Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 04:49 PM JST

PDB ID	:	7F3V
Title	:	Crystal structure of YfiH with C107A mutation in complex with endogenous UDP-MurNAc
Authors	:	Lee, M.S.; Hsieh, K.Y.; Chang, C.I.
Deposited on	:	2021-06-17
Resolution	:	1.47 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

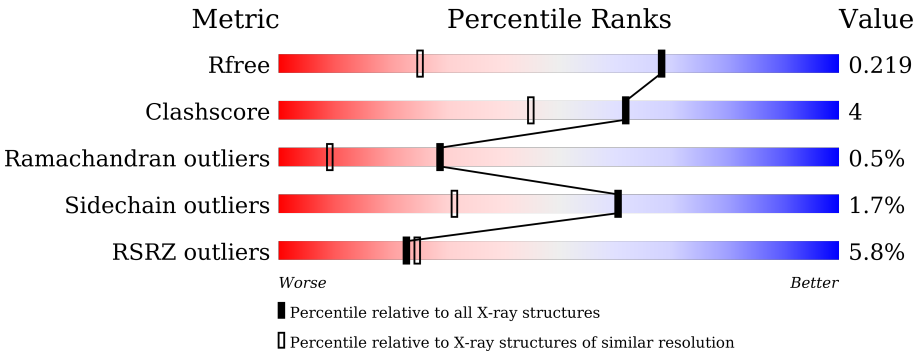
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.47 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	251	5% 88% 8% ·
1	B	251	8% 89% 6% · ·
1	C	251	4% 88% 7% 5%
1	D	251	6% 86% 7% 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8333 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 Purine nucleoside phosphorylase YfiH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	2	0
			1856	1172	330	344	10			
1	B	241	Total	C	N	O	S	0	0	0
			1836	1160	325	341	10			
1	C	238	Total	C	N	O	S	0	1	0
			1812	1143	322	336	11			
1	D	234	Total	C	N	O	S	0	1	0
			1789	1132	318	329	10			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	ALA	CYS	engineered mutation	UNP P33644
A	244	LEU	-	expression tag	UNP P33644
A	245	GLU	-	expression tag	UNP P33644
A	246	HIS	-	expression tag	UNP P33644
A	247	HIS	-	expression tag	UNP P33644
A	248	HIS	-	expression tag	UNP P33644
A	249	HIS	-	expression tag	UNP P33644
A	250	HIS	-	expression tag	UNP P33644
A	251	HIS	-	expression tag	UNP P33644
B	107	ALA	CYS	engineered mutation	UNP P33644
B	244	LEU	-	expression tag	UNP P33644
B	245	GLU	-	expression tag	UNP P33644
B	246	HIS	-	expression tag	UNP P33644
B	247	HIS	-	expression tag	UNP P33644
B	248	HIS	-	expression tag	UNP P33644
B	249	HIS	-	expression tag	UNP P33644
B	250	HIS	-	expression tag	UNP P33644
B	251	HIS	-	expression tag	UNP P33644
C	107	ALA	CYS	engineered mutation	UNP P33644
C	244	LEU	-	expression tag	UNP P33644
C	245	GLU	-	expression tag	UNP P33644

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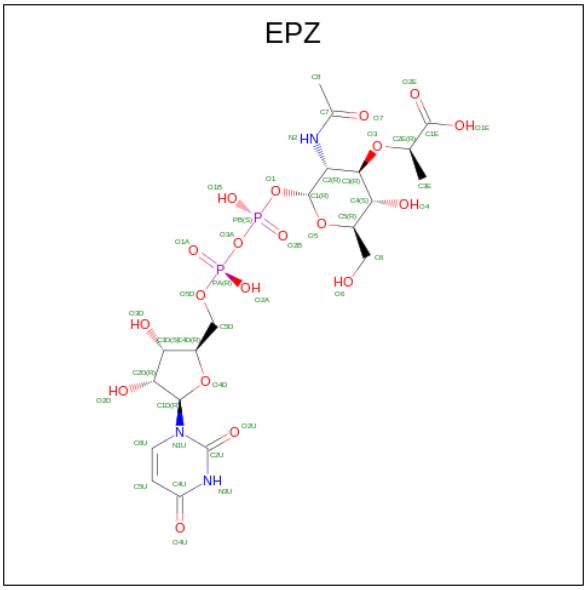
Chain	Residue	Modelled	Actual	Comment	Reference
C	246	HIS	-	expression tag	UNP P33644
C	247	HIS	-	expression tag	UNP P33644
C	248	HIS	-	expression tag	UNP P33644
C	249	HIS	-	expression tag	UNP P33644
C	250	HIS	-	expression tag	UNP P33644
C	251	HIS	-	expression tag	UNP P33644
D	107	ALA	CYS	engineered mutation	UNP P33644
D	244	LEU	-	expression tag	UNP P33644
D	245	GLU	-	expression tag	UNP P33644
D	246	HIS	-	expression tag	UNP P33644
D	247	HIS	-	expression tag	UNP P33644
D	248	HIS	-	expression tag	UNP P33644
D	249	HIS	-	expression tag	UNP P33644
D	250	HIS	-	expression tag	UNP P33644
D	251	HIS	-	expression tag	UNP P33644

- Molecule 2 is (2R)-2-{[(2R,3R,4R,5S,6R)-3-(acetylamino)-2-{[(S)-{[(R)-{[(2R,3S,4R,5R)-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methoxy}(hydroxy)phosphoryl]oxy}(hydroxy)phosphoryl]oxy}-5-hydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-4-yl]oxy}propanoic acid (three-letter code: EPZ) (formula: $C_{20}H_{31}N_3O_{19}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
2	B	1	Total	C	N	O	P	0	0
			44	20	3	19	2		

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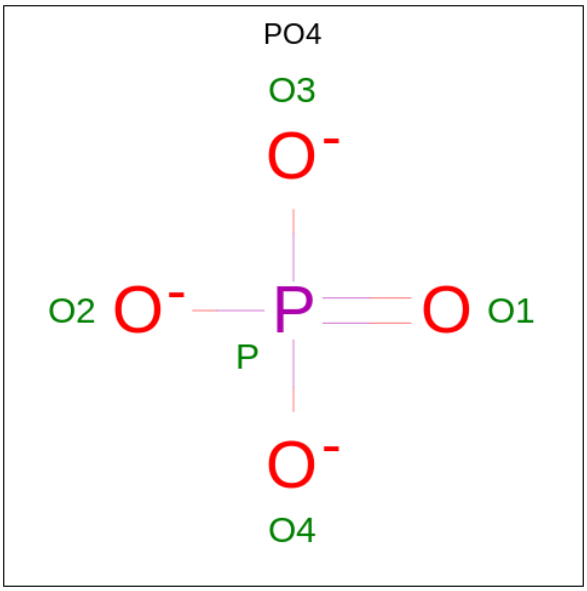
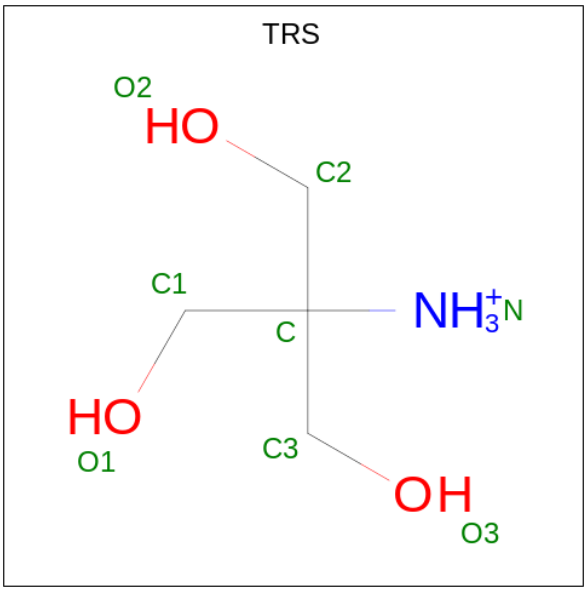
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
2	D	1	Total	C	N	O	P	0	0
			44	20	3	19	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



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			

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C N O 8 4 1 3	0	0
4	D	1	Total C N O 8 4 1 3	0	0

- Molecule 5 is water.

