Full wwPDB X-ray Structure Validation Report (i)

Dec 4, 2023 – 12:33 PM EST

PDB ID	:	8V4A
Title	:	Proteus vulgaris tryptophan indole-lyase complexed with L-ethionine
Authors	:	Phillips, R.S.
Deposited on	:	2023-11-28
Resolution	:	1.96 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 (i) 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 (i)) were used in the production of this report:

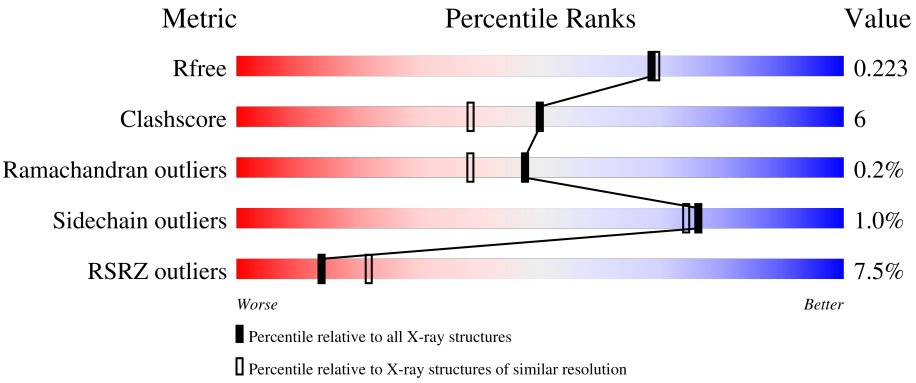
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 <=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	6% 88% 12%
1	B	467	7% 85% 15%
1	C	467	12% 82% 17%
1	D	467	6% 84% 15%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16294 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.

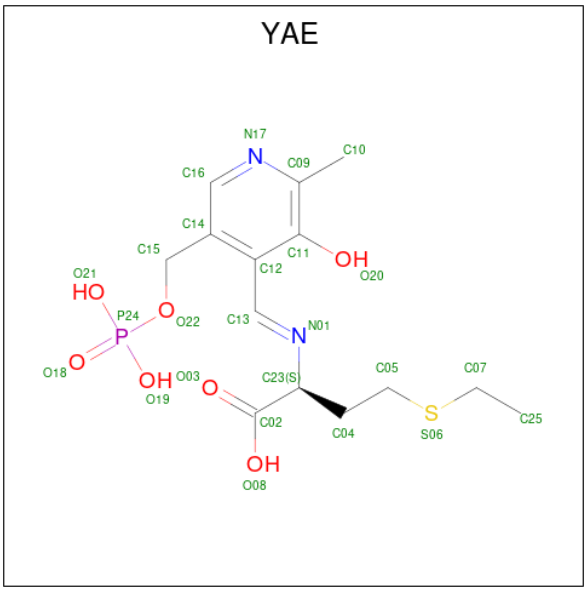
- Molecule 1 is a protein called Tryptophanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	8	0
			3749	2395	640	696	18			
1	B	466	Total	C	N	O	S	0	5	0
			3731	2382	638	693	18			
1	C	465	Total	C	N	O	S	0	9	0
			3735	2390	640	686	19			
1	D	466	Total	C	N	O	S	0	13	0
			3784	2421	642	703	18			

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

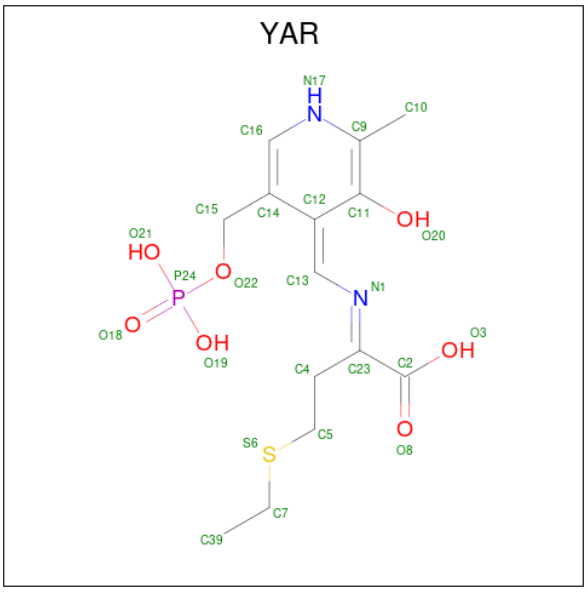
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	K	0	0
			2	2		
2	C	2	Total	K	0	0
			2	2		

- Molecule 3 is (E)-S-ethyl-N-({3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methylidene)-L-homocysteine (three-letter code: YAE) (formula: $C_{14}H_{21}N_2O_7PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			25	14	2	7	1	1		
3	C	1	Total	C	N	O	P	S	0	0
			25	14	2	7	1	1		

- Molecule 4 is (2E)-4-(ethylsulfanyl)-2-{[(Z)-{3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4(1H)-ylidene}methyl]imino}butanoic acid (three-letter code: YAR) (formula: $C_{14}H_{21}N_2O_7PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	S	0	0
			25	14	2	7	1	1		

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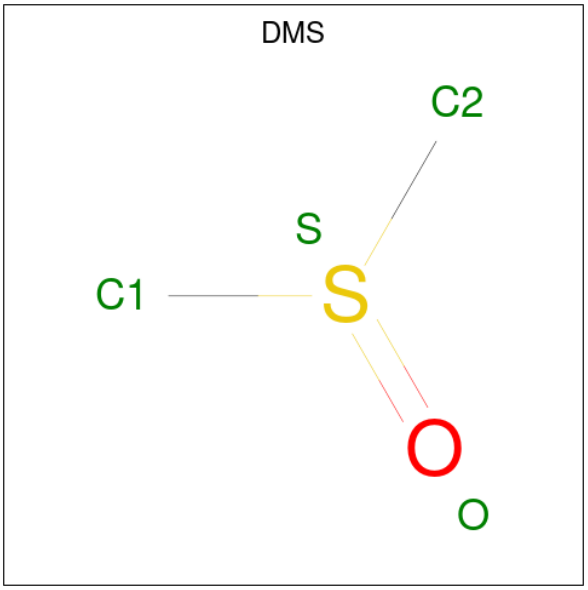
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	S	0	0
			25	14	2	7	1	1		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

- Molecule 6 is water.

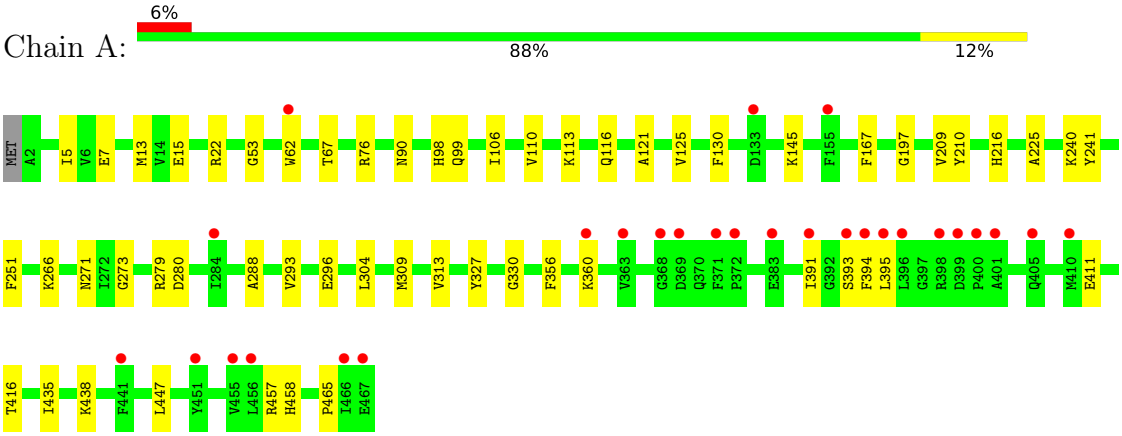
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	266	Total	O	0	13
			266	266		
6	B	314	Total	O	0	8
			314	314		
6	C	280	Total	O	0	8
			280	280		
6	D	327	Total	O	0	10
			327	327		

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.

