



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2022 – 08:04 PM EST

PDB ID : 7LL3  
Title : S-adenosylmethionine synthetase co-crystallized with UppNHp  
Authors : Tan, L.L.; Jackson, C.J.  
Deposited on : 2021-02-03  
Resolution : 2.24 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](mailto: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.

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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 : 2.26  
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) : 2.26

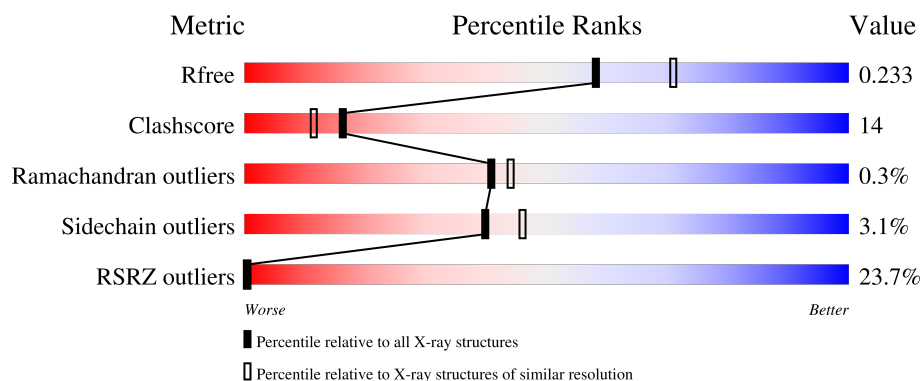
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.24 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	384	
1	B	384	

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	702	-	-	-	X
4	PPK	A	705	-	-	-	X
4	PPK	B	703	-	-	-	X
5	MG	A	707	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6070 atoms, of which 1 is hydrogen 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	376	Total	C	N	O	S	0	4	0
			2923	1847	500	562	14			
1	B	379	Total	C	N	O	S	0	3	0
			2936	1852	499	572	13			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



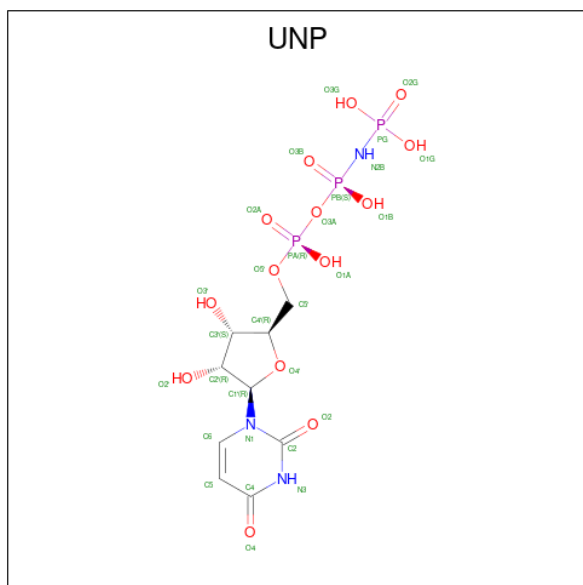
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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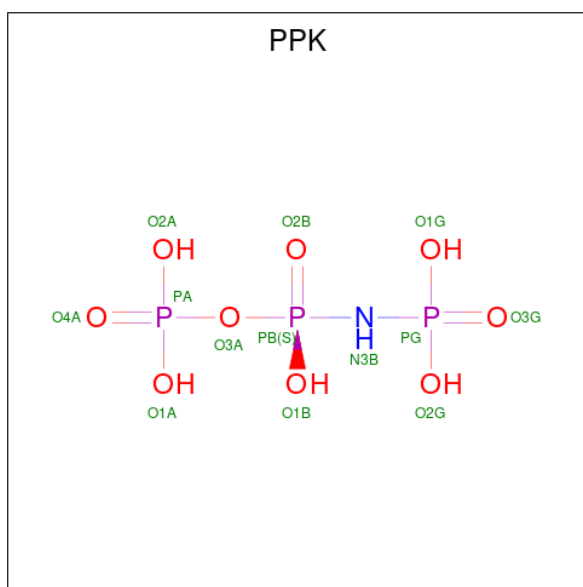
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is 5'-O-[(R)-hydroxy{[(S)-hydroxy(phosphonoamino)phosphoryl]oxy}phosphoryl]uridine (three-letter code: UNP) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>3</sub>O<sub>14</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			29	9	3	14	3		

- Molecule 4 is (DIPHOSPHONO)AMINOPHOSPHONIC ACID (three-letter code: PPK) (formula: H<sub>6</sub>NO<sub>9</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	H	N	O	P	0	0
			14	1	1	9	3		
4	B	1	Total	N	O	P		0	0
			13	1	9	3			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		

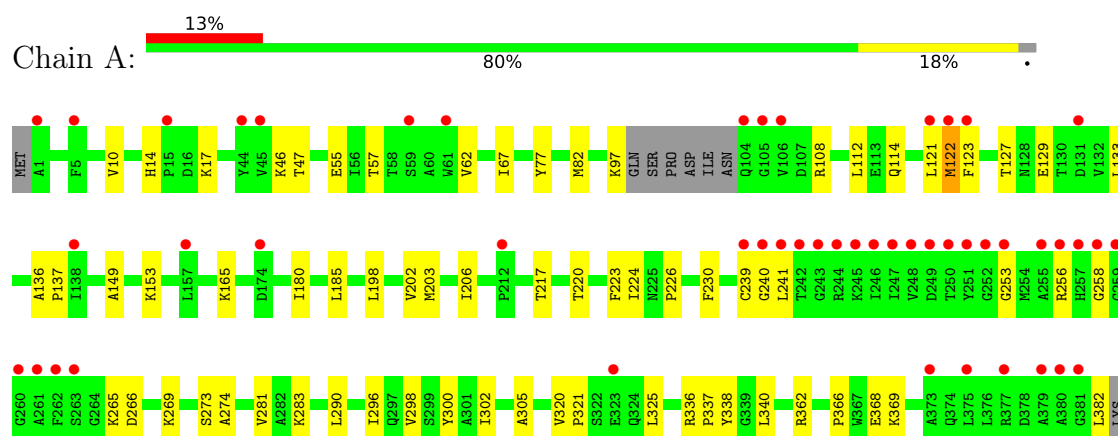
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	72	Total	O	0	0
			72	72		
6	B	61	Total	O	0	0
			61	61		

