



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:06 PM UTC

PDB ID : 7DAH / pdb_00007dah
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

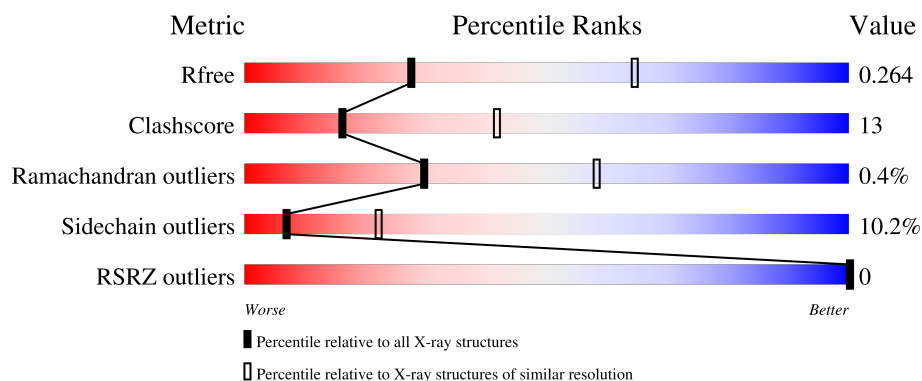
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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}	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (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	
1	B	310	
1	C	310	
1	D	310	
1	E	310	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	310	69% 19% 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:

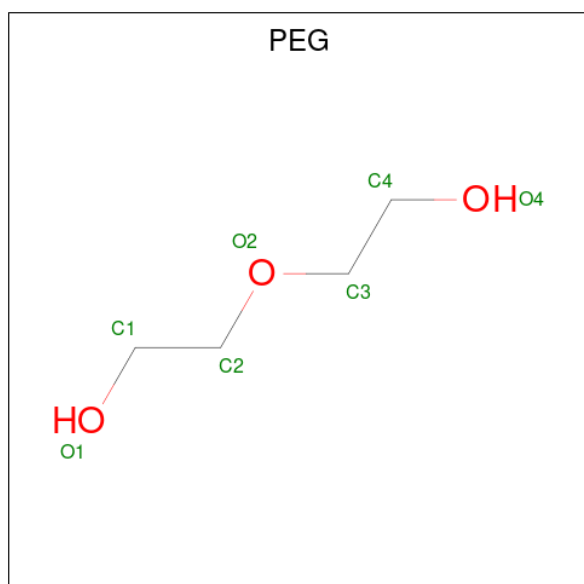
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP C3LU29
A	-4	HIS	-	expression tag	UNP C3LU29
A	-3	HIS	-	expression tag	UNP C3LU29
A	-2	HIS	-	expression tag	UNP C3LU29
A	-1	HIS	-	expression tag	UNP C3LU29
A	0	HIS	-	expression tag	UNP C3LU29
B	-5	HIS	-	expression tag	UNP C3LU29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

Continued on next page...

Continued from previous page...

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 (CCD ID: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



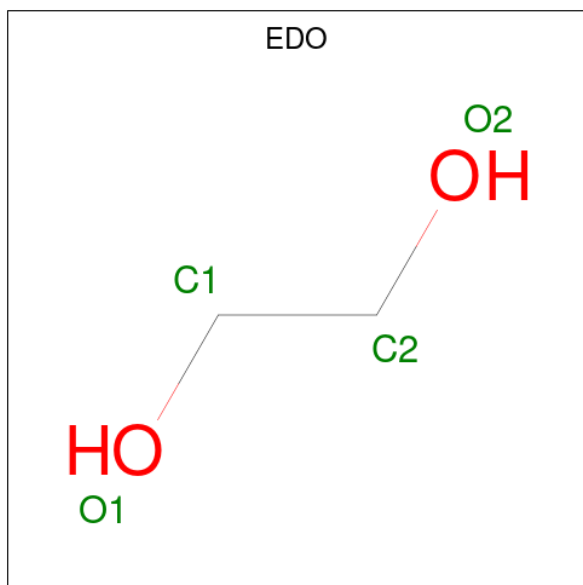
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



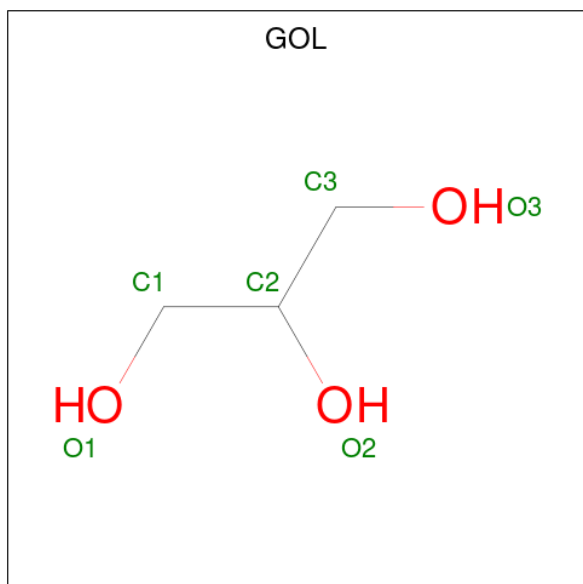
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (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 (CCD ID: 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		

Continued on next page...

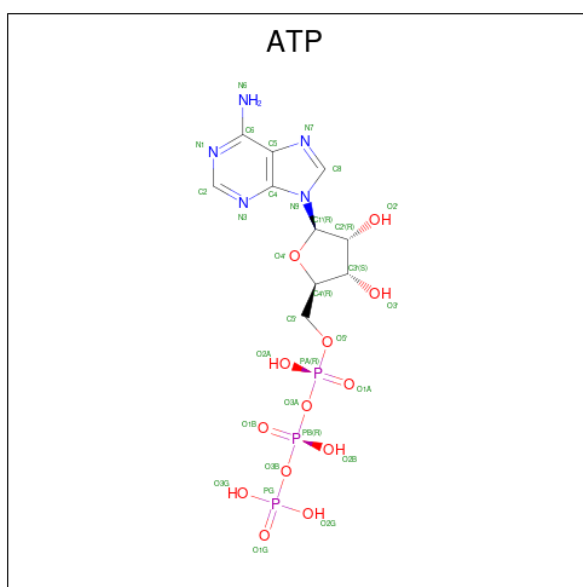
Continued from previous page...

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

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

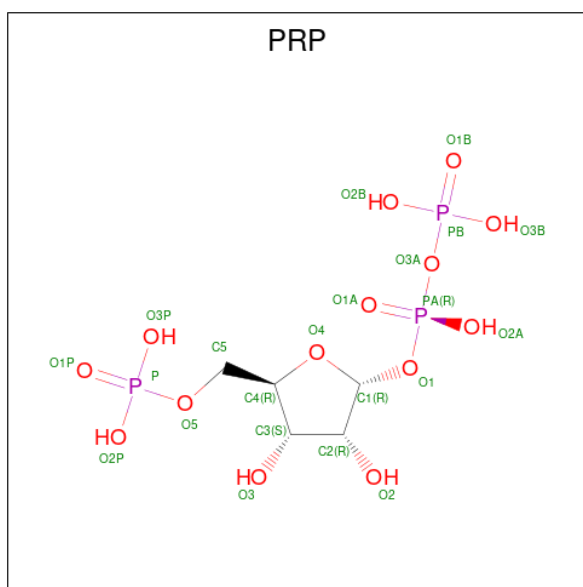
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: 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 (CCD ID: 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		

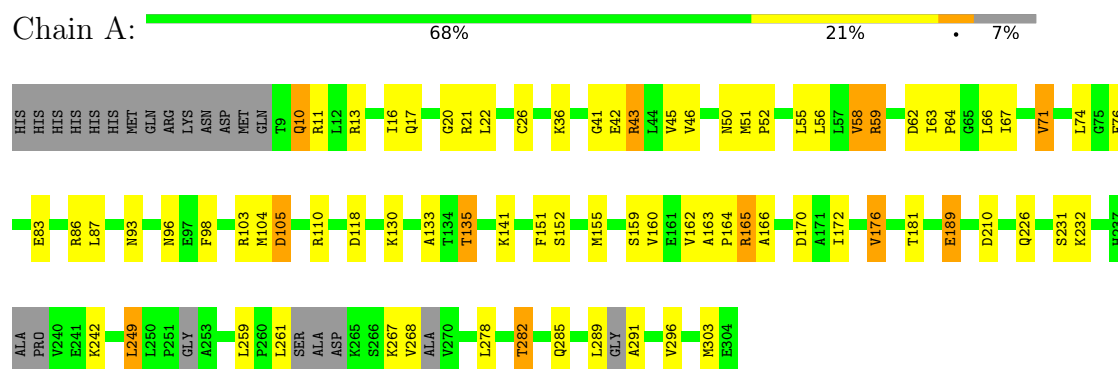
- Molecule 9 is water.

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		

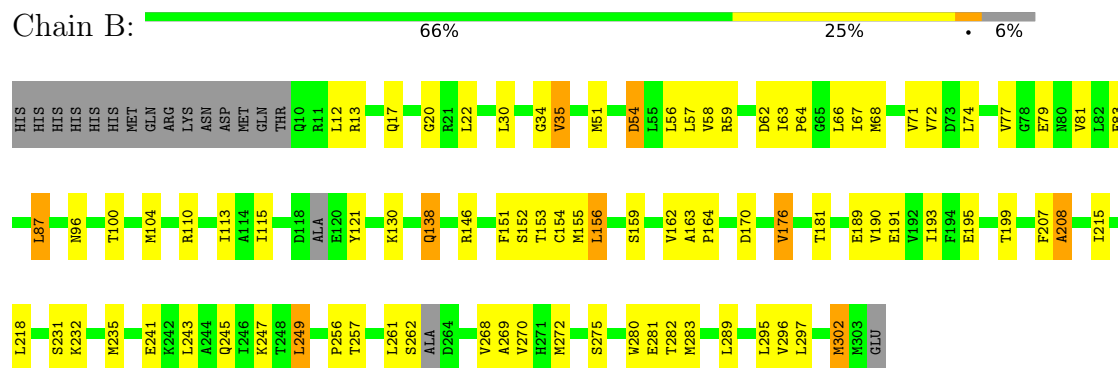
3 Residue-property plots

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.

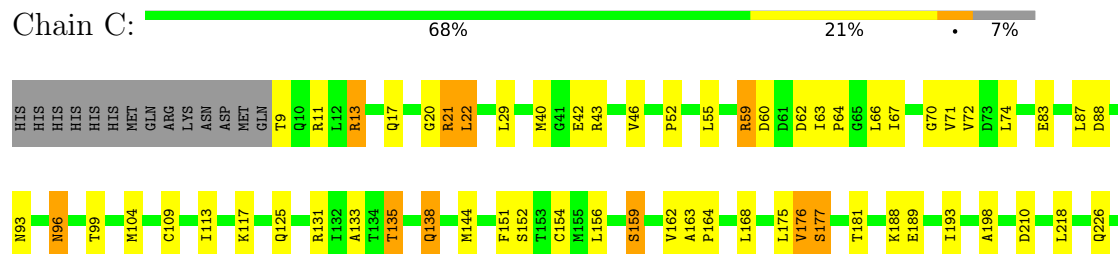
• Molecule 1: ATP phosphoribosyltransferase

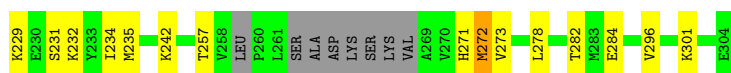


• Molecule 1: ATP phosphoribosyltransferase



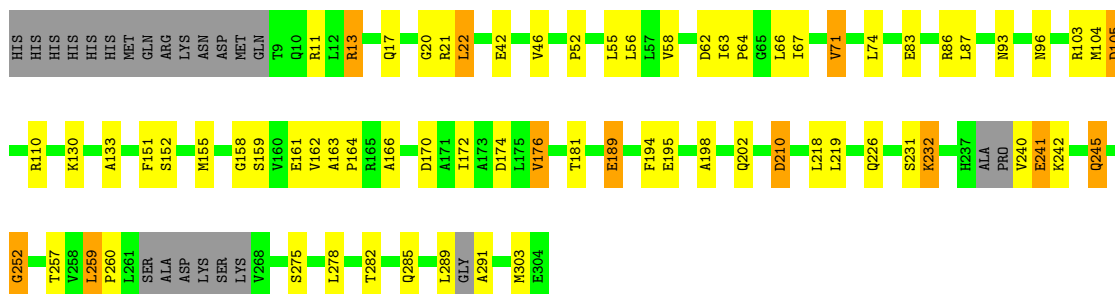
• Molecule 1: ATP phosphoribosyltransferase





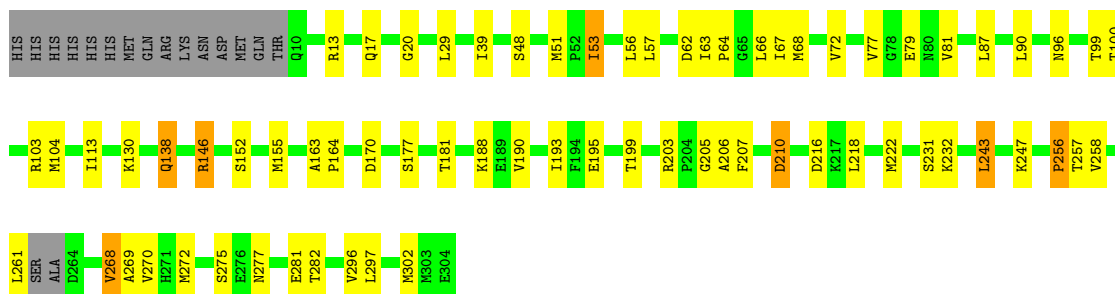
- Molecule 1: ATP phosphoribosyltransferase

Chain D: 70% 19% 7%



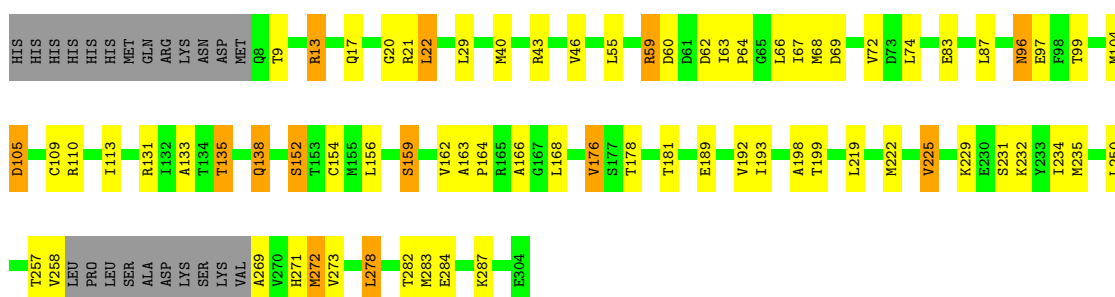
- Molecule 1: ATP phosphoribosyltransferase

Chain E: 72% 20% 5%



- Molecule 1: ATP phosphoribosyltransferase

Chain F: 69% 19% 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 28.32 – 2.92	Depositor EDS
% Data completeness (in resolution range)	99.6 (28.32-2.92) 99.8 (28.32-2.92)	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 (4.62%)	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)	0.27 , 31.4	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	0.96	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: GOL, EDO, ATP, PO4, PRP, PEG, MG

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	1.14	1/2170 (0.0%)	1.55	6/2924 (0.2%)
1	B	1.16	0/2155	1.57	5/2916 (0.2%)
1	C	1.14	0/2157	1.54	2/2911 (0.1%)
1	D	1.17	2/2164 (0.1%)	1.54	9/2917 (0.3%)
1	E	1.18	3/2150 (0.1%)	1.57	6/2912 (0.2%)
1	F	1.15	0/2129	1.56	3/2876 (0.1%)
All	All	1.16	6/12925 (0.0%)	1.56	31/17456 (0.2%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	189	GLU	C-O	-6.65	1.16	1.23
1	A	189	GLU	C-O	-6.44	1.16	1.23
1	E	205	GLY	C-O	6.01	1.28	1.23
1	E	302	MET	C-O	5.55	1.29	1.23
1	D	158	GLY	C-O	5.42	1.30	1.24
1	E	256	PRO	C-O	-5.15	1.18	1.23

