



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:32 AM UTC

PDB ID : 8V9P / pdb_00008v9p
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 : 4-5-2 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

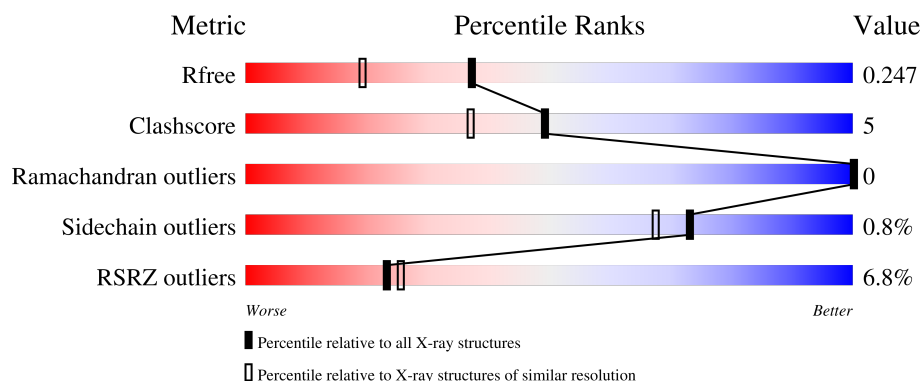
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (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	5% 85% 15%
1	B	467	6% 85% 14%
1	C	467	5% 87% 13%
1	D	467	11% 87% 12%

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.

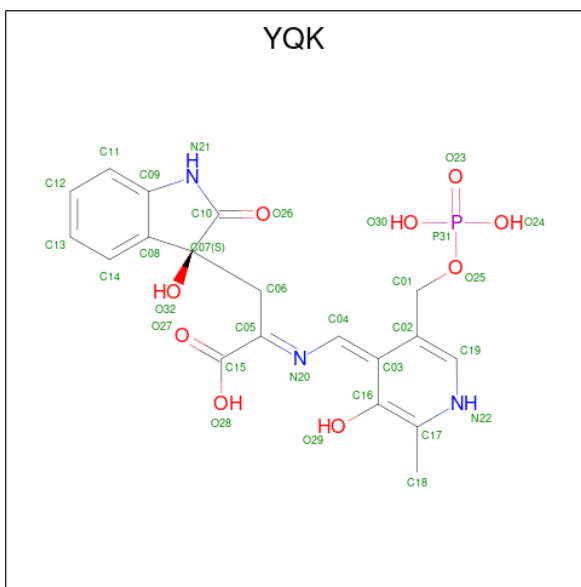
- Molecule 1 is a protein called Tryptophanase.

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

- 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		
2	C	1	Total	K	0	0
			1	1		
2	D	1	Total	K	0	0
			1	1		

- Molecule 3 is (2 {E})-2-[({Z})-[2-methyl-3-oxidanyl-5-[[oxidanyl-bis(oxidanylidene)- $\text{S}^{\wedge}$ {6}-phosphanyl]oxymethyl]-1 {H}-pyridin-4-ylidene]methyl]imino-3-[(3 {S})-3-oxidanyl-2-oxidanylidene-1 {H}-indol-3-yl]propanoic acid (CCD ID: YQK) (formula: $\text{C}_{19}\text{H}_{20}\text{N}_3\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 (CCD ID: DMS) (formula: C_2H_6OS).



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

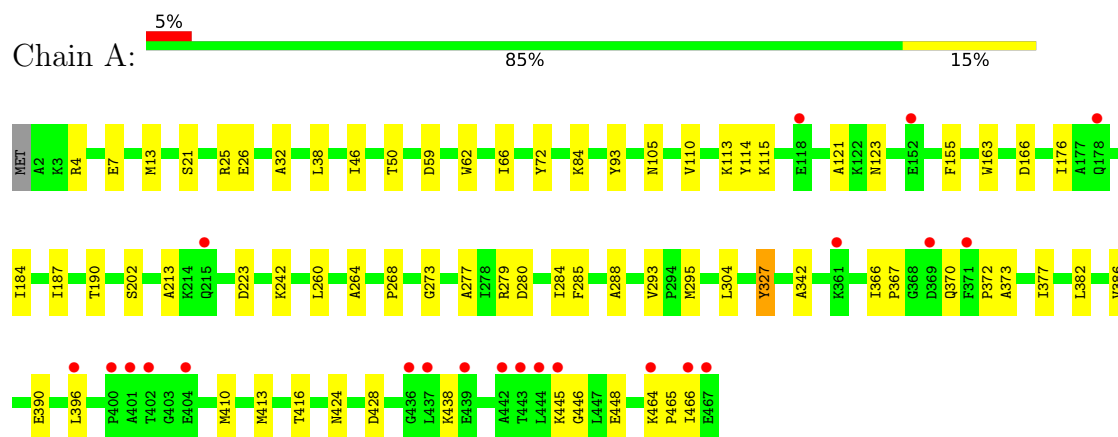
- Molecule 5 is water.

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		

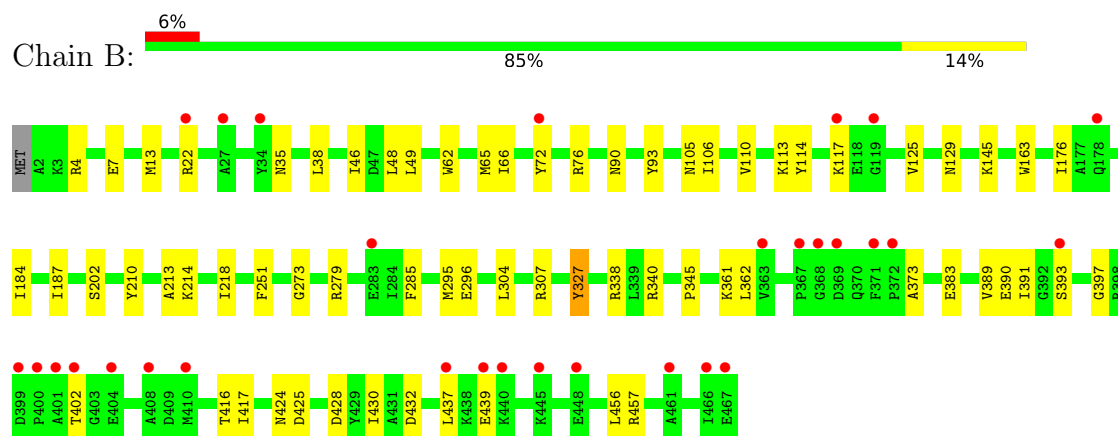
3 Residue-property plots [i](#)

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.

