



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 02:05 PM EST

PDB ID : 8V9P
Title : Proteus vulgaris tryptophan indole-lyase complexed with (3S)-dioxindolyl-L-alanine
Authors : Phillips, R.S.
Deposited on : 2023-12-08
Resolution : 1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

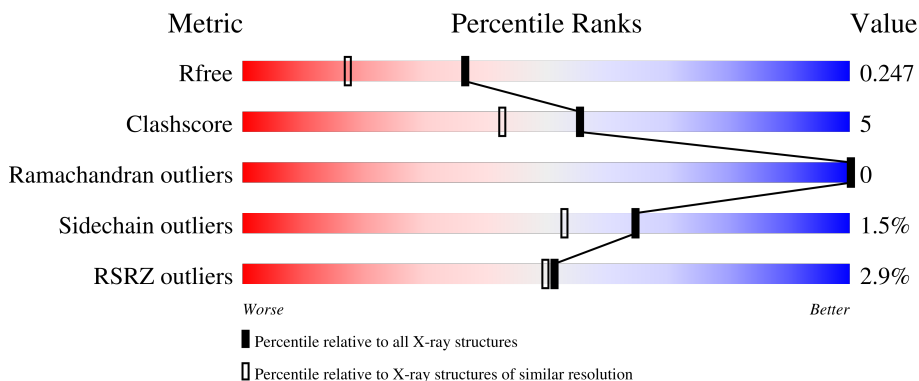
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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% 84% 15%
1	B	467	 2% 85% 14%
1	C	467	 % 86% 13%
1	D	467	 6% 89% 11%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16188 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.

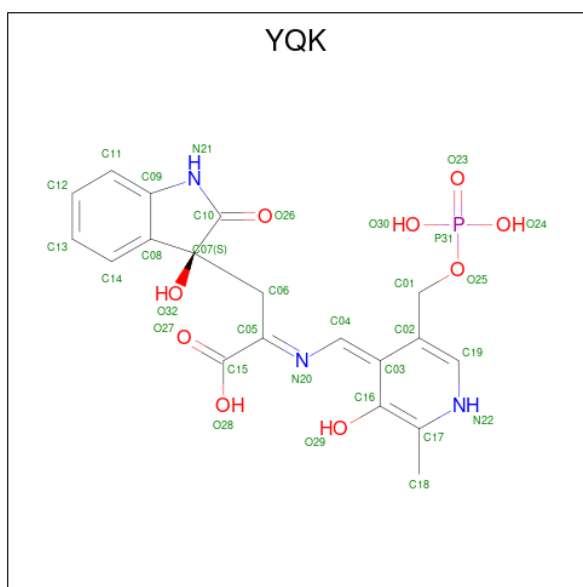
- Molecule 1 is a protein called Tryptophanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	466	3725	2380	633	694	18	0	5	0
1	B	466	3729	2381	635	694	19	0	5	0
1	C	466	3740	2388	639	695	18	0	7	0
1	D	466	3732	2385	634	694	19	0	6	0

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

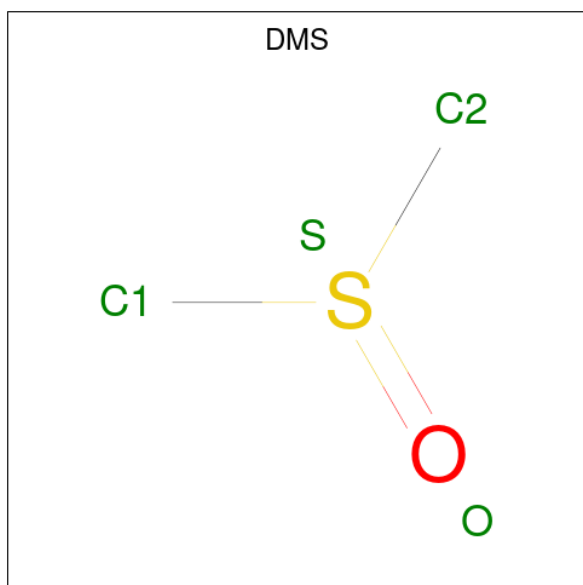
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total K 2 2	0	0
2	C	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0

- Molecule 3 is (2 {E})-2-[({Z})-[2-methyl-3-oxidanyl-5-[[oxidanyl-bis(oxidanylidene)-\$l^{6}\$-phosphanyl]oxymethyl]-1 {H}-pyridin-4-ylidene]methyl]imino-3-[(3 {S})-3-oxidanyl-2-oxidanylidene-1 {H}-indol-3-yl]propanoic acid (three-letter code: YQK) (formula: C₁₉H₂₀N₃O₉P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total	C	N	O	P	0	0
			32	19	3	9	1		
3	B	1	Total	C	N	O	P	0	0
			32	19	3	9	1		
3	C	1	Total	C	N	O	P	0	0
			32	19	3	9	1		
3	D	1	Total	C	N	O	P	0	0
			32	19	3	9	1		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

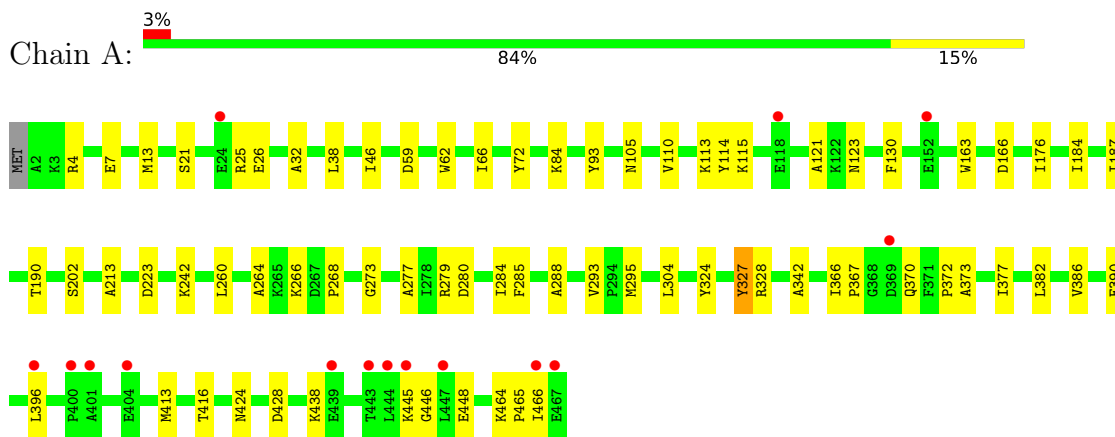
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	306	Total	O	0	8
			306	306		
5	B	293	Total	O	0	7
			293	293		
5	C	264	Total	O	0	4
			264	264		
5	D	263	Total	O	0	4
			263	263		

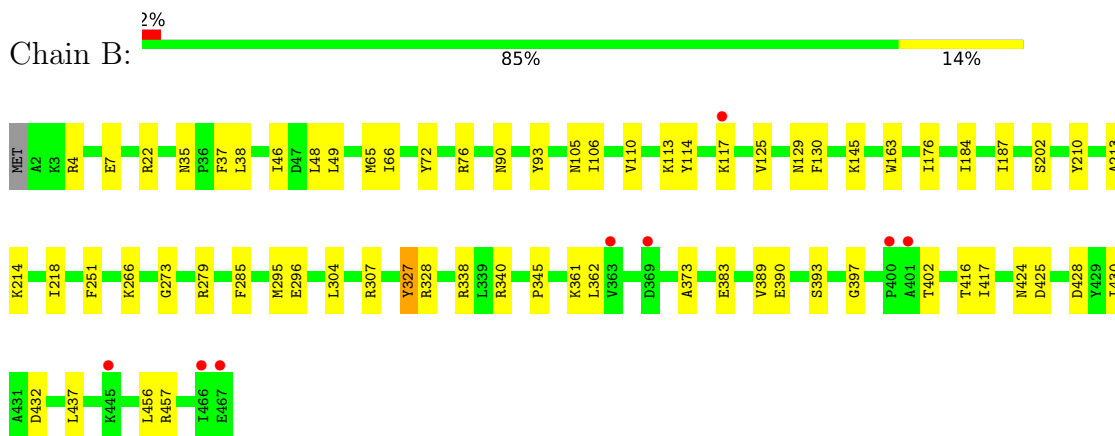
3 Residue-property plots [i](#)

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.