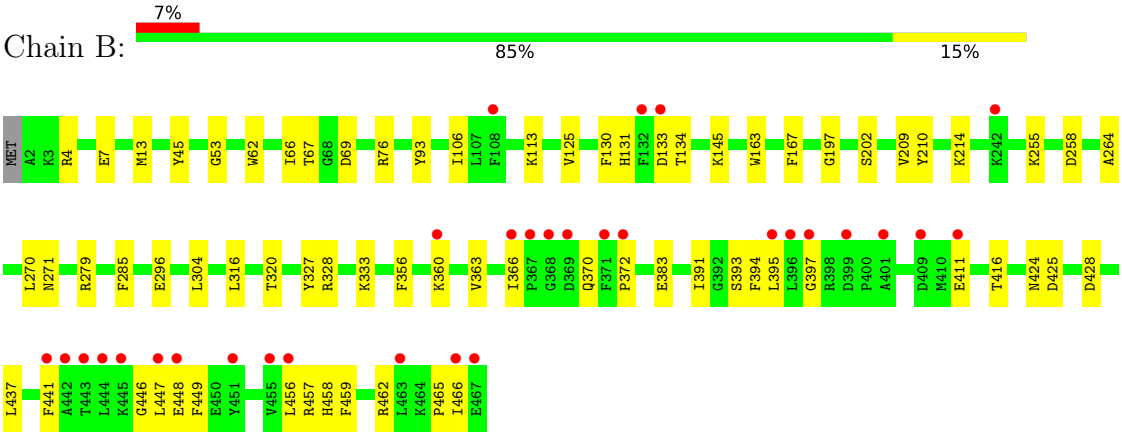
• Molecule 1: Tryptophanase

Chain A:



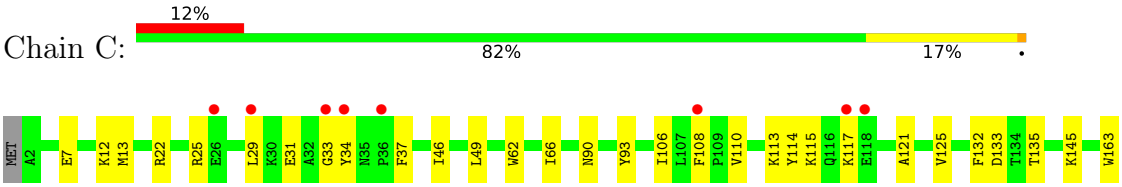
• Molecule 1: Tryptophanase

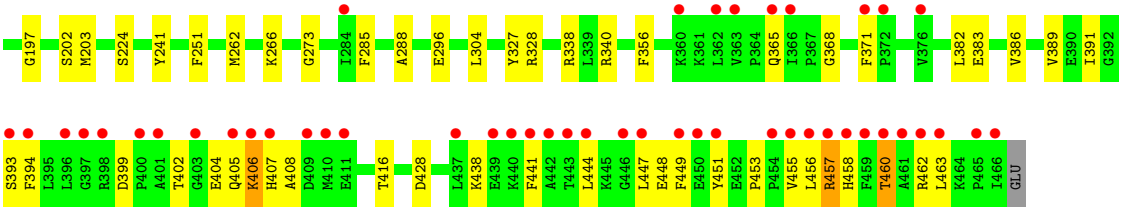
Chain B:



• Molecule 1: Tryptophanase

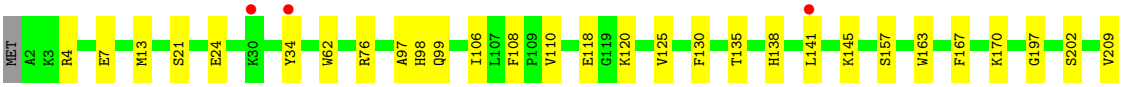
Chain C:

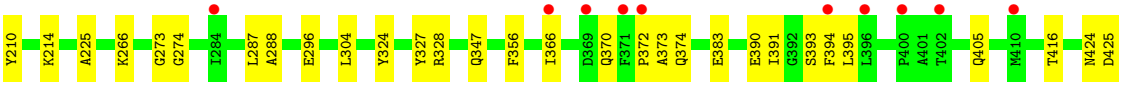


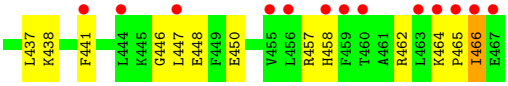


• Molecule 1: Tryptophanase

Chain D:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	150.75Å 207.08Å 60.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.76 – 1.96 62.76 – 1.96	Depositor EDS
% Data completeness (in resolution range)	67.3 (62.76-1.96) 67.3 (62.76-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 1.97Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.177 , 0.224 0.177 , 0.223	Depositor DCC
R_{free} test set	2000 reflections (2.18%)	wwPDB-VP
Wilson B-factor (Å^2)	27.2	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16294	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.38	0/3847	0.58	0/5190
1	B	0.39	0/3820	0.58	0/5155
1	C	0.39	0/3841	0.58	0/5184
1	D	0.39	0/3885	0.64	2/5240 (0.0%)
All	All	0.39	0/15393	0.60	2/20769 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	466[A]	ILE	O-C-N	-14.13	100.08	122.70
1	D	466[B]	ILE	O-C-N	-14.13	100.08	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	466[A]	ILE	Mainchain
1	D	466[B]	ILE	Mainchain

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	3749	0	3741	37	0
1	B	3731	0	3714	46	0
1	C	3735	0	3757	53	0
1	D	3784	0	3788	46	0
2	A	2	0	0	0	0
2	C	2	0	0	0	0
3	A	25	0	0	2	0
3	C	25	0	0	1	0
4	B	25	0	0	0	0
4	D	25	0	0	1	0
5	B	4	0	6	0	0
6	A	266	0	0	7	0
6	B	314	0	0	4	0
6	C	280	0	0	2	0
6	D	327	0	0	7	0
All	All	16294	0	15006	175	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 6.