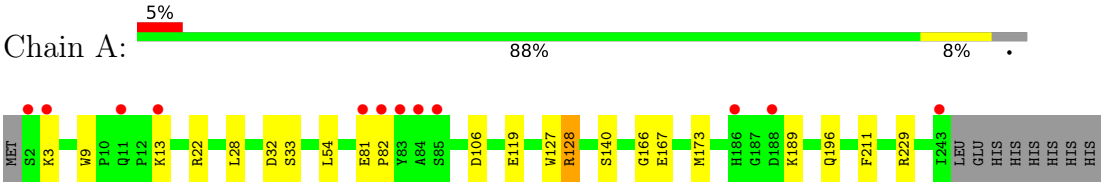
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	240	Total O 240 240	0	0
5	B	173	Total O 173 173	0	0
5	C	222	Total O 222 222	0	0
5	D	203	Total O 203 203	0	0

3 Residue-property plots (i)

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

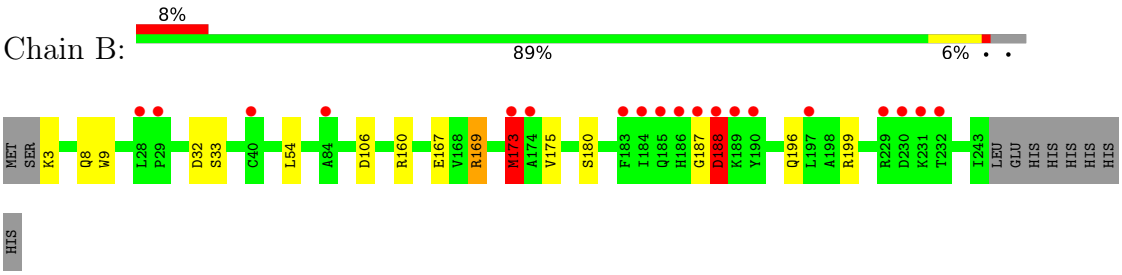
• Molecule 1: Purine nucleoside phosphorylase YfiH

Chain A:



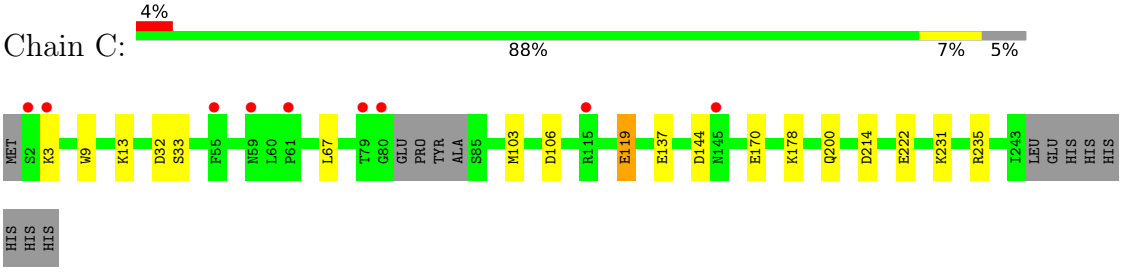
• Molecule 1: Purine nucleoside phosphorylase YfiH

Chain B:



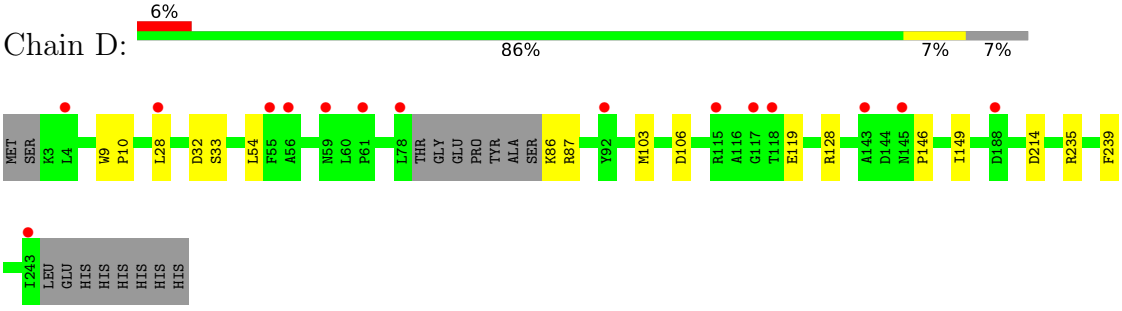
• Molecule 1: Purine nucleoside phosphorylase YfiH

Chain C:



• Molecule 1: Purine nucleoside phosphorylase YfiH

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.95Å 98.83Å 136.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.08 – 1.47 34.06 – 1.47	Depositor EDS
% Data completeness (in resolution range)	92.5 (34.08-1.47) 92.5 (34.06-1.47)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 1.47Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.185 , 0.214 0.192 , 0.219	Depositor DCC
R_{free} test set	7531 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	13.8	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8333	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, EPZ, PO4

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	0.79	0/1906	1.12	6/2592 (0.2%)
1	B	0.75	0/1881	0.93	1/2558 (0.0%)
1	C	0.81	1/1857 (0.1%)	0.96	0/2522
1	D	0.75	0/1836	0.95	1/2495 (0.0%)
All	All	0.78	1/7480 (0.0%)	0.99	8/10167 (0.1%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	170	GLU	CD-OE1	5.55	1.31	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	128[A]	ARG	NE-CZ-NH1	-15.85	112.37	120.30
1	A	128[B]	ARG	NE-CZ-NH1	-15.85	112.37	120.30
1	A	229	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	A	22	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	D	128	ARG	NE-CZ-NH1	-6.41	117.09	120.30
1	A	128[A]	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	A	128[B]	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	B	173	MET	CA-CB-CG	-5.36	104.19	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	231	LYS	Mainchain

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	1856	0	1816	17	0
1	B	1836	0	1792	25	0
1	C	1812	0	1774	17	0
1	D	1789	0	1756	13	0
2	A	44	0	28	1	0
2	B	44	0	28	0	0
2	C	44	0	28	0	0
2	D	44	0	28	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	C	8	0	12	4	0
4	D	8	0	12	5	0
5	A	240	0	0	2	2
5	B	173	0	0	5	0
5	C	222	0	0	7	2
5	D	203	0	0	4	0
All	All	8333	0	7274	65	2

