



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:18 AM UTC

PDB ID : 8V2K / pdb_00008v2k
Title : Proteus vulgaris tryptophan indole-lyase complexed with L-alanine
Authors : Phillips, R.S.
Deposited on : 2023-11-22
Resolution : 1.81 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

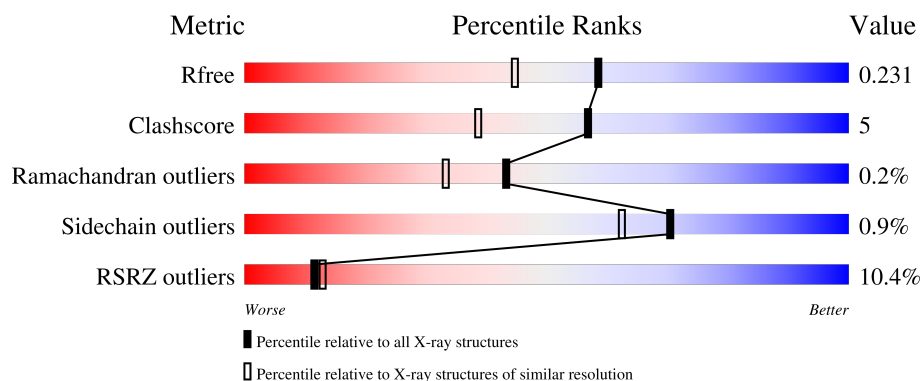
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	467	17% 82% 15% ..
1	B	467	8% 88% 10% .
1	C	467	7% 87% 12%
1	D	467	9% 88% 11% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15904 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.

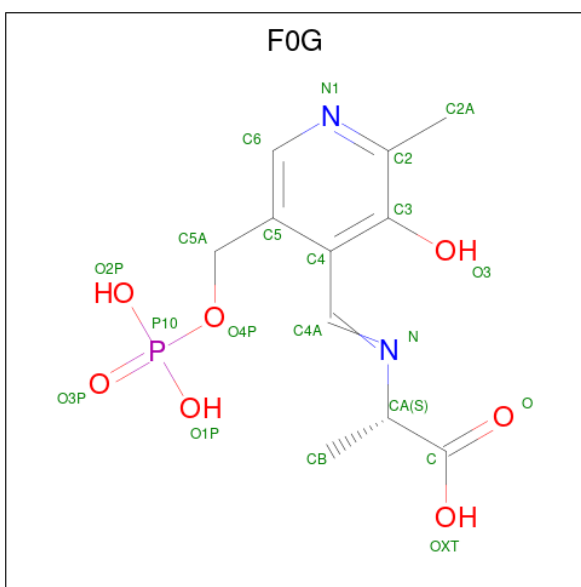
- Molecule 1 is a protein called Tryptophanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	5	0
			3678	2356	624	680	18			
1	B	458	Total	C	N	O	S	0	2	0
			3641	2329	621	673	18			
1	C	465	Total	C	N	O	S	0	6	0
			3726	2381	639	688	18			
1	D	462	Total	C	N	O	S	0	4	0
			3685	2359	623	684	19			

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

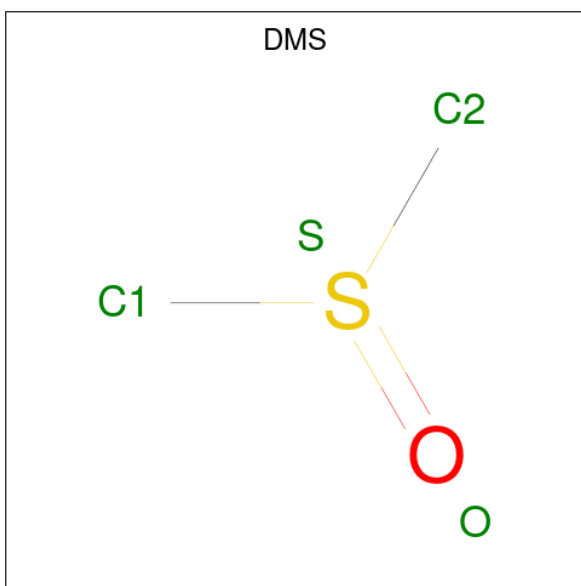
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		
2	C	2	Total	K	0	0
			2	2		

- Molecule 3 is (E)-N-({3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methylidene)-L-alanine (CCD ID: F0G) (formula: C₁₁H₁₅N₂O₇P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 21	C 11	N 2	O 7	P 1	0	0
3	D	1	Total 21	C 11	N 2	O 7	P 1	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: $\text{C}_2\text{H}_6\text{OS}$).



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

- [illegible]

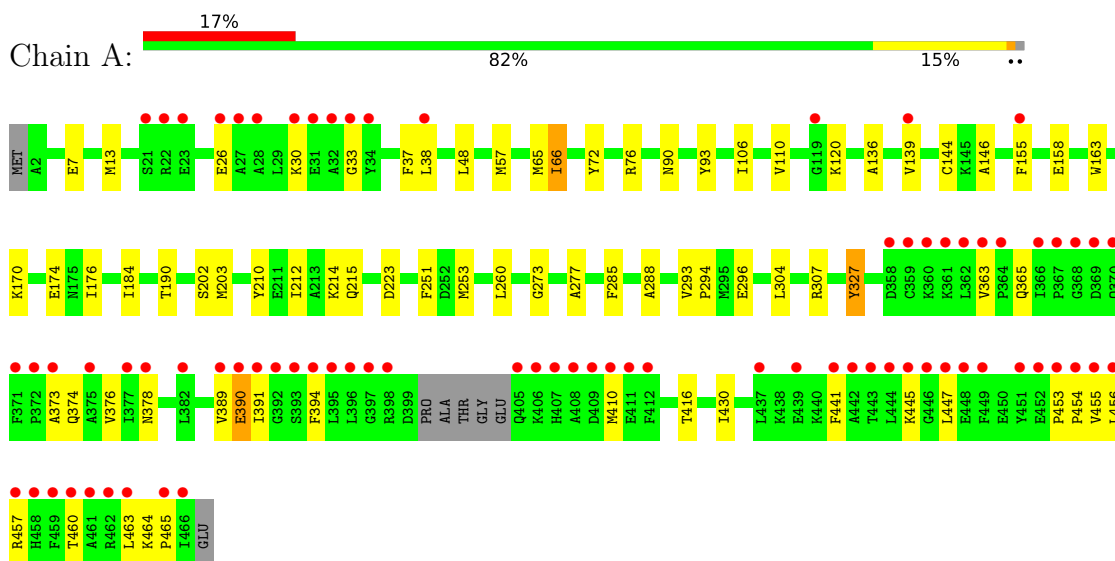
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	226	Total O 226 226	0	4
6	B	249	Total O 249 249	0	2
6	C	303	Total O 303 303	0	1
6	D	300	Total O 300 300	0	8

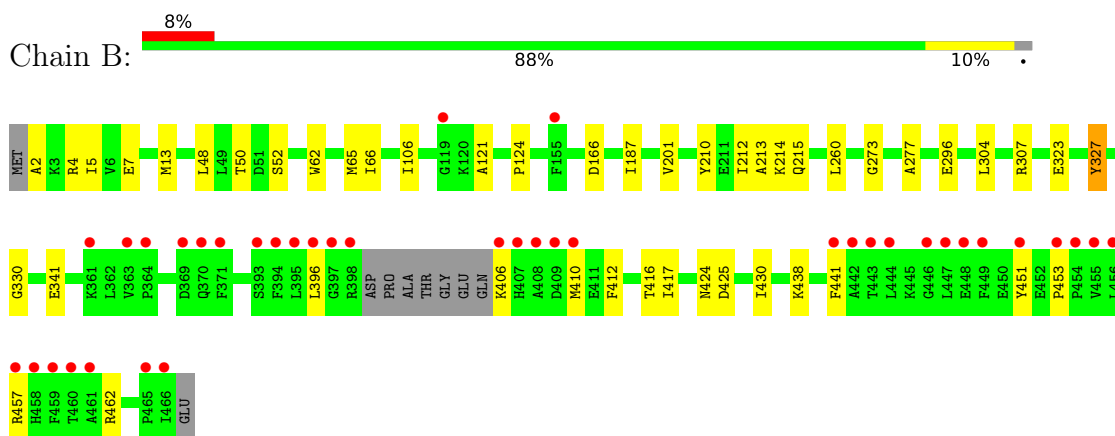
3 Residue-property plots [i](#)

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.