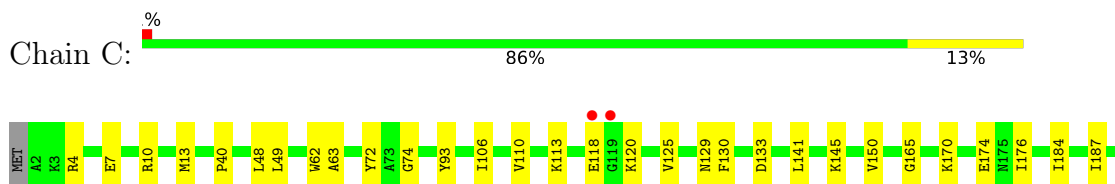
- Molecule 1: Tryptophanase

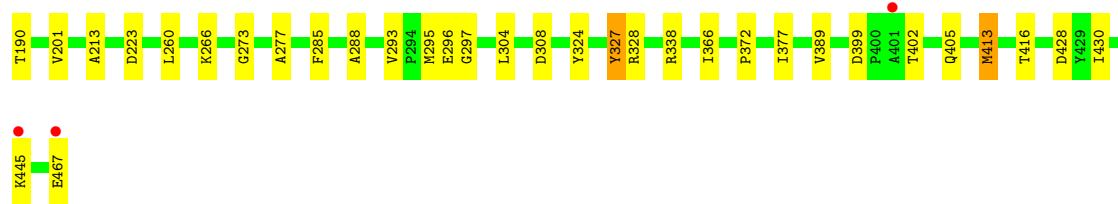


- Molecule 1: Tryptophanase

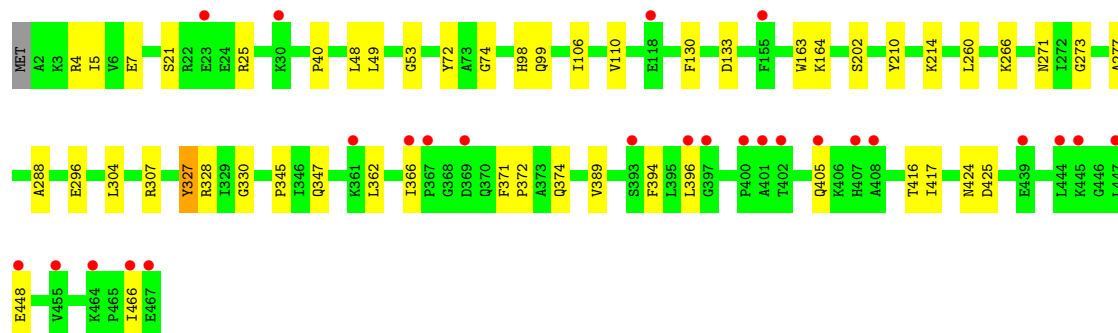
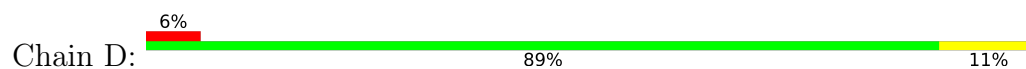


- Molecule 1: Tryptophanase





- 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	67.34Å 112.72Å 119.52Å 90.00° 97.91° 90.00°	Depositor
Resolution (Å)	61.87 – 1.85 61.87 – 1.85	Depositor EDS
% Data completeness (in resolution range)	50.7 (61.87-1.85) 50.7 (61.87-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 1.84Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.199 , 0.247 0.199 , 0.247	Depositor DCC
R_{free} test set	3856 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	12.0	Xtrriage
Anisotropy	0.046	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16188	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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: YQK, 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	0.27	0/3818	0.50	0/5155
1	B	0.28	0/3818	0.51	0/5153
1	C	0.28	0/3835	0.51	0/5176
1	D	0.28	0/3828	0.50	0/5167
All	All	0.28	0/15299	0.50	0/20651

