Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 11:25 PM EDT

PDB ID	:	7LNN
Title	:	E. coli S-adenosyl methionine transferase co-crystallized with guanosine-5'-imidotriphosphate
Authors	:	Tan, L.L.; Jackson, C.J.
Deposited on	:	2021-02-08
Resolution	:	2.50 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:

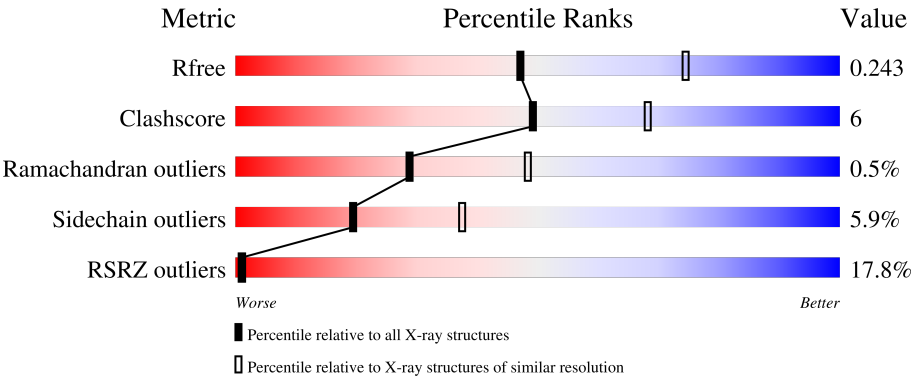
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	384	12% 83% 13%
1	B	384	23% 77% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	B	801	-	-	-	X
3	PPK	B	802	-	-	-	X

2 Entry composition

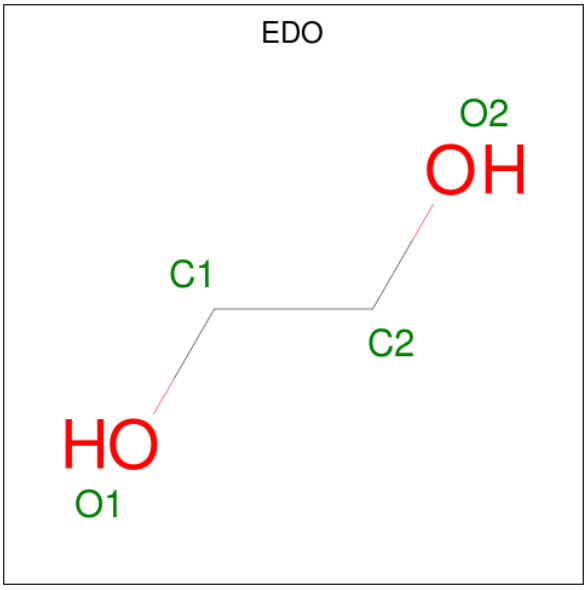
There are 6 unique types of molecules in this entry. The entry contains 6017 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

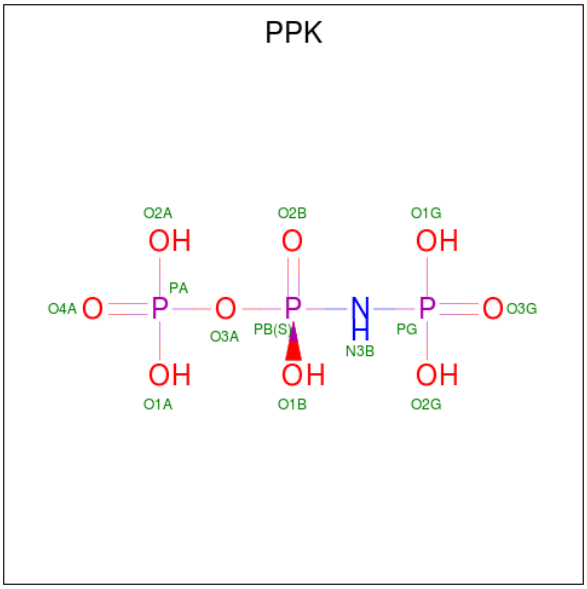
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	6	0
			2940	1857	505	565	13			
1	B	378	Total	C	N	O	S	0	5	0
			2948	1865	501	568	14			

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



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

- Molecule 3 is (DIPHOSPHONO)AMINOPHOSPHONIC ACID (three-letter code: PPK) (formula: $H_6NO_9P_3$).

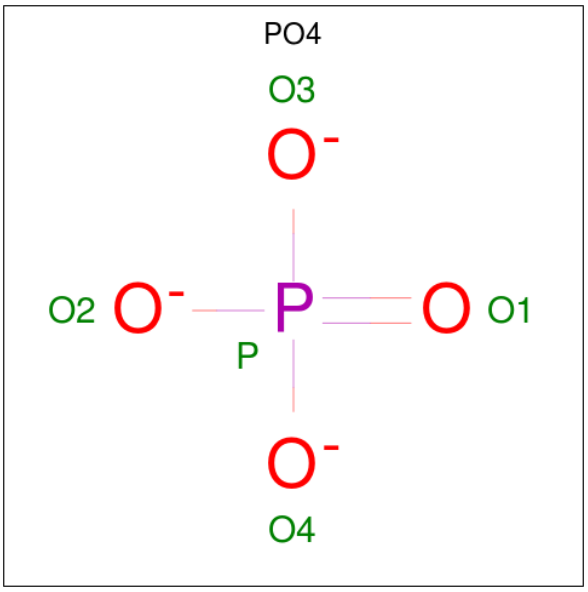


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N O P 13 1 9 3	0	0
3	B	1	Total N O P 13 1 9 3	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 6 is water.