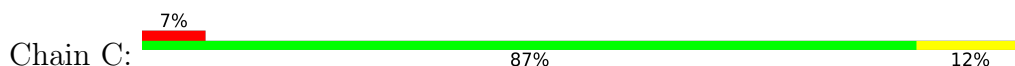
• Molecule 1: Tryptophanase

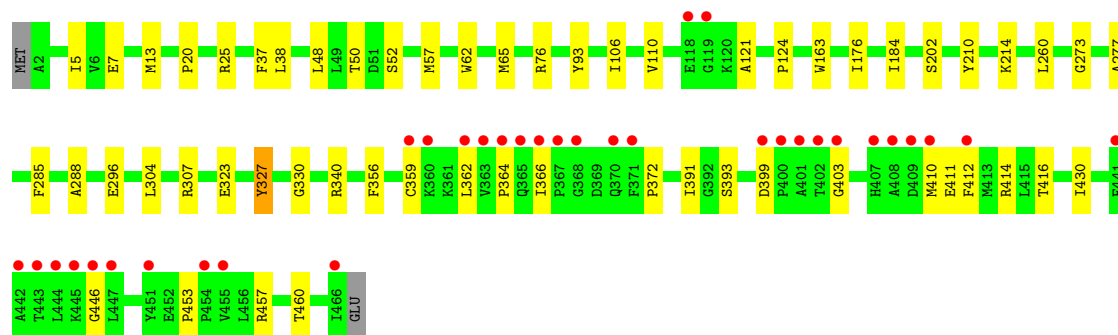


• Molecule 1: Tryptophanase

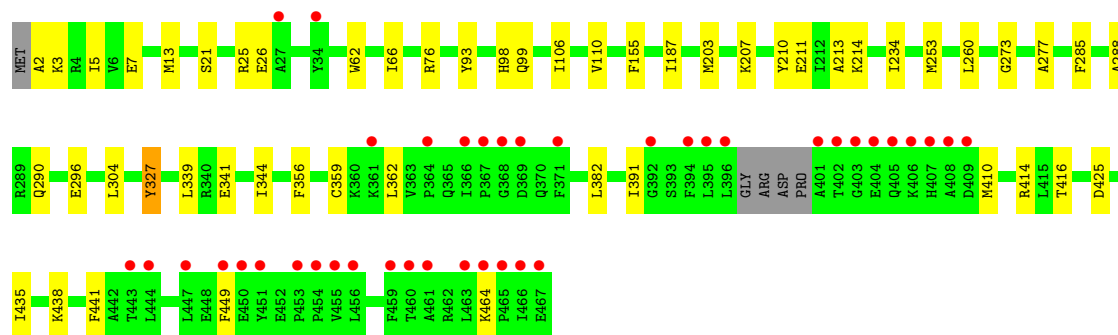
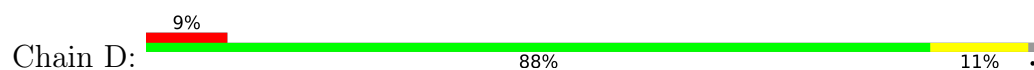


• Molecule 1: Tryptophanase





● Molecule 1: Tryptophanase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.89Å 113.07Å 120.33Å 90.00° 98.33° 90.00°	Depositor
Resolution (Å)	119.06 – 1.81 119.06 – 1.81	Depositor EDS
% Data completeness (in resolution range)	70.5 (119.06-1.81) 70.8 (119.06-1.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.81Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.186 , 0.231 0.187 , 0.231	Depositor DCC
R_{free} test set	5715 reflections (3.53%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15904	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.77% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PLI, F0G, DMS, K

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	0.14	0/3771	0.35	0/5090
1	B	0.13	0/3724	0.33	0/5026
1	C	0.15	0/3821	0.34	0/5158
1	D	0.16	0/3775	0.36	0/5094
All	All	0.15	0/15091	0.34	0/20368

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3678	0	3673	45	0
1	B	3641	0	3636	32	0
1	C	3726	0	3722	33	0
1	D	3685	0	3677	33	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
3	A	21	0	0	1	0
3	D	21	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	6	0	0
4	C	4	0	6	0	0
5	B	21	0	11	0	0
5	C	21	0	11	0	0
6	A	226	0	0	3	0
6	B	249	0	0	2	0
6	C	303	0	0	4	0
6	D	300	0	0	2	0
All	All	15904	0	14742	136	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 5.