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	105	ASP	CA-CB-CG	6.83	119.43	112.60
1	A	10	GLN	N-CA-C	-6.67	106.08	114.56
1	D	105	ASP	CA-CB-CG	5.99	118.59	112.60
1	E	190	VAL	CA-C-O	-5.79	114.95	119.46
1	A	105	ASP	CA-CB-CG	5.77	118.37	112.60
1	E	87	LEU	CA-C-O	-5.73	114.80	120.82
1	B	87	LEU	CA-C-O	-5.71	114.81	120.70
1	D	151	PHE	CA-C-O	-5.61	115.23	121.23
1	D	252	GLY	CA-C-O	-5.55	115.62	121.56
1	F	257	THR	N-CA-C	5.50	116.95	111.07
1	C	42	GLU	CB-CG-CD	5.49	121.93	112.60
1	F	72	VAL	CA-C-O	-5.45	116.11	121.67
1	B	190	VAL	CA-C-O	-5.44	115.22	119.46
1	D	42	GLU	CB-CG-CD	5.43	121.83	112.60
1	A	87	LEU	CA-C-O	-5.43	115.11	120.70
1	B	281	GLU	CB-CG-CD	5.42	121.82	112.60
1	C	72	VAL	CA-C-O	-5.38	116.18	121.67
1	A	151	PHE	CA-C-O	-5.34	115.56	121.33
1	E	257	THR	CB-CA-C	5.30	118.36	109.89
1	E	281	GLU	CB-CG-CD	5.27	121.56	112.60
1	B	257	THR	CB-CA-C	5.26	118.31	109.89
1	A	58	VAL	CA-C-O	-5.20	116.36	121.67
1	D	257	THR	CB-CA-C	5.19	118.30	109.84
1	D	58	VAL	CA-C-O	-5.17	116.19	121.67
1	D	241	GLU	N-CA-CB	-5.17	104.88	112.78
1	E	146	ARG	CB-CA-C	5.16	120.57	110.67
1	E	277	ASN	N-CA-CB	5.14	117.52	109.97
1	B	115	ILE	CA-C-O	-5.13	116.44	121.67
1	A	21	ARG	CA-C-O	-5.11	115.14	120.55
1	D	21	ARG	CA-C-O	-5.05	115.19	120.55
1	D	87	LEU	CA-C-O	-5.04	115.51	120.70

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	57	0
1	B	2131	0	2087	77	0
1	C	2134	0	2101	67	0
1	D	2142	0	2124	48	0
1	E	2123	0	2056	49	0
1	F	2105	0	2057	62	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
9	F	26	0	0	0	0
All	All	13159	0	12679	336	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 13.

All (336) 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:C	1:B:156:LEU:HD13	2.00	0.87
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: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:F:29:LEU:CD2	1:F:104:MET:HE1	2.19	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:35:VAL:HA	1:B:51:MET:HE3	1.74	0.69
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
1:F:96:ASN:C	1:F:96:ASN:HD22	2.00	0.68
1:E:64:PRO:O	1:E:67:ILE:HG22	1.94	0.68
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:E:261:LEU:C	9:E:508:HOH:O	2.38	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:MET:O	1:C:40:MET:HG3	1.94	0.66
1:F:231:SER:O	1:F:232:LYS:HD2	1.97	0.65
1:C:96:ASN:C	1:C:96:ASN:HD22	2.04	0.64
1:B:12:LEU:HD11	1:B:215:ILE:HD11	1.79	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: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:C:29:LEU:CD2	1:C:104:MET:HE1	2.29	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: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:B:231:SER:HB2	1:B:302:MET:HE1	1.83	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: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
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:B:64:PRO:C	1:B:68:MET:HE2	2.28	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:35:VAL:HG12	1:B:51:MET:HE1	1.87	0.57
1:D:93:ASN:HB2	1:E:100:THR:HG21	1.87	0.56
1:E:64:PRO:C	1:E:68:MET:HE2	2.29	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:C:235:MET:HE2	1:C:271:HIS:NE2	2.22	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:105:ASP:CG	1:F:105:ASP:O	2.51	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:C:96:ASN:C	1:C:96:ASN:ND2	2.66	0.53
1:B:104:MET:HA	1:B:104:MET:HE2	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:235:MET:HE2	1:F:271:HIS:NE2	2.24	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:F:96:ASN:C	1:F:96:ASN:ND2	2.64	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:E:104:MET:HE2	1:E:104:MET:HA	1.93	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: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:C:284:GLU:HA	1:D:303:MET:HE1	1.92	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:C:88:ASP:CG	9:C:508:HOH:O	2.55	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:56:LEU:N	1:B:56:LEU:HD12	2.27	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: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:B:280:TRP:CE3	1:B:283:MET:HE3	2.48	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:ILE:HG23	1:E:39:ILE:O	2.14	0.46
1:E:63:ILE:N	1:E:64:PRO:CD	2.79	0.46
1:D:103:ARG:C	1:D:104:MET:HE2	2.41	0.45
1:C:175:LEU:O	8:C:403:PRP:O3	2.31	0.45
1:F:40:MET:CB	1:F:43:ARG:NH2	2.79	0.45
1:F:258:VAL:C	1:F:269:ALA:O	2.59	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:104:MET:HE2	1:A:104:MET:HA	1.98	0.45
1:D:104:MET:HE2	1:D:104:MET:HA	1.98	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: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:104:MET:HE2	1:B:104:MET:CA	2.47	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:A:67:ILE:HD11	1:A:74:LEU:C	2.42	0.44
1:B:30:LEU:HB3	1:B:35:VAL:HG21	1.99	0.44
1:B:67:ILE:HD11	1:B:74:LEU:C	2.42	0.44
1:E:77:VAL:HG22	1:E:81:VAL:CG2	2.47	0.44
1:B:296:VAL:C	1:B:297:LEU:HD12	2.43	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:E:296:VAL:C	1:E:297:LEU:HD12	2.42	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:235:MET:HE2	1:F:271:HIS:CD2	2.53	0.44
1:A:103:ARG:C	1:A:104:MET:HE2	2.42	0.44
1:A:303:MET:HE1	1:F:284:GLU:HG3	1.99	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:D:67:ILE:HD11	1:D:74:LEU:C	2.42	0.44
1:A:249:LEU:CD2	1:A:282:THR:HG23	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:67:ILE:HD11	1:F:74:LEU:C	2.43	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:C:67:ILE:HD11	1:C:74:LEU:C	2.43	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:C:272:MET:HE3	1:C:272:MET:HB3	1.85	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:104:MET:HE2	1:E:104:MET:CA	2.48	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
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:D:104:MET:HE2	1:D:104:MET:N	2.33	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:B:302:MET:HE2	1:B:302:MET:HB3	1.78	0.42
1:D:104:MET:HE2	1:D:104:MET:CA	2.49	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:F:46:VAL:HB	1:F:55:LEU:HB2	2.01	0.42
1:B:235:MET:HE3	1:B:295:LEU:HD12	2.01	0.42
1:B:163:ALA:N	1:B:164:PRO:CD	2.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:MET:HE2	1:C:271:HIS:CD2	2.54	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:B:121:TYR:OH	1:B:191:GLU:OE1	2.34	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:A:104:MET:HE2	1:A:104:MET:N	2.35	0.41
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:A:104:MET:HE2	1:A:104:MET:CA	2.50	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:258:VAL:HG13	1:E:268:VAL:CG1	2.51	0.41
1:A:261:LEU:C	1:A:267:LYS:CB	2.93	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:E:103:ARG:C	1:E:104:MET:HE2	2.45	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
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:E:96:ASN:C	1:E:96:ASN:OD1	2.64	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: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:B:34:GLY:O	1:B:51:MET:HE2	2.21	0.40
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	18	46
1	B	286/310 (92%)	271 (95%)	14 (5%)	1 (0%)	36	64
1	C	282/310 (91%)	269 (95%)	12 (4%)	1 (0%)	30	58
1	D	279/310 (90%)	262 (94%)	15 (5%)	2 (1%)	18	46
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%)	30	58

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%)	193 (91%)	20 (9%)	8	25
1	B	201/263 (76%)	178 (89%)	23 (11%)	5	17
1	C	207/263 (79%)	184 (89%)	23 (11%)	6	19
1	D	212/263 (81%)	195 (92%)	17 (8%)	11	32
1	E	197/263 (75%)	177 (90%)	20 (10%)	7	22
1	F	201/263 (76%)	178 (89%)	23 (11%)	5	17
All	All	1231/1578 (78%)	1105 (90%)	126 (10%)	7	22

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	13	ARG
1	A	22	LEU
1	A	42	GLU
1	A	43	ARG
1	A	59	ARG
1	A	71	VAL
1	A	96	ASN
1	A	105	ASP
1	A	118	ASP
1	A	135	THR
1	A	141	LYS
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	35	VAL
1	B	54	ASP
1	B	96	ASN
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	218	LEU
1	B	241	GLU
1	B	243	LEU
1	B	249	LEU
1	B	262	SER
1	B	268	VAL
1	B	272	MET
1	B	275	SER
1	B	282	THR
1	B	302	MET
1	C	9	THR
1	C	13	ARG
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	272	MET
1	C	278	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	282	THR
1	C	301	LYS
1	D	13	ARG
1	D	22	LEU
1	D	71	VAL
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	210	ASP
1	D	218	LEU
1	D	219	LEU
1	D	232	LYS
1	D	245	GLN
1	D	278	LEU
1	D	282	THR
1	D	285	GLN
1	E	13	ARG
1	E	53	ILE
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	188	LYS
1	E	195	GLU
1	E	199	THR
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	59	ARG
1	F	96	ASN
1	F	97	GLU
1	F	99	THR
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	250	LEU
1	F	272	MET
1	F	278	LEU
1	F	282	THR
1	F	287	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	96	ASN
1	A	125	GLN
1	A	202	GLN
1	A	277	ASN
1	B	17	GLN
1	B	27	GLN
1	B	93	ASN
1	B	94	GLN
1	B	96	ASN
1	B	125	GLN
1	B	138	GLN
1	B	202	GLN
1	B	223	HIS
1	B	271	HIS
1	C	10	GLN
1	C	17	GLN
1	C	27	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	185	ASN
1	C	202	GLN
1	C	226	GLN
1	C	277	ASN
1	D	17	GLN
1	D	96	ASN
1	D	202	GLN
1	D	277	ASN
1	E	17	GLN
1	E	93	ASN
1	E	138	GLN
1	E	237	HIS
1	F	17	GLN
1	F	27	GLN
1	F	138	GLN
1	F	185	ASN
1	F	202	GLN
1	F	226	GLN
1	F	277	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	405	-	3,3,3	0.41	0	2,2,2	0.16	0
4	PO4	A	404	-	4,4,4	1.53	1 (25%)	6,6,6	0.38	0
2	PEG	A	401	-	6,6,6	0.19	0	5,5,5	0.22	0
3	EDO	A	403	-	3,3,3	0.27	0	2,2,2	0.14	0
4	PO4	D	406	-	4,4,4	0.76	0	6,6,6	0.61	0
3	EDO	A	402	-	3,3,3	0.25	0	2,2,2	0.20	0
8	PRP	C	403	-	20,22,22	0.98	1 (5%)	32,35,35	1.33	3 (9%)
3	EDO	F	402	-	3,3,3	0.37	0	2,2,2	0.34	0
3	EDO	C	404	-	3,3,3	0.11	0	2,2,2	0.10	0
3	EDO	E	401	-	3,3,3	0.19	0	2,2,2	0.19	0
7	ATP	F	404	6	32,33,33	0.78	1 (3%)	48,52,52	0.91	2 (4%)
2	PEG	D	401	-	6,6,6	0.23	0	5,5,5	0.18	0
8	PRP	F	403	-	20,22,22	1.44	1 (5%)	32,35,35	1.23	2 (6%)
3	EDO	D	404	-	3,3,3	0.22	0	2,2,2	0.18	0
7	ATP	C	402	6	32,33,33	0.96	3 (9%)	48,52,52	0.95	2 (4%)
3	EDO	D	402	-	3,3,3	0.14	0	2,2,2	0.06	0
5	GOL	D	403	-	5,5,5	0.17	0	5,5,5	0.35	0
5	GOL	A	405	-	5,5,5	0.17	0	5,5,5	0.34	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	405	-	-	1/1/1/1	-
2	PEG	A	401	-	-	0/4/4/4	-
3	EDO	A	403	-	-	1/1/1/1	-
8	PRP	C	403	-	-	4/16/33/33	0/1/1/1
3	EDO	A	402	-	-	1/1/1/1	-
3	EDO	F	402	-	-	0/1/1/1	-
3	EDO	C	404	-	-	1/1/1/1	-
3	EDO	E	401	-	-	1/1/1/1	-
7	ATP	F	404	6	-	5/22/38/38	0/3/3/3
2	PEG	D	401	-	-	3/4/4/4	-
8	PRP	F	403	-	-	3/16/33/33	0/1/1/1
3	EDO	D	404	-	-	0/1/1/1	-
7	ATP	C	402	6	-	8/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	402	-	-	0/1/1/1	-
5	GOL	D	403	-	-	3/4/4/4	-
5	GOL	A	405	-	-	0/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	403	PRP	PA-O3A	5.57	1.65	1.59
8	C	403	PRP	PA-O3A	3.13	1.62	1.59
4	A	404	PO4	P-O1	3.05	1.57	1.50
7	C	402	ATP	PA-O3A	2.92	1.62	1.59
7	C	402	ATP	C1'-N9	2.72	1.53	1.46
7	F	404	ATP	PA-O3A	2.49	1.62	1.59
7	C	402	ATP	PB-O3A	2.04	1.61	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	403	PRP	O5-P-O1P	-4.24	94.98	106.44
8	F	403	PRP	O2P-P-O5	-3.31	98.04	106.67
8	C	403	PRP	O1-C1-C2	3.00	111.52	106.65
7	F	404	ATP	C2'-C1'-N9	2.61	119.78	113.30
7	C	402	ATP	C2'-C1'-N9	2.56	119.66	113.30
8	F	403	PRP	O3P-P-O2P	2.45	116.98	107.80
7	F	404	ATP	O2'-C2'-C1'	2.27	117.91	110.10
8	C	403	PRP	O3P-P-O1P	2.11	119.07	110.83
7	C	402	ATP	O2'-C2'-C1'	2.06	117.19	110.10

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-O2A
7	C	402	ATP	O4'-C4'-C5'-O5'
7	F	404	ATP	PB-O3B-PG-O2G
7	F	404	ATP	O4'-C4'-C5'-O5'
8	C	403	PRP	C1-O1-PA-O3A
8	F	403	PRP	PA-O3A-PB-O2B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	C	402	ATP	C3'-C4'-C5'-O5'
7	F	404	ATP	C3'-C4'-C5'-O5'
3	E	401	EDO	O1-C1-C2-O2
2	D	401	PEG	O2-C3-C4-O4
3	C	404	EDO	O1-C1-C2-O2
5	D	403	GOL	O1-C1-C2-O2
3	D	405	EDO	O1-C1-C2-O2
8	C	403	PRP	C1-O1-PA-O1A
7	C	402	ATP	C5'-O5'-PA-O1A
7	C	402	ATP	C5'-O5'-PA-O3A
7	F	404	ATP	C5'-O5'-PA-O1A
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
7	F	404	ATP	PB-O3B-PG-O3G
8	F	403	PRP	PA-O3A-PB-O3B
3	A	403	EDO	O1-C1-C2-O2
8	F	403	PRP	PA-O3A-PB-O1B
7	C	402	ATP	O4'-C1'-N9-C8
3	A	402	EDO	O1-C1-C2-O2
8	C	403	PRP	PB-O3A-PA-O2A

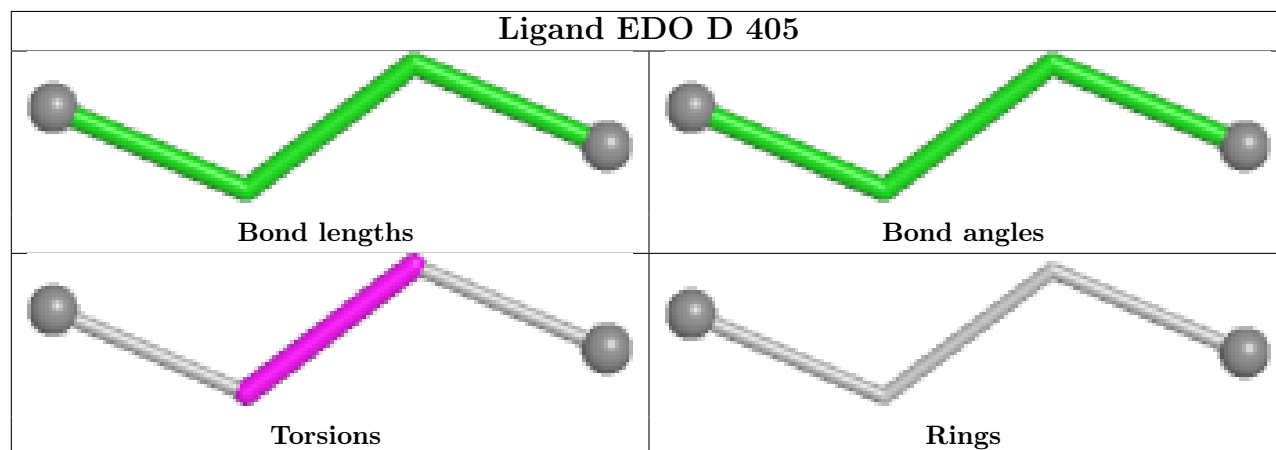
There are no ring outliers.