All (175) 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:C:451:TYR:HB3	1:C:462[A]:ARG:HB3	1.69	0.75
1:D:125:VAL:HG12	1:D:145:LYS:HB2	1.69	0.74
1:D:327[A]:TYR:OH	6:D:601[A]:HOH:O	2.06	0.73
1:C:447:LEU:HB3	1:C:463:LEU:HD13	1.74	0.70
1:D:225:ALA:HB1	1:D:266:LYS:HG3	1.74	0.69
1:C:365:GLN:HB2	1:C:444:LEU:HD13	1.74	0.68
1:B:62:TRP:CD1	1:D:13:MET:HE2	2.29	0.66
1:C:453:PRO:HG2	1:C:457:ARG:HA	1.75	0.66
1:A:125:VAL:HG12	1:A:145:LYS:HB3	1.77	0.66
1:C:25:ARG:NH1	1:C:382:LEU:O	2.28	0.66
1:C:451:TYR:HB3	1:C:462[B]:ARG:HB2	1.78	0.65
1:B:462:ARG:NH2	6:B:603:HOH:O	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:TRP:CD1	1:C:13:MET:HE2	2.34	0.63
1:D:405:GLN:OE1	6:D:603:HOH:O	2.15	0.62
1:B:370:GLN:HB3	1:B:446:GLY:HA3	1.82	0.62
1:A:393:SER:O	1:A:457:ARG:NH2	2.32	0.61
1:C:338:ARG:NH1	1:C:428:ASP:OD1	2.33	0.61
1:D:370:GLN:HB3	1:D:446:GLY:HA3	1.83	0.61
1:A:225:ALA:HB1	1:A:266:LYS:HG3	1.84	0.60
1:A:273:GLY:HA2	1:A:304:LEU:HD21	1.82	0.60
1:B:393:SER:O	1:B:457:ARG:NH2	2.35	0.59
1:C:273:GLY:HA2	1:C:304:LEU:HD21	1.84	0.59
1:D:373:ALA:HB3	1:D:390[A]:GLU:HG3	1.84	0.59
1:D:76:ARG:NH2	6:D:612:HOH:O	2.34	0.59
1:C:125:VAL:HG12	1:C:145:LYS:HB3	1.85	0.58
1:B:366:ILE:HB	1:B:372:PRO:HB3	1.85	0.57
1:B:424:ASN:ND2	1:D:425:ASP:OD2	2.29	0.57
1:D:273:GLY:HA2	1:D:304:LEU:HD21	1.86	0.57
1:C:266:LYS:HZ1	3:C:502:YAE:C13	2.18	0.57
1:C:406:LYS:O	1:C:408:ALA:N	2.31	0.57
1:D:7:GLU:HG3	1:D:327[B]:TYR:CZ	2.41	0.56
1:B:456:LEU:HD22	1:B:459:PHE:HE2	1.70	0.55
1:A:435:ILE:O	1:A:438:LYS:HG2	2.06	0.55
1:B:67:THR:O	1:B:76[A]:ARG:NH2	2.38	0.55
1:D:118:GLU:HB2	1:D:120:LYS:HG3	1.89	0.54
1:B:214:LYS:NZ	1:B:258:ASP:OD2	2.27	0.54
1:C:49:LEU:HD12	1:C:389:VAL:HB	1.91	0.53
1:C:455:VAL:HG22	1:C:456:LEU:HG	1.90	0.53
1:A:67:THR:O	1:A:76[B]:ARG:NH2	2.40	0.53
1:D:383:GLU:HG2	1:D:437:LEU:HD21	1.90	0.53
1:B:13:MET:HE2	1:D:62:TRP:CD1	2.44	0.53
1:A:447:LEU:HD23	1:A:465:PRO:HA	1.90	0.53
1:C:114:TYR:HA	1:C:117:LYS:HD2	1.89	0.52
1:A:360:LYS:HG3	1:A:411:GLU:HB2	1.90	0.52
1:D:7:GLU:HG3	1:D:327[A]:TYR:CZ	2.44	0.52
1:D:447:LEU:HD23	1:D:465[A]:PRO:HA	1.92	0.51
1:A:13:MET:HE2	1:C:62:TRP:CD1	2.46	0.51
1:C:7:GLU:HG3	1:C:327:TYR:CZ	2.46	0.51
1:C:197:GLY:HA2	1:C:356:PHE:CE1	2.46	0.50
1:D:21:SER:OG	1:D:24:GLU:HG3	2.12	0.50
1:A:13:MET:HE2	1:C:62:TRP:CG	2.47	0.50
1:A:106:ILE:HD11	1:A:296:GLU:HG3	1.93	0.49
1:C:404:GLU:HG3	1:C:406:LYS:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:LEU:HG	1:C:34:TYR:HA	1.95	0.49
1:B:13:MET:HE2	1:D:62:TRP:CG	2.47	0.49
1:A:113:LYS:HD3	6:A:819:HOH:O	2.12	0.49
1:A:7:GLU:HG3	1:A:327:TYR:CE1	2.47	0.49
1:B:383:GLU:HG2	1:B:437:LEU:HD21	1.94	0.49
1:C:113:LYS:HD3	6:C:840:HOH:O	2.13	0.49
1:D:106:ILE:HD11	1:D:296:GLU:HG3	1.94	0.49
1:C:404:GLU:CG	1:C:406:LYS:HB3	2.42	0.49
1:C:90:ASN:HB2	1:C:251:PHE:CE1	2.49	0.48
1:B:456:LEU:HB3	1:B:459:PHE:HD2	1.76	0.48
1:C:110:VAL:HG21	1:C:288:ALA:HA	1.96	0.48
1:A:110:VAL:HG21	1:A:288:ALA:HA	1.96	0.47
1:D:138:HIS:HA	1:D:141[B]:LEU:HG	1.96	0.47
1:B:391:ILE:HG23	1:B:395:LEU:HD22	1.96	0.47
1:C:453:PRO:HB3	6:D:858:HOH:O	2.14	0.47
1:A:197:GLY:HA2	1:A:356:PHE:CZ	2.49	0.47
1:D:34:TYR:CD1	1:D:465[B]:PRO:HD3	2.50	0.47
1:D:366:ILE:HB	1:D:372:PRO:HB3	1.96	0.47
1:B:7:GLU:HG3	1:B:327:TYR:CZ	2.50	0.47
1:A:5:ILE:HD12	1:A:330:GLY:HA3	1.97	0.47
1:A:22[A]:ARG:HG3	6:A:662:HOH:O	2.15	0.47
1:A:391:ILE:HD13	1:A:395:LEU:HD13	1.97	0.47
1:B:62:TRP:O	1:B:66:ILE:HG12	2.15	0.47
1:C:163:TRP:CD2	1:C:202:SER:HB3	2.50	0.46
1:C:399:ASP:HB3	1:C:402:THR:HB	1.96	0.46
1:C:406:LYS:C	1:C:408:ALA:H	2.15	0.46
1:A:210:TYR:OH	1:A:279:ARG:NH2	2.49	0.46
1:A:53:GLY:HA2	1:A:271:ASN:HA	1.98	0.46
1:C:46:ILE:HB	1:C:386[B]:VAL:HG12	1.97	0.46
1:B:131:HIS:HB2	6:B:611:HOH:O	2.16	0.46
1:B:316:LEU:O	1:B:320:THR:HG23	2.15	0.46
1:B:106:ILE:HD11	1:B:296:GLU:HG3	1.97	0.46
1:D:448:GLU:HG3	1:D:464[A]:LYS:HG3	1.97	0.46
1:B:397:GLY:HA2	1:B:457:ARG:NE	2.31	0.46
1:C:33:GLY:HA3	1:C:462[A]:ARG:HG3	1.97	0.46
1:D:98:HIS:CD2	1:D:99:GLN:HG2	2.51	0.46
1:D:287:LEU:HD13	6:D:709:HOH:O	2.14	0.46
1:D:394:PHE:CZ	1:D:458:HIS:HA	2.51	0.45
1:B:125:VAL:HG12	1:B:145:LYS:HB3	1.98	0.45
1:C:93:TYR:HB3	1:C:285:PHE:CD1	2.51	0.45
1:D:108:PHE:HE2	1:D:135:THR:HG23	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:LYS:C	1:C:408:ALA:N	2.69	0.45
1:D:197:GLY:HA2	1:D:356:PHE:CE1	2.52	0.45
1:A:280:ASP:O	6:A:602:HOH:O	2.21	0.45
1:A:394:PHE:CZ	1:A:458:HIS:HA	2.52	0.45
1:B:53:GLY:HA2	1:B:271:ASN:HA	1.97	0.45
1:C:7:GLU:HG3	1:C:327:TYR:CE1	2.51	0.45
1:A:98:HIS:CD2	1:A:99:GLN:HG2	2.52	0.45
1:B:163:TRP:CD2	1:B:202:SER:HB3	2.51	0.45
1:B:333:LYS:HE2	6:B:881:HOH:O	2.17	0.44
1:B:449:PHE:CZ	1:B:457:ARG:HD2	2.51	0.44
1:C:31:GLU:O	1:C:462[B]:ARG:NH2	2.41	0.44
1:C:197:GLY:HA2	1:C:356:PHE:CZ	2.52	0.44
1:B:133[B]:ASP:OD1	1:B:134:THR:N	2.50	0.44
1:B:197:GLY:HA2	1:B:356:PHE:CE1	2.52	0.44
1:C:106:ILE:HD11	1:C:296:GLU:HG3	1.99	0.44
1:A:116:GLN:HG2	1:A:121:ALA:HB3	1.99	0.44
1:C:62:TRP:O	1:C:66:ILE:HG12	2.18	0.44
1:C:460:THR:O	1:C:460:THR:OG1	2.33	0.44
1:C:368:GLY:O	1:C:393:SER:OG	2.21	0.44
1:C:108:PHE:HE2	1:C:135:THR:HG23	1.83	0.44
1:D:210:TYR:CE1	1:D:214:LYS:HE3	2.52	0.44
1:A:360:LYS:NZ	6:A:615:HOH:O	2.43	0.44
4:D:501:YAR:O20	4:D:501:YAR:N1	2.49	0.44
1:B:394:PHE:CZ	1:B:458:HIS:HA	2.53	0.44
1:B:69:ASP:HB2	1:B:76[B]:ARG:NH1	2.33	0.43
1:B:93:TYR:HB3	1:B:285:PHE:CD1	2.53	0.43
1:B:167:PHE:CD1	1:B:209:VAL:HG21	2.52	0.43
1:C:438:LYS:HA	1:C:441:PHE:CD2	2.53	0.43
1:D:214:LYS:HD3	1:D:214:LYS:HA	1.79	0.43
1:B:360:LYS:HG3	1:B:411:GLU:HB2	2.00	0.43
1:C:22[B]:ARG:NH2	1:C:383:GLU:OE1	2.51	0.43
1:D:110:VAL:HG21	1:D:288:ALA:HA	2.00	0.43
1:D:167:PHE:CD1	1:D:209:VAL:HG21	2.53	0.43
3:A:502:YAE:N01	3:A:502:YAE:O20	2.52	0.43
1:D:157[B]:SER:HA	1:D:347:GLN:OE1	2.19	0.43
1:C:132:PHE:CG	1:C:133:ASP:N	2.87	0.43
1:B:113:LYS:HD3	6:B:826:HOH:O	2.19	0.42
1:D:438:LYS:HA	1:D:441:PHE:CD2	2.54	0.42
1:A:216:HIS:HD2	6:A:847:HOH:O	2.01	0.42
1:A:393:SER:OG	1:A:411:GLU:OE2	2.27	0.42
1:D:4[B]:ARG:NE	6:D:624[B]:HOH:O	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:GLN:HB2	1:D:390[A]:GLU:OE1	2.19	0.42
1:A:240:LYS:HE2	1:A:241:TYR:CZ	2.54	0.42
1:C:356:PHE:HE2	1:C:391:ILE:HD12	1.84	0.42
1:A:293:VAL:HG12	1:B:456:LEU:HD13	2.02	0.42
1:B:425:ASP:OD2	1:D:424:ASN:ND2	2.42	0.42
1:C:394:PHE:CE2	1:C:458:HIS:HA	2.55	0.42
1:D:97:ALA:O	1:D:274:GLY:N	2.48	0.42
1:D:391:ILE:HD13	1:D:395:LEU:HD13	2.02	0.42
1:D:163:TRP:CD2	1:D:202:SER:HB3	2.55	0.42
1:D:395:LEU:HD12	1:D:458:HIS:CD2	2.55	0.42
1:D:170:LYS:NZ	6:D:606:HOH:O	2.25	0.42
1:D:197:GLY:HA2	1:D:356:PHE:CZ	2.54	0.42
1:D:393:SER:O	1:D:457:ARG:NH2	2.49	0.42
1:A:447:LEU:HD21	6:A:794:HOH:O	2.20	0.41
1:B:447:LEU:HD23	1:B:465:PRO:HA	2.02	0.41
1:B:456:LEU:HB3	1:B:459:PHE:CD2	2.54	0.41
1:C:203:MET:HE3	1:C:241:TYR:CZ	2.55	0.41
1:A:309:MET:O	1:A:313:VAL:HG23	2.20	0.41
1:D:157[A]:SER:HA	1:D:347:GLN:OE1	2.19	0.41
1:A:197:GLY:HA2	1:A:356:PHE:CE1	2.55	0.41
1:B:255:LYS:O	1:B:279:ARG:NH2	2.52	0.41
1:A:167:PHE:CD1	1:A:209:VAL:HG21	2.55	0.41
1:B:448:GLU:HG3	1:B:466:ILE:HD13	2.02	0.41
3:A:502:YAE:O18	6:A:601:HOH:O	2.21	0.41
1:C:448:GLU:O	1:C:463:LEU:HB2	2.20	0.41
1:A:90:ASN:HB2	1:A:251:PHE:CE1	2.56	0.41
1:B:4[B]:ARG:NH2	1:B:428:ASP:OD2	2.46	0.41
1:B:210:TYR:CE1	1:B:214:LYS:HE3	2.56	0.41
1:C:224:SER:HB2	1:C:262[B]:MET:HB3	2.02	0.41
1:C:340:ARG:NH1	6:C:606:HOH:O	2.39	0.41
1:C:371:PHE:HZ	1:C:449:PHE:CE2	2.39	0.40
1:B:133[A]:ASP:OD2	1:B:395:LEU:HG	2.22	0.40
1:B:264:ALA:HB1	1:B:270:LEU:HD12	2.03	0.40
1:C:115:LYS:HG2	1:C:121:ALA:HB2	2.03	0.40
1:A:13:MET:HB2	1:A:13:MET:HE3	1.97	0.40
1:B:304:LEU:HD23	1:B:304:LEU:HA	1.95	0.40
1:B:446:GLY:C	1:B:466:ILE:HG12	2.41	0.40
1:A:15:GLU:HB2	1:C:12[A]:LYS:HD2	2.03	0.40
1:B:363:VAL:HG12	1:B:441:PHE:O	2.21	0.40
1:D:450:GLU:HB2	1:D:462:ARG:O	2.22	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	472/467 (101%)	455 (96%)	17 (4%)	0	100	100
1	B	469/467 (100%)	451 (96%)	17 (4%)	1 (0%)	47	38
1	C	472/467 (101%)	446 (94%)	24 (5%)	2 (0%)	34	22
1	D	476/467 (102%)	458 (96%)	18 (4%)	0	100	100
All	All	1889/1868 (101%)	1810 (96%)	76 (4%)	3 (0%)	47	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	406	LYS
1	C	407	HIS
1	B	45	TYR