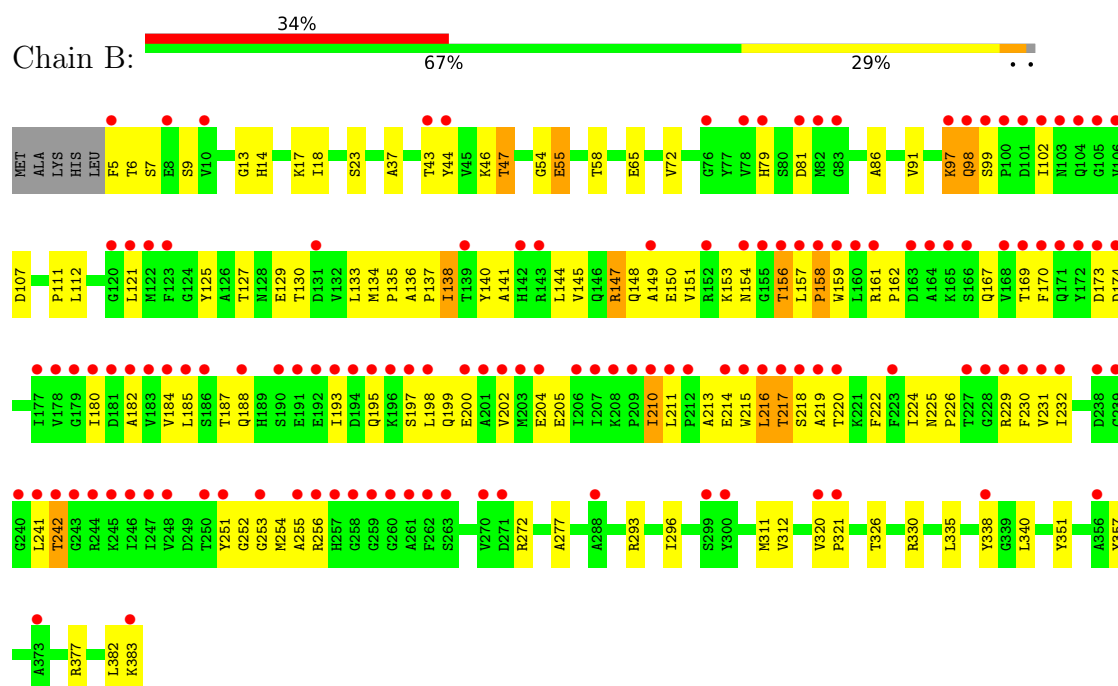
### 3 Residue-property plots [i](#)

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



#### • Molecule 1: S-adenosylmethionine synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.66Å 123.66Å 289.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.98 – 2.24 43.98 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.98-2.24) 99.9 (43.98-2.24)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.211 , 0.234 0.211 , 0.233	Depositor DCC
$R_{free}$ test set	3190 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.6	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 70.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6070	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PPK, EDO, UNP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.29	0/2981	0.47	0/4040
1	B	0.27	0/2995	0.46	0/4062
All	All	0.28	0/5976	0.47	0/8102

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	2923	0	2887	61	0
1	B	2936	0	2886	116	0
2	A	12	0	18	1	0
2	B	8	0	12	0	0
3	A	29	0	12	0	0
4	A	13	1	1	1	0
4	B	13	0	1	0	0
5	A	2	0	0	0	0
6	A	72	0	0	1	0
6	B	61	0	0	3	0
All	All	6069	1	5817	169	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 14.

