OG	2.14	0.48
1:D:195:GLU:H	2:D:401:PEG:H21	1.79	0.48
1:E:77:VAL:CG2	1:E:81:VAL:CG2	2.92	0.48
1:C:62:ASP:O	1:C:66:LEU:HG	2.13	0.48
1:D:62:ASP:O	1:D:66:LEU:HG	2.14	0.48
1:D:210:ASP:HB3	9:D:531:HOH:O	2.12	0.48
1:A:249:LEU:HD22	1:A:282:THR:HG23	1.95	0.48
1:D:71:VAL:CG1	1:F:168:LEU:CD2	2.92	0.48
1:B:62:ASP:O	1:B:66:LEU:HG	2.14	0.48
1:F:113:ILE:HD12	1:F:193:ILE:CG2	2.44	0.48
1:B:297:LEU:N	1:B:297:LEU:CD1	2.77	0.47
1:E:29:LEU:HD21	1:E:222:MET:HG2	1.95	0.47
1:A:165:ARG:HD3	9:A:515:HOH:O	2.15	0.47
1:F:62:ASP:O	1:F:66:LEU:HG	2.15	0.47
1:B:57:LEU:N	1:B:57:LEU:HD12	2.30	0.47
1:C:234:ILE:CD1	1:C:296:VAL:HG22	2.44	0.47
1:E:48:SER:HB2	1:E:53:ILE:HG23	1.95	0.47
1:F:278:LEU:HD23	1:F:283:MET:HG2	1.97	0.47
1:A:130:LYS:HB3	1:A:170:ASP:HB2	1.97	0.47
1:E:62:ASP:O	1:E:66:LEU:HG	2.14	0.47
1:B:153:THR:CG2	9:B:419:HOH:O	2.63	0.46
1:F:131:ARG:CD	1:F:152:SER:HB2	2.43	0.46
1:F:60:ASP:OD1	7:F:404:ATP:O1G	2.33	0.46
1:A:71:VAL:CG1	1:C:168:LEU:HD21	2.46	0.46
1:B:63:ILE:N	1:B:64:PRO:CD	2.79	0.46
1:A:62:ASP:O	1:A:66:LEU:HG	2.15	0.46
1:E:39:ILE:HG23	1:E:39:ILE:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:ILE:N	1:E:64:PRO:CD	2.79	0.46
1:F:40:MET:CB	1:F:43:ARG:NH2	2.79	0.45
1:A:51:MET:HG2	9:A:520:HOH:O	2.16	0.45
1:B:232:LYS:HB3	1:B:296:VAL:HG13	1.98	0.45
1:E:57:LEU:HD12	1:E:57:LEU:N	2.30	0.45
1:A:59:ARG:HG2	1:A:59:ARG:HH21	1.82	0.45
1:B:54:ASP:OD1	1:B:54:ASP:N	2.49	0.45
1:C:88:ASP:CG	9:C:508:HOH:O	2.55	0.45
1:E:51:MET:CB	9:E:518:HOH:O	2.64	0.45
1:B:77:VAL:CG2	1:B:81:VAL:CG2	2.95	0.45
1:A:46:VAL:HB	1:A:55:LEU:HB2	1.99	0.45
1:A:71:VAL:HG11	1:C:168:LEU:HD22	1.98	0.45
1:B:156:LEU:HD13	1:B:156:LEU:N	2.32	0.45
1:C:113:ILE:HD12	1:C:193:ILE:CG2	2.46	0.45
1:D:242:LYS:CB	1:D:245:GLN:HE22	2.30	0.45
1:B:30:LEU:HB3	1:B:35:VAL:HG21	1.99	0.44
1:E:77:VAL:HG22	1:E:81:VAL:CG2	2.47	0.44
1:C:135:THR:HG23	1:C:156:LEU:O	2.18	0.44
1:D:133:ALA:HB3	1:D:172:ILE:HG22	1.99	0.44
1:F:63:ILE:N	1:F:64:PRO:CD	2.80	0.44
1:B:130:LYS:HB3	1:B:170:ASP:HB2	1.99	0.44
1:D:195:GLU:H	2:D:401:PEG:H22	1.83	0.44
1:A:133:ALA:HB3	1:A:172:ILE:HG22	2.00	0.44
1:D:71:VAL:CG1	1:F:168:LEU:HD22	2.48	0.44
1:F:87:LEU:CB	1:F:138:GLN:HG3	2.48	0.44
1:B:261:LEU:HD21	1:B:269:ALA:HB2	2.00	0.44
1:A:249:LEU:CD2	1:A:282:THR:HG23	2.49	0.43
1:C:63:ILE:N	1:C:64:PRO:CD	2.81	0.43
1:D:130:LYS:HB3	1:D:170:ASP:HB2	1.99	0.43
1:E:29:LEU:CD2	1:E:222:MET:HG2	2.48	0.43
1:B:146:ARG:HD3	9:B:413:HOH:O	2.19	0.43
1:E:138:GLN:HA	1:E:138:GLN:NE2	2.26	0.43
1:B:110:ARG:NH1	1:B:176:VAL:CG1	2.81	0.43
1:C:46:VAL:HB	1:C:55:LEU:HB2	2.01	0.43
1:D:63:ILE:N	1:D:64:PRO:CD	2.81	0.43
1:C:59:ARG:HE	1:C:59:ARG:HB3	1.69	0.43
1:F:59:ARG:HE	1:F:59:ARG:HB3	1.72	0.43
1:A:110:ARG:CZ	1:A:176:VAL:HG12	2.49	0.43
1:C:144:MET:HB2	1:C:151:PHE:HE2	1.82	0.43
1:E:232:LYS:HB3	1:E:296:VAL:HG13	2.00	0.43
1:F:131:ARG:HG2	1:F:152:SER:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:297:LEU:N	1:E:297:LEU:CD1	2.81	0.43
1:F:222:MET:HA	1:F:225:VAL:HG13	2.00	0.43
1:F:272:MET:HG2	1:F:273:VAL:N	2.33	0.43
1:B:113:ILE:HD12	1:B:193:ILE:CG2	2.49	0.43
1:C:133:ALA:HA	1:C:154:CYS:O	2.19	0.43
1:A:63:ILE:N	1:A:64:PRO:CD	2.82	0.42
1:A:226:GLN:OE1	1:A:226:GLN:HA	2.18	0.42
1:C:29:LEU:HD22	1:C:104:MET:CE	2.49	0.42
1:C:176:VAL:HG11	1:C:189:GLU:OE1	2.18	0.42
1:E:130:LYS:HB3	1:E:170:ASP:HB2	2.01	0.42
1:A:16:ILE:HD11	1:A:76:PHE:CD2	2.55	0.42
1:F:133:ALA:HA	1:F:154:CYS:O	2.19	0.42
1:F:135:THR:HG23	1:F:156:LEU:O	2.19	0.42
1:A:93:ASN:ND2	1:B:79:GLU:HG2	2.30	0.42
1:D:110:ARG:CZ	1:D:176:VAL:HG12	2.49	0.42
1:B:113:ILE:HD12	1:B:193:ILE:HG21	2.02	0.42
1:B:247:LYS:HE2	1:C:70:GLY:HA3	2.02	0.42
1:C:284:GLU:HA	1:D:303:MET:HE1	2.01	0.42
1:F:46:VAL:HB	1:F:55:LEU:HB2	2.01	0.42
1:B:163:ALA:N	1:B:164:PRO:CD	2.82	0.42
1:F:29:LEU:HD22	1:F:104:MET:CE	2.50	0.42
1:A:16:ILE:HD12	1:A:26:CYS:HB3	2.00	0.42
1:C:11:ARG:NH2	1:C:52:PRO:HA	2.35	0.42
1:C:83:GLU:HA	1:C:83:GLU:OE1	2.20	0.42
1:E:113:ILE:HD12	1:E:193:ILE:CG2	2.48	0.42
1:D:46:VAL:HB	1:D:55:LEU:HB2	2.02	0.42
1:E:163:ALA:N	1:E:164:PRO:CD	2.83	0.42
1:B:110:ARG:CZ	1:B:176:VAL:HG12	2.50	0.42
1:B:71:VAL:HG23	1:B:72:VAL:HG13	2.02	0.42
1:C:235:MET:HE3	1:C:271:HIS:CD2	2.54	0.42
1:B:77:VAL:HG22	1:B:81:VAL:CG2	2.50	0.41
1:E:113:ILE:HD12	1:E:193:ILE:HG21	2.02	0.41
1:F:163:ALA:N	1:F:164:PRO:CD	2.83	0.41
1:C:87:LEU:CB	1:C:138:GLN:HG3	2.48	0.41
1:E:121:TYR:OH	1:E:191:GLU:OE1	2.32	0.41
1:E:258:VAL:HG13	1:E:268:VAL:CG1	2.51	0.41
1:C:22:LEU:HD23	1:C:22:LEU:HA	1.84	0.41
1:F:87:LEU:HB2	1:F:138:GLN:CG	2.50	0.41
1:A:83:GLU:OE1	1:A:86:ARG:NH2	2.54	0.41
1:A:98:PHE:CZ	1:B:146:ARG:HG2	2.55	0.41
1:C:87:LEU:HB2	1:C:138:GLN:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:LYS:HA	1:C:188:LYS:CD	2.50	0.41
1:D:83:GLU:OE1	1:D:86:ARG:NH2	2.54	0.41
1:C:11:ARG:NE	9:C:503:HOH:O	2.53	0.41
1:D:226:GLN:OE1	1:D:226:GLN:HA	2.19	0.41
1:A:16:ILE:HD13	1:A:76:PHE:HD2	1.85	0.41
1:A:163:ALA:N	1:A:164:PRO:CD	2.84	0.41
1:B:87:LEU:CB	1:B:138:GLN:CG	2.90	0.41
1:C:144:MET:HG3	1:C:151:PHE:CE2	2.56	0.41
1:C:175:LEU:O	8:C:403:PRP:O3	2.31	0.41
1:D:71:VAL:CG1	1:F:168:LEU:HD21	2.51	0.41
1:D:163:ALA:N	1:D:164:PRO:CD	2.84	0.41
1:E:77:VAL:HG22	1:E:81:VAL:HG22	2.03	0.41
1:F:258:VAL:C	1:F:269:ALA:O	2.59	0.41
1:F:83:GLU:HA	1:F:83:GLU:OE1	2.21	0.40
1:B:58:VAL:HG12	1:B:59:ARG:N	2.36	0.40
1:C:163:ALA:N	1:C:164:PRO:CD	2.84	0.40
1:A:232:LYS:HB3	1:A:296:VAL:HG13	2.03	0.40
1:B:83:GLU:HA	1:B:83:GLU:OE1	2.20	0.40
1:B:74:LEU:HD21	1:B:215:ILE:HD12	2.04	0.40
1:E:243:LEU:HD22	1:E:247:LYS:HE3	2.02	0.40
1:B:30:LEU:HB3	1:B:35:VAL:CG2	2.52	0.40
1:B:193:ILE:HG21	1:B:193:ILE:HD13	1.84	0.40
1:C:177:SER:N	8:C:403:PRP:O1P	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	276/310 (89%)	260 (94%)	14 (5%)	2 (1%)	22 53
1	B	286/310 (92%)	271 (95%)	14 (5%)	1 (0%)	41 70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	282/310 (91%)	269 (95%)	12 (4%)	1 (0%)	34	65
1	D	279/310 (90%)	262 (94%)	15 (5%)	2 (1%)	22	53
1	E	289/310 (93%)	275 (95%)	14 (5%)	0	100	100
1	F	283/310 (91%)	269 (95%)	14 (5%)	0	100	100
All	All	1695/1860 (91%)	1606 (95%)	83 (5%)	6 (0%)	34	65

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	LYS
1	B	208	ALA
1	C	242	LYS
1	D	260	PRO
1	D	259	LEU
1	A	41	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	213/263 (81%)	196 (92%)	17 (8%)	12	32
1	B	201/263 (76%)	174 (87%)	27 (13%)	4	11
1	C	207/263 (79%)	182 (88%)	25 (12%)	5	14
1	D	212/263 (81%)	198 (93%)	14 (7%)	16	42
1	E	197/263 (75%)	177 (90%)	20 (10%)	7	21
1	F	201/263 (76%)	177 (88%)	24 (12%)	5	14
All	All	1231/1578 (78%)	1104 (90%)	127 (10%)	7	21

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN

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Mol	Chain	Res	Type
1	A	13	ARG
1	A	22	LEU
1	A	42	GLU
1	A	59	ARG
1	A	96	ASN
1	A	105	ASP
1	A	118	ASP
1	A	135	THR
1	A	152	SER
1	A	155	MET
1	A	165	ARG
1	A	176	VAL
1	A	181	THR
1	A	249	LEU
1	A	278	LEU
1	A	282	THR
1	B	13	ARG
1	B	22	LEU
1	B	35	VAL
1	B	54	ASP
1	B	96	ASN
1	B	122	ARG
1	B	138	GLN
1	B	152	SER
1	B	154	CYS
1	B	156	LEU
1	B	176	VAL
1	B	181	THR
1	B	195	GLU
1	B	199	THR
1	B	216	ASP
1	B	218	LEU
1	B	241	GLU
1	B	243	LEU
1	B	247	LYS
1	B	249	LEU
1	B	262	SER
1	B	268	VAL
1	B	271	HIS
1	B	272	MET
1	B	275	SER
1	B	282	THR

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Mol	Chain	Res	Type
1	B	302	MET
1	C	9	THR
1	C	13	ARG
1	C	19	LYS
1	C	21	ARG
1	C	22	LEU
1	C	59	ARG
1	C	71	VAL
1	C	93	ASN
1	C	96	ASN
1	C	99	THR
1	C	135	THR
1	C	138	GLN
1	C	152	SER
1	C	159	SER
1	C	176	VAL
1	C	177	SER
1	C	181	THR
1	C	218	LEU
1	C	226	GLN
1	C	229	LYS
1	C	232	LYS
1	C	272	MET
1	C	278	LEU
1	C	282	THR
1	C	301	LYS
1	D	13	ARG
1	D	40	MET
1	D	43	ARG
1	D	96	ASN
1	D	105	ASP
1	D	152	SER
1	D	155	MET
1	D	176	VAL
1	D	181	THR
1	D	218	LEU
1	D	232	LYS
1	D	245	GLN
1	D	278	LEU
1	D	282	THR
1	E	13	ARG
1	E	53	ILE