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	393/386 (102%)	391 (100%)	2 (0%)	88	88
1	B	390/386 (101%)	387 (99%)	3 (1%)	81	80
1	C	393/386 (102%)	387 (98%)	6 (2%)	65	60
1	D	398/386 (103%)	394 (99%)	4 (1%)	76	74
All	All	1574/1544 (102%)	1559 (99%)	15 (1%)	76	74

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	PHE
1	A	416	THR
1	B	130	PHE
1	B	328	ARG
1	B	416	THR
1	C	37	PHE
1	C	328	ARG
1	C	405	GLN
1	C	416	THR
1	C	457	ARG
1	C	460	THR
1	D	130	PHE
1	D	324	TYR
1	D	328	ARG
1	D	416	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	YAE	C	502	-	25,25,25	1.31	3 (12%)	30,34,34	2.70	7 (23%)
3	YAE	A	502	-	25,25,25	1.20	2 (8%)	30,34,34	2.79	8 (26%)
4	YAR	B	501	-	23,25,25	1.34	2 (8%)	24,34,34	1.88	7 (29%)
4	YAR	D	501	-	23,25,25	1.43	2 (8%)	24,34,34	1.87	5 (20%)
5	DMS	B	502	-	3,3,3	0.65	0	3,3,3	1.02	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	YAE	C	502	-	-	2/20/20/20	0/1/1/1
4	YAR	B	501	-	-	5/17/20/20	0/1/1/1
4	YAR	D	501	-	-	1/17/20/20	0/1/1/1
3	YAE	A	502	-	-	6/20/20/20	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	501	YAR	O8-C2	5.34	1.36	1.22
4	B	501	YAR	O8-C2	4.55	1.34	1.22
3	C	502	YAE	O20-C11	-3.85	1.28	1.37
3	A	502	YAE	O20-C11	-3.49	1.28	1.37
3	C	502	YAE	C23-N01	2.88	1.50	1.46
4	B	501	YAR	O3-C2	-2.77	1.22	1.30
4	D	501	YAR	O3-C2	-2.48	1.23	1.30
3	C	502	YAE	C23-C02	2.22	1.54	1.52
3	A	502	YAE	C23-C02	2.06	1.54	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502	YAE	C23-N01-C13	8.71	129.88	117.31
3	A	502	YAE	C12-C11-C09	-8.50	114.93	120.19
3	C	502	YAE	C12-C11-C09	-7.62	115.47	120.19
3	A	502	YAE	C11-C12-C14	7.45	123.98	118.26
3	C	502	YAE	C11-C12-C14	5.98	122.85	118.26
3	A	502	YAE	C23-N01-C13	5.76	125.62	117.31
4	D	501	YAR	C16-N17-C9	-4.74	120.57	124.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	YAE	C04-C05-S06	-4.56	103.07	113.31
4	B	501	YAR	C16-N17-C9	-4.46	120.79	124.27
4	B	501	YAR	C15-C14-C12	-4.01	119.63	122.20
4	D	501	YAR	C15-C14-C12	-3.95	119.67	122.20
4	D	501	YAR	C11-C12-C14	-3.63	117.20	119.26
4	B	501	YAR	C11-C12-C14	-3.63	117.21	119.26
4	D	501	YAR	C10-C9-C11	-2.85	118.82	122.34
3	C	502	YAE	O08-C02-O03	2.73	130.29	124.09
3	A	502	YAE	O08-C02-O03	2.66	130.14	124.09
3	C	502	YAE	C14-C12-C13	-2.44	117.54	121.56
3	A	502	YAE	O20-C11-C09	2.41	122.74	117.49
3	A	502	YAE	C16-N17-C09	2.41	123.62	119.17
3	C	502	YAE	C16-N17-C09	2.39	123.59	119.17
3	C	502	YAE	C04-C05-S06	-2.34	108.06	113.31
4	B	501	YAR	O3-C2-O8	-2.32	118.30	123.61
4	B	501	YAR	C5-S6-C7	2.22	108.02	101.02
4	D	501	YAR	C11-C9-N17	2.21	121.06	118.57
3	A	502	YAE	O21-P24-O19	2.15	115.85	107.64
4	B	501	YAR	C12-C11-C9	2.08	120.23	118.36
4	B	501	YAR	O19-P24-O22	2.01	112.09	106.73