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	3725	0	3703	48	0
1	B	3729	0	3706	42	0
1	C	3740	0	3728	42	0
1	D	3732	0	3711	30	0
2	A	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	32	0	0	3	0
3	B	32	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	32	0	0	3	0
3	D	32	0	0	2	0
4	B	4	0	6	0	0
5	A	306	0	0	9	0
5	B	293	0	0	7	0
5	C	264	0	0	2	0
5	D	263	0	0	3	0
All	All	16188	0	14854	153	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 (153) 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:361:LYS:NZ	5:B:602:HOH:O	2.21	0.72
1:B:273:GLY:HA2	1:B:304:LEU:HD21	1.75	0.68
1:B:66:ILE:HD11	1:C:63:ALA:HB2	1.76	0.67
1:A:13:MET:HE2	1:C:62:TRP:CD1	2.31	0.66
1:A:62:TRP:CD1	1:C:13:MET:HE2	2.30	0.66
1:C:4[A]:ARG:NH2	1:C:428:ASP:OD2	2.28	0.66
1:A:4[A]:ARG:NH1	5:A:606:HOH:O	2.31	0.64
1:B:125:VAL:HG12	1:B:145:LYS:HB2	1.80	0.62
1:C:113:LYS:NZ	5:C:608:HOH:O	2.30	0.62
1:C:110:VAL:HA	1:C:113:LYS:HE3	1.80	0.62
1:A:273:GLY:HA2	1:A:304:LEU:HD21	1.82	0.61
1:B:110:VAL:HA	1:B:113:LYS:HE3	1.83	0.60
1:C:273:GLY:HA2	1:C:304:LEU:HD21	1.83	0.60
1:A:448:GLU:HG3	1:A:466:ILE:HD11	1.84	0.60
1:A:464:LYS:HD2	1:A:465:PRO:HD2	1.84	0.59
1:D:374:GLN:HB2	5:D:780:HOH:O	2.03	0.58
1:B:76[B]:ARG:NH1	5:B:616:HOH:O	2.37	0.57
1:B:424:ASN:ND2	1:D:425:ASP:OD2	2.38	0.57
1:C:170:LYS:NZ	1:C:174:GLU:OE2	2.37	0.57
1:C:125:VAL:HG12	1:C:145:LYS:HB2	1.86	0.57
1:C:7:GLU:HG3	1:C:327[B]:TYR:CZ	2.40	0.56
1:A:72:TYR:OH	3:B:502:YQK:O32	2.16	0.56
1:A:115:LYS:HG3	1:A:121:ALA:HB2	1.88	0.56
1:B:7:GLU:HG3	1:B:327[B]:TYR:CZ	2.40	0.56
1:D:273:GLY:HA2	1:D:304:LEU:HD21	1.89	0.55
1:C:445:LYS:HD3	1:C:467:GLU:HB2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:ILE:HD11	1:C:296:GLU:HG3	1.90	0.54
1:D:164:LYS:NZ	1:D:347:GLN:OE1	2.33	0.54
1:A:166:ASP:OD2	5:A:601:HOH:O	2.18	0.54
1:A:367:PRO:HG2	1:A:370:GLN:HG3	1.90	0.54
1:B:4[B]:ARG:NH2	1:B:428:ASP:OD2	2.41	0.54
1:D:371:PHE:HB3	5:D:780:HOH:O	2.09	0.53
1:C:266:LYS:HZ1	3:C:502:YQK:C04	2.22	0.53
1:D:210:TYR:CE1	1:D:214:LYS:HE3	2.44	0.53
1:A:123:ASN:ND2	5:A:609:HOH:O	2.35	0.52
1:B:279:ARG:NH2	5:B:607:HOH:O	2.33	0.52
1:A:4[B]:ARG:NH2	1:A:428:ASP:OD2	2.43	0.52
1:B:163:TRP:CD2	1:B:202:SER:HB3	2.45	0.52
1:B:338:ARG:NH2	1:B:432:ASP:OD1	2.40	0.52
1:B:402:THR:O	5:B:601:HOH:O	2.19	0.50
1:A:260:LEU:HG	1:A:277:ALA:HB3	1.94	0.50
1:D:448:GLU:HG3	1:D:466:ILE:HD11	1.92	0.50
1:B:210:TYR:CE1	1:B:214:LYS:HE3	2.46	0.50
1:B:266:LYS:HZ1	3:B:502:YQK:C04	2.25	0.50
1:D:7:GLU:HG3	1:D:327[B]:TYR:CZ	2.47	0.50
1:A:93:TYR:HB3	1:A:285:PHE:CD1	2.47	0.49
1:A:7:GLU:HG3	1:A:327[B]:TYR:CZ	2.48	0.49
1:B:106:ILE:HD11	1:B:296:GLU:HG3	1.93	0.49
1:C:110:VAL:HG21	1:C:288:ALA:HA	1.94	0.49
1:C:366:ILE:HB	1:C:372:PRO:HB3	1.95	0.49
1:C:399:ASP:HB3	1:C:402:THR:HB	1.94	0.49
1:D:110:VAL:HG21	1:D:288:ALA:HA	1.95	0.48
1:A:377:ILE:HG12	1:A:413:MET:HE3	1.96	0.48
1:B:35:ASN:HB3	1:B:38:LEU:HD23	1.94	0.47
1:A:7:GLU:OE1	1:A:7:GLU:N	2.42	0.47
1:D:266:LYS:HZ1	3:D:502:YQK:C04	2.27	0.47
1:B:49:LEU:HD12	1:B:389:VAL:HB	1.96	0.47
1:A:113:LYS:HB3	5:A:821:HOH:O	2.15	0.47
1:A:264:ALA:HA	1:A:268:PRO:HG2	1.96	0.47
1:B:22:ARG:HD3	5:B:745:HOH:O	2.14	0.47
1:C:118:GLU:HB2	1:C:120:LYS:HE2	1.97	0.47
1:B:393:SER:O	1:B:457:ARG:NH2	2.45	0.47
3:B:502:YQK:O29	3:B:502:YQK:N20	2.47	0.47
1:A:26:GLU:HG2	1:A:382:LEU:HD22	1.96	0.47
1:B:383:GLU:HG2	1:B:437:LEU:HD21	1.97	0.46
1:A:279:ARG:HD3	5:A:694:HOH:O	2.15	0.46
1:C:129:ASN:O	1:C:150:VAL:HB	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:502:YQK:O32	1:D:72:TYR:OH	2.18	0.46
1:B:46:ILE:HG21	1:B:430:ILE:HD11	1.98	0.46
1:A:114:TYR:CG	1:A:284:ILE:HD11	2.51	0.45
1:C:190:THR:HA	1:C:223:ASP:HB3	1.96	0.45
1:A:110:VAL:HG21	1:A:288:ALA:HA	1.98	0.45
1:C:74:GLY:HA3	1:D:40:PRO:HA	1.98	0.45
1:D:133:ASP:OD1	1:D:133:ASP:N	2.46	0.45
1:A:46:ILE:HB	1:A:386:VAL:HG22	1.99	0.45
1:C:165:GLY:O	1:C:201:VAL:HG22	2.17	0.45
1:D:260:LEU:HG	1:D:277:ALA:HB3	1.99	0.45
1:B:105:ASN:HD21	1:B:295:MET:HE2	1.81	0.45
1:C:187:ILE:HD12	1:C:213:ALA:HB2	1.98	0.45
1:A:190:THR:HA	1:A:223:ASP:HB3	1.98	0.44
1:B:176:ILE:HA	1:B:184:ILE:HD11	1.98	0.44
1:C:72:TYR:OH	3:D:502:YQK:O32	2.27	0.44
1:C:176:ILE:HA	1:C:184:ILE:HD11	1.99	0.44
1:D:21:SER:O	1:D:25:ARG:HG3	2.17	0.44
1:A:373:ALA:HB3	1:A:390:GLU:HG2	2.00	0.44
1:A:13:MET:HE2	1:C:62:TRP:CG	2.52	0.44
1:B:345:PRO:HD2	1:B:362:LEU:HD13	1.99	0.44
1:B:425:ASP:OD2	1:D:424:ASN:ND2	2.44	0.44
1:A:293:VAL:HG12	1:B:456:LEU:HD13	1.99	0.44
1:A:366:ILE:HB	1:A:372:PRO:HB3	2.00	0.44
1:A:424:ASN:ND2	5:A:630:HOH:O	2.45	0.44
1:D:4[A]:ARG:NH2	1:D:425:ASP:OD1	2.47	0.44
1:C:110:VAL:O	1:C:113:LYS:HG2	2.18	0.43
1:C:48:LEU:HD11	1:C:430:ILE:HD13	2.01	0.43
1:D:5:ILE:HD12	1:D:330:GLY:HA3	1.98	0.43
5:A:606:HOH:O	1:C:4[B]:ARG:NH1	2.51	0.43
1:A:445:LYS:HD2	1:A:466:ILE:O	2.19	0.43
1:B:48:LEU:HD11	1:B:430:ILE:HD13	1.99	0.43
1:D:49:LEU:HD12	1:D:389:VAL:HB	2.01	0.43
1:B:90:ASN:HB2	1:B:251:PHE:CE1	2.54	0.43
1:B:397:GLY:HA2	1:B:457:ARG:NE	2.34	0.43
1:D:405[B]:GLN:H	1:D:405[B]:GLN:HG2	1.42	0.43
1:A:62:TRP:O	1:A:66:ILE:HG12	2.19	0.43
1:A:266:LYS:HZ1	3:A:503:YQK:C04	2.31	0.43
3:A:503:YQK:O32	1:B:72:TYR:OH	2.22	0.42
1:B:113:LYS:NZ	5:B:610:HOH:O	2.34	0.42
1:C:295:MET:HB3	1:C:295:MET:HE2	1.92	0.42
1:A:464:LYS:NZ	1:A:465:PRO:O	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:LEU:HD21	5:D:855:HOH:O	2.19	0.42
1:D:106:ILE:HD11	1:D:296:GLU:HG3	2.01	0.42
1:A:342:ALA:O	1:A:438:LYS:NZ	2.37	0.42
3:A:503:YQK:O29	3:A:503:YQK:N20	2.52	0.42
1:B:129:ASN:N	1:B:129:ASN:OD1	2.52	0.42
1:A:32:ALA:HB1	1:A:38:LEU:HB2	2.01	0.42
1:B:65:MET:HG2	1:B:307:ARG:O	2.19	0.42
1:B:48:LEU:HD22	1:B:417:ILE:HD13	2.01	0.42
1:B:373:ALA:HB3	1:B:390:GLU:HG2	2.01	0.42
1:C:93:TYR:HB3	1:C:285:PHE:CD1	2.55	0.42
1:C:377:ILE:HA	1:C:413:MET:HE3	2.02	0.42
1:C:308:ASP:OD1	1:D:307:ARG:NH2	2.51	0.41
1:A:21:SER:O	1:A:25:ARG:HG3	2.20	0.41
1:A:370:GLN:HB3	1:A:446:GLY:HA3	2.02	0.41
1:C:260:LEU:HG	1:C:277:ALA:HB3	2.02	0.41
1:D:396:LEU:HD23	1:D:396:LEU:HA	1.94	0.41
1:C:133:ASP:N	1:C:133:ASP:OD1	2.52	0.41
3:C:502:YQK:O29	3:C:502:YQK:N20	2.53	0.41
1:D:48:LEU:HD22	1:D:417:ILE:HD13	2.03	0.41
1:B:93:TYR:HB3	1:B:285:PHE:CD1	2.56	0.41
1:D:163:TRP:CD2	1:D:202:SER:HB3	2.55	0.41
1:A:163:TRP:CD2	1:A:202:SER:HB3	2.56	0.41
1:A:242:LYS:HE2	5:A:884:HOH:O	2.19	0.41
1:D:345:PRO:HD2	1:D:362:LEU:HD13	2.03	0.41
5:B:637:HOH:O	1:C:10:ARG:NH2	2.54	0.41
1:C:293:VAL:HA	1:C:297:GLY:O	2.21	0.41
1:C:405[B]:GLN:HG3	5:C:601:HOH:O	2.21	0.41
1:D:366:ILE:HB	1:D:372:PRO:HB3	2.03	0.41
1:A:105:ASN:HD21	1:A:295:MET:HE2	1.85	0.40
1:B:213:ALA:HB1	1:B:218:ILE:HB	2.03	0.40
1:A:396:LEU:HD12	1:A:396:LEU:HA	1.95	0.40
1:D:98:HIS:CD2	1:D:99:GLN:HG2	2.56	0.40
1:A:114:TYR:CD2	1:A:284:ILE:HD11	2.56	0.40
1:B:187:ILE:HD12	1:B:213:ALA:HB2	2.03	0.40
1:C:40:PRO:HA	1:D:74:GLY:HA3	2.04	0.40
1:D:53:GLY:HA2	1:D:271:ASN:HA	2.03	0.40
1:A:187:ILE:HD12	1:A:213:ALA:HB2	2.04	0.40
1:A:280:ASP:HB2	5:A:835:HOH:O	2.20	0.40
1:B:66:ILE:HD11	1:C:63:ALA:CB	2.47	0.40
1:C:49:LEU:HD12	1:C:389:VAL:HB	2.04	0.40
1:A:59:ASP:OD1	1:A:59:ASP:N	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LYS:HA	1:A:84:LYS:HD2	1.94	0.40
1:A:176:ILE:HA	1:A:184:ILE:HD11	2.03	0.40
1:B:66:ILE:HD11	1:C:63:ALA:N	2.37	0.40
1:B:114:TYR:HA	1:B:117:LYS:HE2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	469/467 (100%)	455 (97%)	14 (3%)	0	100	100
1	B	469/467 (100%)	453 (97%)	16 (3%)	0	100	100
1	C	471/467 (101%)	452 (96%)	19 (4%)	0	100	100
1	D	470/467 (101%)	455 (97%)	15 (3%)	0	100	100
All	All	1879/1868 (101%)	1815 (97%)	64 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	390/386 (101%)	384 (98%)	6 (2%)	65	53
1	B	390/386 (101%)	383 (98%)	7 (2%)	59	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	392/386 (102%)	384 (98%)	8 (2%)	55	40
1	D	391/386 (101%)	385 (98%)	6 (2%)	65	53
All	All	1563/1544 (101%)	1536 (98%)	27 (2%)	65	47

