



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:45 AM UTC

PDB ID : 7LL3 / pdb_00007ll3
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

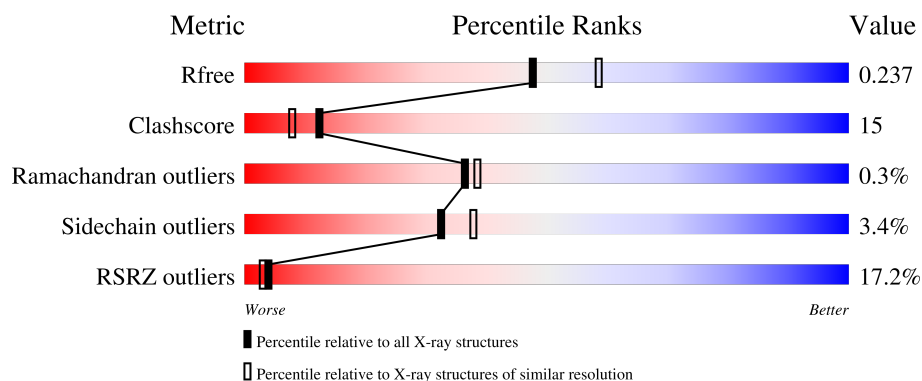
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (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 ≥ 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	5% 79% 18% ..
1	B	384	29% 67% 28% ..

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 (CCD ID: EDO) (formula: C₂H₆O₂).



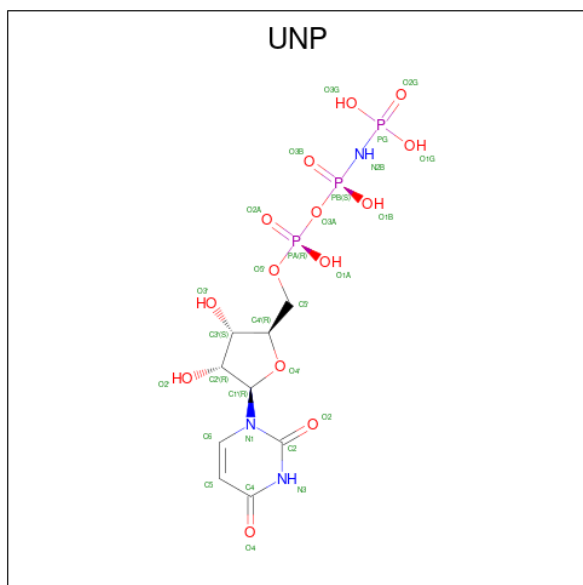
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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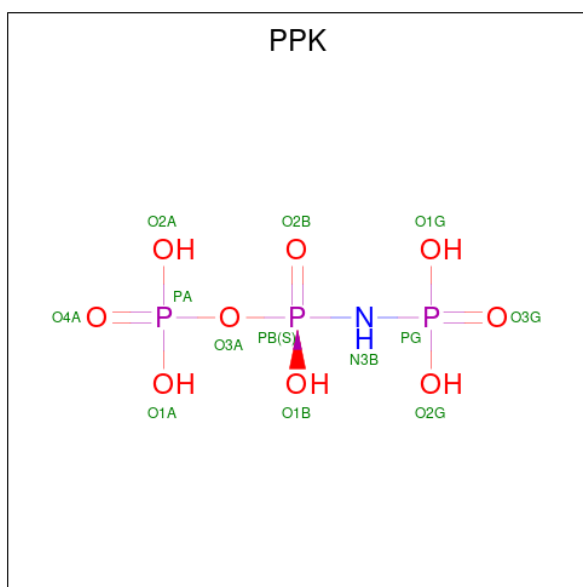
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is 5'-O-[(R)-hydroxy{[(S)-hydroxy(phosphonoamino)phosphoryl]oxy}phosphoryl]uridine (CCD ID: UNP) (formula: C₉H₁₆N₃O₁₄P₃) (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 (CCD ID: PPK) (formula: H₆NO₉P₃).



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 (CCD ID: MG) (formula: Mg).

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

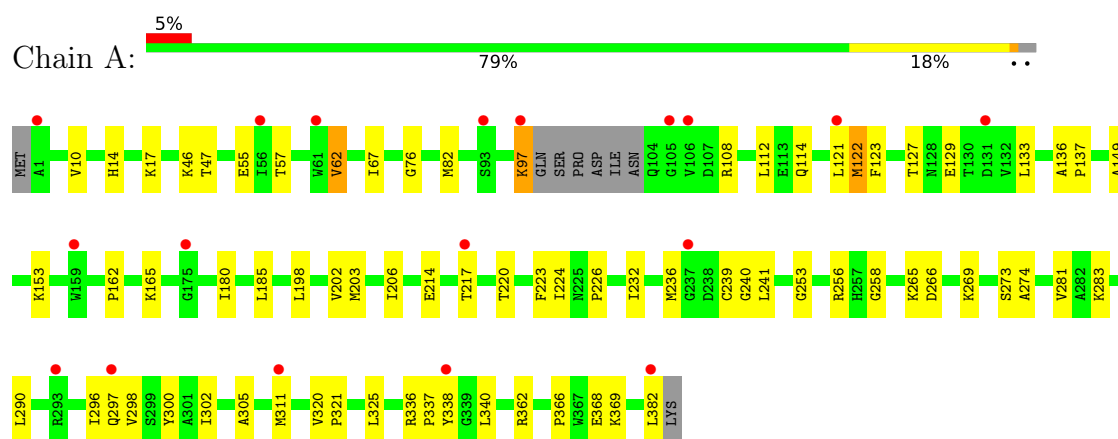
- Molecule 6 is water.

