Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 11:11 AM EDT

PDB ID	:	6O82
Title	:	S. pombe ubiquitin E1 complex with a ubiquitin-AMP mimic
Authors	:	Olsen, S.K.; Lima, C.D.
Deposited on	:	2019-03-08
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

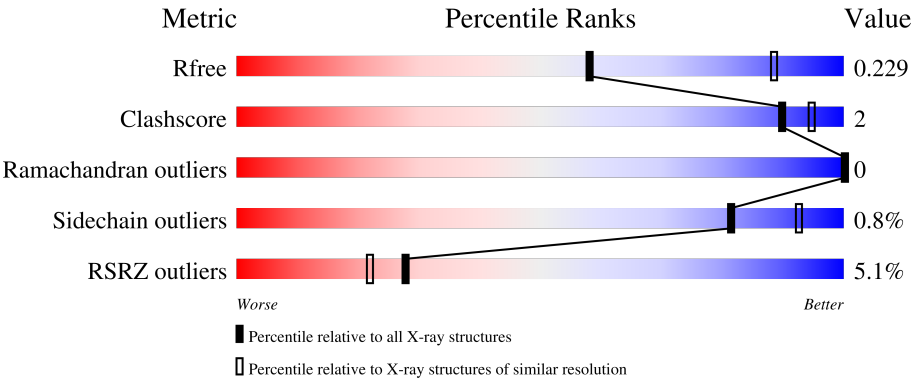
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	1001	2% 94%
1	C	1001	9% 91% 6%
2	B	76	100%
2	D	76	3% 89% 11%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 17008 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 Ubiquitin-activating enzyme E1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	986	Total 7745	C 4953	N 1266	O 1487	S 39	0	0	0
1	C	975	Total 7664	C 4896	N 1255	O 1474	S 39	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	SER	-	expression tag	UNP O94609
C	12	SER	-	expression tag	UNP O94609

- Molecule 2 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total 595	C 372	N 102	O 119	S 2	0	0	0
2	D	76	Total 595	C 372	N 102	O 119	S 2	0	0	0

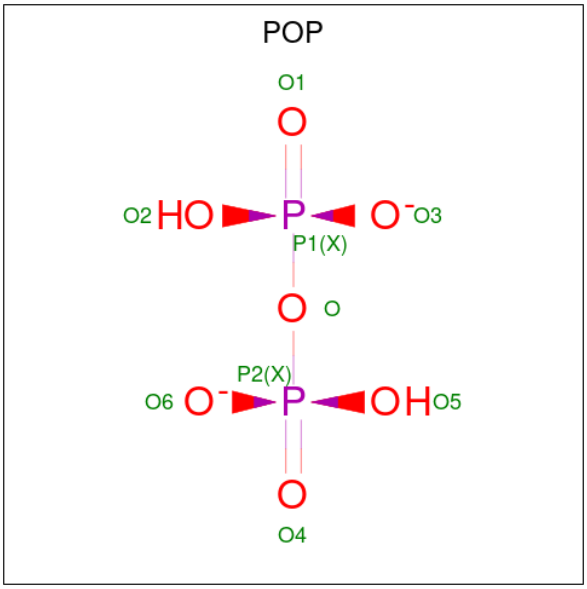
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	74	CYS	ARG	engineered mutation	UNP P0CH07
D	74	CYS	ARG	engineered mutation	UNP P0CH07

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

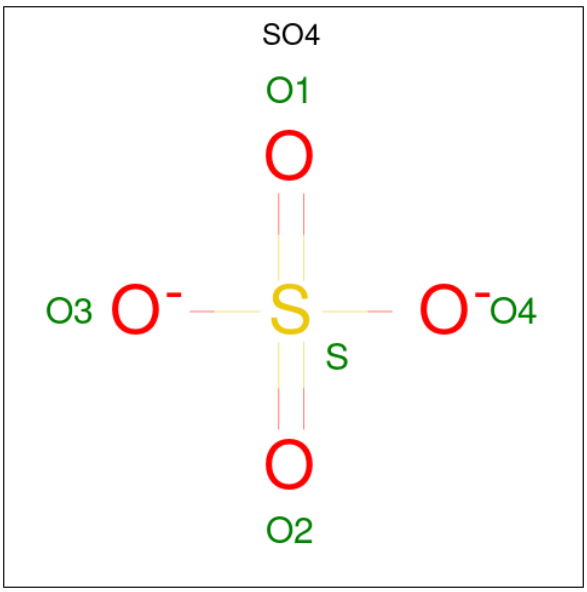
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Mg 2	0	0
3	C	2	Total 2	Mg 2	0	0

- Molecule 4 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$) (labeled as "Ligand of Interest" by depositor).



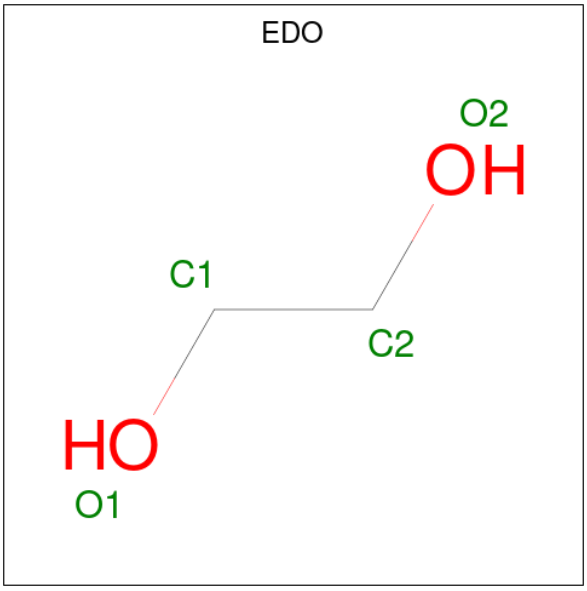
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 9 7 2	0	0
4	A	1	Total O P 9 7 2	0	0
4	C	1	Total O P 9 7 2	0	0

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



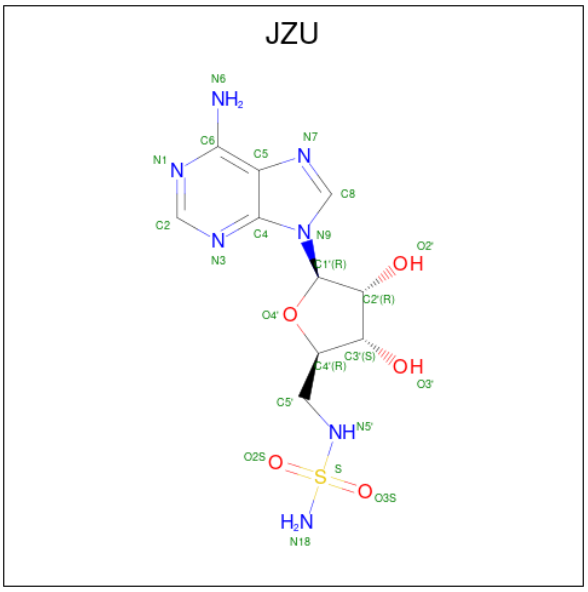
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is 5'-deoxy-5'-(sulfamoylamino)adenosine (three-letter code: JZU) (formula: $C_{10}H_{15}N_7O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			23	10	7	5	1		
7	D	1	Total	C	N	O	S	0	0
			23	10	7	5	1		

- Molecule 8 is water.