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 (65) 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:173:MET:HE1	1:B:180:SER:HB3	1.31	1.12
1:A:140:SER:OG	5:A:401:HOH:O	1.76	1.01
1:B:173:MET:CE	1:B:180:SER:HB3	2.01	0.91
1:C:103:MET:HE2	5:C:407:HOH:O	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:MET:SD	1:B:173:MET:CE	2.66	0.83
4:D:302:TRS:H31	5:D:448:HOH:O	1.78	0.82
1:C:178:LYS:NZ	5:C:402:HOH:O	2.11	0.81
1:A:173:MET:SD	1:B:173:MET:HE1	2.20	0.80
1:B:8:GLN:HG2	5:B:455:HOH:O	1.81	0.80
1:C:235:ARG:HH21	4:C:302:TRS:H11	1.45	0.79
1:C:235:ARG:HH21	4:C:302:TRS:C1	1.99	0.76
4:D:302:TRS:H32	5:D:497:HOH:O	1.84	0.75
1:B:169:ARG:NE	1:B:173:MET:SD	2.59	0.75
1:C:3:LYS:O	5:C:403:HOH:O	2.12	0.68
1:A:13:LYS:NZ	5:A:402:HOH:O	2.27	0.66
4:C:302:TRS:H22	5:C:515:HOH:O	1.97	0.63
1:A:81:GLU:HG2	1:A:82:PRO:HA	1.79	0.63
1:A:173:MET:SD	1:B:173:MET:HE2	2.37	0.63
1:B:8:GLN:CG	5:B:455:HOH:O	2.44	0.61
1:D:86:LYS:N	5:D:403:HOH:O	2.35	0.60
1:B:160:ARG:HG2	1:D:10:PRO:HA	1.82	0.59
1:A:211:PHE:CE1	1:C:222:GLU:HG3	2.38	0.58
1:C:222:GLU:H	1:C:222:GLU:CD	2.05	0.58
1:B:169:ARG:CZ	1:B:173:MET:SD	2.93	0.56
1:B:8:GLN:HG2	1:B:8:GLN:O	2.06	0.56
4:C:302:TRS:H31	5:C:489:HOH:O	2.07	0.55
1:D:54:LEU:HD21	1:D:239:PHE:CE1	2.43	0.54
1:A:127:TRP:CH2	1:A:128[A]:ARG:HG2	2.42	0.54
1:A:127:TRP:CZ3	1:A:128[A]:ARG:HG2	2.44	0.53
1:D:54:LEU:CD2	1:D:239:PHE:CZ	2.92	0.53
1:D:235:ARG:HH21	4:D:302:TRS:C1	2.21	0.52
1:D:54:LEU:HD21	1:D:239:PHE:CZ	2.45	0.52
1:A:196:GLN:HG3	1:C:214:ASP:HB3	1.91	0.51
1:B:3:LYS:O	5:B:402:HOH:O	2.18	0.50
1:D:103:MET:HG3	1:D:235:ARG:HB3	1.94	0.50
1:B:187:GLY:O	1:B:188:ASP:HB2	2.12	0.50
1:D:146:PRO:HA	1:D:149:ILE:HD12	1.95	0.49
1:B:169:ARG:NH1	1:B:173:MET:CE	2.77	0.48
1:C:137:GLU:HG2	5:C:547:HOH:O	2.14	0.47
1:B:199:ARG:NE	5:B:401:HOH:O	2.10	0.47
1:C:119:GLU:OE2	1:C:144:ASP:HB2	2.15	0.47
1:A:54:LEU:C	1:A:54:LEU:HD13	2.34	0.47
1:C:67:LEU:N	5:C:407:HOH:O	2.40	0.47
1:B:175:VAL:CG1	1:C:178:LYS:HD2	2.45	0.47
1:B:175:VAL:HG11	1:C:178:LYS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ARG:NH1	1:B:173:MET:HE2	2.30	0.47
1:A:211:PHE:HE1	1:C:222:GLU:HG3	1.80	0.46
1:B:175:VAL:HA	1:C:200:GLN:HG2	1.96	0.46
1:B:169:ARG:NH1	1:B:173:MET:SD	2.87	0.46
1:C:32:ASP:HA	1:C:33:SER:HA	1.72	0.46
1:A:211:PHE:CZ	1:C:222:GLU:HG3	2.51	0.46
1:A:189:LYS:HD3	2:A:301:EPZ:O2U	2.15	0.45
1:B:3:LYS:N	5:B:409:HOH:O	2.49	0.45
1:A:32:ASP:HA	1:A:33:SER:HA	1.76	0.45
1:B:54:LEU:O	1:B:54:LEU:HG	2.12	0.45
1:B:173:MET:CE	1:B:180:SER:CB	2.85	0.45
1:B:32:ASP:HA	1:B:33:SER:HA	1.72	0.43
1:D:86:LYS:HG2	1:D:87:ARG:O	2.19	0.43
1:D:32:ASP:HA	1:D:33:SER:HA	1.73	0.42
1:A:166:GLY:O	1:A:167:GLU:C	2.57	0.42
1:B:196:GLN:HG3	1:D:214:ASP:HB3	2.02	0.42
1:D:235:ARG:HH21	4:D:302:TRS:H11	1.83	0.41
4:D:302:TRS:O2	5:D:401:HOH:O	1.66	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:467:HOH:O	5:C:577:HOH:O[3_544]	2.11	0.09
5:A:550:HOH:O	5:C:577:HOH:O[3_544]	2.18	0.02

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	242/251 (96%)	233 (96%)	8 (3%)	1 (0%)	34 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	239/251 (95%)	227 (95%)	10 (4%)	2 (1%)	19 4
1	C	235/251 (94%)	229 (97%)	5 (2%)	1 (0%)	34 13
1	D	231/251 (92%)	222 (96%)	8 (4%)	1 (0%)	34 13
All	All	947/1004 (94%)	911 (96%)	31 (3%)	5 (0%)	29 9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	ASP
1	B	106	ASP
1	C	106	ASP
1	D	106	ASP
1	B	188	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	191/198 (96%)	188 (98%)	3 (2%)	62 34
1	B	188/198 (95%)	183 (97%)	5 (3%)	44 14
1	C	187/198 (94%)	184 (98%)	3 (2%)	62 34
1	D	184/198 (93%)	182 (99%)	2 (1%)	73 50
All	All	750/792 (95%)	737 (98%)	13 (2%)	60 31

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	9	TRP
1	A	119	GLU
1	B	9	TRP
1	B	167	GLU
1	B	169	ARG

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Mol	Chain	Res	Type
1	B	173	MET
1	B	188	ASP
1	C	9	TRP
1	C	13	LYS
1	C	119	GLU
1	D	9	TRP
1	D	119	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	C	59	ASN
1	C	209	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)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PO4	A	302	-	4,4,4	0.75	0	6,6,6	0.87	0
2	EPZ	B	301	-	43,46,46	0.67	1 (2%)	60,69,69	0.85	2 (3%)
2	EPZ	C	301	-	43,46,46	0.64	0	60,69,69	0.82	1 (1%)
2	EPZ	A	301	-	43,46,46	0.71	0	60,69,69	0.83	0
4	TRS	C	302	-	7,7,7	0.56	0	9,9,9	1.04	0
2	EPZ	D	301	-	43,46,46	0.57	0	60,69,69	0.89	1 (1%)
4	TRS	D	302	-	7,7,7	0.41	0	9,9,9	1.26	1 (11%)
3	PO4	B	302	-	4,4,4	1.27	1 (25%)	6,6,6	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EPZ	B	301	-	-	4/34/71/71	0/3/3/3
2	EPZ	C	301	-	-	4/34/71/71	0/3/3/3
2	EPZ	A	301	-	-	2/34/71/71	0/3/3/3
2	EPZ	D	301	-	-	4/34/71/71	0/3/3/3
4	TRS	D	302	-	-	6/9/9/9	-
4	TRS	C	302	-	-	0/9/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	EPZ	O2E-C1E	2.44	1.29	1.22
3	B	302	PO4	P-O1	2.16	1.55	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	302	TRS	O3-C3-C	2.74	119.68	111.00
2	C	301	EPZ	O2U-C2U-N3U	2.31	125.81	121.50
2	D	301	EPZ	O3A-PB-O1	2.18	106.87	102.48
2	B	301	EPZ	O1B-PB-O1	2.13	115.20	106.78
2	B	301	EPZ	O1E-C1E-O2E	2.03	128.70	124.09

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	EPZ	C5D-O5D-PA-O1A
2	C	301	EPZ	C5D-O5D-PA-O1A
2	D	301	EPZ	C5D-O5D-PA-O1A
4	D	302	TRS	C1-C-C2-O2
4	D	302	TRS	C3-C-C2-O2
4	D	302	TRS	N-C-C3-O3
4	D	302	TRS	C2-C-C3-O3
2	A	301	EPZ	C5D-O5D-PA-O3A
2	B	301	EPZ	C5D-O5D-PA-O3A
2	C	301	EPZ	C5D-O5D-PA-O3A
2	D	301	EPZ	C5D-O5D-PA-O3A
4	D	302	TRS	N-C-C2-O2
2	B	301	EPZ	C5D-O5D-PA-O2A
2	C	301	EPZ	C5D-O5D-PA-O2A
2	D	301	EPZ	C5D-O5D-PA-O2A
2	B	301	EPZ	C1E-C2E-O3-C3
2	C	301	EPZ	C1E-C2E-O3-C3
4	D	302	TRS	C1-C-C3-O3
2	A	301	EPZ	C3E-C2E-O3-C3
2	D	301	EPZ	C3E-C2E-O3-C3

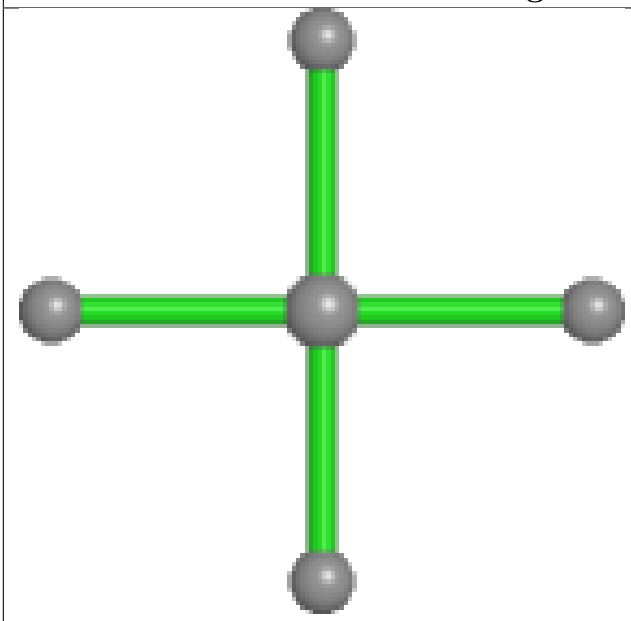
There are no ring outliers.