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

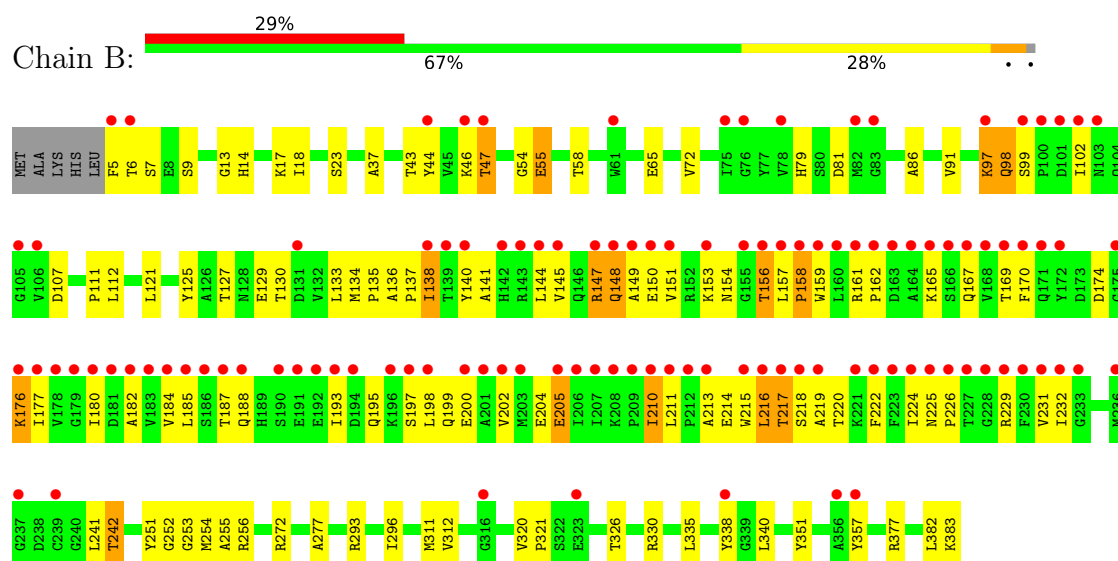
3 Residue-property plots [i](#)

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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.211 , 0.234 0.217 , 0.237	Depositor DCC
R_{free} test set	3192 reflections (4.15%)	wwPDB-VP
Wilson B-factor (Å ²)	67.6	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 75.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.19	0/2981	0.37	0/4040
1	B	0.17	0/2995	0.36	0/4062
All	All	0.18	0/5976	0.36	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	67	0
1	B	2936	0	2886	122	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	1	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	181	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 15.

All (181) 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:A:203:MET:HE2	1:A:224:ILE:HD11	1.53	0.88
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:B:254:MET:HE3	1:B:254:MET:HA	1.63	0.80
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:156:THR:C	1:B:158:PRO:HD2	2.19	0.67
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: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:A:122:MET:HE1	1:A:300:TYR:CE1	2.33	0.62
1:B:147:ARG:NH1	1:B:205:GLU:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ILE:HG12	1:B:252:GLY:CA	2.30	0.62
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:A:240:GLY:C	1:A:241:LEU:HD12	2.25	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:HE3	1:A:274:ALA:HB1	1.86	0.58
1:B:220:THR:HG23	1:B:222:PHE:CE1	2.39	0.57
1:B:216:LEU:HD22	1:B:216:LEU:H	1.69	0.57
1:B:229:ARG:CZ	1:B:231:VAL:HG21	2.35	0.56
1:A:122:MET:HE1	1:A:300:TYR:CD1	2.41	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:B:138:ILE:HG12	1:B:251:TYR:C	2.31	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:A:122:MET:HE3	1:A:274:ALA:CB	2.38	0.54
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:82:MET:HE3	1:A:162:PRO:HD3	1.90	0.53
1:A:121:LEU:HD13	1:B:6:THR:O	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:HIS:O	1:B:18:ILE:HG13	2.11	0.51
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: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:A:76:GLY:O	1:A:82:MET:HE1	2.11	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:B:176:LYS:HZ2	1:B:177:ILE:H	1.59	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:A:203:MET:CE	1:A:224:ILE:HD11	2.34	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:B:185:LEU:C	1:B:185:LEU:HD23	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:198:LEU:C	1:A:198:LEU:HD23	2.41	0.46
1:B:13:GLY:HA3	1:B:162:PRO:HB3	1.98	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:A:214:GLU:H	1:A:214:GLU:CD	2.26	0.44
1:A:232:ILE:HG23	1:A:236:MET:HE3	1.99	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:B:157:LEU:O	1:B:158:PRO:C	2.61	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:165:LYS:NZ	4:B:703:PPK:O1A	2.45	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:A:122:MET:HE1	1:A:300:TYR:HE1	1.81	0.43
1:A:203:MET:HE2	1:A:224:ILE:CD1	2.35	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:297:GLN:CB	1:A:311:MET:HE2	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:232:ILE:C	1:B:232:ILE:HD12	2.45	0.42
1:A:10:VAL:HG12	1:A:165:LYS:HG2	2.01	0.41
1:B:198:LEU:C	1:B:198:LEU:HD23	2.45	0.41
1:A:62:VAL:CG1	1:A:67:ILE:HD12	2.50	0.41
1:A:256:ARG:HD3	1:B:254:MET:O	2.21	0.41
1:B:138:ILE:CD1	1:B:138:ILE:N	2.80	0.41
1:A:82:MET:HE3	1:A:162:PRO:CD	2.51	0.40
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:HD12	1:B:232:ILE:O	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:213:ALA:C	1:B:215:TRP:H	2.29	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	376/384 (98%)	361 (96%)	15 (4%)	0	100	100
1	B	380/384 (99%)	345 (91%)	33 (9%)	2 (0%)	24	23
All	All	756/768 (98%)	706 (93%)	48 (6%)	2 (0%)	36	38