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	PHE
1	A	324	TYR
1	A	327[A]	TYR
1	A	327[B]	TYR
1	A	328	ARG
1	A	416	THR
1	B	37	PHE
1	B	130	PHE
1	B	327[A]	TYR
1	B	327[B]	TYR
1	B	328	ARG
1	B	340	ARG
1	B	416	THR
1	C	130	PHE
1	C	324	TYR
1	C	327[A]	TYR
1	C	327[B]	TYR
1	C	328	ARG
1	C	338	ARG
1	C	413	MET
1	C	416	THR
1	D	130	PHE
1	D	327[A]	TYR
1	D	327[B]	TYR
1	D	328	ARG
1	D	394	PHE
1	D	416	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	C	105	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 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$
3	YQK	D	502	-	32,34,34	1.19	3 (9%)	41,51,51	2.08	10 (24%)
3	YQK	B	502	-	32,34,34	1.21	3 (9%)	41,51,51	2.11	11 (26%)
3	YQK	A	503	-	32,34,34	1.20	3 (9%)	41,51,51	2.31	10 (24%)
4	DMS	B	501	-	3,3,3	0.67	0	3,3,3	0.37	0
3	YQK	C	502	-	32,34,34	1.19	2 (6%)	41,51,51	2.17	11 (26%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	YQK	C	502	-	-	1/17/36/36	0/3/3/3
3	YQK	D	502	-	-	4/17/36/36	0/3/3/3
3	YQK	B	502	-	-	1/17/36/36	0/3/3/3
3	YQK	A	503	-	-	4/17/36/36	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	YQK	P31-O23	3.30	1.61	1.50
3	A	503	YQK	C07-C10	-3.24	1.51	1.55
3	D	502	YQK	P31-O23	3.22	1.60	1.50
3	B	502	YQK	P31-O23	3.19	1.60	1.50
3	A	503	YQK	P31-O23	3.12	1.60	1.50
3	B	502	YQK	C07-C10	-3.07	1.51	1.55
3	D	502	YQK	C07-C10	-3.02	1.51	1.55
3	C	502	YQK	C07-C10	-3.00	1.51	1.55
3	B	502	YQK	C19-N22	-2.20	1.32	1.36
3	D	502	YQK	C19-N22	-2.14	1.32	1.36
3	A	503	YQK	C19-N22	-2.00	1.32	1.36

