



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:47 AM UTC

PDB ID : 7LO2 / pdb_00007lo2
Title : S-adenosylmethionine synthetase cocrystallized with CTP
Authors : Tan, L.L.; Jackson, C.J.
Deposited on : 2021-02-09
Resolution : 1.89 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

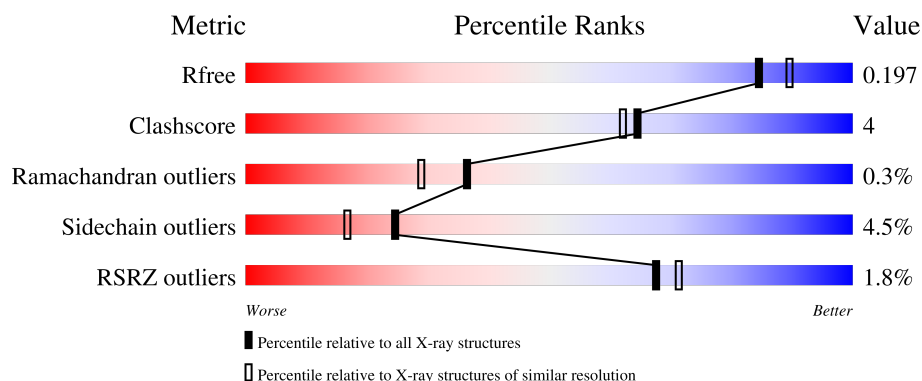
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	384	3% 88% 10% ..
1	B	384	2% 86% 9% ..
1	C	384	86% 11% .
1	D	384	2% 88% 8% ..

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
7	PG4	D	401	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12452 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.

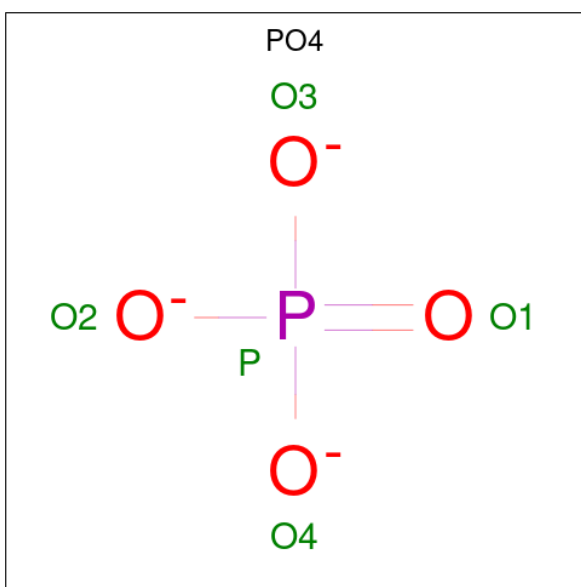
- Molecule 1 is a protein called S-adenosylmethionine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	5	0
			2970	1873	508	575	14			
1	B	372	Total	C	N	O	S	0	3	0
			2880	1818	488	559	15			
1	C	375	Total	C	N	O	S	0	5	0
			2926	1846	501	565	14			
1	D	375	Total	C	N	O	S	0	2	0
			2895	1829	495	557	14			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

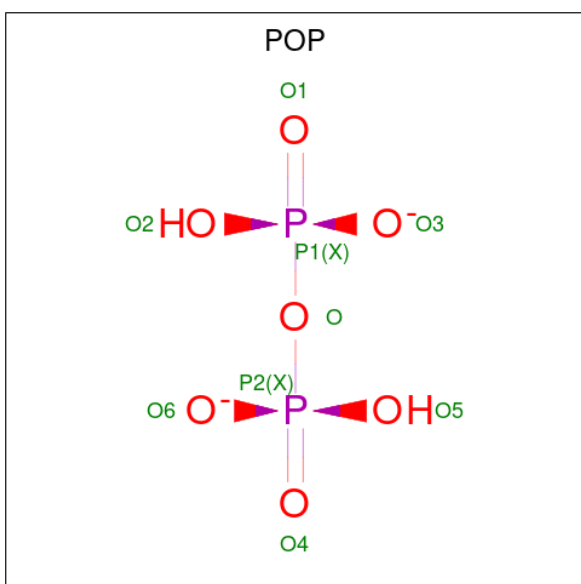
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mg	0	0
			3	3		
2	B	1	Total	Mg	0	0
			1	1		
2	C	3	Total	Mg	0	0
			3	3		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



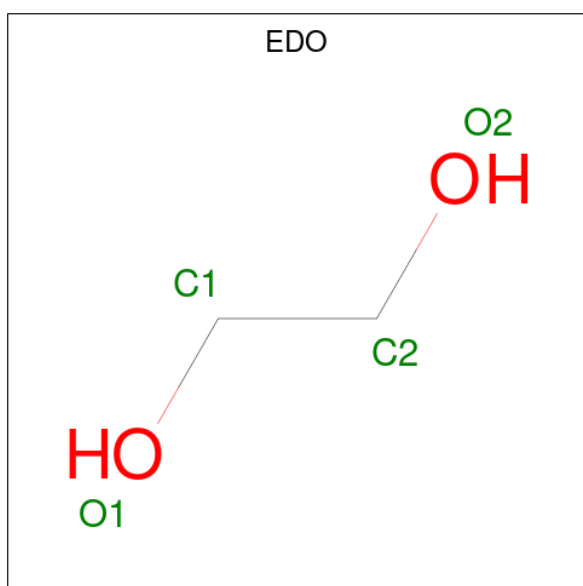
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 9 7 2	0	0
4	B	1	Total O P 9 7 2	0	0
4	C	1	Total O P 9 7 2	0	0
4	D	1	Total O P 9 7 2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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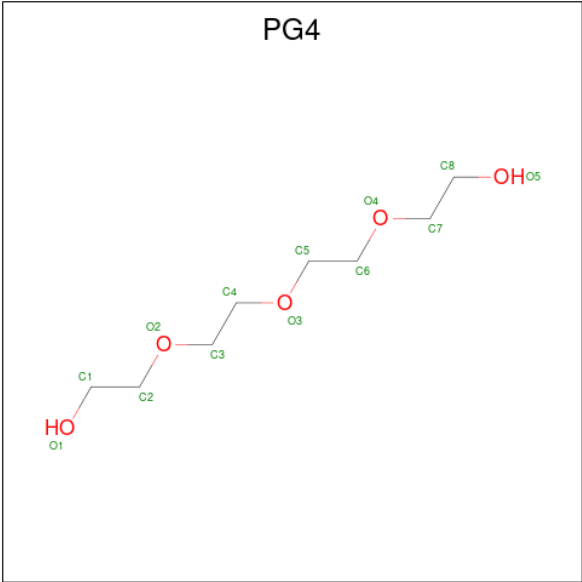
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	2	Total K 2 2	0	0
6	C	1	Total K 1 1	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			13	8	5		