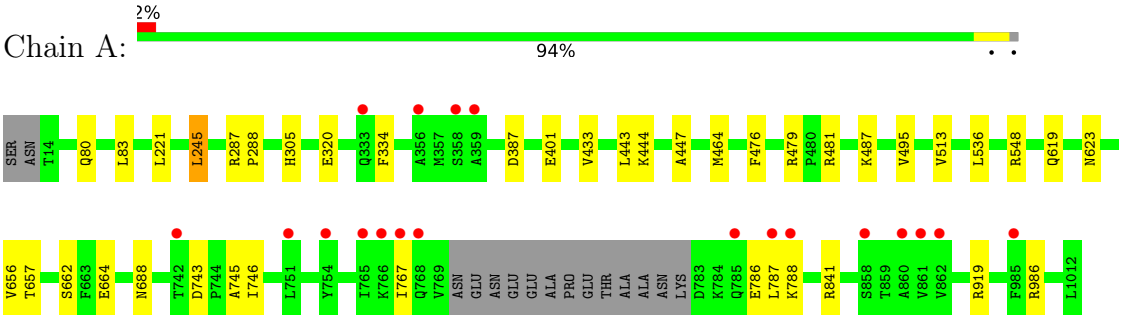
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	197	Total	O	0	0
			197	197		
8	B	22	Total	O	0	0
			22	22		
8	C	57	Total	O	0	0
			57	57		
8	D	13	Total	O	0	0
			13	13		

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.

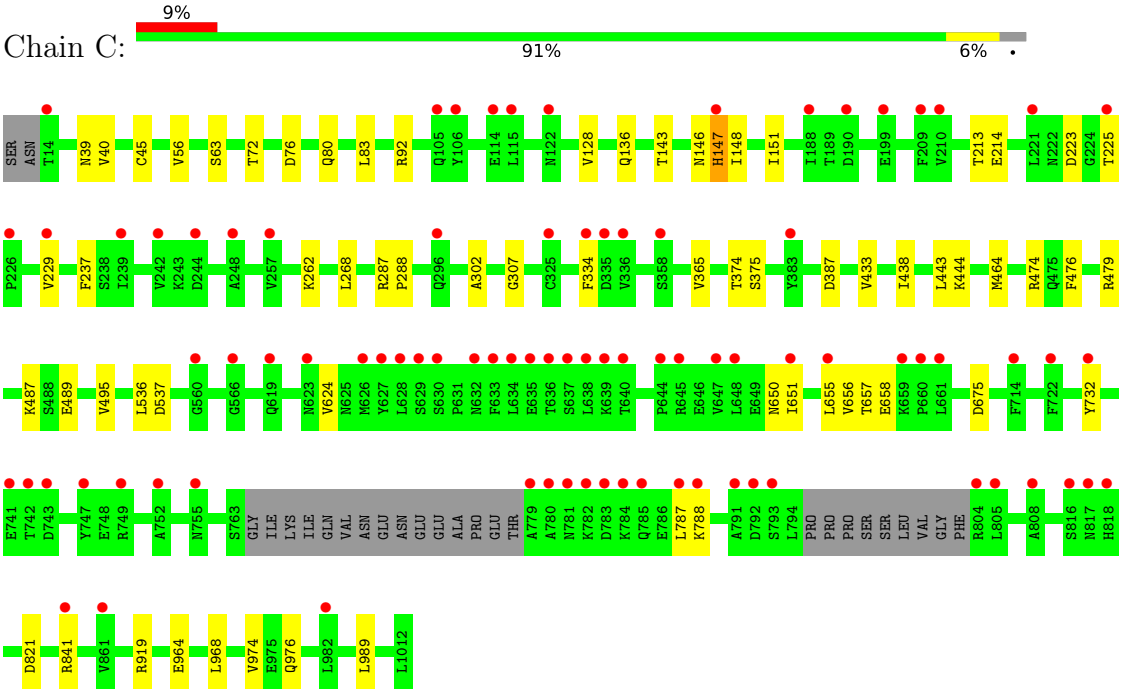
• Molecule 1: Ubiquitin-activating enzyme E1 1

Chain A:



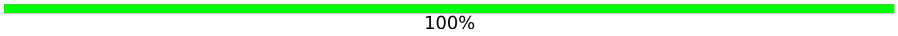
• Molecule 1: Ubiquitin-activating enzyme E1 1

Chain C:



• Molecule 2: Ubiquitin-60S ribosomal protein L40

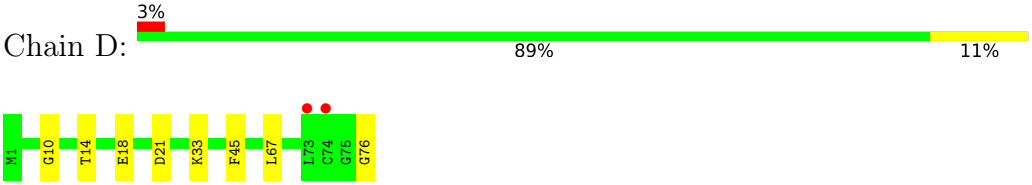
Chain B:



There are no outlier residues recorded for this chain.

• Molecule 2: Ubiquitin-60S ribosomal protein L40

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	182.06Å 114.62Å 125.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.39 – 2.60 42.39 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.39-2.60) 99.9 (42.39-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.14_3211	Depositor
R, R_{free}	0.197 , 0.230 0.198 , 0.229	Depositor DCC
R_{free} test set	4073 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	49.0	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17008	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: MG, EDO, JZU, SO4, POP

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	0.25	0/7916	0.41	0/10713
1	C	0.24	0/7830	0.40	0/10592
2	B	0.25	0/600	0.46	0/806
2	D	0.25	0/600	0.45	0/806
All	All	0.25	0/16946	0.41	0/22917

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

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	7745	0	7688	20	0
1	C	7664	0	7598	36	1
2	B	595	0	617	0	0
2	D	595	0	617	5	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0
4	A	18	0	0	1	0
4	C	9	0	0	2	0
5	A	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	10	0	0	0	0
6	A	4	0	6	1	0
6	C	4	0	6	0	0
7	B	23	0	14	0	0
7	D	23	0	13	1	0
8	A	197	0	0	1	0
8	B	22	0	0	0	0
8	C	57	0	0	2	0
8	D	13	0	0	1	0
All	All	17008	0	16559	60	1

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 2.