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Mol	Chain	Res	Type
1	E	90	LEU
1	E	99	THR
1	E	138	GLN
1	E	146	ARG
1	E	152	SER
1	E	155	MET
1	E	181	THR
1	E	195	GLU
1	E	199	THR
1	E	203	ARG
1	E	210	ASP
1	E	216	ASP
1	E	218	LEU
1	E	243	LEU
1	E	268	VAL
1	E	272	MET
1	E	275	SER
1	E	282	THR
1	F	9	THR
1	F	13	ARG
1	F	22	LEU
1	F	59	ARG
1	F	90	LEU
1	F	96	ASN
1	F	97	GLU
1	F	99	THR
1	F	131	ARG
1	F	135	THR
1	F	138	GLN
1	F	152	SER
1	F	159	SER
1	F	176	VAL
1	F	181	THR
1	F	192	VAL
1	F	199	THR
1	F	219	LEU
1	F	225	VAL
1	F	229	LYS
1	F	232	LYS
1	F	250	LEU
1	F	272	MET
1	F	287	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	96	ASN
1	A	125	GLN
1	B	17	GLN
1	B	27	GLN
1	B	93	ASN
1	B	96	ASN
1	B	125	GLN
1	B	138	GLN
1	C	10	GLN
1	C	17	GLN
1	C	226	GLN
1	D	10	GLN
1	D	17	GLN
1	D	96	ASN
1	E	17	GLN
1	E	93	ASN
1	F	17	GLN
1	F	27	GLN
1	F	185	ASN
1	F	226	GLN

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](#)

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	D	402	-	3,3,3	0.14	0	2,2,2	0.03	0
8	PRP	C	403	-	19,22,22	0.67	0	33,35,35	1.35	4 (12%)
8	PRP	F	403	-	19,22,22	0.71	0	33,35,35	1.26	2 (6%)
3	EDO	C	404	-	3,3,3	0.11	0	2,2,2	0.13	0
7	ATP	F	404	6	26,33,33	0.62	0	31,52,52	1.05	1 (3%)
3	EDO	A	402	-	3,3,3	0.27	0	2,2,2	0.27	0
5	GOL	D	403	-	5,5,5	0.17	0	5,5,5	0.36	0
2	PEG	D	401	-	6,6,6	0.23	0	5,5,5	0.18	0
3	EDO	E	401	-	3,3,3	0.20	0	2,2,2	0.26	0
3	EDO	F	402	-	3,3,3	0.37	0	2,2,2	0.42	0
4	PO4	A	404	-	4,4,4	1.47	1 (25%)	6,6,6	0.36	0
7	ATP	C	402	6	26,33,33	0.61	0	31,52,52	1.11	2 (6%)
3	EDO	D	404	-	3,3,3	0.23	0	2,2,2	0.26	0
2	PEG	A	401	-	6,6,6	0.19	0	5,5,5	0.23	0
3	EDO	D	405	-	3,3,3	0.41	0	2,2,2	0.21	0
3	EDO	A	403	-	3,3,3	0.27	0	2,2,2	0.13	0
5	GOL	A	405	-	5,5,5	0.18	0	5,5,5	0.34	0
4	PO4	D	406	-	4,4,4	0.71	0	6,6,6	0.58	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	EDO	D	402	-	-	0/1/1/1	-
8	PRP	C	403	-	-	3/16/33/33	0/1/1/1
8	PRP	F	403	-	-	4/16/33/33	0/1/1/1
3	EDO	C	404	-	-	1/1/1/1	-
7	ATP	F	404	6	-	6/18/38/38	0/3/3/3
3	EDO	A	402	-	-	0/1/1/1	-
5	GOL	D	403	-	-	3/4/4/4	-
2	PEG	D	401	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	E	401	-	-	1/1/1/1	-
3	EDO	F	402	-	-	0/1/1/1	-
3	EDO	D	404	-	-	0/1/1/1	-
2	PEG	A	401	-	-	0/4/4/4	-
3	EDO	D	405	-	-	1/1/1/1	-
3	EDO	A	403	-	-	1/1/1/1	-
5	GOL	A	405	-	-	1/4/4/4	-
7	ATP	C	402	6	-	7/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	404	PO4	P-O1	2.92	1.57	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	403	PRP	O5-P-O1P	-4.10	94.98	106.47
8	F	403	PRP	O2P-P-O5	-3.27	98.04	106.73
8	C	403	PRP	O1-C1-C2	2.83	111.52	106.72
7	F	404	ATP	C5-C6-N6	2.63	124.35	120.35
7	C	402	ATP	C5-C6-N6	2.63	124.34	120.35
8	F	403	PRP	O3P-P-O2P	2.44	116.98	107.64
8	C	403	PRP	O3P-P-O1P	2.14	119.07	110.68
7	C	402	ATP	PA-O3A-PB	2.06	139.91	132.83
8	C	403	PRP	PA-O3A-PB	-2.06	125.77	132.83

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	403	GOL	C1-C2-C3-O3
5	D	403	GOL	O2-C2-C3-O3
7	C	402	ATP	PB-O3B-PG-O3G
7	C	402	ATP	C5'-O5'-PA-O3A
7	C	402	ATP	O4'-C4'-C5'-O5'
7	C	402	ATP	C3'-C4'-C5'-O5'
7	F	404	ATP	PB-O3B-PG-O2G
7	F	404	ATP	O4'-C4'-C5'-O5'
8	F	403	PRP	PA-O3A-PB-O2B
7	F	404	ATP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	E	401	EDO	O1-C1-C2-O2
2	D	401	PEG	O2-C3-C4-O4
8	C	403	PRP	C1-O1-PA-O3A
3	C	404	EDO	O1-C1-C2-O2
3	D	405	EDO	O1-C1-C2-O2
5	D	403	GOL	O1-C1-C2-O2
7	F	404	ATP	C5'-O5'-PA-O3A
7	C	402	ATP	C5'-O5'-PA-O1A
7	C	402	ATP	C5'-O5'-PA-O2A
7	C	402	ATP	PB-O3B-PG-O1G
2	D	401	PEG	C1-C2-O2-C3
2	D	401	PEG	O1-C1-C2-O2
8	C	403	PRP	PB-O3A-PA-O1A
3	A	403	EDO	O1-C1-C2-O2
7	F	404	ATP	PB-O3B-PG-O3G
8	F	403	PRP	PA-O3A-PB-O3B
8	C	403	PRP	O4-C4-C5-O5
5	A	405	GOL	O1-C1-C2-C3
7	F	404	ATP	C5'-O5'-PA-O1A
8	F	403	PRP	O4-C4-C5-O5
8	F	403	PRP	PA-O3A-PB-O1B

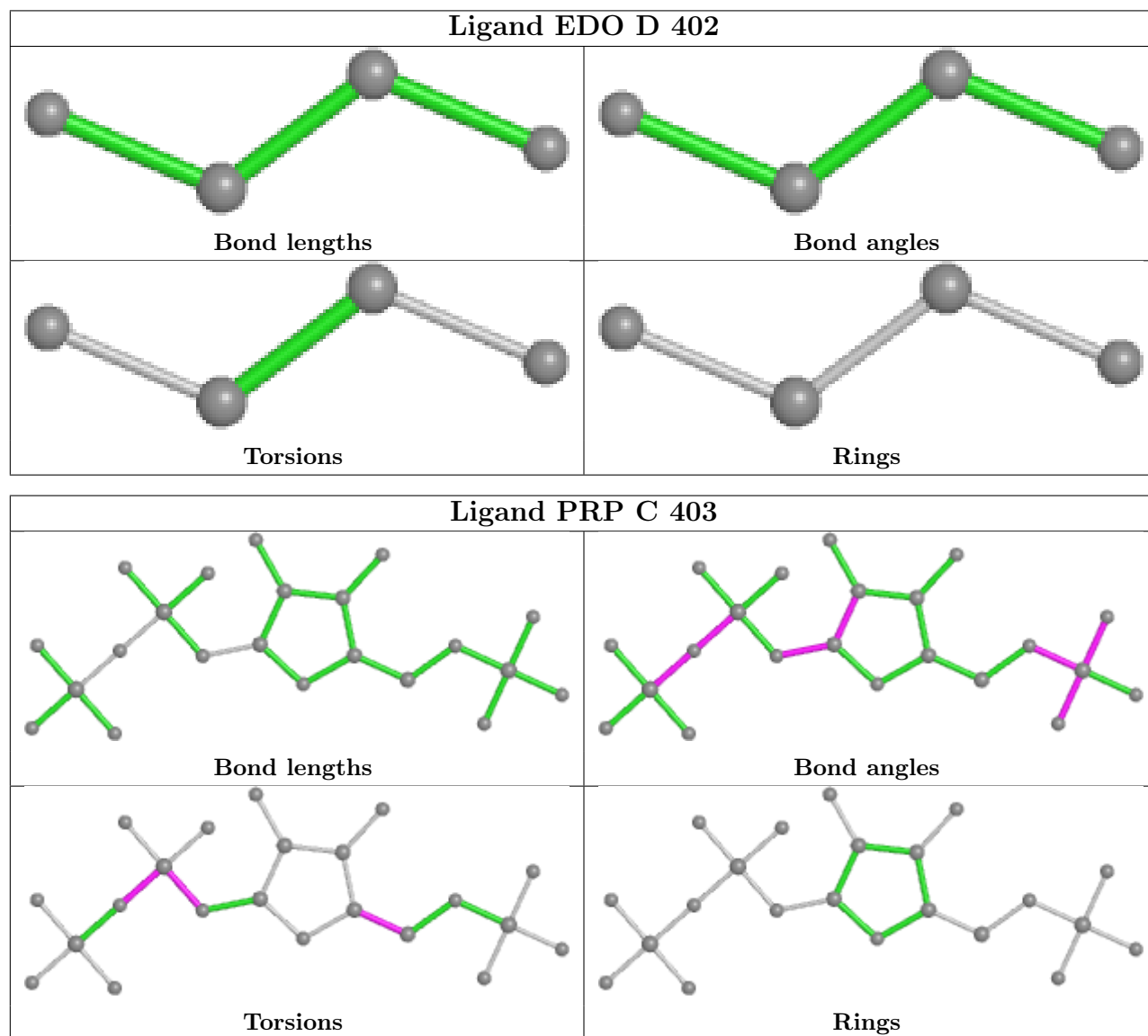
There are no ring outliers.

7 monomers are involved in 14 short contacts:

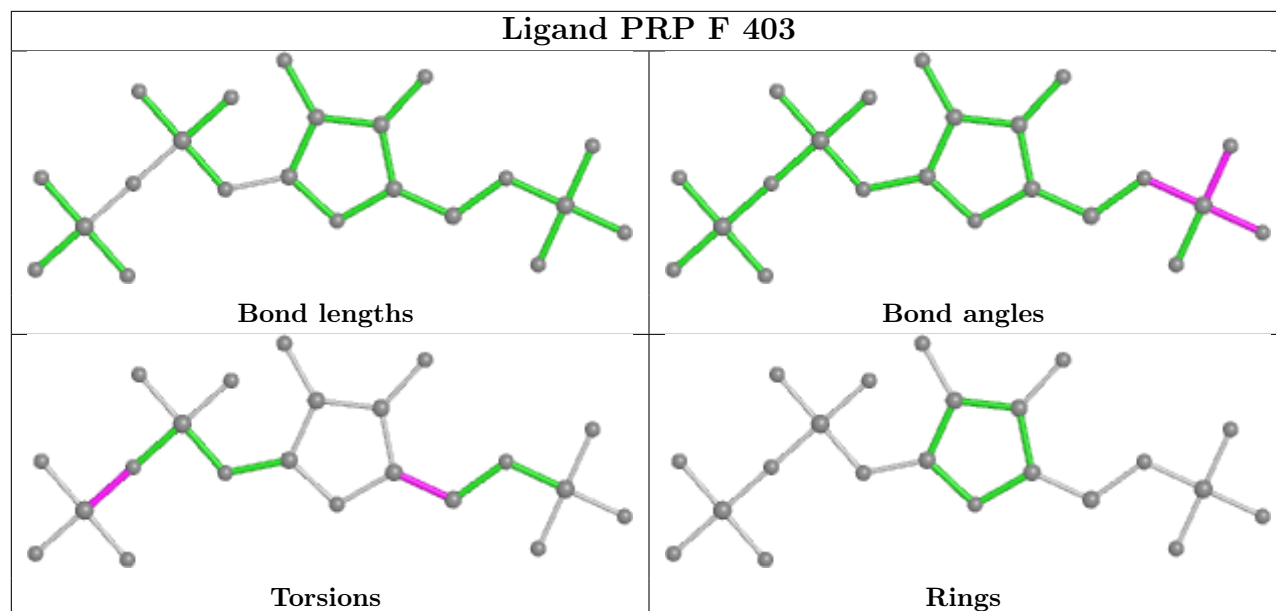
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	EDO	1	0
8	C	403	PRP	2	0
8	F	403	PRP	2	0
7	F	404	ATP	2	0
5	D	403	GOL	1	0
2	D	401	PEG	4	0
7	C	402	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

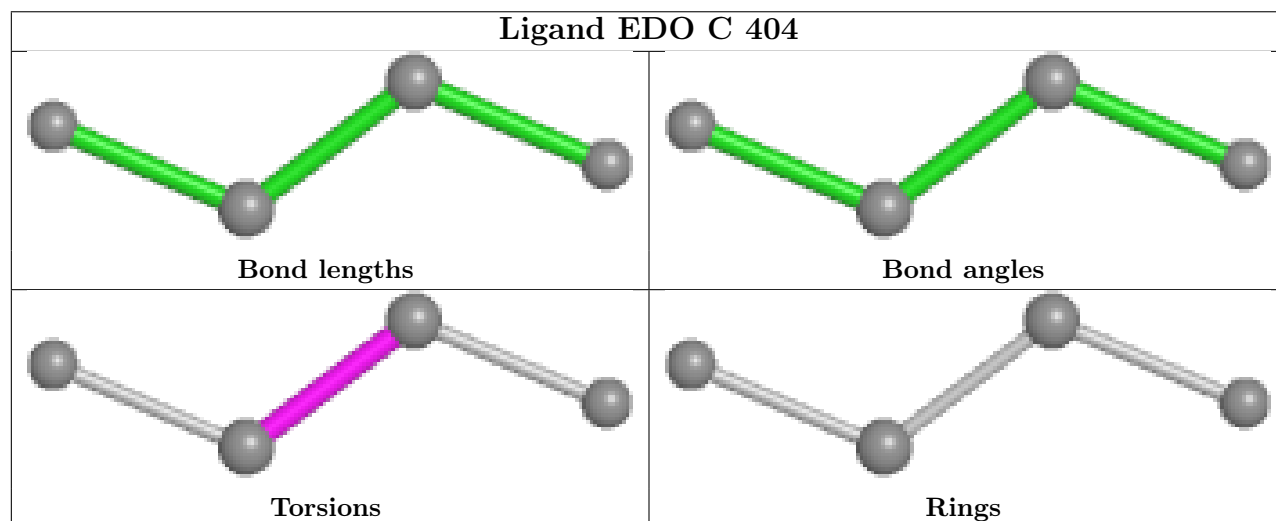
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