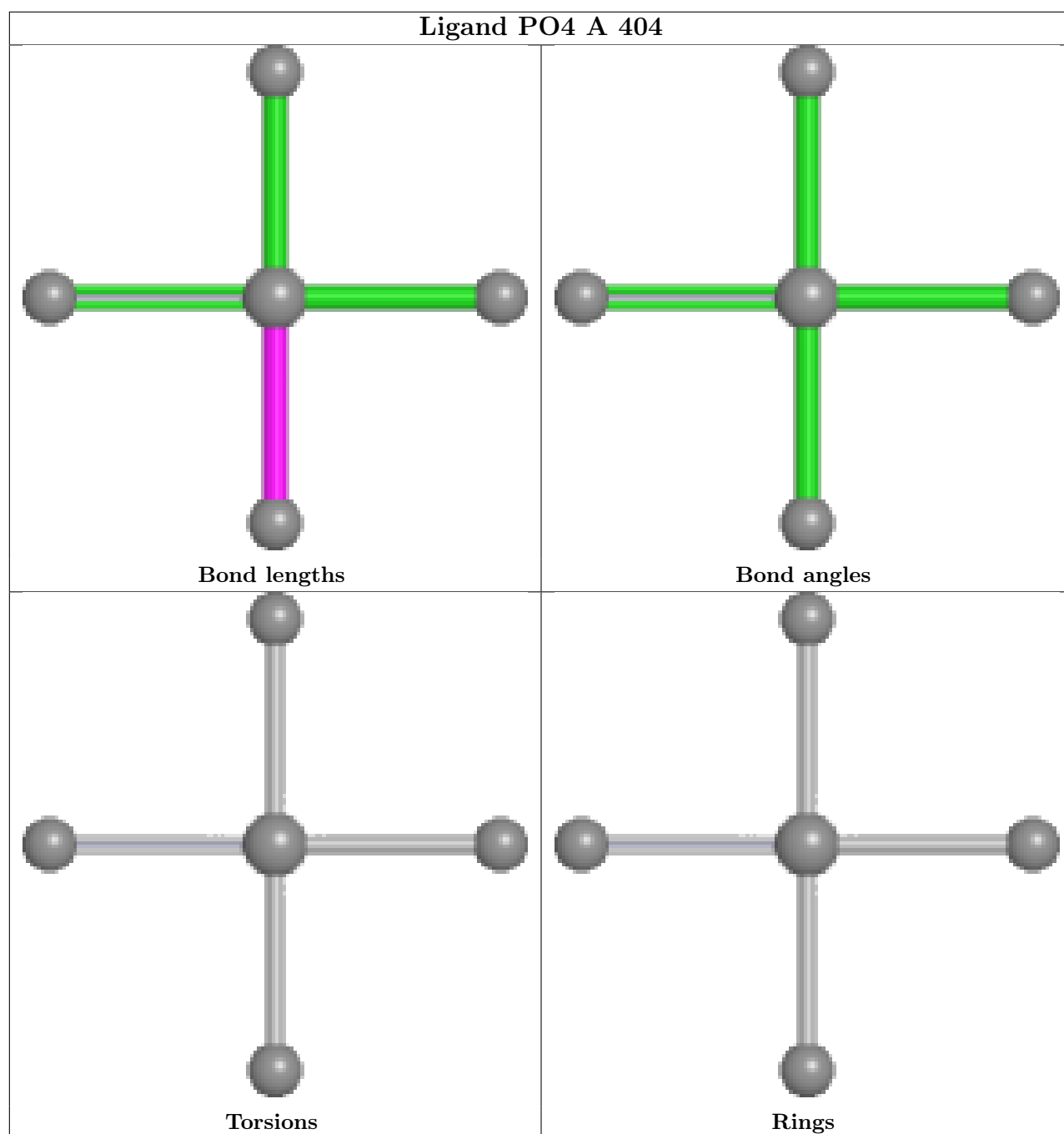
7 monomers are involved in 14 short contacts:

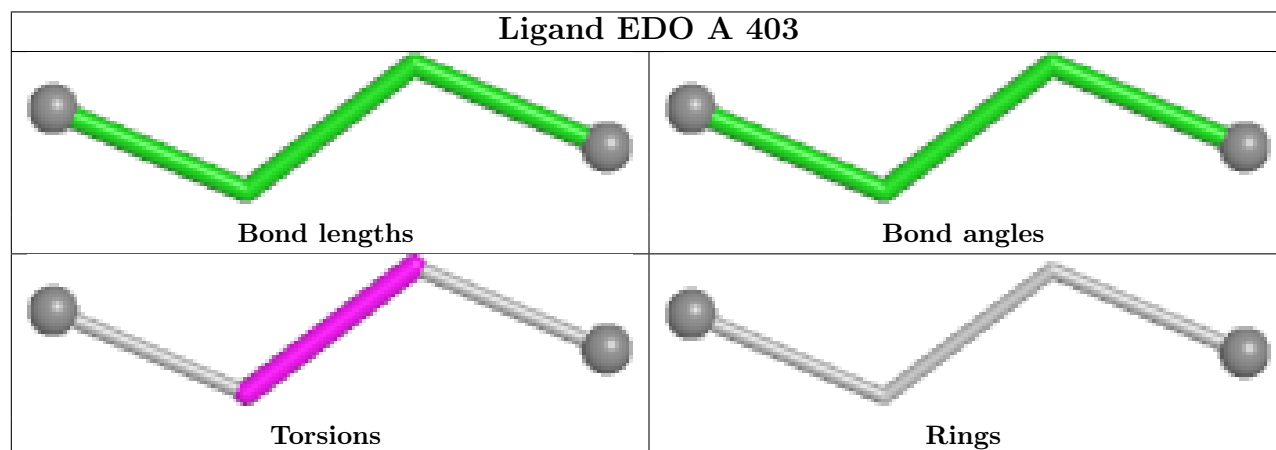
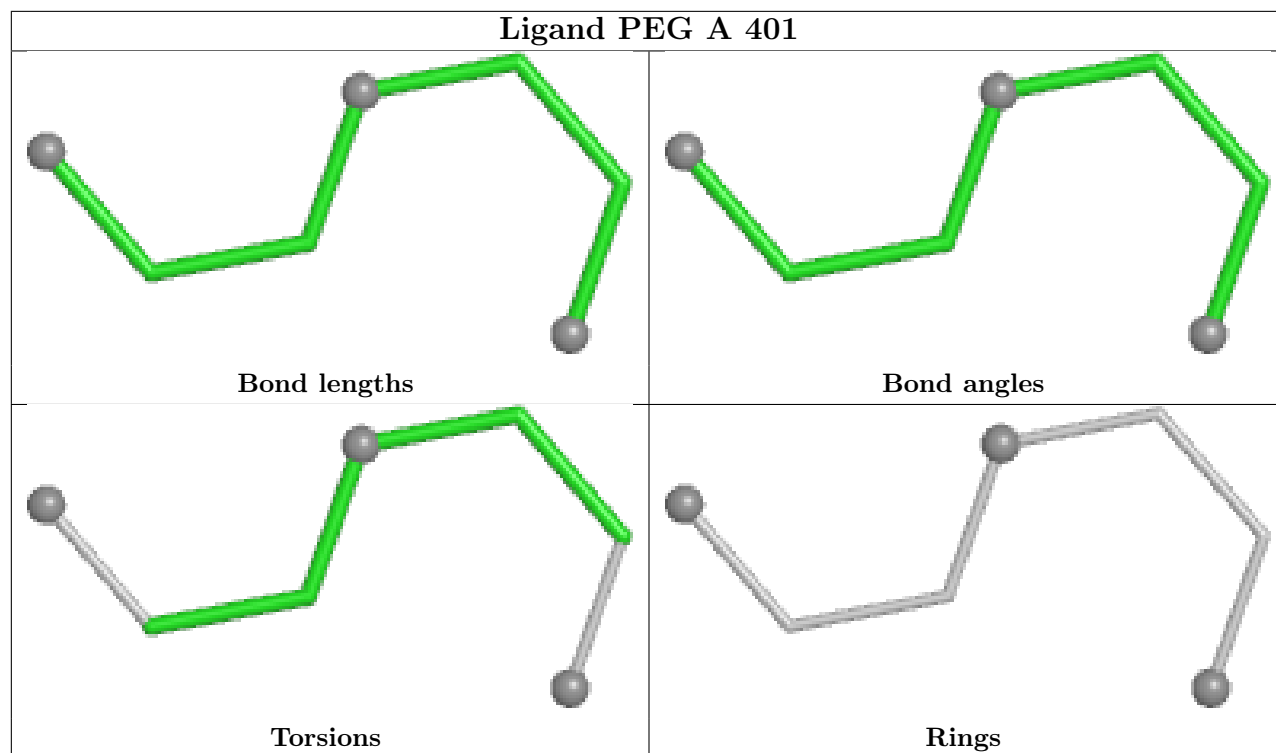
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	403	PRP	2	0
7	F	404	ATP	2	0
2	D	401	PEG	4	0
8	F	403	PRP	2	0
7	C	402	ATP	2	0
3	D	402	EDO	1	0
5	D	403	GOL	1	0

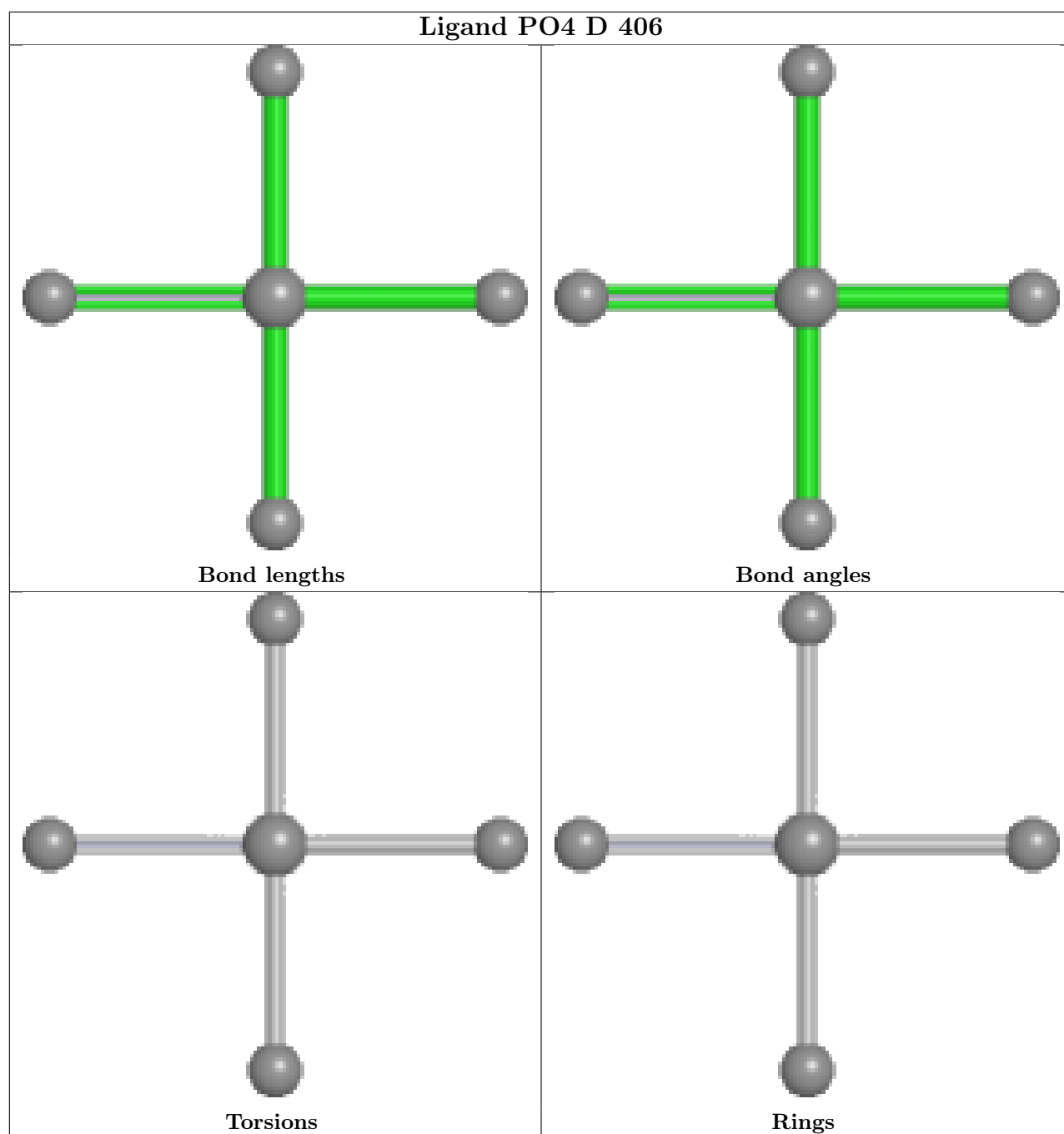
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