All (136) 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:374:GLN:HB2	1:A:391:ILE:HG12	1.72	0.72
1:C:366:ILE:HD12	1:C:446:GLY:HA2	1.74	0.70
1:A:215:GLN:NE2	6:A:601:HOH:O	2.24	0.69
1:A:453:PRO:HG3	1:A:460:THR:HG23	1.74	0.69
1:B:62:TRP:CD1	1:D:13:MET:HE2	2.28	0.68
1:A:65:MET:HE2	1:A:307:ARG:HD2	1.78	0.66
1:C:273:GLY:HA2	1:C:304:LEU:HD21	1.80	0.64
1:A:76:ARG:NH1	6:A:604:HOH:O	2.31	0.62
1:B:13:MET:HE2	1:D:62:TRP:CD1	2.35	0.62
1:A:455:VAL:HG22	1:A:456:LEU:HG	1.82	0.61
1:C:7:GLU:HG3	1:C:327[B]:TYR:CZ	2.36	0.61
1:D:106:ILE:HD11	1:D:296:GLU:HG3	1.83	0.61
1:D:273:GLY:HA2	1:D:304:LEU:HD21	1.82	0.60
1:D:155:PHE:HA	1:D:410[A]:MET:HE2	1.84	0.60
1:A:38:LEU:HD21	1:A:460:THR:HA	1.84	0.59
1:A:106:ILE:HD11	1:A:296:GLU:HG3	1.85	0.58
1:A:155:PHE:HA	1:A:410:MET:HE2	1.85	0.58
1:D:359:CYS:HA	1:D:362:LEU:HB2	1.85	0.57
1:C:366:ILE:HD13	1:C:372:PRO:HA	1.86	0.57
1:A:453:PRO:HG2	1:A:457:ARG:HA	1.87	0.57
1:A:391:ILE:HD13	1:A:394:PHE:HB3	1.87	0.57
1:A:273:GLY:HA2	1:A:304:LEU:HD21	1.88	0.56
1:D:391:ILE:HD11	1:D:414:ARG:HD3	1.88	0.56
1:C:393:SER:OG	1:C:411:GLU:OE2	2.24	0.56
1:D:76[A]:ARG:NH1	6:D:612[A]:HOH:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:GLY:HA2	1:B:304:LEU:HD21	1.86	0.56
1:D:290:GLN:NE2	6:D:607:HOH:O	2.31	0.56
1:A:13:MET:HE2	1:C:62:TRP:CD1	2.41	0.56
1:B:406:LYS:N	6:B:608:HOH:O	2.39	0.56
1:C:65:MET:HE2	1:C:307:ARG:HD2	1.87	0.56
1:A:374:GLN:NE2	1:A:378:ASN:OD1	2.39	0.55
1:A:26:GLU:O	1:A:30:LYS:HG2	2.07	0.55
1:C:76[B]:ARG:NH2	6:C:601:HOH:O	2.40	0.55
1:C:359:CYS:HA	1:C:362:LEU:HB3	1.89	0.54
1:A:48:LEU:HD11	1:A:430:ILE:HD13	1.89	0.54
1:D:26:GLU:HG2	1:D:382:LEU:HD22	1.90	0.54
1:D:207:LYS:NZ	1:D:211:GLU:OE2	2.33	0.53
1:D:210:TYR:CE1	1:D:214:LYS:HE3	2.44	0.53
1:C:5:ILE:HD12	1:C:330:GLY:HA3	1.90	0.53
1:B:5:ILE:HD12	1:B:330:GLY:HA3	1.91	0.52
1:A:376:VAL:HG13	1:A:441:PHE:HE1	1.75	0.52
1:D:449:PHE:O	1:D:464:LYS:NZ	2.43	0.52
1:B:50[A]:THR:HG23	1:B:52:SER:H	1.74	0.52
1:B:106:ILE:HD11	1:B:296:GLU:HG3	1.90	0.52
1:A:374:GLN:H	1:A:391:ILE:HG23	1.74	0.52
1:B:48:LEU:HD11	1:B:430:ILE:HD13	1.91	0.51
1:B:260:LEU:HG	1:B:277:ALA:HB3	1.92	0.51
1:A:7:GLU:HG3	1:A:327[B]:TYR:CZ	2.46	0.51
1:A:389:VAL:HG22	1:A:390:GLU:H	1.75	0.51
1:C:163:TRP:CD2	1:C:202:SER:HB3	2.46	0.50
1:B:187:ILE:HD12	1:B:213:ALA:HB2	1.93	0.50
1:C:340[A]:ARG:NH2	6:C:614:HOH:O	2.44	0.50
1:B:4:ARG:NH2	1:B:425:ASP:OD1	2.44	0.50
1:C:453:PRO:HG2	1:C:457:ARG:HA	1.92	0.49
1:B:424:ASN:ND2	1:D:425:ASP:OD2	2.40	0.49
1:B:121:ALA:HB1	1:B:124:PRO:HB3	1.94	0.49
1:A:203:MET:HE1	1:A:253:MET:HG3	1.95	0.49
1:B:214:LYS:NZ	6:B:617:HOH:O	2.45	0.49
3:D:501:F0G:O3	3:D:501:F0G:N	2.45	0.49
1:D:110:VAL:HG21	1:D:288:ALA:HA	1.93	0.49
1:C:38:LEU:HD21	1:C:460:THR:HA	1.95	0.48
1:B:410:MET:HE3	1:B:412:PHE:CZ	2.47	0.48
1:B:453:PRO:HG2	1:B:457:ARG:HA	1.95	0.48
1:D:260:LEU:HG	1:D:277:ALA:HB3	1.96	0.48
1:D:98:HIS:CD2	1:D:99:GLN:HG2	2.49	0.47
1:A:260:LEU:HG	1:A:277:ALA:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:GLU:H	1:C:323:GLU:CD	2.21	0.47
3:A:502:F0G:N	3:A:502:F0G:O3	2.44	0.47
1:C:399:ASP:O	1:C:403:GLY:N	2.43	0.47
1:D:187:ILE:HD12	1:D:213:ALA:HB2	1.96	0.47
1:D:356:PHE:CE2	1:D:391:ILE:HD12	2.50	0.47
1:B:2:ALA:N	1:B:341:GLU:OE2	2.48	0.47
1:A:139[A]:VAL:HG13	1:A:144:CYS:HB2	1.96	0.46
1:D:7:GLU:HG3	1:D:327[B]:TYR:CZ	2.50	0.46
1:A:176:ILE:HA	1:A:184[A]:ILE:HD11	1.98	0.46
1:A:110:VAL:HG21	1:A:288:ALA:HA	1.97	0.46
1:B:323:GLU:H	1:B:323:GLU:CD	2.23	0.46
1:D:339:LEU:HB3	1:D:344:ILE:HB	1.97	0.46
1:C:76[B]:ARG:NH1	6:C:613:HOH:O	2.44	0.46
1:A:365:GLN:NE2	1:A:441:PHE:O	2.44	0.45
1:D:3:LYS:HE3	1:D:5:ILE:HD11	1.97	0.45
1:D:203:MET:HE1	1:D:253:MET:HG3	1.98	0.45
1:B:48:LEU:HD22	1:B:417:ILE:HD13	1.98	0.45
1:B:396:LEU:HG	1:B:406:LYS:NZ	2.32	0.45
1:D:93:TYR:HB3	1:D:285:PHE:CD1	2.52	0.45
1:B:451:TYR:HD2	1:B:462:ARG:HD3	1.82	0.45
1:B:451:TYR:CD2	1:B:462:ARG:HD3	2.53	0.44
1:C:210:TYR:CE1	1:C:214:LYS:HE3	2.53	0.44
1:C:93:TYR:HB3	1:C:285:PHE:CD1	2.51	0.44
1:C:121:ALA:HB1	1:C:124:PRO:HB3	1.99	0.44
1:C:410:MET:HE3	1:C:412:PHE:CZ	2.53	0.44
1:B:7:GLU:HG3	1:B:327:TYR:CE1	2.53	0.44
1:A:293:VAL:HB	1:A:294:PRO:HD3	2.00	0.44
1:C:106:ILE:HD11	1:C:296:GLU:HG3	2.00	0.43
1:B:65:MET:HE2	1:B:307:ARG:HD2	2.00	0.43
1:A:136:ALA:O	1:A:139[B]:VAL:HG22	2.18	0.43
1:A:464:LYS:HG3	1:A:465:PRO:HD2	2.00	0.43
1:C:366:ILE:CD1	1:C:446:GLY:HA2	2.47	0.43
1:D:362:LEU:HD23	1:D:362:LEU:HA	1.84	0.43
1:A:33:GLY:O	1:A:463:LEU:N	2.50	0.43
1:A:170:LYS:HE2	1:A:174:GLU:OE2	2.19	0.43
1:A:447:LEU:HD23	1:A:465:PRO:HA	2.01	0.43
1:C:260:LEU:HG	1:C:277:ALA:HB3	2.00	0.43
1:D:435:ILE:O	1:D:438:LYS:HG3	2.18	0.43
1:A:212:ILE:O	1:A:215:GLN:HG2	2.19	0.43
1:B:210:TYR:CE1	1:B:214:LYS:HE3	2.54	0.43
1:C:110:VAL:HG21	1:C:288:ALA:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:LEU:HD11	1:C:430:ILE:HD13	2.01	0.43
1:C:414[B]:ARG:NH1	6:C:626:HOH:O	2.51	0.42
1:B:13:MET:HE3	1:D:13:MET:HE3	2.01	0.42
1:A:93:TYR:HB3	1:A:285:PHE:CD1	2.55	0.42
1:A:57:MET:O	1:C:13:MET:HA	2.20	0.42
1:D:203:MET:HE2	1:D:234:ILE:HD13	2.02	0.42
1:C:176:ILE:HA	1:C:184:ILE:HD11	2.02	0.42
1:A:139[B]:VAL:HG21	1:A:146:ALA:HB2	2.01	0.42
1:B:62:TRP:CG	1:D:13:MET:HE2	2.53	0.42
1:A:190:THR:HA	1:A:223:ASP:HB3	2.02	0.41
1:A:373:ALA:HB3	1:A:391:ILE:HA	2.01	0.41
1:C:20:PRO:O	1:C:25:ARG:NH1	2.49	0.41
1:A:120:LYS:HG2	6:A:628:HOH:O	2.21	0.41
1:A:163:TRP:CD2	1:A:202:SER:HB3	2.56	0.41
1:A:210:TYR:CE1	1:A:214:LYS:HE3	2.55	0.41
1:C:356:PHE:HE2	1:C:391:ILE:HD12	1.85	0.41
1:A:90:ASN:HB2	1:A:251:PHE:CE1	2.56	0.41
1:C:50[B]:THR:HG23	1:C:52:SER:H	1.86	0.41
1:C:57:MET:HE1	1:C:65:MET:SD	2.60	0.41
1:A:445:LYS:HE2	1:A:465:PRO:HB3	2.03	0.41
1:B:62:TRP:O	1:B:66:ILE:HG12	2.20	0.41
1:B:438:LYS:HA	1:B:441:PHE:CD2	2.56	0.41
1:D:21:SER:O	1:D:25:ARG:HG3	2.21	0.41
1:B:166:ASP:HA	1:B:201:VAL:HG13	2.03	0.40
1:A:72:TYR:CD2	1:B:50[A]:THR:HG21	2.56	0.40
1:D:438:LYS:HA	1:D:441:PHE:CD2	2.56	0.40
1:D:2:ALA:N	1:D:341:GLU:OE2	2.54	0.40
1:A:66:ILE:HG13	1:D:66[B]:ILE:HD12	2.03	0.40
1:B:212:ILE:O	1:B:215:GLN:HG2	2.22	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	461/467 (99%)	440 (95%)	19 (4%)	2 (0%)	30	19
1	B	456/467 (98%)	439 (96%)	17 (4%)	0	100	100
1	C	469/467 (100%)	453 (97%)	15 (3%)	1 (0%)	43	33
1	D	462/467 (99%)	444 (96%)	18 (4%)	0	100	100
All	All	1848/1868 (99%)	1776 (96%)	69 (4%)	3 (0%)	43	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	454	PRO
1	C	364	PRO
1	A	390	GLU