3 monomers are involved in 10 short contacts:

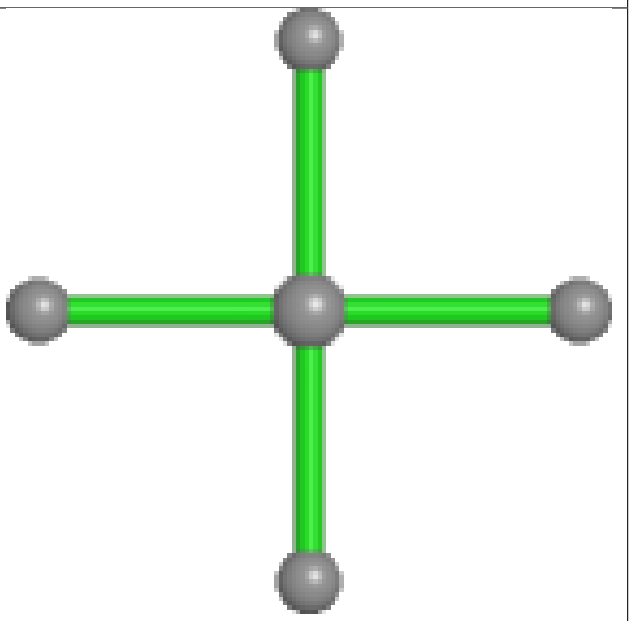
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	EPZ	1	0
4	C	302	TRS	4	0
4	D	302	TRS	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

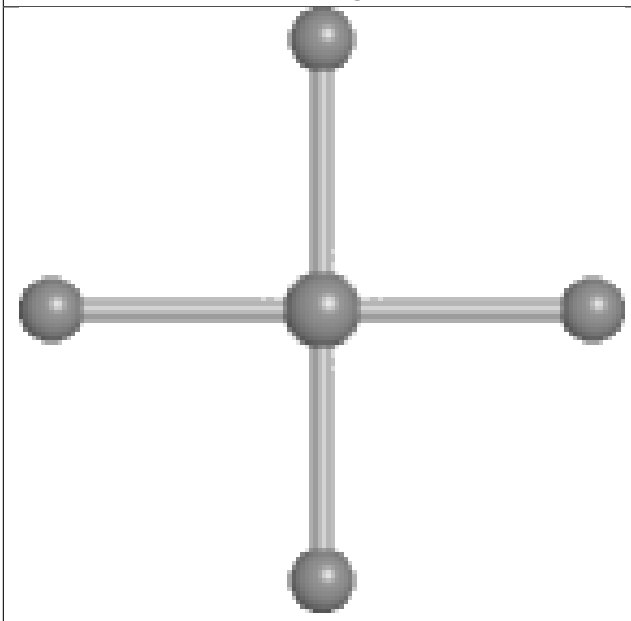
Ligand PO4 A 302



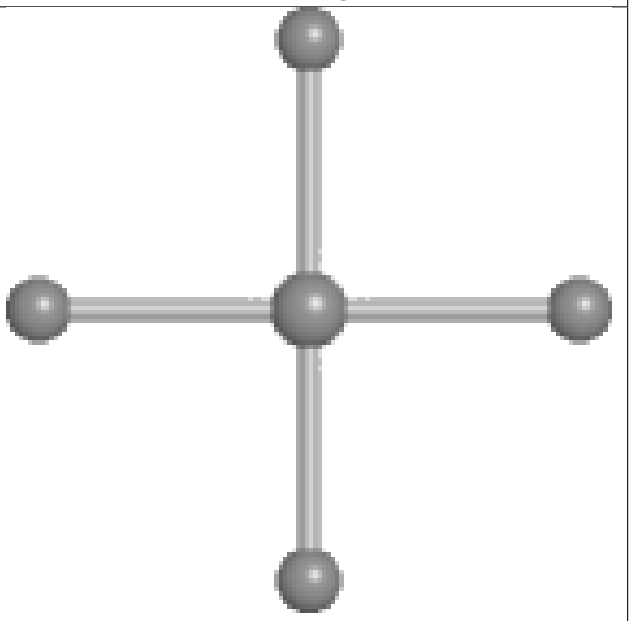
Bond lengths



Bond angles

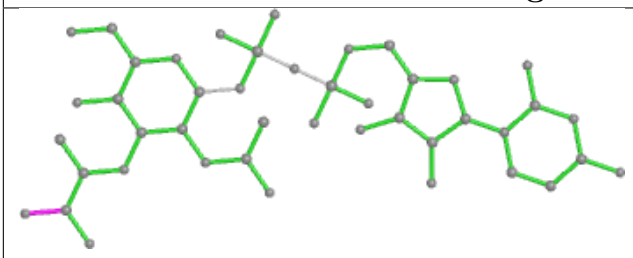


Torsions

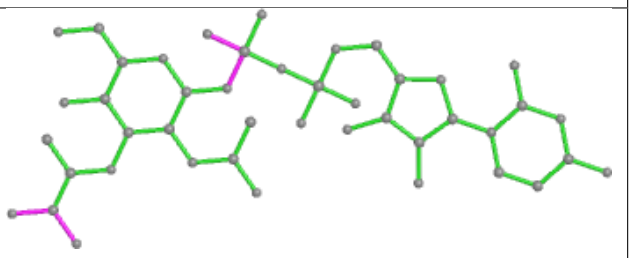


Rings

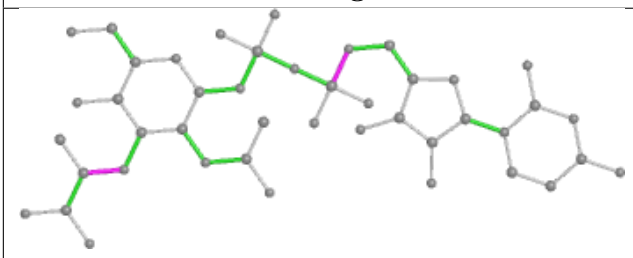
Ligand EPZ B 301



Bond lengths



Bond angles



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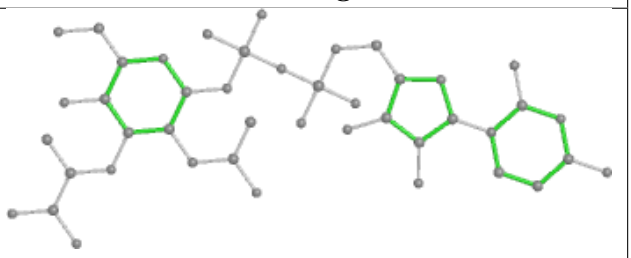
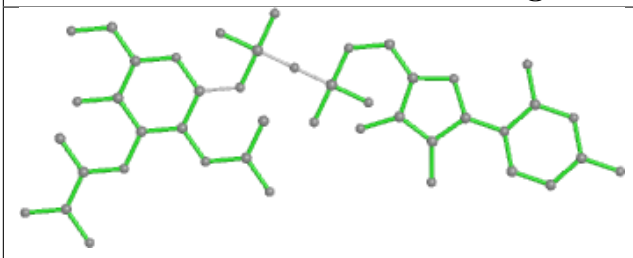
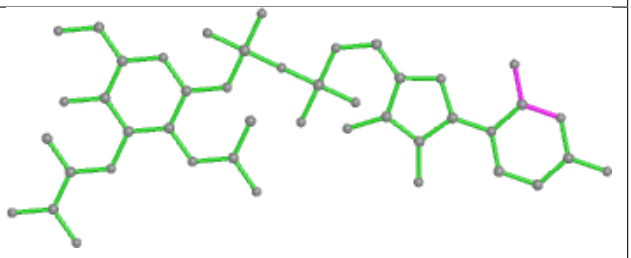