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	YQK	C08-C07-C10	8.82	104.63	101.53
3	C	502	YQK	C08-C07-C10	8.17	104.40	101.53
3	D	502	YQK	C08-C07-C10	7.61	104.20	101.53
3	B	502	YQK	C08-C07-C10	7.58	104.20	101.53
3	A	503	YQK	C07-C08-C09	-7.05	106.03	108.86
3	C	502	YQK	C07-C08-C09	-6.73	106.16	108.86
3	D	502	YQK	C07-C08-C09	-6.62	106.20	108.86
3	B	502	YQK	C07-C08-C09	-6.47	106.26	108.86
3	A	503	YQK	C01-C02-C03	-4.49	119.32	122.20
3	C	502	YQK	C01-C02-C03	-3.62	119.88	122.20
3	B	502	YQK	C01-C02-C03	-3.28	120.09	122.20
3	C	502	YQK	C18-C17-C16	-3.28	118.30	122.34
3	D	502	YQK	C19-N22-C17	-3.07	121.87	124.27
3	D	502	YQK	C16-C03-C02	-3.05	117.53	119.26
3	D	502	YQK	C01-C02-C03	-3.02	120.27	122.20
3	D	502	YQK	C18-C17-C16	-3.00	118.64	122.34
3	B	502	YQK	C11-C09-C08	-2.91	119.15	121.91
3	C	502	YQK	C11-C09-C08	-2.90	119.15	121.91
3	A	503	YQK	C11-C09-C08	-2.85	119.19	121.91
3	D	502	YQK	C11-C09-C08	-2.74	119.31	121.91
3	A	503	YQK	C19-N22-C17	-2.72	122.14	124.27
3	B	502	YQK	C18-C17-C16	-2.70	119.01	122.34
3	B	502	YQK	O29-C16-C17	2.70	121.17	118.43
3	A	503	YQK	C07-C10-N21	-2.67	106.79	108.41
3	A	503	YQK	O29-C16-C17	2.66	121.13	118.43
3	B	502	YQK	C19-N22-C17	-2.60	122.24	124.27
3	A	503	YQK	C16-C03-C02	-2.53	117.83	119.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	YQK	C19-N22-C17	-2.43	122.37	124.27
3	A	503	YQK	C01-C02-C19	2.42	121.56	118.98
3	B	502	YQK	C16-C17-N22	2.36	121.22	118.57
3	D	502	YQK	C16-C17-N22	2.33	121.19	118.57
3	C	502	YQK	C07-C10-N21	-2.29	107.02	108.41
3	C	502	YQK	C01-C02-C19	2.22	121.35	118.98
3	A	503	YQK	C18-C17-C16	-2.12	119.73	122.34
3	D	502	YQK	C14-C08-C07	2.11	133.50	130.62
3	B	502	YQK	C07-C10-N21	-2.09	107.14	108.41
3	D	502	YQK	O28-C15-O27	-2.08	118.86	123.61
3	C	502	YQK	C16-C17-N22	2.07	120.89	118.57
3	B	502	YQK	C16-C03-C02	-2.06	118.10	119.26
3	B	502	YQK	O28-C15-O27	-2.04	118.95	123.61
3	C	502	YQK	O29-C16-C17	2.00	120.46	118.43
3	C	502	YQK	C06-C07-C08	-2.00	111.33	115.24

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	YQK	C06-C05-C15-O27
3	C	502	YQK	C02-C03-C04-N20
3	D	502	YQK	C06-C05-C15-O28
3	D	502	YQK	N20-C05-C15-O27
3	D	502	YQK	N20-C05-C15-O28
3	D	502	YQK	C06-C05-C15-O27
3	A	503	YQK	N20-C05-C15-O28
3	B	502	YQK	N20-C05-C15-O28
3	A	503	YQK	C06-C05-C15-O28
3	A	503	YQK	N20-C05-C15-O27

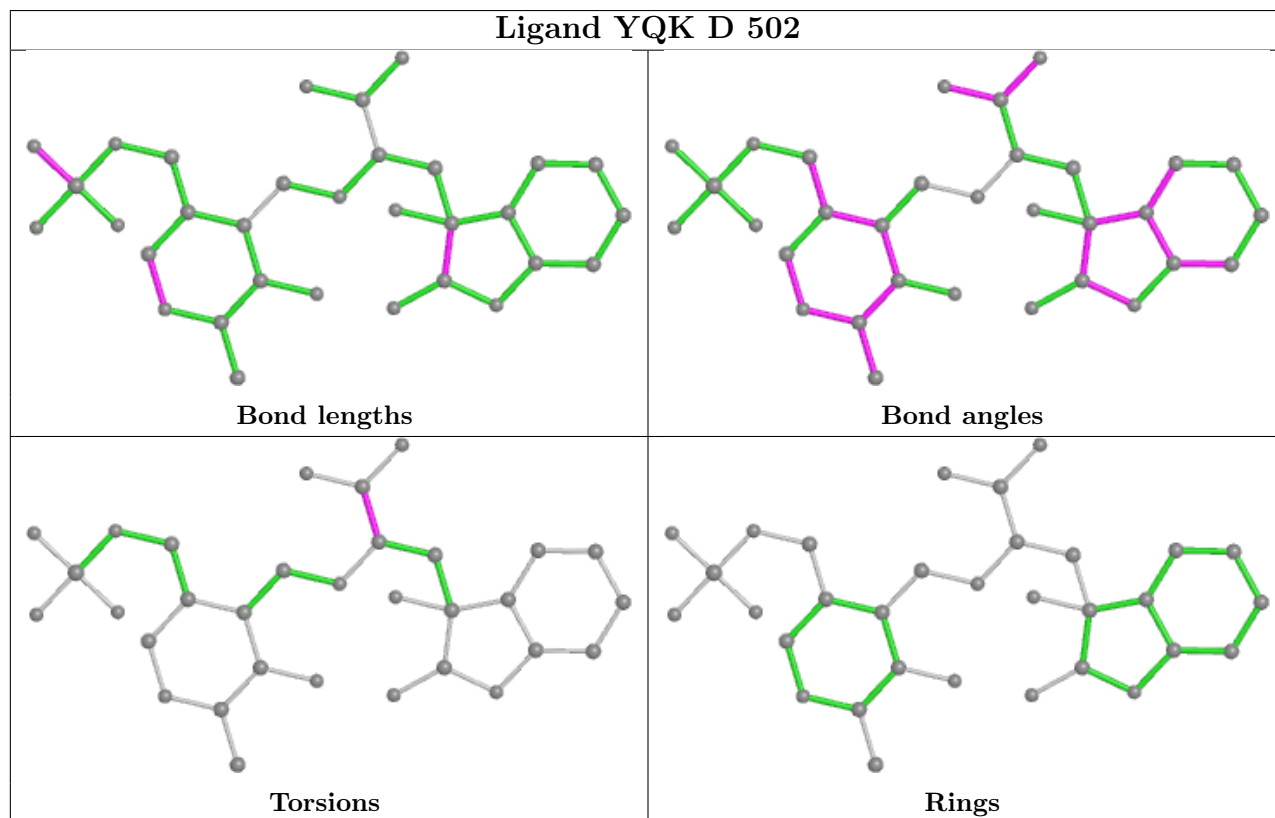
There are no ring outliers.