All (169) 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:138:ILE:H	1:B:138:ILE:HD12	1.29	0.95
1:B:135:PRO:HG2	1:B:138:ILE:HD13	1.57	0.85
1:B:138:ILE:HG12	1:B:252:GLY:HA3	1.62	0.81
1:A:122:MET:HE2	1:A:298:VAL:HG23	1.65	0.79
1:B:43:THR:H	1:B:242:THR:CG2	1.97	0.78
1:B:157:LEU:N	1:B:158:PRO:HD2	1.98	0.77
1:B:180:ILE:H	1:B:215:TRP:HB3	1.50	0.77
1:A:122:MET:CE	1:A:298:VAL:HG23	2.15	0.77
1:B:46:LYS:HE3	1:B:47:THR:HG22	1.68	0.75
1:B:148:GLN:O	1:B:151:VAL:HG22	1.86	0.75
1:A:223:PHE:HB3	1:A:226:PRO:HG3	1.71	0.73
1:B:7:SER:OG	1:B:138:ILE:HG13	1.87	0.73
1:B:99:SER:HB2	1:B:102:ILE:HD12	1.71	0.73
1:A:55:GLU:OE2	1:A:97:LYS:HB2	1.88	0.72
1:B:167:GLN:HB3	1:B:184:VAL:HB	1.71	0.72
1:B:7:SER:HB3	1:B:137:PRO:HB2	1.71	0.72
1:A:185[A]:LEU:HD23	1:A:202:VAL:CG1	2.22	0.70
1:B:217:THR:HG23	1:B:219:ALA:H	1.56	0.70
1:B:55:GLU:OE2	6:B:801:HOH:O	2.12	0.68
1:B:138:ILE:CG1	1:B:252:GLY:HA3	2.22	0.68
1:B:43:THR:H	1:B:242:THR:HG23	1.57	0.68
1:B:145:VAL:HG23	1:B:357:TYR:CE1	2.29	0.67
1:B:335:LEU:HA	1:B:340:LEU:HD21	1.77	0.66
1:B:125:TYR:OH	1:B:293:ARG:HD2	1.95	0.66
1:A:302:ILE:CG2	1:B:226:PRO:HG2	2.25	0.66
1:B:217:THR:O	1:B:220:THR:HG22	1.95	0.65
1:B:112:LEU:HD23	1:B:338[B]:TYR:CD2	2.30	0.65
1:B:148:GLN:N	1:B:148:GLN:OE1	2.29	0.64
1:A:122:MET:HE1	1:A:300:TYR:CE1	2.31	0.64
1:B:377:ARG:HE	1:B:383:LYS:HD3	1.61	0.64
1:B:377:ARG:HH21	1:B:383:LYS:HG3	1.62	0.64
1:B:202:VAL:HG11	1:B:224:ILE:HG23	1.79	0.63
1:B:205:GLU:HA	1:B:205:GLU:OE1	1.97	0.63
1:B:156:THR:C	1:B:158:PRO:HD2	2.19	0.62
1:A:203:MET:HE1	1:A:224:ILE:HD11	1.81	0.62
1:B:147:ARG:NH1	1:B:205:GLU:O	2.33	0.62
1:B:138:ILE:HG12	1:B:252:GLY:CA	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:VAL:HG23	1:B:357:TYR:CD1	2.35	0.62
1:B:216:LEU:HB3	1:B:220:THR:HG21	1.81	0.61
1:B:13:GLY:HA3	1:B:162:PRO:CB	2.31	0.61
1:A:265:LYS:HB3	1:A:269:LYS:HG3	1.82	0.61
1:A:10:VAL:HG23	1:A:17:LYS:HG3	1.82	0.60
1:A:302:ILE:HG23	1:B:226:PRO:HG2	1.82	0.60
1:B:72:VAL:HG12	1:B:86:ALA:HB2	1.82	0.60
1:B:320:VAL:HG22	1:B:321:PRO:HD2	1.83	0.60
1:B:277:ALA:CB	1:B:340:LEU:HD22	2.31	0.59
1:A:253:GLY:O	1:B:256:ARG:HD2	2.01	0.59
1:A:46:LYS:NZ	1:B:55:GLU:OE1	2.34	0.59
1:B:135:PRO:CG	1:B:138:ILE:HD13	2.32	0.58
1:A:320:VAL:HB	1:A:321:PRO:HD2	1.85	0.58
1:A:122:MET:HE1	1:A:300:TYR:CD1	2.39	0.57
1:A:203:MET:CE	1:A:224:ILE:HD11	2.34	0.57
1:B:220:THR:HG23	1:B:222:PHE:CE1	2.39	0.57
1:A:122:MET:HE3	1:A:274:ALA:HB1	1.87	0.57
1:B:216:LEU:HD22	1:B:216:LEU:H	1.69	0.57
1:A:240:GLY:C	1:A:241:LEU:HD12	2.25	0.56
1:B:229:ARG:CZ	1:B:231:VAL:HG21	2.35	0.56
1:B:7:SER:HB3	1:B:137:PRO:CB	2.35	0.56
1:B:43:THR:H	1:B:242:THR:HG21	1.71	0.56
1:A:180:ILE:O	1:A:220:THR:HG22	2.05	0.56
1:B:320:VAL:CG2	1:B:321:PRO:HD2	2.36	0.56
1:B:13:GLY:HA3	1:B:162:PRO:HB2	1.88	0.55
1:A:77:TYR:HA	1:A:82:MET:HE2	1.89	0.55
1:B:213:ALA:HA	6:B:833:HOH:O	2.06	0.55
1:B:377:ARG:HH21	1:B:383:LYS:CG	2.19	0.55
1:A:185[B]:LEU:HD13	1:A:202:VAL:CG1	2.36	0.55
1:B:79:HIS:ND1	1:B:81:ASP:HB2	2.22	0.54
1:B:202:VAL:HB	1:B:224:ILE:HG21	1.90	0.54
1:A:256:ARG:HD2	1:B:253:GLY:O	2.08	0.53
1:A:121:LEU:HD13	1:B:6:THR:O	2.08	0.53
1:A:122:MET:HE3	1:A:274:ALA:CB	2.39	0.53
1:A:46:LYS:HD3	1:A:239[A]:CYS:SG	2.49	0.52
1:B:5:PHE:N	1:B:170:PHE:O	2.42	0.52
1:B:9:SER:HB3	1:B:141:ALA:HB1	1.91	0.52
1:B:127:THR:OG1	1:B:129:GLU:HG3	2.09	0.52
1:B:277:ALA:HB2	1:B:340:LEU:HD22	1.92	0.51
1:A:55:GLU:HB3	1:A:97:LYS:NZ	2.25	0.51
1:B:14:HIS:O	1:B:18:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:THR:CG2	1:B:134:MET:H	2.24	0.51
1:B:216:LEU:CA	1:B:220:THR:HG21	2.39	0.51
1:B:138:ILE:HG12	1:B:251:TYR:C	2.31	0.51
1:B:224:ILE:N	1:B:224:ILE:HD12	2.27	0.50
1:B:200:GLU:O	1:B:204:GLU:HG2	2.12	0.50
1:B:130:THR:HG22	1:B:134:MET:O	2.12	0.50
1:B:193:ILE:HD11	1:B:197:SER:OG	2.12	0.50
1:B:377:ARG:HE	1:B:383:LYS:CD	2.25	0.49
1:B:72:VAL:CG1	1:B:86:ALA:HB2	2.42	0.49
1:B:136:ALA:HB3	1:B:137:PRO:HD3	1.94	0.49
1:B:326:THR:O	1:B:330:ARG:HG3	2.12	0.49
1:A:127:THR:OG1	1:A:129:GLU:HG3	2.12	0.49
1:B:216:LEU:HB3	1:B:222:PHE:HZ	1.77	0.49
1:A:62:VAL:HG13	1:A:67:ILE:CD1	2.43	0.49
1:B:335:LEU:HA	1:B:340:LEU:CD2	2.42	0.48
1:A:127:THR:O	1:A:133:LEU:HA	2.14	0.48
1:A:185[B]:LEU:HD11	1:A:206:ILE:HG21	1.94	0.48
1:A:266:ASP:OD1	1:A:269:LYS:NZ	2.47	0.48
1:A:57:THR:CG2	1:A:97:LYS:HG2	2.43	0.48
1:B:149:ALA:O	1:B:153:LYS:HG2	2.13	0.48
1:A:273:SER:HB2	1:A:340:LEU:CD1	2.43	0.48
1:B:65:GLU:HA	1:B:91:VAL:HG11	1.96	0.47
1:A:14:HIS:CE1	4:A:705:PPK:O4A	2.66	0.47
1:B:157:LEU:N	1:B:158:PRO:CD	2.72	0.47
1:B:159:TRP:CD2	1:B:193:ILE:HG21	2.50	0.47
1:A:46:LYS:HD2	1:A:47:THR:H	1.78	0.47
1:A:362:ARG:O	1:A:368:GLU:HG3	2.15	0.47
1:A:336:ARG:NH1	2:A:701:EDO:O2	2.38	0.47
1:B:377:ARG:HH21	1:B:383:LYS:CD	2.28	0.47
1:B:169:THR:HB	1:B:182:ALA:HB3	1.96	0.46
1:B:216:LEU:CB	1:B:220:THR:HG21	2.46	0.46
1:B:127:THR:O	1:B:133:LEU:HA	2.15	0.46
1:A:121:LEU:O	1:A:258:GLY:HA3	2.15	0.46
1:B:150:GLU:HG2	1:B:151:VAL:N	2.30	0.46
1:B:161:ARG:HD2	1:B:188:GLN:NE2	2.31	0.46
1:A:290:LEU:HB3	1:A:325:LEU:HD21	1.98	0.46
1:B:377:ARG:HH21	1:B:383:LYS:HD2	1.81	0.46
1:A:55:GLU:HB3	1:A:97:LYS:HZ2	1.81	0.46
1:A:112:LEU:HD23	1:A:338[B]:TYR:HD2	1.80	0.46
1:B:13:GLY:HA3	1:B:162:PRO:HB3	1.98	0.45
1:B:254:MET:CE	1:B:254:MET:HA	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:MET:HE1	1:A:300:TYR:HE1	1.79	0.45
1:B:140:TYR:O	1:B:144:LEU:HG	2.16	0.45
1:B:138:ILE:H	1:B:138:ILE:CD1	2.04	0.45
1:B:5:PHE:O	1:B:170:PHE:N	2.47	0.45
1:B:97:LYS:HA	1:B:97:LYS:HE3	1.99	0.45
1:B:220:THR:HG23	1:B:222:PHE:HE1	1.78	0.45
1:B:180:ILE:HB	1:B:216:LEU:HD13	2.00	0.44
1:B:198:LEU:HD11	6:B:836:HOH:O	2.16	0.44
1:B:210:ILE:O	1:B:211:LEU:HB2	2.18	0.44
1:B:154:ASN:OD1	1:B:157:LEU:HD13	2.17	0.44
1:B:272:ARG:NH2	1:B:351:TYR:HB3	2.32	0.44
1:A:123:PHE:HA	1:A:296:ILE:O	2.17	0.44
1:B:44:TYR:CD2	1:B:241:LEU:HD21	2.52	0.44
1:A:149:ALA:O	1:A:153:LYS:HG3	2.18	0.44
1:B:198:LEU:HD21	1:B:225:ASN:OD1	2.18	0.43
1:A:133:LEU:HD12	1:A:283:LYS:HG3	2.01	0.43
1:B:217:THR:OG1	1:B:218:SER:N	2.50	0.43
1:A:62:VAL:HG13	1:A:67:ILE:HD11	2.00	0.43
1:A:239[A]:CYS:SG	1:B:54:GLY:HA2	2.59	0.43
1:B:125:TYR:CG	1:B:255:ALA:HB2	2.53	0.43
1:A:108:ARG:HG3	1:A:114:GLN:HA	1.99	0.43
1:B:216:LEU:HD22	1:B:216:LEU:N	2.30	0.43
1:B:220:THR:HG23	1:B:220:THR:O	2.19	0.43
1:A:121:LEU:H	1:A:121:LEU:HD23	1.82	0.43
1:A:281:VAL:HG13	1:A:296:ILE:HG13	2.01	0.43
1:A:305:ALA:O	1:A:337:PRO:HD3	2.18	0.43
1:B:98:GLN:H	1:B:98:GLN:HG3	1.42	0.42
1:A:382:LEU:HD23	1:A:382:LEU:HA	1.90	0.42
1:B:382:LEU:O	1:B:383:LYS:HB2	2.20	0.42
1:B:17:LYS:HD3	1:B:17:LYS:HA	1.56	0.42
1:B:195:GLN:O	1:B:199:GLN:HG3	2.18	0.42
1:B:185:LEU:C	1:B:185:LEU:HD23	2.40	0.42
1:B:296:ILE:CD1	1:B:312:VAL:HG22	2.49	0.42
1:B:145:VAL:HG23	1:B:357:TYR:HE1	1.78	0.42
1:B:187:THR:HG22	1:B:188:GLN:O	2.20	0.42
1:A:366:PRO:O	1:A:369:LYS:HE2	2.20	0.42
1:A:122:MET:CE	1:A:300:TYR:HE1	2.33	0.42
1:A:258:GLY:O	6:A:801:HOH:O	2.22	0.42
1:B:37:ALA:HB1	1:B:58:THR:HB	2.01	0.42
1:A:10:VAL:HG12	1:A:165:LYS:HG2	2.01	0.41
1:A:62:VAL:CG1	1:A:67:ILE:HD12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ARG:HD3	1:B:254:MET:O	2.21	0.41
1:A:198:LEU:C	1:A:198:LEU:HD23	2.41	0.41
1:B:138:ILE:CD1	1:B:138:ILE:N	2.80	0.41
1:A:136:ALA:HB3	1:A:137:PRO:HD3	2.02	0.40
1:B:111:PRO:HB2	1:B:338[B]:TYR:CE2	2.56	0.40
1:B:232:ILE:O	1:B:232:ILE:HD12	2.22	0.40
1:A:217:THR:H	1:A:220:THR:CG2	2.34	0.40
1:B:44:TYR:CE1	1:B:46:LYS:HB2	2.56	0.40
1:B:23:SER:OG	1:B:242:THR:HG21	2.21	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	376/384 (98%)	361 (96%)	15 (4%)	0	100	100
1	B	380/384 (99%)	345 (91%)	33 (9%)	2 (0%)	29	28
All	All	756/768 (98%)	706 (93%)	48 (6%)	2 (0%)	41	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	158	PRO
1	B	217	THR