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	308/312 (99%)	305 (99%)	3 (1%)	68	76
1	B	311/312 (100%)	293 (94%)	18 (6%)	18	17
All	All	619/624 (99%)	598 (97%)	21 (3%)	32	38

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	97	LYS
1	A	122	MET
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	148	GLN
1	B	156	THR
1	B	174	ASP
1	B	176	LYS
1	B	205	GLU
1	B	210	ILE
1	B	214	GLU
1	B	216	LEU
1	B	242	THR
1	B	311	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	114	GLN
1	B	188	GLN
1	B	195	GLN
1	B	342	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 oligosaccharides 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	$\# Z > 2$
3	UNP	A	704	-	30,30,30	4.28	19 (63%)	40,47,47	1.75	8 (20%)
2	EDO	B	702	-	3,3,3	0.45	0	2,2,2	0.35	0
2	EDO	A	701	-	3,3,3	0.34	0	2,2,2	0.59	0
4	PPK	A	705	5	11,12,12	2.94	6 (54%)	14,20,20	1.26	1 (7%)
2	EDO	B	701	-	3,3,3	0.49	0	2,2,2	0.28	0
2	EDO	A	703	-	3,3,3	0.44	0	2,2,2	0.41	0
2	EDO	A	702	-	3,3,3	0.48	0	2,2,2	0.26	0
4	PPK	B	703	-	11,12,12	2.75	6 (54%)	14,20,20	1.14	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
3	UNP	A	704	-	-	4/18/38/38	0/2/2/2
2	EDO	B	702	-	-	0/1/1/1	-
2	EDO	A	701	-	-	1/1/1/1	-
4	PPK	A	705	5	-	6/8/12/12	-
2	EDO	B	701	-	-	0/1/1/1	-
2	EDO	A	703	-	-	0/1/1/1	-
2	EDO	A	702	-	-	0/1/1/1	-
4	PPK	B	703	-	-	3/8/12/12	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	704	UNP	C3'-C4'	-7.97	1.32	1.53
3	A	704	UNP	PB-O3A	7.32	1.68	1.59
3	A	704	UNP	O4'-C4'	7.15	1.60	1.45
3	A	704	UNP	C2-N1	6.71	1.49	1.38
3	A	704	UNP	C6-C5	6.68	1.50	1.35
3	A	704	UNP	C2-N3	6.54	1.49	1.38
3	A	704	UNP	PA-O3A	6.33	1.66	1.59
4	A	705	PPK	PB-O3A	5.72	1.66	1.59
3	A	704	UNP	C2'-C1'	-5.36	1.36	1.53
3	A	704	UNP	O4'-C1'	5.24	1.54	1.42
4	B	703	PPK	PB-O3A	5.19	1.65	1.59
3	A	704	UNP	PG-N2B	4.76	1.75	1.63
3	A	704	UNP	PG-O2G	4.53	1.53	1.46
3	A	704	UNP	C2'-C3'	4.35	1.65	1.53
3	A	704	UNP	C4-N3	4.02	1.45	1.38
4	A	705	PPK	PB-O2B	3.95	1.52	1.46
4	B	703	PPK	PB-O2B	3.55	1.51	1.46
4	B	703	PPK	PG-O3G	3.49	1.51	1.46
3	A	704	UNP	PB-N2B	3.46	1.72	1.63
4	A	705	PPK	PG-O3G	3.44	1.51	1.46
3	A	704	UNP	PB-O3B	3.31	1.51	1.46
4	A	705	PPK	PB-N3B	3.28	1.71	1.63
4	A	705	PPK	PG-N3B	3.28	1.71	1.63
3	A	704	UNP	PG-O1G	-3.13	1.48	1.56
3	A	704	UNP	C6-N1	3.08	1.45	1.38
4	B	703	PPK	PG-N3B	2.96	1.71	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	703	PPK	PB-N3B	2.95	1.71	1.63
3	A	704	UNP	PB-O1B	-2.57	1.50	1.56
3	A	704	UNP	C5-C4	2.43	1.49	1.43
4	B	703	PPK	PG-O2G	-2.06	1.51	1.56
4	A	705	PPK	PB-O1B	-2.02	1.51	1.56

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	704	UNP	C4-N3-C2	-4.87	120.57	126.61
3	A	704	UNP	N3-C2-N1	3.82	119.87	114.89
3	A	704	UNP	C5-C4-N3	3.60	119.84	114.80
3	A	704	UNP	O4-C4-C5	-3.07	119.86	125.16
3	A	704	UNP	C4'-O4'-C1'	-3.06	102.70	109.47
3	A	704	UNP	C3'-C2'-C1'	2.67	106.52	101.46
3	A	704	UNP	C2'-C3'-C4'	2.64	107.71	102.61
3	A	704	UNP	O3B-PB-N2B	-2.51	108.08	111.77
4	A	705	PPK	O1G-PG-O3G	-2.04	108.32	113.45

There are no chirality outliers.