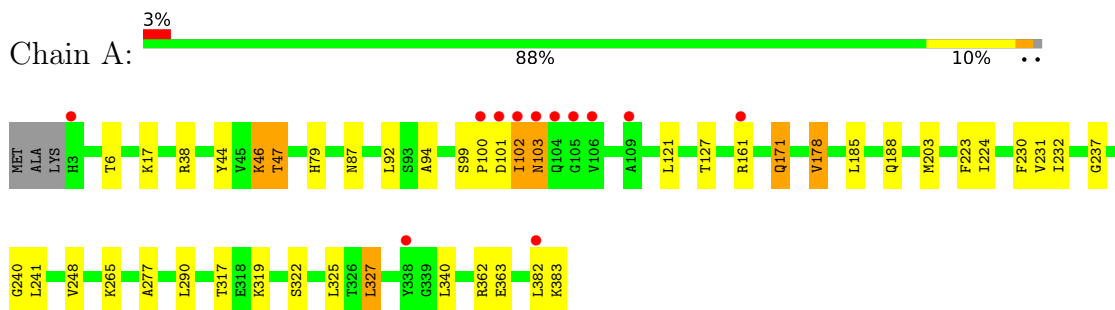
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	182	Total	O	0	0
			182	182		
8	B	141	Total	O	0	0
			141	141		
8	C	168	Total	O	0	0
			168	168		
8	D	142	Total	O	0	0
			142	142		

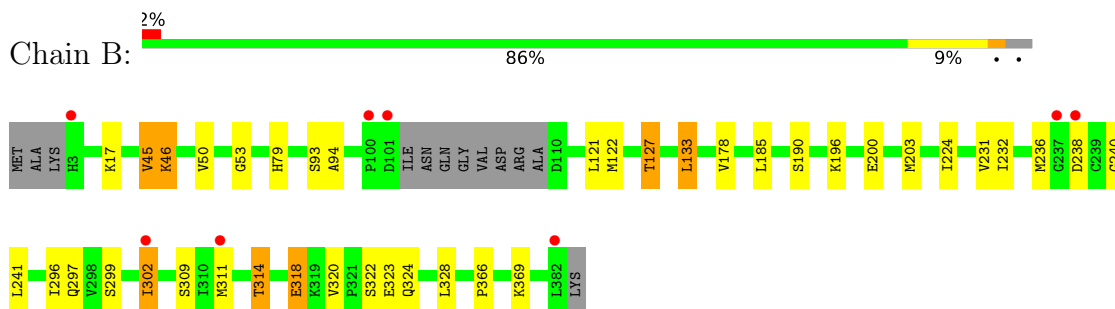
3 Residue-property plots

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.

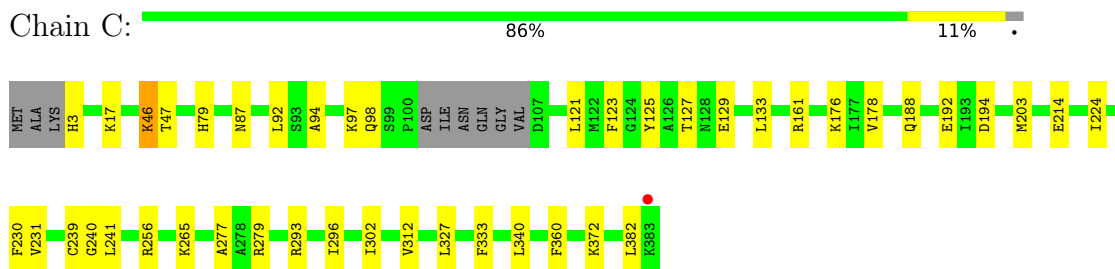
- Molecule 1: S-adenosylmethionine synthase



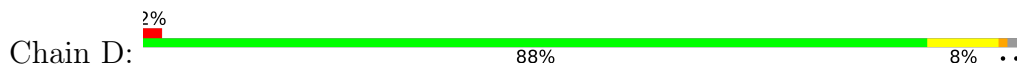
- Molecule 1: S-adenosylmethionine synthase

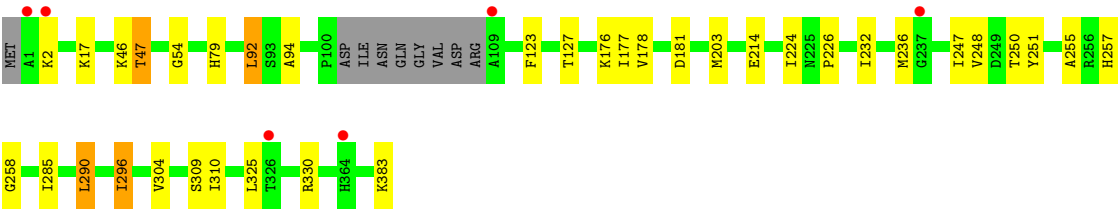


- Molecule 1: S-adenosylmethionine synthase



- Molecule 1: S-adenosylmethionine synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.14Å 118.32Å 144.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.22 – 1.89 38.22 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.22-1.89) 99.8 (38.22-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874, PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.166 , 0.195 0.167 , 0.197	Depositor DCC
R_{free} test set	6979 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12452	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: MG, K, POP, PO4, EDO, PG4

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	0.47	0/3030	0.63	0/4109
1	B	0.43	0/2938	0.58	0/3984
1	C	0.45	0/2984	0.59	0/4042
1	D	0.42	0/2953	0.59	0/4003
All	All	0.44	0/11905	0.60	0/16138

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2970	0	2924	29	0
1	B	2880	0	2830	25	0
1	C	2926	0	2886	25	0
1	D	2895	0	2866	26	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	C	3	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	1	0
3	D	10	0	0	1	0
4	A	9	0	0	1	0
4	B	9	0	0	0	0
4	C	9	0	0	0	0
4	D	9	0	0	0	0
5	A	32	0	48	3	0
5	B	12	0	18	2	0
5	C	24	0	36	4	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
7	D	13	0	18	10	0
8	A	182	0	0	2	0
8	B	141	0	0	2	0
8	C	168	0	0	2	0
8	D	142	0	0	0	0
All	All	12452	0	11626	91	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 4.