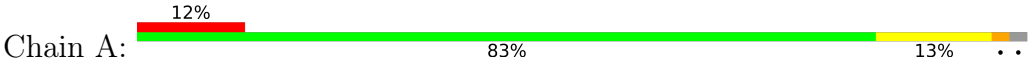
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	46	Total O 46 46	0	0
6	B	34	Total O 34 34	0	0

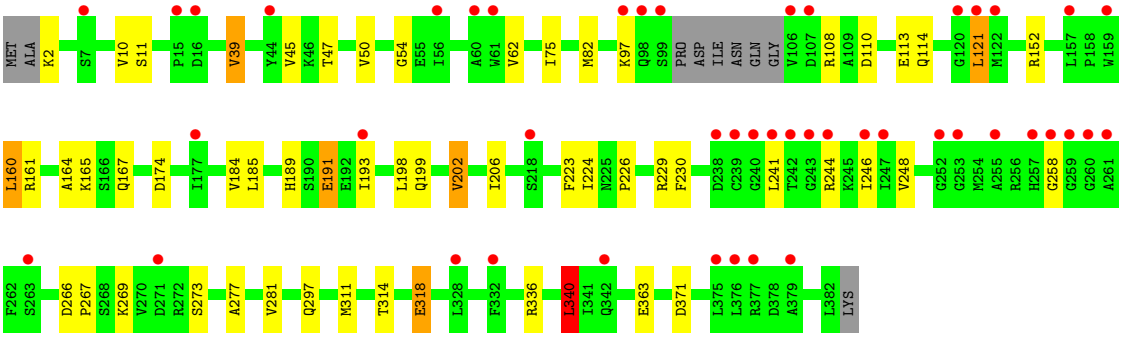
3 Residue-property plots (i)

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: S-adenosylmethionine synthase

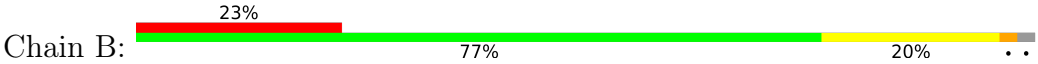
Chain A:

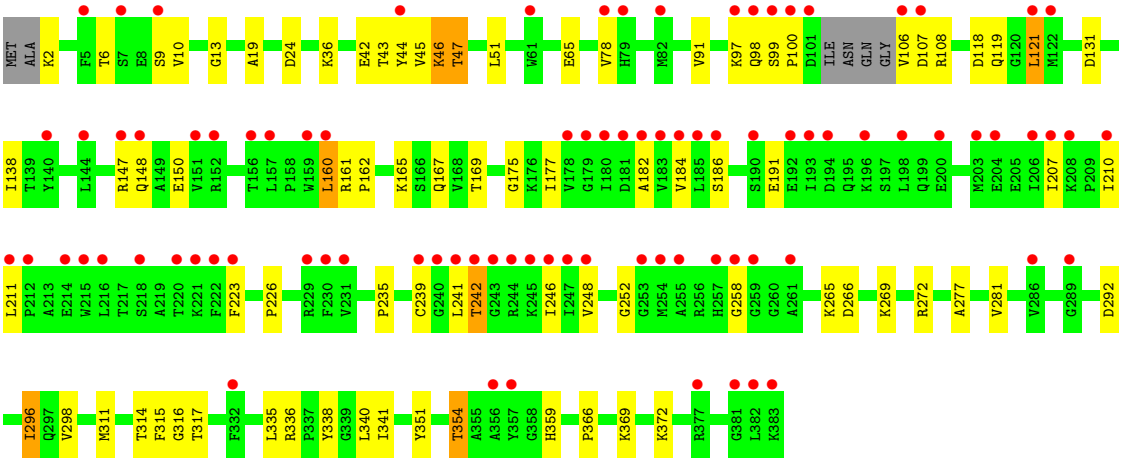




• Molecule 1: S-adenosylmethionine synthase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	122.34Å 122.34Å 287.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.63 – 2.50 43.63 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.63-2.50) 99.4 (43.63-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.222 , 0.243 0.222 , 0.243	Depositor DCC
R_{free} test set	2229 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	71.0	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 69.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6017	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: PPK, PO4, MG, EDO

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	0/2998	0.47	1/4064 (0.0%)
1	B	0.25	0/3007	0.44	0/4077
All	All	0.25	0/6005	0.45	1/8141 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	340	LEU	CA-CB-CG	7.00	131.40	115.30

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	2940	0	2903	33	0
1	B	2948	0	2911	41	0
2	A	12	0	18	1	0
2	B	4	0	6	1	0
3	A	13	0	1	1	0
3	B	13	0	1	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	5	0	0	0	0
6	A	46	0	0	0	0
6	B	34	0	0	0	0
All	All	6017	0	5840	69	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 6.