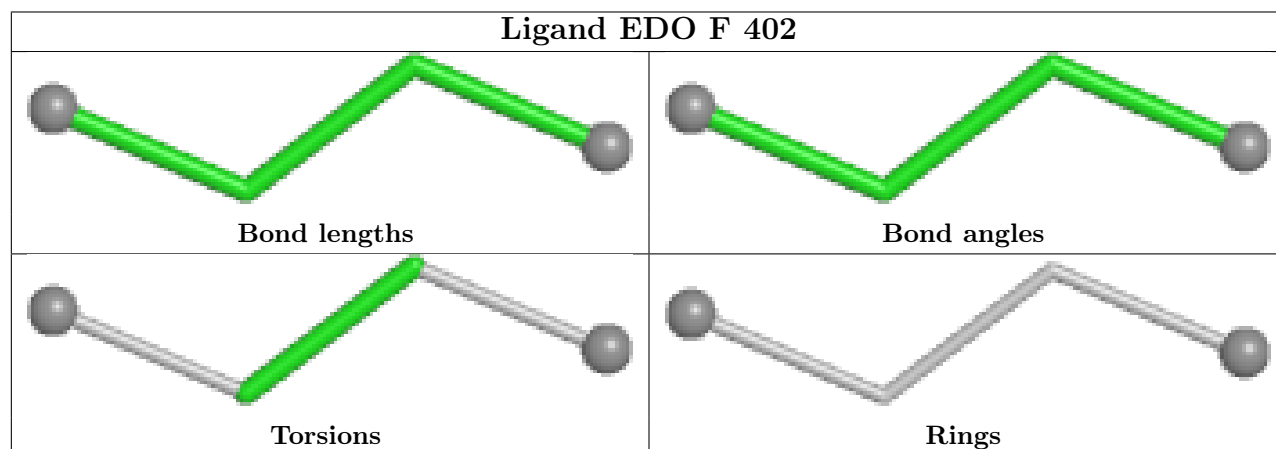
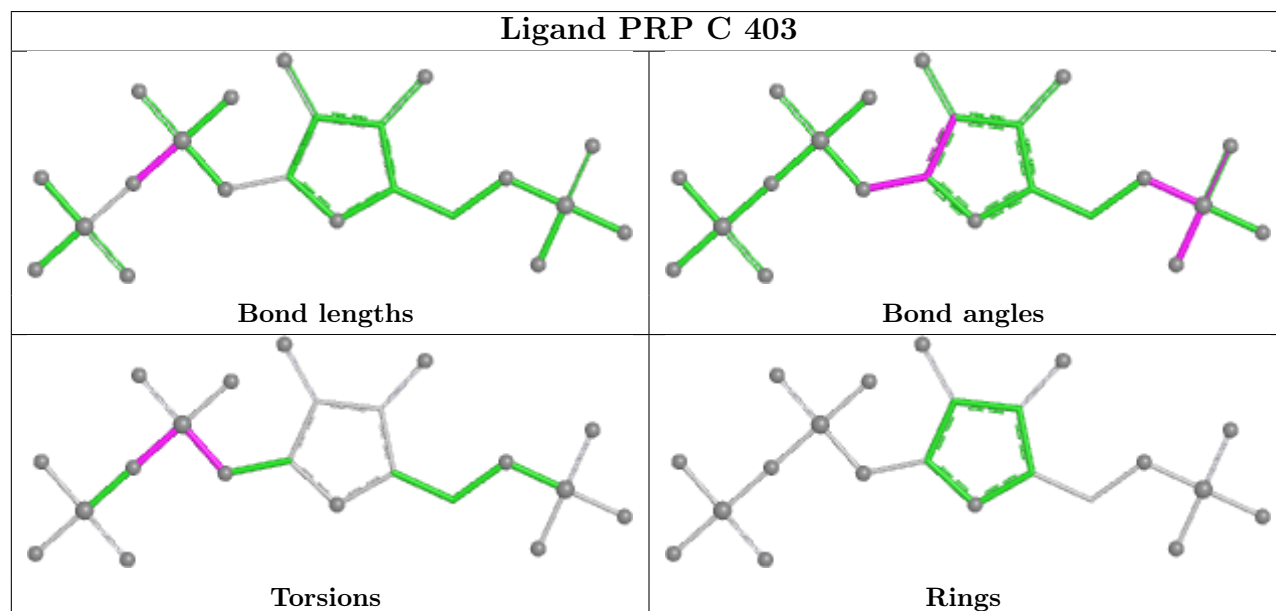
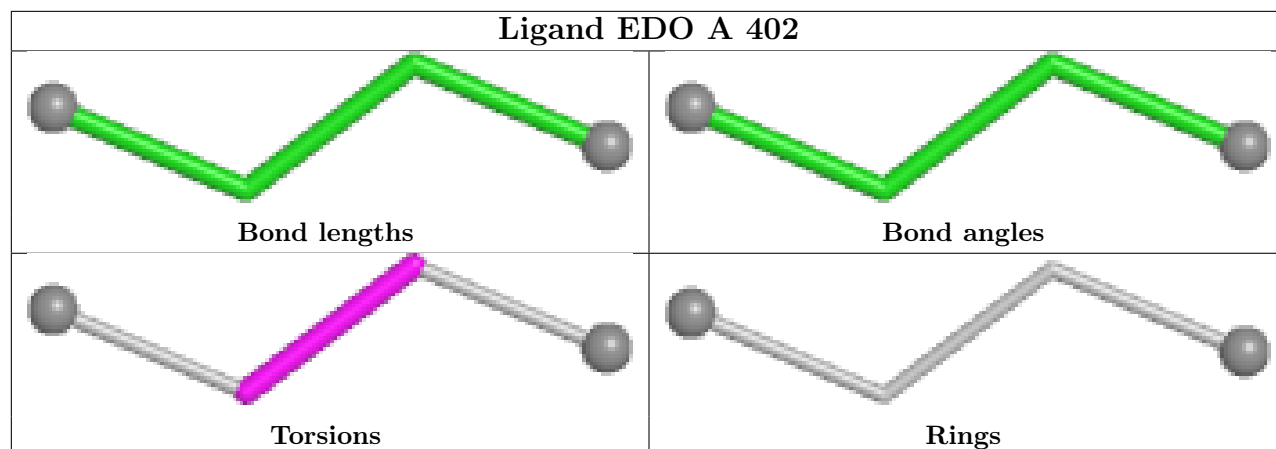
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

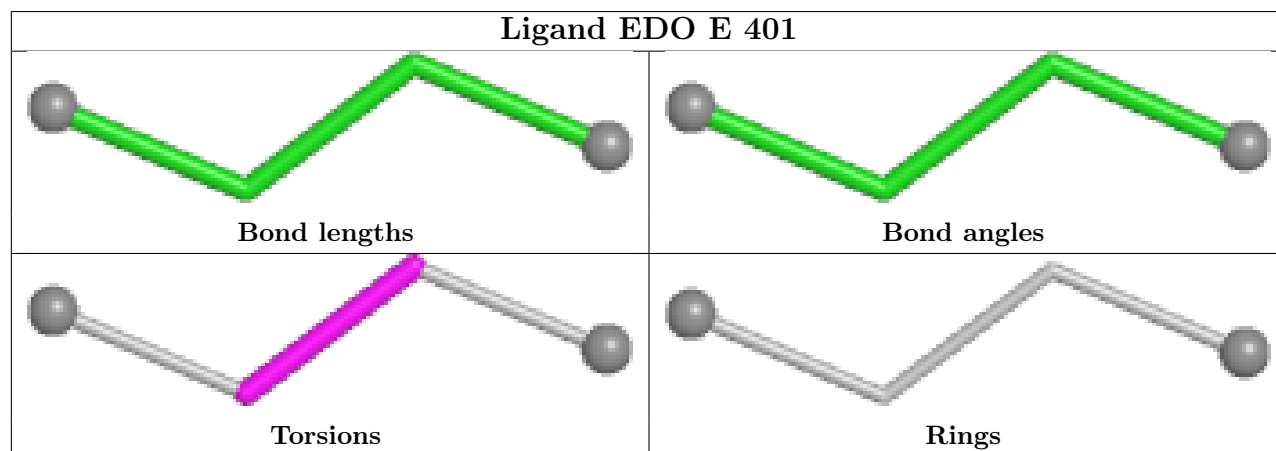
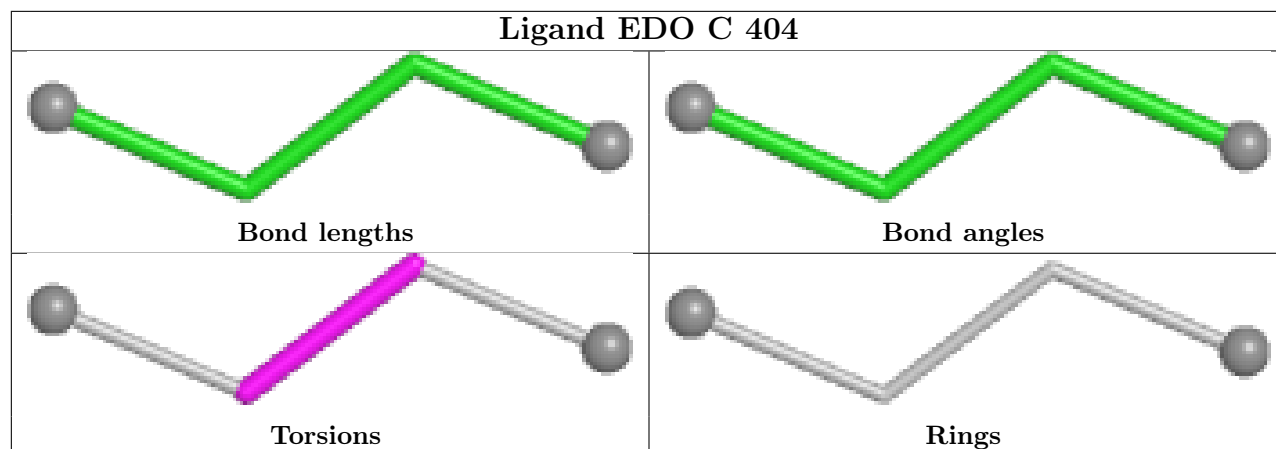




