



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:21 PM UTC

PDB ID : 8V6P / pdb_00008v6p
Title : Proteus vulgaris tryptophan indole-lyase complexed with 7-aza-L-tryptophan
Authors : Phillips, R.S.
Deposited on : 2023-12-02
Resolution : 1.74 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

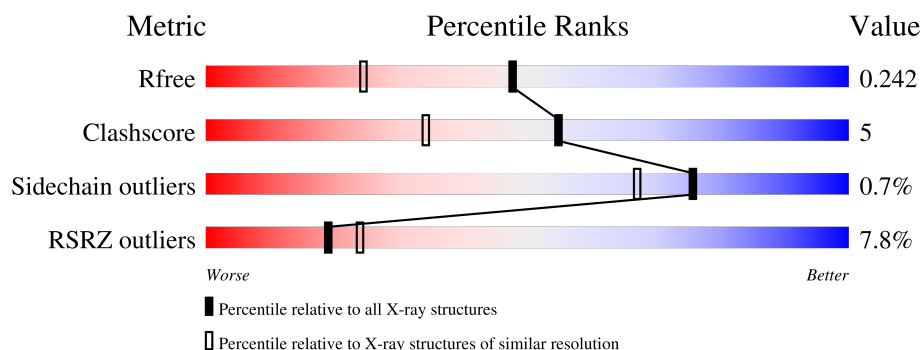
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	3% 92% 7%
1	B	467	9% 86% 13%
1	C	467	12% 78% 20% •
1	D	467	7% 88% 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17340 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.

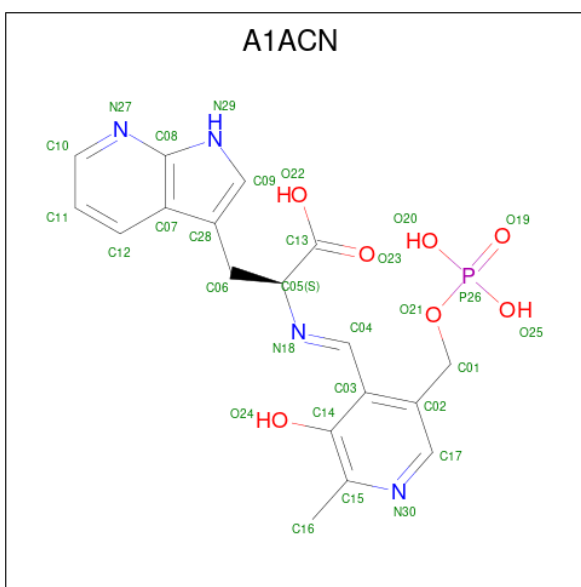
- Molecule 1 is a protein called Tryptophanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	5	0
			3716	2377	633	687	19			
1	B	466	Total	C	N	O	S	0	10	0
			3759	2406	637	695	21			
1	C	459	Total	C	N	O	S	0	124	0
			4623	2974	780	846	23			
1	D	465	Total	C	N	O	S	0	9	0
			3734	2389	635	690	20			

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

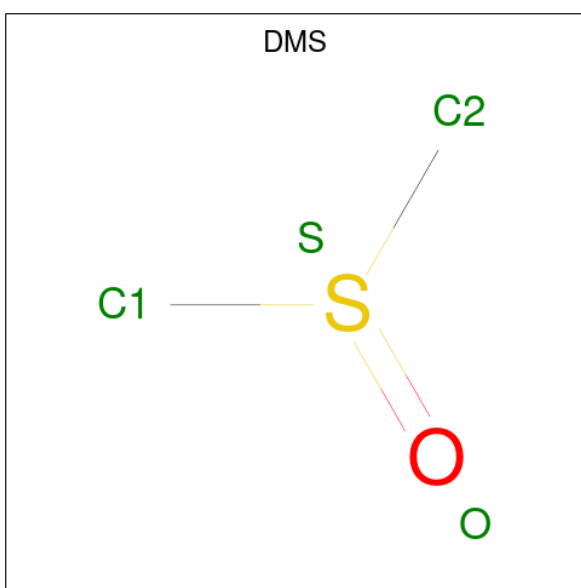
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	K	0	0
			2	2		

- Molecule 3 is (E)-N-({3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl}methylidene)-3-(1H-pyrrolo[2,3-b]pyridin-3-yl)-L-alanine (CCD ID: A1ACN) (formula: C₁₈H₁₉N₄O₇P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			30	18	4	7	1		
3	C	1	Total	C	N	O	P	0	0
			30	18	4	7	1		

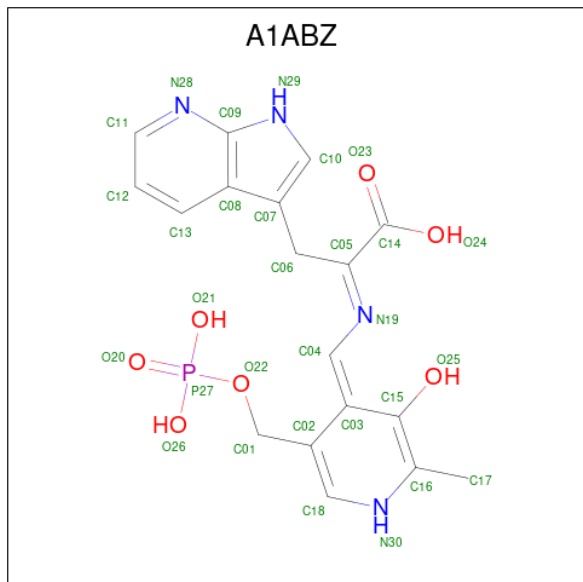
- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

- Molecule 5 is (2E)-2-{[(Z)-{3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4(1H)-y

lidene)methyl]imino}-3-(1H-pyrrolo[2,3-b]pyridin-3-yl)propanoic acid (CCD ID: A1ABZ)
(formula: C₁₈H₁₉N₄O₇P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			30	18	4	7	1		
5	D	1	Total	C	N	O	P	0	0
			30	18	4	7	1		

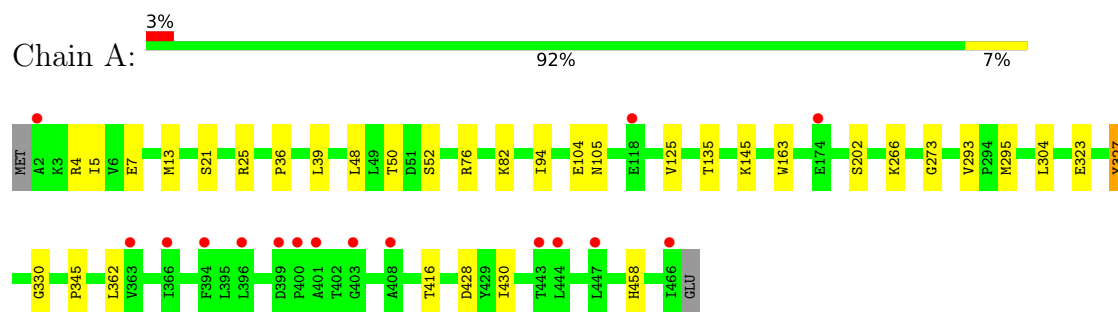
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	319	Total	O	0	2
			319	319		
6	B	356	Total	O	0	5
			356	356		
6	C	335	Total	O	0	13
			335	335		
6	D	372	Total	O	0	11
			372	372		

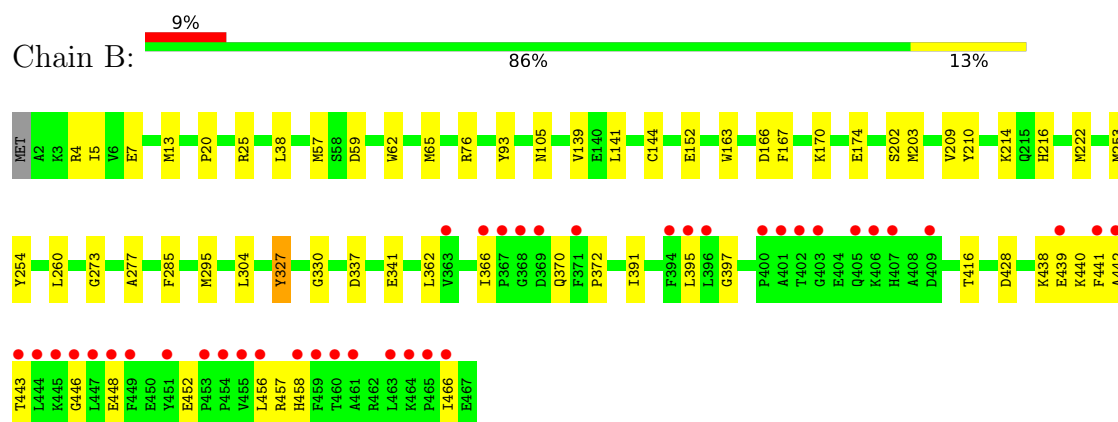
3 Residue-property plots [i](#)

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.