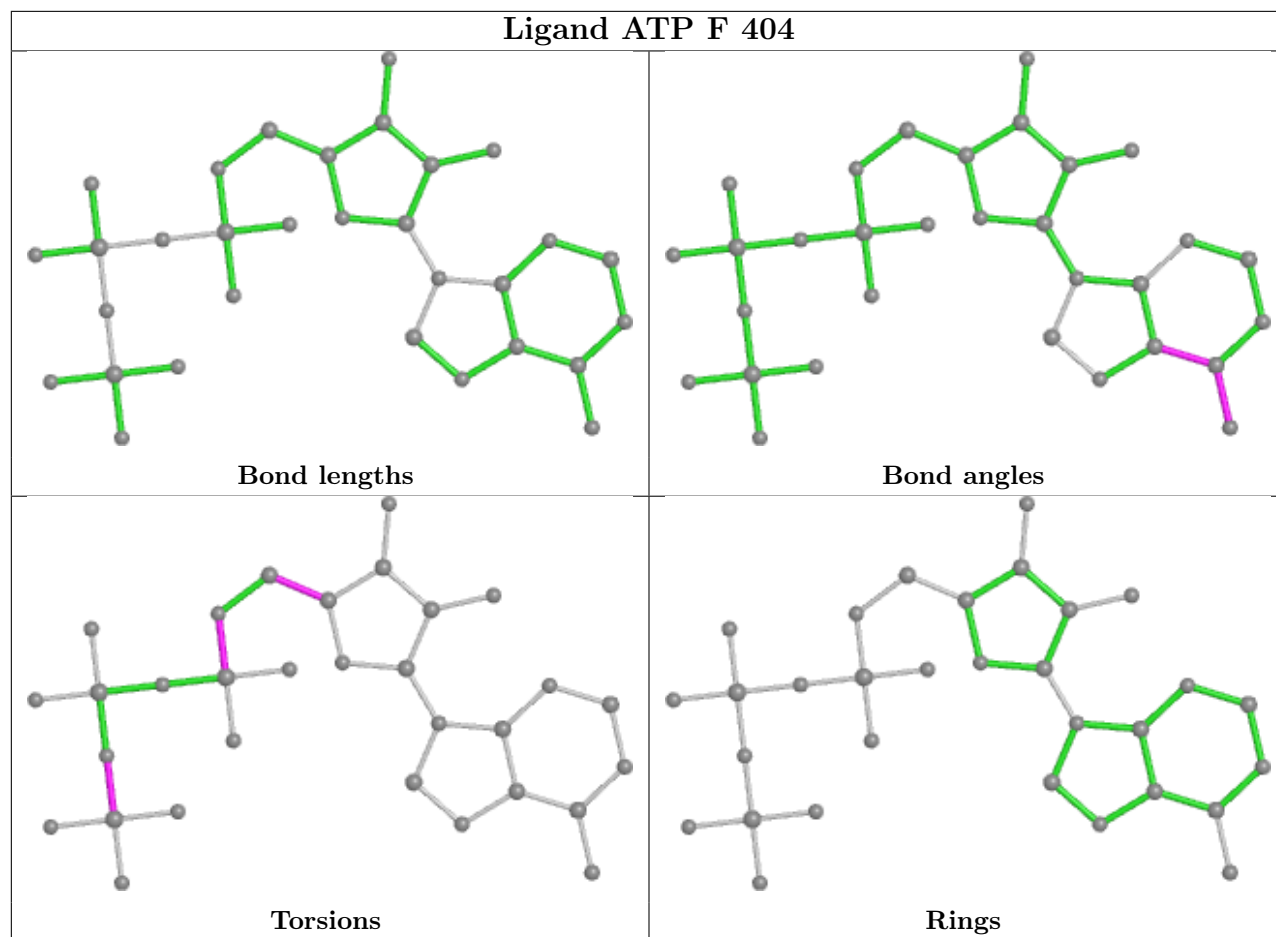
Ligand PRP F 403



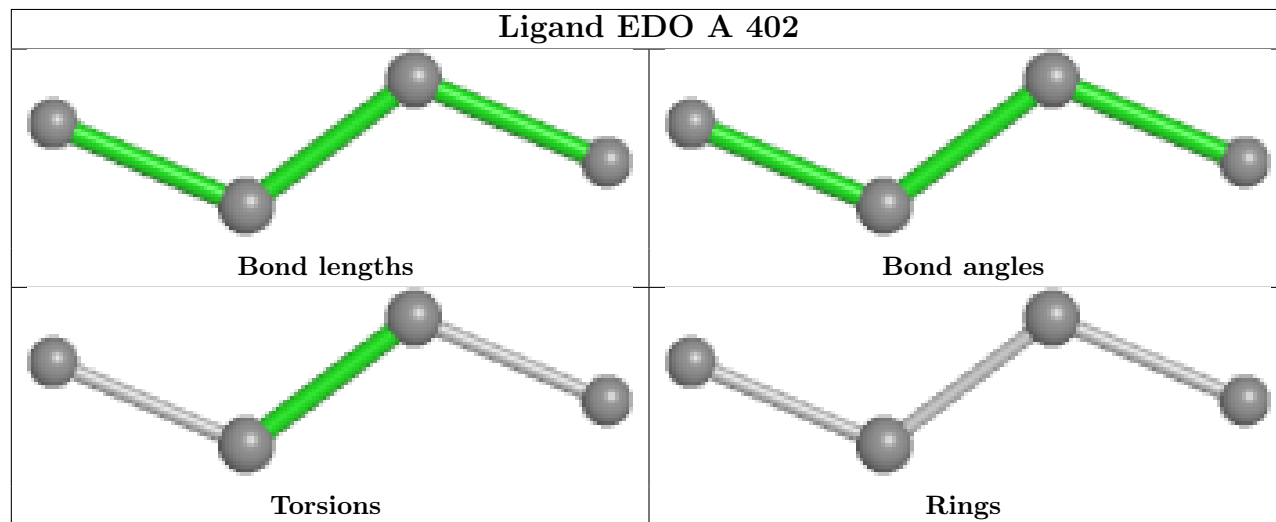
Ligand EDO C 404

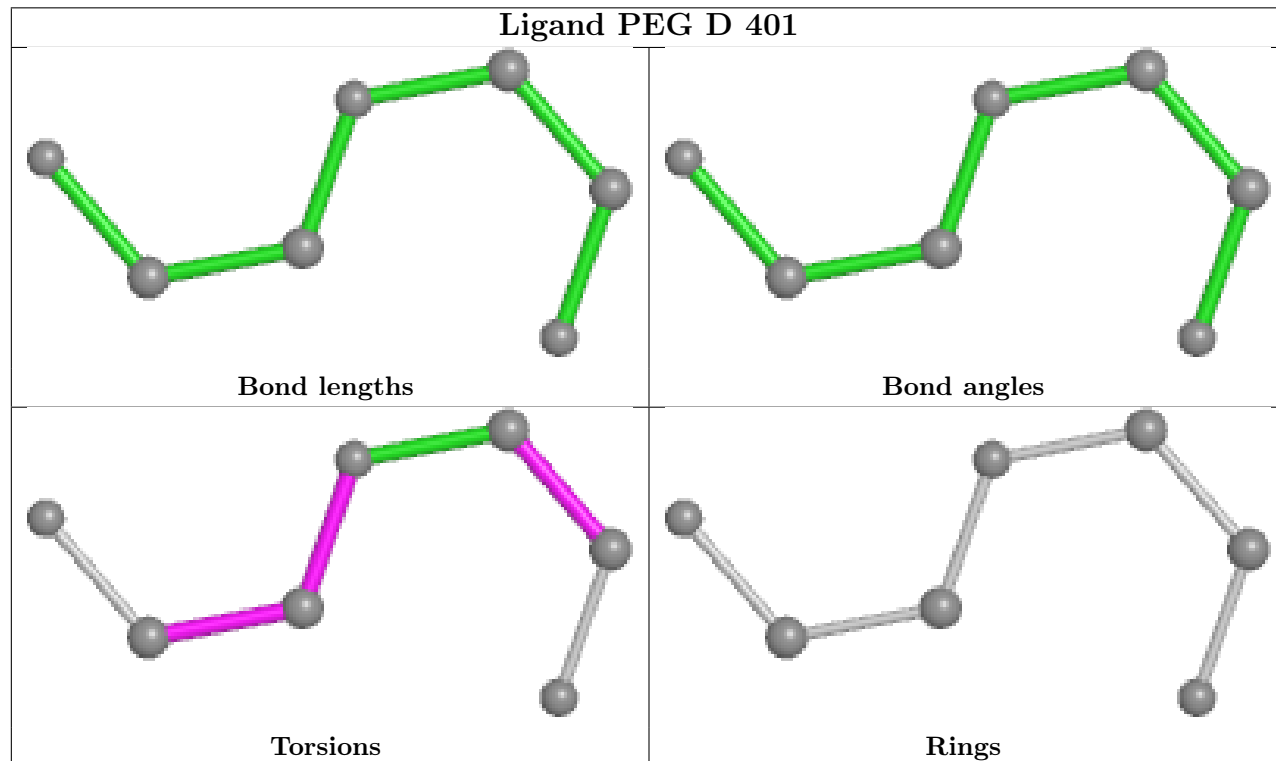
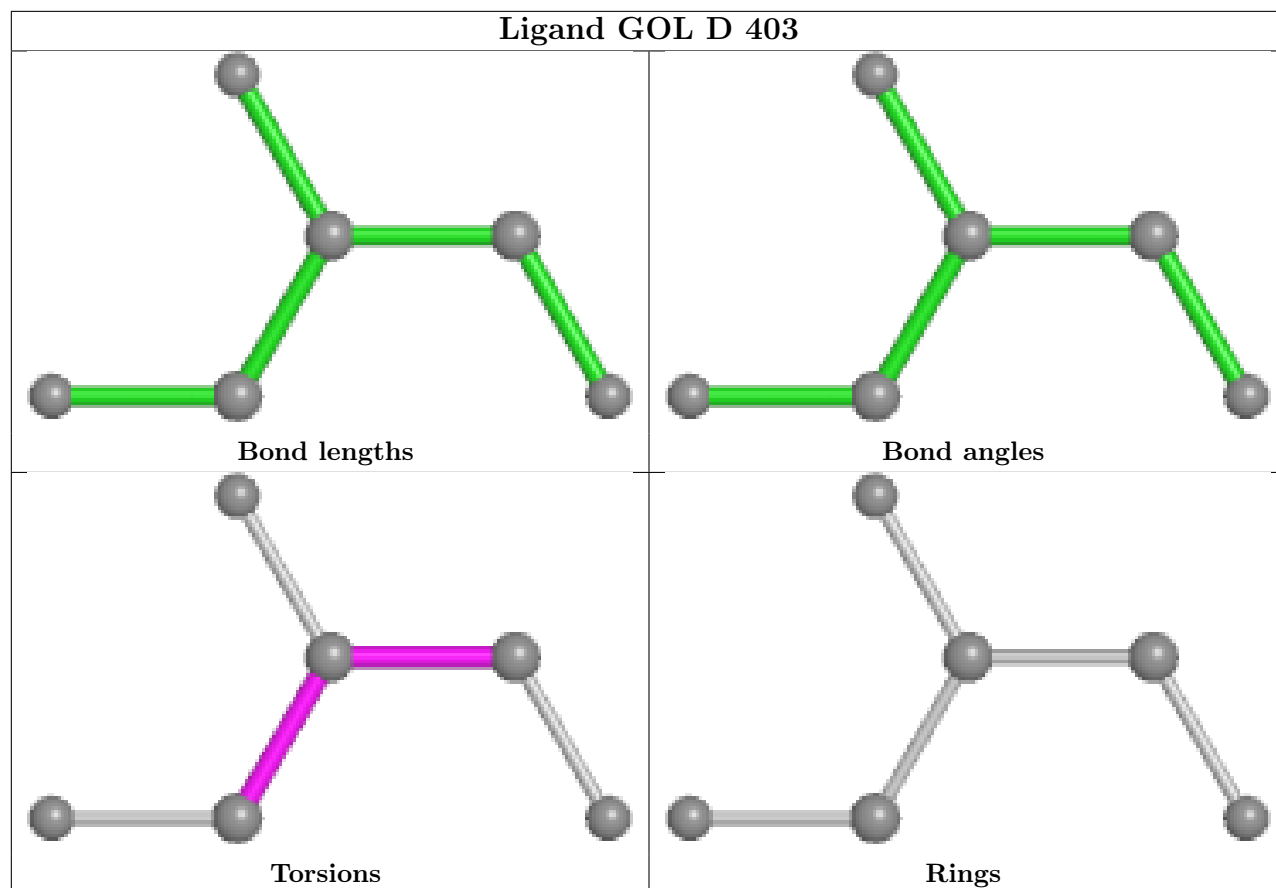