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	YAE	O03-C02-C23-C04
3	A	502	YAE	C23-C04-C05-S06
3	A	502	YAE	C02-C23-N01-C13
3	A	502	YAE	C04-C23-N01-C13
3	C	502	YAE	C23-C04-C05-S06
3	C	502	YAE	C04-C23-N01-C13
4	B	501	YAR	C14-C12-C13-N1
4	B	501	YAR	O3-C2-C23-C4
4	B	501	YAR	O8-C2-C23-C4
4	B	501	YAR	C39-C7-S6-C5
3	A	502	YAE	O08-C02-C23-C04
4	B	501	YAR	C23-C4-C5-S6
4	D	501	YAR	O3-C2-C23-N1
3	A	502	YAE	C04-C05-S06-C07

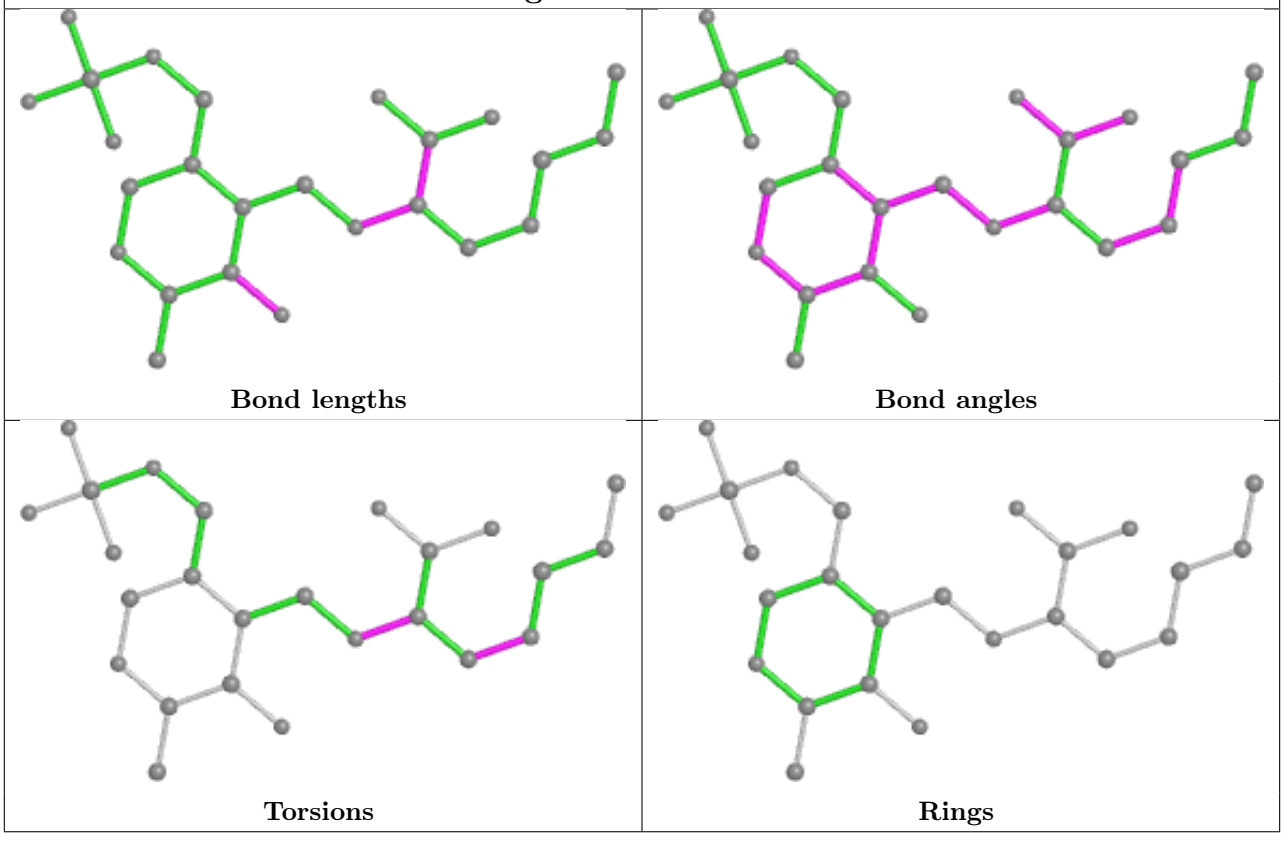
There are no ring outliers.

3 monomers are involved in 4 short contacts:

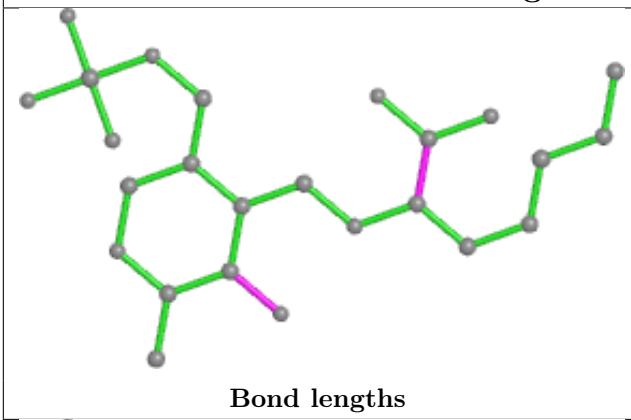
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	YAE	1	0
3	A	502	YAE	2	0
4	D	501	YAR	1	0