### 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	308/312 (99%)	306 (99%)	2 (1%)	86	90
1	B	311/312 (100%)	294 (94%)	17 (6%)	21	20
All	All	619/624 (99%)	600 (97%)	19 (3%)	40	46

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	MET
1	A	230	PHE
1	B	47	THR
1	B	55	GLU
1	B	97	LYS
1	B	98	GLN
1	B	107	ASP
1	B	121	LEU
1	B	138	ILE
1	B	147	ARG
1	B	156	THR
1	B	173	ASP
1	B	174	ASP
1	B	210	ILE
1	B	214	GLU
1	B	216	LEU
1	B	230	PHE
1	B	242	THR
1	B	311	MET

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	195	GLN

### 5.3.3 RNA ⓘ

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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	A	703	-	3,3,3	0.47	0	2,2,2	0.36	0
2	EDO	B	701	-	3,3,3	0.52	0	2,2,2	0.23	0
4	PPK	B	703	-	11,12,12	2.69	6 (54%)	15,20,20	1.24	1 (6%)
3	UNP	A	704	-	25,30,30	5.17	16 (64%)	27,47,47	1.46	4 (14%)
2	EDO	A	701	-	3,3,3	0.37	0	2,2,2	0.56	0
4	PPK	A	705	5	11,12,12	2.88	5 (45%)	15,20,20	1.33	2 (13%)
2	EDO	B	702	-	3,3,3	0.48	0	2,2,2	0.31	0
2	EDO	A	702	-	3,3,3	0.51	0	2,2,2	0.21	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	A	703	-	-	0/1/1/1	-
2	EDO	B	701	-	-	0/1/1/1	-
4	PPK	B	703	-	-	4/8/12/12	-
3	UNP	A	704	-	-	6/16/38/38	0/2/2/2
2	EDO	A	701	-	-	1/1/1/1	-
4	PPK	A	705	5	-	6/8/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	702	-	-	0/1/1/1	-
2	EDO	A	702	-	-	0/1/1/1	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	704	UNP	C2'-C1'	-11.28	1.36	1.53
3	A	704	UNP	O4'-C1'	9.34	1.54	1.41
3	A	704	UNP	C3'-C4'	-7.92	1.32	1.53
3	A	704	UNP	C6-N1	7.78	1.45	1.35
3	A	704	UNP	PB-O3A	7.23	1.68	1.59
3	A	704	UNP	C4-N3	7.16	1.45	1.33
3	A	704	UNP	O4'-C4'	7.11	1.60	1.45
3	A	704	UNP	C6-C5	5.66	1.50	1.38
4	A	705	PPK	PB-O3A	5.64	1.66	1.59
3	A	704	UNP	C2-N3	5.64	1.49	1.38
4	B	703	PPK	PB-O3A	5.13	1.65	1.59
3	A	704	UNP	PG-N2B	4.76	1.75	1.63
3	A	704	UNP	PG-O2G	4.34	1.53	1.46
3	A	704	UNP	C2'-C3'	4.31	1.65	1.53
4	A	705	PPK	PB-O2B	3.79	1.52	1.46
3	A	704	UNP	PB-N2B	3.46	1.72	1.63
4	B	703	PPK	PB-O2B	3.41	1.51	1.46
4	B	703	PPK	PG-O3G	3.35	1.51	1.46
4	A	705	PPK	PG-O3G	3.31	1.51	1.46
4	A	705	PPK	PG-N3B	3.29	1.72	1.63
4	A	705	PPK	PB-N3B	3.28	1.71	1.63
3	A	704	UNP	PB-O3B	3.18	1.51	1.46
3	A	704	UNP	PG-O1G	-3.07	1.48	1.56
4	B	703	PPK	PG-N3B	2.96	1.71	1.63
4	B	703	PPK	PB-N3B	2.95	1.71	1.63
3	A	704	UNP	PB-O1B	-2.52	1.50	1.56
4	B	703	PPK	PG-O2G	-2.01	1.51	1.56