All (60) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:SER:OG	1:A:664:GLU:OE1	2.04	0.75
2:D:10:GLY:O	8:D:201:HOH:O	2.07	0.71
1:C:374:THR:O	1:C:375:SER:OG	2.11	0.68
2:D:45:PHE:HB2	2:D:67:LEU:HD22	1.77	0.67
1:C:80:GLN:HG2	1:C:83:LEU:HD22	1.77	0.66
1:C:72:THR:HG23	1:C:83:LEU:HD23	1.79	0.65
1:A:487:LYS:NZ	4:A:1103:POP:O4	2.25	0.62
1:C:45:CYS:O	1:C:80:GLN:NE2	2.33	0.61
1:C:650:ASN:OD1	1:C:651:ILE:N	2.36	0.59
1:C:443:LEU:HB3	1:C:495:VAL:HG11	1.85	0.58
1:C:223:ASP:OD1	1:C:225:THR:N	2.35	0.58
1:A:787:LEU:HD12	1:A:788:LYS:N	2.20	0.57
1:C:476:PHE:O	1:C:479:ARG:NH1	2.34	0.57
1:C:976:GLN:NE2	8:C:1204:HOH:O	2.38	0.57
1:A:443:LEU:HB3	1:A:495:VAL:HG21	1.88	0.56
1:A:743:ASP:O	1:A:746:ILE:HG22	2.05	0.56
2:D:18:GLU:N	2:D:21:ASP:OD1	2.37	0.55
1:C:537:ASP:OD1	7:D:101:JZU:H8	2.07	0.55
1:A:619:GLN:O	1:A:623:ASN:ND2	2.42	0.53
1:C:143:THR:HB	1:C:148:ILE:HG23	1.91	0.53
1:A:433:VAL:HG12	1:A:536:LEU:HD21	1.93	0.51
1:C:76:ASP:OD2	1:C:92:ARG:NH1	2.44	0.50
1:C:964:GLU:OE1	1:C:964:GLU:N	2.35	0.50
1:C:474:ARG:NH2	4:C:1103:POP:O2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:675:ASP:OD1	8:C:1201:HOH:O	2.18	0.50
1:C:821:ASP:OD1	1:C:841:ARG:NH1	2.45	0.49
1:C:213:THR:HG22	1:C:214:GLU:HG3	1.94	0.49
1:C:487:LYS:NZ	4:C:1103:POP:O6	2.39	0.49
1:A:656:VAL:HG23	1:A:657:THR:HG23	1.95	0.48
1:A:433:VAL:HG13	1:A:513:VAL:HG21	1.96	0.47
1:C:128:VAL:HG11	1:C:136:GLN:HG2	1.97	0.46
1:A:80:GLN:HG2	1:A:83:LEU:HD12	1.97	0.46
1:C:624:VAL:HG13	1:C:655:LEU:HD21	1.97	0.46
1:C:656:VAL:HG23	1:C:657:THR:N	2.31	0.45
1:A:786:GLU:OE1	1:A:786:GLU:N	2.42	0.45
1:C:433:VAL:HG12	1:C:536:LEU:HD21	1.98	0.45
1:C:658:GLU:O	1:C:732:TYR:OH	2.30	0.45
1:C:80:GLN:CG	1:C:83:LEU:HD13	2.46	0.45
1:A:841:ARG:HB2	6:A:1110:EDO:H22	1.99	0.45
1:C:40:VAL:HG11	1:C:56:VAL:HG11	1.99	0.44
1:C:974:VAL:HG21	1:C:989:LEU:HD21	2.00	0.44
1:A:447:ALA:HB2	1:A:495:VAL:HG13	2.00	0.43
1:A:221:LEU:N	1:A:245:LEU:HD21	2.33	0.43
1:C:964:GLU:O	1:C:968:LEU:HD13	2.19	0.43
1:A:476:PHE:O	1:A:479:ARG:NH2	2.44	0.43
1:C:39:ASN:OD1	1:C:63:SER:OG	2.22	0.42
1:C:229:VAL:HG13	1:C:237:PHE:CD1	2.54	0.42
1:C:302:ALA:O	1:C:307:GLY:N	2.48	0.42
1:A:688:ASN:OD1	1:A:767:ILE:HD12	2.20	0.42
1:C:268:LEU:HD23	1:C:268:LEU:O	2.19	0.42
1:C:151:ILE:HG21	1:C:365:VAL:HG13	2.01	0.41
1:A:287:ARG:N	1:A:288:PRO:CD	2.83	0.41
1:C:287:ARG:N	1:C:288:PRO:CD	2.84	0.41
1:C:146:ASN:O	1:C:147:HIS:C	2.59	0.41
2:D:14:THR:O	2:D:33:LYS:NZ	2.51	0.41
1:C:438:ILE:HD12	2:D:76:GLY:HA3	2.02	0.41
1:A:481:ARG:NH1	8:A:1208:HOH:O	2.43	0.41
1:A:743:ASP:OD2	1:A:745:ALA:HB3	2.21	0.40
1:C:787:LEU:HD12	1:C:788:LYS:N	2.36	0.40
1:A:305:HIS:HE2	1:A:320:GLU:CD	2.24	0.40

All (1) 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)
1:C:262:LYS:NZ	1:C:489:GLU:OE1[3_546]	2.17	0.03

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	982/1001 (98%)	945 (96%)	37 (4%)	0	100	100
1	C	969/1001 (97%)	924 (95%)	45 (5%)	0	100	100
2	B	74/76 (97%)	74 (100%)	0	0	100	100
2	D	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
All	All	2099/2154 (97%)	2016 (96%)	83 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	865/877 (99%)	856 (99%)	9 (1%)	76	90
1	C	854/877 (97%)	848 (99%)	6 (1%)	84	94
2	B	69/69 (100%)	69 (100%)	0	100	100
2	D	69/69 (100%)	69 (100%)	0	100	100
All	All	1857/1892 (98%)	1842 (99%)	15 (1%)	81	92

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	LEU
1	A	334	PHE
1	A	387	ASP
1	A	401	GLU
1	A	444	LYS
1	A	464	MET
1	A	548	ARG
1	A	919	ARG
1	A	986	ARG
1	C	147	HIS
1	C	334	PHE
1	C	387	ASP
1	C	444	LYS
1	C	464	MET
1	C	919	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	144	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
6	EDO	A	1110	-	3,3,3	0.47	0	2,2,2	0.27	0
4	POP	A	1104	-	6,8,8	0.74	0	13,13,13	1.21	1 (7%)
5	SO4	A	1107	-	4,4,4	0.14	0	6,6,6	0.05	0
4	POP	A	1103	3	6,8,8	0.72	0	13,13,13	1.15	1 (7%)
5	SO4	A	1105	-	4,4,4	0.13	0	6,6,6	0.05	0
6	EDO	C	1106	-	3,3,3	0.46	0	2,2,2	0.33	0
7	JZU	B	101	3,2	22,25,25	0.96	1 (4%)	22,38,38	1.70	3 (13%)
7	JZU	D	101	3,2	22,25,25	0.97	1 (4%)	22,38,38	1.83	4 (18%)
5	SO4	A	1106	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	A	1108	-	4,4,4	0.14	0	6,6,6	0.05	0
4	POP	C	1103	3	6,8,8	0.73	0	13,13,13	1.33	1 (7%)
5	SO4	C	1105	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	C	1104	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	A	1109	-	4,4,4	0.14	0	6,6,6	0.05	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
6	EDO	A	1110	-	-	0/1/1/1	-
4	POP	A	1104	-	-	0/6/6/6	-
4	POP	A	1103	3	-	3/6/6/6	-
6	EDO	C	1106	-	-	0/1/1/1	-
7	JZU	B	101	3,2	-	2/5/26/26	0/3/3/3
4	POP	C	1103	3	-	1/6/6/6	-
7	JZU	D	101	3,2	-	2/5/26/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	101	JZU	S-N5'	-2.55	1.52	1.62
7	B	101	JZU	S-N5'	-2.40	1.53	1.62