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	386/386 (100%)	379 (98%)	7 (2%)	51	39
1	B	381/386 (99%)	379 (100%)	2 (0%)	81	77
1	C	390/386 (101%)	386 (99%)	4 (1%)	68	60
1	D	386/386 (100%)	383 (99%)	3 (1%)	73	67
All	All	1543/1544 (100%)	1527 (99%)	16 (1%)	70	60

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	PHE
1	A	66	ILE
1	A	158	GLU
1	A	327[A]	TYR
1	A	327[B]	TYR
1	A	363	VAL
1	A	416	THR
1	B	327	TYR

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Mol	Chain	Res	Type
1	B	416	THR
1	C	37	PHE
1	C	327[A]	TYR
1	C	327[B]	TYR
1	C	416	THR
1	D	327[A]	TYR
1	D	327[B]	TYR
1	D	416	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	175	ASN
1	C	123	ASN
1	C	175	ASN
1	C	374	GLN
1	C	407	HIS
1	D	175	ASN

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, 4 are monoatomic - leaving 6 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	F0G	D	501	-	20,21,21	1.71	2 (10%)	26,30,30	1.17	2 (7%)
4	DMS	C	503	-	3,3,3	0.66	0	3,3,3	0.50	0
3	F0G	A	502	-	20,21,21	1.71	2 (10%)	26,30,30	1.20	3 (11%)
5	PLI	B	503	-	20,21,21	2.66	4 (20%)	27,30,30	2.73	14 (51%)
5	PLI	C	504	-	20,21,21	2.48	4 (20%)	27,30,30	2.81	12 (44%)
4	DMS	B	502	-	3,3,3	0.64	0	3,3,3	0.33	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	F0G	D	501	-	-	2/15/15/15	0/1/1/1
5	PLI	B	503	-	-	2/14/15/15	0/1/1/1
5	PLI	C	504	-	-	4/14/15/15	0/1/1/1
3	F0G	A	502	-	-	4/15/15/15	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	503	PLI	OP4-C5A	-7.39	1.36	1.43
5	C	504	PLI	OP4-C5A	-6.03	1.37	1.43
3	A	502	F0G	C4-C4A	-5.71	1.34	1.46
5	B	503	PLI	C2-N1	5.70	1.40	1.34
5	C	504	PLI	C2-N1	5.66	1.40	1.34
3	D	501	F0G	C4-C4A	-5.63	1.34	1.46
5	C	504	PLI	P-OP4	5.45	1.77	1.60
5	B	503	PLI	P-OP4	5.39	1.77	1.60
5	B	503	PLI	C6-N1	2.35	1.40	1.36
5	C	504	PLI	C6-N1	2.19	1.39	1.36
3	D	501	F0G	C4A-N	2.08	1.31	1.27
3	A	502	F0G	C4A-N	2.05	1.31	1.27

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	504	PLI	C3-C4-C5	-8.01	115.06	119.28
5	B	503	PLI	C3-C4-C5	-7.33	115.41	119.28
5	C	504	PLI	C6-N1-C2	-5.25	119.84	124.20
5	B	503	PLI	C6-N1-C2	-5.11	119.96	124.20
5	B	503	PLI	O-C-CA	-5.01	115.23	121.35
5	C	504	PLI	O-C-CA	-4.70	115.60	121.35
5	C	504	PLI	CB-CA-C	-3.82	114.51	118.11
5	B	503	PLI	C6-C5-C4	3.29	121.56	119.00
5	C	504	PLI	C6-C5-C4	3.27	121.54	119.00
5	C	504	PLI	C4-C3-C2	3.07	121.03	118.34
5	B	503	PLI	O3A-C3-C2	3.05	121.22	118.40
5	C	504	PLI	O3A-C3-C2	3.02	121.19	118.40
5	B	503	PLI	C4-C3-C2	2.96	120.94	118.34
5	B	503	PLI	CB-CA-C	-2.92	115.36	118.11
5	C	504	PLI	CB-CA-N	-2.92	118.48	124.67
5	B	503	PLI	CB-CA-N	-2.71	118.91	124.67
5	B	503	PLI	C5A-C5-C4	-2.70	120.38	122.19
3	A	502	F0G	C5-C6-N1	-2.58	119.63	123.83
5	C	504	PLI	OP4-P-OP2	-2.53	99.61	106.44
5	C	504	PLI	C3-C2-N1	2.44	121.33	118.63
3	D	501	F0G	C5-C6-N1	-2.44	119.87	123.83
5	B	503	PLI	OP4-P-OP2	-2.39	99.98	106.44
5	C	504	PLI	OP1-P-OP4	-2.37	100.49	106.67
3	A	502	F0G	C4-C3-C2	-2.26	118.87	120.14
5	B	503	PLI	OP1-P-OP4	-2.23	100.84	106.67
5	B	503	PLI	OP3-P-OP4	-2.22	100.88	106.67
5	C	504	PLI	OP3-P-OP1	2.09	115.65	107.80
5	B	503	PLI	OP3-P-OP1	2.07	115.58	107.80
3	A	502	F0G	OXT-C-O	-2.05	119.42	124.08
3	D	501	F0G	OXT-C-O	-2.05	119.43	124.08
5	B	503	PLI	C3-C2-N1	2.02	120.86	118.63

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	501	F0G	C-CA-N-C4A
5	B	503	PLI	CB-CA-N-C4A
5	B	503	PLI	OXT-C-CA-CB
5	C	504	PLI	CB-CA-N-C4A
5	C	504	PLI	OXT-C-CA-CB
3	D	501	F0G	CB-CA-N-C4A
5	C	504	PLI	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
5	C	504	PLI	C5-C4-C4A-N
3	A	502	F0G	CB-CA-N-C4A
3	A	502	F0G	OXT-C-CA-CB
3	A	502	F0G	C-CA-N-C4A
3	A	502	F0G	O-C-CA-N