Rings

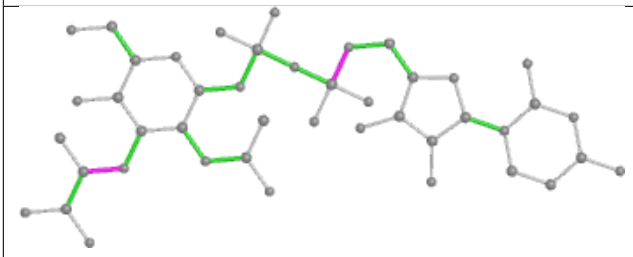
Ligand EPZ C 301



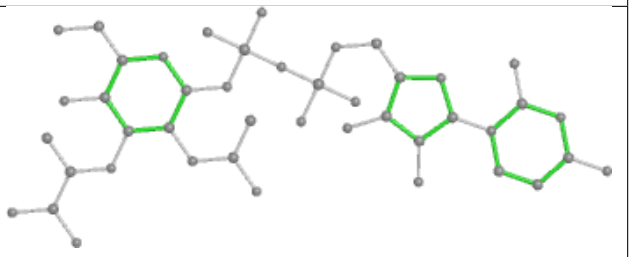
Bond lengths



Bond angles

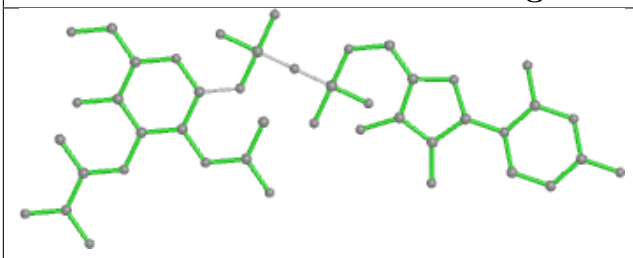


Torsions

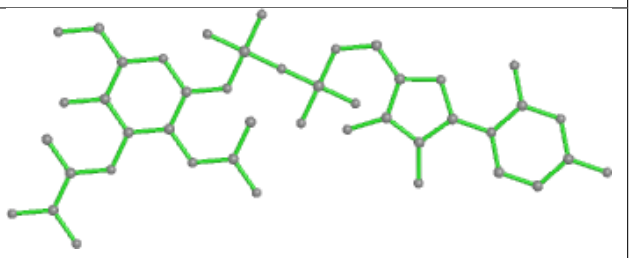


Rings

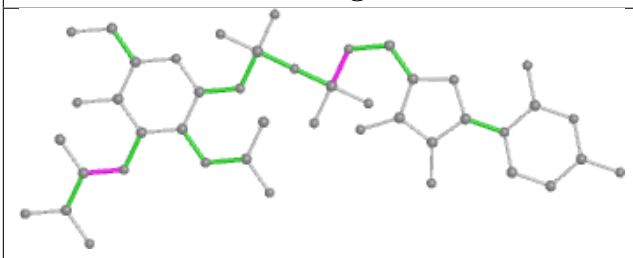
Ligand EPZ A 301



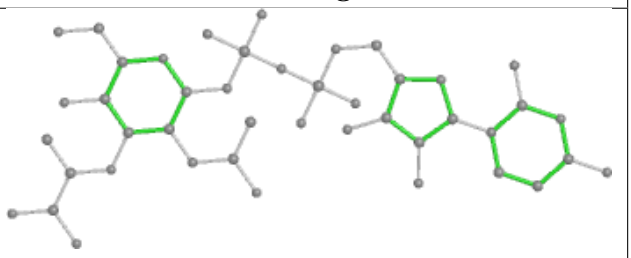
Bond lengths



Bond angles

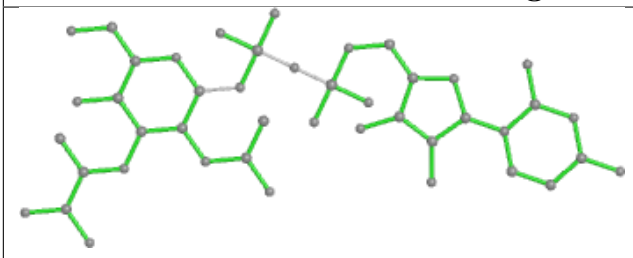


Torsions

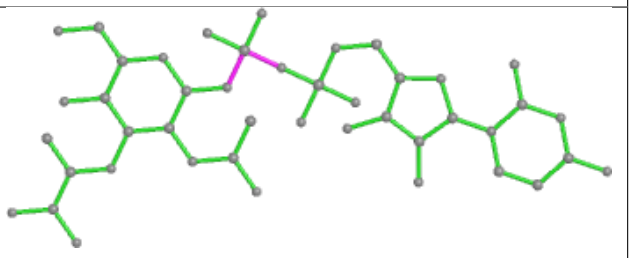


Rings

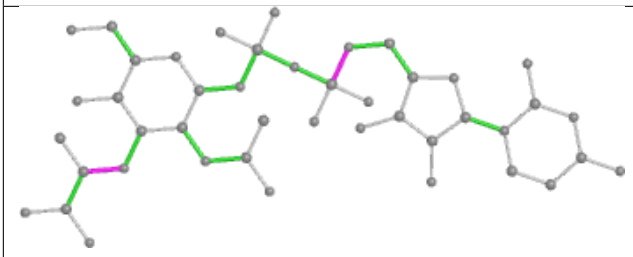
Ligand EPZ D 301



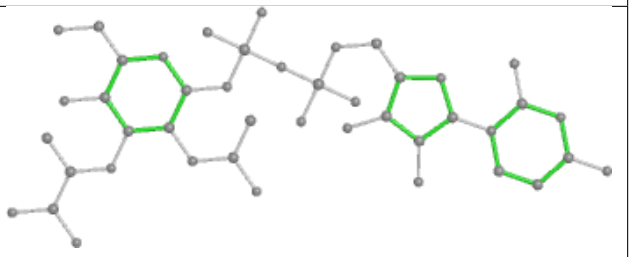
Bond lengths



Bond angles

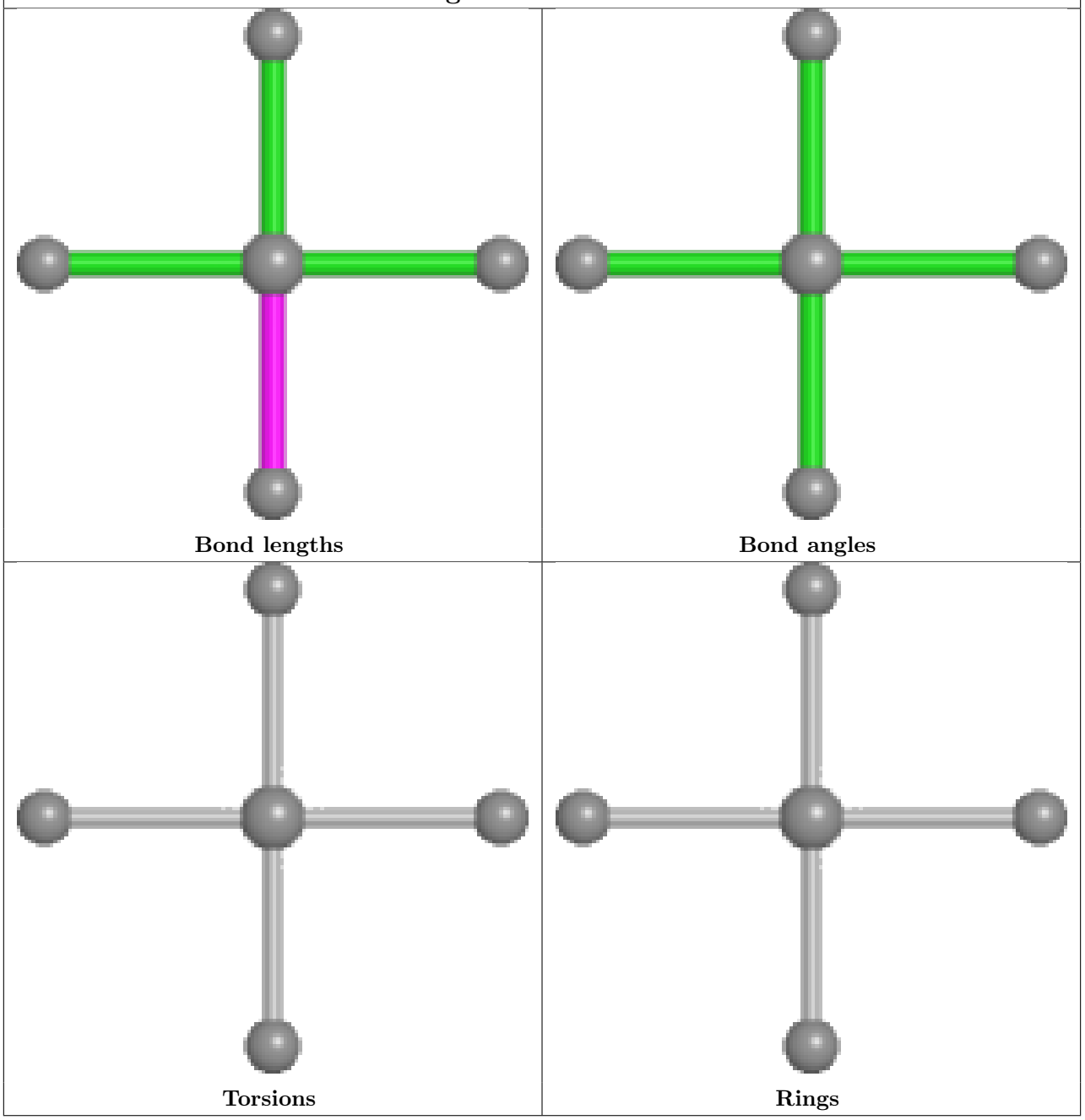


Torsions



Rings

Ligand PO4 B 302



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	242/251 (96%)	0.35	12 (4%)	28	31	7, 13, 28, 61	0
1	B	241/251 (96%)	0.45	19 (7%)	12	13	8, 16, 33, 52	0
1	C	238/251 (94%)	0.28	9 (3%)	40	44	6, 13, 26, 52	0
1	D	234/251 (93%)	0.44	15 (6%)	19	20	9, 17, 32, 48	0
All	All	955/1004 (95%)	0.38	55 (5%)	23	25	6, 14, 31, 61	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	188	ASP	5.4
1	C	2	SER	4.3
1	A	2	SER	4.3
1	A	188	ASP	4.1
1	A	83	TYR	4.0
1	D	145	ASN	3.9
1	C	79	THR	3.9
1	A	84	ALA	3.8
1	B	187	GLY	3.8
1	C	145	ASN	3.7
1	D	115	ARG	3.7
1	D	59	ASN	3.7
1	A	3	LYS	3.6
1	B	185	GLN	3.3
1	D	117	GLY	3.1