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	101	JZU	O3S-S-O2S	-4.42	109.84	119.96
7	D	101	JZU	O3S-S-O2S	-4.35	109.99	119.96
7	D	101	JZU	N3-C2-N1	-4.02	122.39	128.68
7	B	101	JZU	N3-C2-N1	-3.91	122.57	128.68
7	D	101	JZU	C4'-C5'-N5'	-3.87	104.75	112.51
4	C	1103	POP	P2-O-P1	-3.52	120.76	132.83
4	A	1104	POP	P2-O-P1	-3.17	121.96	132.83
7	B	101	JZU	C4'-C5'-N5'	-2.99	106.52	112.51
4	A	1103	POP	P2-O-P1	-2.75	123.41	132.83
7	D	101	JZU	C3'-C2'-C1'	2.35	104.52	100.98

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1103	POP	P2-O-P1-O2
4	C	1103	POP	P2-O-P1-O3
7	B	101	JZU	C5'-N5'-S-O2S
7	D	101	JZU	C5'-N5'-S-O2S
7	B	101	JZU	C5'-N5'-S-O3S
7	D	101	JZU	C5'-N5'-S-O3S
4	A	1103	POP	P2-O-P1-O3
4	A	1103	POP	P2-O-P1-O1

There are no ring outliers.

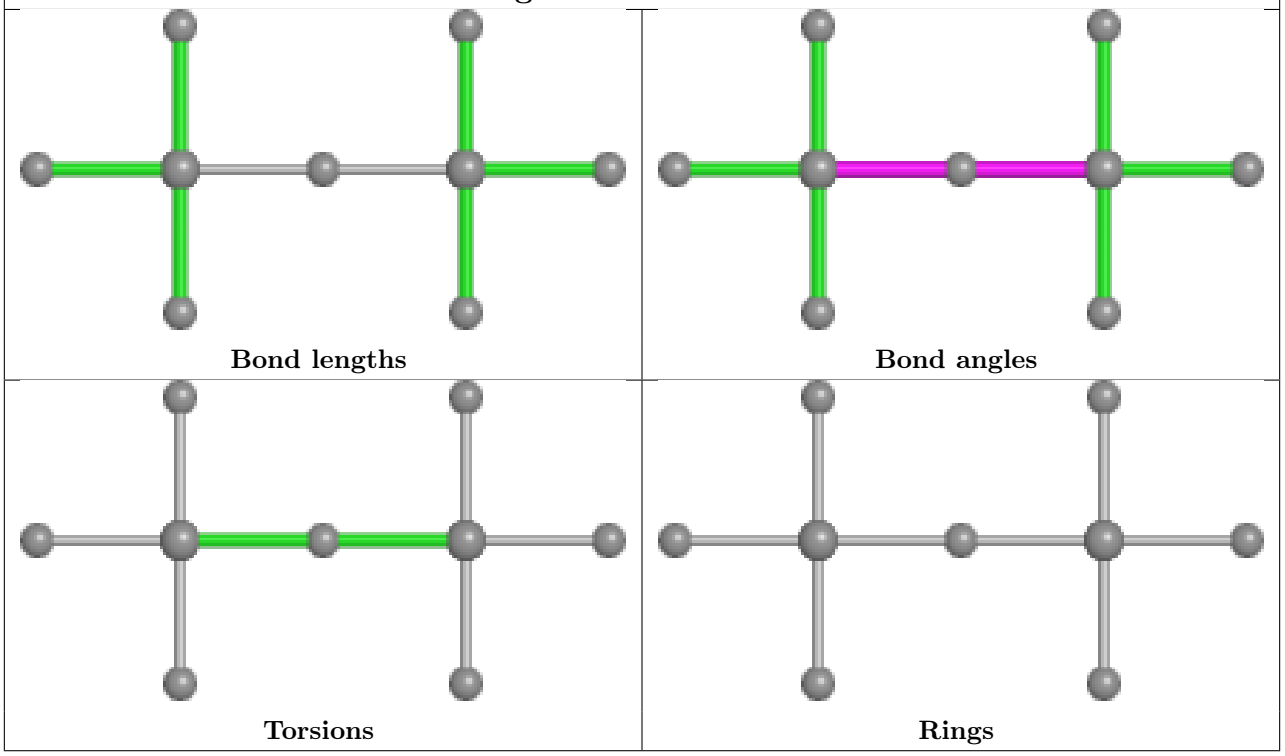
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1110	EDO	1	0
4	A	1103	POP	1	0
7	D	101	JZU	1	0
4	C	1103	POP	2	0

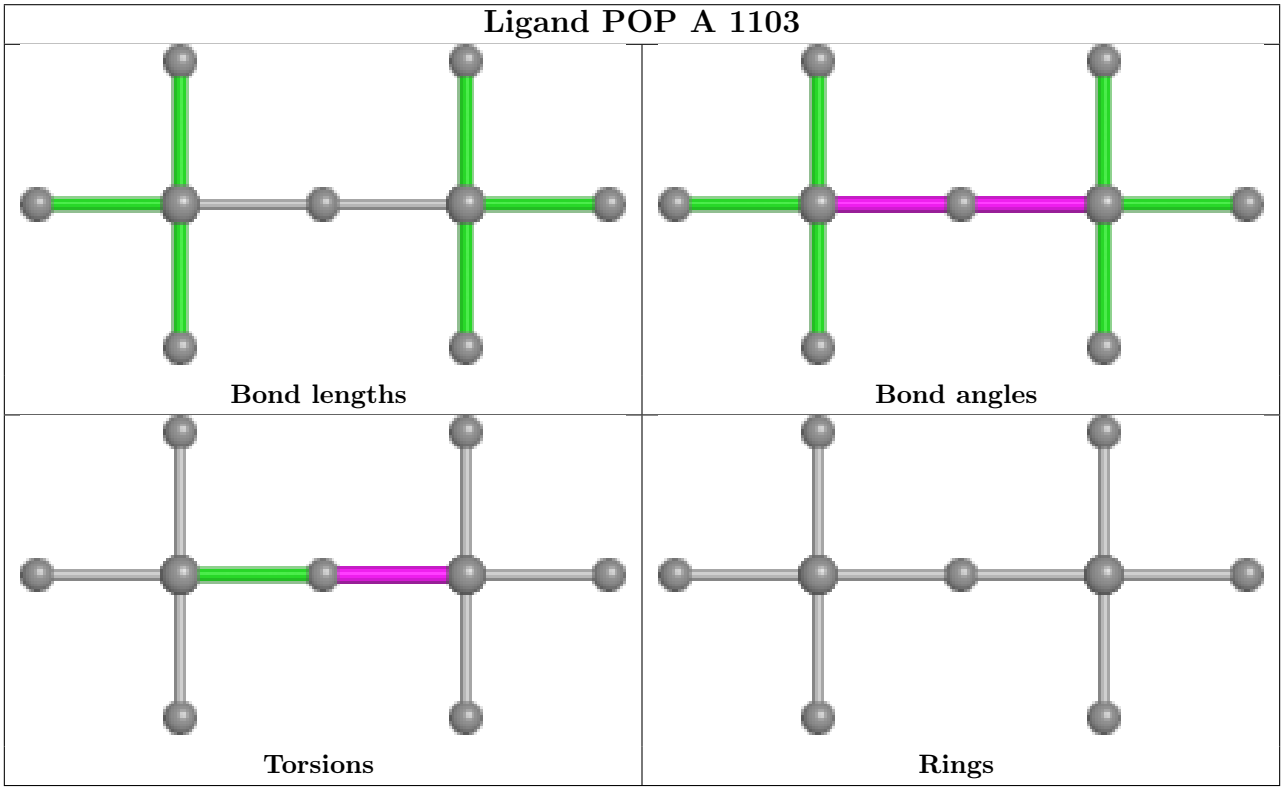
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