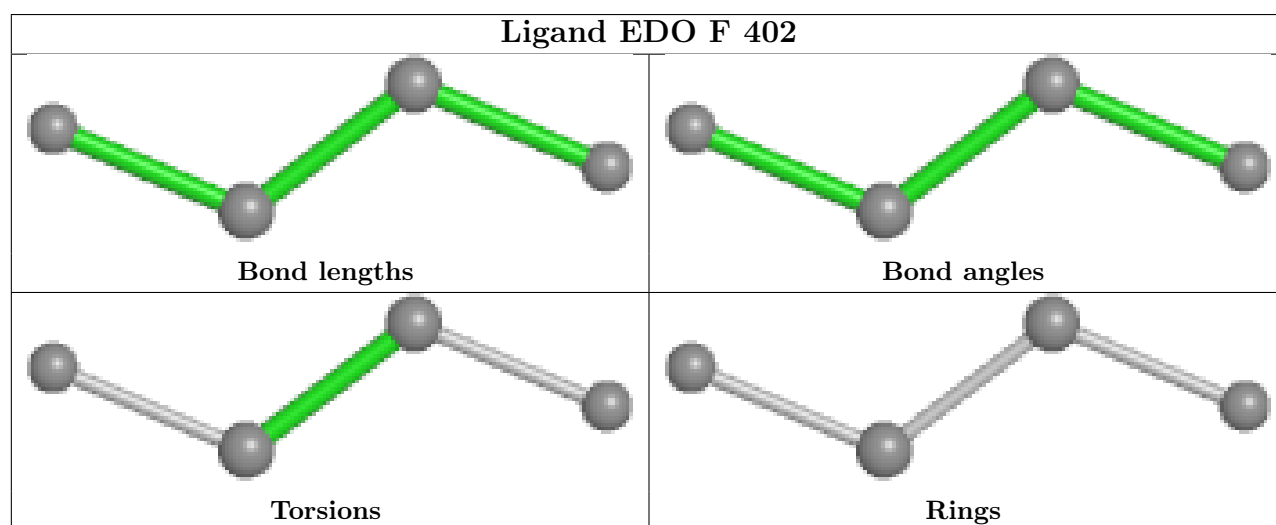
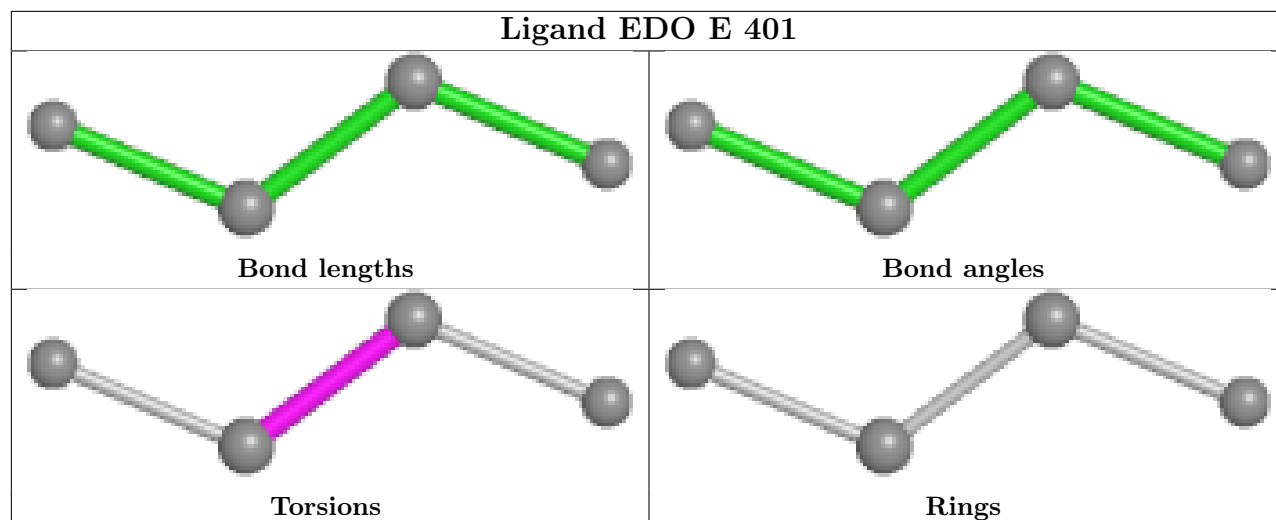
Ligand ATP F 404