All (91) 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:B:190:SER:HA	5:B:408:EDO:H12	1.68	0.73
1:B:121:LEU:HD21	1:B:297:GLN:HG3	1.72	0.71
1:A:362:ARG:HA	5:A:410:EDO:H12	1.73	0.70
1:D:255:ALA:O	7:D:401:PG4:H82	1.91	0.70
4:A:405:POP:O2	8:A:501:HOH:O	2.09	0.70
1:C:46:LYS:HE2	1:D:94:ALA:HB1	1.74	0.69
1:A:38:ARG:NH1	8:A:502:HOH:O	2.25	0.68
1:C:203:MET:HE2	1:C:224:ILE:HD11	1.78	0.66
1:B:314:THR:HG21	1:B:318:GLU:HB3	1.77	0.66
1:D:257:HIS:HA	7:D:401:PG4:H51	1.78	0.66
1:B:203:MET:HE2	1:B:224:ILE:HD11	1.78	0.65
1:A:102:ILE:HG23	1:A:103:ASN:H	1.64	0.62
1:B:231:VAL:HG13	5:B:408:EDO:H11	1.82	0.62
1:B:299:SER:HB2	1:B:309:SER:HB3	1.82	0.62
1:B:366:PRO:O	1:B:369:LYS:HE2	1.99	0.62
1:D:247:ILE:HD12	7:D:401:PG4:H81	1.80	0.61
1:D:251:TYR:HD2	7:D:401:PG4:H71	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:MET:HE2	1:D:224:ILE:HD11	1.83	0.60
1:C:129:GLU:HB2	5:C:407:EDO:H12	1.84	0.60
1:A:92:LEU:HD23	1:C:94:ALA:HB2	1.84	0.58
1:C:94:ALA:O	1:D:46:LYS:HE2	2.03	0.58
1:D:251:TYR:CD2	7:D:401:PG4:H61	2.39	0.57
1:A:47:THR:HG21	8:B:511:HOH:O	2.03	0.57
1:D:251:TYR:CE2	7:D:401:PG4:H61	2.41	0.56
1:D:258:GLY:H	7:D:401:PG4:C3	2.19	0.55
1:A:171:GLN:O	1:A:178:VAL:HG13	2.08	0.54
1:B:318:GLU:OE1	1:B:322:SER:OG	2.25	0.54
1:C:231:VAL:HG13	5:C:406:EDO:H12	1.90	0.54
1:A:223:PHE:CD2	1:B:302:ILE:HD11	2.44	0.53
1:D:250:THR:OG1	7:D:401:PG4:H72	2.09	0.53
1:B:238[A]:ASP:N	1:B:238[A]:ASP:OD1	2.39	0.52
1:D:232:ILE:HG23	1:D:236:MET:HG2	1.92	0.52
1:C:333:PHE:CE2	1:C:372:LYS:HD2	2.45	0.52
1:C:240:GLY:O	1:C:241:LEU:HD23	2.11	0.51
1:B:232:ILE:CG2	1:B:236:MET:HG2	2.41	0.51
1:C:302:ILE:HG23	1:D:226:PRO:HG2	1.93	0.51
1:D:123:PHE:HB2	7:D:401:PG4:H52	1.92	0.50
1:A:223:PHE:CE2	1:B:302:ILE:HD11	2.46	0.50
1:B:196:LYS:HE2	1:B:200:GLU:OE2	2.12	0.50
1:B:232:ILE:HG23	1:B:236:MET:HG2	1.93	0.50
1:D:176:LYS:HD2	1:D:177:ILE:O	2.13	0.49
1:A:94:ALA:HB2	1:C:92:LEU:HD23	1.94	0.48
1:B:94:ALA:HB2	1:D:92:LEU:HD13	1.94	0.48
1:A:87:ASN:O	1:D:236:MET:HE1	2.15	0.47
1:D:310:ILE:HD12	1:D:330:ARG:HD3	1.97	0.47
1:A:44:TYR:HE1	1:A:46:LYS:HD2	1.80	0.47
1:A:290:LEU:HD23	1:A:382:LEU:HD22	1.96	0.47
1:C:97:LYS:HD3	8:C:644:HOH:O	2.14	0.47
1:A:47:THR:HG22	1:A:237:GLY:H	1.79	0.46
1:A:327:LEU:HA	1:A:327:LEU:HD22	1.72	0.45
1:A:203:MET:HE2	1:A:224:ILE:HD11	1.99	0.45
1:B:46:LYS:HD2	8:B:622:HOH:O	2.16	0.45
1:A:6:THR:H	1:B:121:LEU:HD12	1.81	0.45
1:C:277:ALA:CB	1:C:340:LEU:HD22	2.47	0.45
1:B:324:GLN:O	1:B:328:LEU:HD23	2.16	0.44
1:C:125:TYR:OH	1:C:293[A]:ARG:HD2	2.17	0.44
1:D:232:ILE:CG2	1:D:236:MET:HG2	2.48	0.44
1:A:102:ILE:HG23	1:A:103:ASN:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:LYS:HB2	1:C:176:LYS:HE2	1.82	0.44
1:A:265:LYS:NZ	3:B:402:PO4:O2	2.44	0.44
1:A:277:ALA:CB	1:A:340:LEU:HD22	2.48	0.44
1:B:236:MET:HE1	1:C:87:ASN:O	2.17	0.44
1:A:47:THR:CG2	1:A:237:GLY:H	2.31	0.44
1:B:240:GLY:C	1:B:241:LEU:HD12	2.43	0.44
1:D:251:TYR:CD2	7:D:401:PG4:H71	2.50	0.44
1:D:290:LEU:HB3	1:D:325:LEU:HD21	1.99	0.44
1:A:363:GLU:H	5:A:410:EDO:H12	1.83	0.43
1:C:161:ARG:NE	5:C:406:EDO:O2	2.47	0.43
1:C:161:ARG:HG3	5:C:406:EDO:O1	2.18	0.43
1:D:46:LYS:O	1:D:47:THR:C	2.62	0.43
1:B:127:THR:O	1:B:133:LEU:HA	2.18	0.43
1:A:188:GLN:HA	1:A:230:PHE:O	2.19	0.43
1:A:231:VAL:HG23	1:A:232:ILE:HG23	2.01	0.43
1:A:363:GLU:H	5:A:410:EDO:C1	2.31	0.43
1:B:121:LEU:HD23	1:B:122:MET:N	2.33	0.43
1:C:98:GLN:HG3	8:C:530:HOH:O	2.19	0.43
1:A:317:THR:O	1:A:319:LYS:HE3	2.18	0.43
1:D:46:LYS:HG2	1:D:47:THR:H	1.84	0.43
1:C:239[B]:CYS:SG	1:D:54:GLY:HA2	2.59	0.42
1:A:79:HIS:CE1	1:D:79:HIS:CE1	3.07	0.42
1:A:240:GLY:C	1:A:241:LEU:HD12	2.43	0.42
1:A:325:LEU:HD23	1:A:325:LEU:HA	1.88	0.42
1:C:188:GLN:HA	1:C:230:PHE:O	2.20	0.42
1:C:279:ARG:HG2	1:C:360:PHE:CD1	2.55	0.41
1:B:79:HIS:CE1	1:C:79:HIS:CE1	3.09	0.41
1:D:285:ILE:HD12	1:D:296:ILE:HD11	2.02	0.41
1:C:127:THR:O	1:C:133:LEU:HA	2.20	0.41
1:C:265:LYS:NZ	3:D:404:PO4:O4	2.45	0.41
1:C:123:PHE:HA	1:C:296:ILE:O	2.21	0.41
1:B:45:VAL:HG22	1:B:50:VAL:HG22	2.02	0.40
1:A:44:TYR:OH	1:B:53:GLY:HA3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	384/384 (100%)	370 (96%)	11 (3%)	3 (1%)	16	8
1	B	371/384 (97%)	363 (98%)	8 (2%)	0	100	100
1	C	376/384 (98%)	369 (98%)	6 (2%)	1 (0%)	36	29
1	D	373/384 (97%)	362 (97%)	10 (3%)	1 (0%)	36	29
All	All	1504/1536 (98%)	1464 (97%)	35 (2%)	5 (0%)	36	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	PRO
1	A	102	ILE
1	A	101	ASP
1	C	47	THR
1	D	47	THR