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

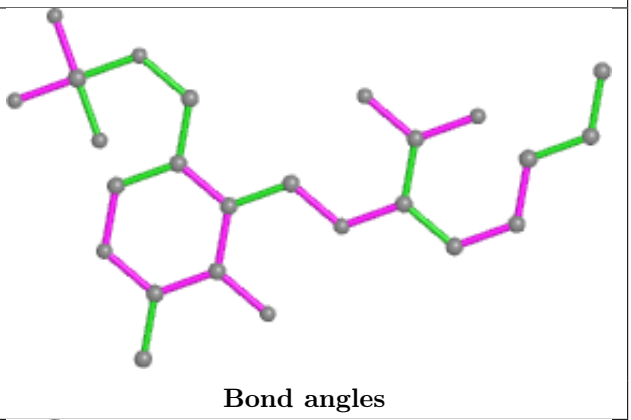
Ligand YAE C 502



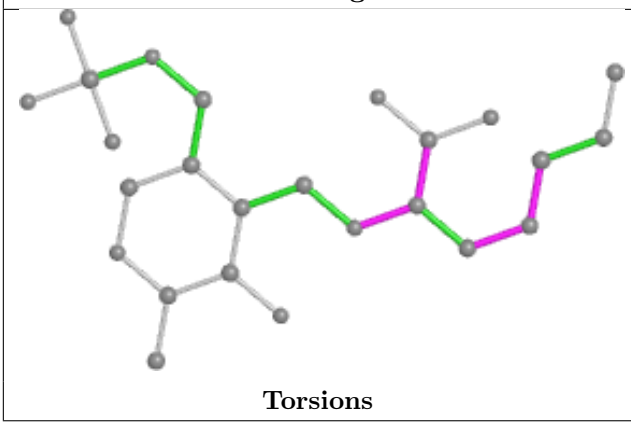
Ligand YAE A 502



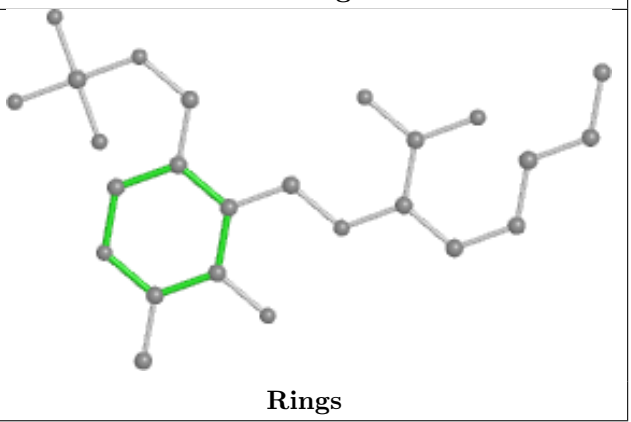
Bond lengths



Bond angles

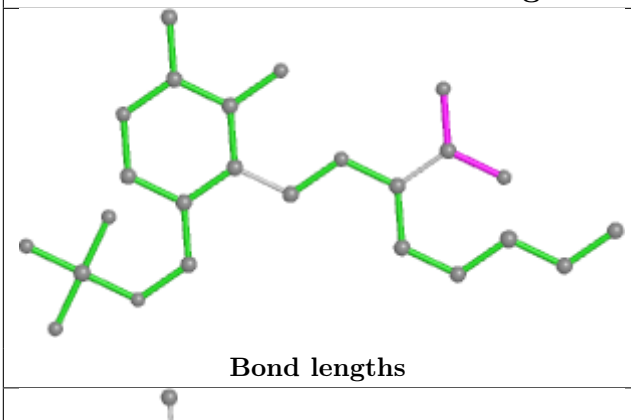


Torsions

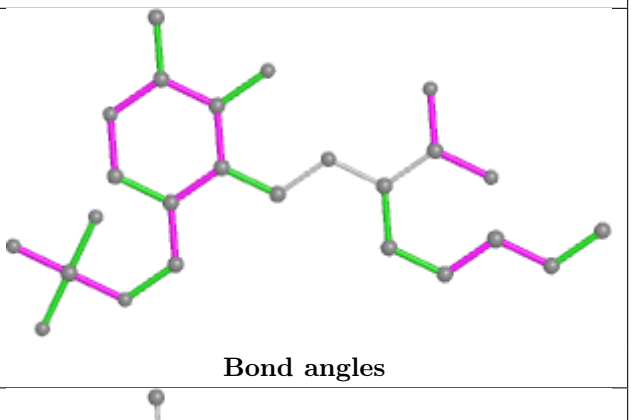


Rings

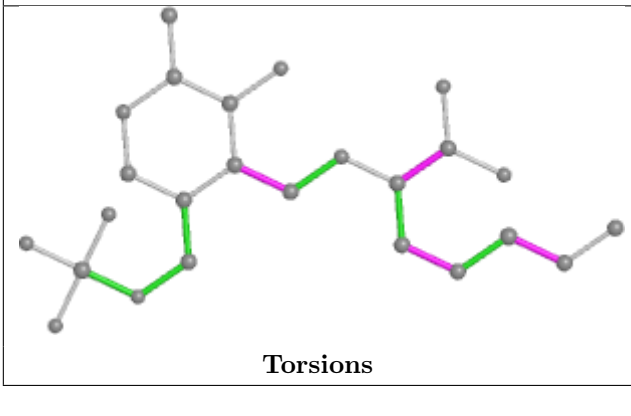
Ligand YAR B 501



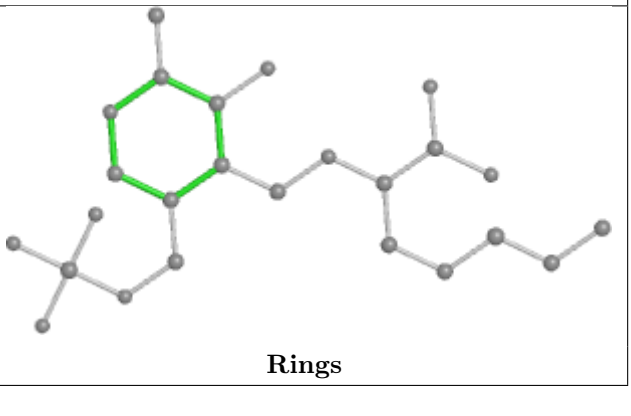
Bond lengths



Bond angles

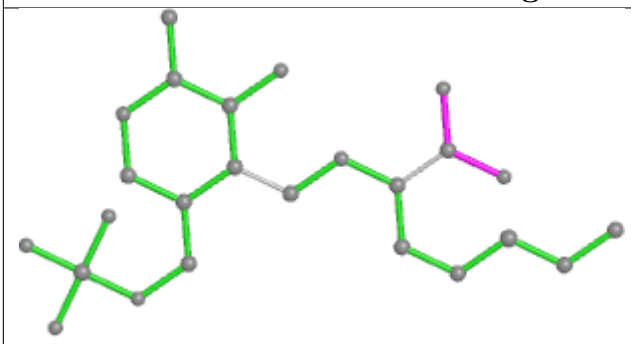


Torsions

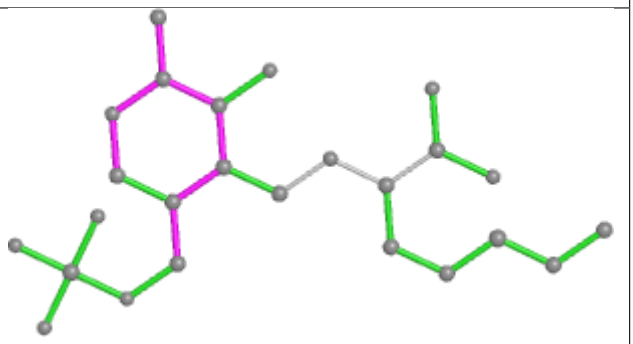


Rings

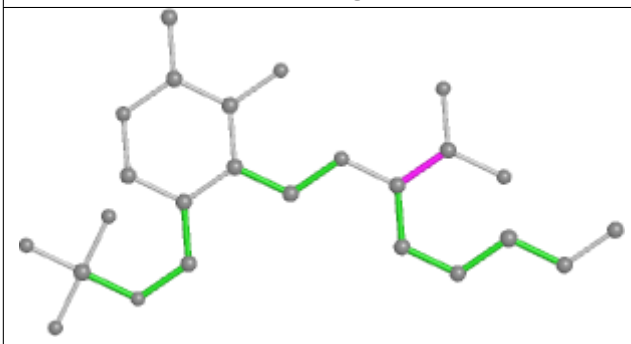
Ligand YAR D 501



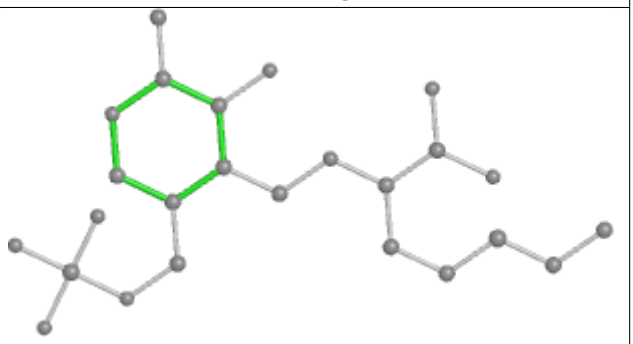
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	0.55	28 (6%)	21	30	19, 33, 71, 147	0
1	B	466/467 (99%)	0.49	31 (6%)	17	26	17, 28, 78, 155	0
1	C	465/467 (99%)	0.73	55 (11%)	4	7	17, 30, 95, 159	0
1	D	466/467 (99%)	0.42	26 (5%)	24	33	16, 29, 74, 135	0
All	All	1863/1868 (99%)	0.55	140 (7%)	14	22	16, 30, 80, 159	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	456	LEU	9.6
1	B	401	ALA	9.0
1	B	369	ASP	7.6
1	C	401	ALA	7.5
1	D	447	LEU	7.4
1	A	401	ALA	7.3
1	C	394	PHE	7.0
1	B	447	LEU	6.7
1	C	463	LEU	6.4
1	C	410	MET	6.4
1	C	442	ALA	6.3
1	C	406	LYS	6.2
1	C	449	PHE	6.0
1	D	402	THR	5.9
1	B	445	LYS	5.8
1	A	455	VAL	5.7
1	B	444	LEU	5.5
1	B	456	LEU	5.2
1	C	363	VAL	5.1
1	D	369	ASP	5.1
1	C	409	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	456	LEU	4.9
1	B	366	ILE	4.8
1	C	371	PHE	4.8
1	B	396	LEU	4.8
1	A	467	GLU	4.7
1	D	466[A]	ILE	4.7
1	C	396	LEU	4.7
1	C	451	TYR	4.5
1	B	395	LEU	4.5
1	C	454	PRO	4.5
1	C	462[A]	ARG	4.5
1	C	466	ILE	4.5
1	B	466	ILE	4.4
1	C	439	GLU	4.3
1	D	441	PHE	4.3
1	A	369	ASP	4.3
1	C	443	THR	4.3
1	A	393	SER	4.2
1	A	371	PHE	4.2
1	A	399	ASP	4.2
1	D	455	VAL	4.2
1	C	450	GLU	4.2
1	C	444	LEU	4.2
1	C	365	GLN	4.1
1	A	394	PHE	4.1
1	B	467	GLU	3.9
1	C	400	PRO	3.9
1	C	441	PHE	3.9
1	A	368	GLY	3.9
1	C	393	SER	3.8
1	C	108	PHE	3.8
1	A	396	LEU	3.8
1	A	456	LEU	3.8
1	A	360	LYS	3.7
1	C	366	ILE	3.7
1	C	360	LYS	3.7
1	C	437	LEU	3.6
1	C	34	TYR	3.5
1	D	444	LEU	3.4
1	A	410	MET	3.4
1	C	447	LEU	3.3
1	D	371	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	371	PHE	3.2
1	C	403	GLY	3.2
1	D	396	LEU	3.1
1	D	372	PRO	3.1
1	A	451	TYR	3.1
1	C	118	GLU	3.1
1	C	440	LYS	3.1
1	B	448	GLU	3.0
1	B	132[A]	PHE	3.0
1	C	411	GLU	3.0
1	A	372	PRO	3.0
1	B	442	ALA	2.9
1	D	366	ILE	2.9
1	D	463[A]	LEU	2.9
1	D	467[A]	GLU	2.8
1	A	363	VAL	2.8
1	B	411	GLU	2.8
1	C	455	VAL	2.8
1	C	460	THR	2.8
1	D	464[A]	LYS	2.8
1	B	360	LYS	2.7
1	D	34	TYR	2.7
1	C	397	GLY	2.7
1	D	400	PRO	2.7
1	B	455	VAL	2.7
1	B	399	ASP	2.7
1	A	405	GLN	2.6
1	B	133[A]	ASP	2.6
1	B	441	PHE	2.6
1	B	367	PRO	2.5
1	A	133[A]	ASP	2.5
1	B	397	GLY	2.5
1	C	398	ARG	2.5
1	A	400	PRO	2.5
1	C	458	HIS	2.5
1	B	463	LEU	2.5
1	C	465	PRO	2.4
1	A	395	LEU	2.4
1	B	242	LYS	2.4
1	A	62	TRP	2.4
1	A	155	PHE	2.4
1	C	362	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	29	LEU	2.4
1	C	459	PHE	2.4
1	C	33	GLY	2.4
1	D	141[A]	LEU	2.4
1	C	407	HIS	2.4
1	B	409	ASP	2.3
1	C	372	PRO	2.3
1	C	457	ARG	2.3
1	B	108	PHE	2.3
1	C	26	GLU	2.2
1	C	284[A]	ILE	2.2
1	C	446	GLY	2.2
1	A	391	ILE	2.2
1	C	405	GLN	2.2
1	A	466	ILE	2.2
1	A	284	ILE	2.2
1	B	372	PRO	2.2
1	D	410	MET	2.2
1	A	398	ARG	2.2
1	A	383[A]	GLU	2.1
1	D	30	LYS	2.1
1	D	460	THR	2.1
1	D	465[A]	PRO	2.1
1	B	368	GLY	2.1
1	A	441	PHE	2.1
1	B	443	THR	2.1
1	C	117	LYS	2.1
1	C	461	ALA	2.1
1	D	284	ILE	2.1
1	B	451	TYR	2.1
1	D	394	PHE	2.1
1	D	459	PHE	2.1
1	D	458	HIS	2.1
1	C	36	PRO	2.1
1	C	376	VAL	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 (i)