All (14) torsion outliers are listed below:

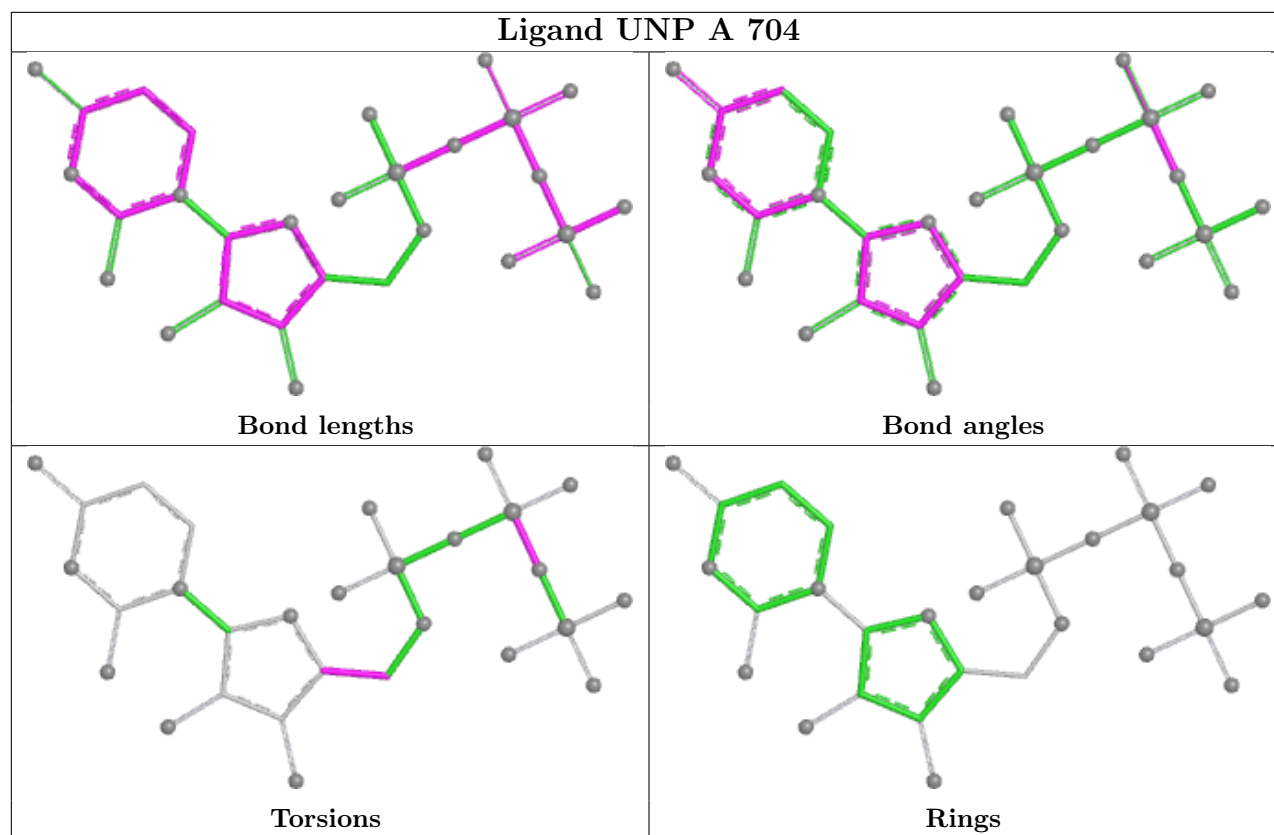
Mol	Chain	Res	Type	Atoms
3	A	704	UNP	PG-N2B-PB-O3B
3	A	704	UNP	PG-N2B-PB-O3A
4	A	705	PPK	PB-N3B-PG-O3G
4	A	705	PPK	PG-N3B-PB-O2B
4	A	705	PPK	PG-N3B-PB-O3A
4	B	703	PPK	PB-N3B-PG-O3G
4	B	703	PPK	PA-O3A-PB-O1B
3	A	704	UNP	C3'-C4'-C5'-O5'
3	A	704	UNP	O4'-C4'-C5'-O5'
4	A	705	PPK	PB-O3A-PA-O4A
4	B	703	PPK	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