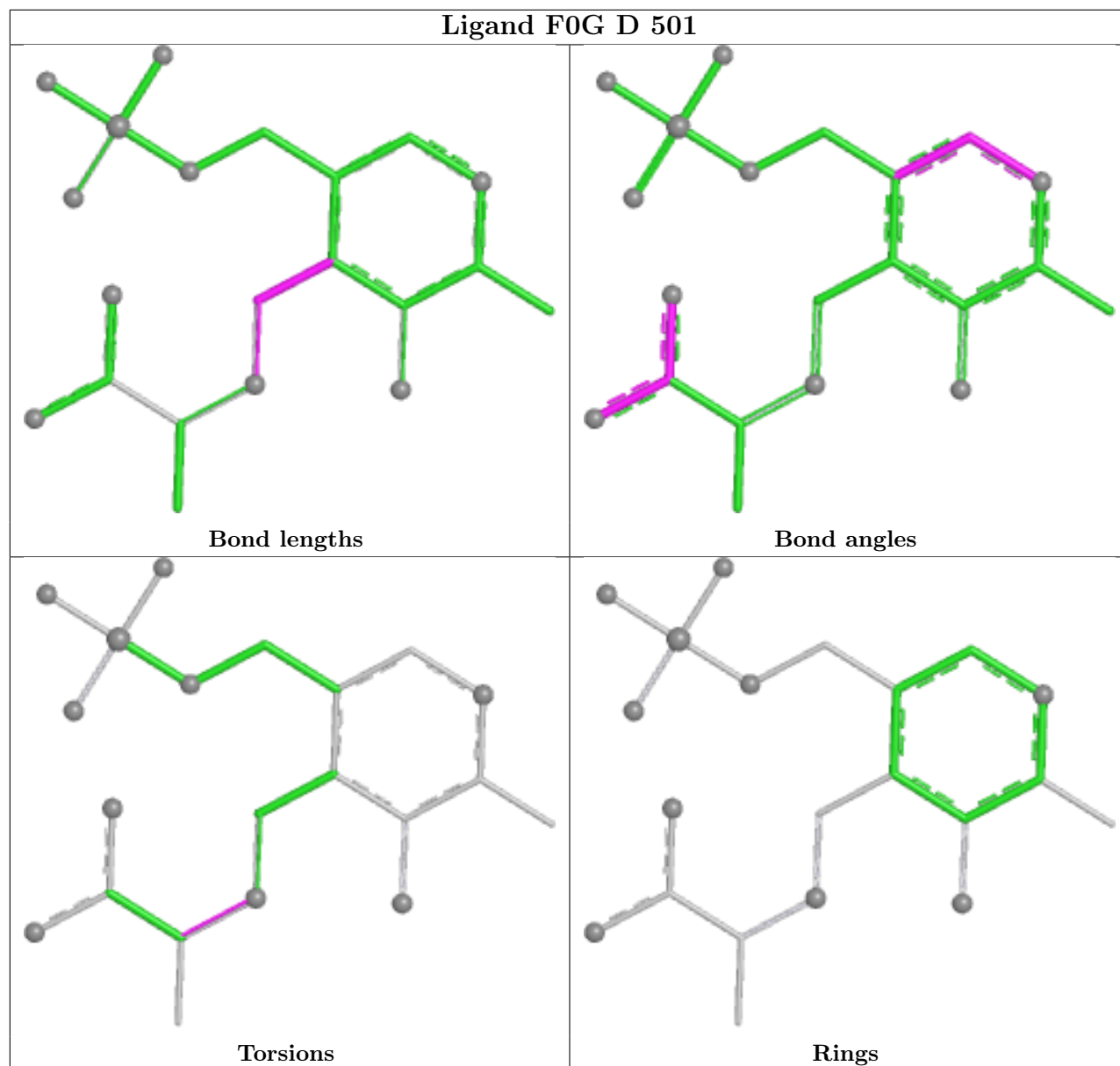
There are no ring outliers.

2 monomers are involved in 2 short contacts:

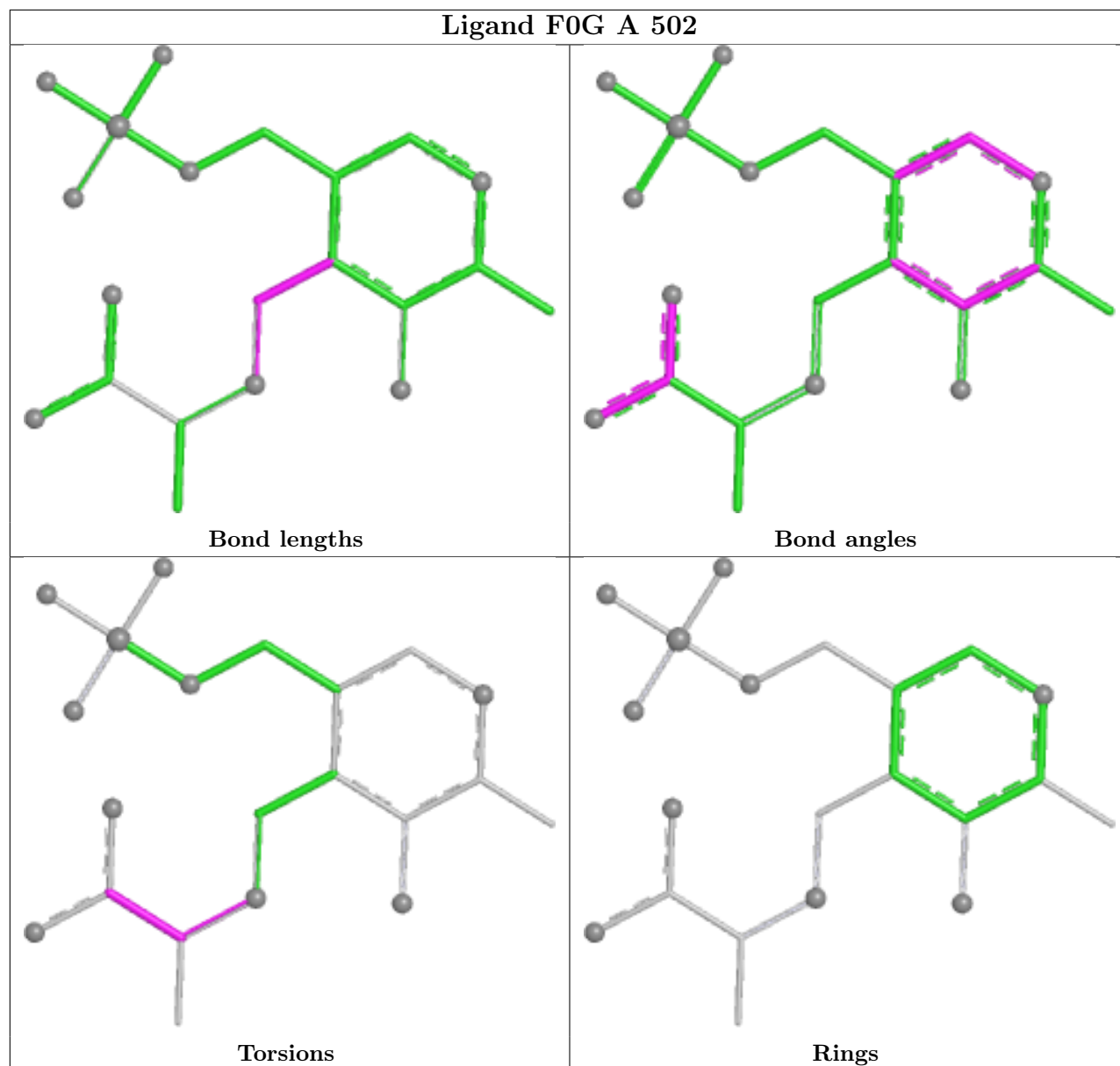
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	F0G	1	0
3	A	502	F0G	1	0

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.