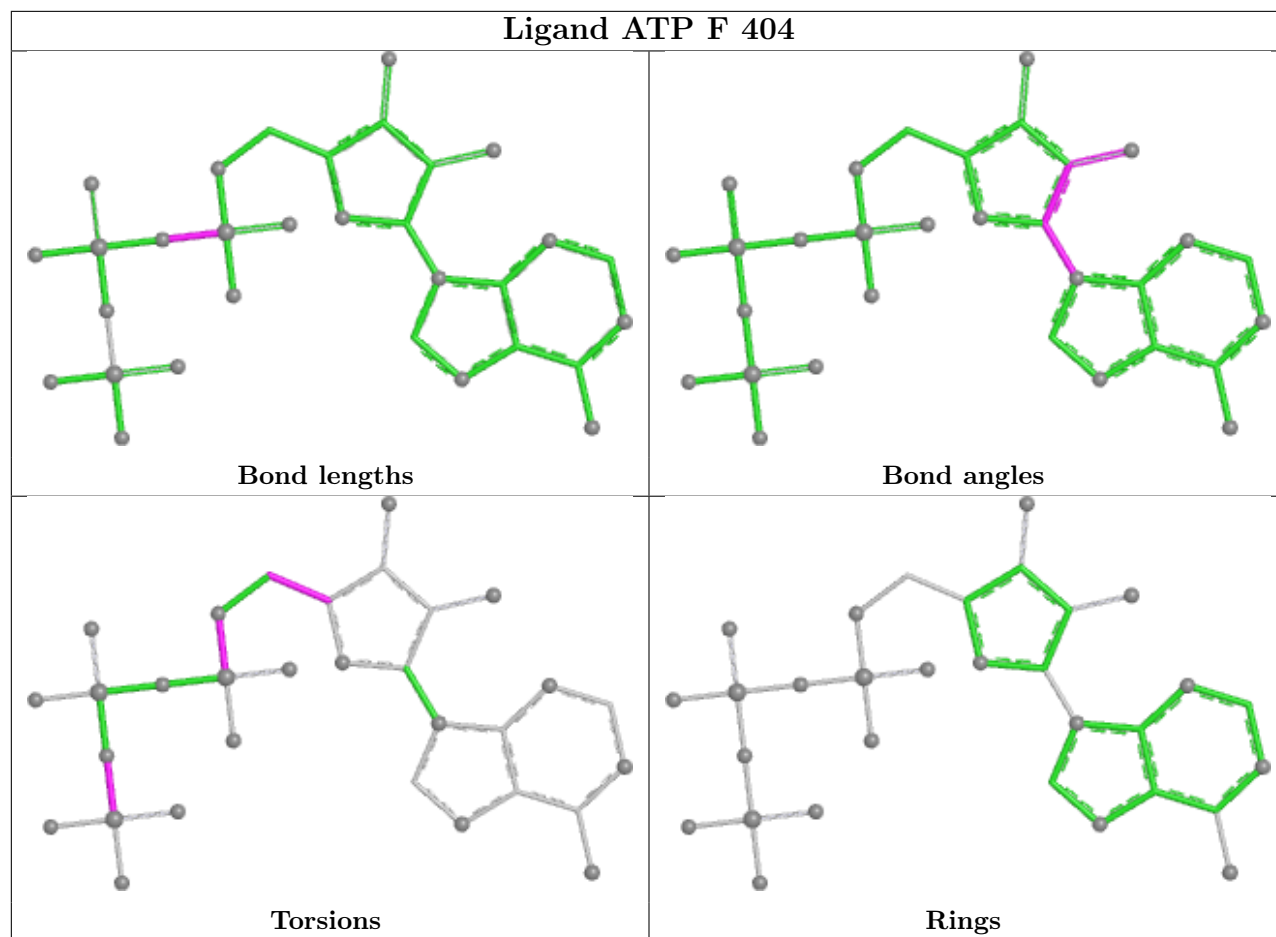




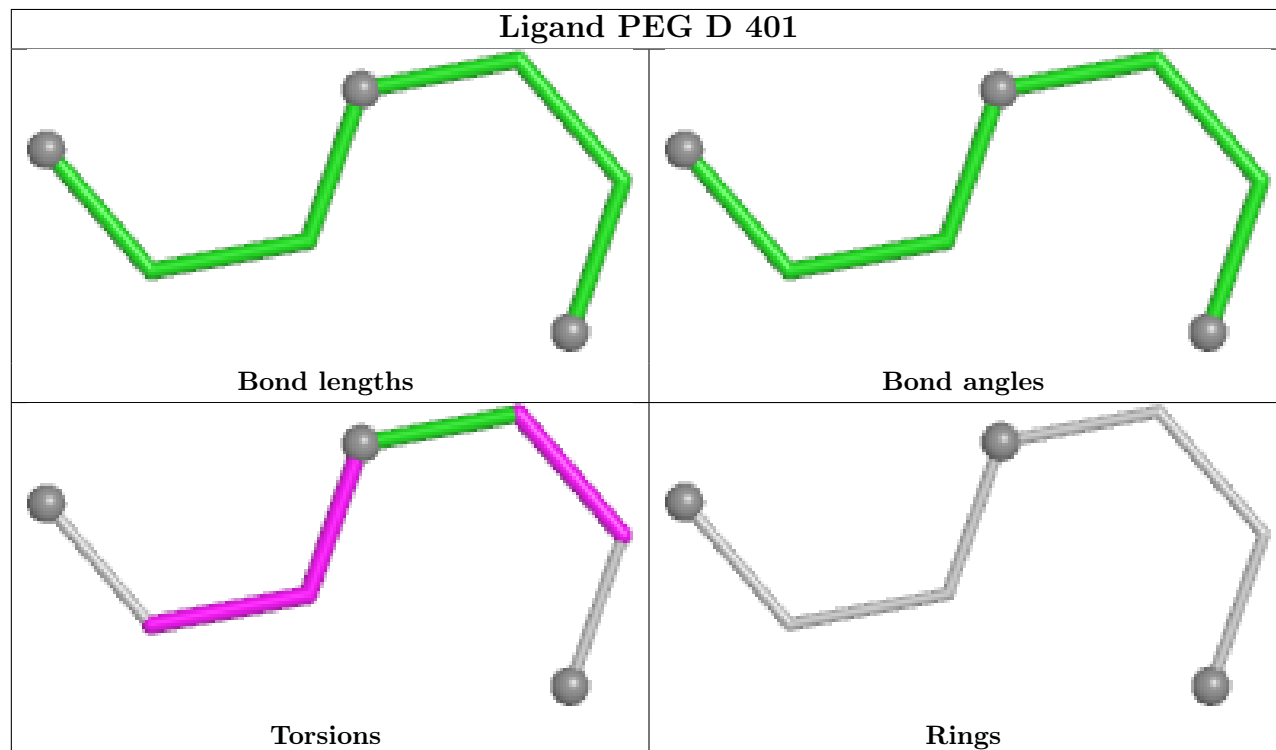




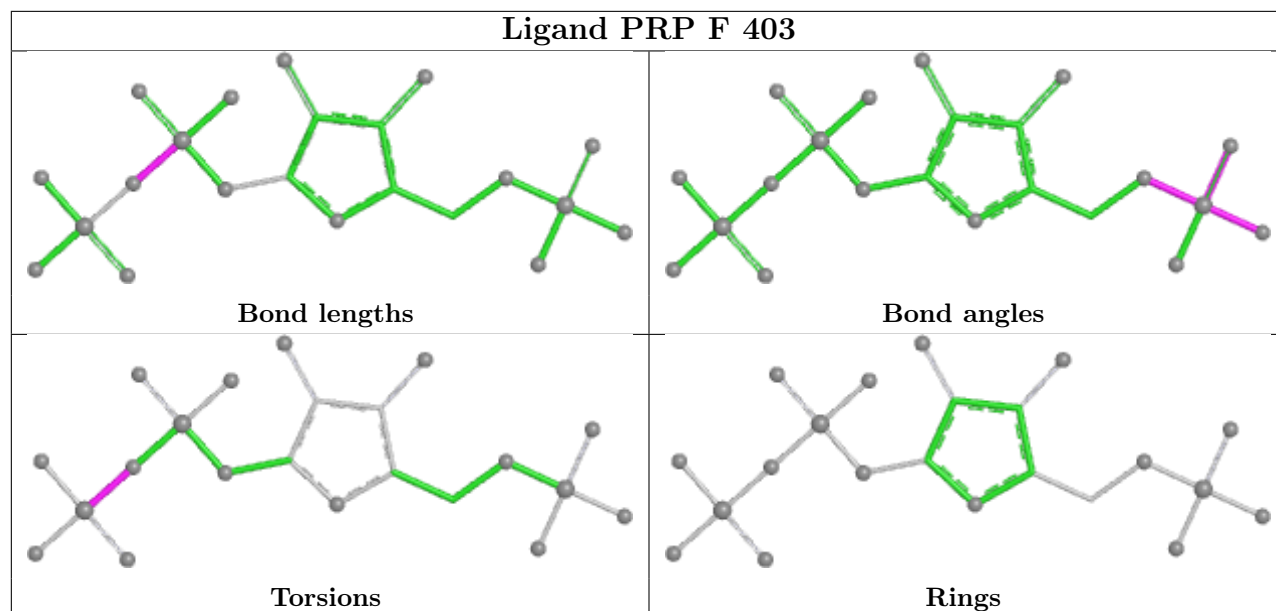
Ligand ATP F 404



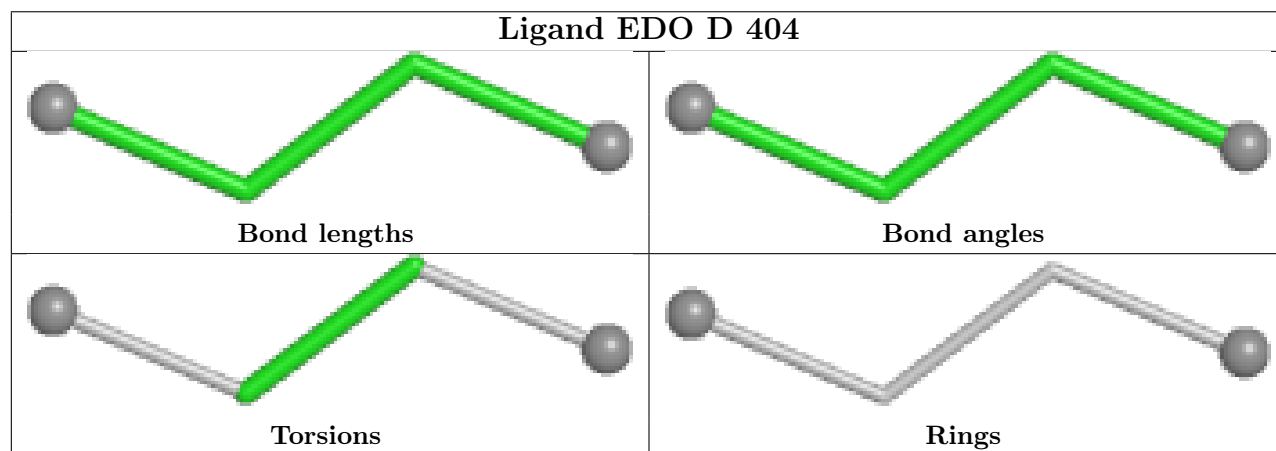
Ligand PEG D 401



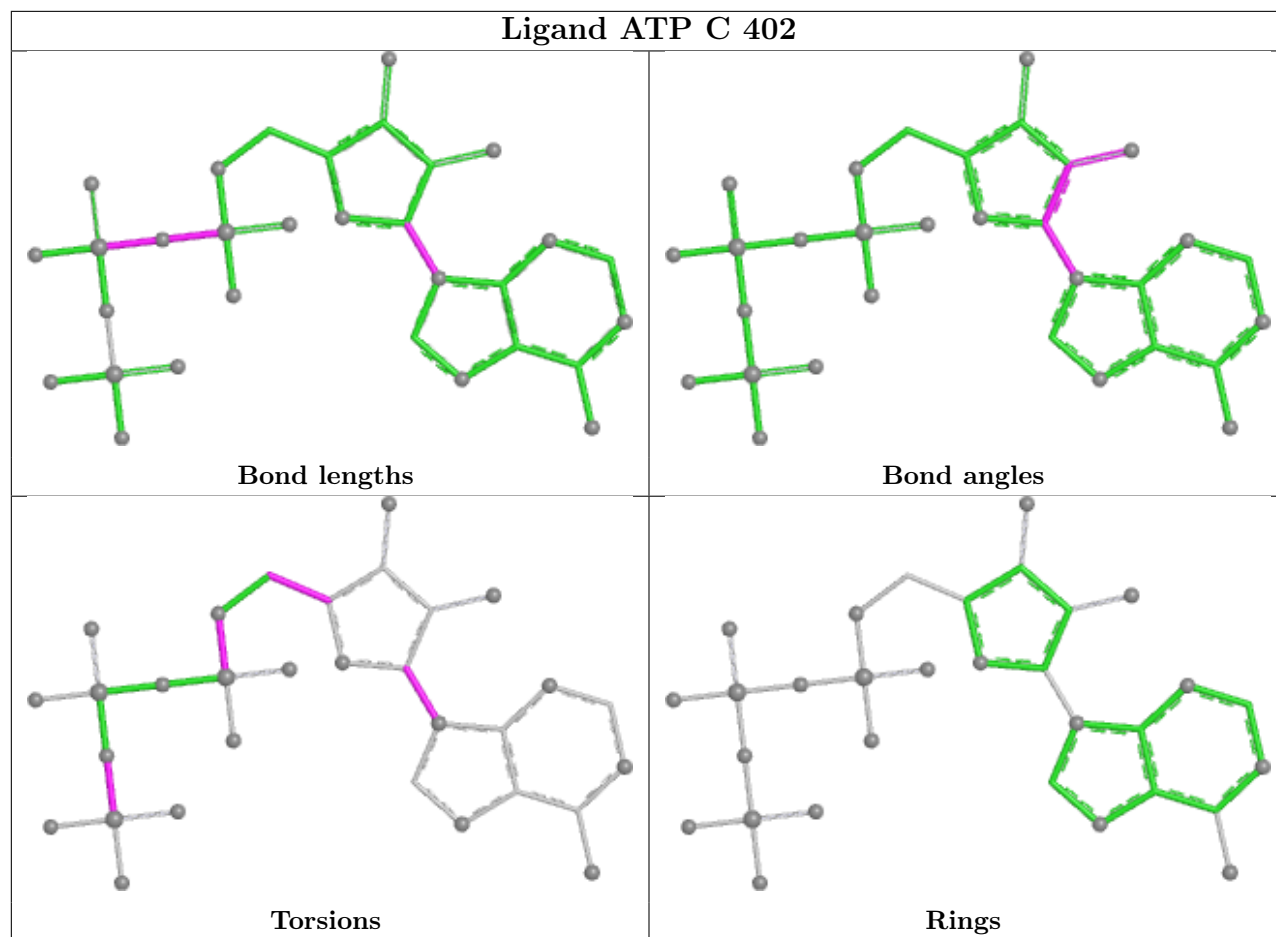
Ligand PRP F 403



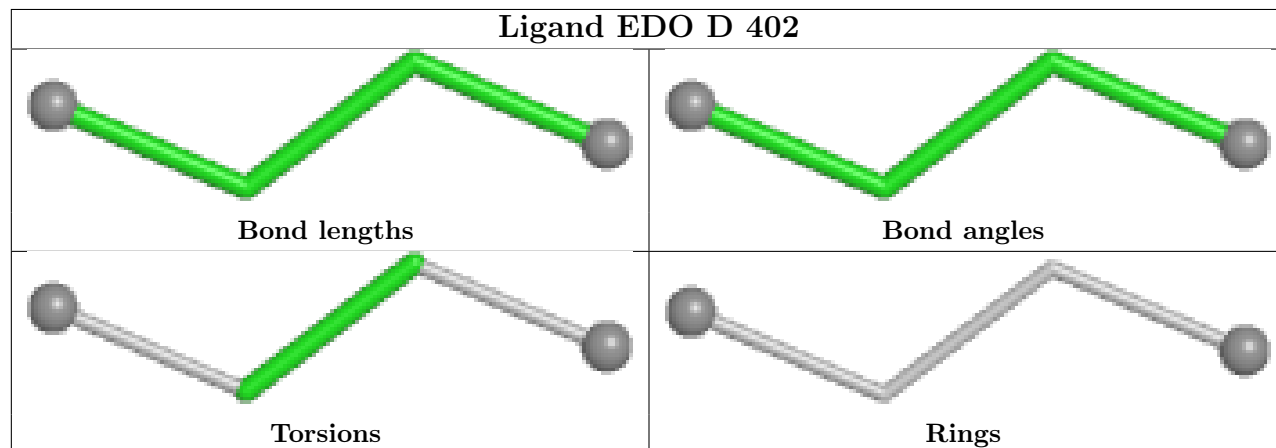
Ligand EDO D 404

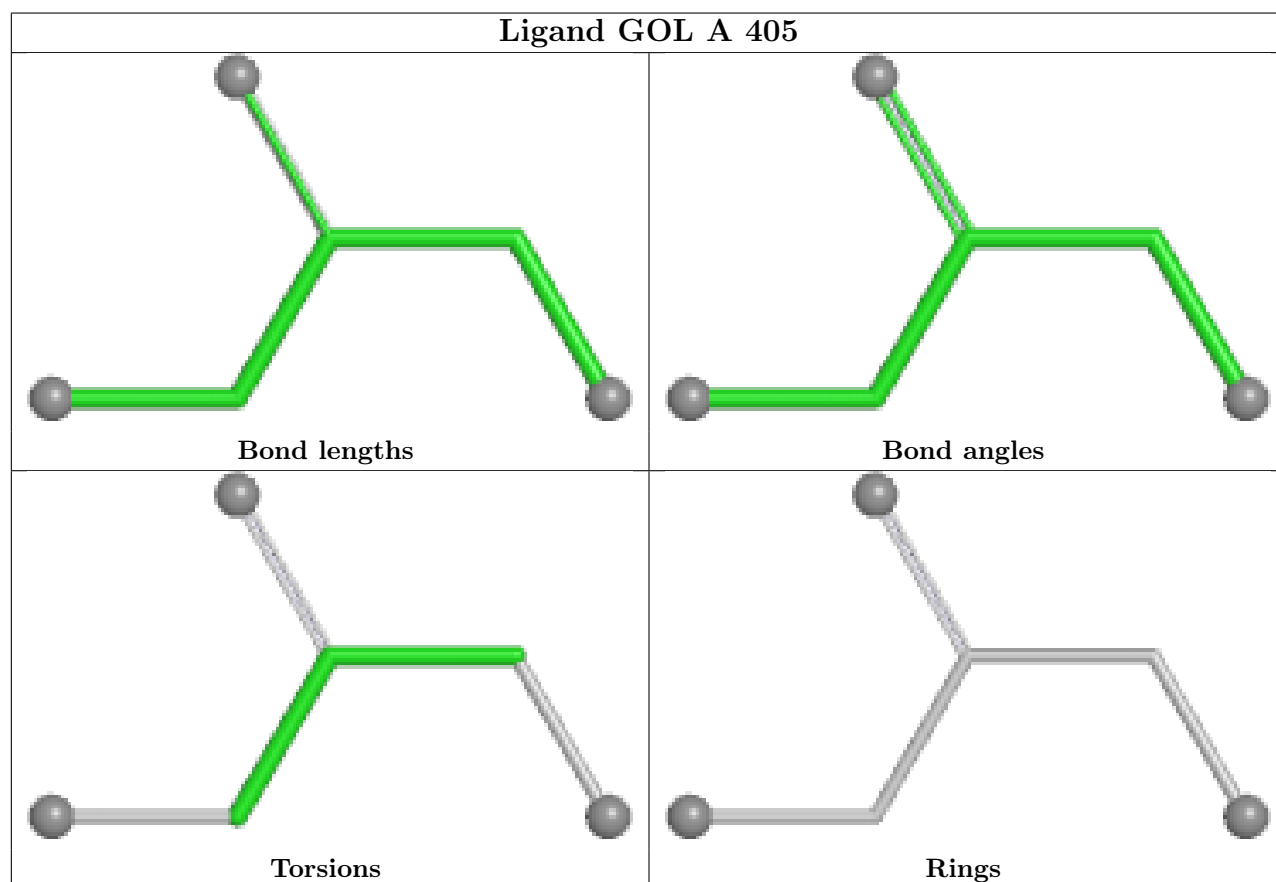
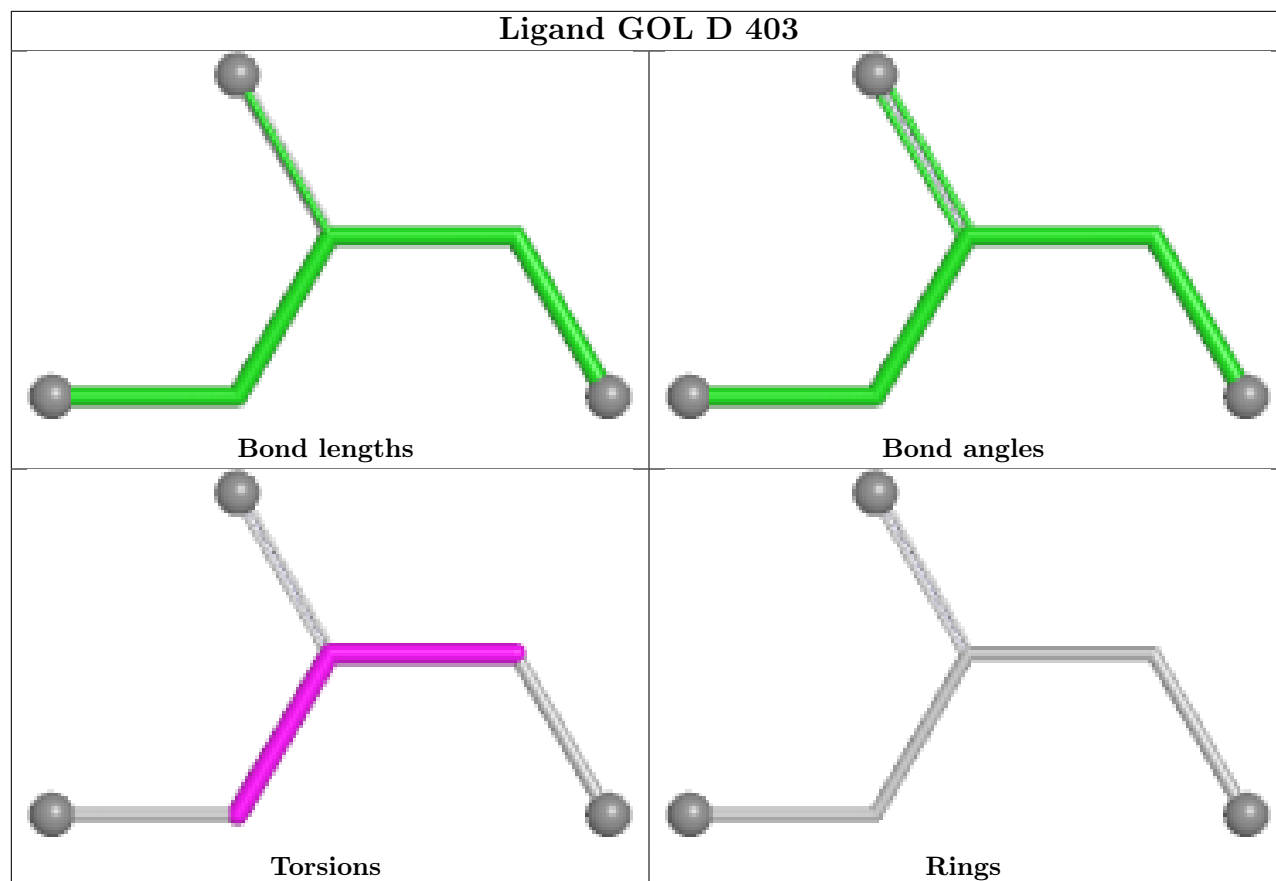