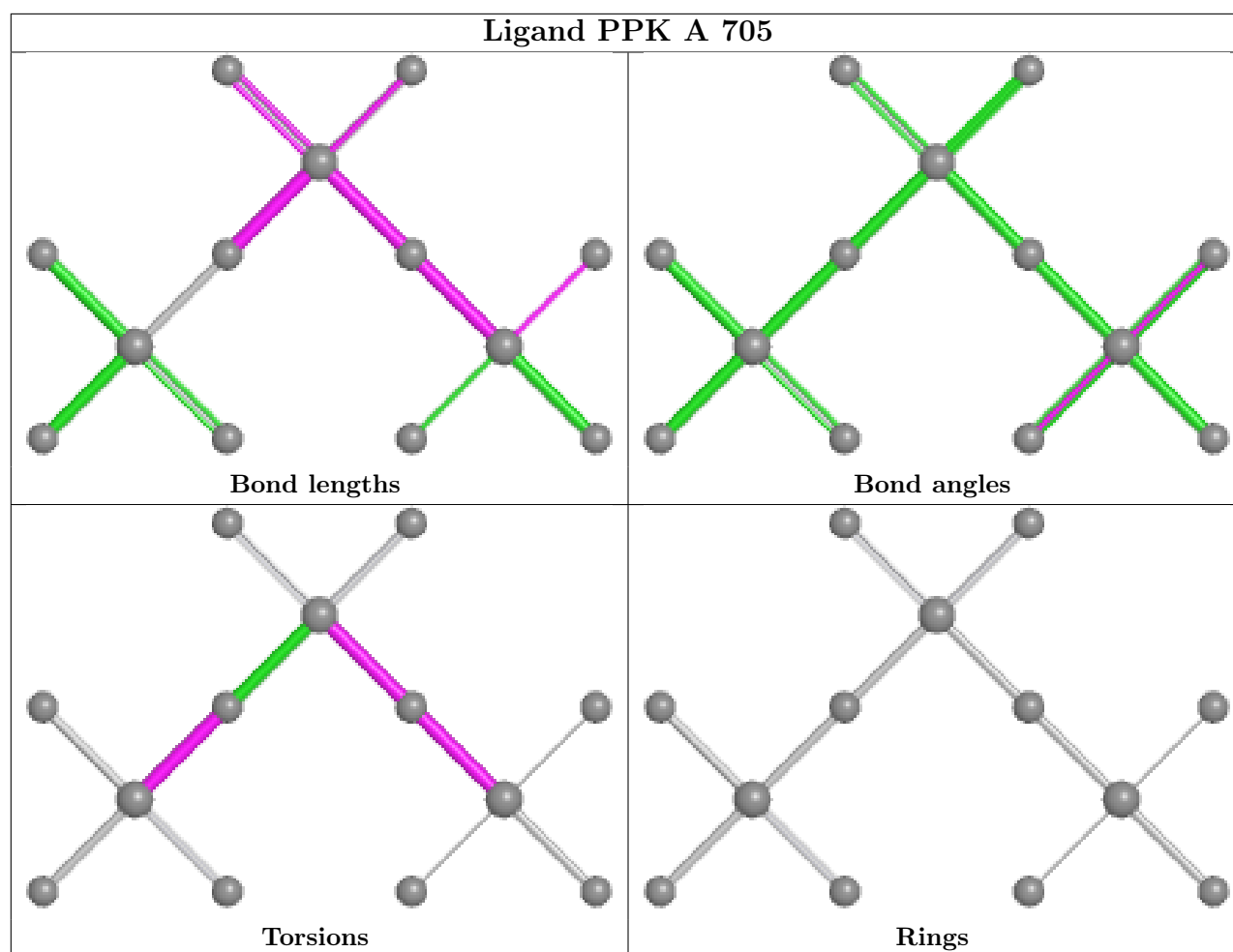
There are no ring outliers.