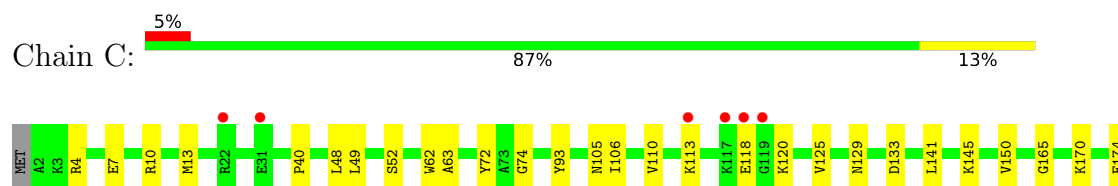
• Molecule 1: Tryptophanase

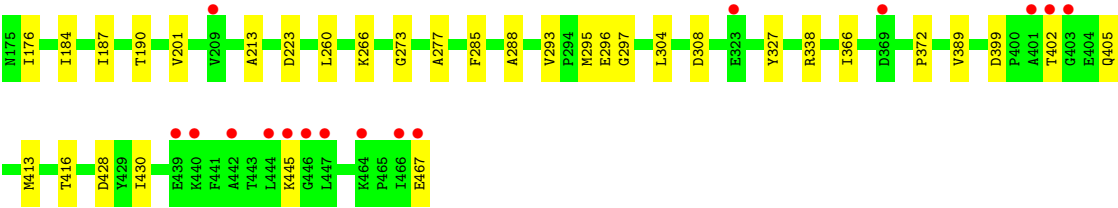


• Molecule 1: Tryptophanase

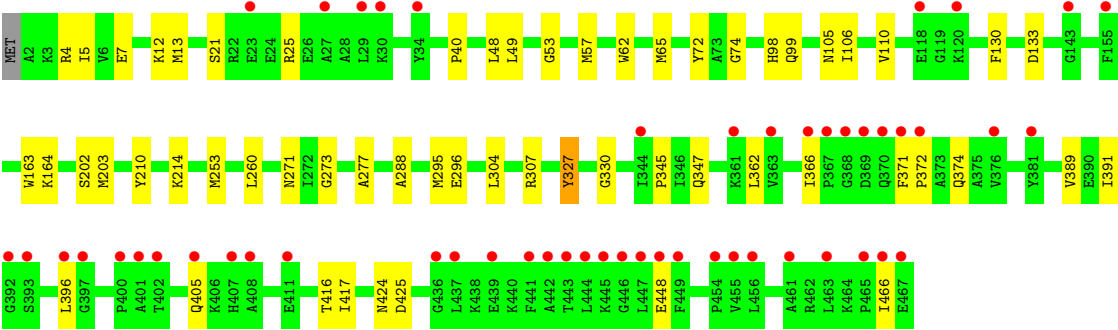
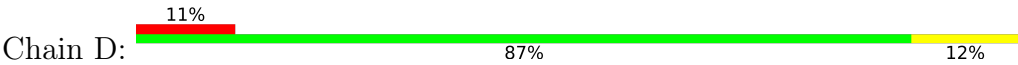


• Molecule 1: Tryptophanase





● 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) 51.1 (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)	Xtriage
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	3861 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å ²)	12.0	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16188	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage'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	0.16	0/3818	0.35	0/5155
1	B	0.17	0/3818	0.36	0/5153
1	C	0.16	0/3835	0.34	0/5176
1	D	0.16	0/3828	0.35	0/5167
All	All	0.16	0/15299	0.35	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	50	0
1	B	3729	0	3706	46	0
1	C	3740	0	3728	41	0
1	D	3732	0	3711	36	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	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	32	0	0	2	0
3	D	32	0	0	1	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	161	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 (161) 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:C:105:ASN:HD21	1:C:295:MET:HE2	1.55	0.70
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:C:113:LYS:NZ	5:C:608:HOH:O	2.30	0.63
1:B:125:VAL:HG12	1:B:145:LYS:HB2	1.80	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:B:62:TRP:CD1	1:D:13:MET:HE2	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:SER:OG	1:C:266:LYS:NZ	2.40	0.55
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
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: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:65:MET:HE2	1:B:307:ARG:HD2	1.92	0.51
1:A:105:ASN:HD21	1:A:295:MET:HE2	1.73	0.51
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: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: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:105:ASN:HD21	1:D:295:MET:HE2	1.79	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:113:LYS:NZ	5:B:610:HOH:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:105:ASN:HD21	1:B:295:MET:HE2	1.78	0.46
1:A:155:PHE:HD1	1:A:410:MET:HE3	1.81	0.46
1:C:129:ASN:O	1:C:150:VAL:HB	2.15	0.46
3:C:502:YQK:O32	1:D:72:TYR:OH	2.18	0.46
1:A:342:ALA:O	1:A:438:LYS:NZ	2.37	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: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:50:THR:OG1	3:A:503:YQK:O28	2.26	0.44
1:A:377:ILE:HA	1:A:413:MET:HE3	1.98	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:377:ILE:HG12	1:A:413:MET:HE3	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:A:13:MET:HE2	1:C:62:TRP:CG	2.53	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:B:439:GLU:CD	1:B:439:GLU:H	2.26	0.43
1:D:57:MET:HE1	1:D:65[B]:MET:SD	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:65[B]:MET:HE2	1:D:307:ARG:HD2	2.00	0.43
3:A:503:YQK:O32	1:B:72:TYR:OH	2.22	0.42
1:A:464:LYS:NZ	1:A:465:PRO:O	2.52	0.42
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
3:A:503:YQK:O29	3:A:503:YQK:N20	2.52	0.42
1:B:13[B]:MET:HE3	1:D:12:LYS:HD3	2.01	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:D:203:MET:HE1	1:D:253:MET:HG3	2.02	0.42
1:B:13[A]:MET:HE2	1:D:62:TRP:CD1	2.55	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 ⓘ