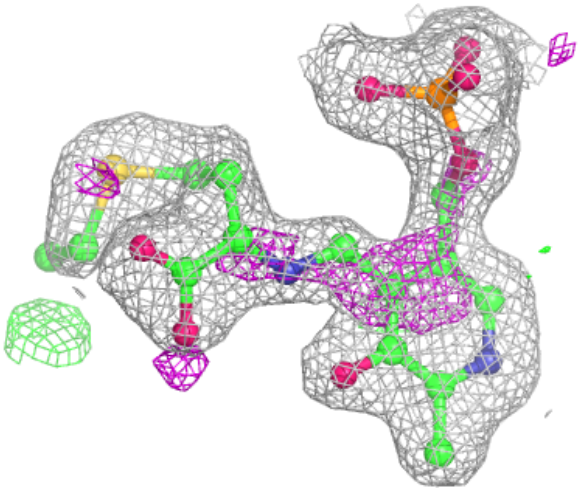
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

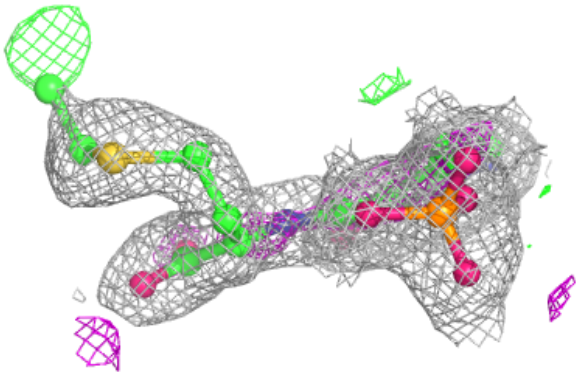
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	B	502	4/4	0.90	0.51	37,44,49,62	0
4	YAR	B	501	25/25	0.95	0.17	18,32,41,56	0
3	YAE	A	502	25/25	0.96	0.17	20,33,43,55	0
4	YAR	D	501	25/25	0.97	0.14	16,29,36,48	0
3	YAE	C	502	25/25	0.98	0.12	22,31,44,63	0
2	K	C	501	1/1	0.98	0.07	28,28,28,28	0
2	K	C	503	1/1	0.99	0.06	25,25,25,25	0
2	K	A	503	1/1	0.99	0.07	27,27,27,27	0
2	K	A	501	1/1	0.99	0.06	25,25,25,25	0

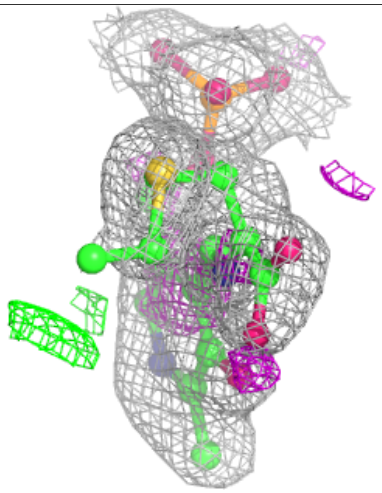
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around YAR 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)