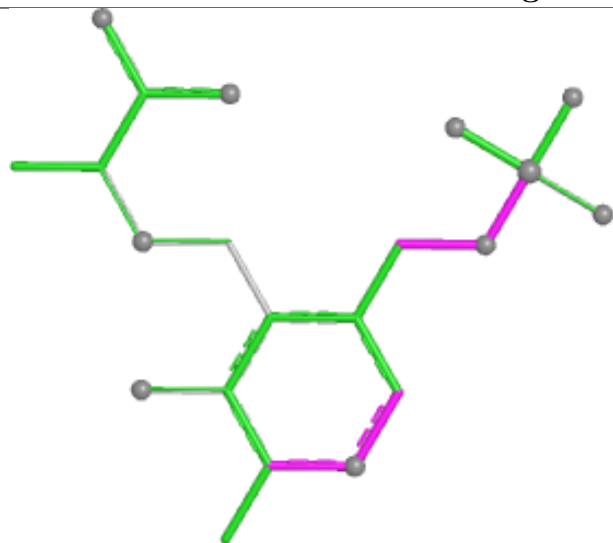
Ligand F0G D 501



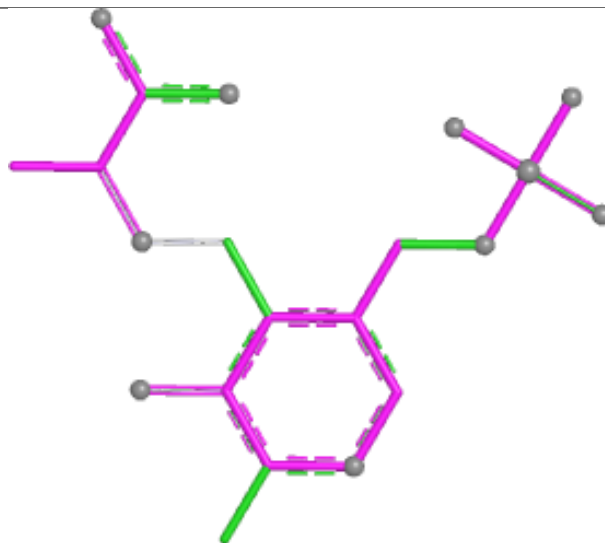
Ligand F0G A 502



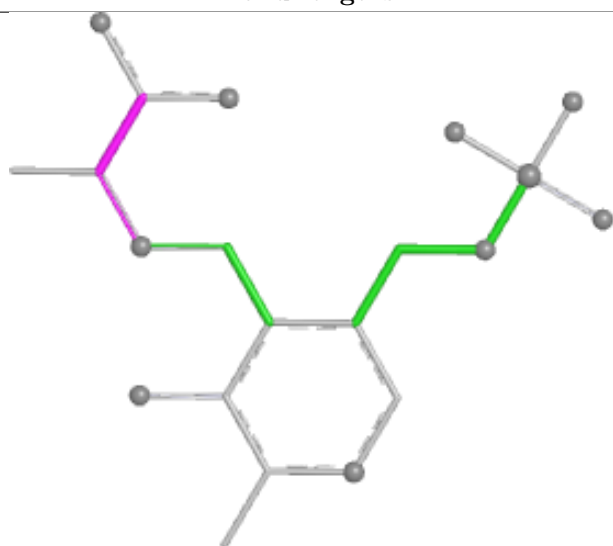
Ligand PLI B 503



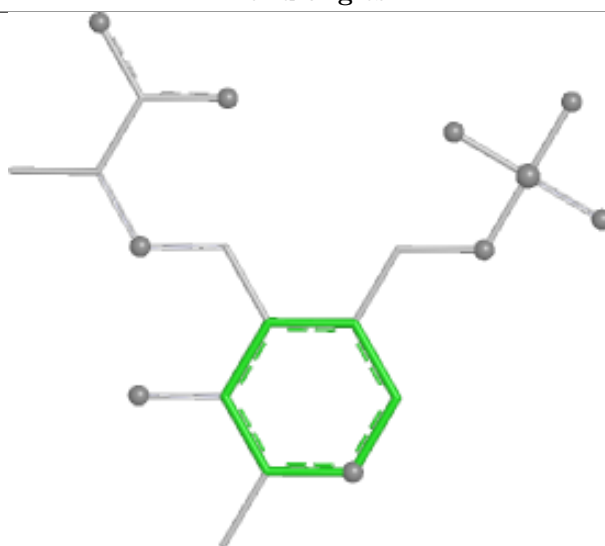
Bond lengths



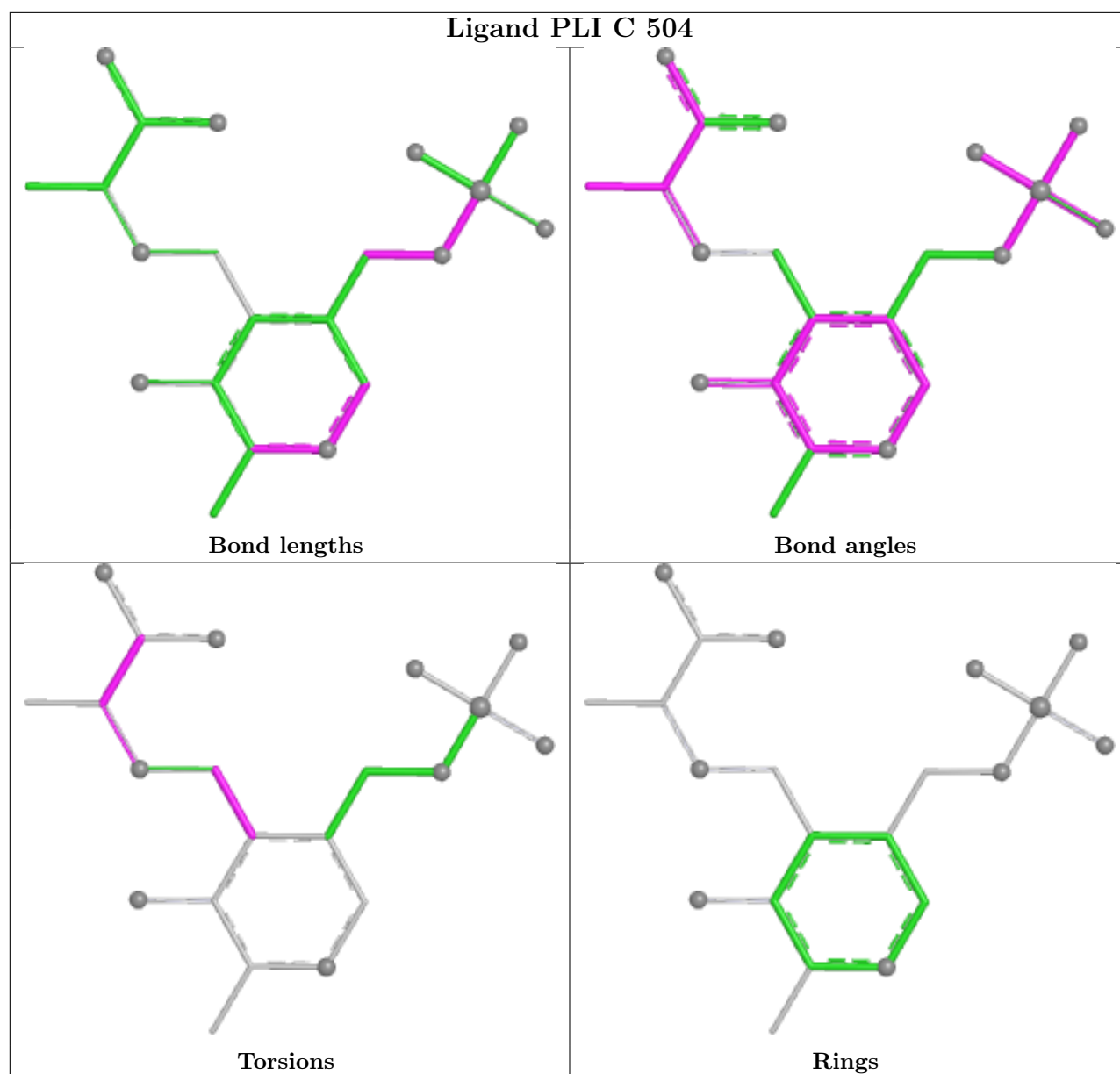
Bond angles



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, 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	460/467 (98%)	0.68	78 (16%) 4 4	11, 30, 82, 129	5 (1%)
1	B	458/467 (98%)	0.36	39 (8%) 16 18	15, 30, 69, 104	2 (0%)
1	C	465/467 (99%)	0.13	34 (7%) 21 24	9, 24, 66, 101	6 (1%)
1	D	462/467 (98%)	0.09	40 (8%) 16 18	11, 22, 62, 123	4 (0%)
All	All	1845/1868 (98%)	0.32	191 (10%) 11 13	9, 27, 71, 129	17 (0%)