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	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 ⓘ

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%)	387 (99%)	3 (1%)	73	67
1	B	390/386 (101%)	385 (99%)	5 (1%)	61	51
1	C	392/386 (102%)	389 (99%)	3 (1%)	73	67
1	D	391/386 (101%)	386 (99%)	5 (1%)	61	51
All	All	1563/1544 (101%)	1547 (99%)	16 (1%)	73	60

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

Mol	Chain	Res	Type
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	340	ARG
1	B	391	ILE
1	B	416	THR
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	391	ILE
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	A	407	HIS
1	B	142	ASN
1	B	175	ASN
1	B	290	GLN
1	C	105	ASN
1	D	175	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	503	-	32,34,34	1.22	3 (9%)	44,51,51	2.24	10 (22%)
3	YQK	C	502	-	32,34,34	1.20	2 (6%)	44,51,51	2.16	12 (27%)
4	DMS	B	501	-	3,3,3	0.68	0	3,3,3	0.38	0
3	YQK	D	502	-	32,34,34	1.21	3 (9%)	44,51,51	2.04	11 (25%)
3	YQK	B	502	-	32,34,34	1.22	3 (9%)	44,51,51	2.05	12 (27%)

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	YQK	D	502	-	-	4/18/36/36	0/3/3/3
3	YQK	B	502	-	-	2/18/36/36	0/3/3/3
3	YQK	A	503	-	-	4/18/36/36	0/3/3/3
3	YQK	C	502	-	-	1/18/36/36	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	3.44	1.61	1.50
3	D	502	YQK	P31-O23	3.36	1.60	1.50
3	A	503	YQK	C07-C10	-3.35	1.51	1.55
3	B	502	YQK	P31-O23	3.34	1.60	1.50
3	A	503	YQK	P31-O23	3.26	1.60	1.50
3	B	502	YQK	C07-C10	-3.18	1.51	1.55
3	D	502	YQK	C07-C10	-3.12	1.51	1.55
3	C	502	YQK	C07-C10	-3.11	1.51	1.55
3	B	502	YQK	C19-N22	-2.28	1.32	1.36
3	D	502	YQK	C19-N22	-2.22	1.32	1.36
3	A	503	YQK	C19-N22	-2.08	1.32	1.36

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	YQK	C08-C07-C10	8.88	104.63	101.51
3	C	502	YQK	C08-C07-C10	8.22	104.40	101.51
3	D	502	YQK	C08-C07-C10	7.66	104.20	101.51
3	B	502	YQK	C08-C07-C10	7.64	104.20	101.51
3	A	503	YQK	C07-C08-C09	-6.92	106.03	108.86
3	C	502	YQK	C07-C08-C09	-6.61	106.16	108.86
3	D	502	YQK	C07-C08-C09	-6.51	106.20	108.86
3	B	502	YQK	C07-C08-C09	-6.36	106.26	108.86
3	A	503	YQK	C01-C02-C03	-4.28	119.32	122.19
3	C	502	YQK	C01-C02-C03	-3.45	119.88	122.19
3	D	502	YQK	C16-C03-C02	-3.31	117.53	119.28
3	C	502	YQK	C07-C06-C05	-3.31	110.75	115.08
3	C	502	YQK	C18-C17-C16	-3.24	118.30	122.27
3	B	502	YQK	C01-C02-C03	-3.13	120.09	122.19
3	B	502	YQK	O29-C16-C17	2.99	121.17	118.40
3	B	502	YQK	C11-C09-C08	-2.97	119.15	121.92
3	C	502	YQK	C11-C09-C08	-2.97	119.15	121.92
3	D	502	YQK	C18-C17-C16	-2.95	118.64	122.27
3	A	503	YQK	O29-C16-C17	2.95	121.12	118.40
3	A	503	YQK	C11-C09-C08	-2.91	119.20	121.92
3	D	502	YQK	C01-C02-C03	-2.87	120.26	122.19
3	D	502	YQK	C19-N22-C17	-2.81	121.87	124.20
3	D	502	YQK	C11-C09-C08	-2.80	119.31	121.92
3	A	503	YQK	C16-C03-C02	-2.75	117.83	119.28
3	A	503	YQK	C07-C10-N21	-2.74	106.79	108.43
3	B	502	YQK	C18-C17-C16	-2.66	119.01	122.27
3	A	503	YQK	C01-C02-C19	2.57	121.56	118.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	YQK	C19-N22-C17	-2.48	122.14	124.20
3	C	502	YQK	C01-C02-C19	2.36	121.35	118.95
3	B	502	YQK	C19-N22-C17	-2.36	122.24	124.20
3	C	502	YQK	C07-C10-N21	-2.35	107.03	108.43
3	B	502	YQK	C16-C17-N22	2.33	121.22	118.63
3	D	502	YQK	C16-C17-N22	2.31	121.19	118.63
3	B	502	YQK	C16-C03-C02	-2.24	118.10	119.28
3	C	502	YQK	O29-C16-C17	2.23	120.46	118.40
3	C	502	YQK	C06-C07-C08	-2.21	111.33	115.28
3	C	502	YQK	C19-N22-C17	-2.21	122.37	124.20
3	B	502	YQK	C07-C10-N21	-2.16	107.14	108.43
3	D	502	YQK	C14-C08-C07	2.13	133.50	130.69
3	D	502	YQK	O28-C15-O27	-2.12	118.86	123.90
3	B	502	YQK	O28-C15-O27	-2.08	118.95	123.90
3	A	503	YQK	C18-C17-C16	-2.07	119.73	122.27
3	D	502	YQK	C07-C10-N21	-2.06	107.19	108.43
3	C	502	YQK	C16-C17-N22	2.04	120.89	118.63
3	B	502	YQK	C06-C07-C08	-2.04	111.64	115.28

There are no chirality outliers.

All (11) 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-O27
3	A	503	YQK	N20-C05-C15-O28
3	B	502	YQK	N20-C05-C15-O27
3	B	502	YQK	N20-C05-C15-O28
3	A	503	YQK	C06-C05-C15-O28

There are no ring outliers.