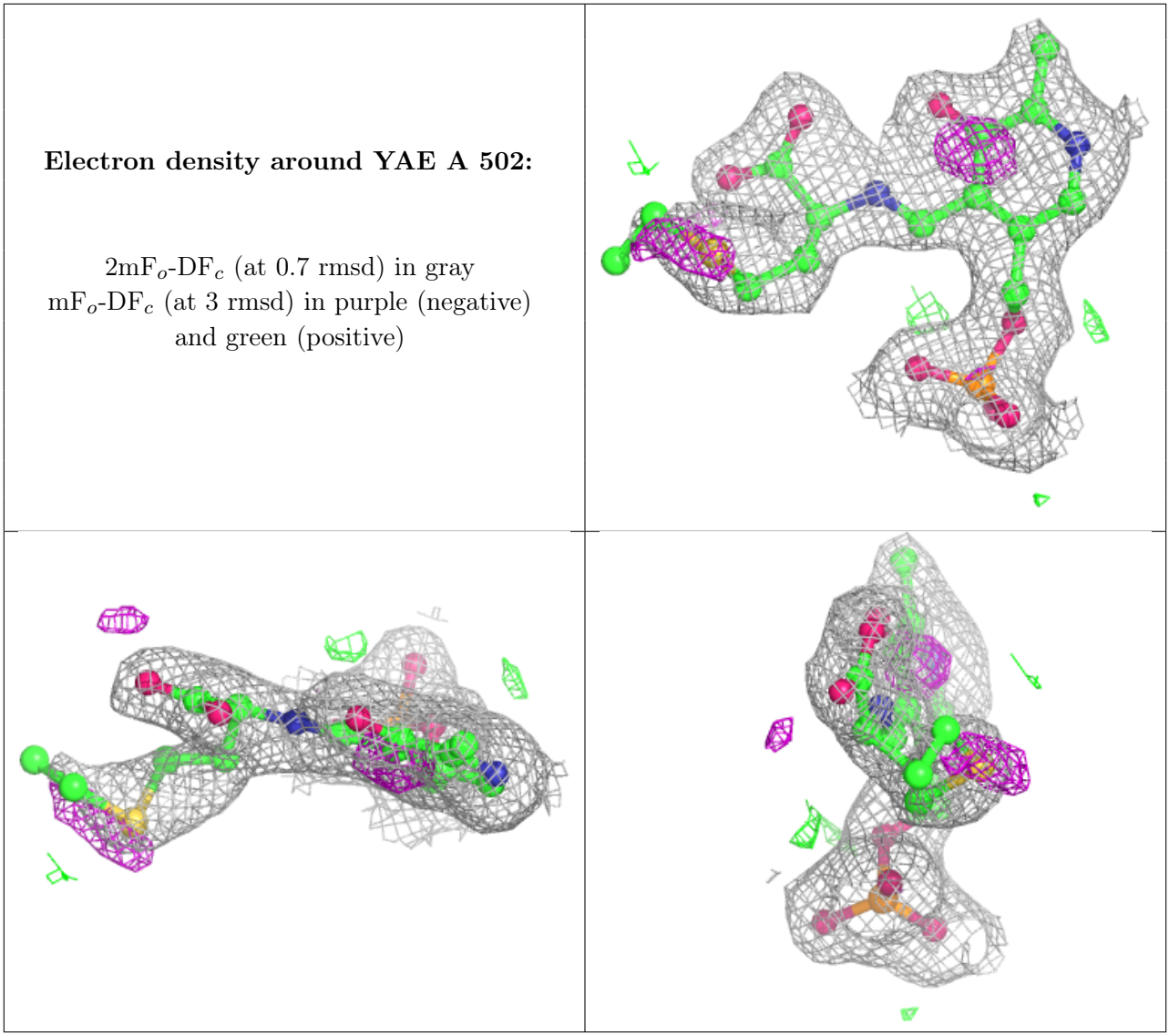






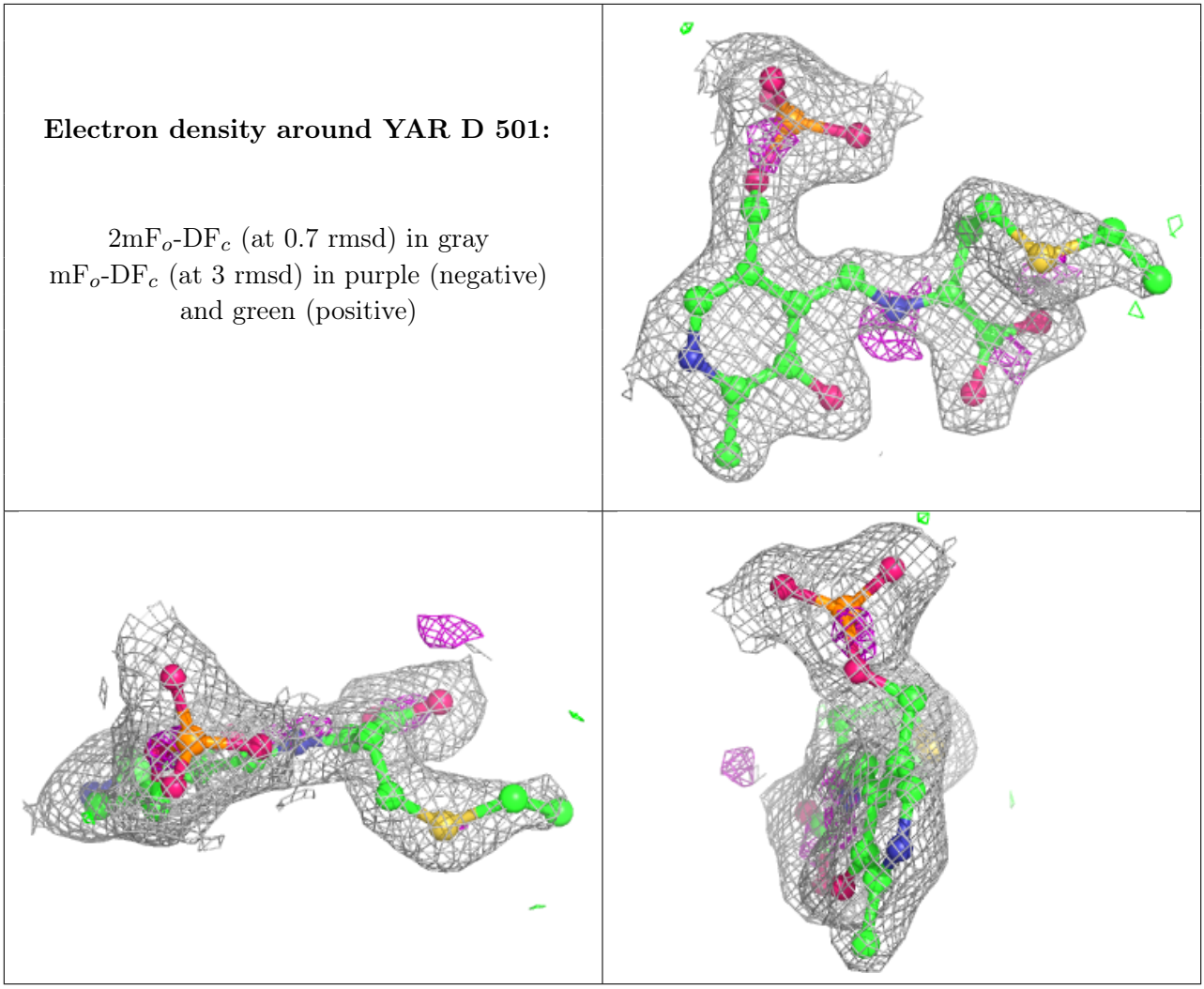
Electron density around YAE A 502:

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



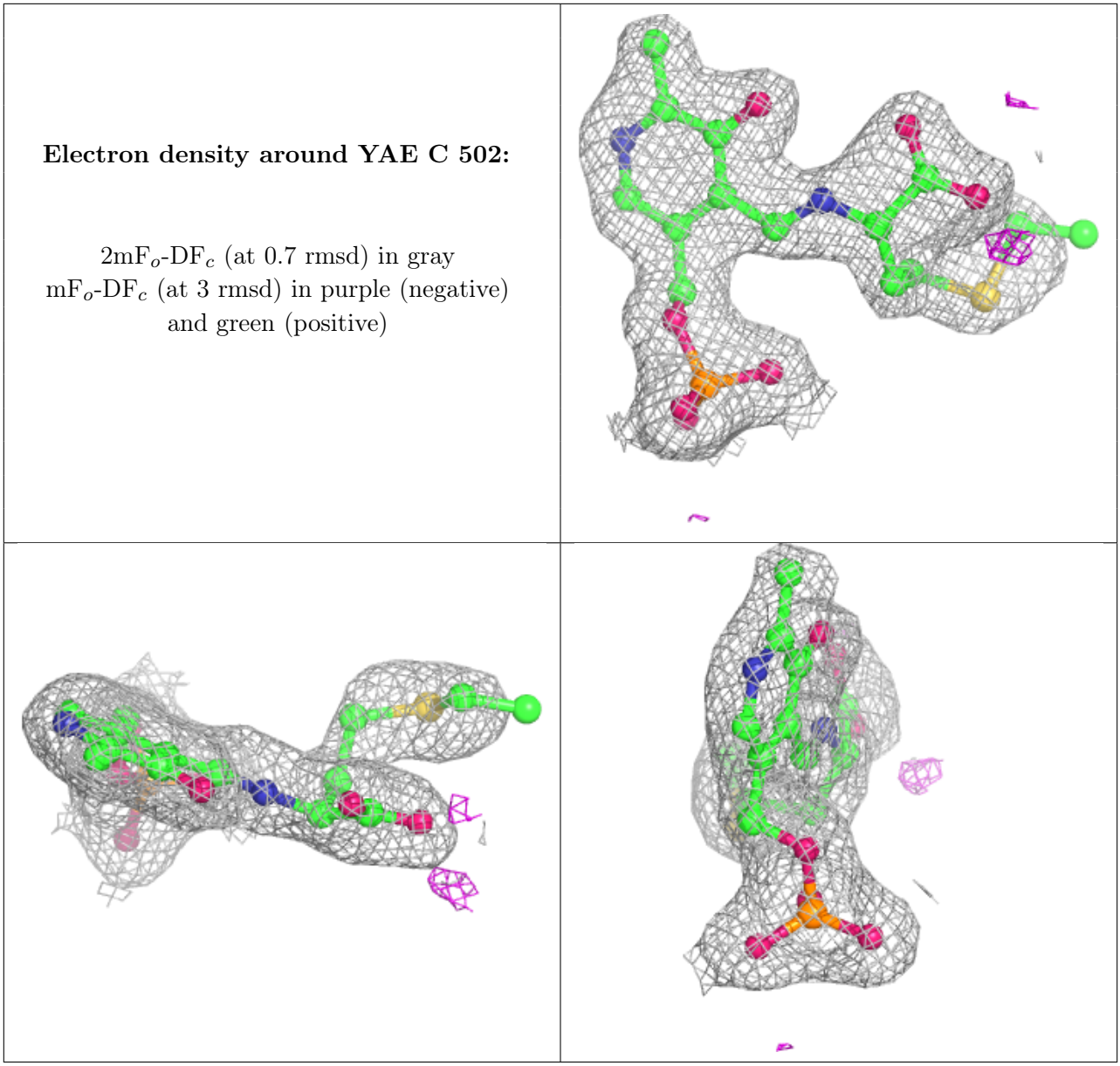
Electron density around YAR D 501:

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



Electron density around YAE 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)



6.5 Other polymers (i)

There are no such residues in this entry.