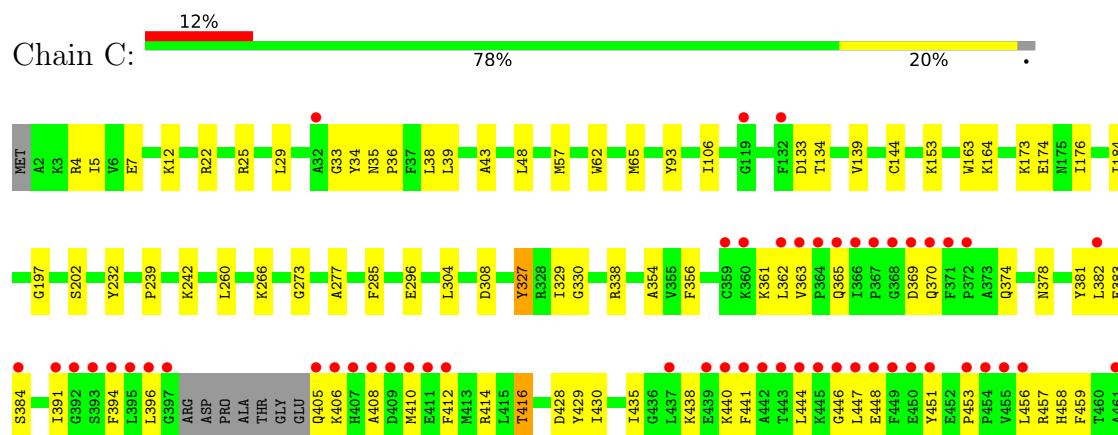
• Molecule 1: Tryptophanase



• Molecule 1: Tryptophanase

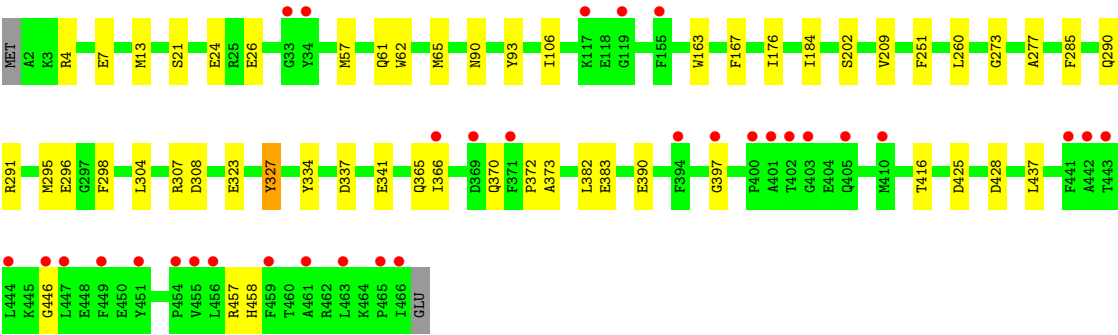
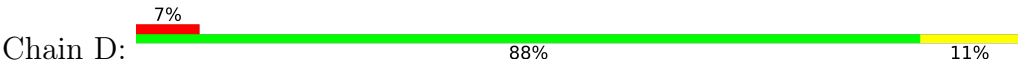


• Molecule 1: Tryptophanase





● Molecule 1: Tryptophanase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	151.63Å 211.34Å 60.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.60 – 1.74 61.60 – 1.74	Depositor EDS
% Data completeness (in resolution range)	67.9 (61.60-1.74) 66.2 (61.60-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.74Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.185 , 0.228 (Not available) , 0.242	Depositor DCC
R_{free} test set	6819 reflections (3.38%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17340	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 2.49% 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: A1ABZ, K, A1ACN, DMS

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	0.21	0/3809	0.41	0/5142
1	B	0.22	0/3860	0.45	0/5208
1	C	0.19	0/4744	0.37	0/6396
1	D	0.24	0/3842	0.44	0/5186
All	All	0.22	0/16255	0.41	0/21932