4 monomers are involved in 8 short contacts:

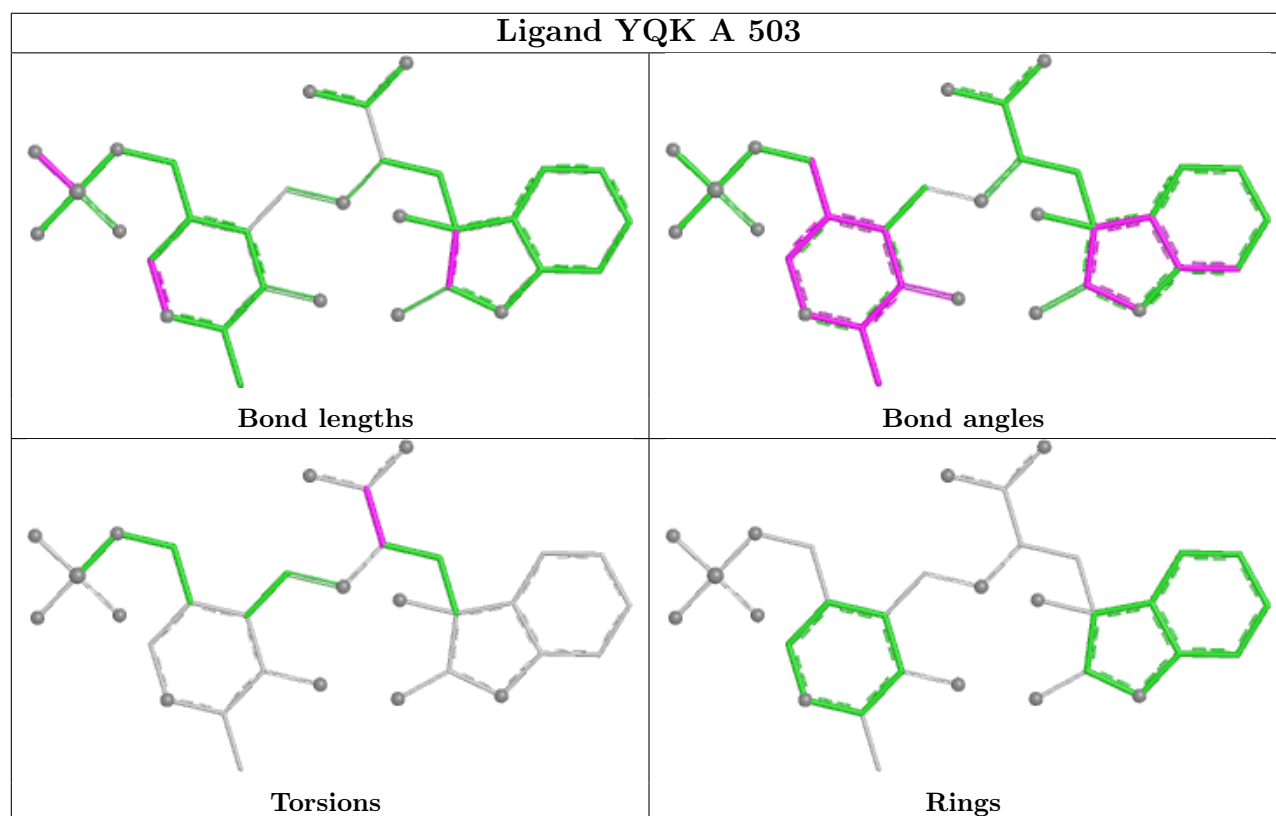
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	YQK	3	0
3	C	502	YQK	2	0