All (69) 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:273:SER:HB3	1:A:340:LEU:HD21	1.66	0.78
1:A:244:ARG:NH2	1:B:42:GLU:OE1	2.23	0.71
1:B:24:ASP:OD1	1:B:272:ARG:NH2	2.31	0.63
1:B:223:PHE:HB3	1:B:226:PRO:HG3	1.84	0.59
1:B:46:LYS:HD3	1:B:47:THR:HG23	1.85	0.58
1:B:44:TYR:HB3	1:B:51:LEU:HB3	1.85	0.57
1:B:351:TYR:O	1:B:354:THR:HG22	2.04	0.57
1:A:39:VAL:HG13	1:A:266:ASP:HB3	1.88	0.55
1:A:160:LEU:HA	1:A:189:HIS:HA	1.88	0.55
1:A:202:VAL:HB	1:A:206:ILE:HD12	1.89	0.54
1:A:297:GLN:HE22	1:B:6:THR:H	1.56	0.53
1:A:273:SER:HB3	1:A:340:LEU:CD2	2.38	0.52
1:A:198:LEU:O	1:A:202:VAL:HG13	2.10	0.52
1:B:338[B]:TYR:HD1	1:B:341:ILE:HD12	1.74	0.52
1:B:354:THR:HG23	1:B:359:HIS:CE1	2.45	0.52
1:A:10:VAL:HG12	1:A:165:LYS:HG2	1.91	0.51
1:A:371:ASP:OD1	1:A:371:ASP:N	2.43	0.51
1:B:43:THR:H	1:B:242:THR:CG2	2.23	0.51
1:B:314:THR:O	1:B:316:GLY:N	2.43	0.51
1:B:169:THR:HB	1:B:182:ALA:HB3	1.91	0.51
1:B:65:GLU:HA	1:B:91:VAL:HG11	1.93	0.50
1:A:108:ARG:HG3	1:A:114:GLN:HA	1.94	0.49
1:B:298:VAL:HG11	1:B:335:LEU:HD13	1.94	0.49
1:A:191:GLU:OE2	1:A:229:ARG:NH2	2.40	0.49
1:A:75:ILE:O	1:A:152:ARG:NH2	2.46	0.49
1:A:45[A]:VAL:HG12	1:A:50:VAL:HG22	1.93	0.48
1:B:167:GLN:HB3	1:B:184:VAL:HB	1.96	0.48
1:A:223:PHE:HB3	1:A:226:PRO:HG3	1.95	0.48
1:A:336:ARG:O	1:A:340:LEU:HD13	2.14	0.47
1:A:167:GLN:HB3	1:A:184:VAL:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ASP:OD1	1:A:269:LYS:NZ	2.43	0.47
1:B:366:PRO:O	1:B:369:LYS:HG2	2.14	0.47
1:B:19:ALA:HB1	1:B:242:THR:HG22	1.97	0.46
1:B:277:ALA:O	1:B:281[A]:VAL:HG13	2.15	0.46
1:A:241:LEU:HD23	1:B:241:LEU:HB3	1.96	0.46
1:B:45:VAL:HG22	1:B:235:PRO:HB3	1.98	0.46
1:A:297:GLN:HB3	1:A:311:MET:HB3	1.99	0.45
1:B:36:LYS:NZ	1:B:338[B]:TYR:OH	2.49	0.45
1:B:46:LYS:HD3	1:B:47:THR:H	1.81	0.45
1:B:43:THR:H	1:B:242:THR:HG23	1.81	0.45
1:B:9:SER:HA	1:B:248:VAL:HG22	1.99	0.45
1:A:246:ILE:HD11	1:B:246:ILE:HD11	2.00	0.44
1:B:266:ASP:OD2	1:B:269:LYS:NZ	2.49	0.44
1:A:11:SER:HB3	1:A:164:ALA:HB3	1.99	0.44
1:A:121:LEU:O	1:A:258:GLY:HA3	2.17	0.44
1:B:207:ILE:HG23	1:B:211:LEU:HD12	2.00	0.44
1:A:336:ARG:NH1	2:A:701:EDO:O2	2.50	0.44
3:A:704:PPK:O2G	1:B:265:LYS:NZ	2.44	0.44
1:A:267:PRO:O	1:A:273:SER:OG	2.18	0.43
1:B:138:ILE:HB	1:B:252:GLY:HA3	2.00	0.43
1:A:110:ASP:HB3	1:A:113:GLU:HG3	1.99	0.43
1:A:277:ALA:O	1:A:281:VAL:HG12	2.19	0.43
1:B:336:ARG:O	1:B:340[B]:LEU:HG	2.19	0.43
1:A:82:MET:HE3	1:A:161[A]:ARG:HD2	2.00	0.42
1:A:199:GLN:HA	1:A:224:ILE:HG21	2.00	0.42
1:B:147:ARG:CB	1:B:210:ILE:HD11	2.48	0.42
1:B:121:LEU:O	1:B:258:GLY:HA3	2.19	0.42
1:B:296:ILE:O	1:B:296:ILE:HG13	2.18	0.42
1:A:54:GLY:HA2	1:B:239[B]:CYS:SG	2.60	0.42
1:B:118:ASP:OD1	1:B:119:GLN:N	2.52	0.42
1:A:314:THR:OG1	1:A:318:GLU:OE1	2.35	0.41
1:B:147:ARG:HA	1:B:150:GLU:HB3	2.02	0.41
1:B:10:VAL:HG12	1:B:165:LYS:HG2	2.02	0.41
1:B:13:GLY:HA3	1:B:162:PRO:HB2	2.02	0.41
1:B:175:GLY:HA2	2:B:801:EDO:H22	2.03	0.41
1:B:292:ASP:HB2	1:B:317:THR:HB	2.03	0.41
1:A:2:LYS:HE2	1:A:2:LYS:HB2	1.88	0.40
1:A:363:GLU:H	1:A:363:GLU:HG2	1.75	0.40
1:B:160:LEU:HD12	1:B:160:LEU:HA	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	377/384 (98%)	361 (96%)	15 (4%)	1 (0%)	41 61
1	B	379/384 (99%)	357 (94%)	19 (5%)	3 (1%)	19 35
All	All	756/768 (98%)	718 (95%)	34 (4%)	4 (0%)	29 48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	315	PHE
1	B	98	GLN
1	A	47	THR
1	B	100	PRO