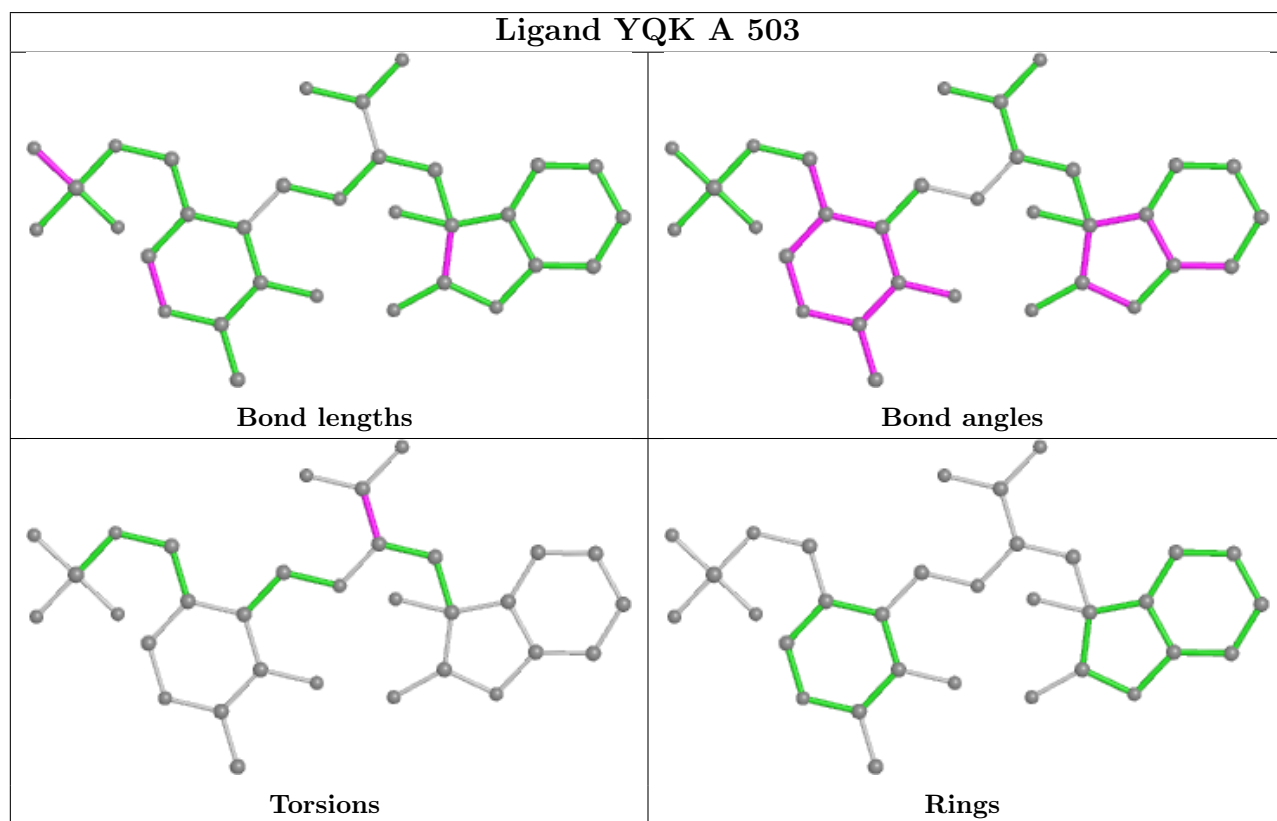
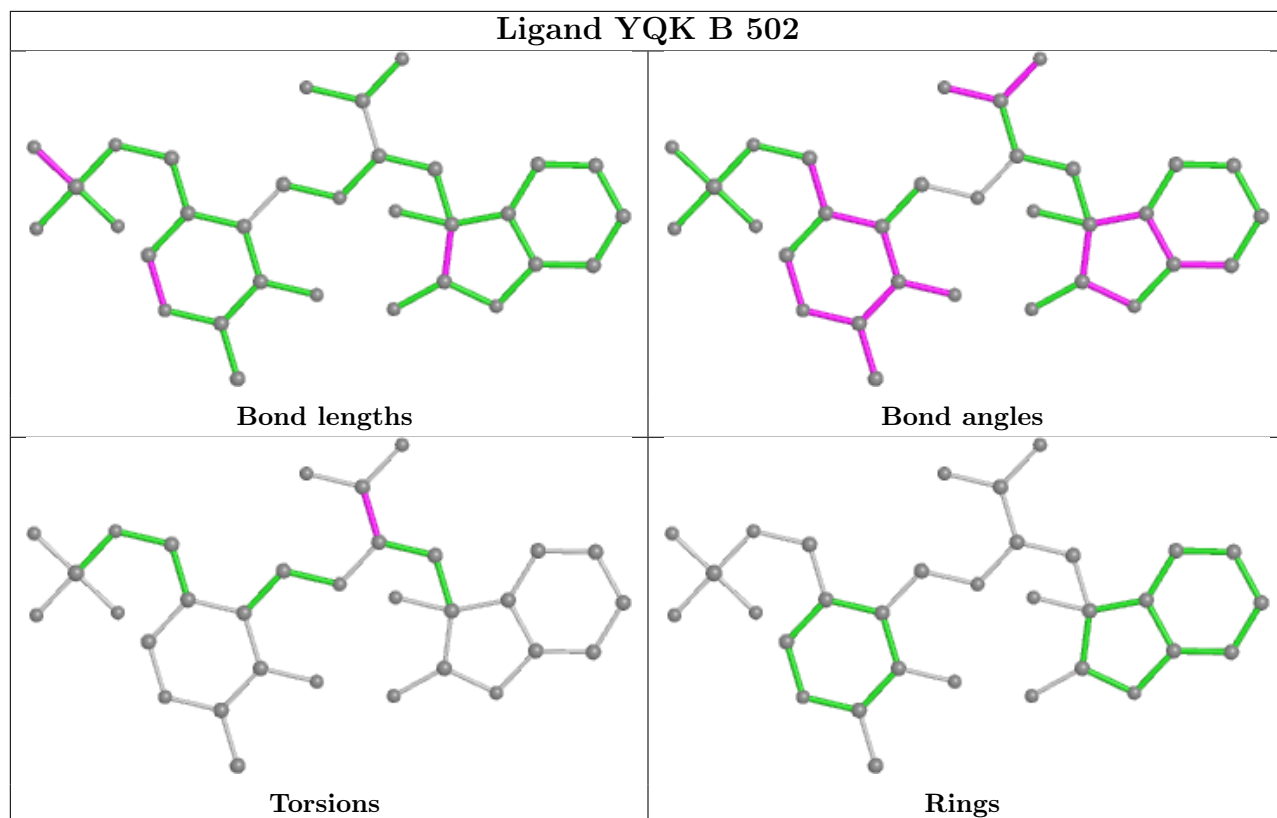
4 monomers are involved in 11 short contacts:

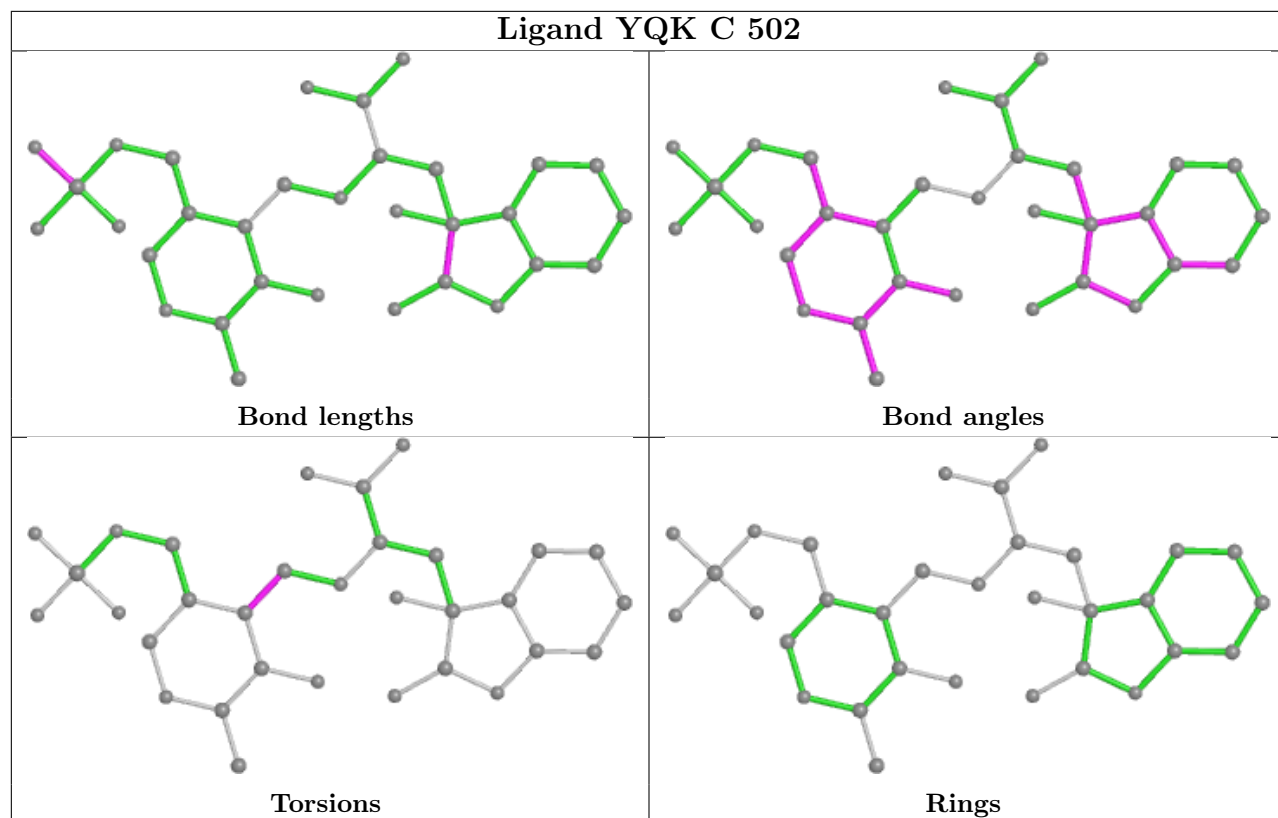
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	YQK	2	0
3	B	502	YQK	3	0
3	A	503	YQK	3	0
3	C	502	YQK	3	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	466/467 (99%)	-0.02	15 (3%) 47 45	7, 14, 38, 64	0
1	B	466/467 (99%)	-0.03	8 (1%) 70 70	6, 15, 35, 55	0
1	C	466/467 (99%)	-0.07	5 (1%) 80 81	7, 16, 35, 68	0
1	D	466/467 (99%)	0.15	26 (5%) 24 23	7, 16, 45, 80	0
All	All	1864/1868 (99%)	0.01	54 (2%) 51 50	6, 16, 39, 80	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	467	GLU	6.2
1	D	467	GLU	6.2
1	D	401	ALA	6.1
1	B	401	ALA	5.6
1	D	400	PRO	5.2
1	A	401	ALA	4.6
1	A	445	LYS	4.6
1	D	447	LEU	4.4
1	B	363	VAL	4.4
1	A	400	PRO	4.3
1	C	445	LYS	4.2
1	D	444	LEU	4.2
1	C	467	GLU	4.1
1	D	393	SER	4.1
1	A	466	ILE	4.0
1	D	397	GLY	4.0
1	B	467	GLU	3.9
1	A	396	LEU	3.9
1	D	439[A]	GLU	3.9
1	C	118	GLU	3.6
1	B	466	ILE	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	445	LYS	3.4
1	D	369	ASP	3.4
1	A	444	LEU	3.4
1	D	455	VAL	3.2
1	C	401	ALA	3.1
1	D	407	HIS	3.0
1	B	445	LYS	2.9
1	D	366	ILE	2.9
1	D	402	THR	2.9
1	B	400	PRO	2.8
1	D	408	ALA	2.8
1	D	448	GLU	2.7
1	C	119	GLY	2.7
1	D	396	LEU	2.7
1	B	369[A]	ASP	2.6
1	D	464	LYS	2.6
1	A	152	GLU	2.6
1	D	367	PRO	2.6
1	D	405[A]	GLN	2.5
1	A	369	ASP	2.4
1	A	404	GLU	2.4
1	D	466	ILE	2.3
1	B	117	LYS	2.3
1	A	24	GLU	2.3
1	D	361	LYS	2.3
1	A	447	LEU	2.2
1	A	439	GLU	2.2
1	D	23	GLU	2.2
1	D	118	GLU	2.2
1	D	155	PHE	2.2
1	A	118	GLU	2.0
1	D	30	LYS	2.0
1	A	443	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

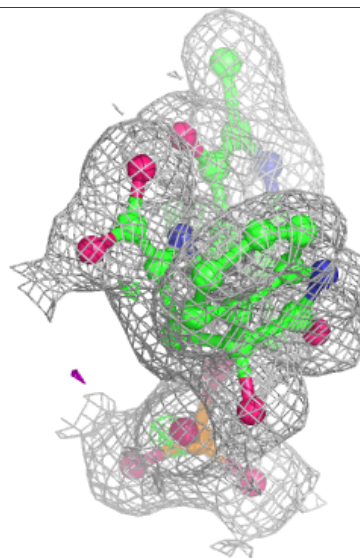
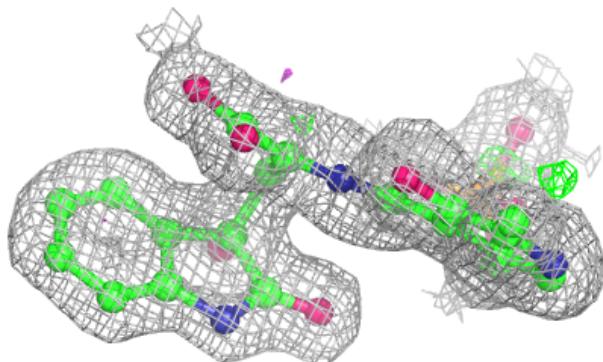
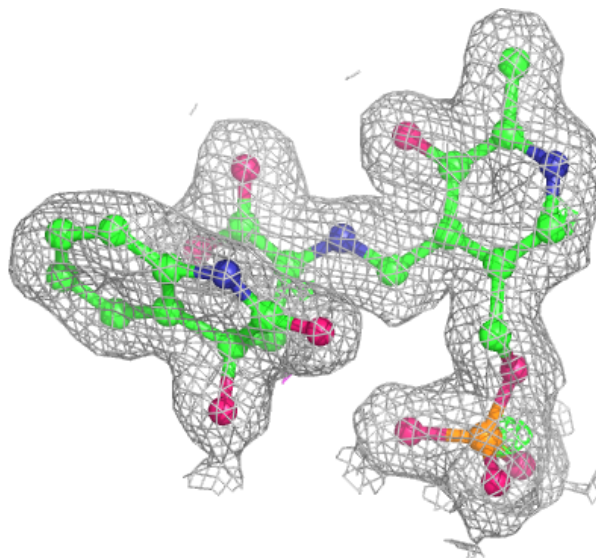
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	YQK	A	503	32/32	0.96	0.09	8,11,14,15	0
3	YQK	B	502	32/32	0.96	0.09	8,11,14,14	0
3	YQK	D	502	32/32	0.96	0.10	10,14,18,19	0
3	YQK	C	502	32/32	0.97	0.08	10,14,16,16	0
4	DMS	B	501	4/4	0.99	0.07	19,20,20,21	0
2	K	A	502	1/1	1.00	0.02	9,9,9,9	0
2	K	C	501	1/1	1.00	0.03	11,11,11,11	0
2	K	D	501	1/1	1.00	0.02	11,11,11,11	0
2	K	A	501	1/1	1.00	0.02	11,11,11,11	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.