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	315/312 (101%)	299 (95%)	16 (5%)	21	13
1	B	306/312 (98%)	290 (95%)	16 (5%)	21	13
1	C	310/312 (99%)	298 (96%)	12 (4%)	28	21
1	D	306/312 (98%)	293 (96%)	13 (4%)	26	19
All	All	1237/1248 (99%)	1180 (95%)	57 (5%)	24	16

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	46	LYS
1	A	47	THR
1	A	99	SER
1	A	103	ASN
1	A	121	LEU
1	A	127	THR
1	A	161[A]	ARG
1	A	161[B]	ARG
1	A	171	GLN
1	A	178	VAL
1	A	185	LEU
1	A	248	VAL
1	A	322	SER
1	A	327	LEU
1	A	383	LYS
1	B	17	LYS
1	B	45	VAL
1	B	46	LYS
1	B	93	SER
1	B	127	THR
1	B	133	LEU
1	B	178	VAL
1	B	185	LEU
1	B	296	ILE
1	B	302	ILE
1	B	311[A]	MET
1	B	311[B]	MET
1	B	314	THR
1	B	318	GLU
1	B	320	VAL
1	B	323	GLU
1	C	3	HIS
1	C	17	LYS
1	C	46	LYS
1	C	121	LEU
1	C	178	VAL
1	C	192	GLU
1	C	194	ASP
1	C	214	GLU
1	C	256	ARG
1	C	312	VAL

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Mol	Chain	Res	Type
1	C	327	LEU
1	C	382	LEU
1	D	2	LYS
1	D	17	LYS
1	D	92	LEU
1	D	127	THR
1	D	178	VAL
1	D	181	ASP
1	D	214	GLU
1	D	248	VAL
1	D	290	LEU
1	D	296	ILE
1	D	304	VAL
1	D	309	SER
1	D	383	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	104	GLN
1	A	114	GLN
1	A	146	GLN
1	A	171	GLN
1	C	195	GLN
1	D	3	HIS
1	D	195	GLN
1	D	297	GLN

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 37 ligands modelled in this entry, 11 are monoatomic - leaving 26 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	$\# Z > 2$
5	EDO	C	411	-	3,3,3	0.44	0	2,2,2	0.32	0
5	EDO	A	413	-	3,3,3	0.50	0	2,2,2	0.63	0
3	PO4	B	402	2	4,4,4	1.37	0	6,6,6	1.21	1 (16%)
5	EDO	A	411	-	3,3,3	0.46	0	2,2,2	0.39	0
5	EDO	B	406	-	3,3,3	0.42	0	2,2,2	0.43	0
5	EDO	A	410	-	3,3,3	0.54	0	2,2,2	0.22	0
5	EDO	B	408	-	3,3,3	0.32	0	2,2,2	0.25	0
5	EDO	C	406	-	3,3,3	0.43	0	2,2,2	0.49	0
5	EDO	C	409	-	3,3,3	0.68	0	2,2,2	0.64	0
3	PO4	D	403	2	4,4,4	0.83	0	6,6,6	1.01	0
5	EDO	C	408	-	3,3,3	0.47	0	2,2,2	0.64	0
5	EDO	B	407	-	3,3,3	0.48	0	2,2,2	0.44	0
5	EDO	C	407	-	3,3,3	0.41	0	2,2,2	0.44	0
5	EDO	A	408	-	3,3,3	0.46	0	2,2,2	0.37	0
4	POP	D	405	2	6,8,8	0.75	0	12,13,13	1.11	1 (8%)
4	POP	B	405	2,6	6,8,8	0.81	0	12,13,13	0.91	1 (8%)
5	EDO	A	406	-	3,3,3	0.42	0	2,2,2	0.50	0
3	PO4	A	404	2	4,4,4	1.16	0	6,6,6	0.94	0
5	EDO	A	409	-	3,3,3	0.51	0	2,2,2	0.33	0
5	EDO	A	412	-	3,3,3	0.51	0	2,2,2	0.63	0
5	EDO	C	410	-	3,3,3	0.34	0	2,2,2	0.62	0
5	EDO	A	407	-	3,3,3	0.45	0	2,2,2	0.43	0
3	PO4	D	404	2	4,4,4	0.98	0	6,6,6	0.83	0
4	POP	A	405	2	6,8,8	0.89	0	12,13,13	1.14	1 (8%)
7	PG4	D	401	-	12,12,12	0.53	0	11,11,11	0.75	0
4	POP	C	405	2,6	6,8,8	0.85	0	12,13,13	1.19	2 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	411	-	-	1/1/1/1	-
5	EDO	A	413	-	-	1/1/1/1	-
5	EDO	A	411	-	-	1/1/1/1	-
5	EDO	B	406	-	-	1/1/1/1	-
5	EDO	A	410	-	-	1/1/1/1	-
5	EDO	B	408	-	-	1/1/1/1	-
5	EDO	C	406	-	-	1/1/1/1	-
5	EDO	C	409	-	-	1/1/1/1	-
5	EDO	C	408	-	-	0/1/1/1	-
5	EDO	B	407	-	-	0/1/1/1	-
5	EDO	C	407	-	-	0/1/1/1	-
5	EDO	A	408	-	-	1/1/1/1	-
4	POP	D	405	2	-	0/6/6/6	-
4	POP	B	405	2,6	-	0/6/6/6	-
5	EDO	A	406	-	-	1/1/1/1	-
5	EDO	A	409	-	-	1/1/1/1	-
5	EDO	A	412	-	-	0/1/1/1	-
5	EDO	C	410	-	-	0/1/1/1	-
5	EDO	A	407	-	-	0/1/1/1	-
4	POP	A	405	2	-	5/6/6/6	-
7	PG4	D	401	-	-	6/10/10/10	-
4	POP	C	405	2,6	-	2/6/6/6	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	405	POP	O6-P2-O	2.77	113.92	104.64
4	B	405	POP	O2-P1-O	2.43	112.77	104.64
4	A	405	POP	O2-P1-O	2.33	112.44	104.64
4	C	405	POP	O3-P1-O	2.32	112.41	104.64
4	C	405	POP	O5-P2-O	2.14	111.80	104.64
3	B	402	PO4	O2-P-O1	-2.02	103.83	110.95

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	405	POP	P1-O-P2-O5
4	A	405	POP	P1-O-P2-O6
4	C	405	POP	P1-O-P2-O6