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	311/312 (100%)	297 (96%)	14 (4%)	27 51
1	B	313/312 (100%)	291 (93%)	22 (7%)	15 29
All	All	624/624 (100%)	588 (94%)	36 (6%)	19 38

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	VAL
1	A	62	VAL

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Mol	Chain	Res	Type
1	A	97	LYS
1	A	121	LEU
1	A	160	LEU
1	A	174	ASP
1	A	185	LEU
1	A	191	GLU
1	A	193	ILE
1	A	202	VAL
1	A	230	PHE
1	A	248	VAL
1	A	318	GLU
1	A	340	LEU
1	B	2	LYS
1	B	46	LYS
1	B	47	THR
1	B	78	VAL
1	B	97	LYS
1	B	99	SER
1	B	106	VAL
1	B	107	ASP
1	B	108	ARG
1	B	121	LEU
1	B	131	ASP
1	B	148	GLN
1	B	160	LEU
1	B	161	ARG
1	B	177	ILE
1	B	186	SER
1	B	191	GLU
1	B	242	THR
1	B	296	ILE
1	B	311	MET
1	B	354	THR
1	B	372	LYS

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

Mol	Chain	Res	Type
1	B	148	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
2	EDO	B	801	-	3,3,3	0.45	0	2,2,2	0.35	0
5	PO4	A	706	-	4,4,4	0.88	0	6,6,6	0.43	0
3	PPK	B	802	4	11,12,12	2.65	5 (45%)	15,20,20	1.38	1 (6%)
2	EDO	A	702	-	3,3,3	0.45	0	2,2,2	0.36	0
2	EDO	A	701	-	3,3,3	0.42	0	2,2,2	0.40	0
3	PPK	A	704	4	11,12,12	2.71	5 (45%)	15,20,20	1.26	1 (6%)
2	EDO	A	703	-	3,3,3	0.46	0	2,2,2	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	801	-	-	0/1/1/1	-
3	PPK	B	802	4	-	1/8/12/12	-
2	EDO	A	702	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	701	-	-	1/1/1/1	-
3	PPK	A	704	4	-	3/8/12/12	-
2	EDO	A	703	-	-	0/1/1/1	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	704	PPK	PB-O3A	5.15	1.65	1.59
3	B	802	PPK	PB-O3A	4.93	1.65	1.59
3	A	704	PPK	PB-O2B	3.42	1.51	1.46
3	A	704	PPK	PG-O3G	3.40	1.51	1.46
3	B	802	PPK	PB-O2B	3.33	1.51	1.46
3	B	802	PPK	PG-O3G	3.24	1.51	1.46
3	A	704	PPK	PG-N3B	3.01	1.71	1.63
3	B	802	PPK	PB-N3B	2.99	1.71	1.63
3	B	802	PPK	PG-N3B	2.99	1.71	1.63
3	A	704	PPK	PB-N3B	2.98	1.71	1.63

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	802	PPK	PB-O3A-PA	-2.53	123.72	132.62
3	A	704	PPK	PB-O3A-PA	-2.28	124.58	132.62

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	704	PPK	PB-N3B-PG-O3G
3	A	704	PPK	PG-N3B-PB-O2B
3	A	704	PPK	PB-O3A-PA-O4A
2	A	701	EDO	O1-C1-C2-O2
3	B	802	PPK	PB-O3A-PA-O2A