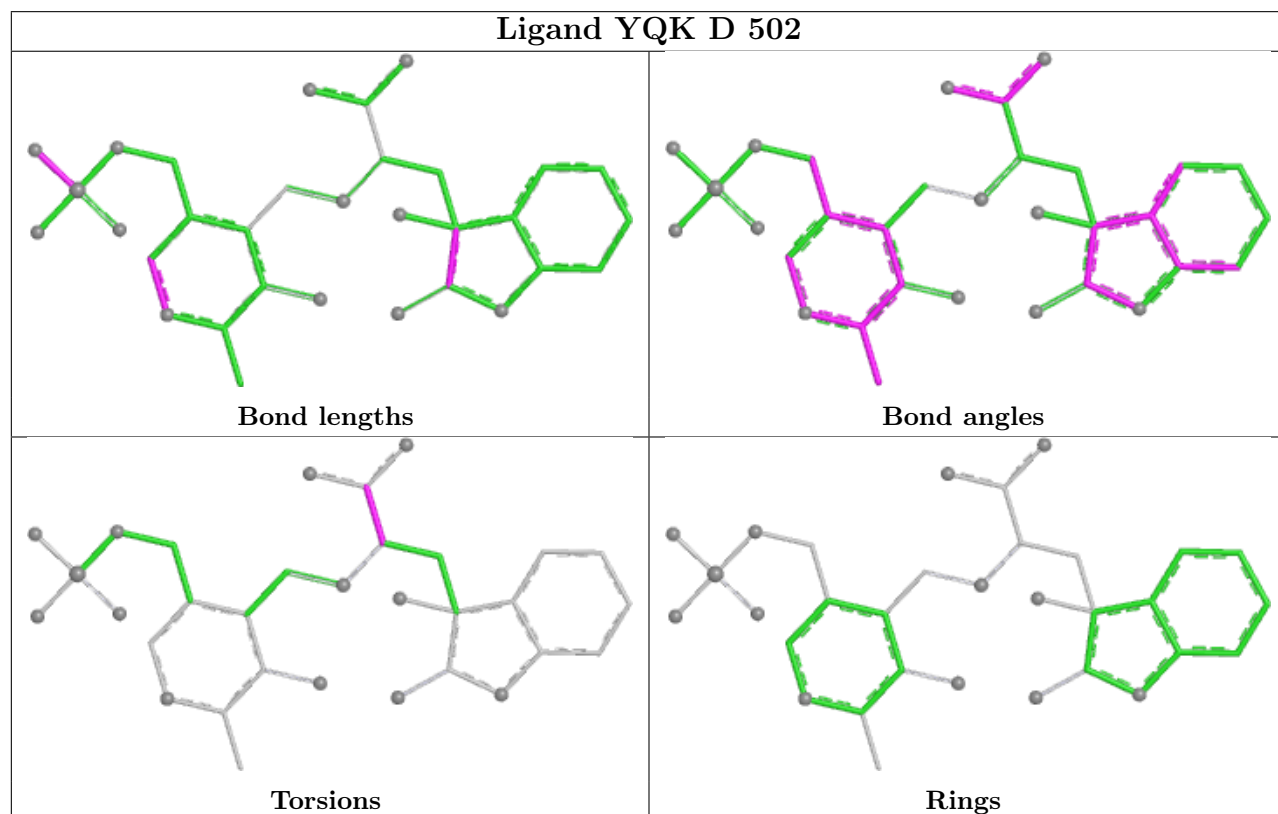
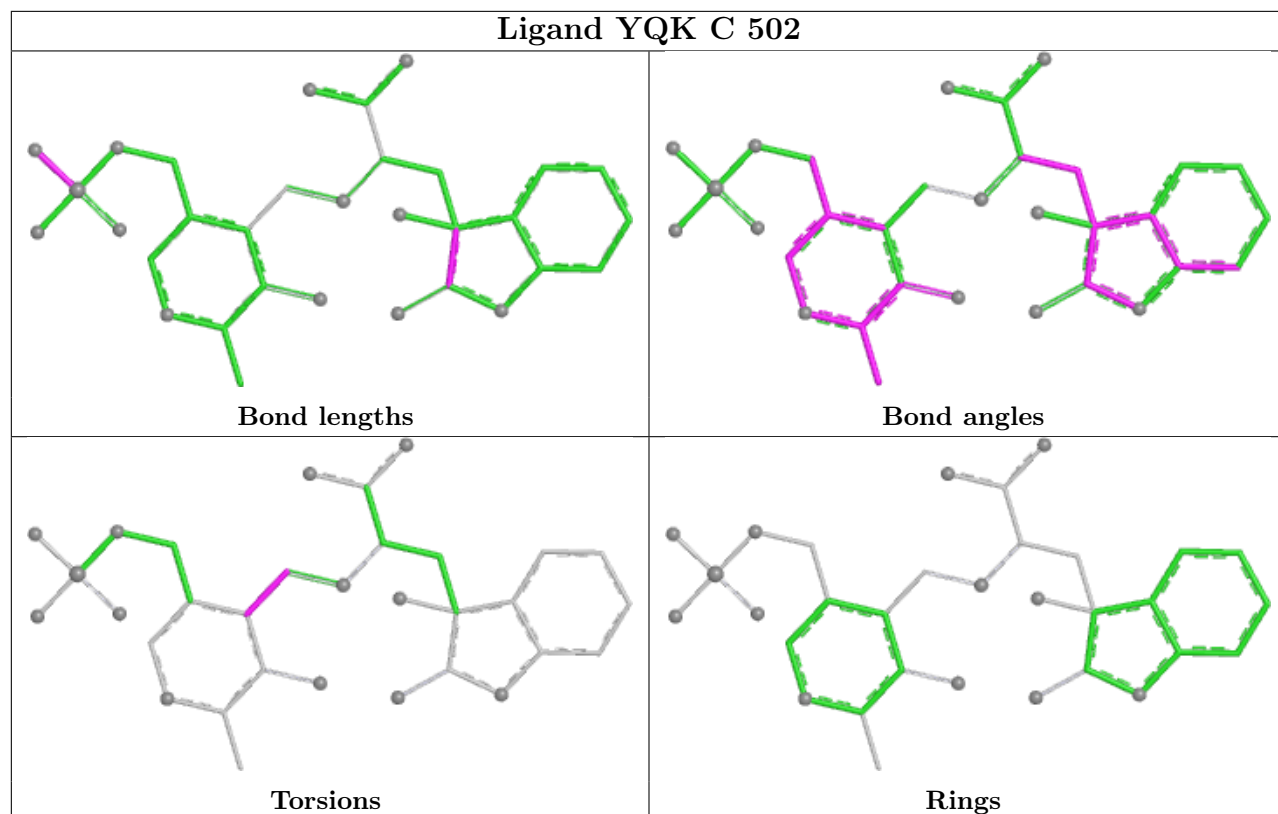
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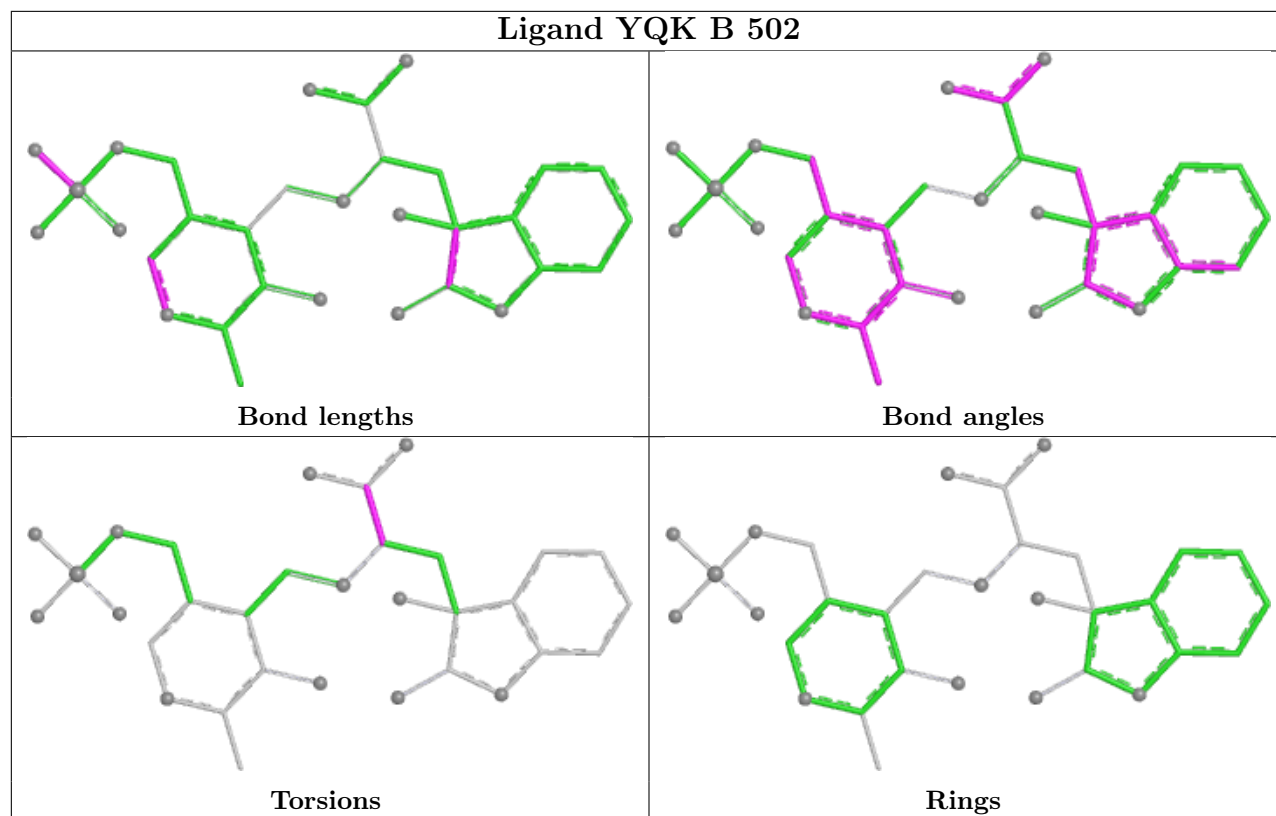
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	YQK	1	0
3	B	502	YQK	2	0