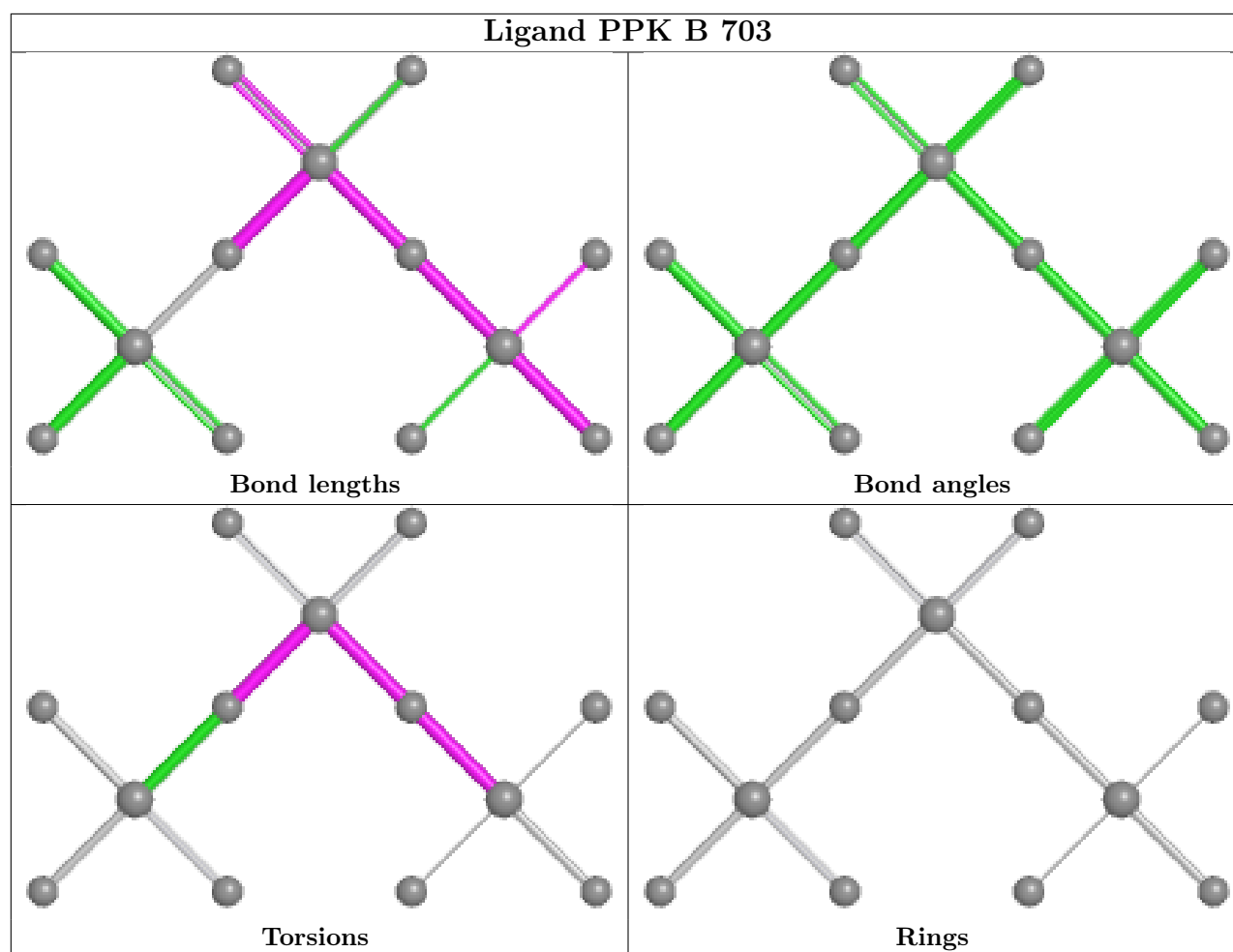
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	EDO	1	0
4	A	705	PPK	1	0
4	B	703	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	376/384 (97%)	0.41	18 (4%)	35 34	34, 77, 115, 191	4 (1%)
1	B	379/384 (98%)	1.43	112 (29%)	1 1	37, 98, 198, 227	3 (0%)
All	All	755/768 (98%)	0.93	130 (17%)	4 3	34, 84, 181, 227	7 (0%)

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	LEU	10.2
1	B	183	VAL	8.6
1	B	159	TRP	6.9
1	B	106	VAL	6.7
1	B	186	SER	6.6
1	B	182	ALA	6.4
1	B	185	LEU	6.3
1	B	202	VAL	5.9
1	A	382	LEU	5.8
1	B	149	ALA	5.7
1	B	157	LEU	5.6
1	B	151	VAL	5.6
1	B	213	ALA	5.5
1	B	211	LEU	5.5
1	B	215	TRP	5.4
1	B	180	ILE	5.4
1	B	207	ILE	5.4
1	B	156	THR	5.4
1	B	100	PRO	5.4
1	B	198	LEU	5.4
1	B	356	ALA	5.3
1	B	209	PRO	5.2
1	B	168	VAL	4.8
1	B	184	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	210	ILE	4.7
1	B	219	ALA	4.7
1	B	223	PHE	4.7
1	B	203	MET	4.7
1	B	179	GLY	4.6
1	B	166	SER	4.4
1	B	155	GLY	4.4
1	B	172	TYR	4.3
1	B	164	ALA	4.3
1	B	169	THR	4.3
1	B	226	PRO	4.1
1	B	192[A]	GLU	4.1
1	B	206	ILE	4.1
1	B	232	ILE	4.1
1	B	193	ILE	4.0
1	B	227	THR	4.0
1	B	201	ALA	4.0
1	B	187	THR	4.0
1	B	230	PHE	4.0
1	B	224	ILE	4.0
1	B	178	VAL	3.9
1	B	181	ASP	3.9
1	B	99	SER	3.9
1	B	102	ILE	3.8
1	B	103	ASN	3.7
1	B	222	PHE	3.7
1	B	212	PRO	3.6
1	B	239	CYS	3.6
1	A	106	VAL	3.6
1	B	139	THR	3.5
1	B	338[A]	TYR	3.3
1	B	158	PRO	3.2
1	B	138	ILE	3.2
1	B	148	GLN	3.2
1	B	150	GLU	3.1
1	B	167	GLN	3.1
1	B	76	GLY	3.1
1	B	145	VAL	3.1
1	B	225	ASN	3.0
1	B	82	MET	3.0
1	A	338[A]	TYR	3.0
1	B	97	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	101	ASP	3.0
1	B	78	VAL	2.9
1	A	217	THR	2.9
1	B	216	LEU	2.9
1	A	97	LYS	2.9
1	B	221	LYS	2.9
1	A	293[A]	ARG	2.9
1	B	175	GLY	2.9
1	B	231	VAL	2.9
1	B	190	SER	2.9
1	B	163	ASP	2.9
1	B	171	GLN	2.8
1	B	194	ASP	2.8
1	B	5	PHE	2.8
1	A	56	ILE	2.7
1	B	196	LYS	2.7
1	A	1	ALA	2.7
1	B	188	GLN	2.7
1	B	147	ARG	2.7
1	B	153	LYS	2.6
1	B	170	PHE	2.6
1	B	142	HIS	2.6
1	B	205	GLU	2.6
1	B	161	ARG	2.6
1	B	233	GLY	2.6
1	B	229	ARG	2.6
1	B	208	LYS	2.6
1	A	131	ASP	2.5
1	A	311	MET	2.5
1	B	144	LEU	2.5
1	A	237	GLY	2.5
1	B	228	GLY	2.5
1	B	165	LYS	2.5
1	B	176	LYS	2.5
1	A	297	GLN	2.4
1	B	83	GLY	2.4
1	B	61	TRP	2.4
1	B	6	THR	2.4
1	B	177	ILE	2.4
1	B	200	GLU	2.3
1	B	44	TYR	2.3
1	B	162	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	236	MET	2.3
1	A	159	TRP	2.2
1	B	191	GLU	2.2
1	B	323	GLU	2.2
1	A	105	GLY	2.2
1	B	105	GLY	2.2
1	B	46	LYS	2.2
1	A	61	TRP	2.1
1	A	121	LEU	2.1
1	A	175	GLY	2.1
1	B	47	THR	2.1
1	B	218	SER	2.1
1	B	143	ARG	2.1
1	B	140	TYR	2.1
1	B	316	GLY	2.1
1	B	75	ILE	2.1
1	B	357	TYR	2.1
1	B	217	THR	2.1
1	B	237	GLY	2.1
1	B	197	SER	2.0
1	A	93	SER	2.0
1	B	131	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