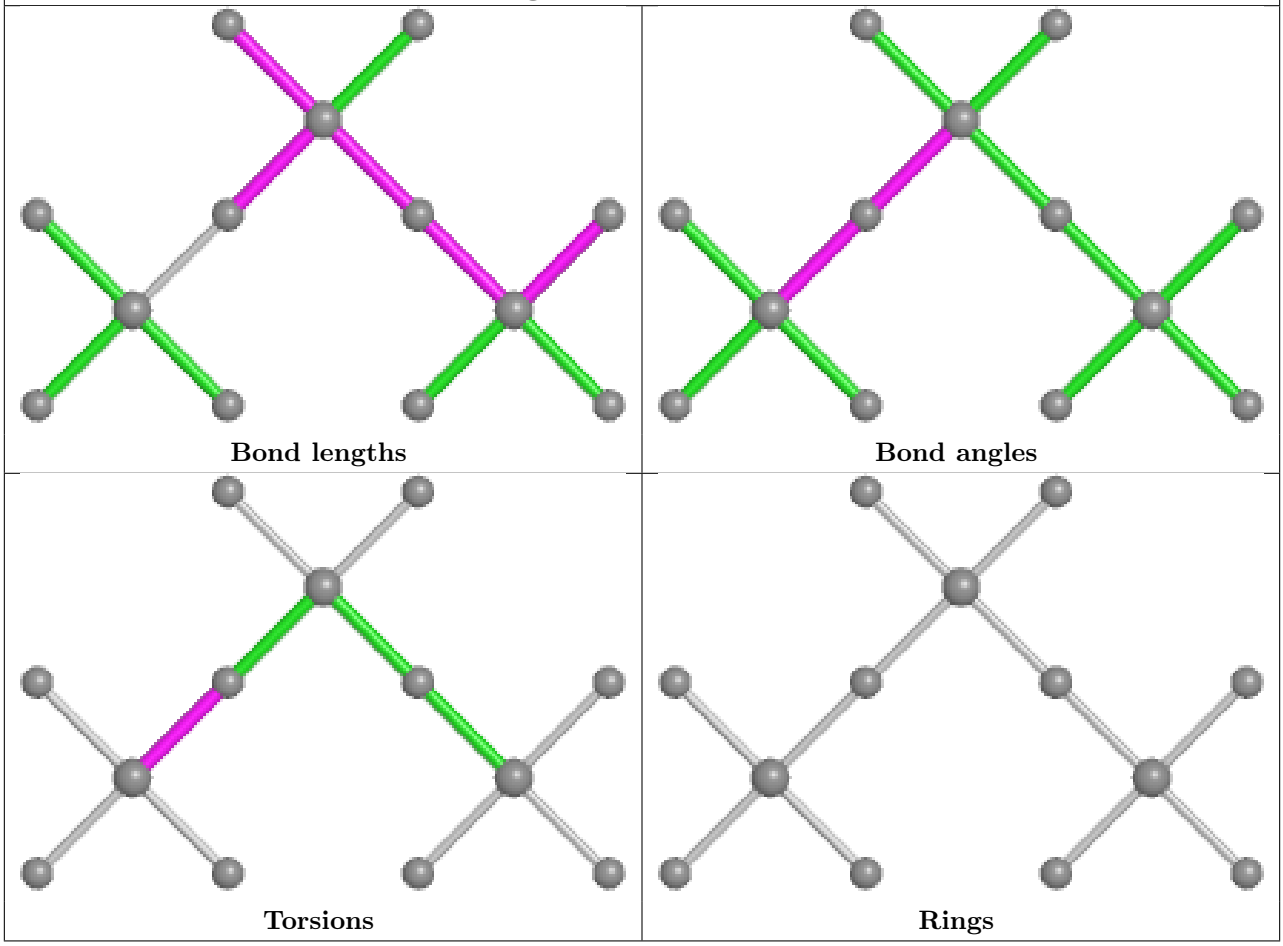
There are no ring outliers.

3 monomers are involved in 3 short contacts:

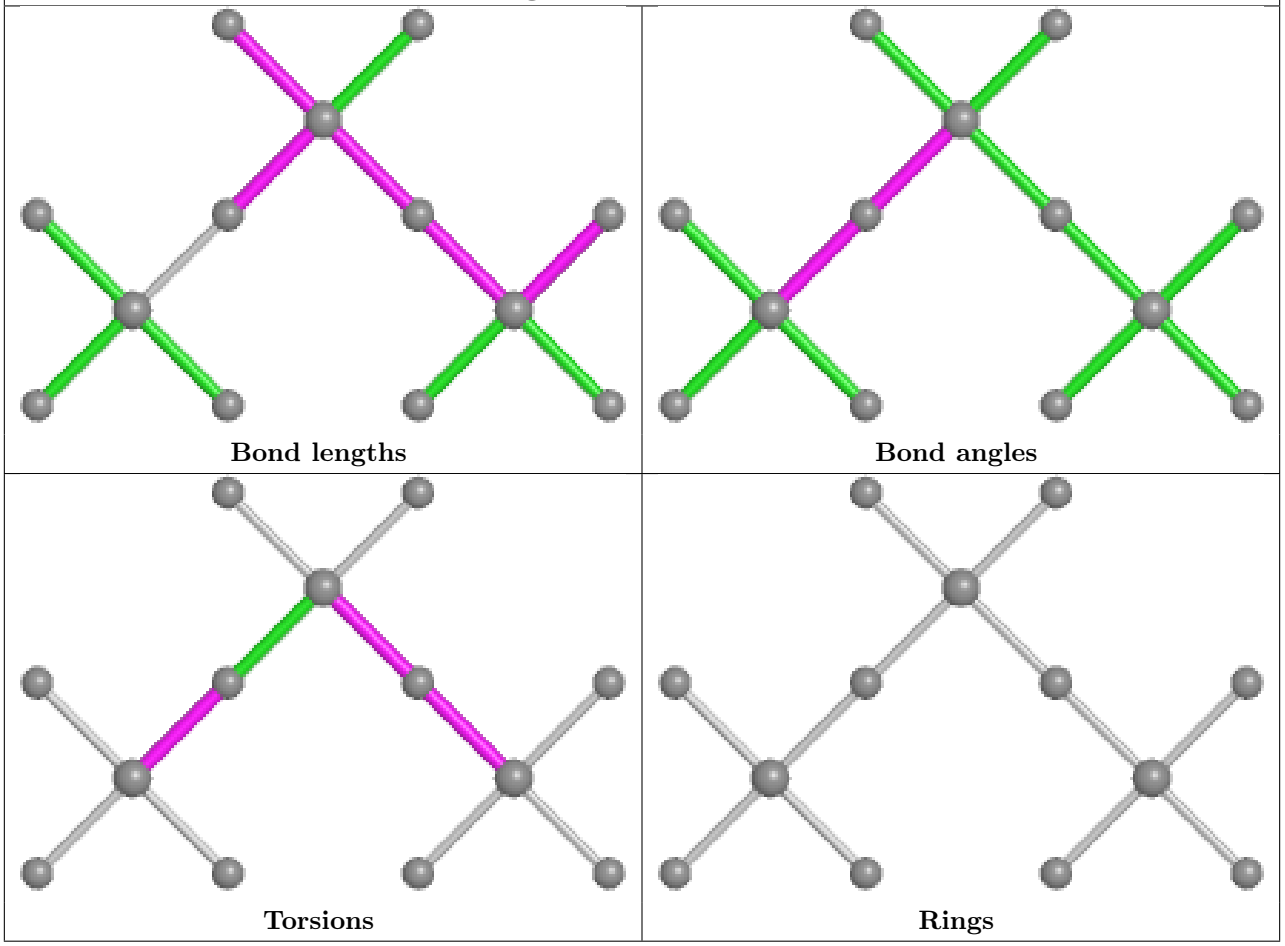
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	EDO	1	0
2	A	701	EDO	1	0
3	A	704	PPK	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 PPK B 802



Ligand PPK A 704



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	375/384 (97%)	0.55	46 (12%)	4 3	55, 80, 113, 160	0
1	B	378/384 (98%)	1.11	88 (23%)	0 0	61, 97, 170, 224	0
All	All	753/768 (98%)	0.83	134 (17%)	1 1	55, 85, 160, 224	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	206	ILE	8.3
1	B	157	LEU	7.8
1	B	100	PRO	7.6
1	B	183	VAL	7.1
1	B	211	LEU	7.1
1	B	151	VAL	6.8
1	B	258	GLY	6.3
1	B	215	TRP	6.0
1	B	356	ALA	5.9
1	A	259	GLY	5.7
1	B	159	TRP	5.6
1	B	140	TYR	5.5
1	A	99	SER	5.2
1	B	207	ILE	5.1
1	B	101	ASP	5.0
1	B	61	TRP	4.9
1	B	239[A]	CYS	4.7
1	B	259	GLY	4.6
1	B	212	PRO	4.5
1	B	208	LYS	4.3
1	B	106	VAL	4.3
1	B	179	GLY	4.3
1	B	160	LEU	4.2
1	B	214	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	258	GLY	4.2
1	B	223	PHE	4.1
1	A	244	ARG	4.1
1	B	144	LEU	3.9
1	B	198	LEU	3.9
1	A	106	VAL	3.9
1	A	243	GLY	3.8
1	B	148	GLN	3.8
1	A	261	ALA	3.8
1	B	193	ILE	3.8
1	B	182	ALA	3.7
1	A	260	GLY	3.7
1	B	178	VAL	3.6
1	A	241	LEU	3.6
1	A	239	CYS	3.5
1	A	121	LEU	3.4
1	B	180	ILE	3.3
1	A	159	TRP	3.3
1	B	377	ARG	3.3
1	B	242	THR	3.2
1	B	243	GLY	3.1
1	B	383	LYS	3.1
1	A	193	ILE	3.1
1	A	252	GLY	3.1
1	B	121	LEU	3.1
1	A	44	TYR	3.1
1	B	221	LYS	3.1
1	B	286	VAL	3.1
1	B	7	SER	3.0
1	B	255	ALA	3.0
1	A	61	TRP	3.0
1	B	332	PHE	3.0
1	B	241	LEU	3.0
1	B	381	GLY	3.0
1	A	16	ASP	3.0
1	A	332	PHE	2.9
1	B	229	ARG	2.9
1	B	210	ILE	2.9
1	B	216	LEU	2.9
1	A	257	HIS	2.8
1	B	231	VAL	2.8
1	B	181	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	242	THR	2.8
1	B	261	ALA	2.8
1	B	196	LYS	2.8
1	B	253	GLY	2.8
1	B	82	MET	2.8
1	B	257	HIS	2.8
1	A	255	ALA	2.7
1	A	376	LEU	2.7
1	B	44	TYR	2.7
1	B	230	PHE	2.7
1	A	7	SER	2.7
1	B	203	MET	2.7
1	B	190	SER	2.7
1	B	200	GLU	2.7
1	B	247[A]	ILE	2.7
1	B	122	MET	2.7
1	B	98	GLN	2.6
1	A	240	GLY	2.6
1	A	56	ILE	2.6
1	A	122	MET	2.6
1	B	185	LEU	2.6
1	B	244	ARG	2.6
1	A	120	GLY	2.5
1	A	247	ILE	2.5
1	A	238	ASP	2.5
1	B	204	GLU	2.5
1	A	246	ILE	2.5
1	B	9	SER	2.5
1	B	152	ARG	2.5
1	A	271	ASP	2.4
1	A	177	ILE	2.4
1	A	328	LEU	2.4
1	B	78	VAL	2.4
1	B	99	SER	2.4
1	B	5	PHE	2.4
1	B	147	ARG	2.4
1	B	220	THR	2.4
1	B	246	ILE	2.3
1	A	253	GLY	2.3
1	B	254	MET	2.3
1	B	97	LYS	2.3
1	B	248	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	97	LYS	2.3
1	B	218	SER	2.2
1	A	98	GLN	2.2
1	A	60	ALA	2.2
1	B	156	THR	2.2
1	B	194	ASP	2.2
1	A	157	LEU	2.2
1	B	382	LEU	2.2
1	B	245	LYS	2.2
1	B	79	HIS	2.1
1	B	192	GLU	2.1
1	B	186	SER	2.1
1	A	377	ARG	2.1
1	A	263	SER	2.1
1	B	184	VAL	2.1
1	A	375	LEU	2.1
1	B	289	GLY	2.1
1	A	107	ASP	2.1
1	A	379	ALA	2.1
1	B	222	PHE	2.1
1	B	107	ASP	2.0
1	A	218	SER	2.0
1	A	342[A]	GLN	2.0
1	B	240	GLY	2.0
1	B	357	TYR	2.0
1	A	15	PRO	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)