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.







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%)	0.41	22 (4%)	36	39	5, 14, 38, 64	5 (1%)
1	B	466/467 (99%)	0.45	30 (6%)	25	27	4, 15, 35, 55	5 (1%)
1	C	466/467 (99%)	0.44	22 (4%)	36	39	7, 16, 35, 68	7 (1%)
1	D	466/467 (99%)	0.59	52 (11%)	10	9	5, 16, 45, 80	6 (1%)
All	All	1864/1868 (99%)	0.47	126 (6%)	23	25	4, 15, 39, 80	23 (1%)

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	401	ALA	5.0
1	D	401	ALA	5.0
1	C	445	LYS	4.9
1	A	467	GLU	4.9
1	D	455	VAL	4.5
1	B	363	VAL	4.2
1	D	393	SER	4.2
1	D	400	PRO	4.1
1	C	401	ALA	3.9
1	C	118	GLU	3.9
1	B	369[A]	ASP	3.9
1	A	401	ALA	3.8
1	D	467	GLU	3.8
1	A	400	PRO	3.7
1	D	408	ALA	3.7
1	D	447	LEU	3.5
1	D	466	ILE	3.4
1	C	119	GLY	3.4
1	B	445	LYS	3.4
1	D	397	GLY	3.3
1	A	396	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	444	LEU	3.3
1	D	443	THR	3.3
1	A	466	ILE	3.3
1	C	439	GLU	3.3
1	D	444	LEU	3.3
1	A	445	LYS	3.2
1	D	120	LYS	3.2
1	B	402	THR	3.2
1	D	29	LEU	3.2
1	D	371	PHE	3.2
1	D	436	GLY	3.2
1	B	117	LYS	3.1
1	B	461	ALA	3.1
1	D	381	TYR	3.1
1	C	467	GLU	3.1
1	B	440	LYS	3.1
1	D	445	LYS	3.1
1	C	402	THR	3.1
1	B	27	ALA	3.1
1	A	404	GLU	3.1
1	D	118	GLU	3.1
1	A	118	GLU	3.0
1	D	366	ILE	3.0
1	C	447	LEU	2.9
1	A	152	GLU	2.9
1	B	467	GLU	2.9
1	A	464	LYS	2.9
1	B	119	GLY	2.9
1	D	405[A]	GLN	2.9
1	A	439	GLU	2.9
1	B	466	ILE	2.9
1	C	22[A]	ARG	2.8
1	D	439[A]	GLU	2.8
1	B	178	GLN	2.8
1	D	437	LEU	2.8
1	D	456	LEU	2.8
1	C	113	LYS	2.8
1	B	400	PRO	2.8
1	D	23	GLU	2.8
1	D	392	GLY	2.7
1	D	367	PRO	2.7
1	B	439	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	464	LYS	2.6
1	D	454	PRO	2.6
1	C	323	GLU	2.6
1	A	444	LEU	2.5
1	D	396	LEU	2.5
1	D	407	HIS	2.5
1	D	402	THR	2.5
1	D	411	GLU	2.5
1	D	30	LYS	2.5
1	B	368	GLY	2.5
1	A	361	LYS	2.5
1	D	449	PHE	2.4
1	D	463	LEU	2.4
1	D	461	ALA	2.4
1	C	209	VAL	2.4
1	D	465	PRO	2.4
1	C	446	GLY	2.4
1	D	34	TYR	2.4
1	C	31	GLU	2.4
1	D	376	VAL	2.4
1	D	448	GLU	2.4
1	D	155	PHE	2.3
1	A	442	ALA	2.3
1	B	283	GLU	2.3
1	A	178	GLN	2.3
1	A	215	GLN	2.3
1	D	369	ASP	2.3
1	B	371	PHE	2.3
1	B	408	ALA	2.3
1	B	22	ARG	2.3
1	D	143	GLY	2.3
1	A	371	PHE	2.2
1	D	446	GLY	2.2
1	C	369	ASP	2.2
1	D	344	ILE	2.2
1	A	437	LEU	2.2
1	A	369	ASP	2.2
1	B	367	PRO	2.2
1	B	393	SER	2.2
1	A	443	THR	2.2
1	B	34	TYR	2.2
1	C	466	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	361	LYS	2.2
1	B	404	GLU	2.2
1	D	363	VAL	2.2
1	B	372	PRO	2.2
1	D	372	PRO	2.2
1	D	441	PHE	2.1
1	C	440	LYS	2.1
1	C	442	ALA	2.1
1	D	442	ALA	2.1
1	C	117	LYS	2.1
1	B	72	TYR	2.0
1	A	402	THR	2.0
1	B	410	MET	2.0
1	D	368	GLY	2.0
1	B	437	LEU	2.0
1	D	27	ALA	2.0
1	B	399	ASP	2.0
1	B	448	GLU	2.0
1	A	436	GLY	2.0
1	C	403	GLY	2.0
1	D	370	GLN	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
3	YQK	A	503	32/32	0.94	0.08	8,11,14,15	0
3	YQK	B	502	32/32	0.94	0.07	8,11,14,14	0