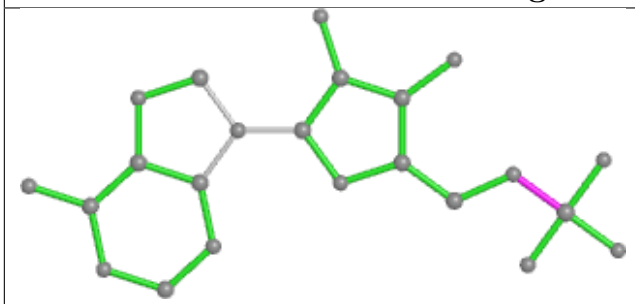
Ligand POP A 1104



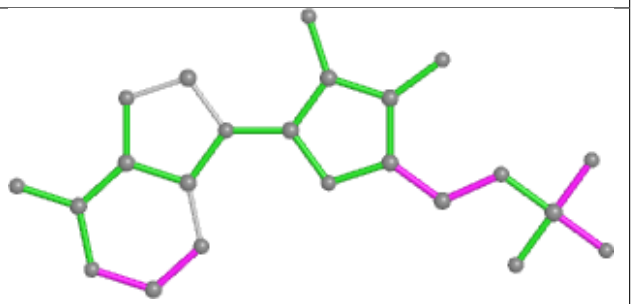
Ligand POP A 1103



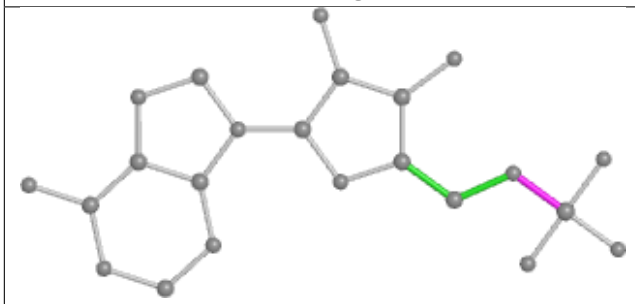
Ligand JZU B 101



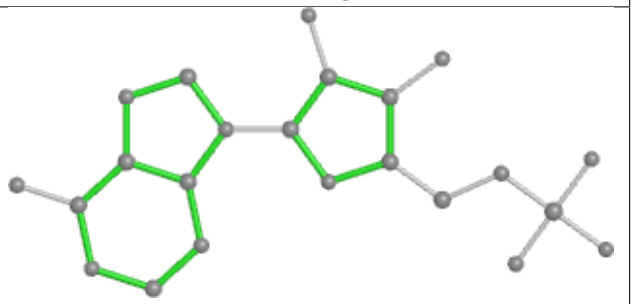
Bond lengths



Bond angles

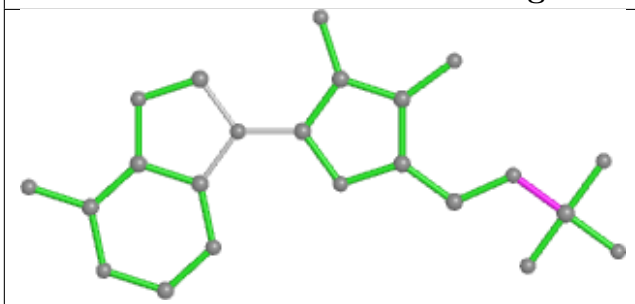


Torsions

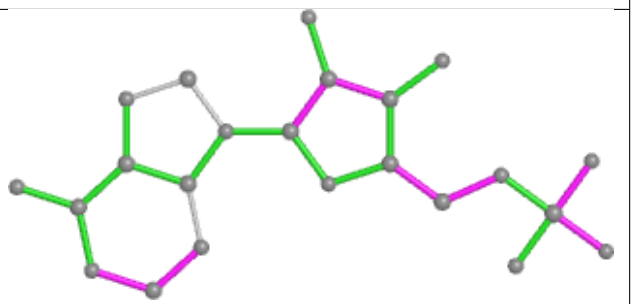


Rings

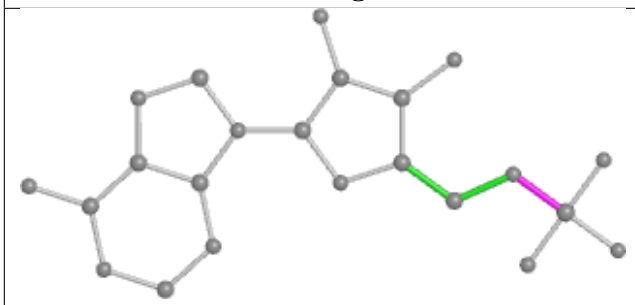
Ligand JZU D 101



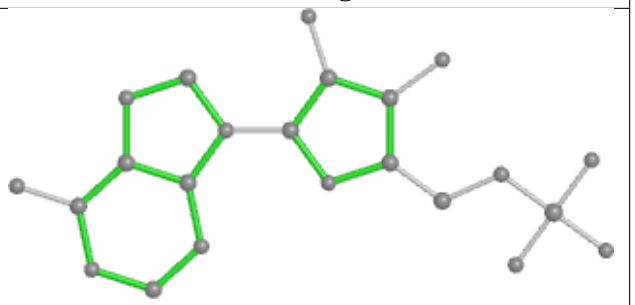
Bond lengths



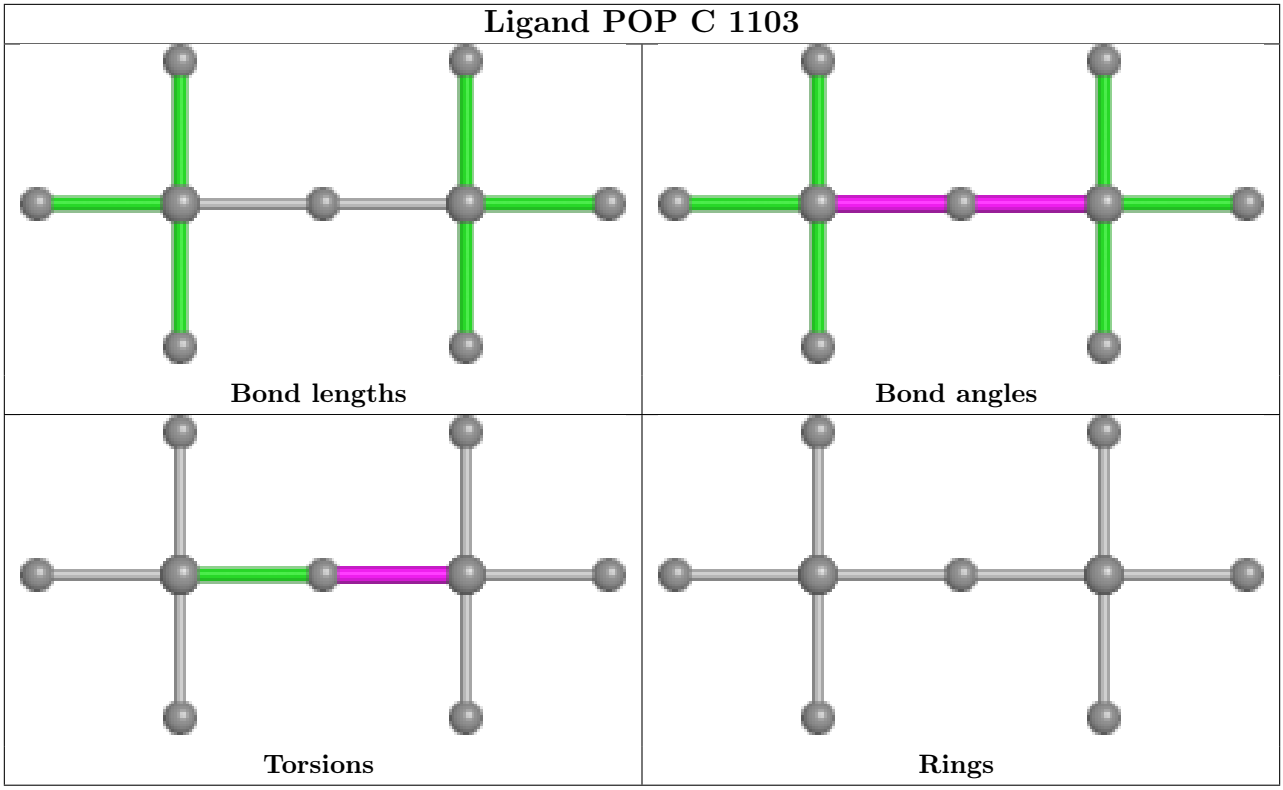
Bond angles



Torsions



Rings



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	986/1001 (98%)	-0.03	19 (1%) 66 62	28, 51, 90, 145	0
1	C	975/1001 (97%)	0.51	86 (8%) 10 7	30, 82, 132, 176	0
2	B	76/76 (100%)	-0.13	0 100 100	26, 38, 59, 67	0
2	D	76/76 (100%)	0.15	2 (2%) 56 50	39, 56, 92, 104	0
All	All	2113/2154 (98%)	0.23	107 (5%) 28 22	26, 62, 120, 176	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	779	ALA	12.4
1	C	787	LEU	7.1
1	C	747	TYR	6.8
1	C	334	PHE	6.7
1	C	780	ALA	6.0
1	C	788	LYS	5.8
1	C	244	ASP	4.8
1	C	793	SER	4.3
1	C	752	ALA	4.2
1	C	781	ASN	3.9
1	C	636	THR	3.9
1	C	655	LEU	3.9
1	C	638	LEU	3.7
1	C	239	ILE	3.7
1	C	742	THR	3.7
1	C	784	LYS	3.7
1	C	640	THR	3.7
1	C	242	VAL	3.7
1	C	633	PHE	3.6
1	C	783	ASP	3.6
1	C	257	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	765	ILE	3.5
1	C	635	GLU	3.4
1	C	648	LEU	3.4
1	C	661	LEU	3.3
1	C	732	TYR	3.2
1	A	768	GLN	3.2