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Mol	Chain	Res	Type	Atoms
7	D	401	PG4	C3-C4-O3-C5
7	D	401	PG4	O1-C1-C2-O2
7	D	401	PG4	O3-C5-C6-O4
7	D	401	PG4	O4-C7-C8-O5
5	A	410	EDO	O1-C1-C2-O2
5	C	409	EDO	O1-C1-C2-O2
5	B	408	EDO	O1-C1-C2-O2
4	A	405	POP	P2-O-P1-O1
5	A	411	EDO	O1-C1-C2-O2
5	A	409	EDO	O1-C1-C2-O2
5	C	406	EDO	O1-C1-C2-O2
7	D	401	PG4	C4-C3-O2-C2
5	A	408	EDO	O1-C1-C2-O2
5	B	406	EDO	O1-C1-C2-O2
4	A	405	POP	P2-O-P1-O2
4	A	405	POP	P2-O-P1-O3
4	C	405	POP	P1-O-P2-O5
5	A	406	EDO	O1-C1-C2-O2
5	C	411	EDO	O1-C1-C2-O2
7	D	401	PG4	O2-C3-C4-O3
5	A	413	EDO	O1-C1-C2-O2

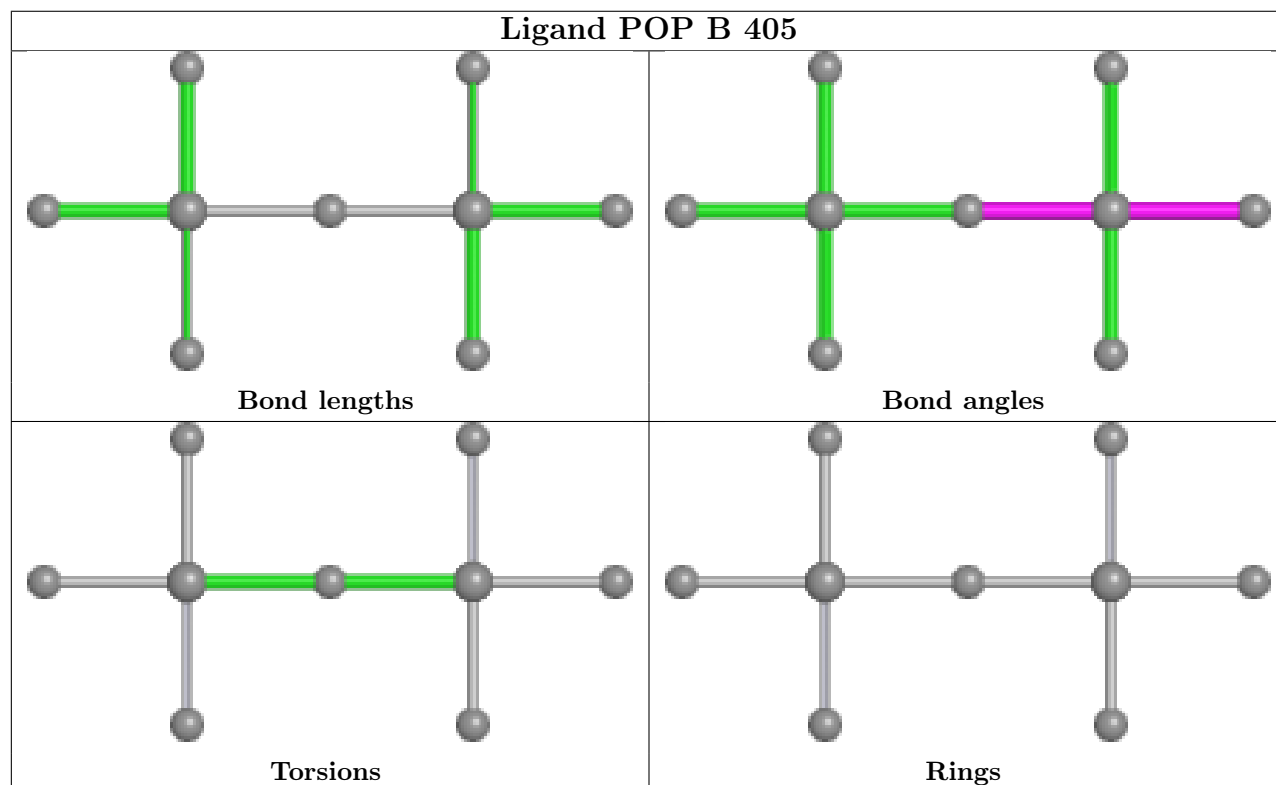
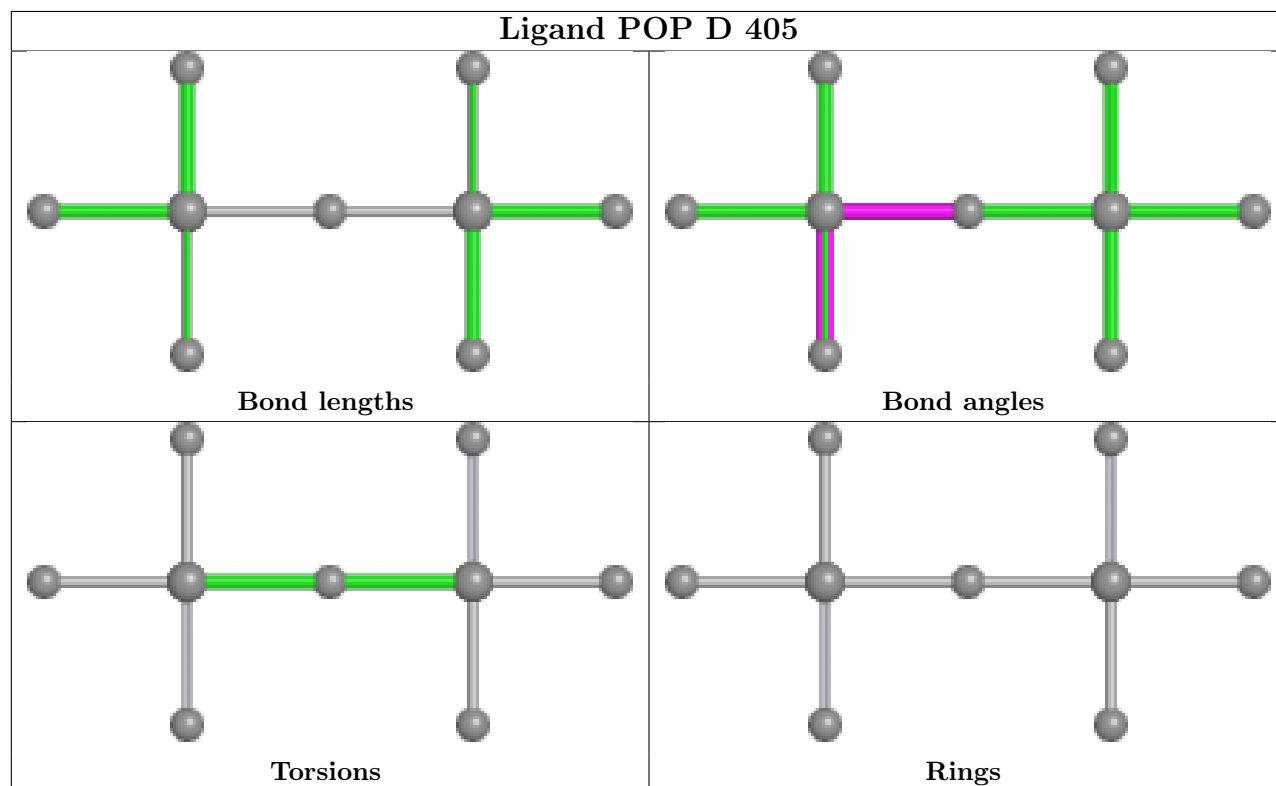
There are no ring outliers.