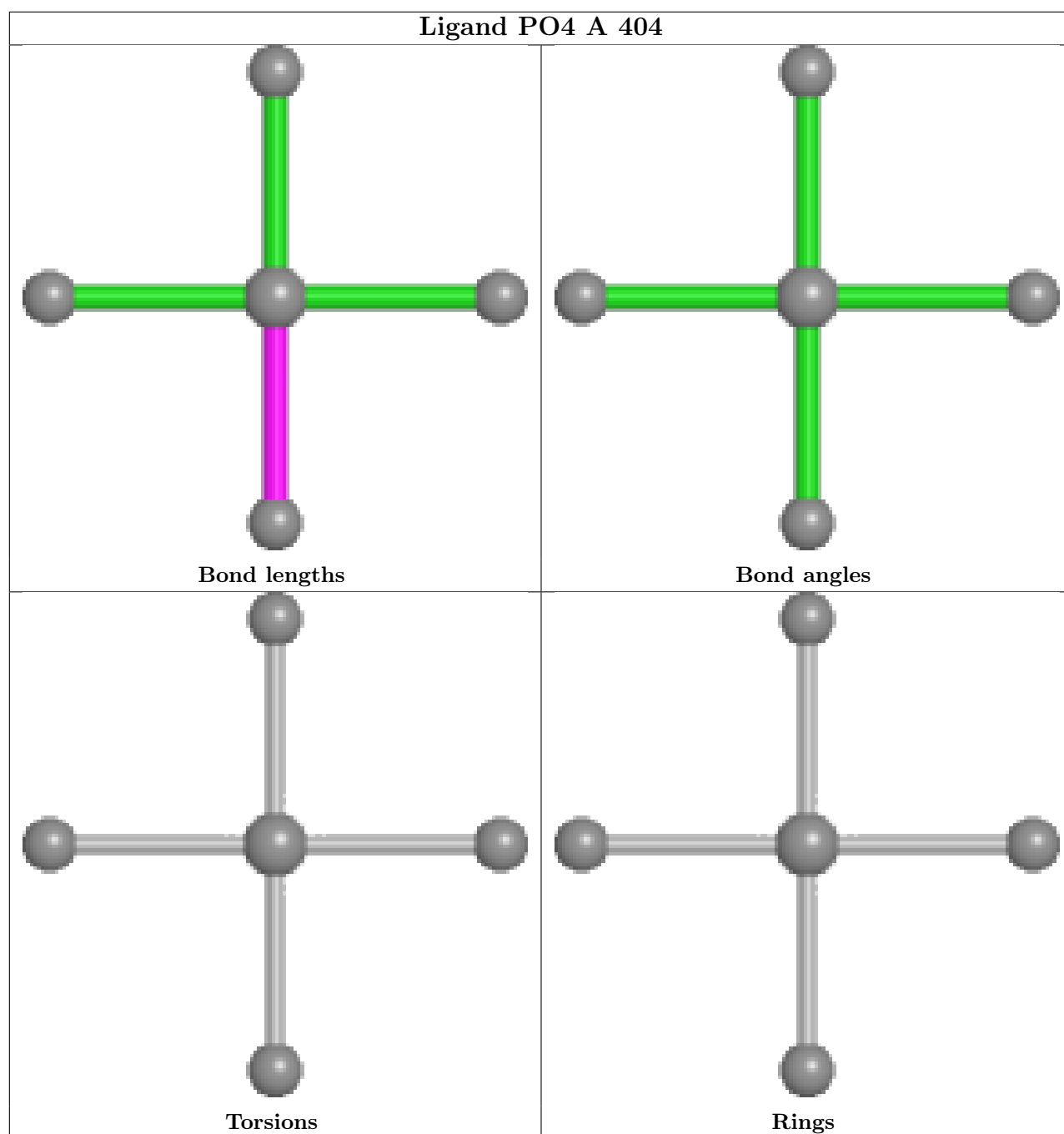


Ligand EDO A 402

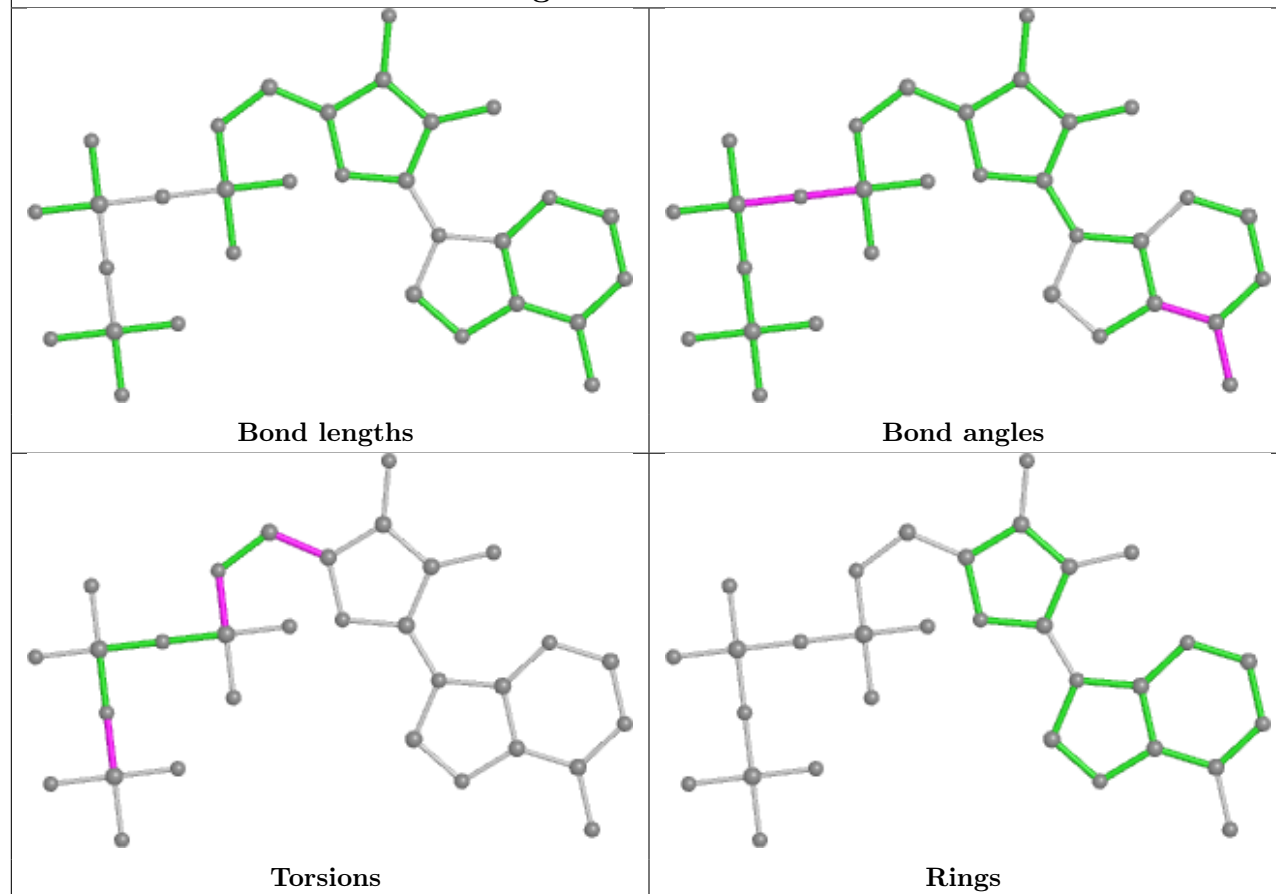




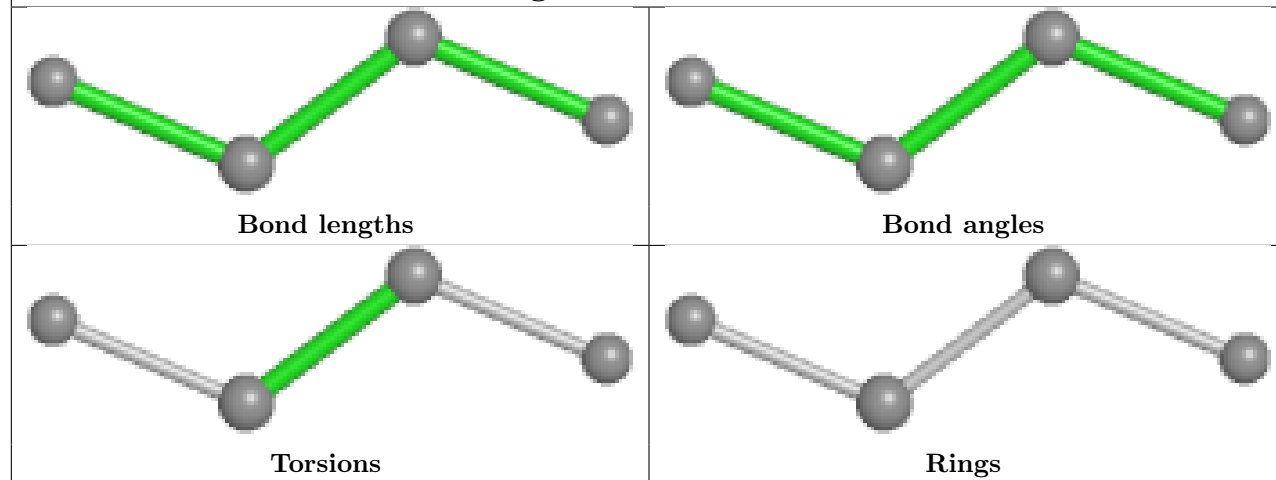


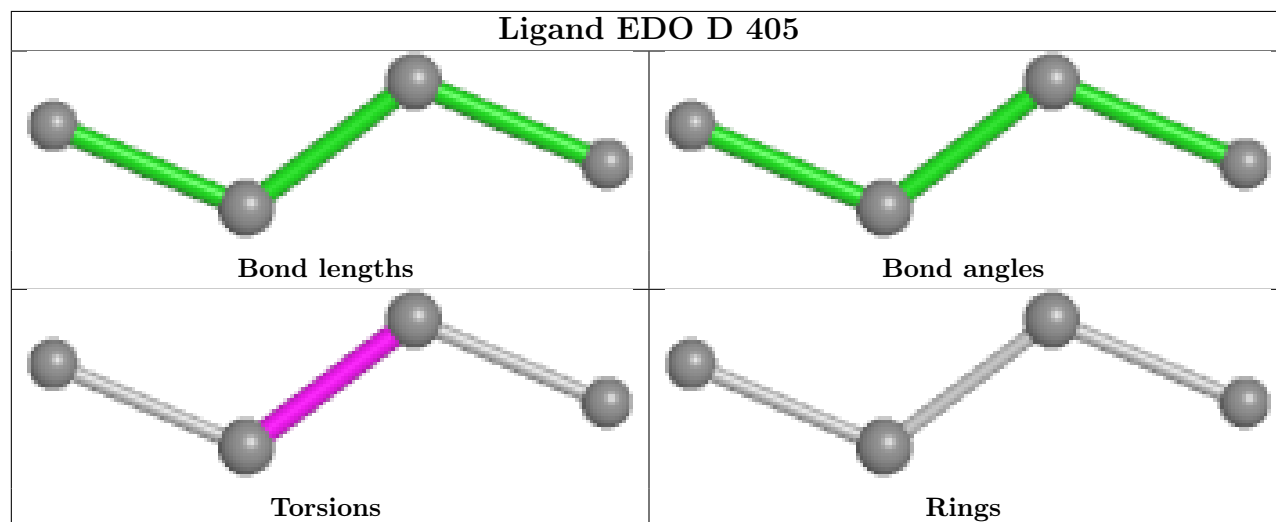
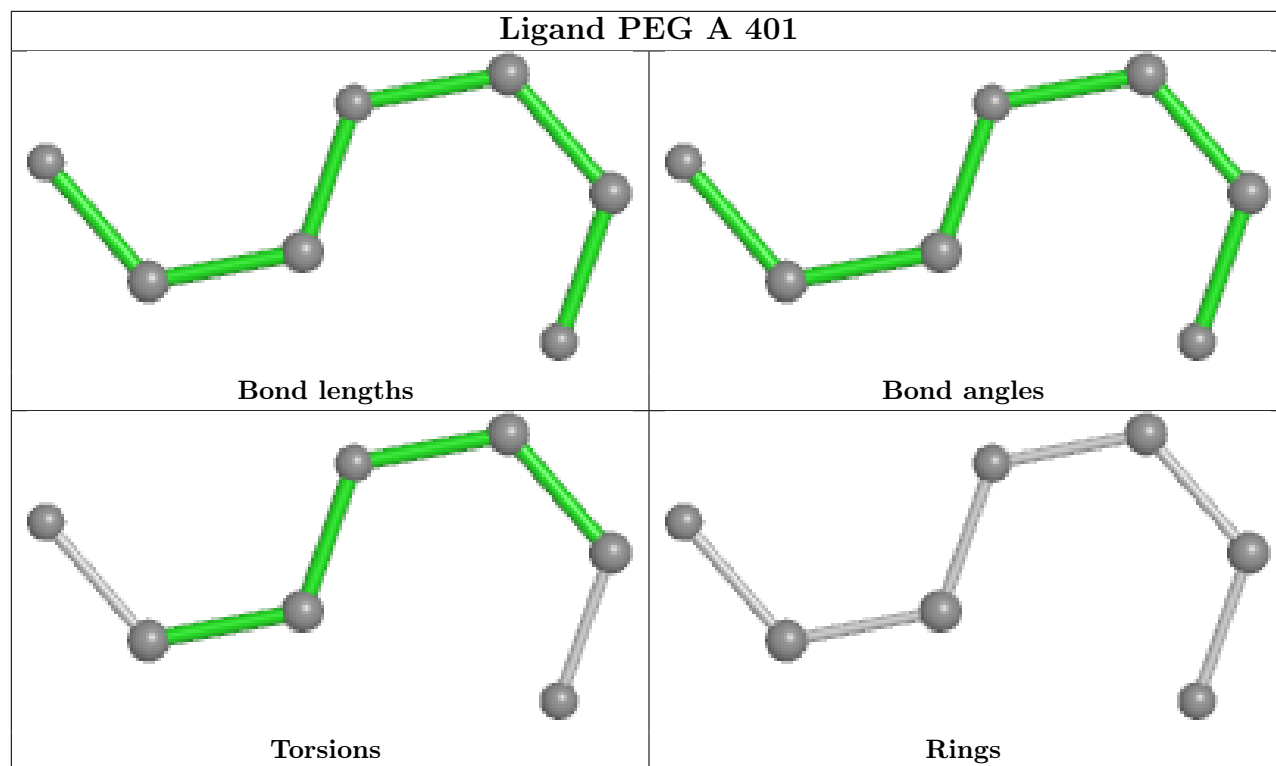


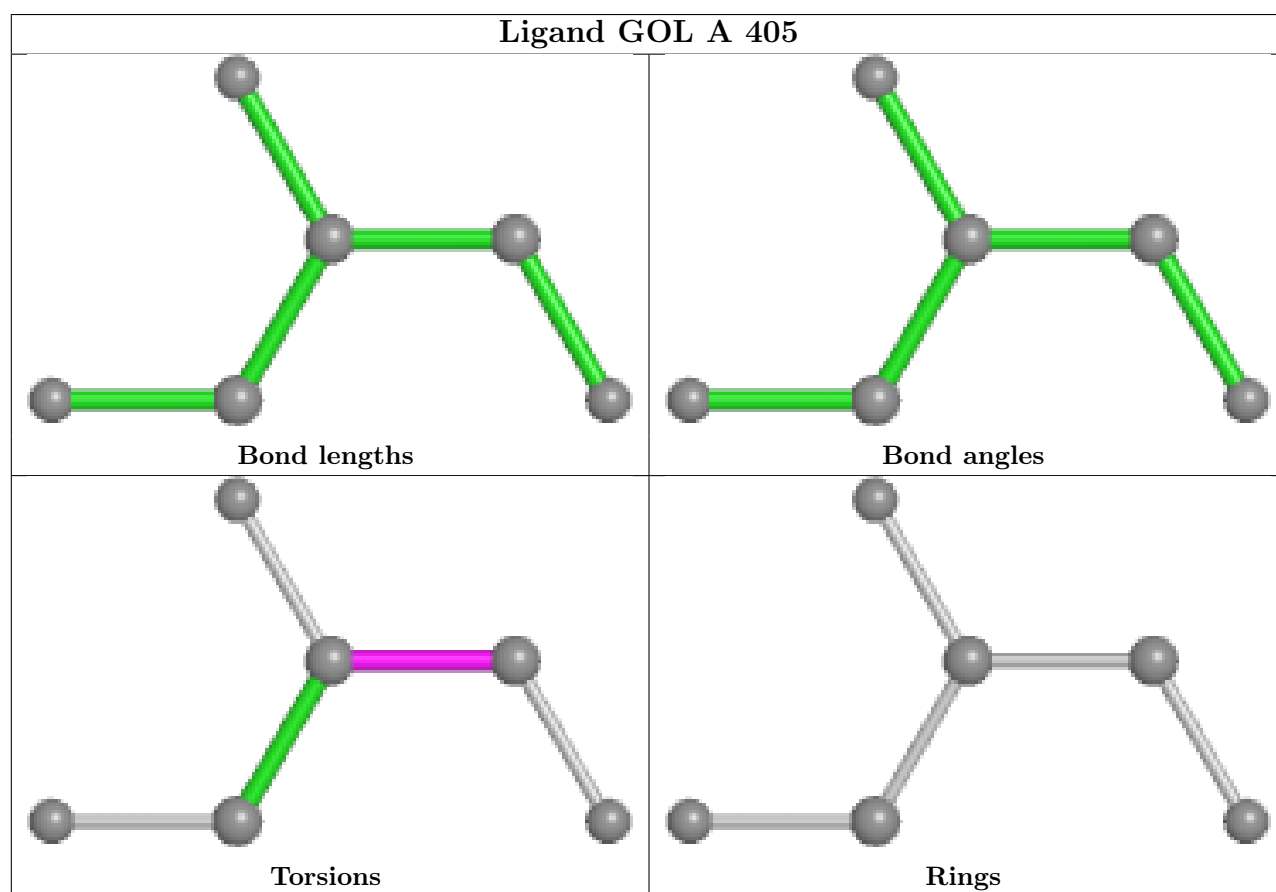
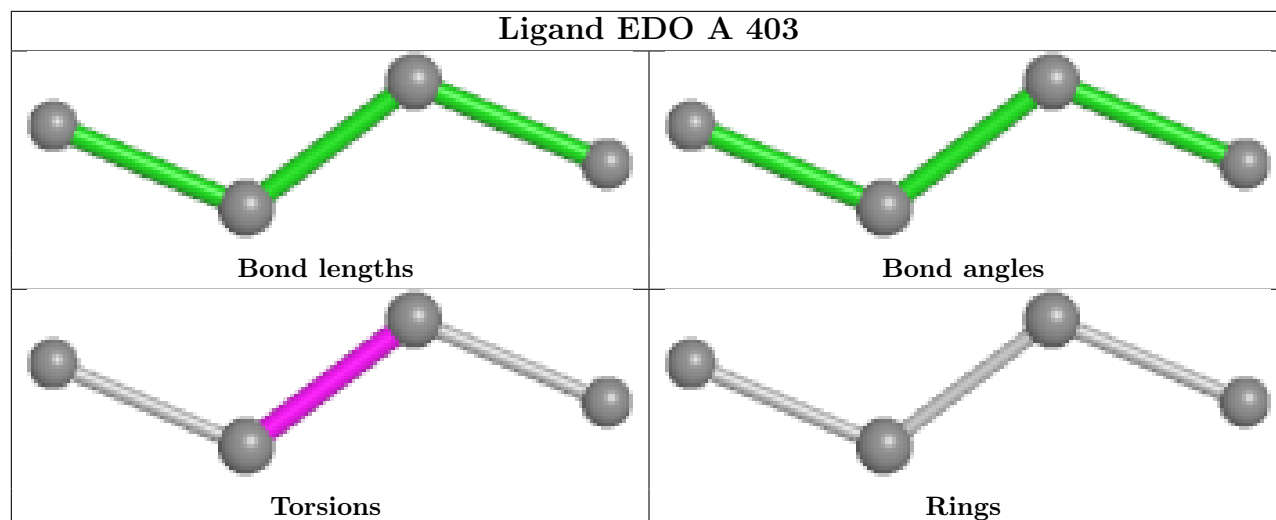
Ligand ATP C 402

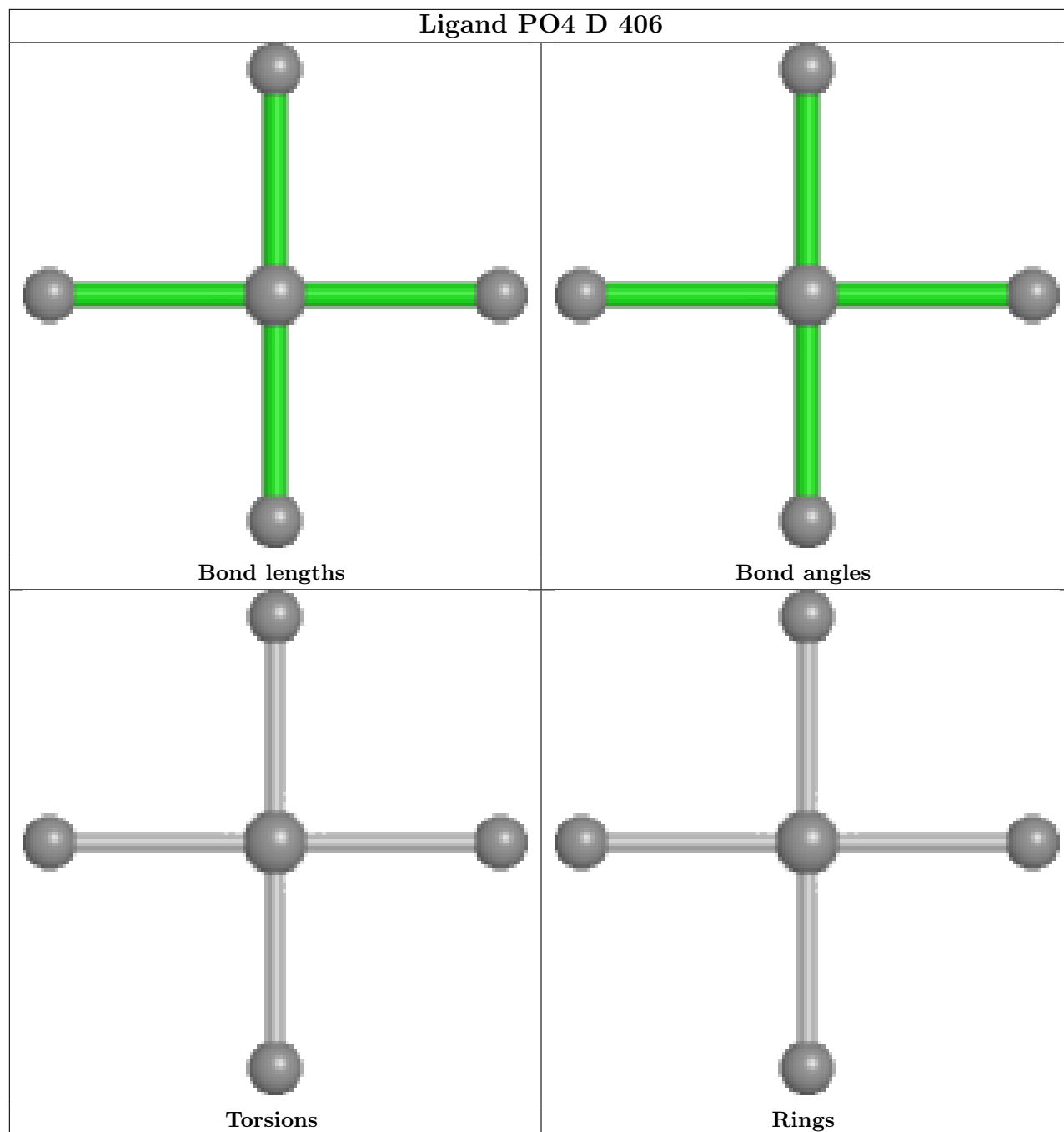


Ligand EDO D 404









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	288/310 (92%)	-0.35	1 (0%) 94 94	39, 62, 110, 136	1 (0%)
1	B	292/310 (94%)	-0.23	0 100 100	45, 78, 111, 128	1 (0%)
1	C	288/310 (92%)	-0.33	1 (0%) 94 94	43, 67, 109, 137	0
1	D	287/310 (92%)	-0.35	0 100 100	38, 61, 108, 130	0
1	E	293/310 (94%)	-0.26	1 (0%) 94 94	47, 78, 112, 125	1 (0%)
1	F	287/310 (92%)	-0.35	1 (0%) 94 94	42, 68, 108, 138	1 (0%)
All	All	1735/1860 (93%)	-0.31	4 (0%) 95 95	38, 69, 111, 138	4 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	170	ASP	2.8
1	A	237	HIS	2.1
1	E	261	LEU	2.1
1	C	93	ASN	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,