1	C	296	GLN	3.2
1	A	985	PHE	3.2
1	A	787	LEU	3.1
1	C	632	ASN	3.1
1	C	335	ASP	3.1
1	C	645	ARG	3.0
1	C	722	PHE	3.0
1	C	639	LYS	3.0
1	C	805	LEU	3.0
1	C	637	SER	3.0
1	C	785	GLN	3.0
1	C	804	ARG	3.0
1	C	627	TYR	2.9
1	A	766	LYS	2.9
1	C	114	GLU	2.9
1	C	629	SER	2.8
1	C	209	PHE	2.8
1	A	861	VAL	2.8
1	C	226	PRO	2.8
1	C	749	ARG	2.8
1	C	626	MET	2.8
1	A	356	ALA	2.7
2	D	74	CYS	2.7
1	C	818	HIS	2.7
1	C	982	LEU	2.7
1	C	336	VAL	2.6
1	A	751	LEU	2.6
1	C	741	GLU	2.6
1	C	782	LYS	2.6
1	C	743	ASP	2.6
1	C	383	TYR	2.6
1	C	651	ILE	2.6
1	C	14	THR	2.6
1	C	644	PRO	2.6
1	C	791	ALA	2.6
1	C	660	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	210	VAL	2.5
1	C	248	ALA	2.5
1	A	742	THR	2.5
1	C	190	ASP	2.4
1	C	623	ASN	2.4
1	C	634	LEU	2.4
1	A	788	LYS	2.4
1	C	619	GLN	2.4
1	A	333	GLN	2.4
1	C	358	SER	2.4
1	C	229	VAL	2.3
1	C	861	VAL	2.3
1	C	816	SER	2.3
1	A	358	SER	2.3
1	C	221	LEU	2.3
1	C	560	GLY	2.2
1	A	860	ALA	2.2
1	C	808	ALA	2.2
1	C	225	THR	2.2
1	C	792	ASP	2.2
1	C	115	LEU	2.2
1	C	105	GLN	2.2
1	C	199	GLU	2.2
1	A	785	GLN	2.2
1	A	862	VAL	2.1
1	C	659	LYS	2.1
1	C	147	HIS	2.1
1	C	628	LEU	2.1
1	A	359	ALA	2.1
1	C	817	ASN	2.1
1	A	767	ILE	2.1
1	C	188	ILE	2.1
1	A	858	SER	2.1
1	C	630	SER	2.1
1	C	714	PHE	2.1
1	C	566	GLY	2.1
2	D	73	LEU	2.1
1	C	647	VAL	2.0
1	A	754	TYR	2.0
1	C	325	CYS	2.0
1	C	106	TYR	2.0
1	C	122	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	755	ASN	2.0
1	C	841	ARG	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.