Ligand ATP C 402



Ligand EDO D 402





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%)	-1.56	0 100 100	35, 62, 110, 136	1 (0%)
1	B	292/310 (94%)	-1.42	0 100 100	45, 78, 111, 128	1 (0%)
1	C	288/310 (92%)	-1.51	0 100 100	43, 67, 109, 137	0
1	D	287/310 (92%)	-1.56	0 100 100	38, 61, 108, 130	0
1	E	293/310 (94%)	-1.43	0 100 100	47, 78, 112, 125	1 (0%)
1	F	287/310 (92%)	-1.53	0 100 100	42, 68, 108, 138	1 (0%)
All	All	1735/1860 (93%)	-1.50	0 100 100	35, 69, 111, 138	4 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides 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
2	PEG	A	401	7/7	0.97	0.10	84,87,89,90	0

Continued on next page...

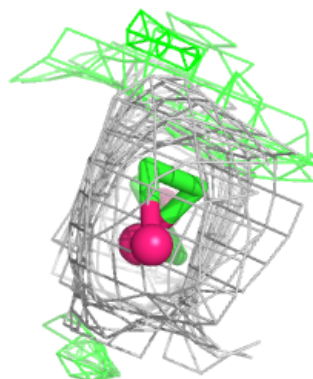
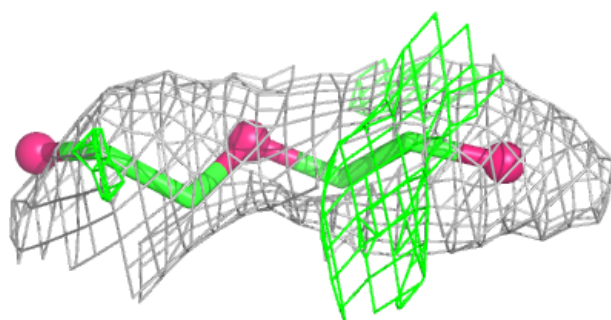
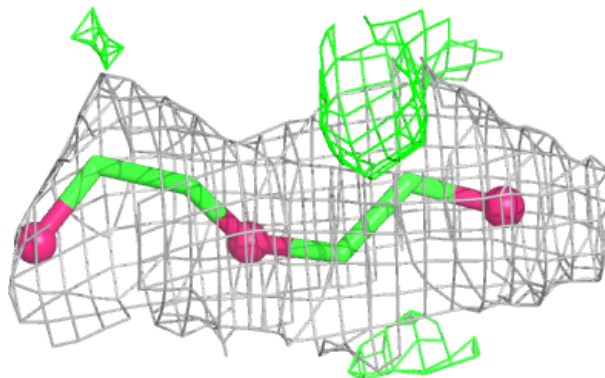
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PEG	D	401	7/7	0.97	0.08	80,89,102,102	0
3	EDO	C	404	4/4	0.98	0.07	91,91,92,92	0
3	EDO	F	402	4/4	0.98	0.06	77,82,85,85	0
3	EDO	A	402	4/4	0.99	0.07	74,75,77,77	0
3	EDO	D	402	4/4	0.99	0.07	91,96,96,97	0
3	EDO	D	405	4/4	0.99	0.05	71,76,81,87	0
3	EDO	E	401	4/4	0.99	0.05	89,89,89,90	0
3	EDO	A	403	4/4	0.99	0.06	74,75,76,77	0
4	PO4	A	404	5/5	0.99	0.04	97,104,113,114	0
4	PO4	D	406	5/5	0.99	0.04	106,116,123,123	0
5	GOL	A	405	6/6	0.99	0.04	69,72,77,80	0
5	GOL	D	403	6/6	0.99	0.04	67,68,70,71	0
7	ATP	C	402	31/31	0.99	0.04	81,111,120,124	1
7	ATP	F	404	31/31	0.99	0.04	78,97,116,118	12
8	PRP	C	403	22/22	0.99	0.04	104,159,200,202	0
8	PRP	F	403	22/22	0.99	0.03	106,168,191,198	0
6	MG	C	401	1/1	1.00	0.03	71,71,71,71	0
6	MG	F	401	1/1	1.00	0.02	76,76,76,76	0
3	EDO	D	404	4/4	1.00	0.04	69,75,78,79	0

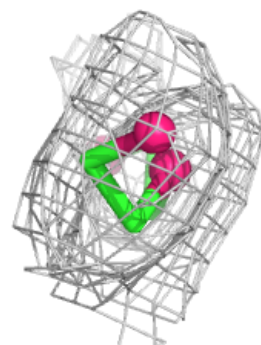
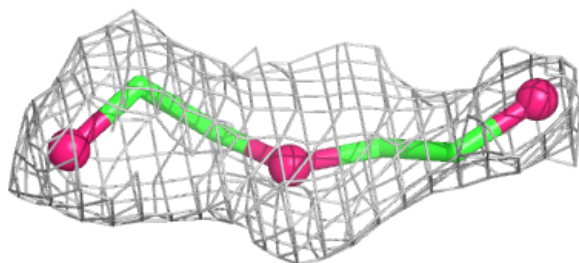
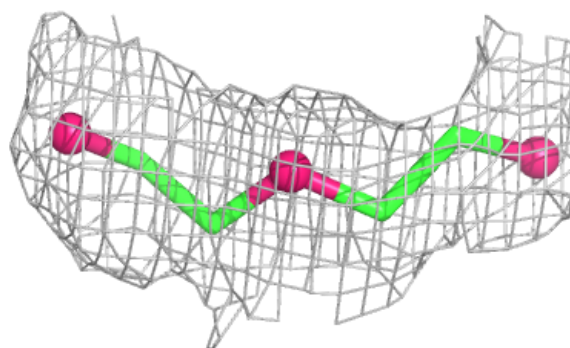
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

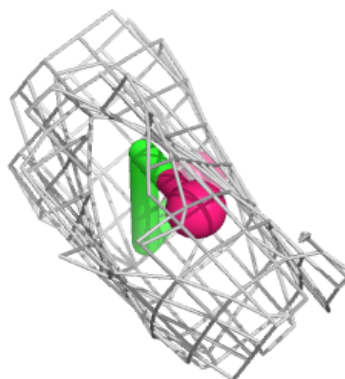
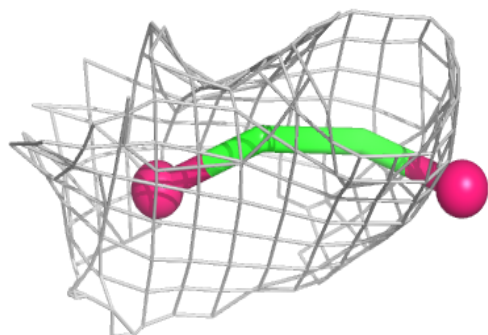
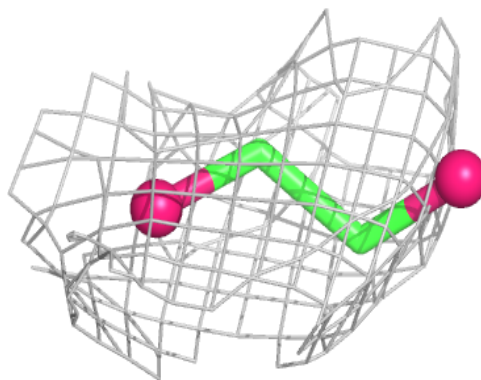
**Electron density around PEG D 401:**

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

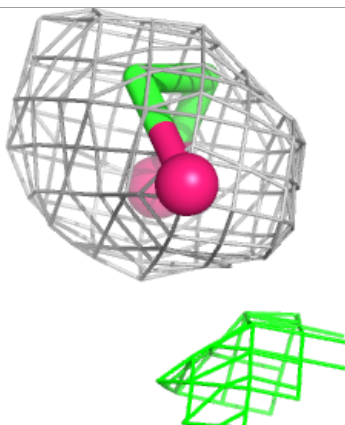
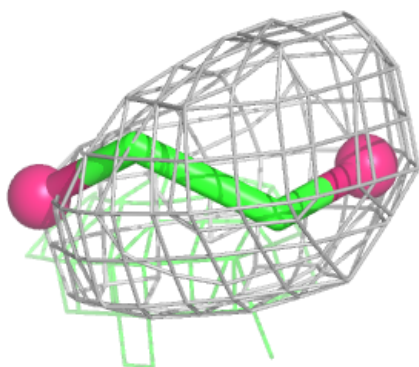
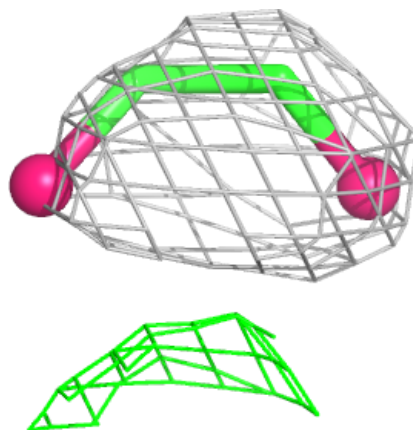


Electron density around EDO C 404:

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

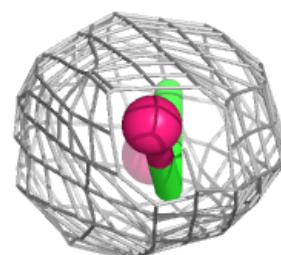
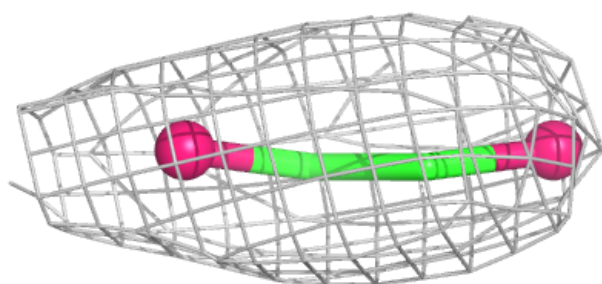
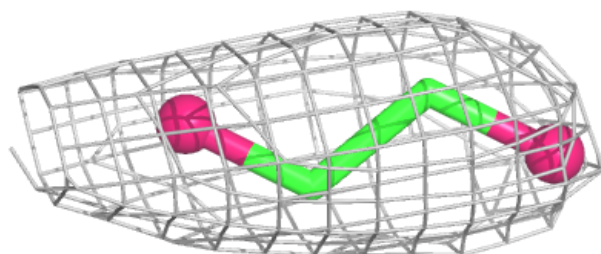
**Electron density around EDO F 402:**

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

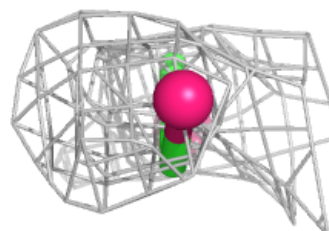
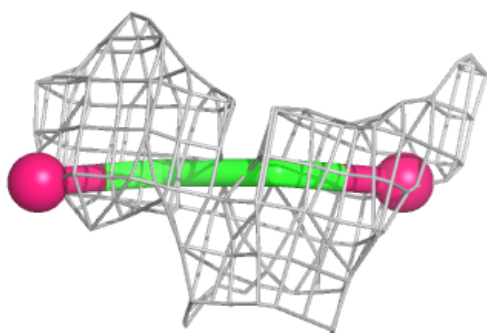
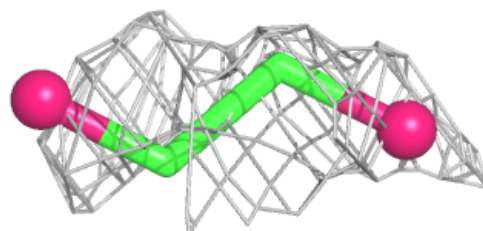


Electron density around EDO A 402:

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

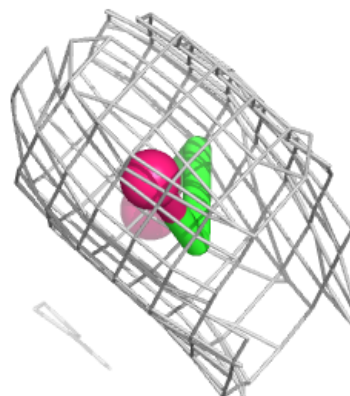
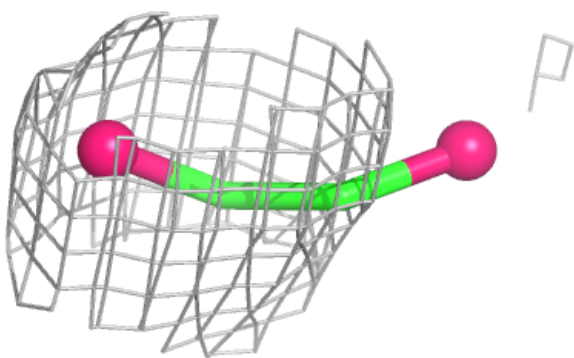
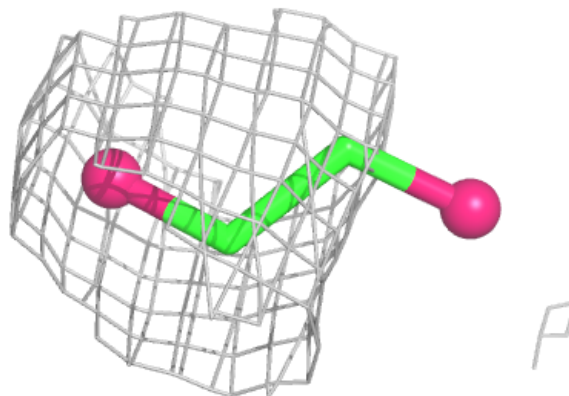
**Electron density around EDO D 402:**