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	704	UNP	C3'-C2'-C1'	3.68	106.52	100.98
3	A	704	UNP	O4'-C1'-C2'	-2.80	102.83	106.93
3	A	704	UNP	C2'-C3'-C4'	2.61	107.71	102.64
3	A	704	UNP	O3B-PB-N2B	-2.51	108.08	111.77
4	B	703	PPK	PB-O3A-PA	-2.24	124.74	132.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	705	PPK	PB-O3A-PA	-2.08	125.29	132.62
4	A	705	PPK	O1G-PG-O3G	-2.04	108.33	113.45

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	704	UNP	PG-N2B-PB-O3B
3	A	704	UNP	PG-N2B-PB-O3A
3	A	704	UNP	C3'-C4'-C5'-O5'
3	A	704	UNP	C2'-C1'-N1-C6
3	A	704	UNP	O4'-C1'-N1-C6
4	A	705	PPK	PB-N3B-PG-O3G
4	A	705	PPK	PG-N3B-PB-O2B
4	A	705	PPK	PG-N3B-PB-O3A
4	B	703	PPK	PB-N3B-PG-O3G
4	B	703	PPK	PA-O3A-PB-O1B
4	B	703	PPK	PA-O3A-PB-O2B
3	A	704	UNP	O4'-C4'-C5'-O5'
4	A	705	PPK	PB-O3A-PA-O4A
4	B	703	PPK	PG-N3B-PB-O2B
4	A	705	PPK	PB-O3A-PA-O1A
4	A	705	PPK	PB-O3A-PA-O2A
2	A	701	EDO	O1-C1-C2-O2

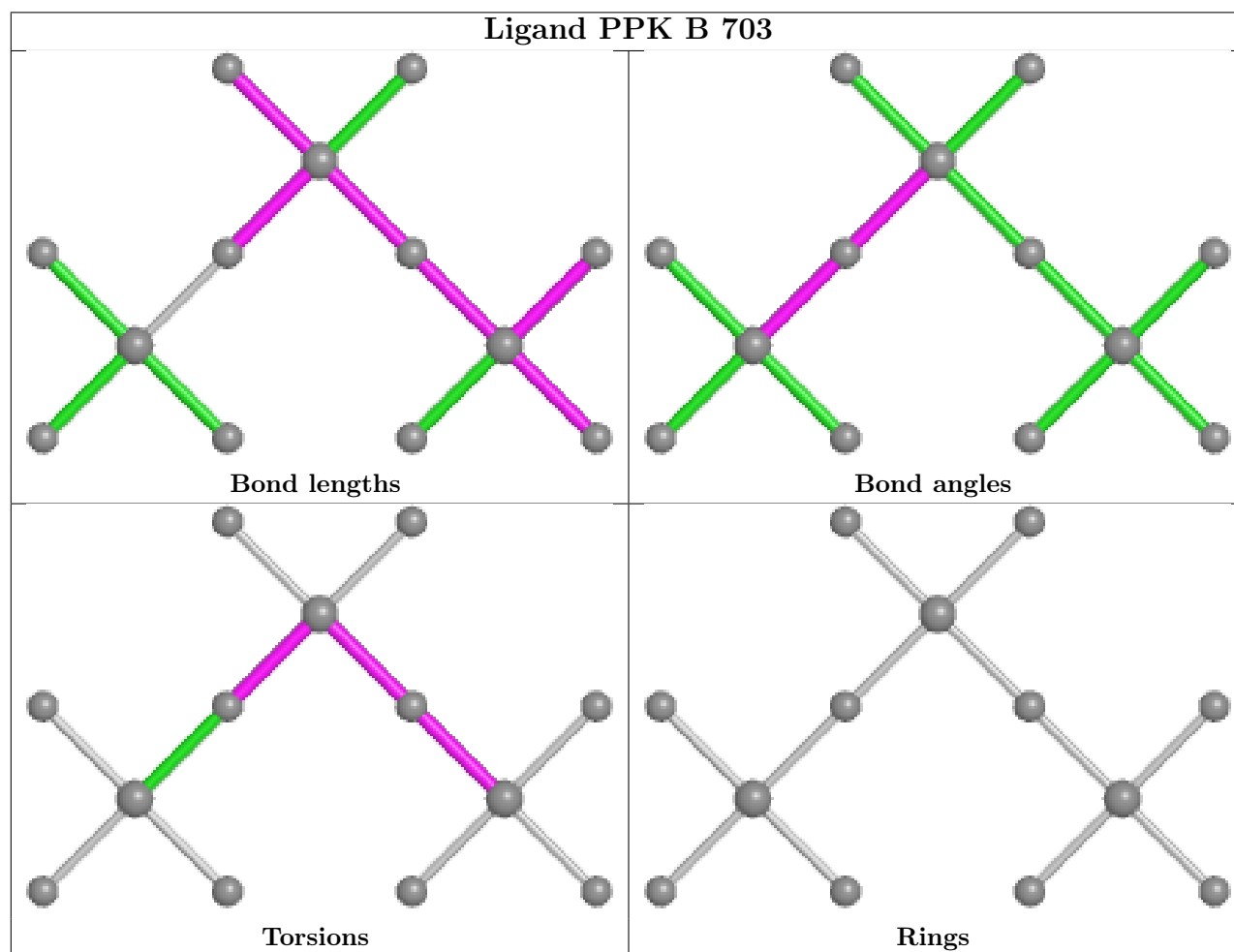
There are no ring outliers.