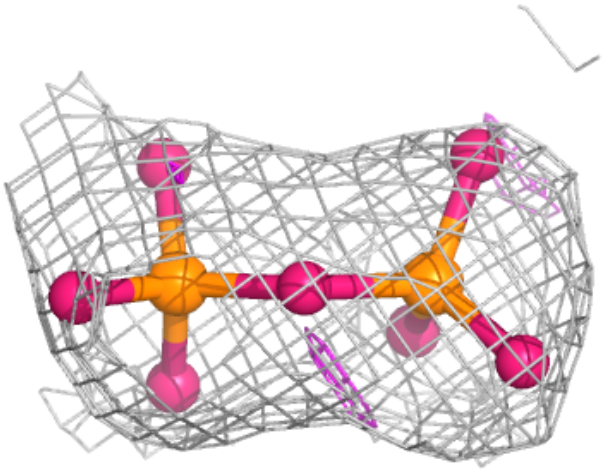
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	A	1108	5/5	0.83	0.44	134,135,135,135	0
5	SO4	C	1104	5/5	0.87	0.21	99,99,99,100	0
5	SO4	A	1107	5/5	0.90	0.36	134,134,134,134	0
5	SO4	A	1109	5/5	0.91	0.26	115,115,115,116	0
4	POP	A	1104	9/9	0.91	0.18	99,100,102,102	0
6	EDO	C	1106	4/4	0.92	0.12	61,61,62,62	0
6	EDO	A	1110	4/4	0.93	0.11	57,58,58,58	0
3	MG	C	1102	1/1	0.93	0.05	34,34,34,34	0
4	POP	C	1103	9/9	0.94	0.13	54,65,67,67	0
5	SO4	C	1105	5/5	0.94	0.20	107,108,108,108	0
7	JZU	D	101	23/23	0.94	0.15	26,44,47,47	0
3	MG	C	1101	1/1	0.95	0.08	41,41,41,41	0
3	MG	A	1102	1/1	0.96	0.13	29,29,29,29	0
5	SO4	A	1105	5/5	0.96	0.08	71,72,72,72	0
7	JZU	B	101	23/23	0.97	0.18	24,33,35,35	0
5	SO4	A	1106	5/5	0.97	0.11	68,69,69,70	0
4	POP	A	1103	9/9	0.98	0.15	35,38,40,41	0
3	MG	A	1101	1/1	0.98	0.11	32,32,32,32	0

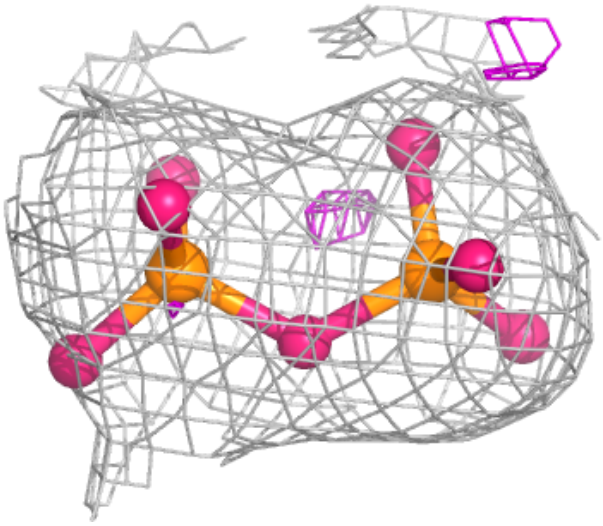
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

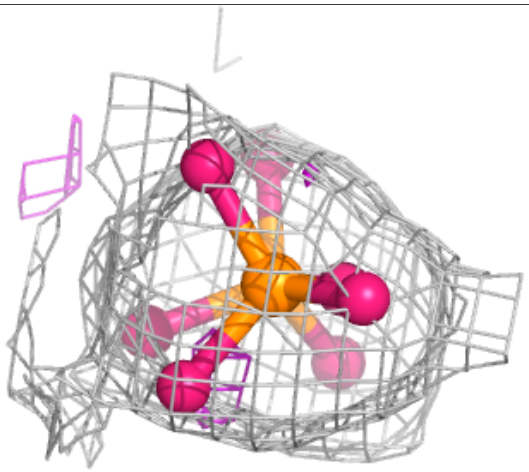
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around POP A 1104:

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

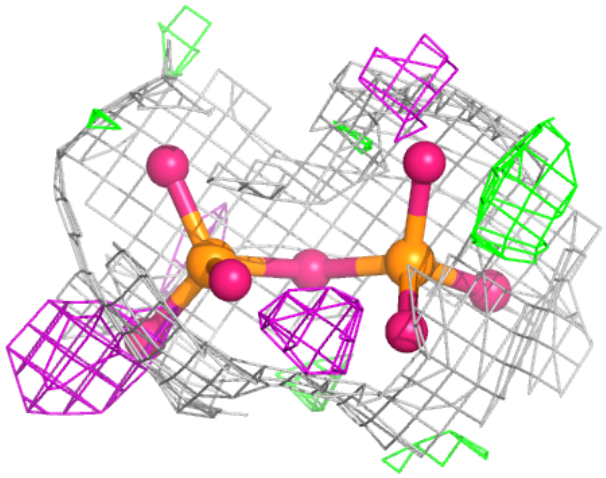


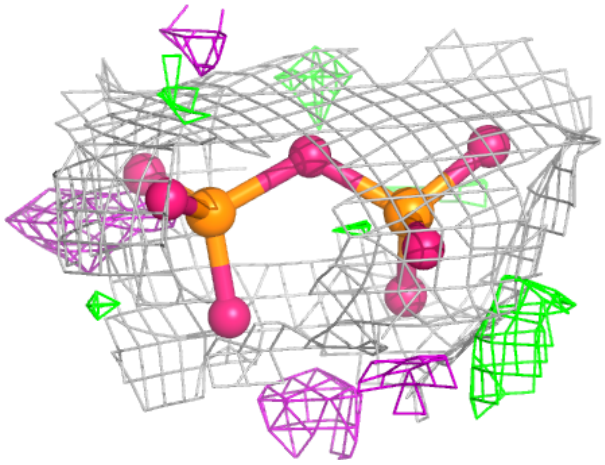


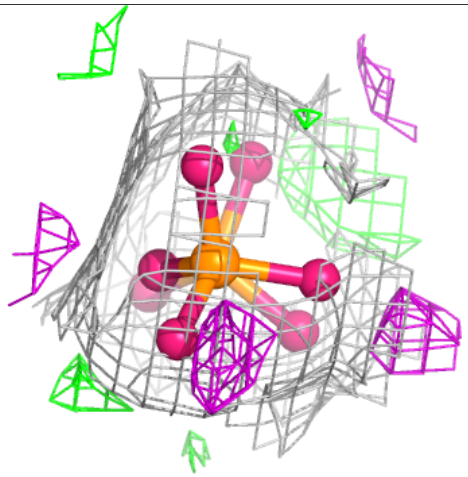


Electron density around POP C 1103:

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

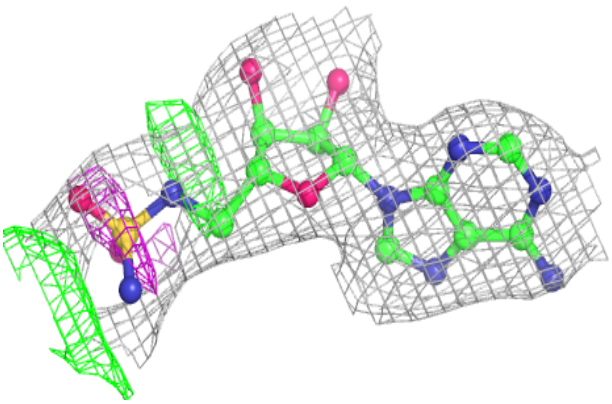


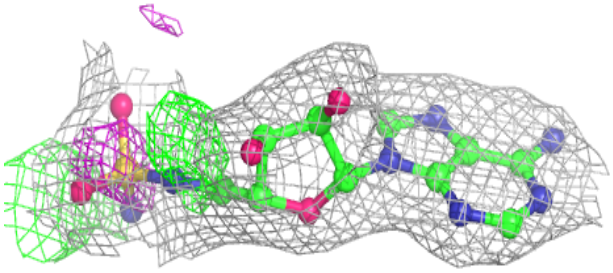


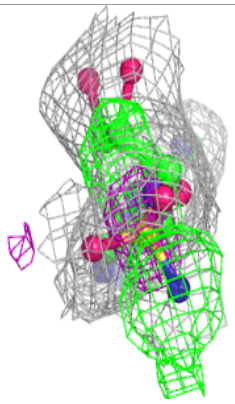


Electron density around JZU D 101:

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

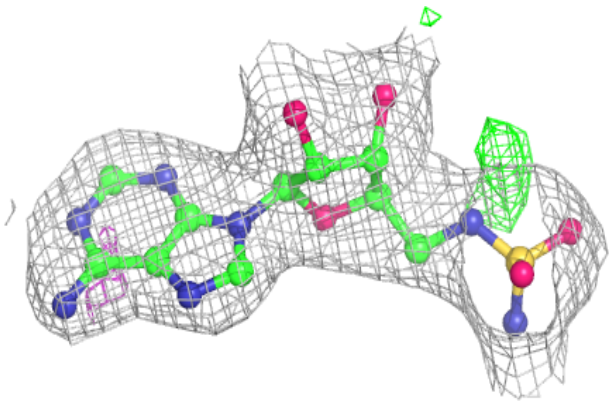


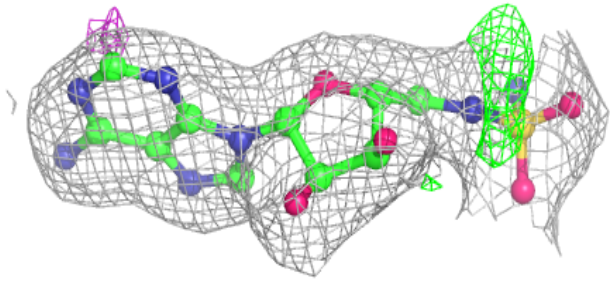


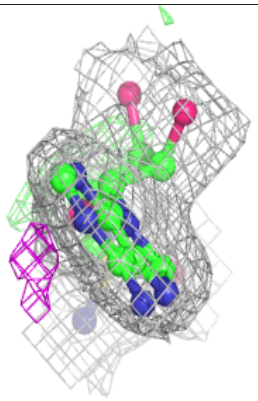


Electron density around JZU B 101:

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

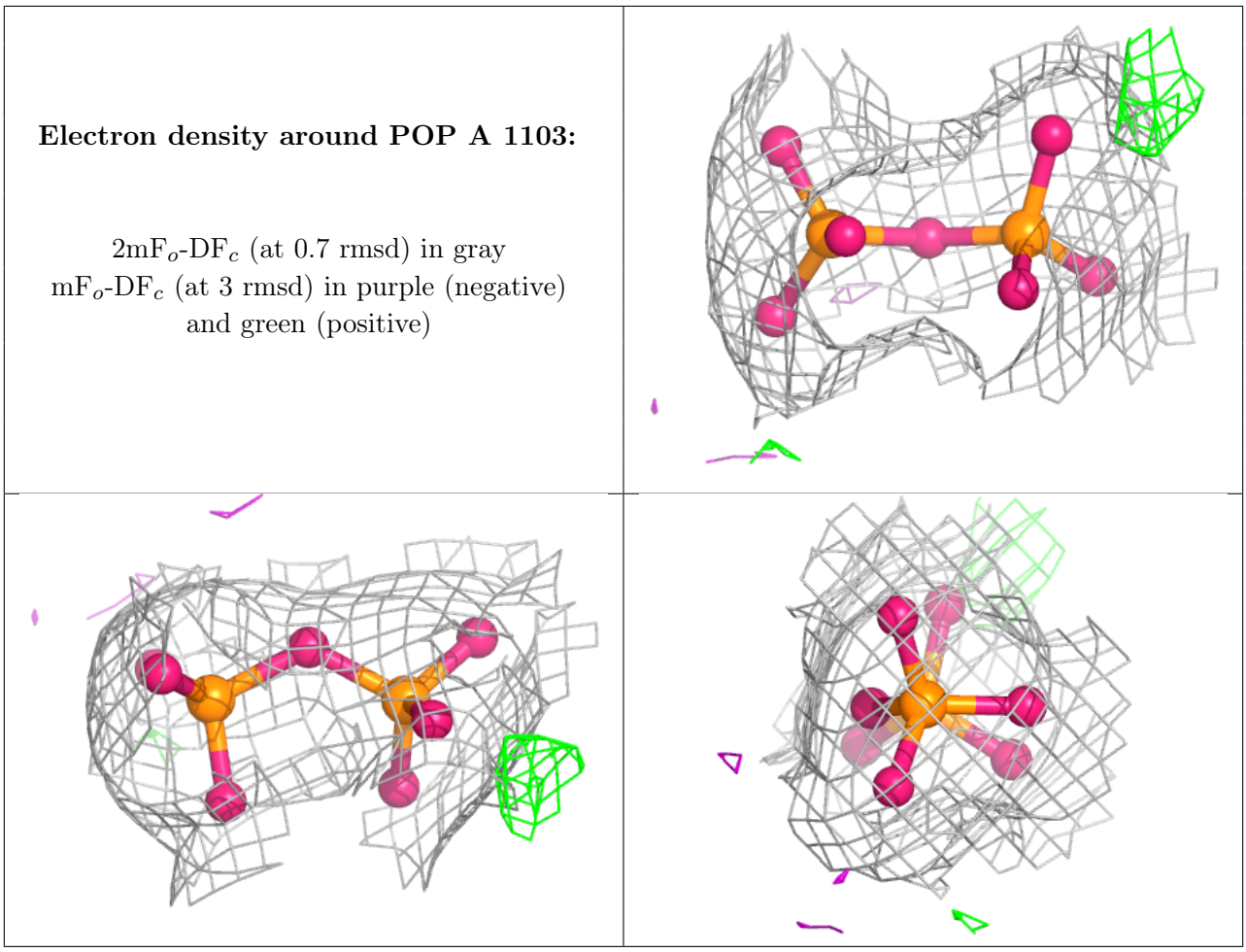






Electron density around POP A 1103:

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



6.5 Other polymers

There are no such residues in this entry.