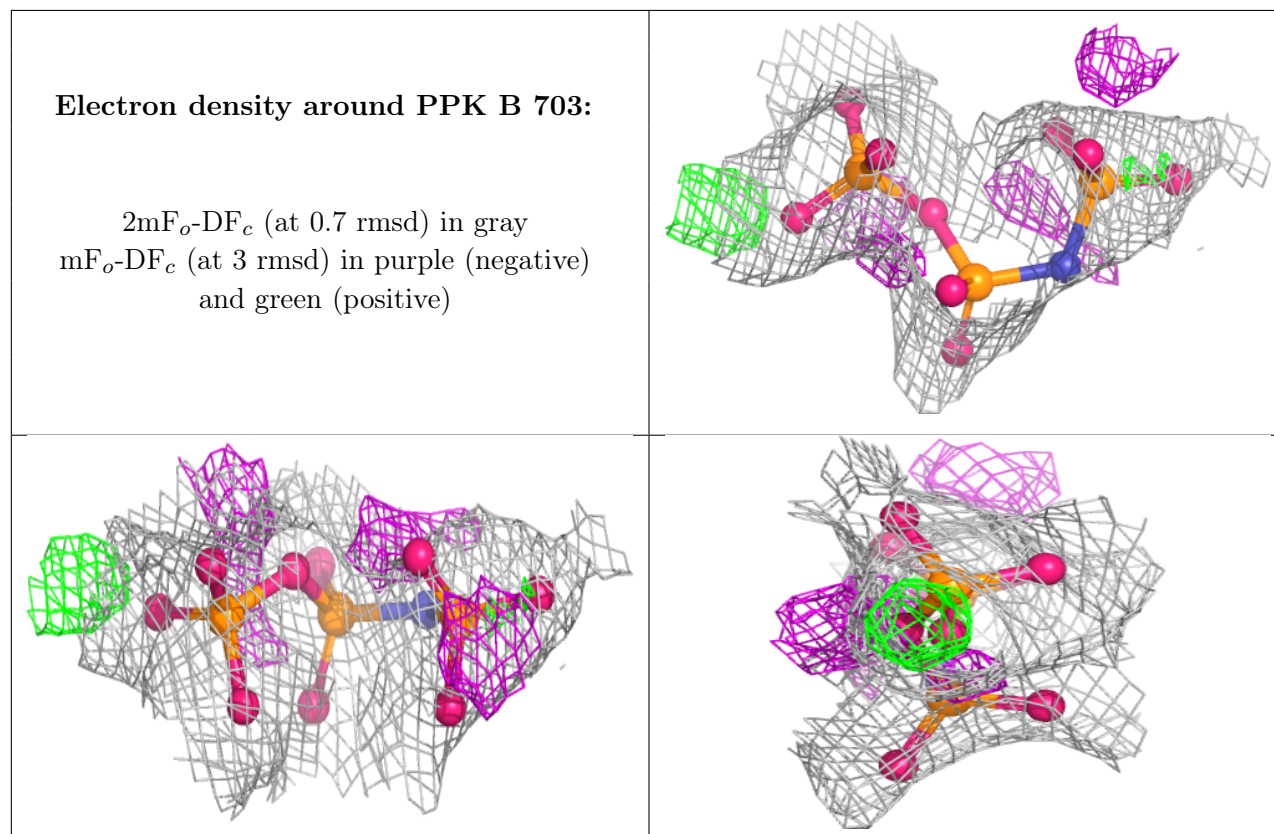
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PPK	B	703	13/13	0.67	0.17	172,180,191,191	0