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	3716	0	3704	21	0
1	B	3759	0	3763	41	0
1	C	4623	0	4640	68	0
1	D	3734	0	3734	33	0
2	A	2	0	0	0	0
3	A	30	0	0	1	0
3	C	30	0	0	0	0
4	A	4	0	6	2	0
5	B	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	30	0	0	0	0
6	A	319	0	0	1	0
6	B	356	0	0	6	0
6	C	335	0	0	7	0
6	D	372	0	0	2	0
All	All	17340	0	15847	154	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 (154) 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:D:4[B]:ARG:NH1	6:D:602[B]:HOH:O	2.21	0.73
1:B:366:ILE:HB	1:B:372:PRO:HB3	1.74	0.70
1:C:25[A]:ARG:NH1	1:C:382[A]:LEU:O	2.26	0.68
1:A:13[B]:MET:HE3	1:C:12:LYS:HG2	1.76	0.68
1:D:370[B]:GLN:HG2	1:D:446:GLY:HA3	1.76	0.66
1:D:366:ILE:HB	1:D:372:PRO:HB3	1.79	0.65
1:B:170:LYS:NZ	1:B:174:GLU:OE2	2.31	0.63
1:A:50:THR:OG1	3:A:503:A1ACN:O22	2.14	0.62
1:C:7:GLU:HG3	1:C:327[B]:TYR:CZ	2.35	0.61
1:D:106:ILE:HD11	1:D:296:GLU:HG3	1.82	0.61
1:B:391:ILE:HD13	1:B:395:LEU:HD13	1.83	0.60
1:D:273:GLY:HA2	1:D:304:LEU:HD21	1.82	0.59
1:D:26:GLU:HG2	1:D:382:LEU:HD22	1.83	0.59
1:D:308:ASP:OD2	6:D:601:HOH:O	2.17	0.59
1:C:106:ILE:HD11	1:C:296:GLU:HG3	1.85	0.58
1:C:451[A]:TYR:HB3	1:C:462[A]:ARG:HB2	1.84	0.58
1:C:4[B]:ARG:NH1	6:C:812[B]:HOH:O	2.36	0.58
1:A:125:VAL:HG12	1:A:145:LYS:HB3	1.85	0.58
1:C:57:MET:HE1	1:C:65[B]:MET:SD	2.43	0.58
1:A:7:GLU:HG3	1:A:327[B]:TYR:CZ	2.39	0.58
1:C:29[B]:LEU:HD13	1:C:382[B]:LEU:HD21	1.85	0.58
1:C:370[B]:GLN:HG3	1:C:466[B]:ILE:HD12	1.85	0.58
1:C:163:TRP:CD2	1:C:202:SER:HB3	2.39	0.57
1:B:5:ILE:HD12	1:B:330:GLY:HA3	1.88	0.56
1:C:453[B]:PRO:HB3	1:D:290:GLN:HG2	1.88	0.56
1:A:5:ILE:HD12	1:A:330:GLY:HA3	1.88	0.55
1:C:133[B]:ASP:OD1	1:C:134:THR:N	2.40	0.55
1:A:273:GLY:HA2	1:A:304:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4[B]:ARG:NH2	1:A:428:ASP:OD2	2.39	0.55
4:A:504:DMS:H11	1:B:76[B]:ARG:HH21	1.71	0.54
1:B:448:GLU:HG3	1:B:466:ILE:HD11	1.89	0.54
1:D:383:GLU:HG2	1:D:437:LEU:HD11	1.90	0.54
1:B:4[B]:ARG:NH2	1:B:428:ASP:OD2	2.36	0.54
1:B:166:ASP:OD2	6:B:601:HOH:O	2.18	0.54
4:A:504:DMS:H11	1:B:76[B]:ARG:NH2	2.23	0.53
1:C:239:PRO:HA	1:C:242:LYS:HG2	1.90	0.53
1:B:62:TRP:CD1	1:D:13[A]:MET:HE2	2.44	0.53
1:C:34[A]:TYR:HB2	1:C:463[A]:LEU:HB2	1.91	0.53
1:C:362[B]:LEU:HD22	1:C:441[B]:PHE:HD2	1.73	0.53
1:A:48:LEU:HD11	1:A:430:ILE:HD13	1.91	0.53
1:B:273:GLY:HA2	1:B:304:LEU:HD21	1.91	0.53
1:B:93:TYR:HB3	1:B:285:PHE:CD1	2.44	0.52
1:C:456[B]:LEU:HB3	1:C:459[B]:PHE:CE2	2.44	0.52
1:B:370:GLN:HB3	1:B:446:GLY:HA3	1.92	0.52
1:C:176:ILE:HA	1:C:184[A]:ILE:HD11	1.92	0.52
1:B:13[A]:MET:HE2	1:D:62:TRP:CD1	2.45	0.52
1:C:36[B]:PRO:HA	1:C:39[B]:LEU:HG	1.92	0.52
1:B:57:MET:HE1	1:B:65[B]:MET:SD	2.50	0.52
1:D:93:TYR:HB3	1:D:285:PHE:CD1	2.46	0.51
1:A:105:ASN:HD21	1:A:295:MET:HE2	1.75	0.51
1:B:7:GLU:HG3	1:B:327[B]:TYR:CZ	2.45	0.51
1:B:337:ASP:O	1:B:341:GLU:HG3	2.12	0.50
1:C:25[A]:ARG:HD3	1:C:381[A]:TYR:O	2.12	0.50
1:B:452:GLU:O	6:B:603:HOH:O	2.20	0.50
1:D:7:GLU:HG3	1:D:327[B]:TYR:CZ	2.47	0.50
1:B:38:LEU:O	6:B:602:HOH:O	2.20	0.50
1:B:260:LEU:HG	1:B:277:ALA:HB3	1.94	0.50
1:D:163:TRP:CD2	1:D:202:SER:HB3	2.47	0.49
1:C:308:ASP:OD1	1:D:307:ARG:NH2	2.40	0.49
1:C:448[B]:GLU:N	1:C:464[B]:LYS:O	2.45	0.49
1:C:440[A]:LYS:O	1:C:444[A]:LEU:HG	2.12	0.49
1:C:139:VAL:HG13	1:C:144:CYS:HB2	1.93	0.49
1:C:369[B]:ASP:HA	1:C:406[B]:LYS:HD2	1.95	0.48
1:A:163:TRP:CD2	1:A:202:SER:HB3	2.48	0.48
1:C:153:LYS:O	1:C:164:LYS:HE2	2.13	0.48
1:C:197:GLY:HA2	1:C:356[A]:PHE:CE1	2.49	0.48
1:C:396[A]:LEU:HD21	6:C:900:HOH:O	2.13	0.48
1:C:369[A]:ASP:OD1	1:C:405[A]:GLN:NE2	2.47	0.48
1:A:50:THR:HG23	1:A:52:SER:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:MET:HE1	1:D:65[B]:MET:SD	2.54	0.48
1:C:5:ILE:HD12	1:C:330:GLY:HA3	1.96	0.47
1:C:370[A]:GLN:HG2	1:C:446[A]:GLY:HA3	1.95	0.47
1:B:4[A]:ARG:HD2	1:D:425:ASP:OD1	2.14	0.47
1:D:260:LEU:HG	1:D:277:ALA:HB3	1.97	0.47
1:B:458:HIS:H	1:B:458:HIS:CD2	2.33	0.46
1:B:59:ASP:OD1	1:B:59:ASP:N	2.49	0.46
1:D:291:ARG:O	1:D:295:MET:HG2	2.15	0.46
1:C:36[B]:PRO:HG2	6:C:914:HOH:O	2.16	0.46
1:C:391[B]:ILE:HD11	1:C:412[B]:PHE:HD2	1.81	0.46
1:C:405[B]:GLN:O	1:C:406[B]:LYS:HE3	2.16	0.46
1:C:391[A]:ILE:HD11	1:C:414[A]:ARG:HD3	1.96	0.46
1:B:222:MET:HG2	1:B:254:TYR:CE2	2.50	0.45
1:C:4[A]:ARG:NH1	1:C:428:ASP:OD2	2.50	0.45
1:C:43:ALA:O	1:C:381[A]:TYR:OH	2.28	0.45
1:C:260:LEU:HG	1:C:277:ALA:HB3	1.97	0.45
1:B:167:PHE:CD1	1:B:209:VAL:HG21	2.51	0.45
1:B:105:ASN:HD21	1:B:295:MET:HE3	1.82	0.45
1:C:232:TYR:CD2	1:C:329:ILE:HD12	2.52	0.45
1:C:354[B]:ALA:HB2	1:C:416:THR:HA	1.98	0.45
1:B:152:GLU:HG3	6:B:688:HOH:O	2.17	0.45
1:B:141[A]:LEU:HG	6:B:661:HOH:O	2.16	0.44
1:D:373:ALA:HB3	1:D:390:GLU:HG2	1.98	0.44
1:C:435[A]:ILE:O	1:C:438[A]:LYS:HG2	2.17	0.44
1:A:21:SER:O	1:A:25:ARG:HG3	2.17	0.44
1:C:362[B]:LEU:HD22	1:C:441[B]:PHE:CD2	2.53	0.44
1:D:365:GLN:H	1:D:365:GLN:CD	2.25	0.44
1:B:210:TYR:CE1	1:B:214:LYS:HE3	2.53	0.44
1:D:61:GLN:O	1:D:65[B]:MET:HG3	2.17	0.44
1:D:337:ASP:O	1:D:341:GLU:HG3	2.17	0.44
1:C:22[A]:ARG:HH21	1:C:383[A]:GLU:HG2	1.82	0.44
1:C:447[A]:LEU:HD23	1:C:465[A]:PRO:HA	1.99	0.44
1:D:176:ILE:HA	1:D:184:ILE:HD11	2.00	0.44
1:D:90:ASN:HB2	1:D:251:PHE:CE1	2.53	0.44
1:D:334:TYR:OH	1:D:428:ASP:OD1	2.34	0.43
1:B:438:LYS:NZ	1:B:439[B]:GLU:OE2	2.51	0.43
1:B:203:MET:HE1	1:B:253:MET:HG3	1.99	0.43
1:B:105:ASN:HD21	1:B:295:MET:CE	2.32	0.43
1:C:363[B]:VAL:HG12	1:C:441[B]:PHE:O	2.18	0.43
1:B:362:LEU:HD21	1:B:441:PHE:CZ	2.54	0.43
1:C:33[A]:GLY:O	1:C:463[A]:LEU:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:PRO:HD2	1:A:362:LEU:HD13	2.00	0.42
1:C:378[B]:ASN:O	1:C:382[B]:LEU:HG	2.19	0.42
1:A:13[A]:MET:HE2	1:C:62:TRP:CD1	2.55	0.42
1:B:216:HIS:HD2	6:B:919:HOH:O	2.02	0.42
1:C:48:LEU:HD11	1:C:430:ILE:HD13	2.00	0.42
1:C:456[B]:LEU:HB3	1:C:459[B]:PHE:CD2	2.55	0.42
1:B:139:VAL:HG13	1:B:144:CYS:HB2	2.01	0.42
1:C:197:GLY:HA2	1:C:356[B]:PHE:CE2	2.54	0.42
1:C:361[A]:LYS:HB2	1:C:361[A]:LYS:HE3	1.81	0.42
1:C:453[B]:PRO:HD2	1:C:457[B]:ARG:HA	2.02	0.42
1:D:323:GLU:H	1:D:323:GLU:CD	2.27	0.42
1:B:442:ALA:O	1:B:443:THR:OG1	2.29	0.42
1:C:173:LYS:NZ	6:C:823:HOH:O	2.46	0.42
1:C:405[B]:GLN:O	1:C:406[B]:LYS:HB2	2.19	0.42
1:D:21:SER:OG	1:D:24:GLU:HG3	2.20	0.42
1:C:29[B]:LEU:HD22	1:C:382[B]:LEU:HD21	2.02	0.42
1:C:273:GLY:HA2	1:C:304:LEU:HD21	2.02	0.42
1:D:65[B]:MET:HE2	1:D:307:ARG:HD2	2.01	0.42
1:C:38[B]:LEU:HD23	1:D:298:PHE:HZ	1.85	0.42
1:C:374[B]:GLN:NE2	6:C:817:HOH:O	2.39	0.41
1:A:76:ARG:NH1	6:A:604:HOH:O	2.30	0.41
1:B:20:PRO:O	1:B:25:ARG:NH1	2.51	0.41
1:C:35[A]:ASN:ND2	1:C:458[A]:HIS:O	2.41	0.41
1:C:174:GLU:HG3	6:C:833:HOH:O	2.19	0.41
1:C:406[A]:LYS:HA	1:C:406[A]:LYS:HD3	1.75	0.41
1:C:408[A]:ALA:C	1:C:410[A]:MET:H	2.27	0.41
1:D:458:HIS:H	1:D:458:HIS:CD2	2.38	0.41
1:A:323:GLU:H	1:A:323:GLU:CD	2.28	0.41
1:A:104:GLU:OE2	1:A:135:THR:OG1	2.34	0.41
1:D:397:GLY:HA2	1:D:457:ARG:CZ	2.51	0.41
1:B:439[A]:GLU:HG2	1:B:440:LYS:HG3	2.02	0.41
1:B:397:GLY:HA2	1:B:457:ARG:CZ	2.50	0.41
1:C:363[A]:VAL:C	1:C:365[A]:GLN:H	2.29	0.41
1:C:384[A]:SER:HB2	1:C:429:TYR:CE1	2.56	0.41
1:A:36:PRO:HA	1:A:39:LEU:HG	2.03	0.41
1:C:448[A]:GLU:HB2	1:C:466[A]:ILE:HG12	2.03	0.41
1:A:293:VAL:HG12	1:B:456:LEU:HD13	2.04	0.41
1:A:458:HIS:CD2	1:A:458:HIS:H	2.38	0.40
1:B:163:TRP:CD2	1:B:202:SER:HB3	2.56	0.40
1:A:82:LYS:HG3	1:A:94:ILE:HG12	2.02	0.40
1:C:338:ARG:NH1	1:C:428:ASP:OD1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:PHE:CD1	1:D:209:VAL:HG21	2.56	0.40
1:C:93:TYR:HB3	1:C:285:PHE:CD1	2.57	0.40
1:C:242:LYS:HG3	6:C:1040:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	389/386 (101%)	385 (99%)	4 (1%)	68	54
1	B	395/386 (102%)	392 (99%)	3 (1%)	73	64
1	C	487/386 (126%)	480 (99%)	7 (1%)	59	41
1	D	393/386 (102%)	390 (99%)	3 (1%)	73	64
All	All	1664/1544 (108%)	1647 (99%)	17 (1%)	76	54