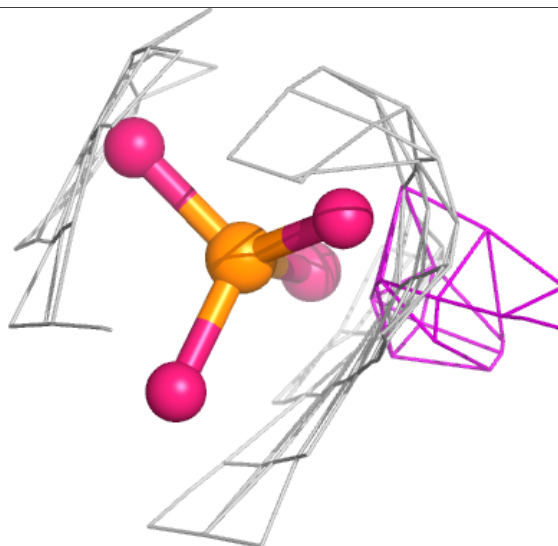
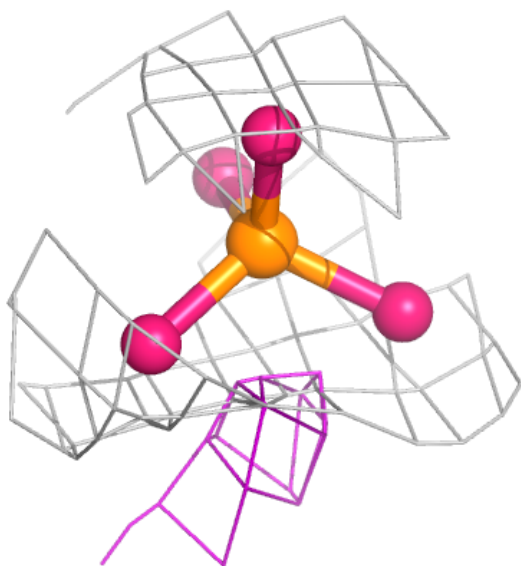
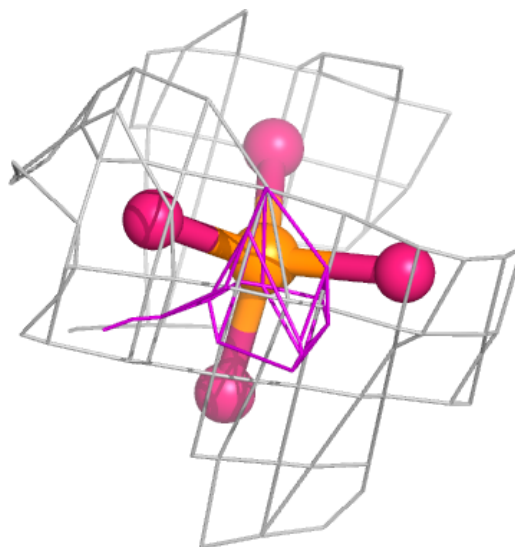
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PO4	D	406	5/5	0.82	0.12	106,116,123,123	0
8	PRP	F	403	22/22	0.82	0.21	106,168,191,198	0
3	EDO	E	401	4/4	0.84	0.24	89,89,89,90	0
8	PRP	C	403	22/22	0.85	0.19	104,159,200,202	0
3	EDO	D	405	4/4	0.85	0.14	71,76,81,87	0
7	ATP	F	404	31/31	0.86	0.16	78,97,116,118	12
3	EDO	F	402	4/4	0.87	0.25	77,82,85,85	0
3	EDO	D	402	4/4	0.88	0.31	91,96,96,97	0
2	PEG	A	401	7/7	0.89	0.15	84,87,89,90	0
2	PEG	D	401	7/7	0.89	0.17	80,89,102,102	0
7	ATP	C	402	31/31	0.90	0.16	81,111,120,124	1
5	GOL	D	403	6/6	0.91	0.17	67,68,70,71	0
4	PO4	A	404	5/5	0.92	0.09	97,104,113,114	0
3	EDO	D	404	4/4	0.92	0.26	69,75,78,79	0
3	EDO	C	404	4/4	0.92	0.17	91,91,92,92	0
6	MG	F	401	1/1	0.92	0.09	76,76,76,76	0
3	EDO	A	402	4/4	0.94	0.15	74,75,77,77	0
5	GOL	A	405	6/6	0.95	0.21	69,72,77,80	0
6	MG	C	401	1/1	0.98	0.06	71,71,71,71	0
3	EDO	A	403	4/4	0.98	0.17	74,75,76,77	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.

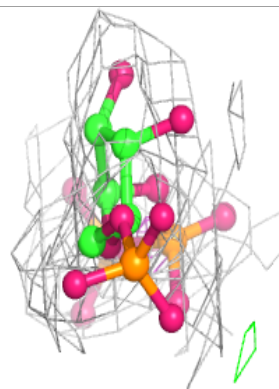
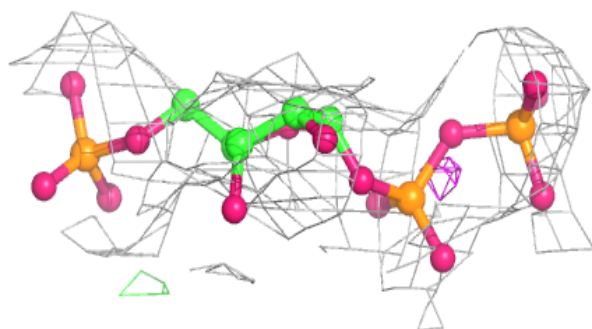
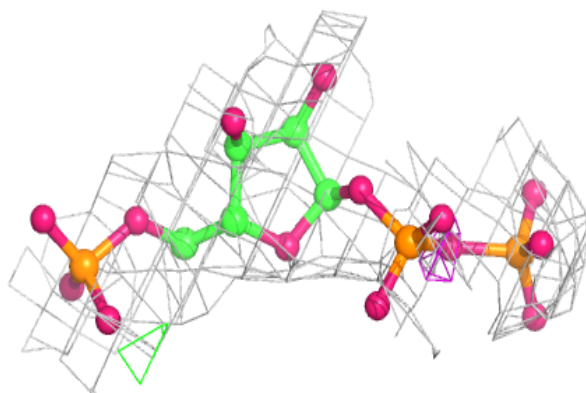
Electron density around PO4 D 406:

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

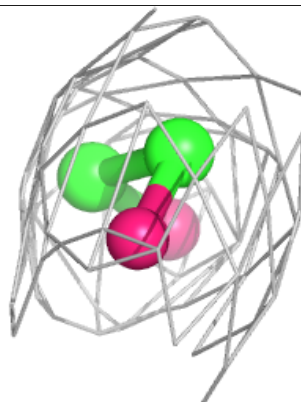
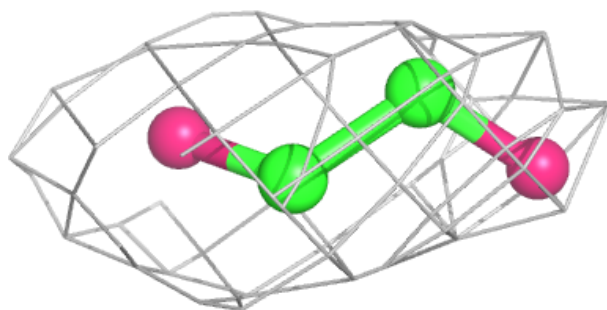
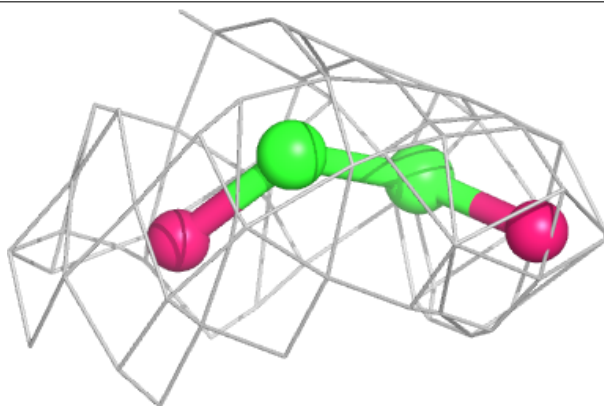


Electron density around PRP F 403:

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

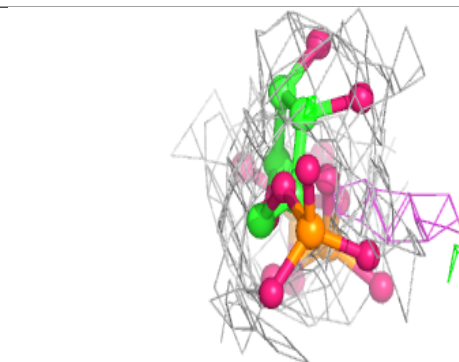
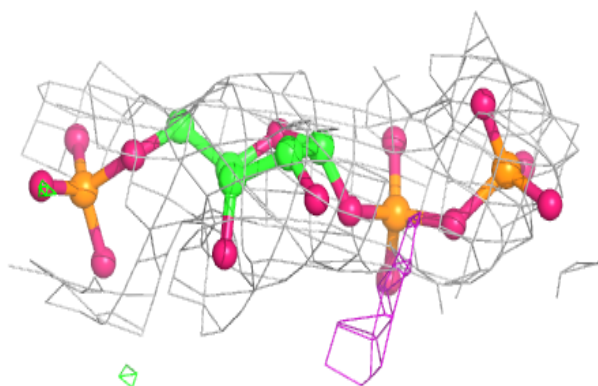
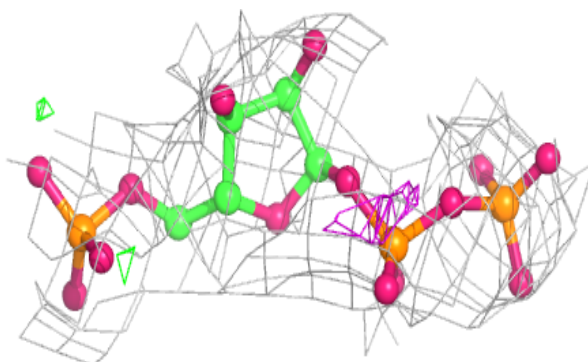
**Electron density around EDO E 401:**

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

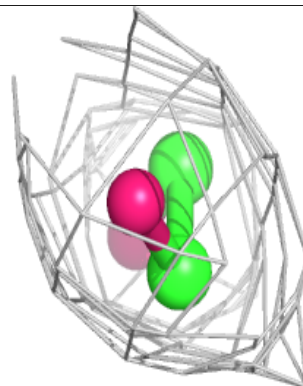
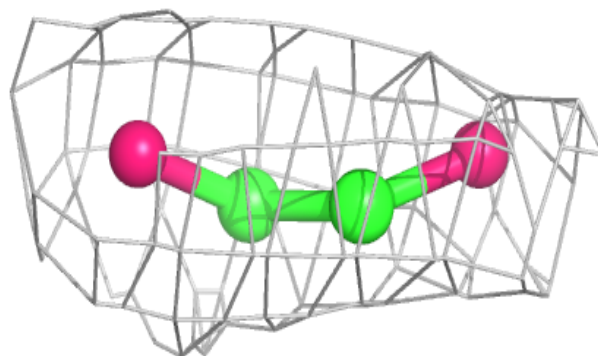
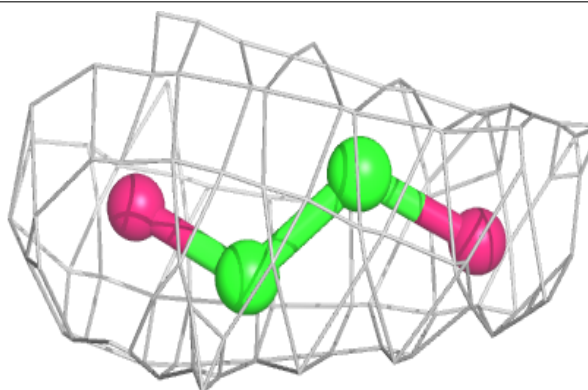


Electron density around PRP C 403:

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

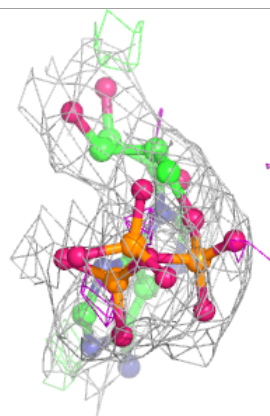
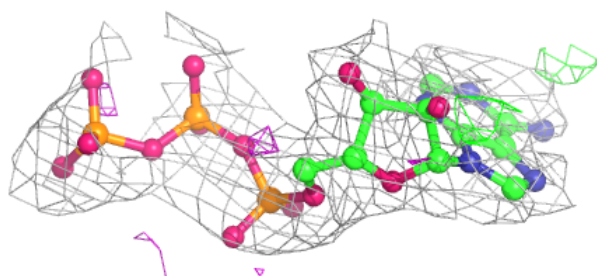
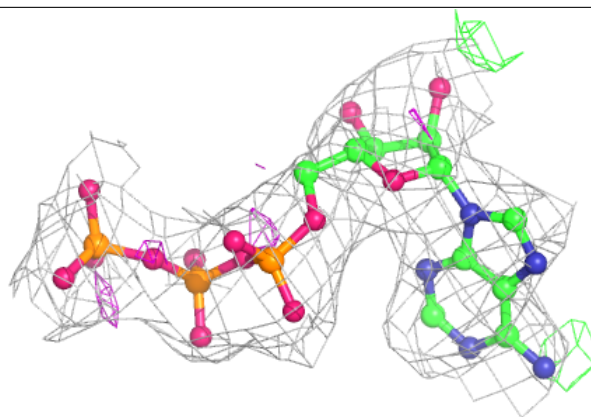
**Electron density around EDO D 405:**