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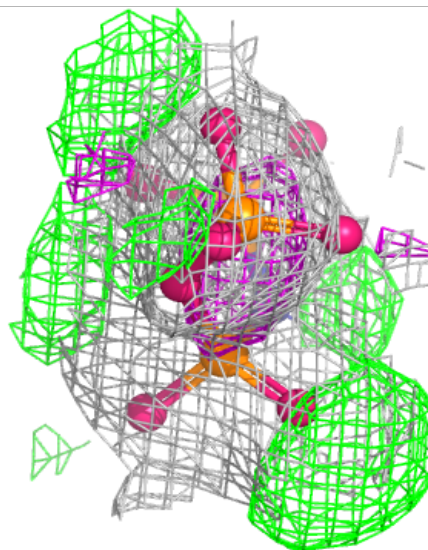
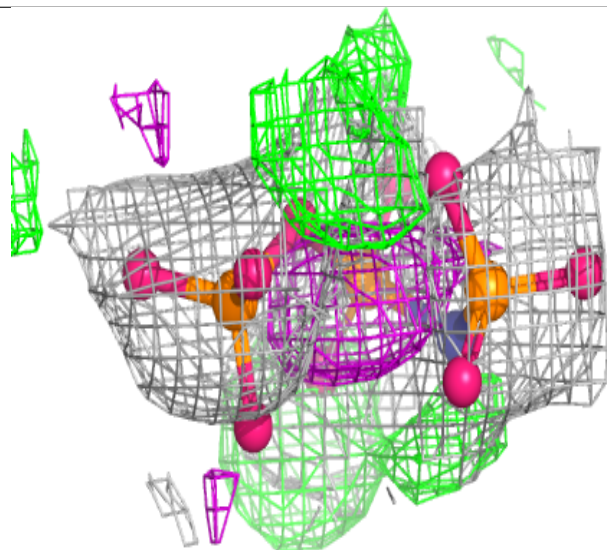
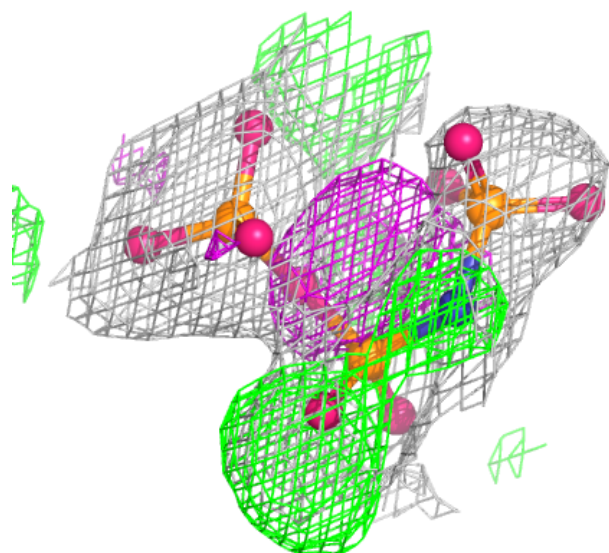
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PPK	A	705	13/13	0.68	0.25	90,109,125,140	14
2	EDO	B	702	4/4	0.74	0.27	126,128,129,129	0
5	MG	A	707	1/1	0.78	0.30	97,97,97,97	0
3	UNP	A	704	29/29	0.82	0.19	111,150,183,188	0
2	EDO	A	703	4/4	0.82	0.17	115,116,119,121	0
2	EDO	B	701	4/4	0.87	0.26	111,111,112,114	0
5	MG	A	706	1/1	0.92	0.11	87,87,87,87	0
2	EDO	A	702	4/4	0.92	0.14	91,95,98,98	0
2	EDO	A	701	4/4	0.93	0.17	60,69,74,86	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.



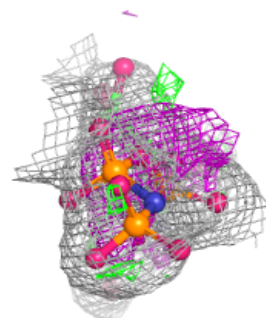
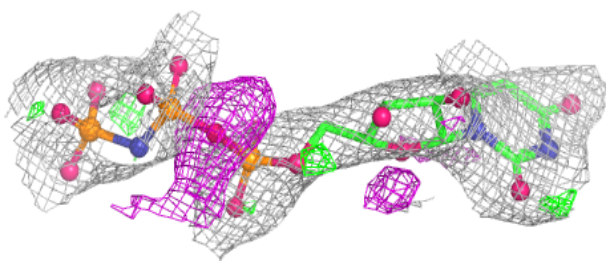
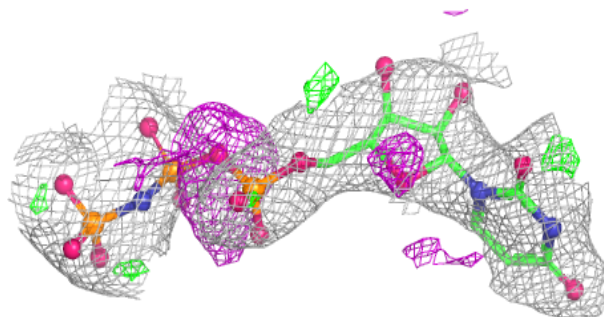
Electron density around PPK A 705:

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



Electron density around 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.