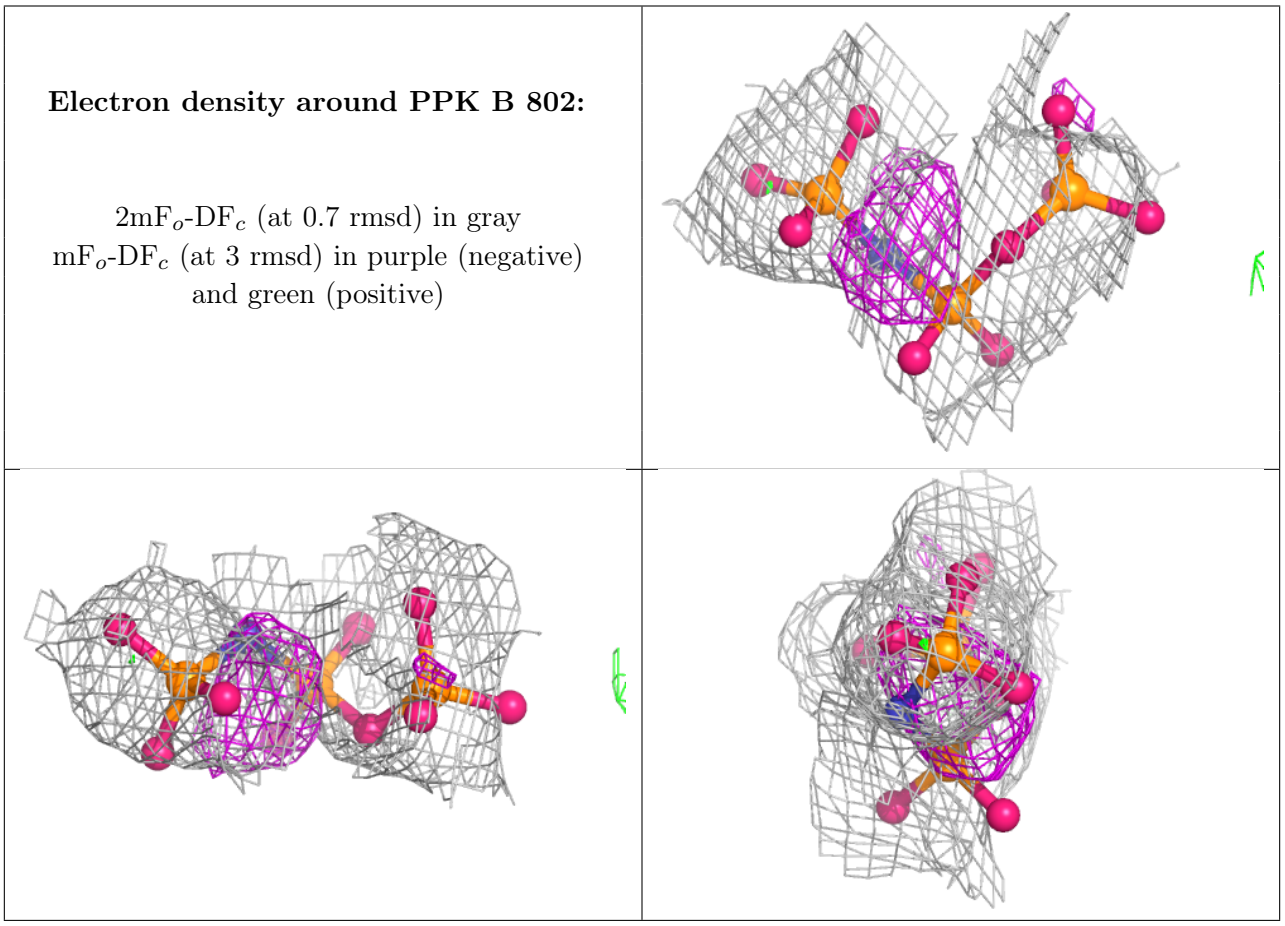
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	EDO	B	801	4/4	0.61	0.46	116,116,117,117	0
3	PPK	B	802	13/13	0.70	0.48	102,135,140,141	13
5	PO4	A	706	5/5	0.78	0.24	138,138,138,139	0
2	EDO	A	703	4/4	0.82	0.21	102,103,104,106	0
3	PPK	A	704	13/13	0.83	0.29	100,125,133,135	0
4	MG	A	705	1/1	0.84	0.15	77,77,77,77	0
2	EDO	A	702	4/4	0.91	0.25	86,88,88,89	0
2	EDO	A	701	4/4	0.92	0.29	72,73,74,81	0
4	MG	B	803	1/1	0.94	0.60	98,98,98,98	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.