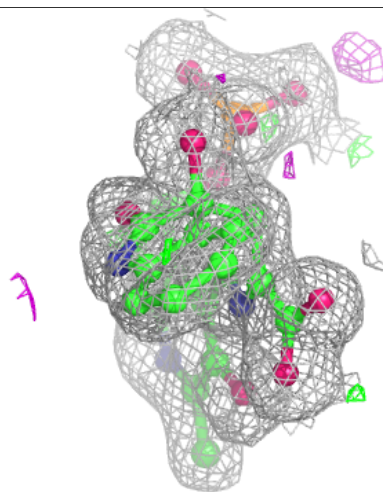
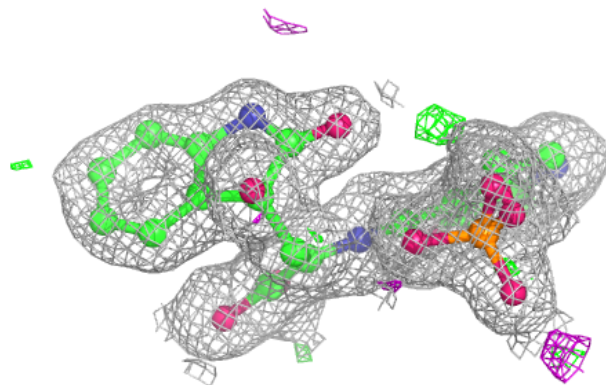
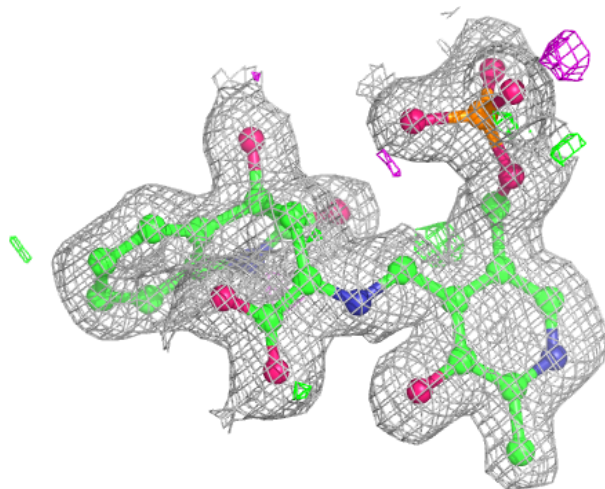
Electron density around YQK A 503:

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



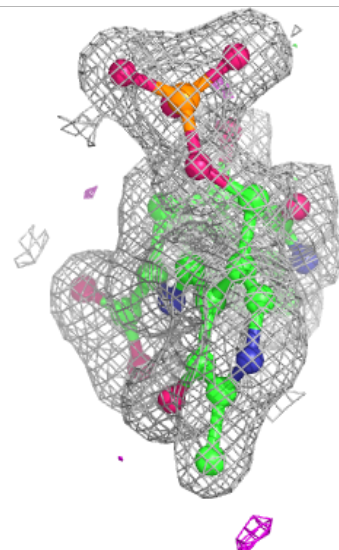
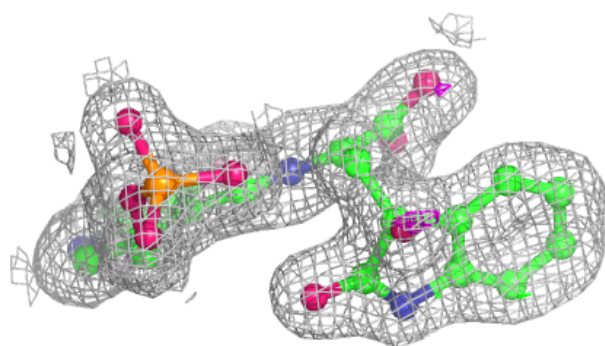
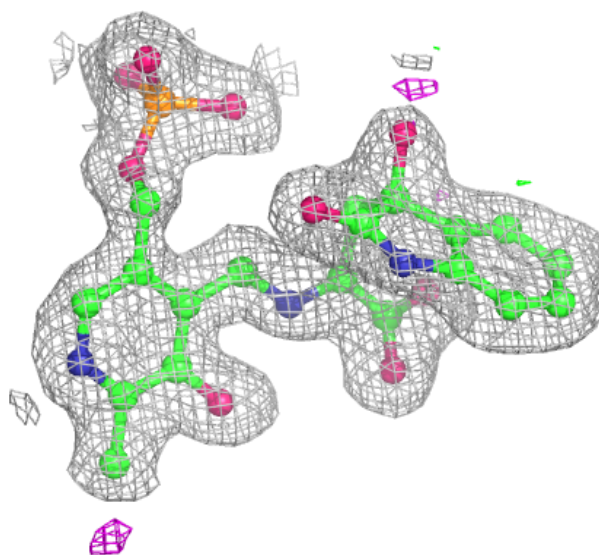
Electron density around YQK B 502:

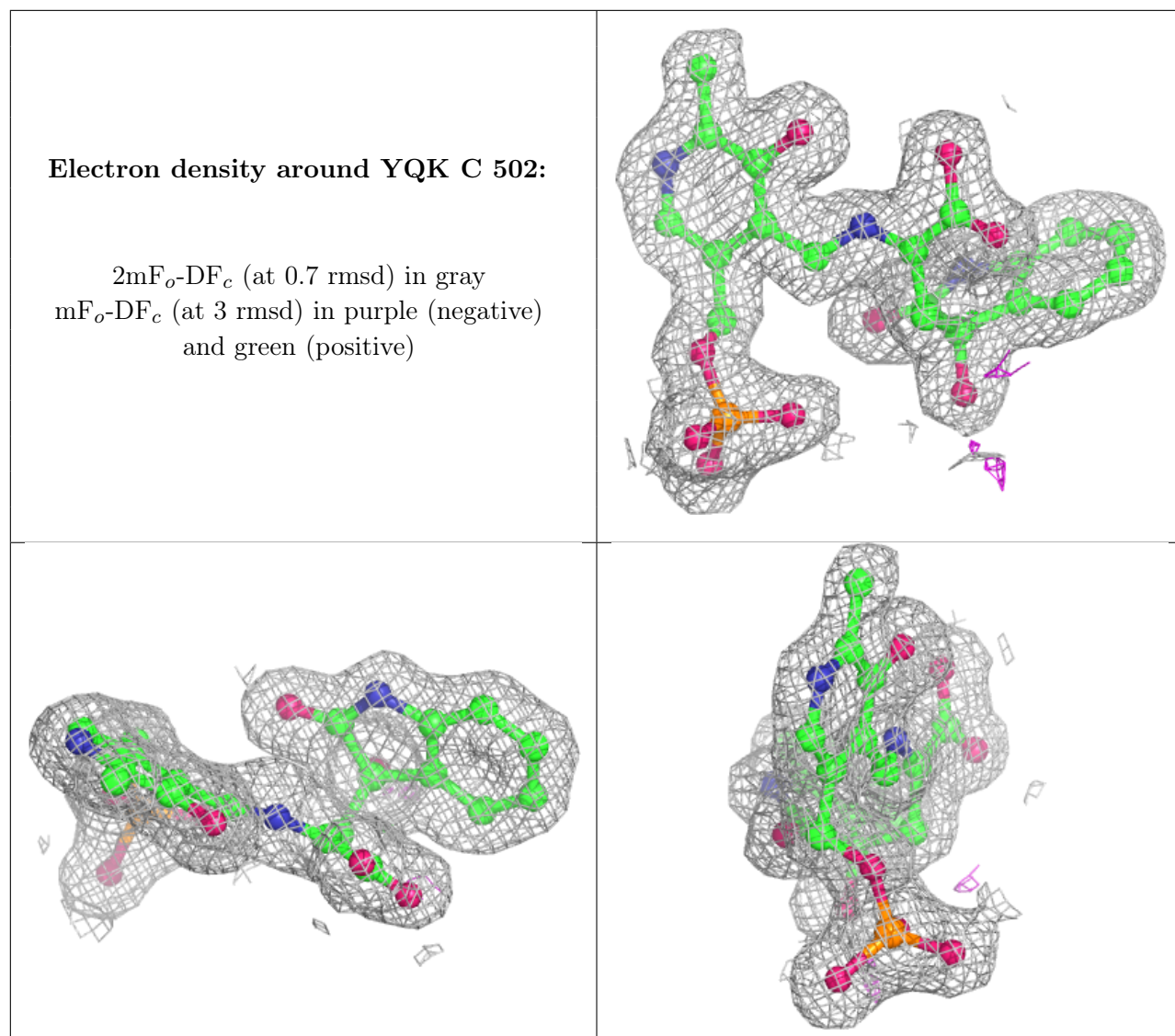
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around YQK D 502:

$2mF_o-DF_c$ (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.