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	266	LYS
1	A	327[A]	TYR
1	A	327[B]	TYR
1	A	416	THR
1	B	327[A]	TYR
1	B	327[B]	TYR
1	B	416	THR
1	C	266[A]	LYS

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Mol	Chain	Res	Type
1	C	266[B]	LYS
1	C	327[A]	TYR
1	C	327[B]	TYR
1	C	394[A]	PHE
1	C	394[B]	PHE
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 (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	290	GLN
1	A	458	HIS
1	B	175	ASN
1	B	216	HIS
1	B	458	HIS
1	C	216	HIS
1	C	290	GLN
1	D	60	HIS
1	D	243	ASN
1	D	458	HIS

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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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
5	A1ABZ	B	501	-	30,32,32	3.31	12 (40%)	37,46,46	2.64	10 (27%)
3	A1ACN	C	701	-	31,32,32	2.67	12 (38%)	42,46,46	2.45	12 (28%)
5	A1ABZ	D	501	-	30,32,32	3.35	12 (40%)	37,46,46	2.85	11 (29%)
3	A1ACN	A	503	-	31,32,32	2.66	14 (45%)	42,46,46	2.39	11 (26%)
4	DMS	A	504	-	3,3,3	0.68	0	3,3,3	0.59	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
5	A1ABZ	B	501	-	-	1/17/19/19	0/3/3/3
3	A1ACN	C	701	-	-	3/19/19/19	0/3/3/3
5	A1ABZ	D	501	-	-	2/17/19/19	0/3/3/3
3	A1ACN	A	503	-	-	2/19/19/19	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	A1ABZ	C10-C07	10.91	1.53	1.36
5	D	501	A1ABZ	C10-C07	10.60	1.52	1.36
5	B	501	A1ABZ	C09-N29	6.55	1.46	1.36
3	A	503	A1ACN	C07-C08	6.33	1.48	1.41
3	C	701	A1ACN	C07-C08	6.28	1.48	1.41
5	D	501	A1ABZ	C16-N30	6.25	1.40	1.34
3	C	701	A1ACN	C05-C13	6.12	1.59	1.52
5	D	501	A1ABZ	C09-N29	6.11	1.45	1.36
3	A	503	A1ACN	C05-C13	5.86	1.59	1.52
5	B	501	A1ABZ	C16-N30	5.68	1.40	1.34
5	D	501	A1ABZ	C08-C07	5.35	1.52	1.44
5	B	501	A1ABZ	C08-C07	5.25	1.52	1.44
3	A	503	A1ACN	O24-C14	-5.08	1.25	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501	A1ABZ	P27-O22	5.03	1.76	1.60
5	B	501	A1ABZ	P27-O22	4.91	1.75	1.60
3	C	701	A1ACN	O24-C14	-4.63	1.26	1.36
5	D	501	A1ABZ	C18-C02	4.58	1.43	1.36
5	D	501	A1ABZ	C06-C07	4.38	1.55	1.50
3	C	701	A1ACN	C03-C14	4.25	1.48	1.41
3	A	503	A1ACN	C03-C14	4.18	1.48	1.41
5	B	501	A1ABZ	C06-C07	4.08	1.55	1.50
3	C	701	A1ACN	P26-O21	3.91	1.72	1.60
5	B	501	A1ABZ	C18-C02	3.83	1.41	1.36
5	D	501	A1ABZ	C15-C16	3.80	1.42	1.37
3	A	503	A1ACN	C08-N29	3.71	1.42	1.36
3	C	701	A1ACN	C08-N29	3.70	1.42	1.36
3	C	701	A1ACN	C05-N18	3.67	1.51	1.46
3	A	503	A1ACN	P26-O21	3.64	1.71	1.60
3	C	701	A1ACN	C15-N30	3.47	1.40	1.33
3	A	503	A1ACN	C15-N30	3.31	1.39	1.33
5	B	501	A1ABZ	C15-C16	3.22	1.41	1.37
3	A	503	A1ACN	P26-O25	3.06	1.66	1.54
3	A	503	A1ACN	C09-C28	3.04	1.41	1.36
3	C	701	A1ACN	C09-C28	2.94	1.41	1.36
3	C	701	A1ACN	C04-N18	2.92	1.32	1.27
5	D	501	A1ABZ	C08-C09	2.86	1.44	1.41
3	A	503	A1ACN	C05-N18	2.81	1.49	1.46
3	C	701	A1ACN	P26-O25	2.81	1.65	1.54
3	A	503	A1ACN	C04-N18	2.72	1.32	1.27
5	B	501	A1ABZ	C08-C09	2.62	1.44	1.41
3	A	503	A1ACN	C17-C02	2.48	1.42	1.37
3	C	701	A1ACN	C17-C02	2.45	1.42	1.37
3	A	503	A1ACN	C14-C15	2.27	1.43	1.41
5	B	501	A1ABZ	C11-N28	2.25	1.39	1.34
5	D	501	A1ABZ	C11-N28	2.22	1.39	1.34
5	D	501	A1ABZ	C03-C02	-2.20	1.39	1.44
5	B	501	A1ABZ	O25-C15	-2.18	1.26	1.33
5	D	501	A1ABZ	O25-C15	-2.17	1.26	1.33
3	A	503	A1ACN	C03-C02	-2.16	1.39	1.42
5	B	501	A1ABZ	C03-C02	-2.11	1.39	1.44

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	501	A1ABZ	C06-C07-C10	-9.47	113.89	126.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	A1ABZ	C06-C07-C10	-9.46	113.91	126.84
3	A	503	A1ACN	C07-C08-N29	-8.54	105.30	108.42
3	C	701	A1ACN	C07-C08-N29	-8.49	105.32	108.42
5	B	501	A1ABZ	C06-C07-C08	-7.77	116.31	126.43
5	D	501	A1ABZ	C06-C07-C08	-7.20	117.04	126.43
5	D	501	A1ABZ	C09-N29-C10	6.37	111.48	108.48
3	C	701	A1ACN	C05-N18-C04	6.01	125.70	116.77
5	D	501	A1ABZ	C08-C09-N29	-5.71	106.33	108.42
3	A	503	A1ACN	C05-N18-C04	5.56	125.03	116.77
3	A	503	A1ACN	C08-N29-C09	5.52	111.08	108.48
5	B	501	A1ABZ	C09-N29-C10	5.48	111.06	108.48
3	C	701	A1ACN	C03-C14-C15	-5.31	117.15	120.14
3	C	701	A1ACN	C08-N29-C09	4.85	110.77	108.48
5	B	501	A1ABZ	C08-C09-N29	-4.51	106.77	108.42
3	A	503	A1ACN	C03-C14-C15	-4.44	117.64	120.14
5	D	501	A1ABZ	O25-C15-C16	4.32	122.39	118.40
3	A	503	A1ACN	O25-P26-O21	-4.03	96.16	106.67
3	C	701	A1ACN	C06-C05-N18	3.85	115.39	109.56
5	D	501	A1ABZ	C08-C07-C10	-3.40	102.68	106.16
5	B	501	A1ABZ	C08-C07-C10	-3.37	102.71	106.16
5	D	501	A1ABZ	C01-C02-C03	-3.32	119.97	122.19
3	C	701	A1ACN	O25-P26-O21	-3.31	98.04	106.67
3	A	503	A1ACN	C12-C07-C28	2.94	138.24	133.85
3	C	701	A1ACN	C12-C07-C28	2.78	138.00	133.85
5	D	501	A1ABZ	O26-P27-O22	-2.64	99.78	106.67
3	C	701	A1ACN	C17-N30-C15	2.62	123.94	119.20
3	C	701	A1ACN	O20-P26-O19	2.61	120.98	110.83
3	A	503	A1ACN	C07-C28-C09	2.60	108.82	106.16
5	D	501	A1ABZ	C18-N30-C16	-2.54	122.09	124.20
3	A	503	A1ACN	O24-C14-C15	2.46	122.68	117.58
5	D	501	A1ABZ	C07-C10-N29	-2.43	107.64	110.31
3	A	503	A1ACN	C17-N30-C15	2.40	123.55	119.20
3	C	701	A1ACN	O24-C14-C15	2.39	122.54	117.58
3	C	701	A1ACN	C07-C28-C09	2.34	108.56	106.16
3	A	503	A1ACN	O20-P26-O19	2.34	119.96	110.83
5	B	501	A1ABZ	O26-P27-O22	-2.31	100.65	106.67
5	B	501	A1ABZ	O25-C15-C16	2.27	120.50	118.40
5	B	501	A1ABZ	C18-N30-C16	-2.21	122.37	124.20
5	B	501	A1ABZ	C17-C16-C15	-2.19	119.59	122.27
5	B	501	A1ABZ	O21-P27-O20	2.11	119.07	110.83
5	D	501	A1ABZ	C17-C16-C15	-2.10	119.69	122.27
3	A	503	A1ACN	C12-C07-C08	-2.04	115.12	117.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	701	A1ACN	C12-C07-C08	-2.01	115.15	117.16