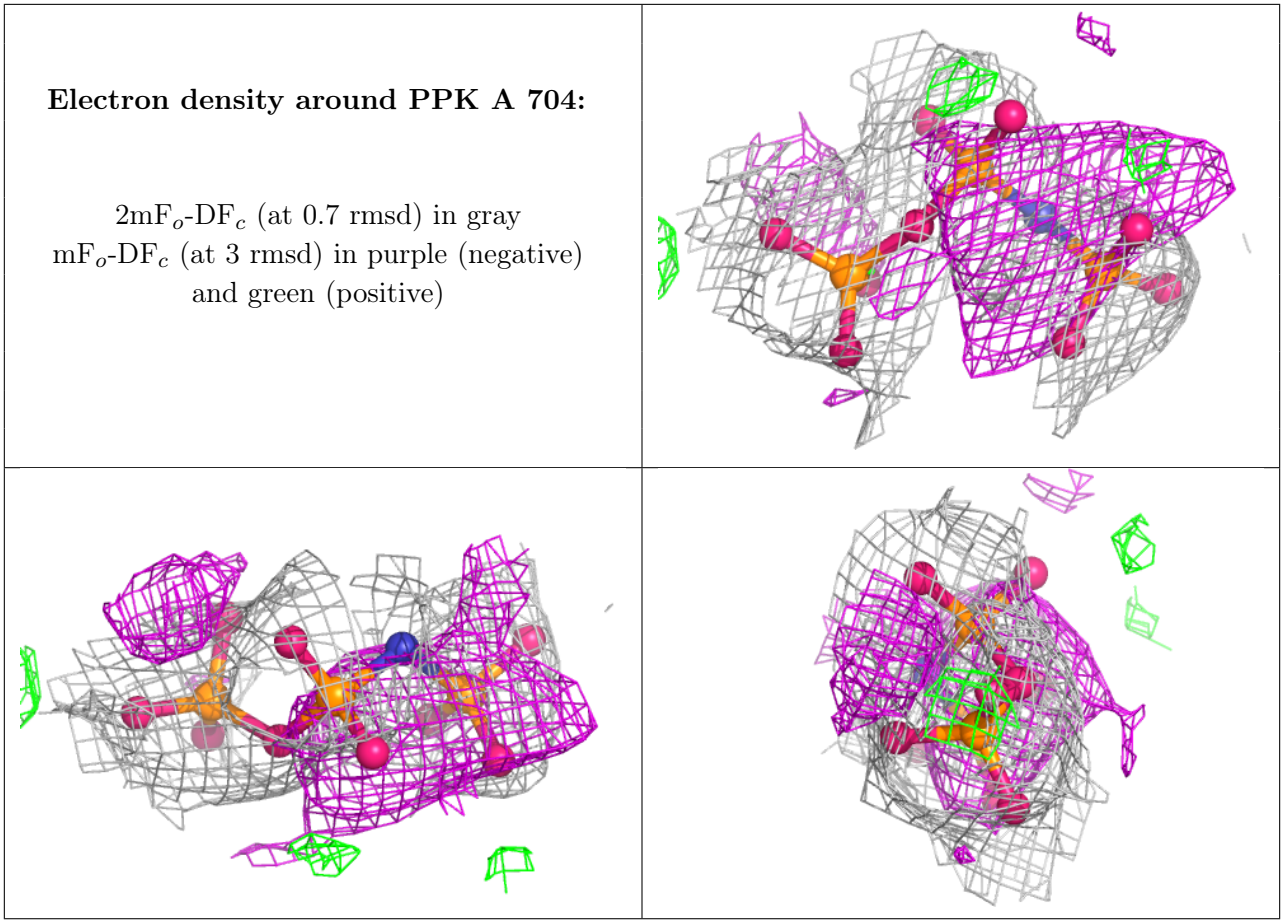
Electron density around PPK B 802:

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



Electron density around PPK A 704:

$2mF_o$-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.