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	363	VAL	8.5
1	A	391	ILE	8.1
1	A	447	LEU	6.2
1	A	394	PHE	6.0
1	A	363	VAL	5.8
1	A	455	VAL	5.7
1	A	449	PHE	5.7
1	B	408	ALA	5.6
1	A	456	LEU	5.5
1	B	454	PRO	5.4
1	C	366	ILE	5.4
1	A	392	GLY	5.3
1	A	371	PHE	5.3
1	A	458	HIS	5.3
1	B	459	PHE	4.8
1	A	406	LYS	4.8
1	A	441	PHE	4.7
1	B	458	HIS	4.7
1	B	396	LEU	4.7
1	B	453	PRO	4.7
1	B	466	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	451	TYR	4.6
1	D	401	ALA	4.6
1	A	408	ALA	4.6
1	A	461	ALA	4.5
1	C	444	LEU	4.5
1	A	396	LEU	4.5
1	A	390	GLU	4.4
1	A	442	ALA	4.4
1	A	407	HIS	4.4
1	A	445	LYS	4.3
1	A	466	ILE	4.2
1	A	444	LEU	4.2
1	A	451	TYR	4.2
1	A	457	ARG	4.2
1	C	466	ILE	4.2
1	A	459	PHE	4.1
1	D	449	PHE	4.1
1	B	397	GLY	4.1
1	B	455	VAL	4.1
1	A	27	ALA	4.1
1	B	449	PHE	4.0
1	A	34	TYR	4.0
1	A	463	LEU	3.9
1	B	447	LEU	3.9
1	A	395	LEU	3.9
1	D	396	LEU	3.9
1	C	360	LYS	3.9
1	A	453	PRO	3.8
1	C	364	PRO	3.8
1	B	446	GLY	3.8
1	B	456	LEU	3.8
1	C	410	MET	3.8
1	C	368	GLY	3.7
1	A	366	ILE	3.7
1	D	443	THR	3.7
1	C	401	ALA	3.6
1	A	368	GLY	3.6
1	D	394	PHE	3.6
1	D	403	GLY	3.6
1	A	465	PRO	3.6
1	B	407	HIS	3.6
1	D	407	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	466	ILE	3.5
1	A	397	GLY	3.5
1	A	446	GLY	3.5
1	B	371	PHE	3.4
1	B	395	LEU	3.3
1	A	30	LYS	3.3
1	A	443	THR	3.3
1	D	402	THR	3.3
1	C	400	PRO	3.3
1	C	442	ALA	3.3
1	A	454	PRO	3.3
1	D	371	PHE	3.3
1	C	407	HIS	3.2
1	D	366	ILE	3.2
1	C	443	THR	3.2
1	A	393	SER	3.2
1	B	442	ALA	3.2
1	D	447	LEU	3.2
1	C	403	GLY	3.2
1	C	402	THR	3.1
1	A	410	MET	3.1
1	D	451	TYR	3.1
1	C	119	GLY	3.1
1	A	412	PHE	3.1
1	A	460	THR	3.1
1	C	408	ALA	3.1
1	B	457	ARG	3.1
1	A	33	GLY	3.1
1	A	389	VAL	3.1
1	D	467	GLU	3.1
1	A	364	PRO	3.1
1	A	411	GLU	3.1
1	B	410	MET	3.0
1	C	446	GLY	3.0
1	D	405	GLN	3.0
1	C	447	LEU	3.0
1	D	454	PRO	3.0
1	A	362	LEU	2.9
1	C	362	LEU	2.9
1	A	361	LYS	2.9
1	B	461	ALA	2.9
1	D	463	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	372	PRO	2.9
1	B	119	GLY	2.9
1	C	412	PHE	2.9
1	A	32	ALA	2.8
1	A	155	PHE	2.8
1	D	395	LEU	2.8
1	A	367	PRO	2.8
1	B	394	PHE	2.7
1	C	441	PHE	2.7
1	A	437	LEU	2.7
1	A	369	ASP	2.7
1	C	365	GLN	2.7
1	D	368	GLY	2.7
1	D	459	PHE	2.7
1	A	38	LEU	2.7
1	D	455	VAL	2.7
1	A	373	ALA	2.7
1	B	409	ASP	2.6
1	B	406	LYS	2.6
1	B	155	PHE	2.6
1	B	444	LEU	2.6
1	A	462	ARG	2.6
1	C	409	ASP	2.6
1	D	408	ALA	2.6
1	C	445	LYS	2.6
1	B	443	THR	2.6
1	D	465	PRO	2.6
1	D	444	LEU	2.6
1	A	405	GLN	2.6
1	D	450	GLU	2.6
1	A	378	ASN	2.6
1	C	454	PRO	2.5
1	B	441	PHE	2.5
1	A	382	LEU	2.5
1	A	409	ASP	2.5
1	A	377	ILE	2.5
1	D	367	PRO	2.5
1	C	451	TYR	2.5
1	A	31	GLU	2.5
1	A	139[A]	VAL	2.5
1	D	364	PRO	2.5
1	A	398	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	461	ALA	2.5
1	A	26	GLU	2.4
1	D	369	ASP	2.4
1	B	363	VAL	2.4
1	D	406	LYS	2.4
1	B	460	THR	2.4
1	B	364	PRO	2.4
1	A	359	CYS	2.4
1	C	399	ASP	2.4
1	D	404	GLU	2.4
1	B	465	PRO	2.4
1	C	370	GLN	2.4
1	D	453	PRO	2.4
1	D	456	LEU	2.3
1	D	27	ALA	2.3
1	C	367	PRO	2.3
1	D	464	LYS	2.3
1	A	28	ALA	2.3
1	A	375	ALA	2.3
1	C	359	CYS	2.3
1	A	22	ARG	2.3
1	C	455	VAL	2.3
1	A	370	GLN	2.2
1	A	448	GLU	2.2
1	B	369	ASP	2.2
1	B	370	GLN	2.2
1	A	452	GLU	2.2
1	D	460	THR	2.2
1	A	119	GLY	2.2
1	A	358	ASP	2.2
1	B	448	GLU	2.1
1	A	21	SER	2.1
1	A	360	LYS	2.1
1	D	34	TYR	2.1
1	D	409	ASP	2.1
1	B	393	SER	2.1
1	D	361	LYS	2.1
1	A	439	GLU	2.0
1	B	361	LYS	2.0
1	B	398	ARG	2.0
1	A	23	GLU	2.0
1	C	118	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	371	PHE	2.0
1	D	392	GLY	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](#)

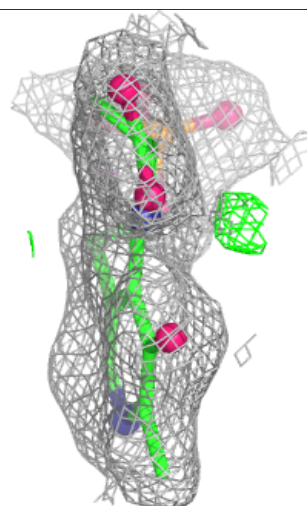
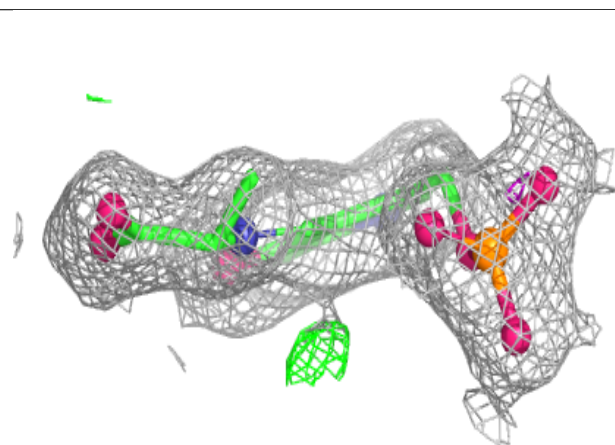
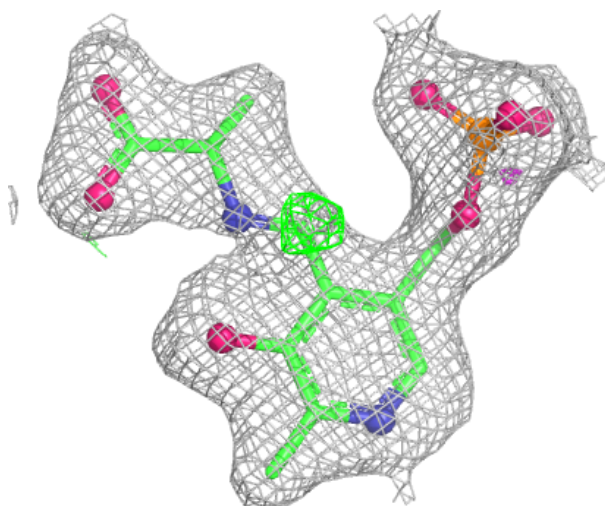
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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	DMS	B	502	4/4	0.89	0.14	40,43,52,52	0
4	DMS	C	503	4/4	0.91	0.14	38,45,49,50	0
3	F0G	A	502	21/21	0.96	0.07	23,27,34,42	0
5	PLI	B	503	21/21	0.97	0.07	20,29,34,36	0
5	PLI	C	504	21/21	0.97	0.08	14,23,31,33	0
3	F0G	D	501	21/21	0.98	0.05	14,19,26,27	0
2	K	C	501	1/1	0.99	0.04	22,22,22,22	0
2	K	C	502	1/1	0.99	0.04	19,19,19,19	0
2	K	A	501	1/1	0.99	0.03	24,24,24,24	0
2	K	B	501	1/1	0.99	0.05	22,22,22,22	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.