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	A1ACN	C06-C05-N18-C04
3	A	503	A1ACN	C13-C05-N18-C04
3	C	701	A1ACN	C06-C05-N18-C04
5	B	501	A1ABZ	C02-C03-C04-N19
5	D	501	A1ABZ	C02-C03-C04-N19
5	D	501	A1ABZ	C06-C05-C14-O23
3	C	701	A1ACN	C14-C03-C04-N18
3	C	701	A1ACN	C13-C05-N18-C04

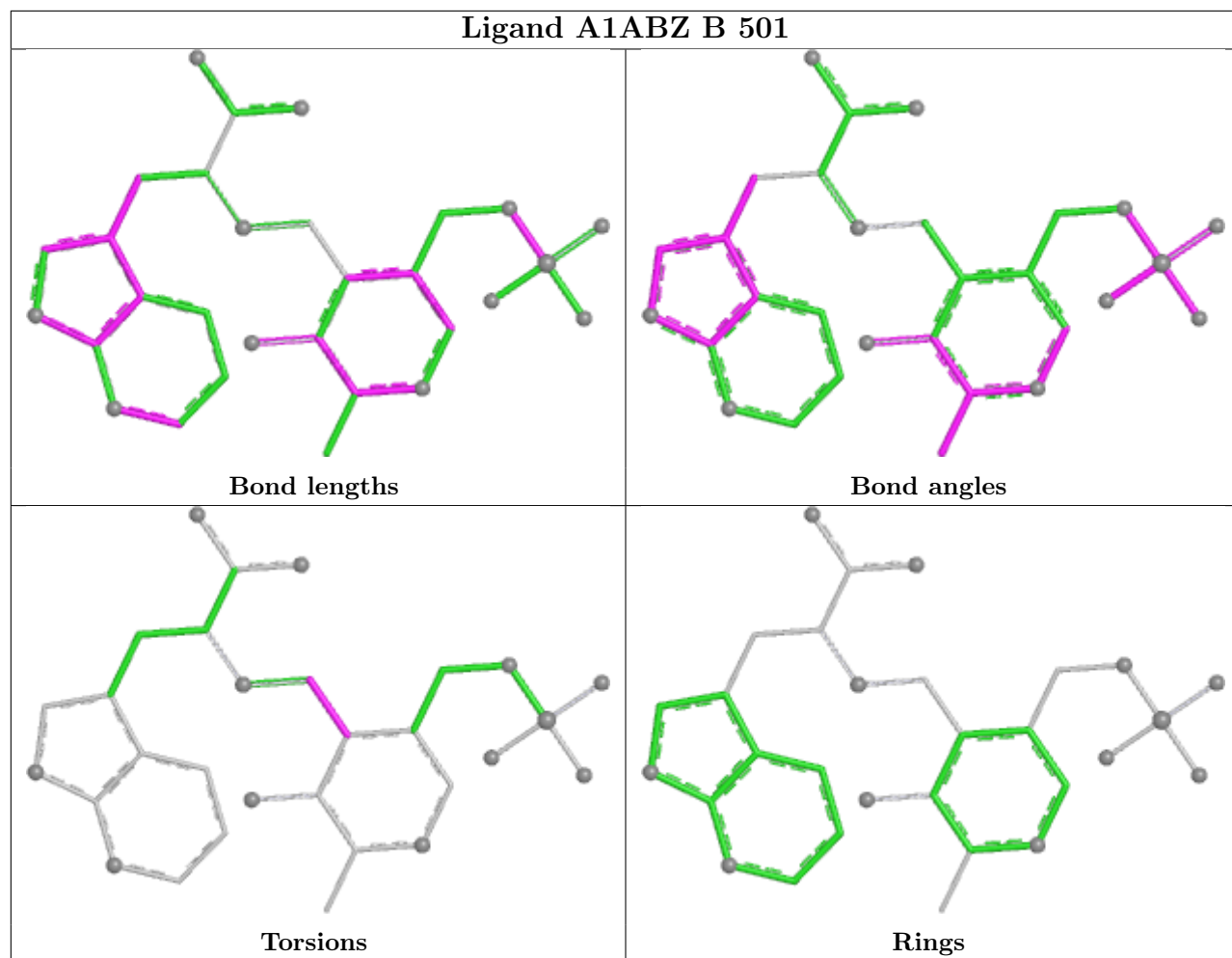
There are no ring outliers.

2 monomers are involved in 3 short contacts:

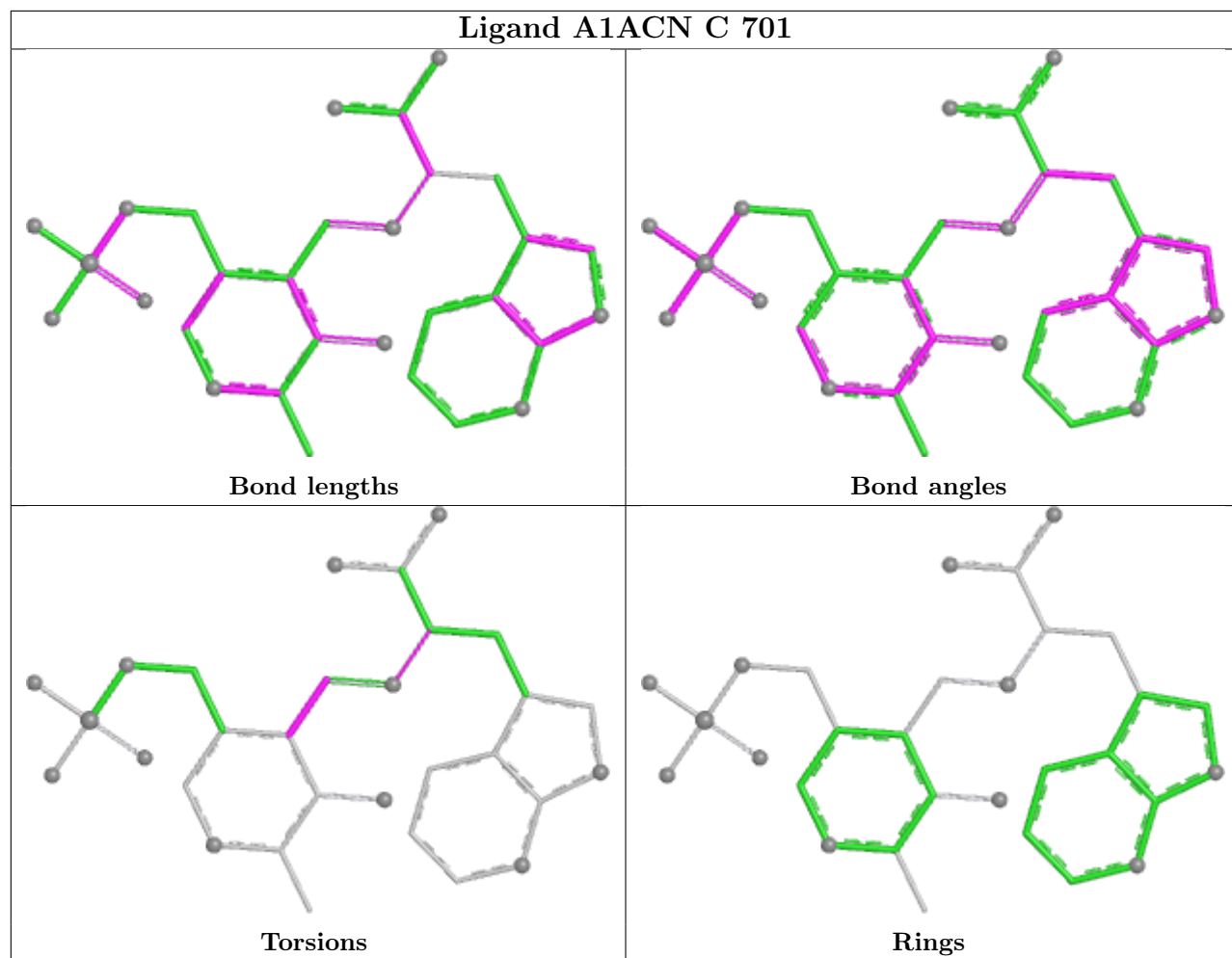
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	A1ACN	1	0
4	A	504	DMS	2	0