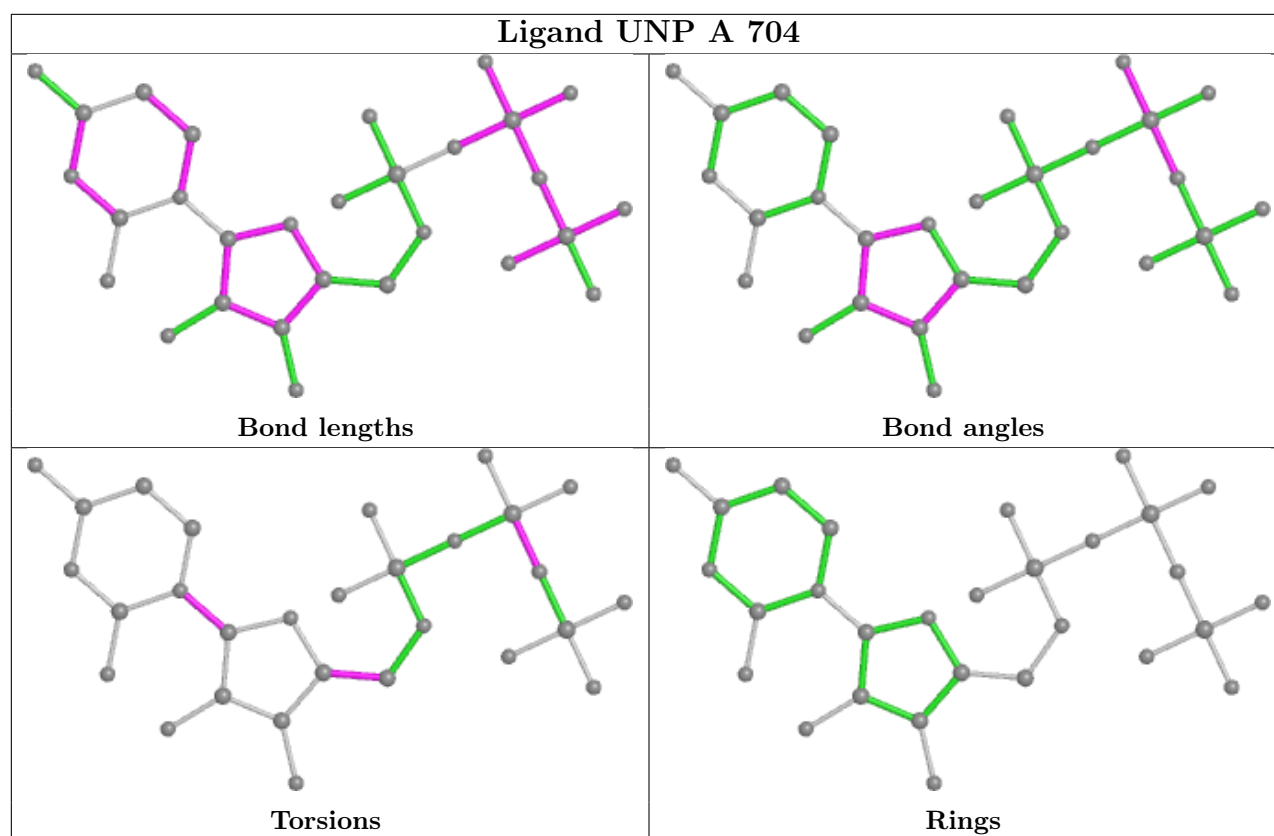
2 monomers are involved in 2 short contacts:

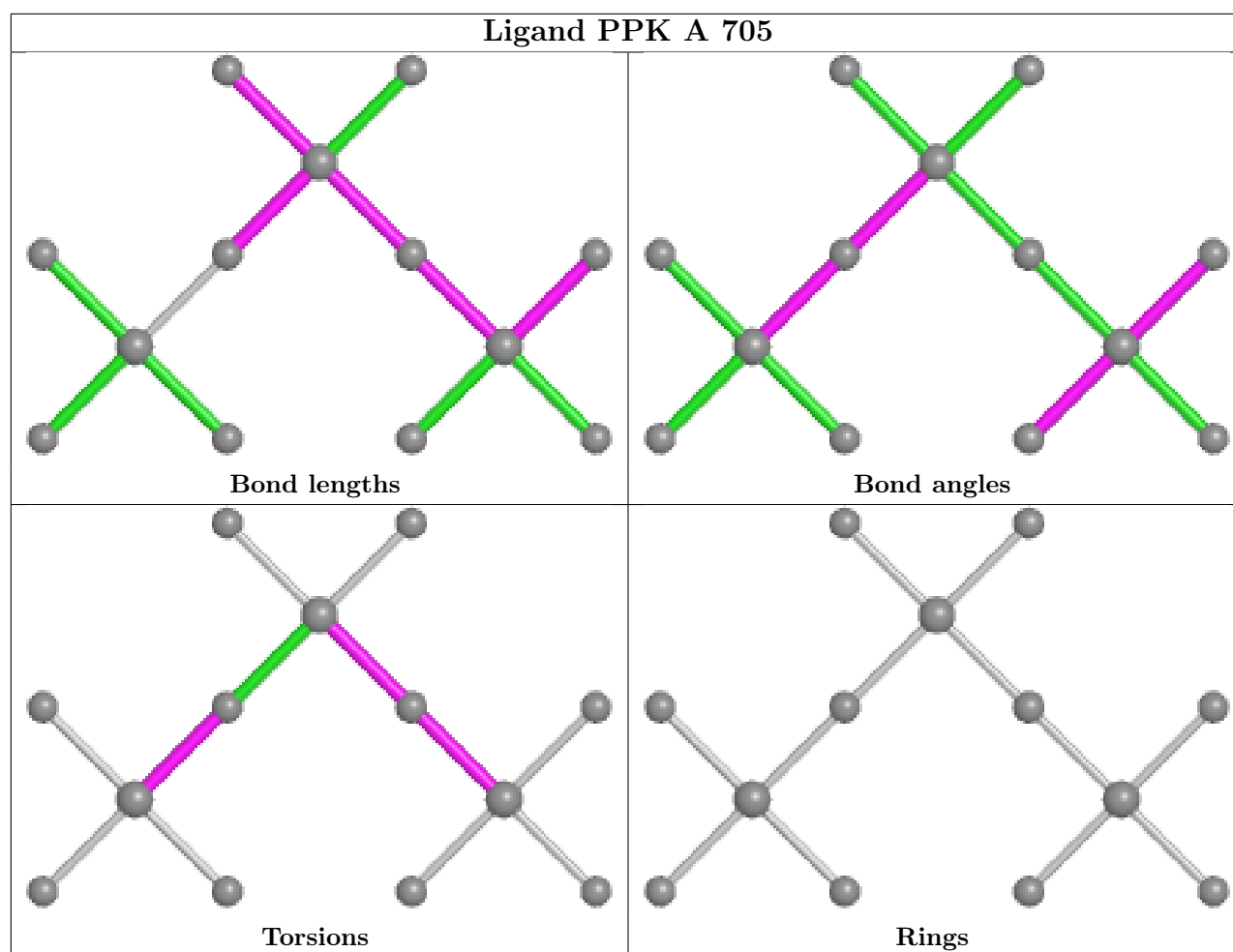
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	EDO	1	0
4	A	705	PPK	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	376/384 (97%)	0.66	49 (13%) <b>3</b> <b>2</b>	55, 77, 115, 191	0
1	B	379/384 (98%)	1.65	130 (34%) <b>0</b> <b>0</b>	58, 98, 200, 227	0
All	All	755/768 (98%)	1.16	179 (23%) <b>0</b> <b>0</b>	55, 84, 182, 227	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	101	ASP	11.5
1	B	160	LEU	10.5
1	B	215	TRP	8.2
1	B	209	PRO	7.6
1	B	105	GLY	7.3
1	B	100	PRO	6.9
1	B	203	MET	6.9
1	B	229	ARG	6.8
1	B	211	LEU	6.7
1	B	246	ILE	6.7
1	B	179	GLY	6.7
1	B	183	VAL	6.5
1	B	198	LEU	6.4
1	A	259	GLY	6.2
1	B	218	SER	6.0
1	A	246	ILE	5.8
1	B	258	GLY	5.8
1	B	182	ALA	5.8
1	B	159	TRP	5.7
1	B	207	ILE	5.6
1	A	260	GLY	5.6
1	A	241	LEU	5.6
1	B	149	ALA	5.5
1	B	190	SER	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	219	ALA	5.3
1	B	121	LEU	5.3
1	B	245	LYS	5.1
1	B	241	LEU	5.1
1	B	155	GLY	5.1
1	A	105	GLY	5.0
1	B	259	GLY	5.0
1	B	230	PHE	5.0
1	B	178	VAL	4.9
1	B	202	VAL	4.9
1	B	103	ASN	4.9
1	B	257	HIS	4.9
1	A	258	GLY	4.8
1	B	239	CYS	4.8
1	A	104	GLN	4.8
1	B	82	MET	4.7
1	A	121	LEU	4.7
1	B	196	LYS	4.7
1	B	184	VAL	4.7
1	B	194	ASP	4.6
1	B	260	GLY	4.6
1	A	106	VAL	4.6
1	B	197	SER	4.5
1	B	106	VAL	4.5
1	B	76	GLY	4.5
1	A	257	HIS	4.4
1	A	174	ASP	4.4
1	B	193	ILE	4.4
1	B	223	PHE	4.4
1	B	158	PRO	4.4
1	B	250	THR	4.3
1	B	227	THR	4.3
1	B	244	ARG	4.2
1	B	217	THR	4.2
1	A	255	ALA	4.2
1	B	216	LEU	4.1
1	B	243	GLY	4.1
1	B	174	ASP	4.1
1	A	261	ALA	4.0
1	B	122	MET	4.0
1	B	102	ILE	4.0
1	B	143	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	104	GLN	4.0
1	B	212	PRO	4.0
1	B	154	ASN	3.9
1	B	186	SER	3.9
1	B	247	ILE	3.8
1	A	239[A]	CYS	3.7
1	B	169	THR	3.7
1	A	379	ALA	3.7
1	B	185	LEU	3.7
1	B	242	THR	3.7
1	A	373	ALA	3.6
1	A	248	VAL	3.6
1	B	320	VAL	3.6
1	B	248	VAL	3.6
1	B	173	ASP	3.6
1	A	61	TRP	3.6
1	B	383	LYS	3.5
1	B	123	PHE	3.4
1	B	261	ALA	3.4
1	B	231	VAL	3.4
1	A	250	THR	3.3
1	B	180	ILE	3.3
1	A	240	GLY	3.3
1	A	243	GLY	3.2
1	A	245	LYS	3.2
1	B	253	GLY	3.2
1	B	262	PHE	3.2
1	B	81	ASP	3.2
1	B	172	TYR	3.1
1	B	157	LEU	3.1
1	B	208	LYS	3.1
1	A	247	ILE	3.1
1	A	323	GLU	3.0
1	A	212	PRO	3.0
1	B	228	GLY	3.0
1	B	99	SER	3.0
1	B	238	ASP	3.0
1	A	263	SER	3.0
1	B	120	GLY	3.0
1	A	244	ARG	3.0
1	A	251	TYR	3.0
1	B	188	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	253	GLY	3.0
1	A	377	ARG	3.0
1	B	161	ARG	3.0
1	A	59	SER	2.9
1	A	380	ALA	2.9
1	B	256	ARG	2.9
1	B	270	VAL	2.9
1	B	255	ALA	2.9
1	A	123	PHE	2.9
1	A	122	MET	2.9
1	B	177	ILE	2.9
1	B	44	TYR	2.9
1	B	240	GLY	2.8
1	B	192[A]	GLU	2.8
1	B	220	THR	2.8
1	B	43	THR	2.8
1	B	171	GLN	2.7
1	B	164	ALA	2.7
1	A	249	ASP	2.7
1	B	5	PHE	2.7
1	A	252	GLY	2.7
1	B	210	ILE	2.7
1	A	242	THR	2.6
1	B	168	VAL	2.6
1	B	170	PHE	2.6
1	B	165	LYS	2.6
1	B	131	ASP	2.6
1	B	152	ARG	2.5
1	A	5	PHE	2.5
1	B	191	GLU	2.5
1	B	8	GLU	2.5
1	B	356	ALA	2.5
1	B	232	ILE	2.5
1	B	204	GLU	2.4
1	B	142	HIS	2.4
1	B	271	ASP	2.4
1	A	44	TYR	2.4
1	B	299	SER	2.4
1	B	288	ALA	2.4
1	B	156	THR	2.4
1	B	166	SER	2.4
1	B	195	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	206	ILE	2.4
1	B	139	THR	2.4
1	B	214	GLU	2.4
1	A	262	PHE	2.3
1	B	79	HIS	2.3
1	A	15	PRO	2.3
1	B	181	ASP	2.3
1	A	375	LEU	2.3
1	B	78	VAL	2.2
1	B	321	PRO	2.2
1	A	256	ARG	2.2
1	B	98	GLN	2.2
1	B	97	LYS	2.2
1	B	163	ASP	2.2
1	A	45	VAL	2.2
1	A	138	ILE	2.2
1	B	338[A]	TYR	2.1
1	A	381	GLY	2.1
1	B	10	VAL	2.1
1	B	200	GLU	2.1
1	B	300	TYR	2.1
1	B	201	ALA	2.1
1	B	83	GLY	2.1
1	B	263	SER	2.1
1	A	1	ALA	2.1
1	B	251	TYR	2.1
1	A	131	ASP	2.0
1	A	157	LEU	2.0
1	B	373	ALA	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