1	A	81	GLU	3.0
1	D	55	PHE	2.9
1	B	40	CYS	2.9
1	A	13	LYS	2.8
1	A	243	ILE	2.8
1	B	84	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	232	THR	2.7
1	C	115	ARG	2.7
1	D	56	ALA	2.7
1	B	190	TYR	2.7
1	A	85	SER	2.7
1	C	80	GLY	2.7
1	C	55	PHE	2.6
1	B	189	LYS	2.6
1	D	4	LEU	2.6
1	D	143	ALA	2.5
1	B	184	ILE	2.4
1	D	61	PRO	2.4
1	A	186	HIS	2.4
1	C	3	LYS	2.4
1	B	231	LYS	2.3
1	B	230	ASP	2.3
1	D	243	ILE	2.3
1	B	197	LEU	2.3
1	D	188	ASP	2.3
1	B	186	HIS	2.2
1	D	28[A]	LEU	2.2
1	D	78	LEU	2.2
1	D	92	TYR	2.2
1	D	118	THR	2.1
1	B	174	ALA	2.1
1	C	61	PRO	2.1
1	A	82	PRO	2.1
1	B	173	MET	2.1
1	C	59	ASN	2.1
1	B	183	PHE	2.1
1	B	28	LEU	2.1
1	B	29	PRO	2.0
1	B	229	ARG	2.0
1	A	11	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

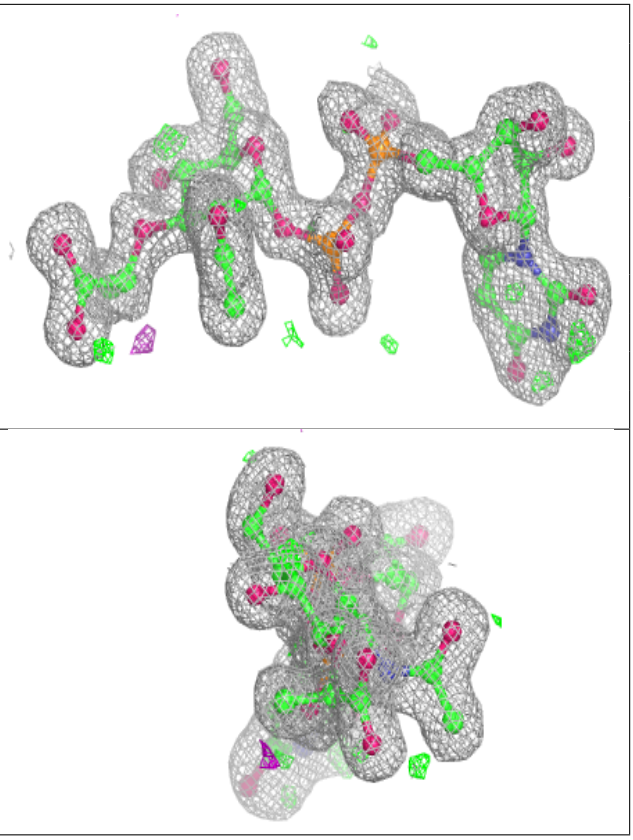
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

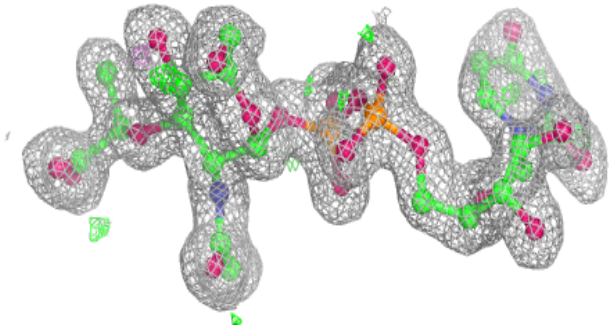
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	TRS	C	302	8/8	0.76	0.23	16,25,28,35	0
4	TRS	D	302	8/8	0.77	0.23	23,29,32,36	0
2	EPZ	B	301	44/44	0.94	0.10	12,16,28,36	0
3	PO4	B	302	5/5	0.95	0.19	19,25,30,32	0
2	EPZ	D	301	44/44	0.97	0.07	8,10,14,19	0
2	EPZ	A	301	44/44	0.97	0.08	7,10,18,26	0
3	PO4	A	302	5/5	0.98	0.11	16,17,23,26	0
2	EPZ	C	301	44/44	0.98	0.07	7,8,16,23	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 EPZ B 301:

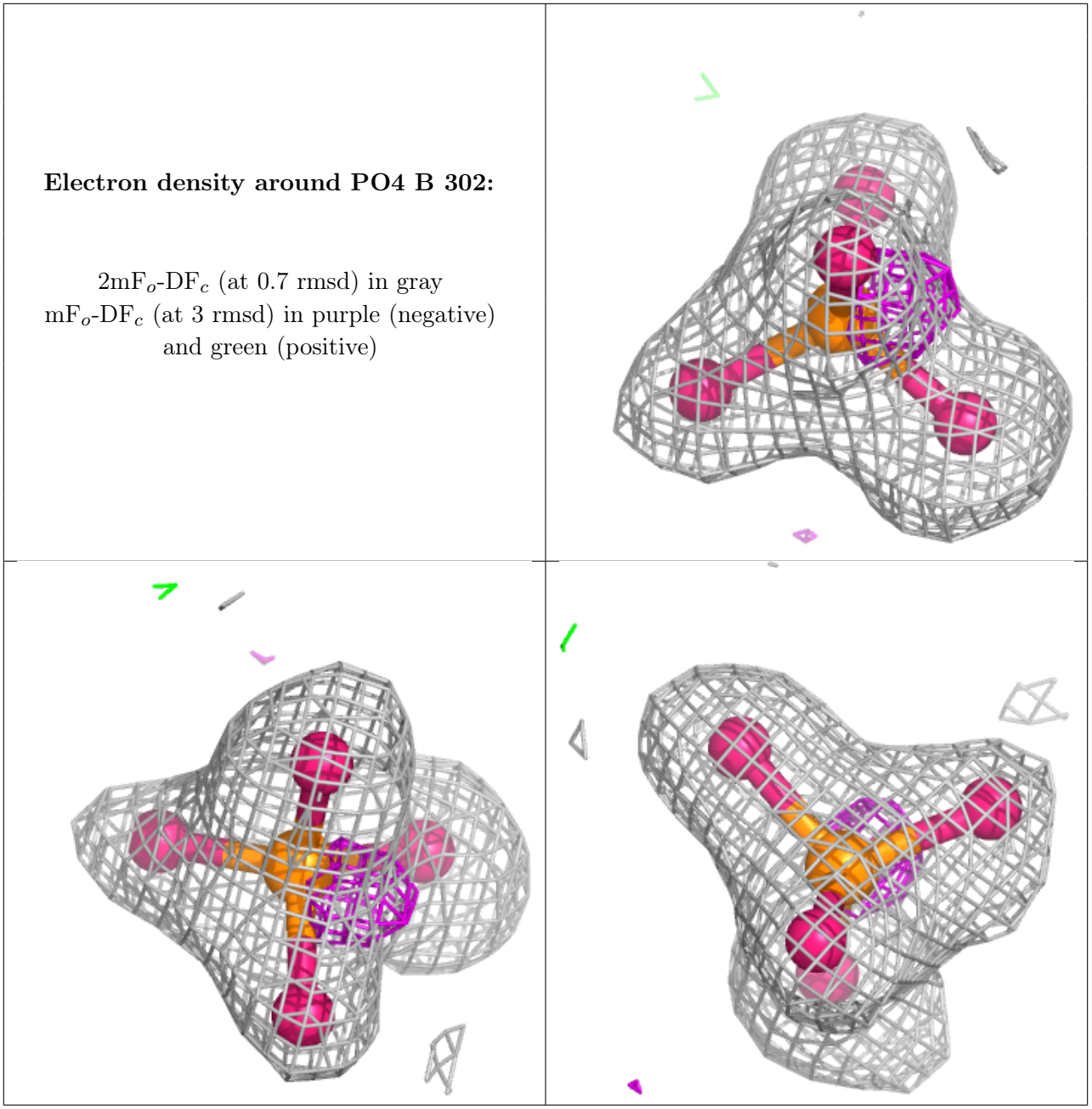
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





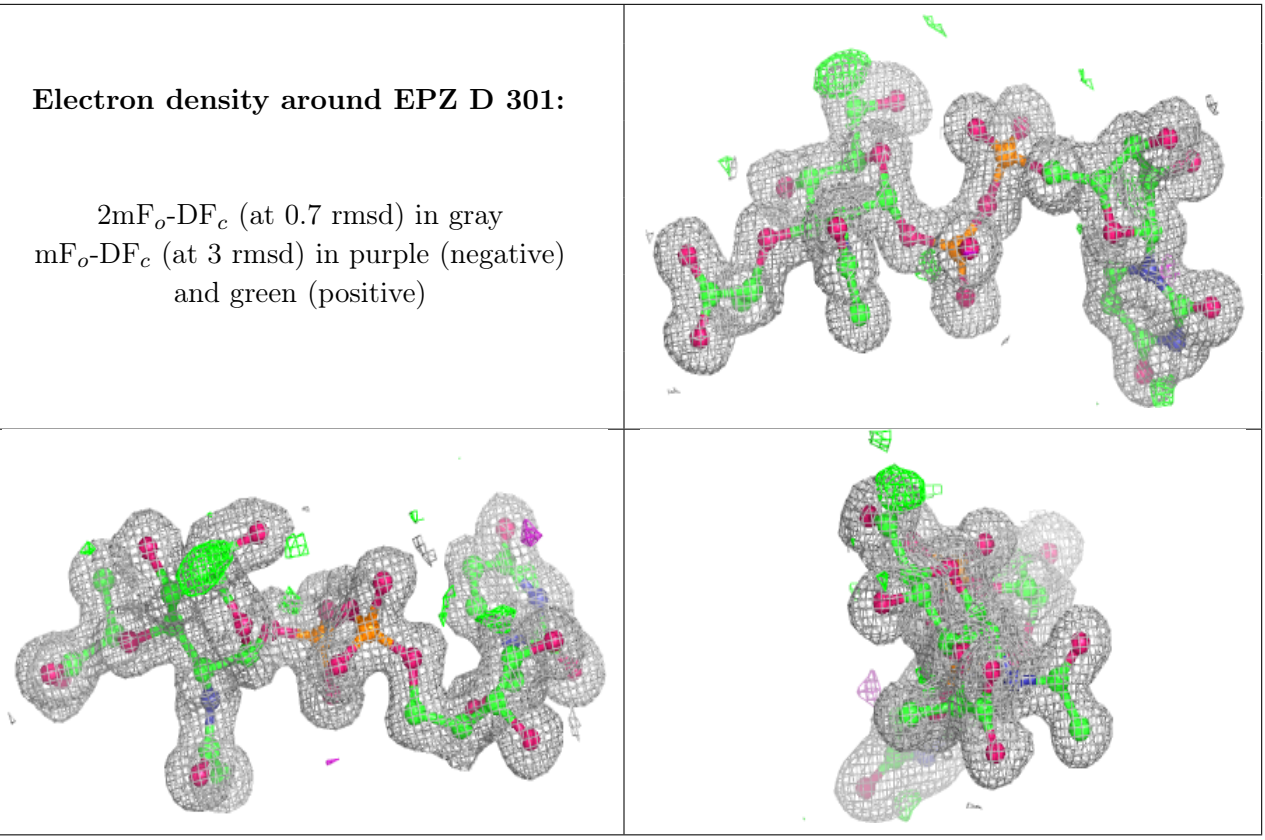
Electron density around PO4 B 302:

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



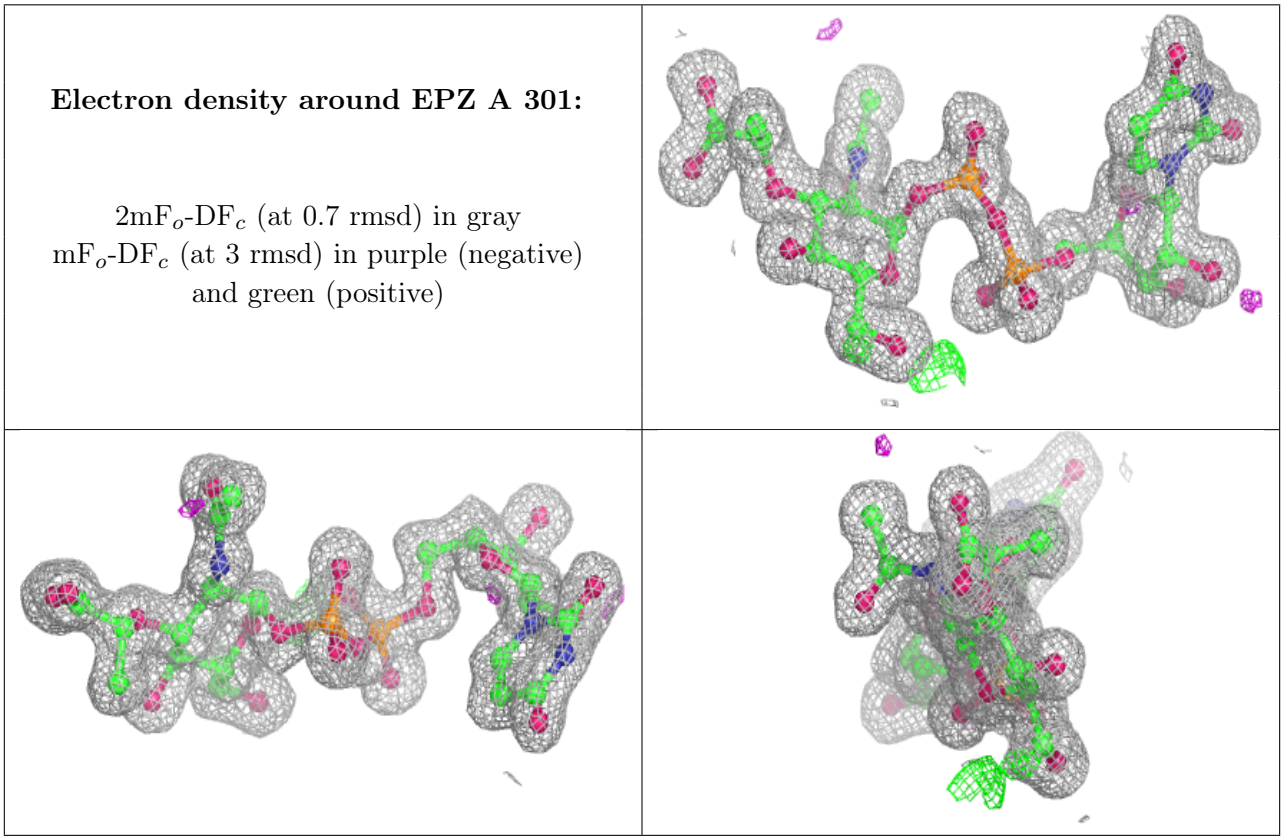
Electron density around EPZ D 301:

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



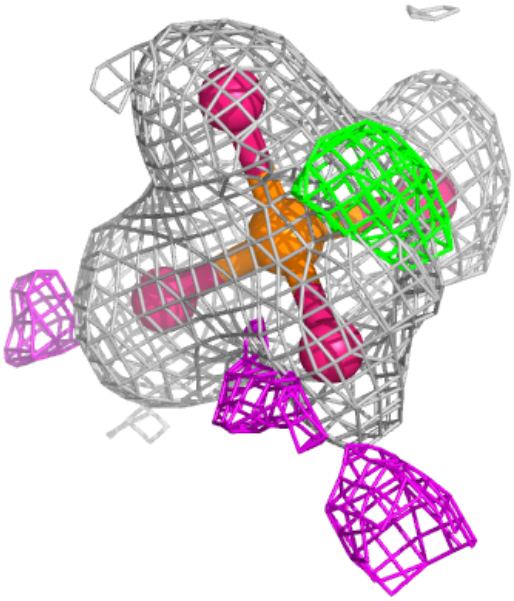
Electron density around EPZ A 301:

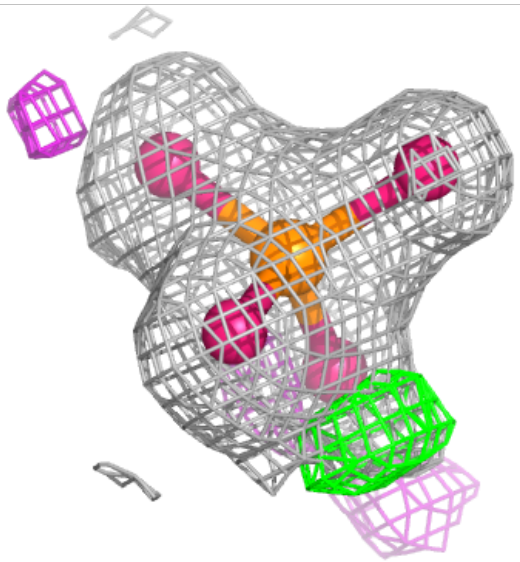
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

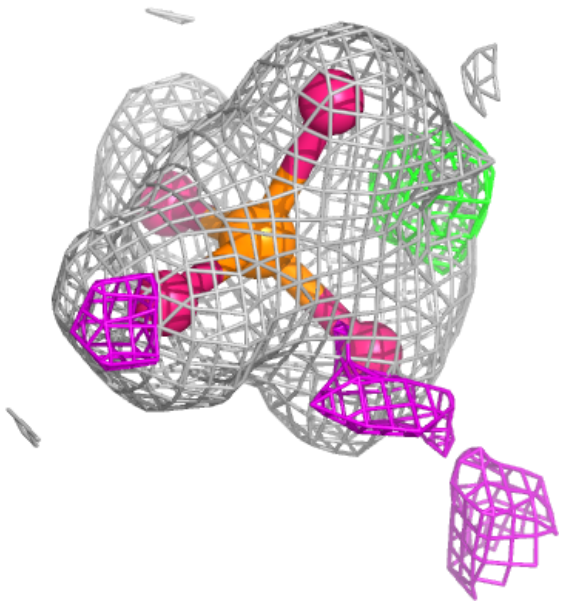


Electron density around PO4 A 302:

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

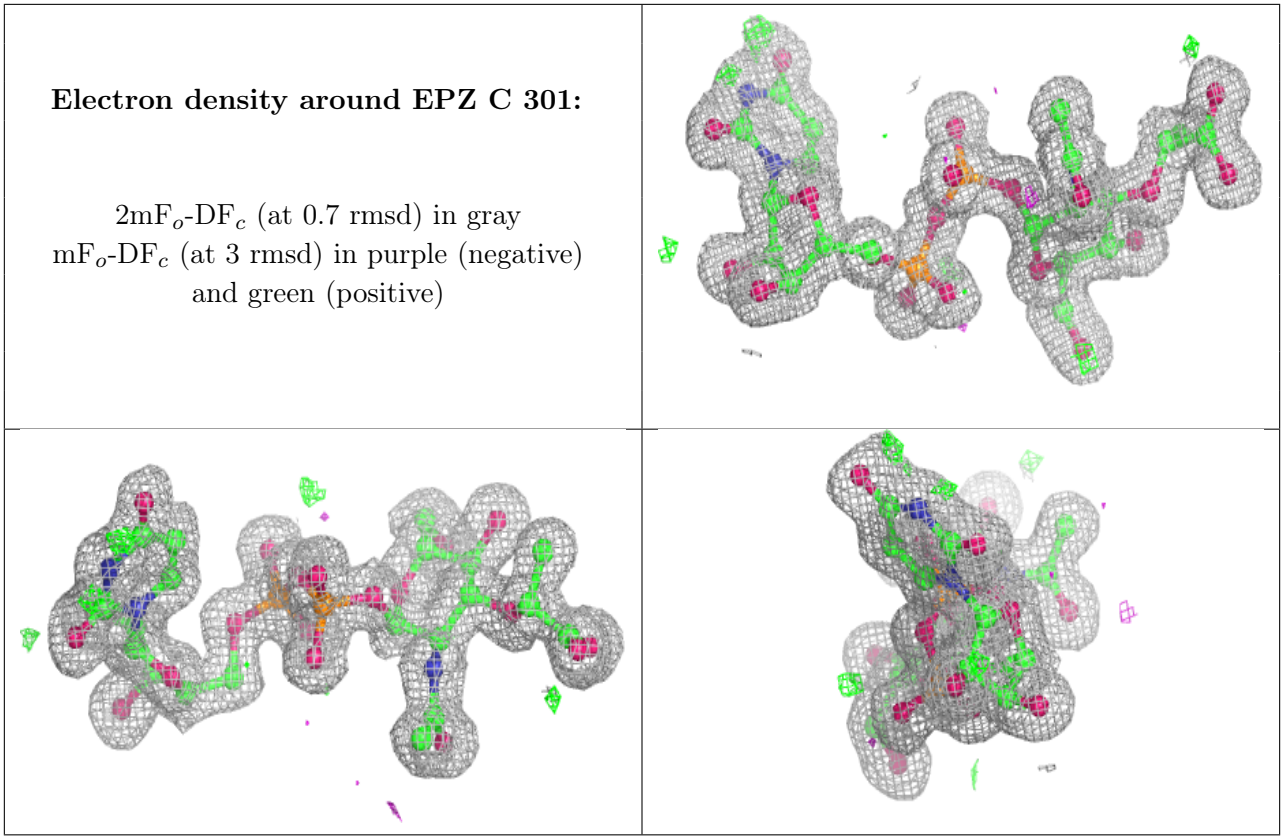






Electron density around EPZ C 301:

$2mF_o$-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.