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

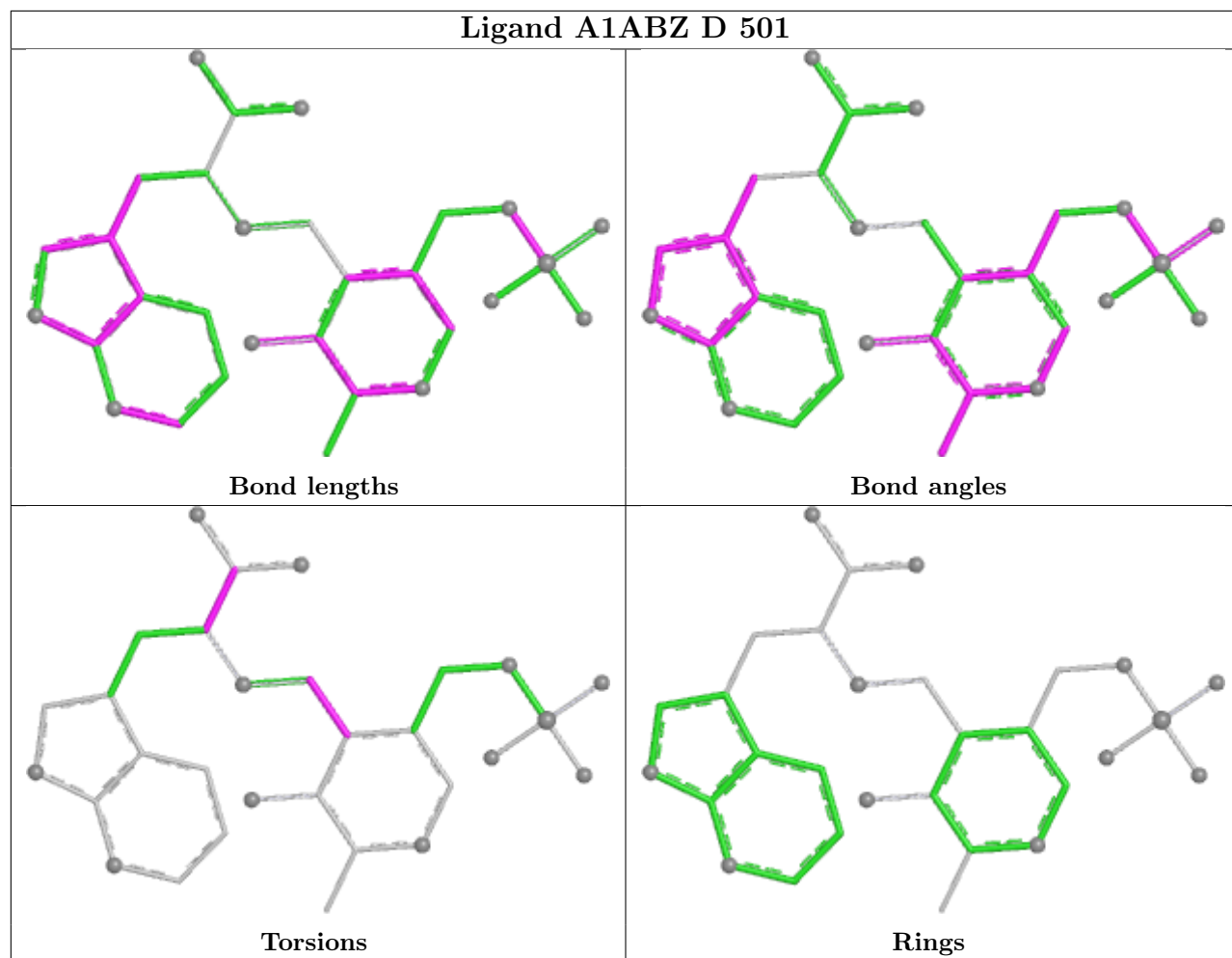
Ligand A1ABZ B 501

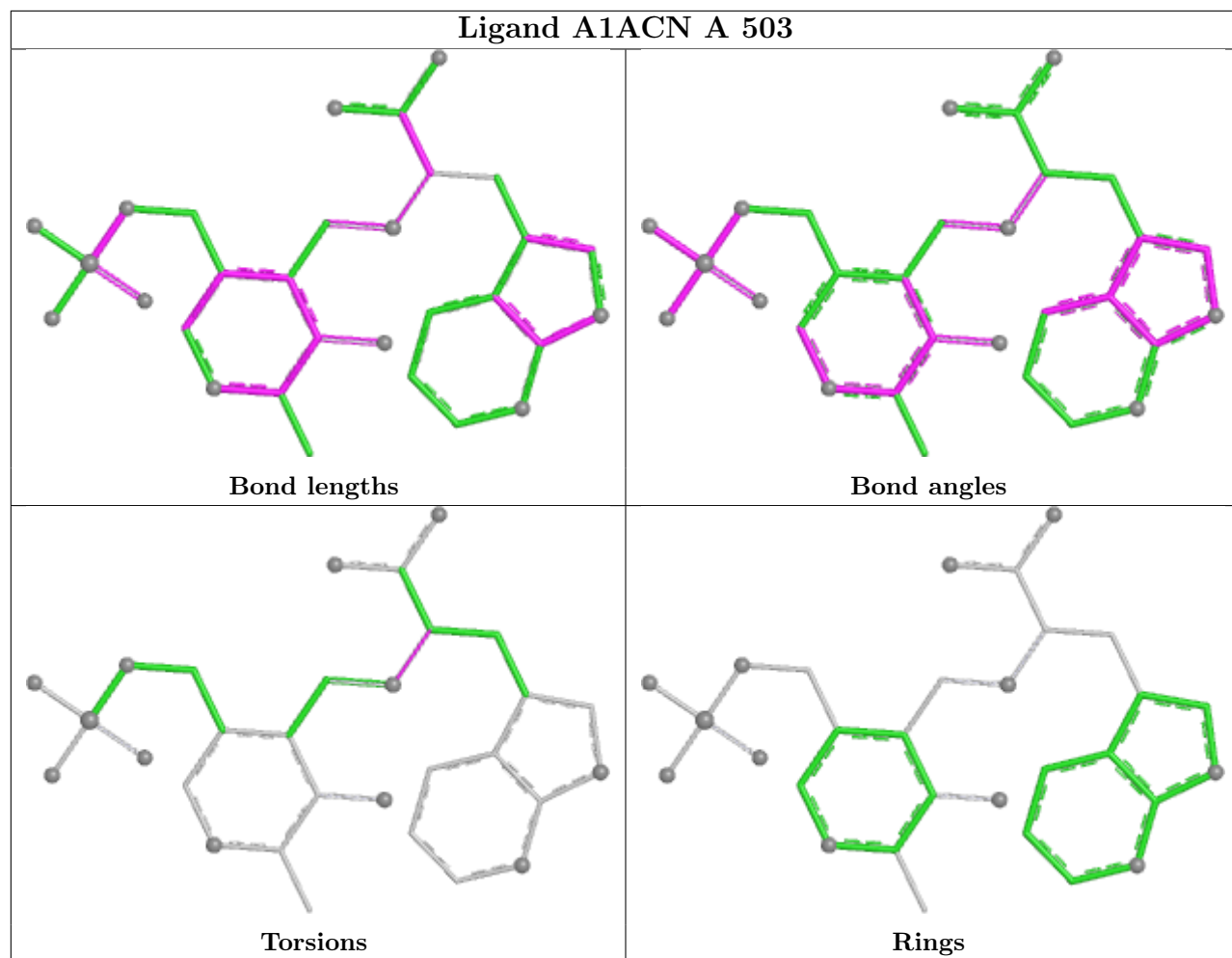


Ligand A1ACN C 701



Ligand A1ABZ D 501





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	465/467 (99%)	0.25	16 (3%)	48	56	9, 30, 55, 85	5 (1%)
1	B	466/467 (99%)	0.18	40 (8%)	16	21	8, 25, 72, 114	10 (2%)
1	C	459/467 (98%)	0.47	57 (12%)	8	11	6, 23, 43, 85	124 (27%)
1	D	465/467 (99%)	0.14	32 (6%)	23	28	9, 25, 58, 95	9 (1%)
All	All	1855/1868 (99%)	0.26	145 (7%)	19	24	6, 26, 59, 114	148 (7%)