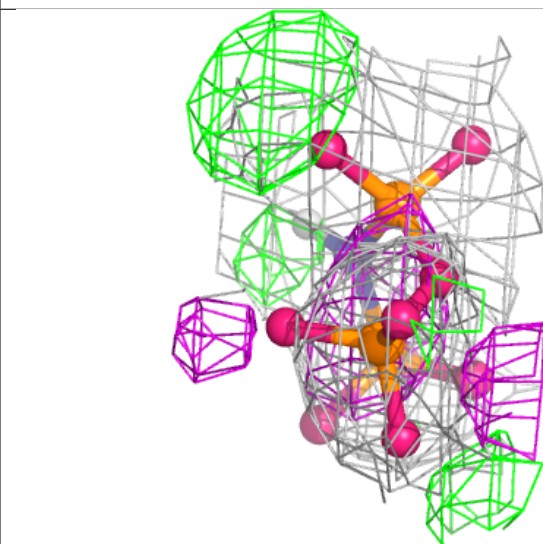
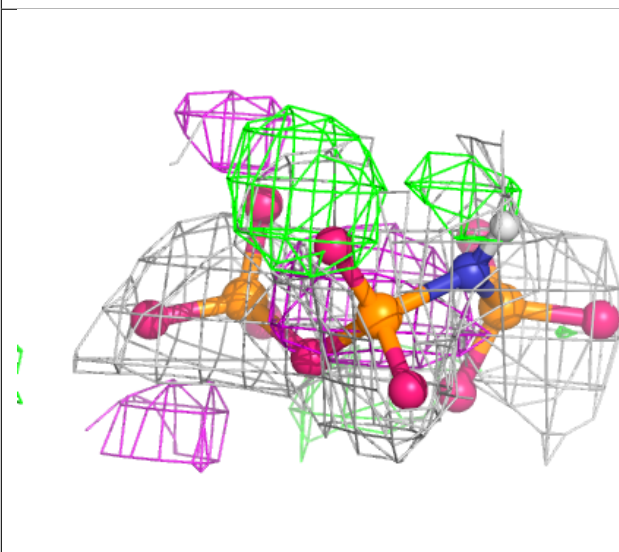
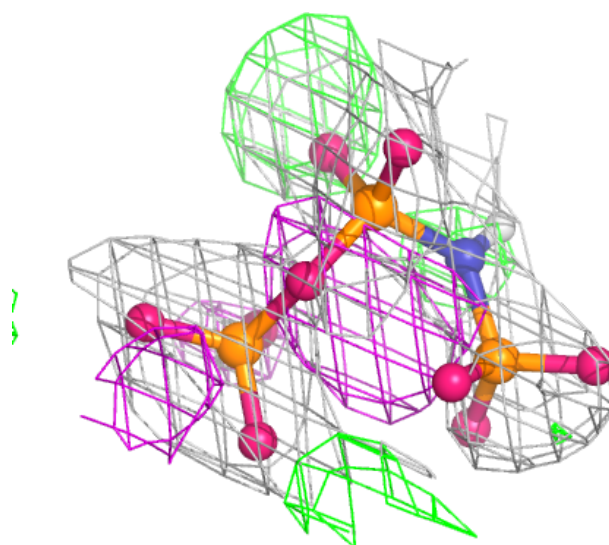
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	EDO	B	702	4/4	0.55	0.41	126,128,129,129	0
4	PPK	A	705	13/13	0.57	0.57	90,109,125,140	14
4	PPK	B	703	13/13	0.58	0.49	172,180,191,191	0
3	UNP	A	704	29/29	0.64	0.23	111,150,183,188	0
2	EDO	B	701	4/4	0.67	0.23	111,111,112,114	0
5	MG	A	707	1/1	0.78	1.50	97,97,97,97	0
2	EDO	A	701	4/4	0.86	0.28	60,69,74,86	0
2	EDO	A	702	4/4	0.88	0.20	91,95,98,98	0
2	EDO	A	703	4/4	0.90	0.10	115,116,119,121	0
5	MG	A	706	1/1	0.91	0.51	87,87,87,87	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.

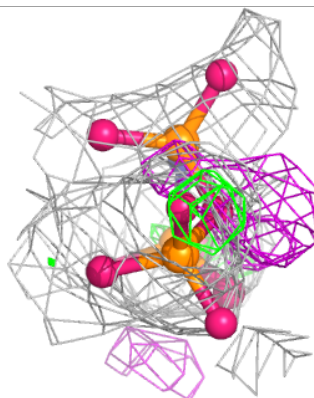
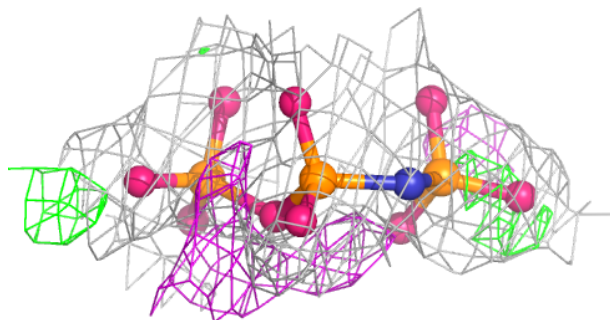
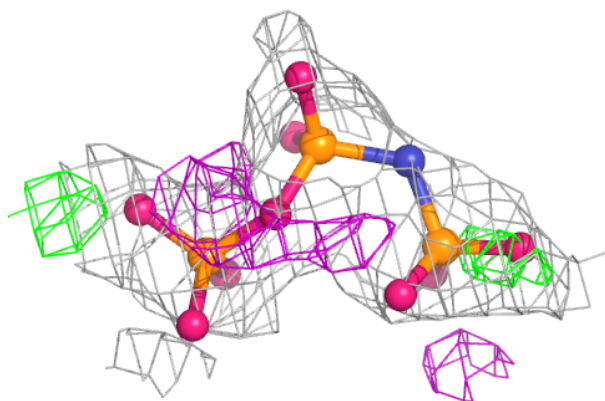
**Electron density around PPK A 705:**

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

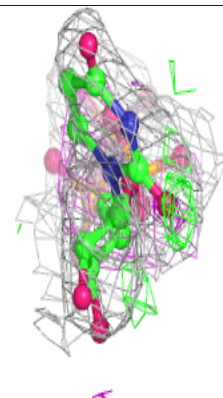
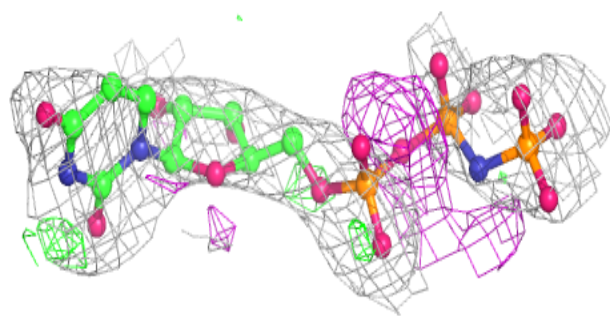
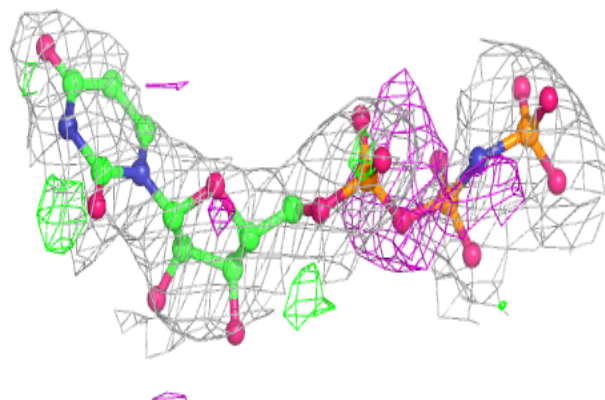


**Electron density around PPK B 703:**

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

**Electron density around UNP 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.