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

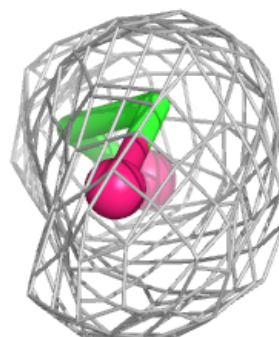
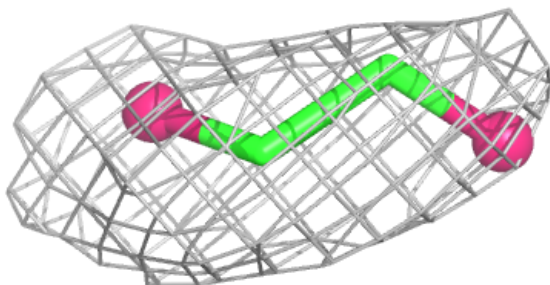
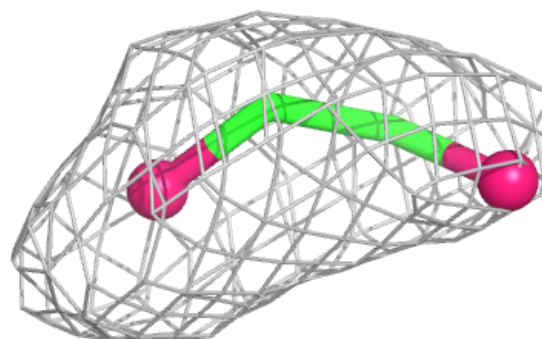


Electron density around EDO D 405:

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

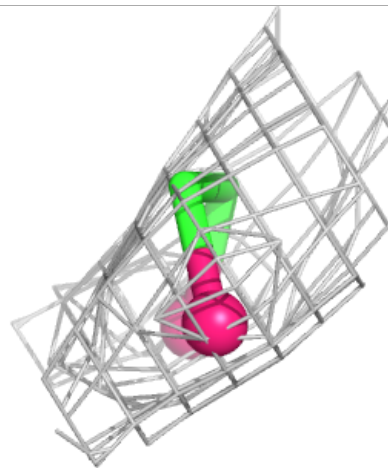
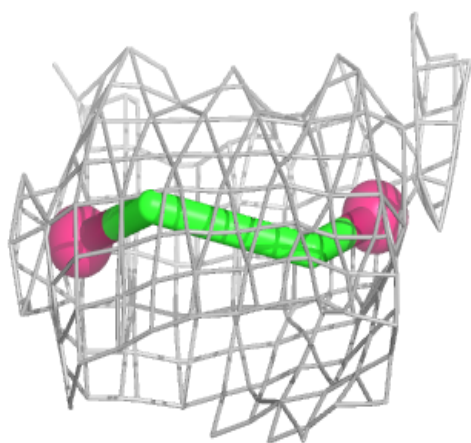
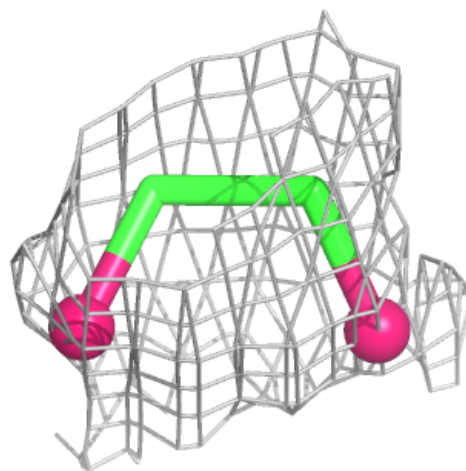
**Electron density around EDO E 401:**

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



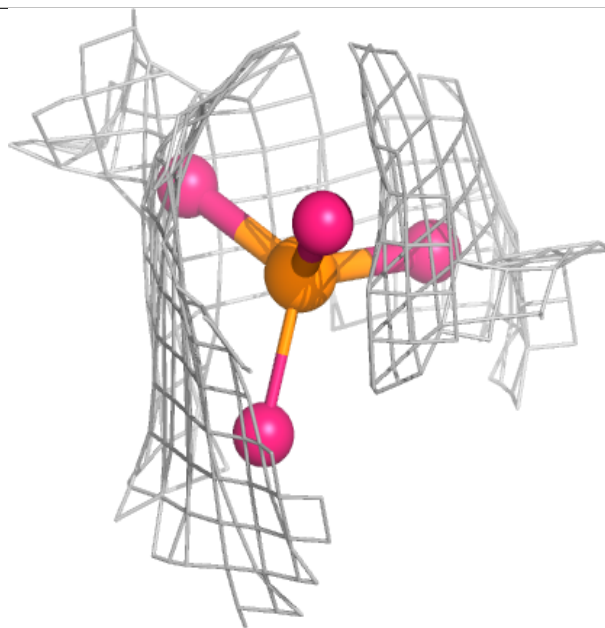
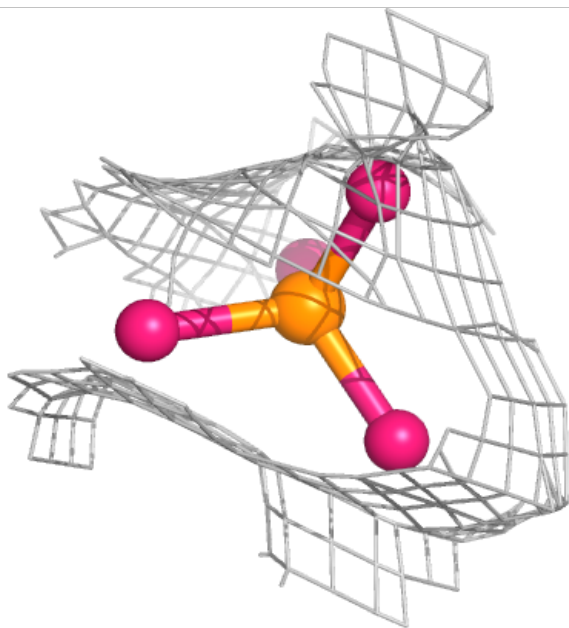
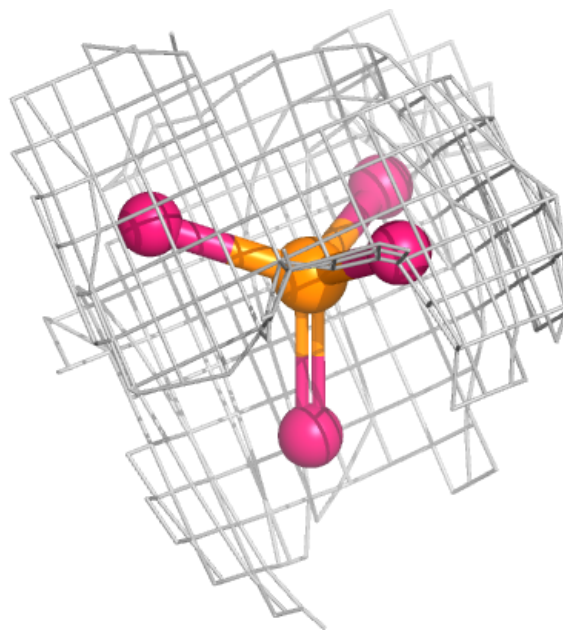
Electron density around EDO A 403:

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



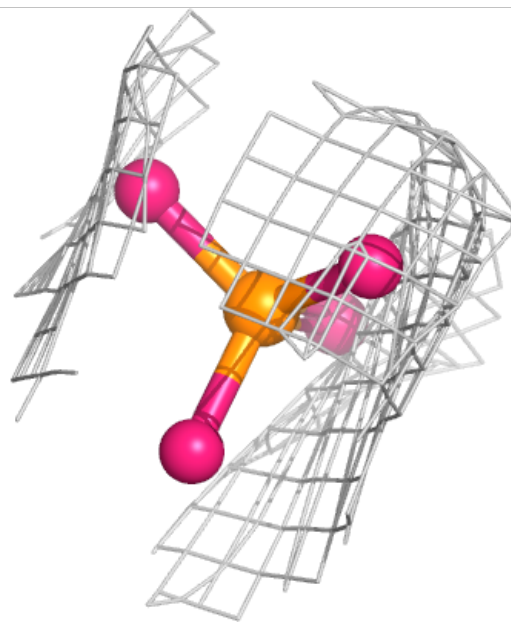
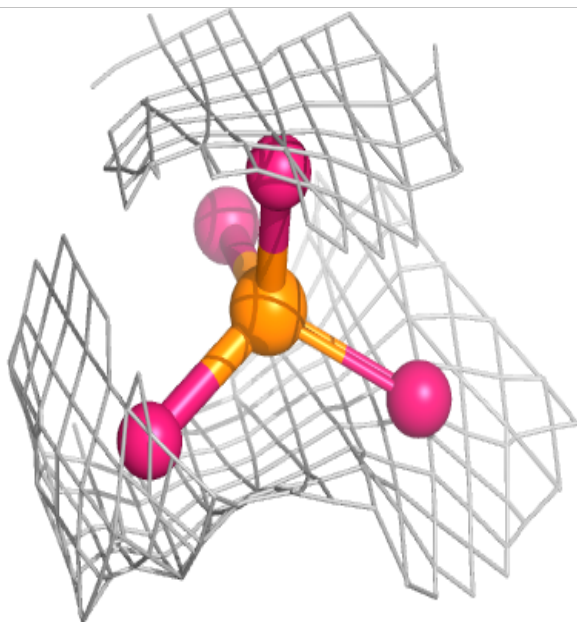
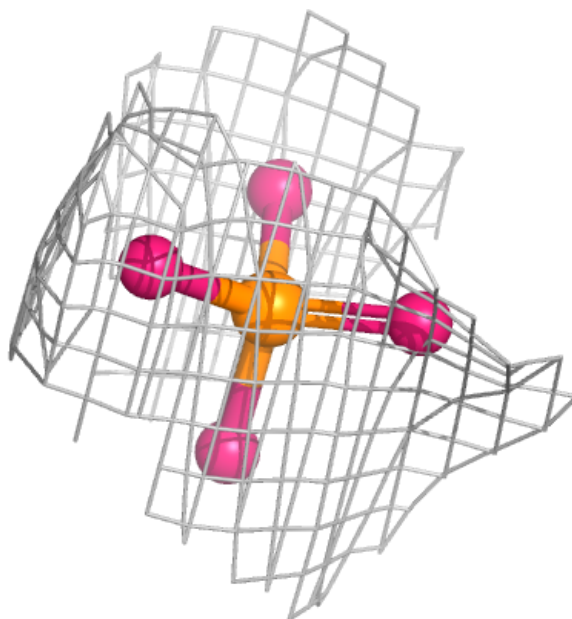
Electron density around PO4 A 404:

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



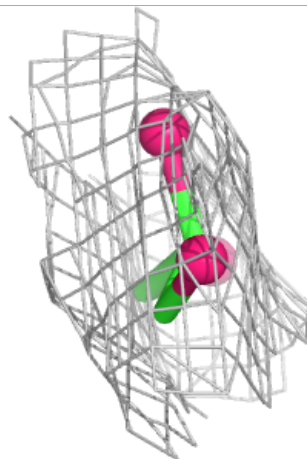
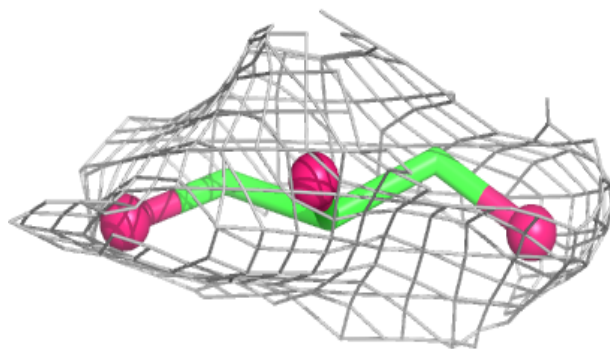
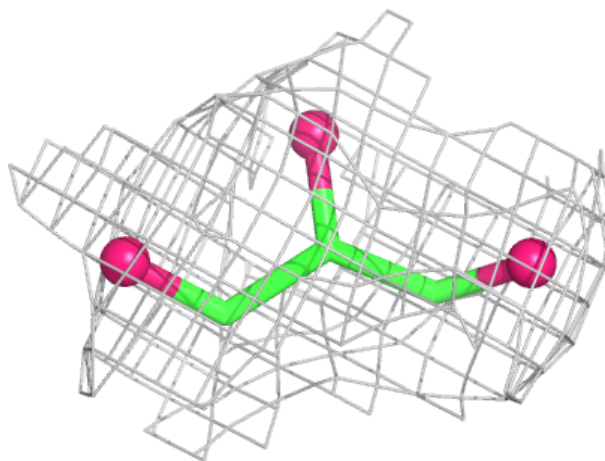
Electron density around PO4 D 406:

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



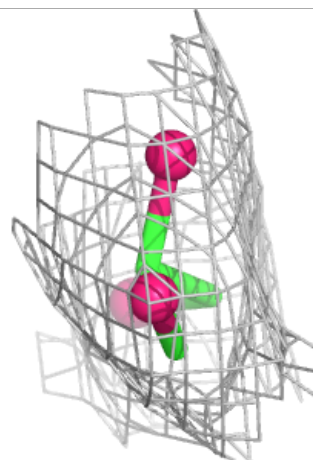
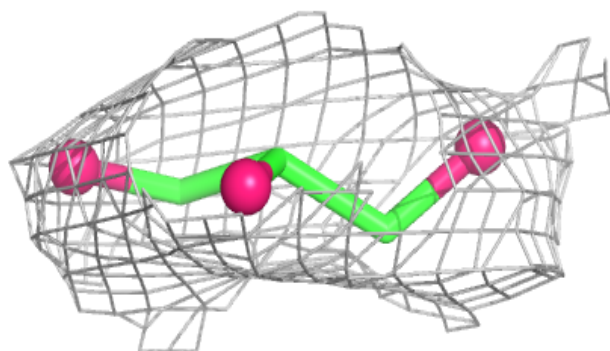
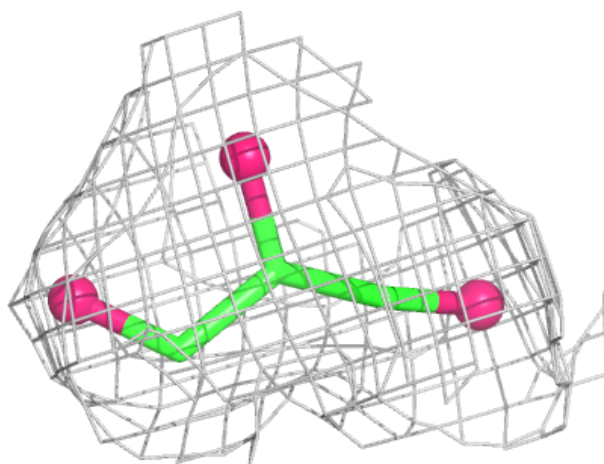
Electron density around GOL A 405:

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



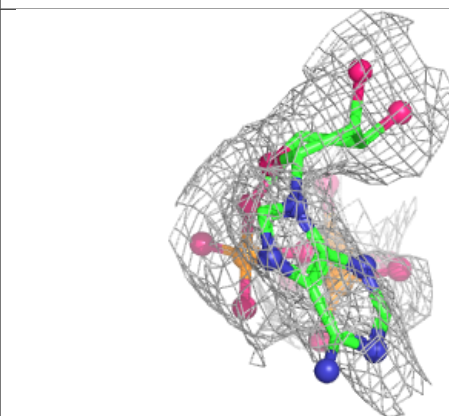
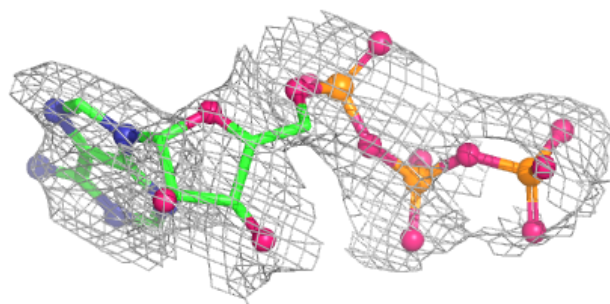
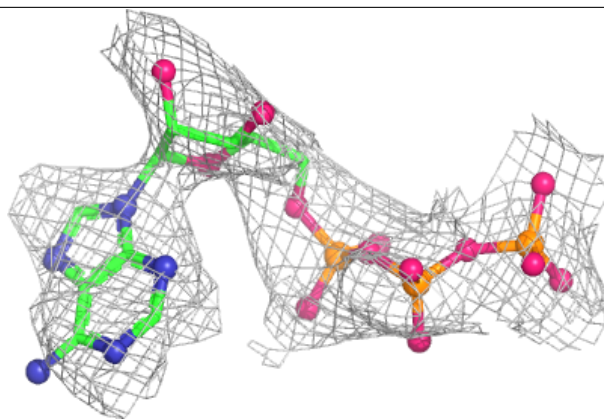
Electron density around GOL D 403:

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

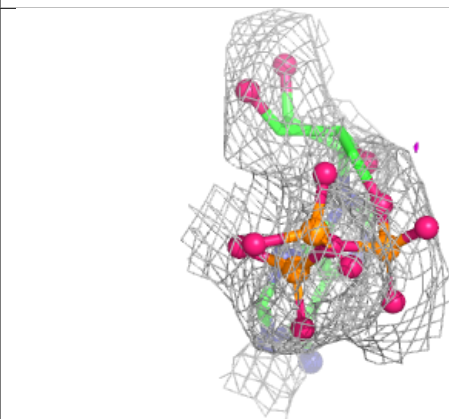
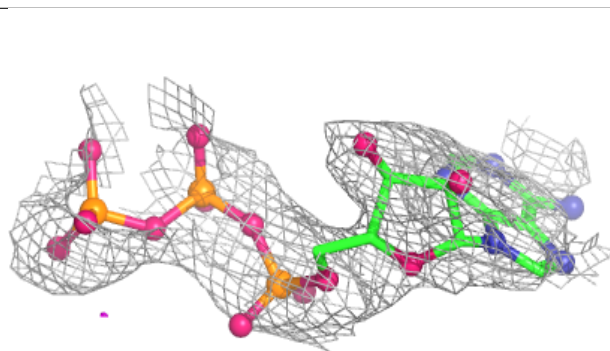
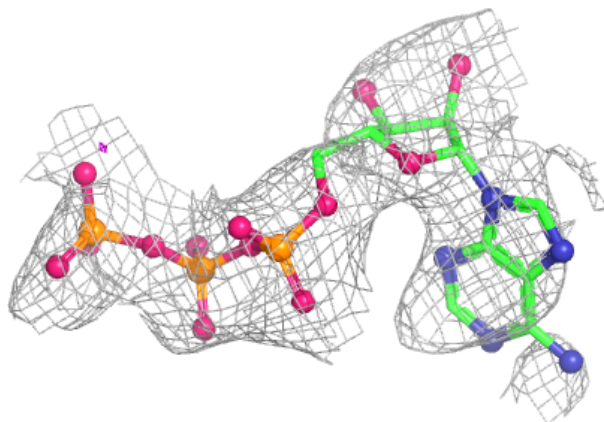


Electron density around ATP C 402:

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

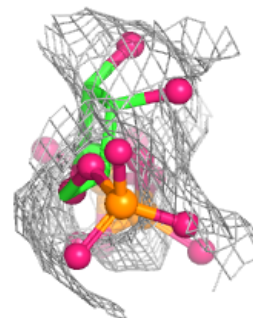
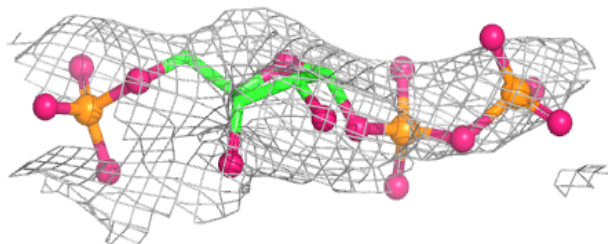
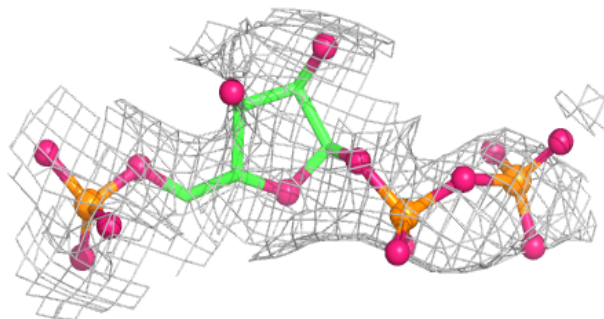
**Electron density around ATP F 404:**

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

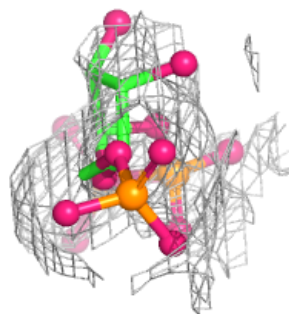
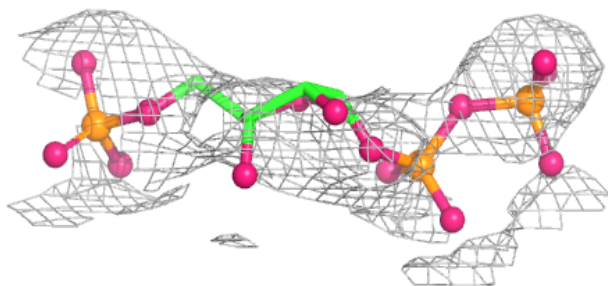
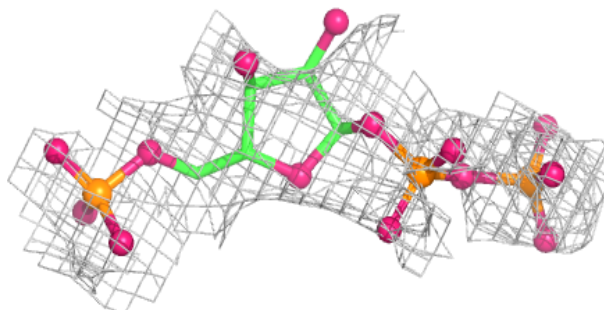


Electron density around PRP C 403:

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

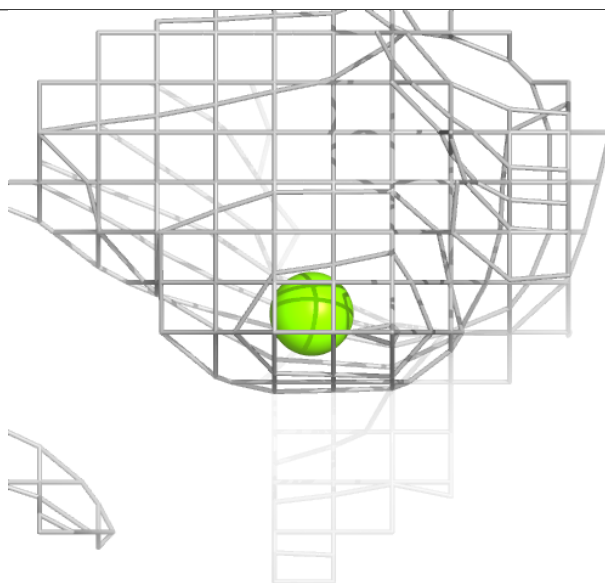
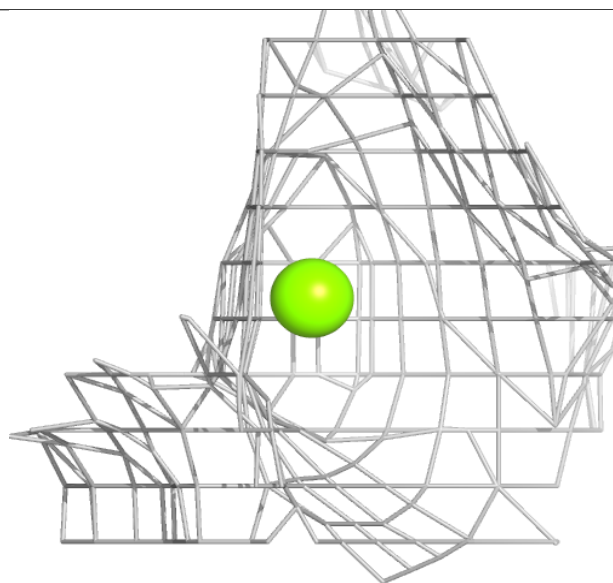
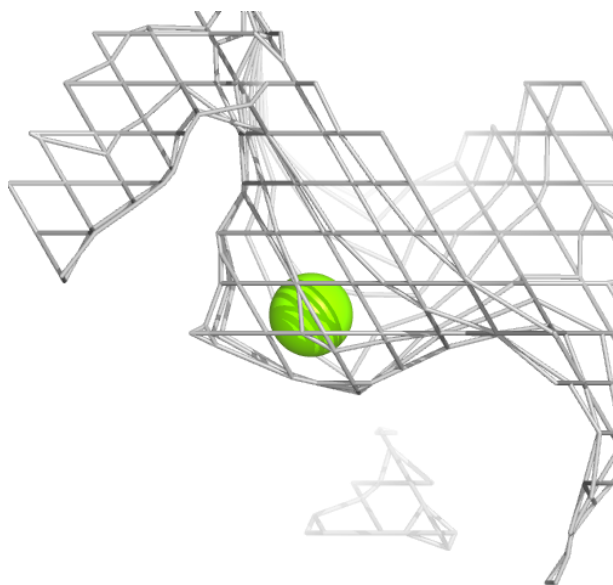
**Electron density around PRP F 403:**

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



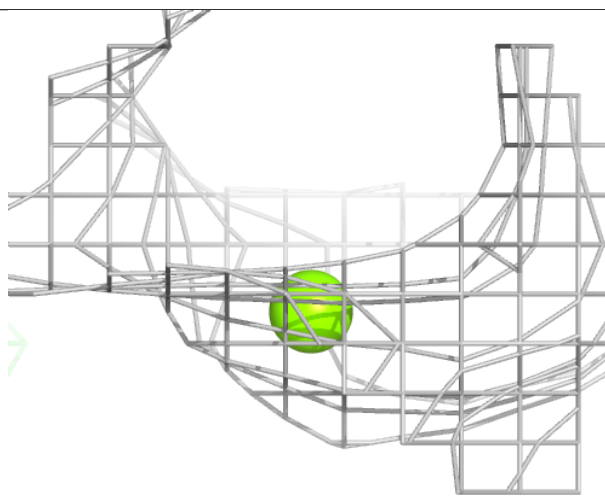
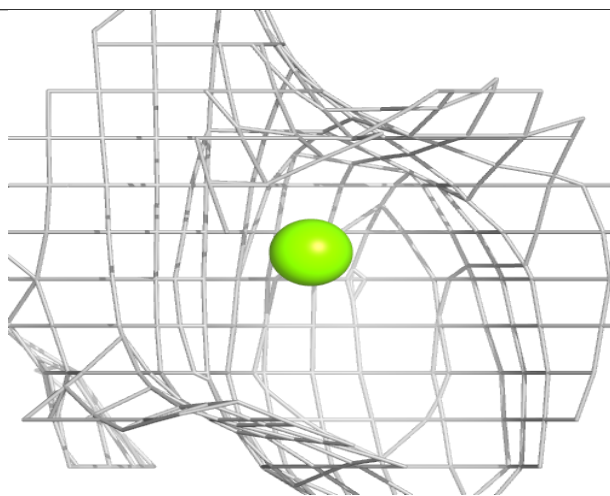
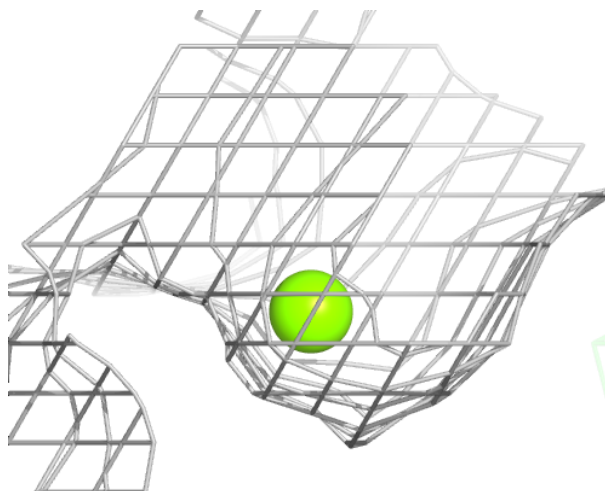
Electron density around MG C 401:

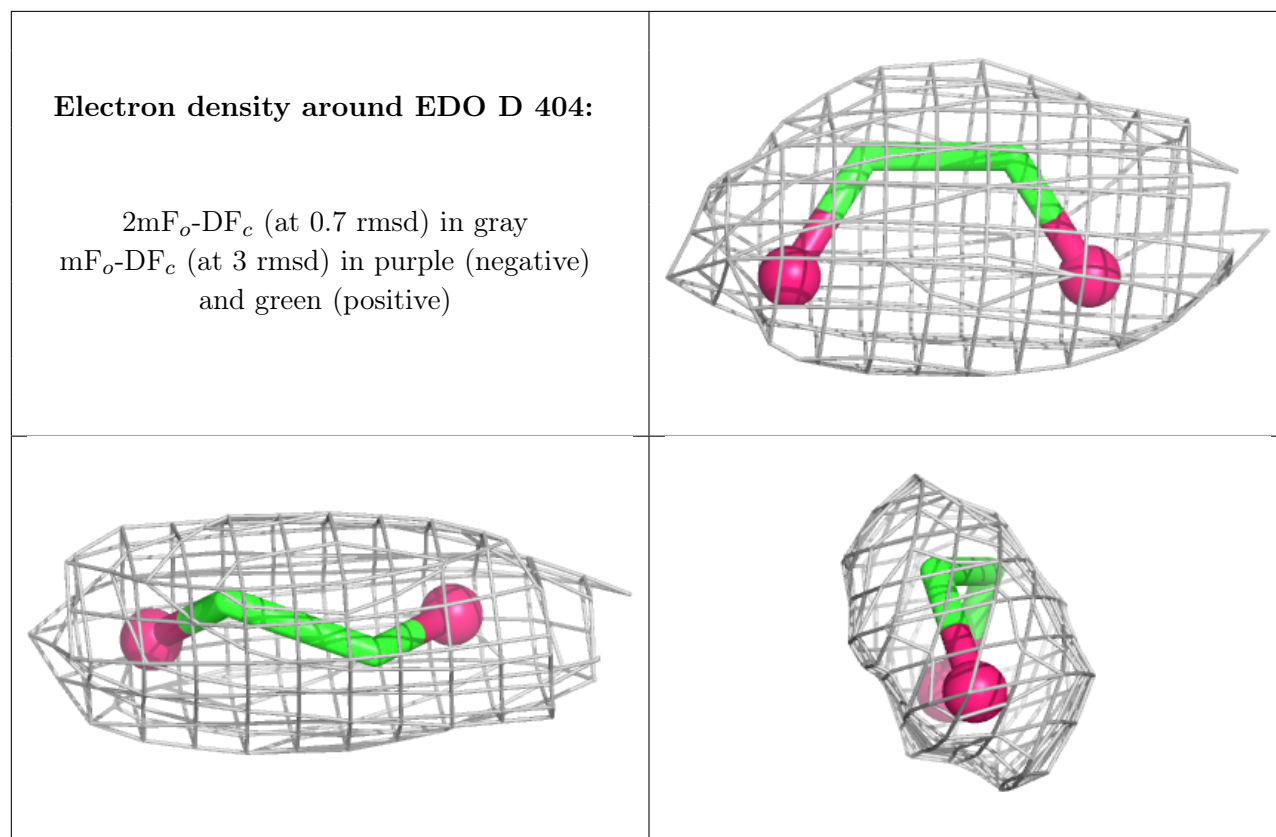
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.