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	396[A]	LEU	8.3
1	C	395[A]	LEU	7.5
1	C	466[A]	ILE	6.5
1	C	442[A]	ALA	6.4
1	C	363[A]	VAL	6.1
1	C	369[A]	ASP	6.0
1	C	359[A]	CYS	5.9
1	C	444[A]	LEU	5.8
1	C	364[A]	PRO	5.5
1	C	443[A]	THR	5.4
1	C	367[A]	PRO	5.3
1	C	451[A]	TYR	5.3
1	B	455	VAL	5.1
1	C	449[A]	PHE	5.1
1	C	465[A]	PRO	5.0
1	C	394[A]	PHE	5.0
1	C	463[A]	LEU	4.9
1	C	454[A]	PRO	4.8
1	C	447[A]	LEU	4.6
1	B	401	ALA	4.5
1	D	466	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	397[A]	GLY	4.3
1	C	393[A]	SER	4.2
1	C	445[A]	LYS	4.2
1	C	410[A]	MET	4.0
1	D	33	GLY	3.9
1	C	467[A]	GLU	3.8
1	C	405[A]	GLN	3.8
1	D	444	LEU	3.7
1	C	370[A]	GLN	3.7
1	B	371	PHE	3.7
1	C	406[A]	LYS	3.7
1	B	442	ALA	3.7
1	B	447	LEU	3.7
1	C	407[A]	HIS	3.6
1	C	446[A]	GLY	3.6
1	B	463	LEU	3.6
1	B	465	PRO	3.5
1	B	456	LEU	3.5
1	B	461	ALA	3.5
1	B	466	ILE	3.5
1	D	401	ALA	3.4
1	C	456[A]	LEU	3.4
1	B	394	PHE	3.4
1	C	371[A]	PHE	3.4
1	C	437[A]	LEU	3.4
1	C	439[A]	GLU	3.3
1	C	362[A]	LEU	3.3
1	B	369	ASP	3.3
1	A	401	ALA	3.3
1	B	366	ILE	3.2
1	B	400	PRO	3.2
1	B	448	GLU	3.2
1	C	408[A]	ALA	3.2
1	C	365[A]	GLN	3.1
1	A	400	PRO	3.1
1	C	464[A]	LYS	3.1
1	B	454	PRO	3.1
1	A	447	LEU	3.1
1	D	465	PRO	3.0
1	C	119	GLY	3.0
1	C	382[A]	LEU	3.0
1	D	366	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	412[A]	PHE	3.0
1	C	366[A]	ILE	3.0
1	D	463	LEU	3.0
1	C	440[A]	LYS	3.0
1	C	372[A]	PRO	3.0
1	C	392[A]	GLY	3.0
1	A	443	THR	3.0
1	A	466	ILE	3.0
1	C	409[A]	ASP	2.9
1	B	441	PHE	2.8
1	D	454	PRO	2.8
1	C	448[A]	GLU	2.8
1	B	458	HIS	2.8
1	A	444	LEU	2.8
1	B	396	LEU	2.8
1	B	444	LEU	2.8
1	B	445	LYS	2.8
1	B	402	THR	2.8
1	B	407	HIS	2.8
1	D	369[A]	ASP	2.7
1	D	447	LEU	2.7
1	B	443	THR	2.7
1	C	368[A]	GLY	2.7
1	C	461[A]	ALA	2.7
1	D	119	GLY	2.7
1	B	459	PHE	2.6
1	D	394	PHE	2.6
1	B	403	GLY	2.6
1	B	451	TYR	2.6
1	D	455	VAL	2.6
1	D	371	PHE	2.6
1	D	442	ALA	2.6
1	C	455[A]	VAL	2.6
1	D	400	PRO	2.5
1	D	461	ALA	2.5
1	B	367	PRO	2.5
1	C	391[A]	ILE	2.5
1	B	449	PHE	2.5
1	A	403	GLY	2.5
1	C	411[A]	GLU	2.5
1	C	450[A]	GLU	2.4
1	D	34	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	384[A]	SER	2.4
1	A	396	LEU	2.4
1	D	456	LEU	2.4
1	C	441[A]	PHE	2.4
1	A	366	ILE	2.4
1	A	408	ALA	2.4
1	A	394	PHE	2.3
1	C	132[A]	PHE	2.3
1	D	459	PHE	2.3
1	C	360[A]	LYS	2.3
1	A	363	VAL	2.3
1	B	464	LYS	2.3
1	D	397	GLY	2.3
1	B	363	VAL	2.3
1	D	443	THR	2.2
1	B	406	LYS	2.2
1	D	117	LYS	2.2
1	D	446	GLY	2.2
1	D	449	PHE	2.2
1	D	410	MET	2.2
1	D	403	GLY	2.2
1	A	118	GLU	2.2
1	B	439[A]	GLU	2.2
1	B	453	PRO	2.2
1	A	399	ASP	2.2
1	D	441	PHE	2.2
1	A	2	ALA	2.1
1	B	368	GLY	2.1
1	B	460	THR	2.1
1	A	174	GLU	2.1
1	D	405	GLN	2.1
1	D	155	PHE	2.1
1	B	446	GLY	2.1
1	D	402	THR	2.1
1	C	453[A]	PRO	2.1
1	D	451	TYR	2.1
1	C	32[A]	ALA	2.0
1	B	395	LEU	2.0
1	B	405	GLN	2.0
1	B	409	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](#)

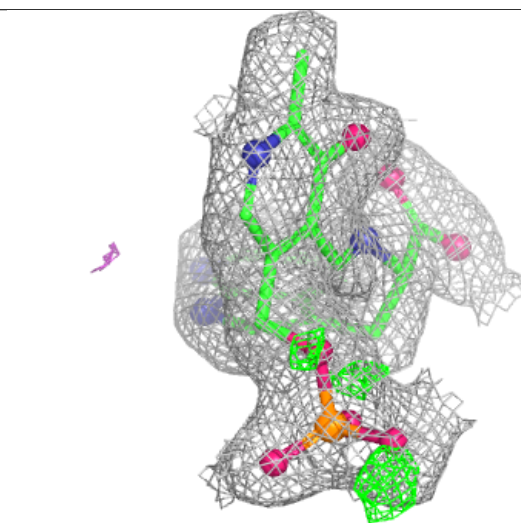
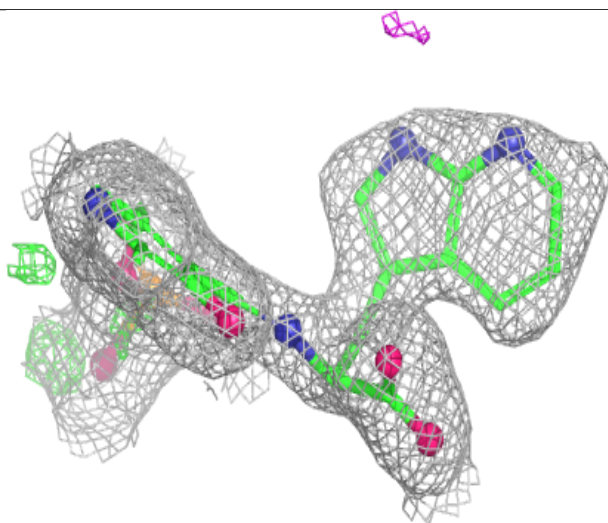
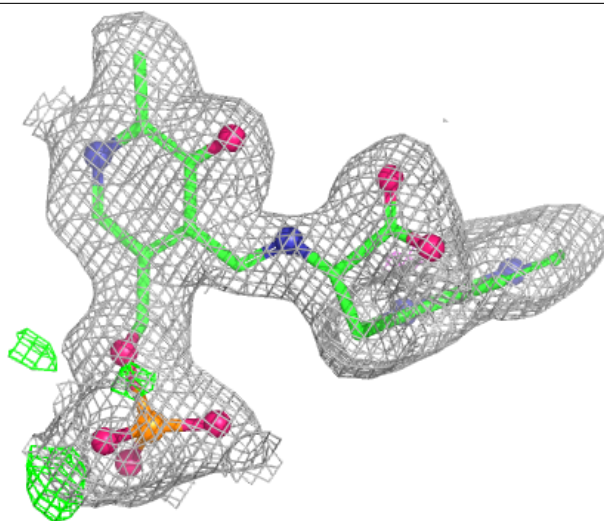
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DMS	A	504	4/4	0.81	0.16	41,42,46,68	0
3	A1ACN	A	503	30/30	0.96	0.08	17,26,41,45	0
3	A1ACN	C	701	30/30	0.97	0.07	13,25,40,52	0
5	A1ABZ	D	501	30/30	0.97	0.06	11,23,33,37	0
5	A1ABZ	B	501	30/30	0.98	0.07	13,23,40,45	0
2	K	A	502	1/1	0.99	0.02	17,17,17,17	1
2	K	A	501	1/1	1.00	0.02	12,12,12,12	1

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.