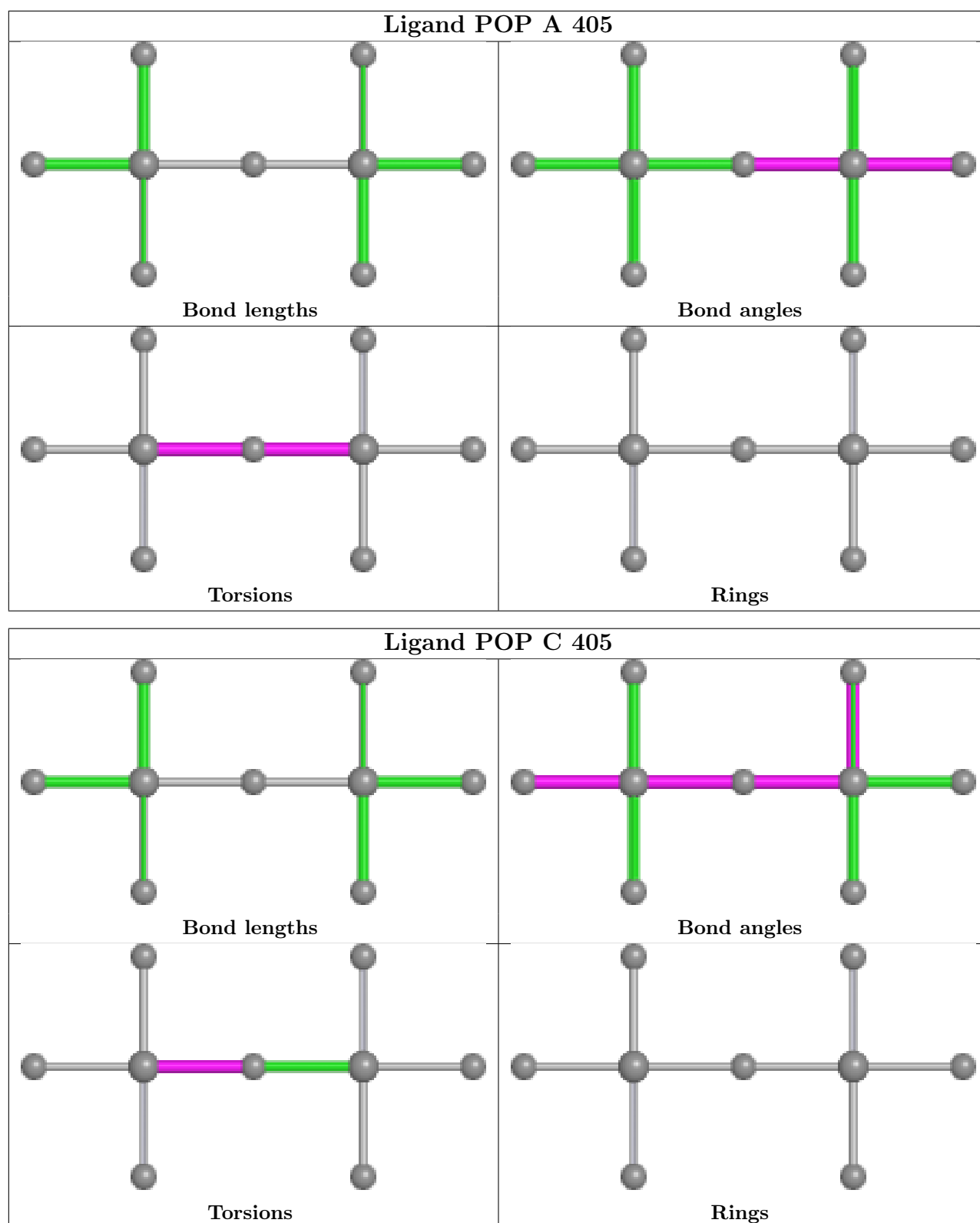
8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	PO4	1	0
5	A	410	EDO	3	0
5	B	408	EDO	2	0
5	C	406	EDO	3	0
5	C	407	EDO	1	0
3	D	404	PO4	1	0
4	A	405	POP	1	0
7	D	401	PG4	10	0

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

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	381/384 (99%)	-0.12	12 (3%) 51 55	14, 38, 70, 140	5 (1%)
1	B	372/384 (96%)	0.01	8 (2%) 62 66	19, 43, 83, 126	3 (0%)
1	C	375/384 (97%)	-0.21	1 (0%) 90 91	15, 38, 72, 103	5 (1%)
1	D	375/384 (97%)	-0.05	6 (1%) 70 74	17, 44, 80, 123	2 (0%)
All	All	1503/1536 (97%)	-0.09	27 (1%) 67 71	14, 41, 77, 140	15 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	102	ILE	6.5
1	A	106	VAL	5.4
1	A	100	PRO	5.0
1	D	109	ALA	4.8
1	A	101	ASP	4.8
1	B	311[A]	MET	4.4
1	A	338[A]	TYR	4.2
1	A	161[A]	ARG	4.0
1	B	382	LEU	3.6
1	C	383	LYS	3.3
1	A	3	HIS	3.3
1	A	105	GLY	3.3
1	B	302	ILE	3.2
1	A	109	ALA	3.1
1	D	1	ALA	3.0
1	A	103	ASN	3.0
1	B	3	HIS	2.6
1	B	100	PRO	2.4
1	D	364	HIS	2.3
1	B	238[A]	ASP	2.3
1	D	237	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	104	GLN	2.1
1	D	2	LYS	2.1
1	B	237	GLY	2.1
1	A	382	LEU	2.1
1	B	101	ASP	2.0
1	D	326	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
5	EDO	A	409	4/4	0.56	0.22	64,68,73,78	0
5	EDO	A	410	4/4	0.62	0.21	46,63,64,72	0
4	POP	A	405	9/9	0.63	0.17	49,63,82,83	9
4	POP	C	405	9/9	0.69	0.18	33,56,64,66	9
5	EDO	A	408	4/4	0.71	0.15	56,61,69,75	0
5	EDO	C	407	4/4	0.75	0.14	63,64,64,69	0
7	PG4	D	401	13/13	0.76	0.16	42,57,67,68	0
5	EDO	B	406	4/4	0.77	0.13	62,65,66,68	0
5	EDO	C	408	4/4	0.79	0.17	50,59,59,62	0
5	EDO	A	411	4/4	0.79	0.13	46,49,55,65	0
5	EDO	A	407	4/4	0.82	0.12	51,57,58,63	0
6	K	C	404	1/1	0.84	0.28	81,81,81,81	0
5	EDO	C	406	4/4	0.84	0.14	53,53,57,62	0
5	EDO	C	410	4/4	0.85	0.11	50,51,57,64	0
2	MG	C	402	1/1	0.86	0.18	55,55,55,55	0
5	EDO	A	406	4/4	0.86	0.13	49,52,55,73	0
5	EDO	B	408	4/4	0.86	0.17	48,50,53,56	0