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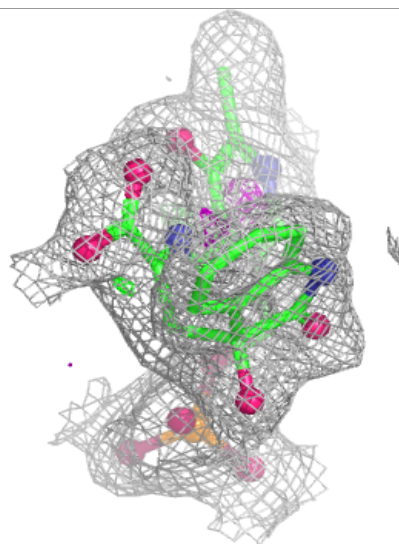
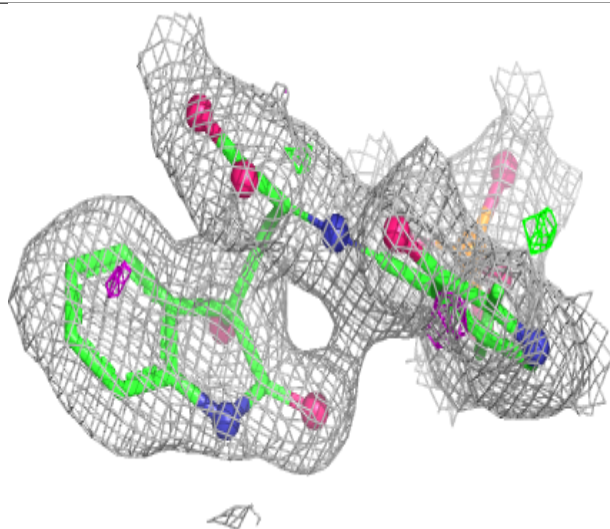
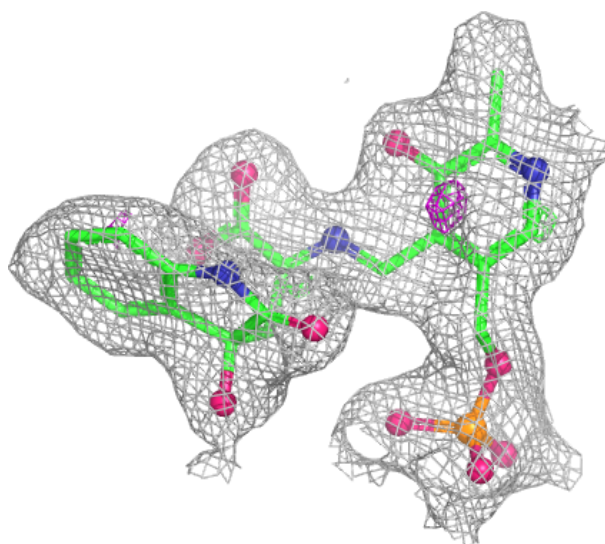
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	YQK	C	502	32/32	0.95	0.07	10,14,16,16	0
3	YQK	D	502	32/32	0.95	0.07	10,14,18,19	0
4	DMS	B	501	4/4	0.97	0.08	19,20,20,21	0
2	K	A	502	1/1	0.99	0.08	9,9,9,9	0
2	K	C	501	1/1	0.99	0.09	11,11,11,11	0
2	K	D	501	1/1	0.99	0.06	11,11,11,11	0
2	K	A	501	1/1	0.99	0.07	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.

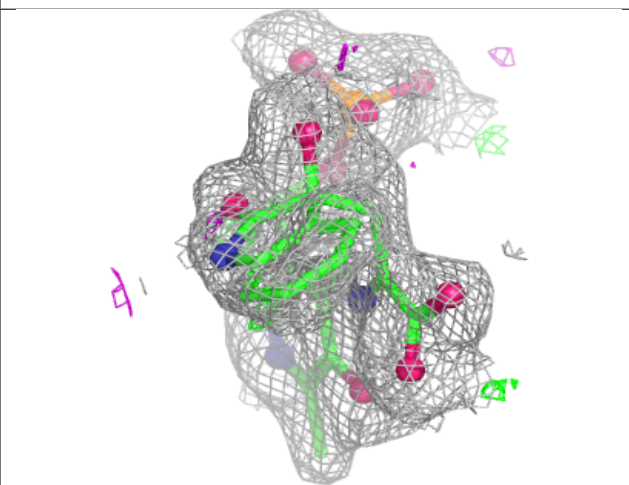
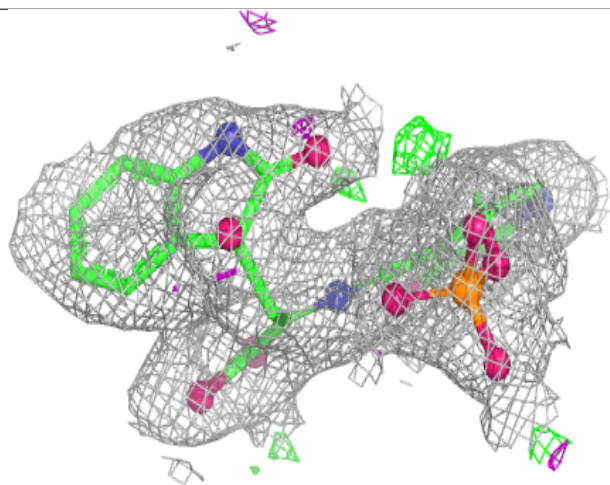
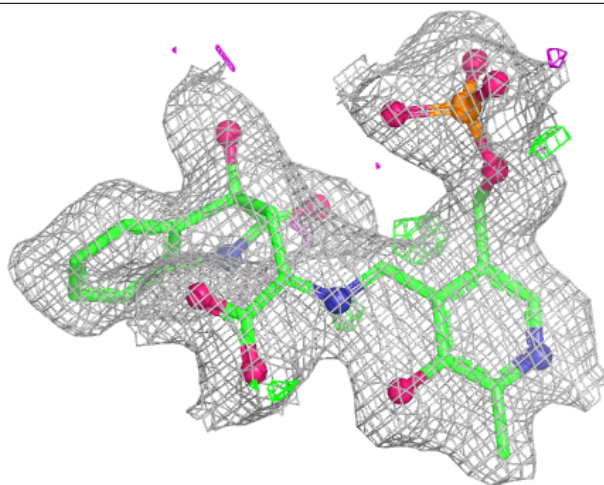
Electron density around YQK A 503:

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



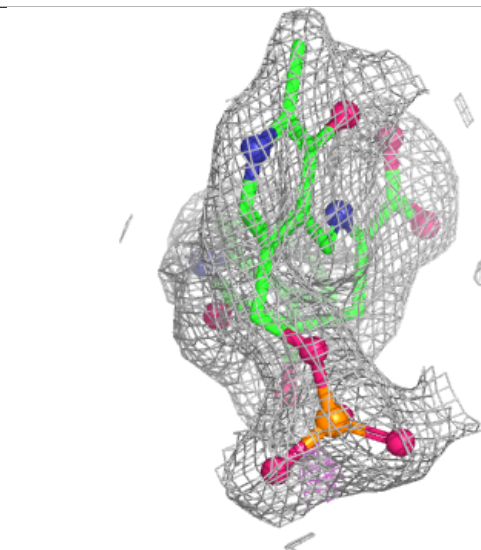
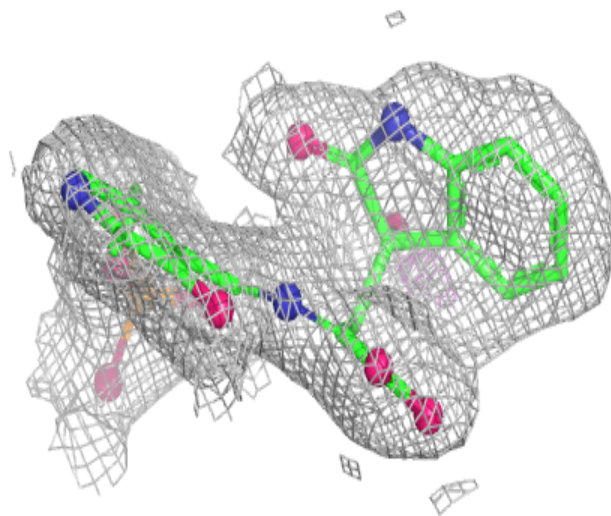
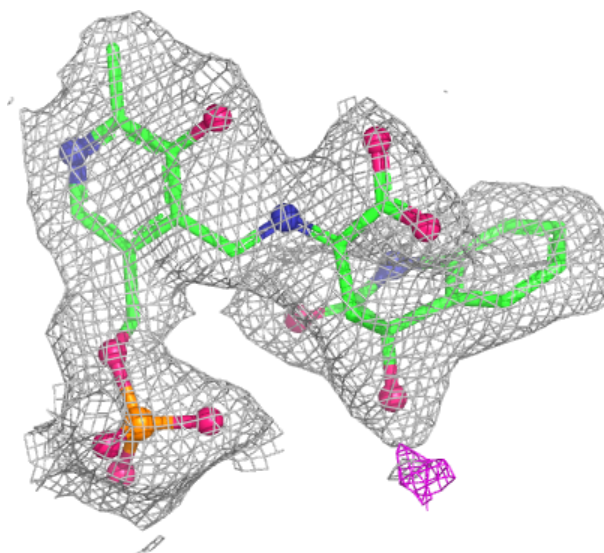
Electron density around YQK B 502:

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



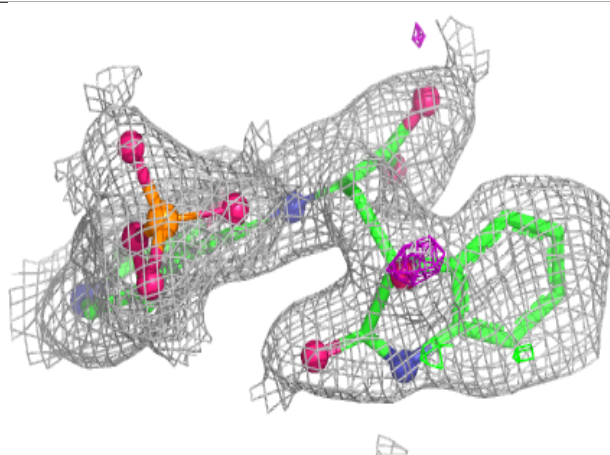
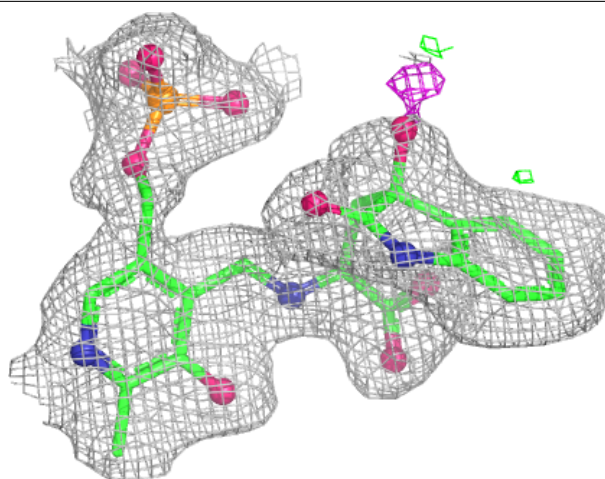
Electron density around YQK C 502:

$2mF_o-DF_c$ (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.