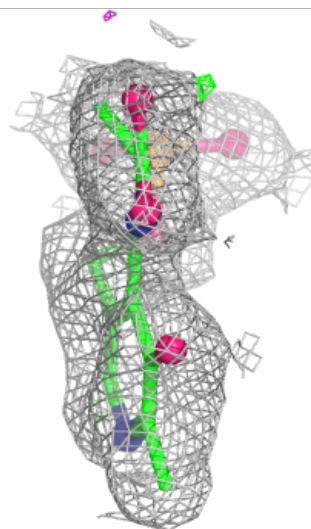
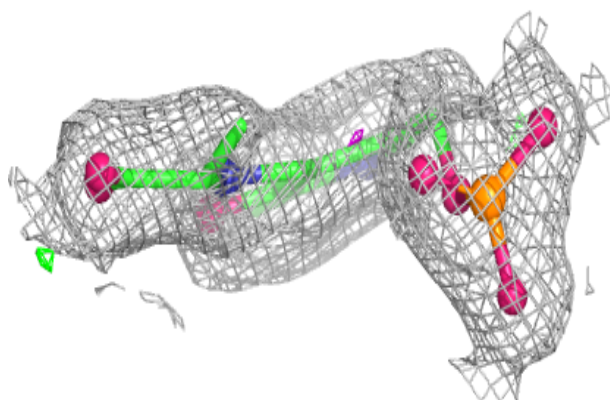
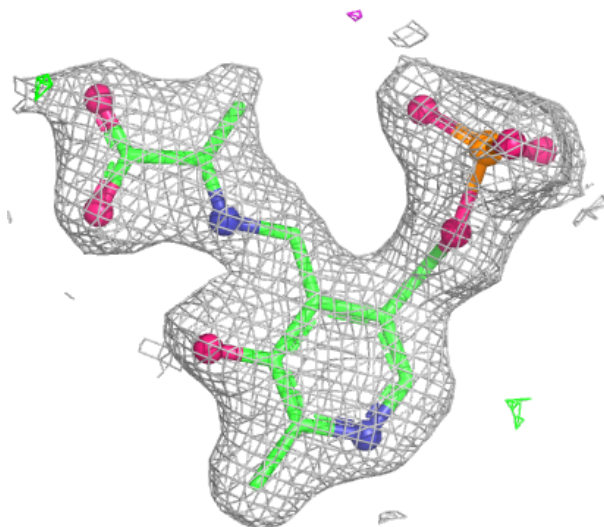
Electron density around F0G A 502:

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



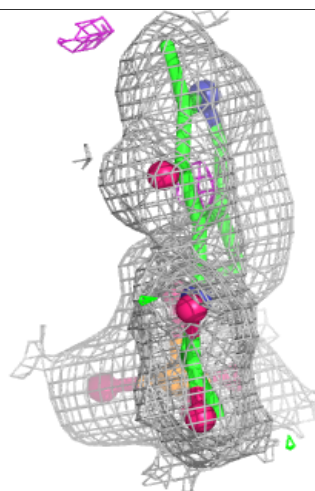
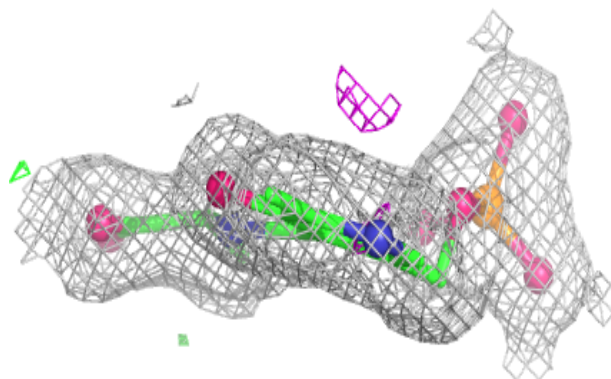
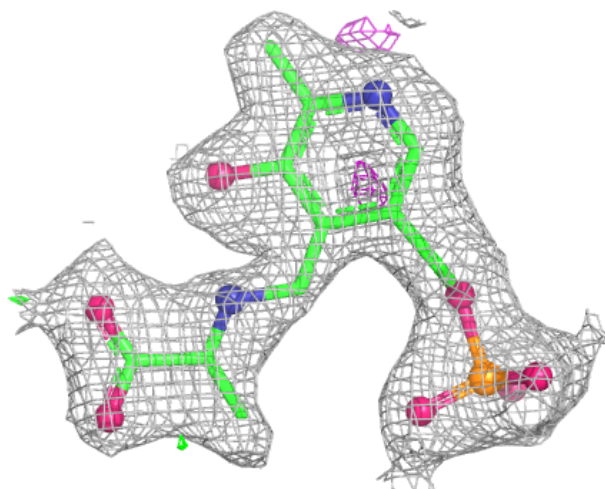
Electron density around PLI B 503:

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



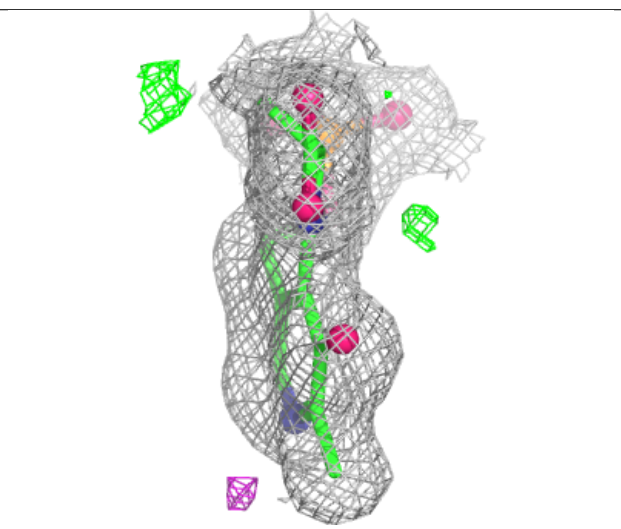
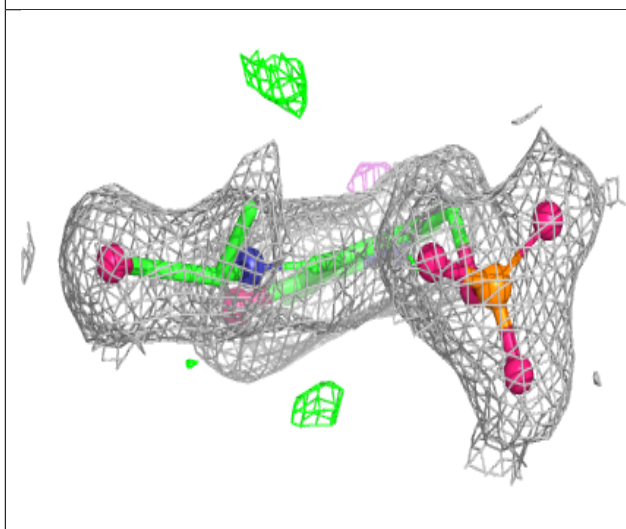
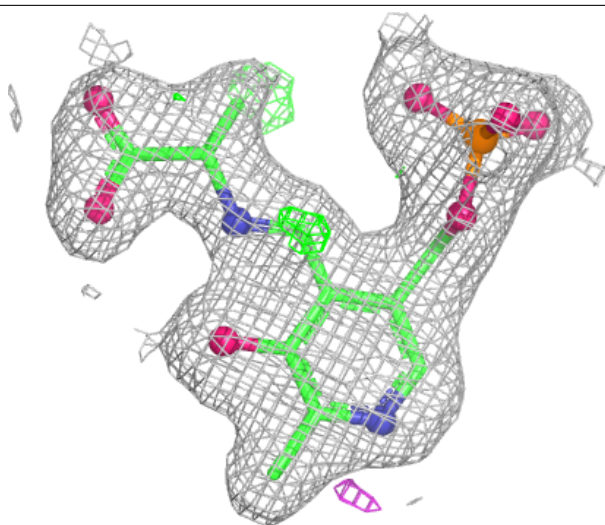
Electron density around PLI C 504:

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



Electron density around F0G D 501:

$2mF_o-DF_c$ (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.