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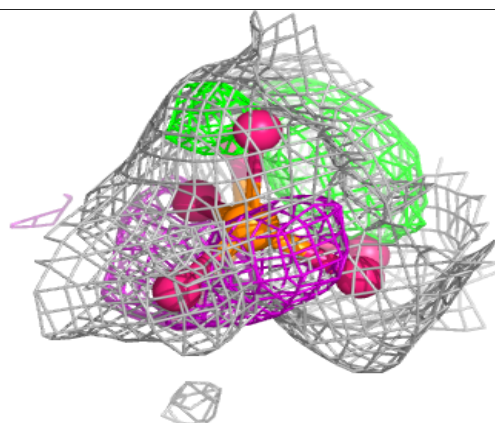
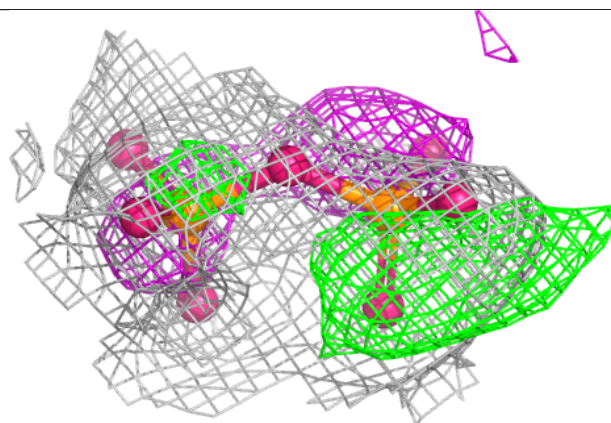
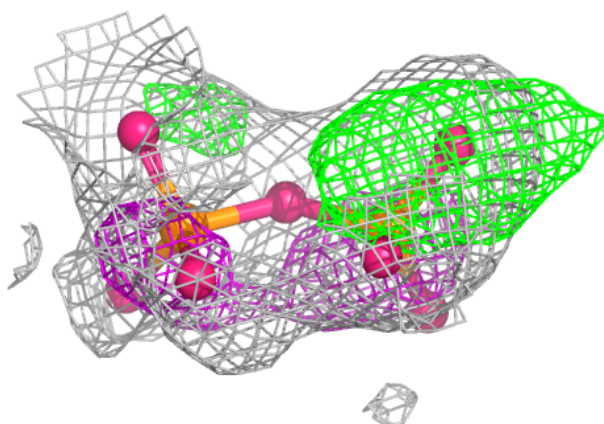
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	402	1/1	0.87	0.23	56,56,56,56	0
5	EDO	C	411	4/4	0.87	0.10	49,51,51,70	0
5	EDO	B	407	4/4	0.89	0.15	46,50,51,58	0
6	K	B	404	1/1	0.89	0.19	79,79,79,79	0
5	EDO	C	409	4/4	0.90	0.16	26,43,44,45	0
5	EDO	A	413	4/4	0.91	0.16	44,53,53,56	0
3	PO4	D	403	5/5	0.93	0.08	41,43,56,57	0
5	EDO	A	412	4/4	0.94	0.08	33,40,41,43	0
6	K	B	403	1/1	0.95	0.12	70,70,70,70	0
3	PO4	A	404	5/5	0.96	0.07	35,37,50,53	5
3	PO4	D	404	5/5	0.97	0.06	26,31,36,36	5
3	PO4	B	402	5/5	0.98	0.05	27,29,31,33	5
4	POP	B	405	9/9	0.98	0.04	30,31,35,36	0
2	MG	A	403	1/1	0.98	0.04	33,33,33,33	0
4	POP	D	405	9/9	0.98	0.04	29,33,36,37	0
2	MG	C	401	1/1	0.98	0.04	43,43,43,43	0
2	MG	B	401	1/1	0.99	0.06	27,27,27,27	0
2	MG	C	403	1/1	0.99	0.03	33,33,33,33	1
2	MG	D	402	1/1	0.99	0.04	31,31,31,31	0
2	MG	A	401	1/1	0.99	0.04	39,39,39,39	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.

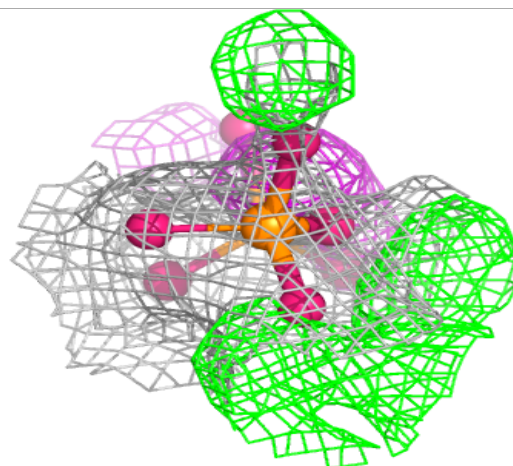
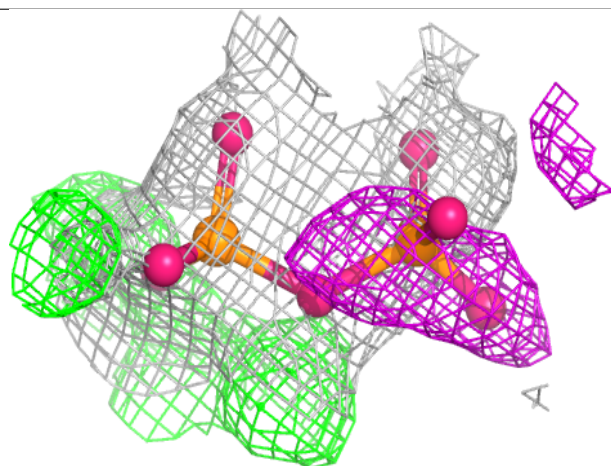
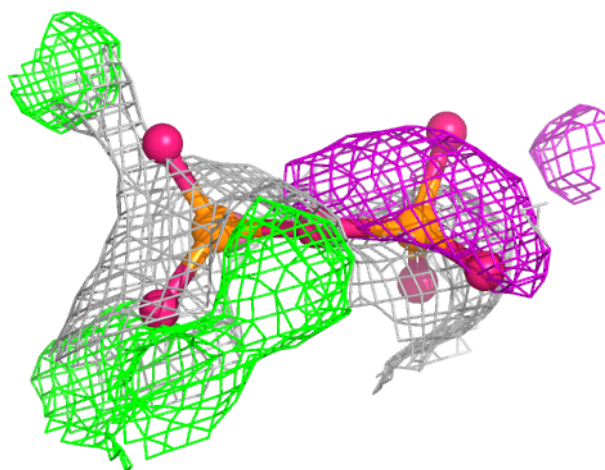
Electron density around POP A 405:

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



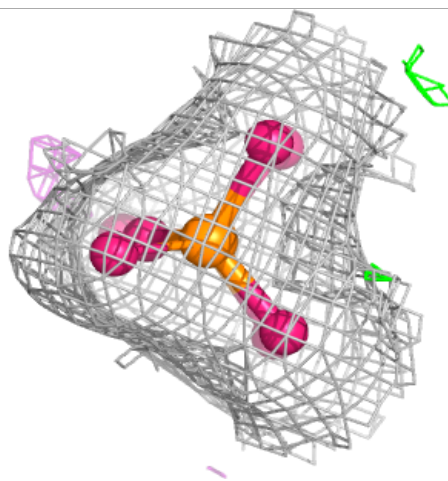
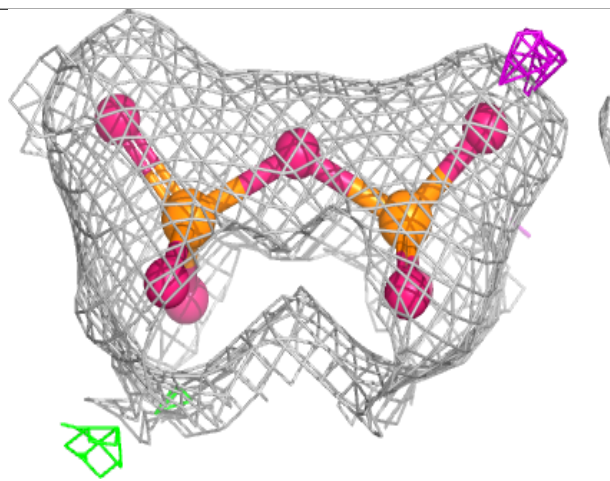
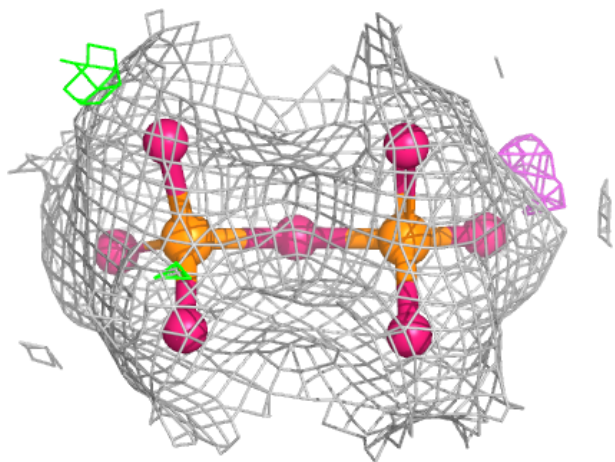
Electron density around POP C 405:

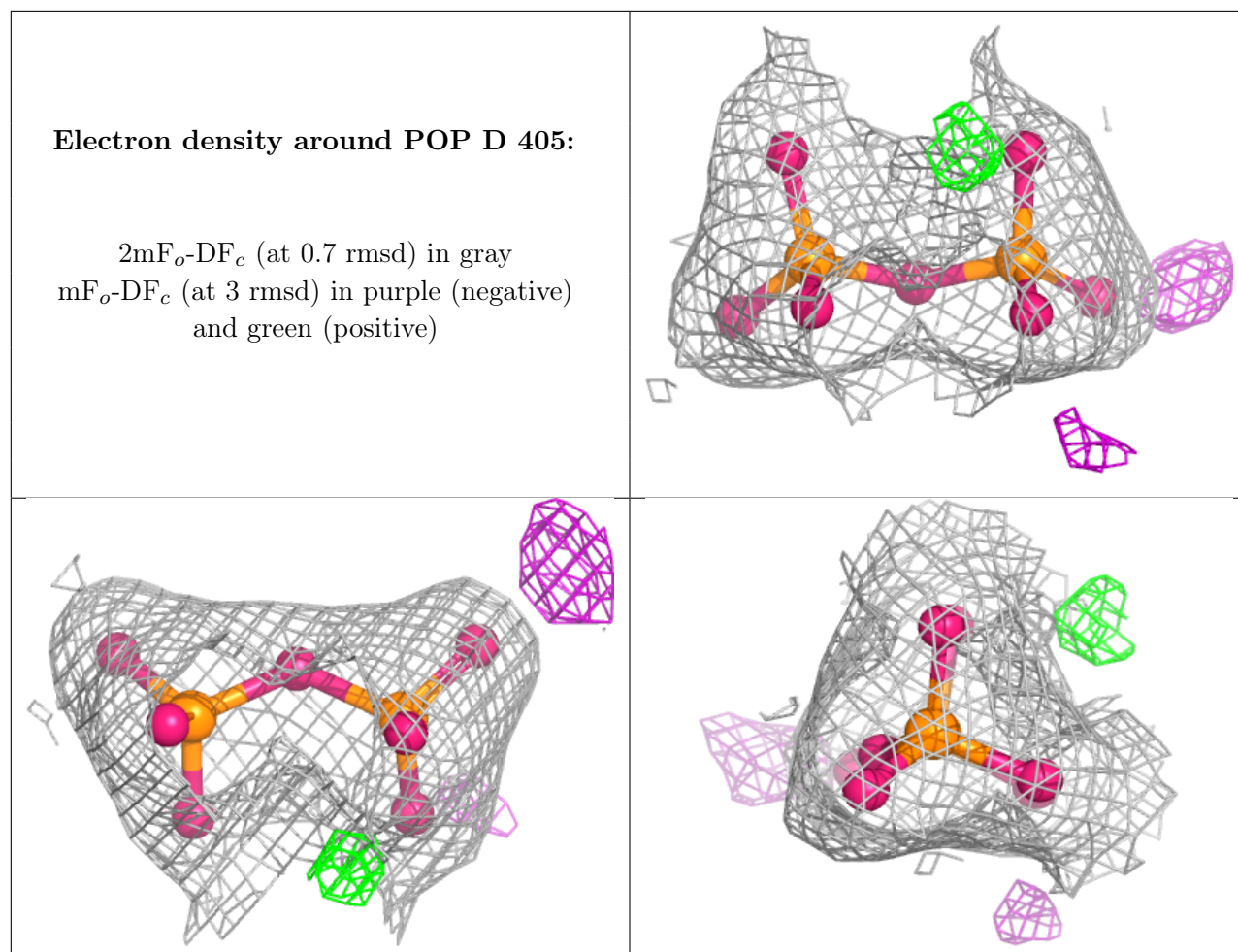
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around POP B 405:

$2mF_o-DF_c$ (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.