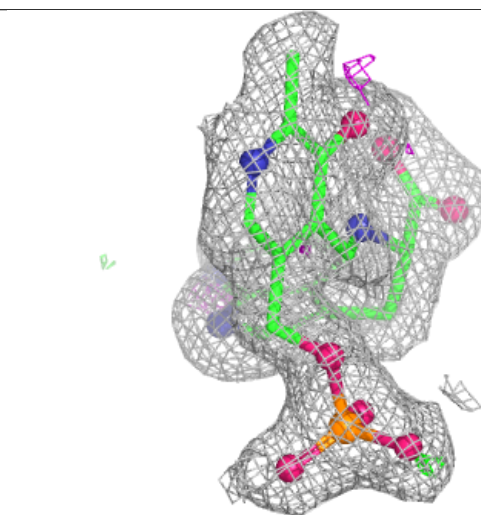
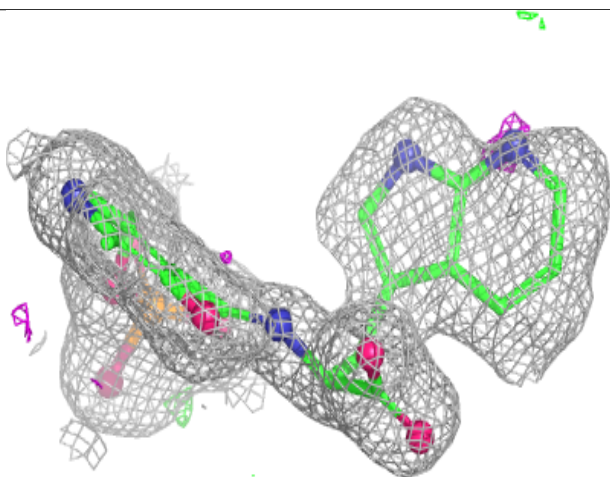
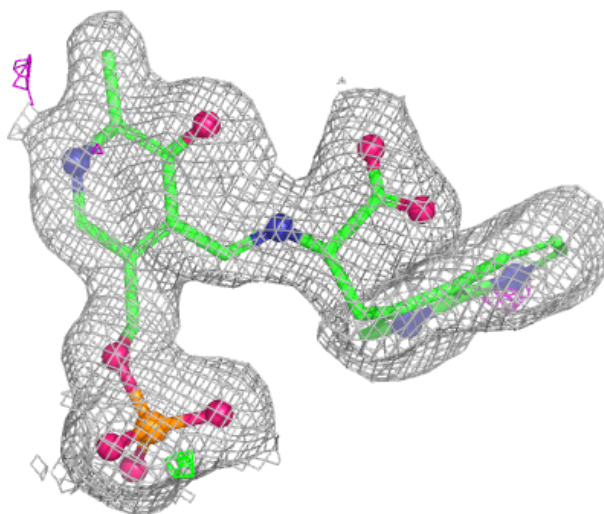
Electron density around A1ACN A 503:

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



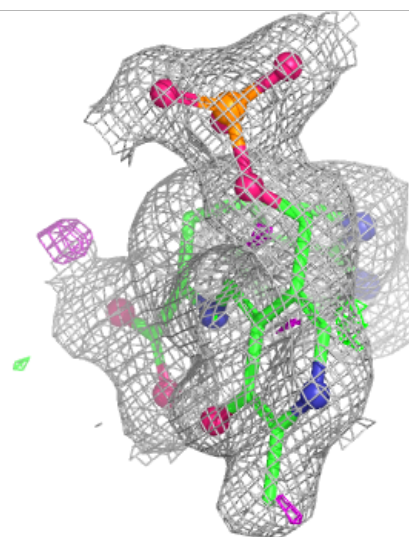
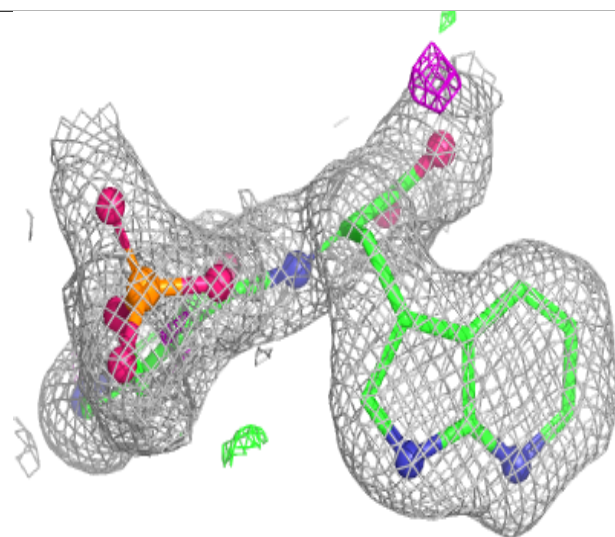
Electron density around A1ACN C 701:

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



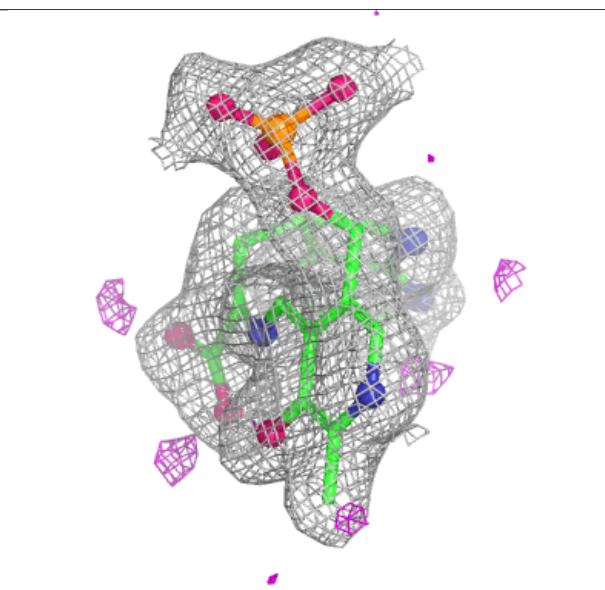
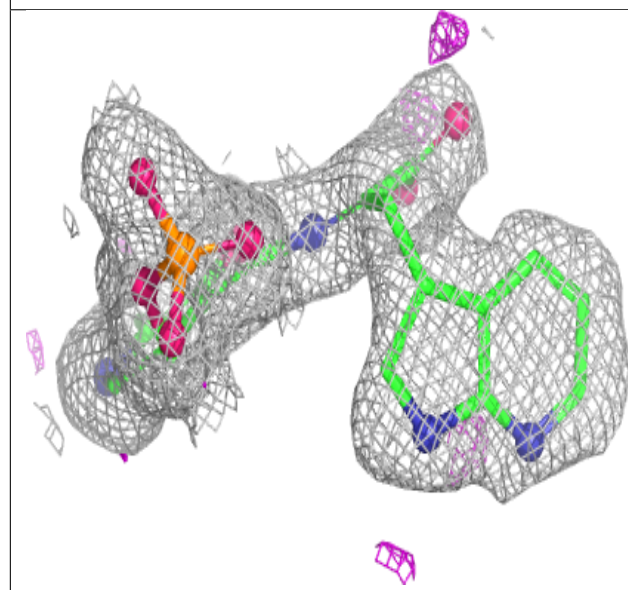
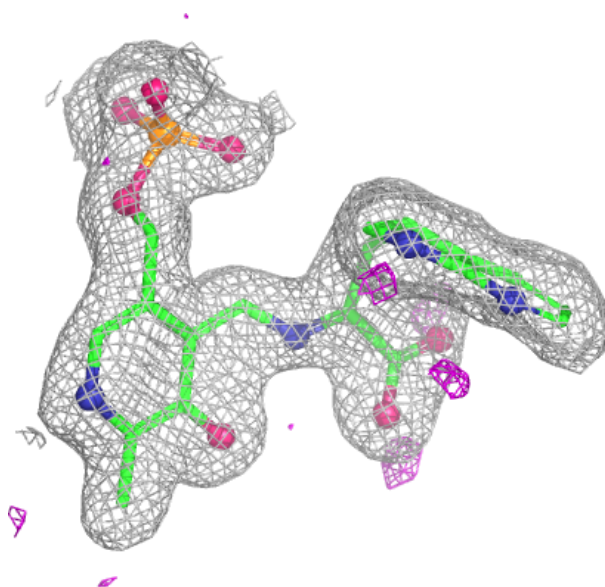
Electron density around A1ABZ D 501:

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



Electron density around A1ABZ B 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 ⓘ

There are no such residues in this entry.