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

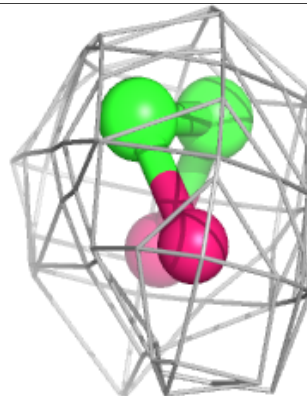
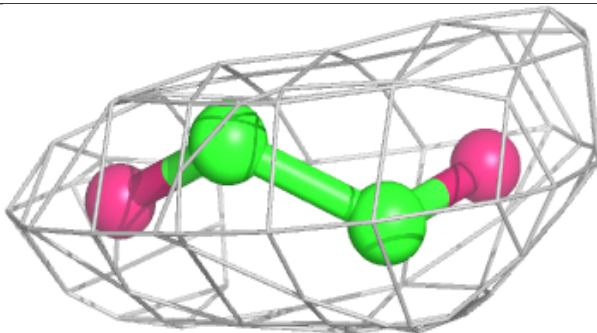
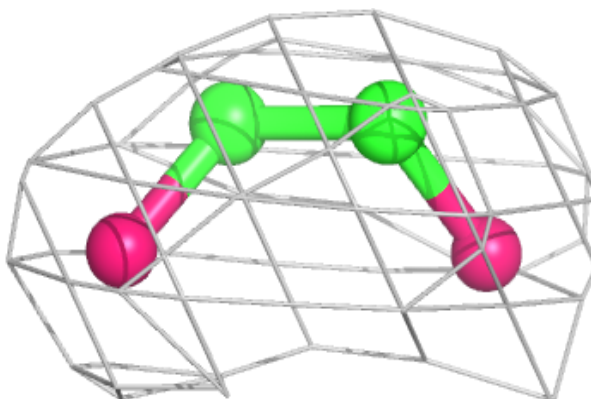


Electron density around ATP F 404:

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

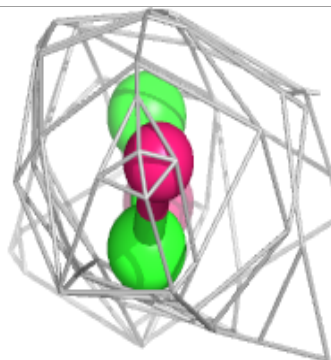
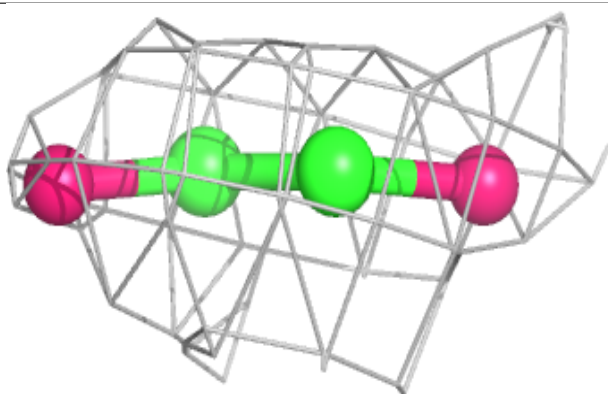
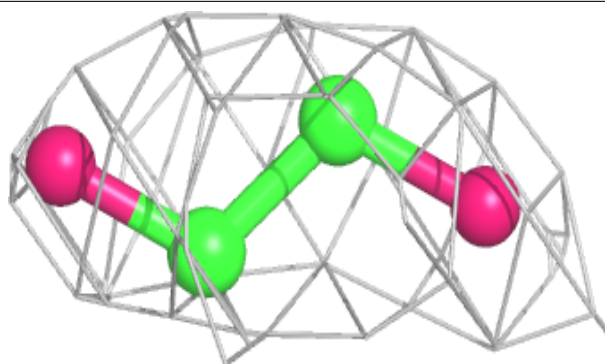
**Electron density around EDO F 402:**

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

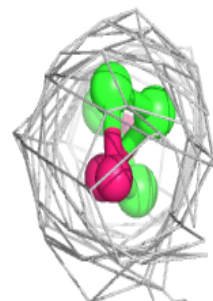
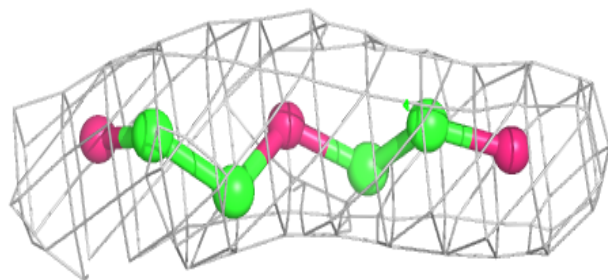
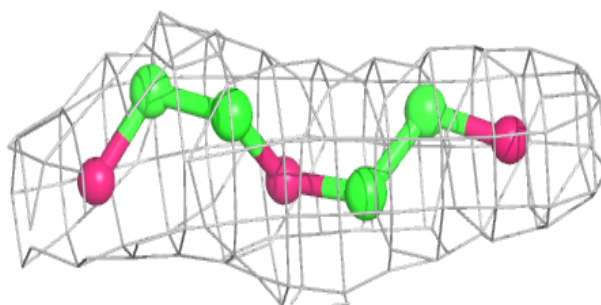


Electron density around EDO D 402:

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

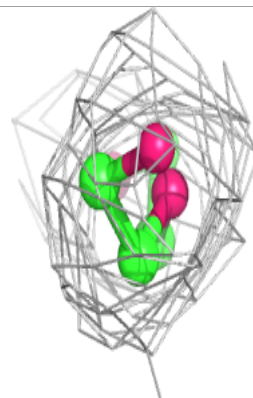
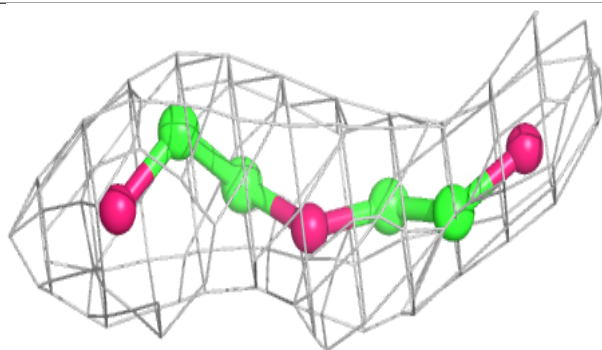
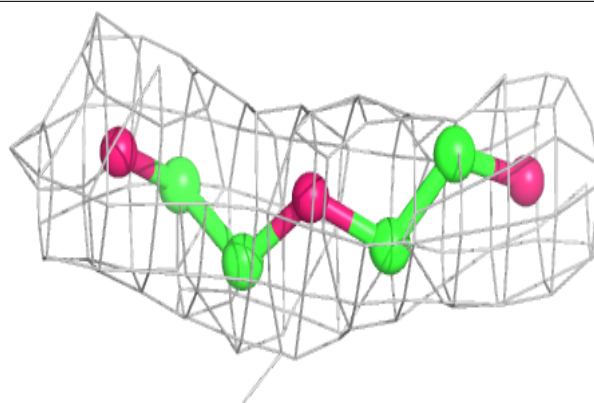
**Electron density around PEG A 401:**

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

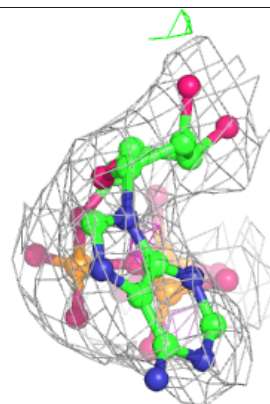
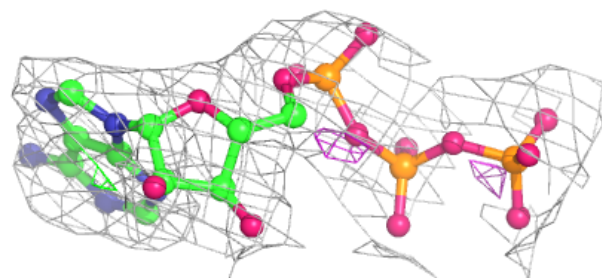
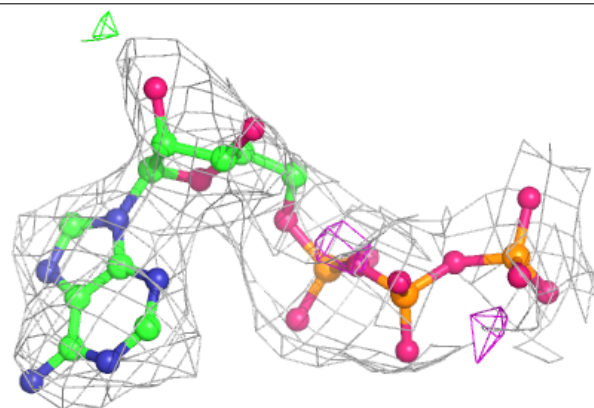


Electron density around PEG D 401:

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

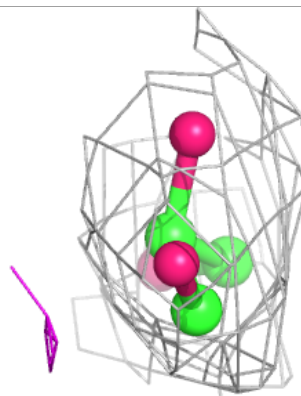
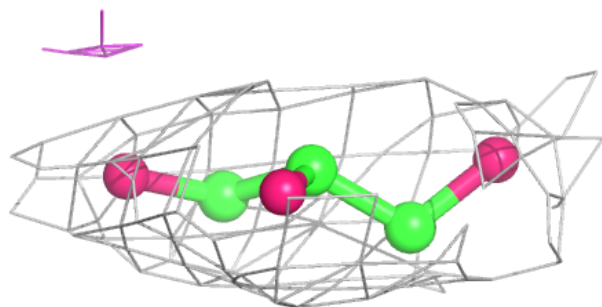
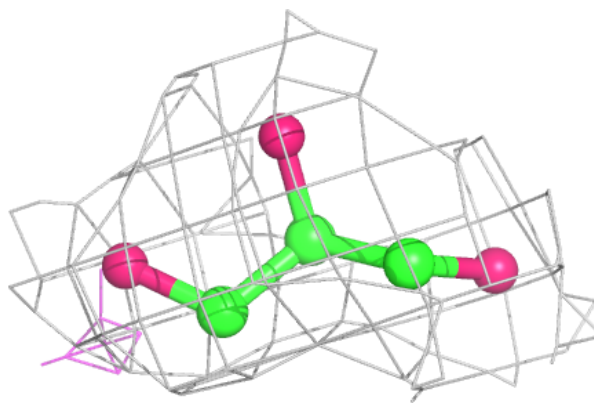
**Electron density around ATP C 402:**

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



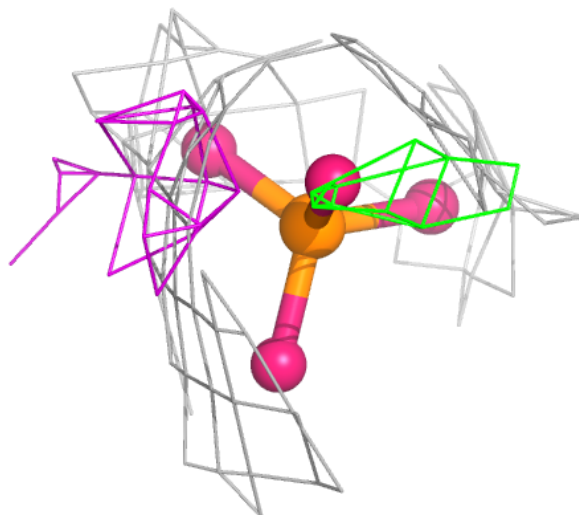
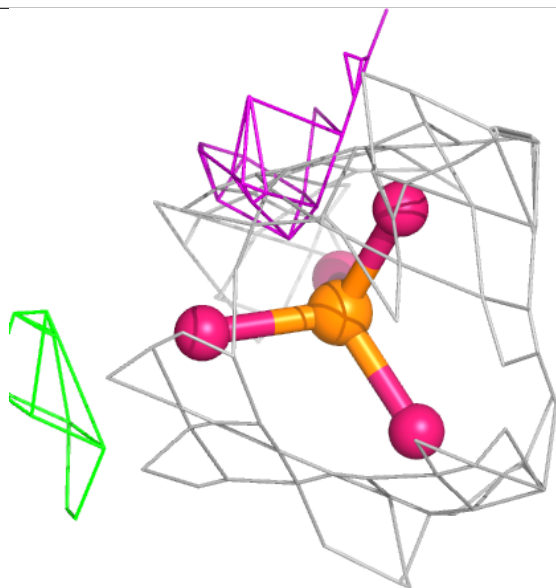
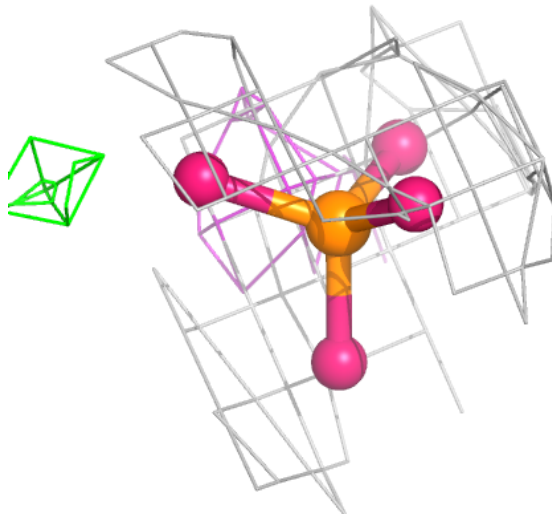
Electron density around GOL D 403:

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



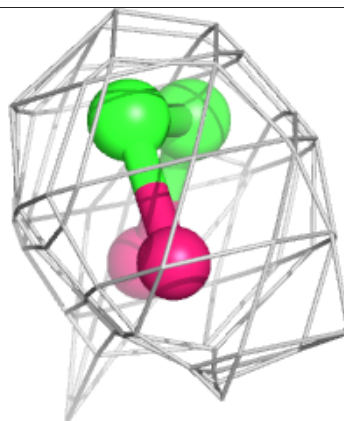
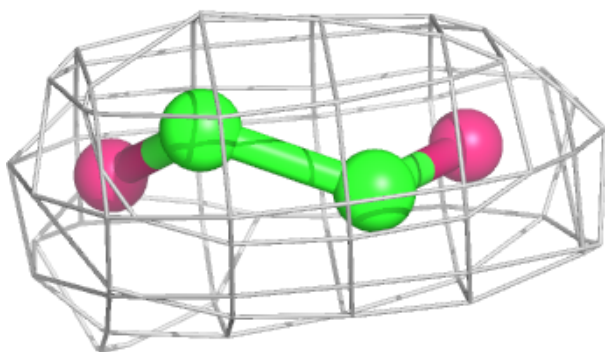
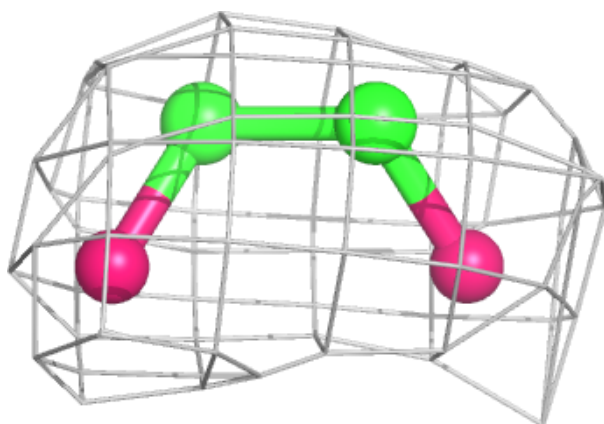
Electron density around PO4 A 404:

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

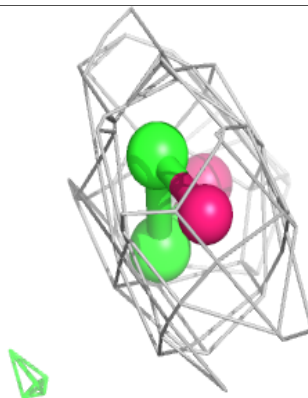
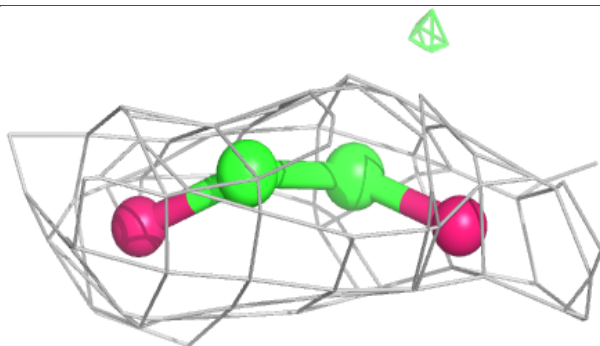
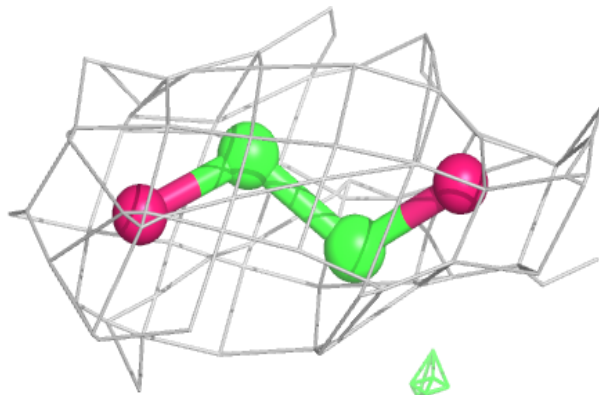


Electron density around EDO D 404:

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

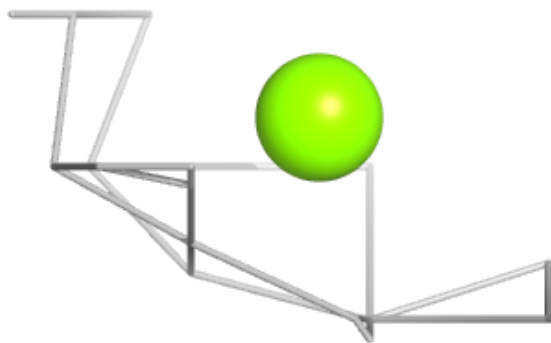
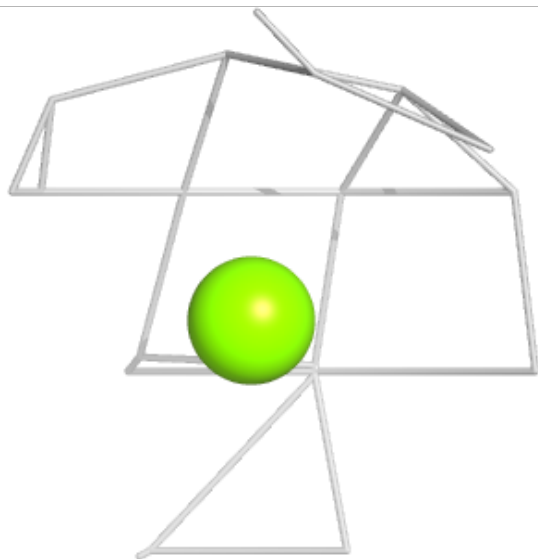
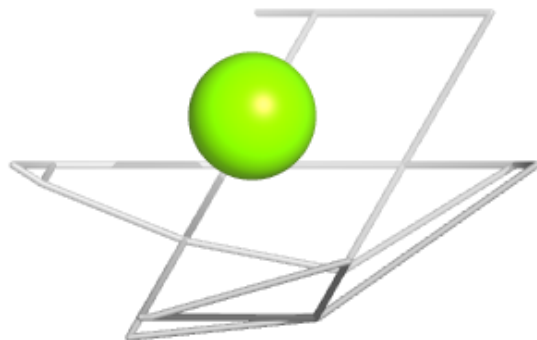
**Electron density around EDO C 404:**

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



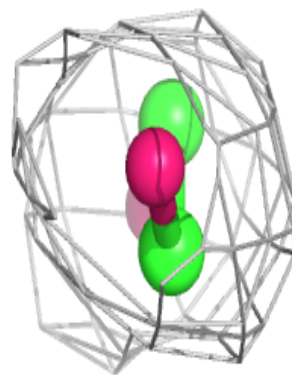
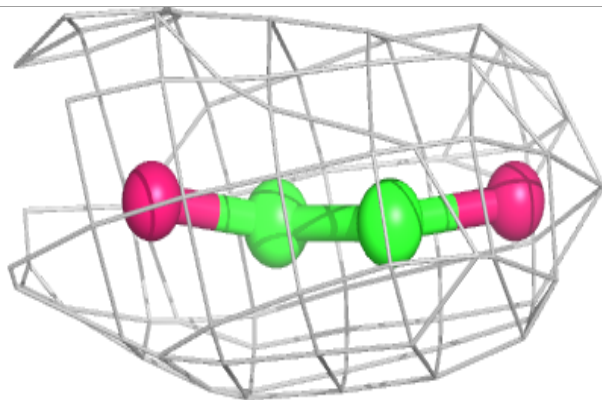
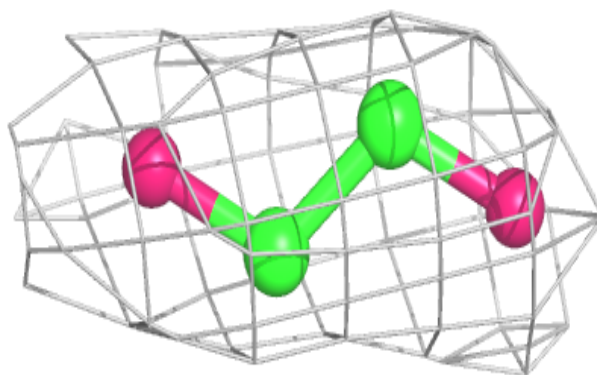
Electron density around MG F 401:

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

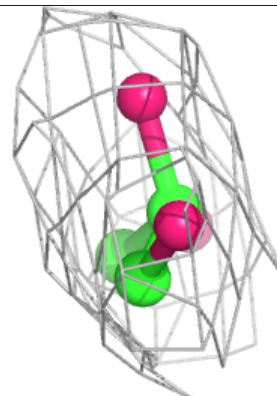
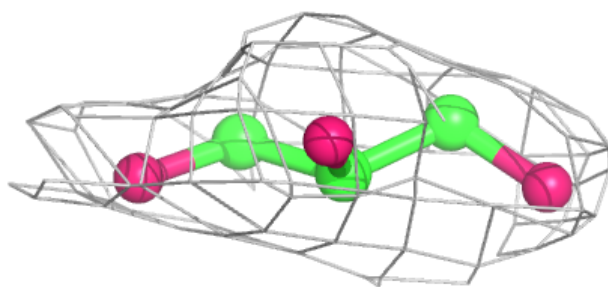
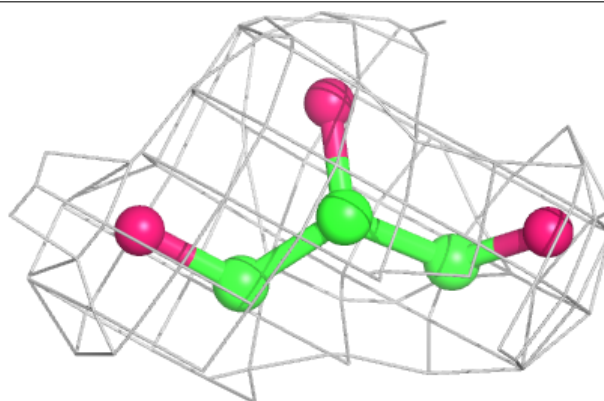


Electron density around EDO A 402:

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

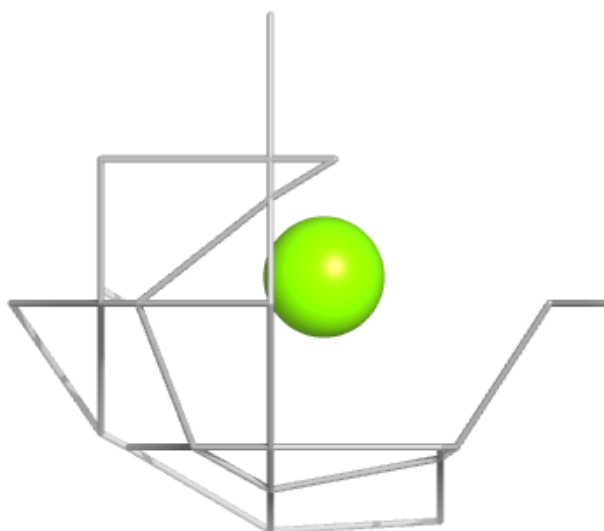
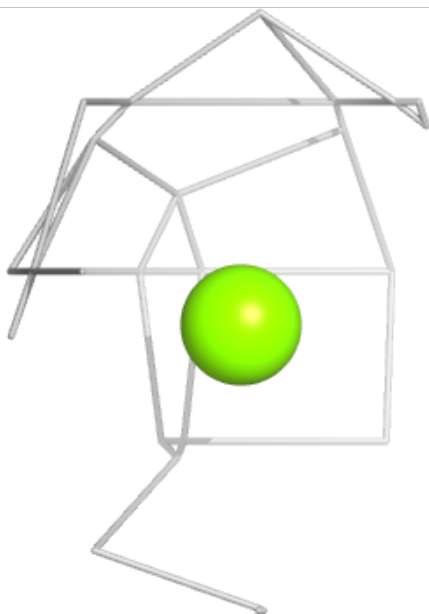
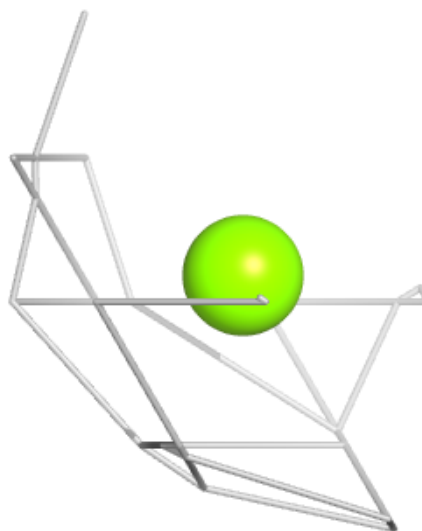
**Electron density around GOL A 405:**

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



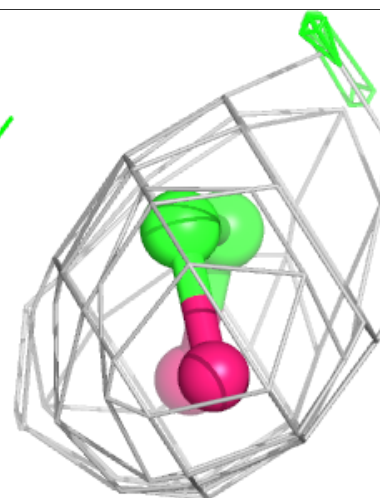
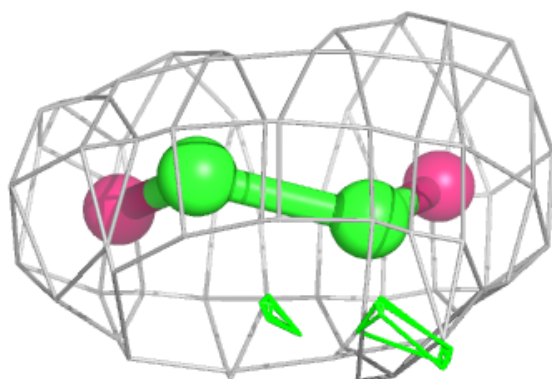
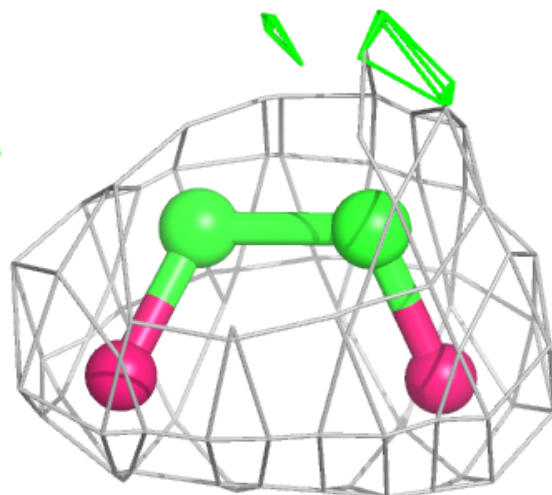
Electron density around MG C 401:

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



Electron density around EDO A 403:

$2mF_o-DF_c$ (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.