



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 10, 2025 – 04:14 PM EDT

PDB ID : 9DY7 / pdb_00009dy7
Title : Proteus vulgaris tryptophan indole-lyase complexed with L-ethionine and Na⁺
Authors : Phillips, R.S.
Deposited on : 2024-10-13
Resolution : 1.87 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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

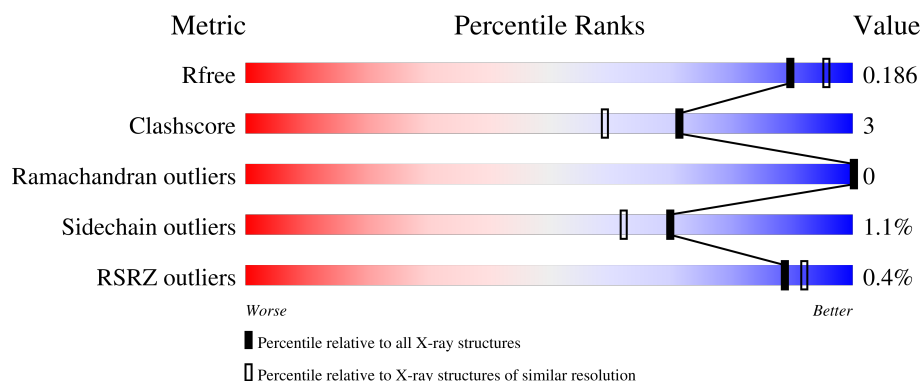
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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}	164625	1090 (1.88-1.88)
Clashscore	180529	1144 (1.88-1.88)
Ramachandran outliers	177936	1135 (1.88-1.88)
Sidechain outliers	177891	1135 (1.88-1.88)
RSRZ outliers	164620	1090 (1.88-1.88)

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	466	<div><div></div><div>92%</div><div>8%</div></div>
1	C	466	<div><div></div><div>90%</div><div>10%</div></div>
2	B	466	<div><div></div><div>87%</div><div>13%</div></div>
2	D	466	<div><div></div><div>90%</div><div>10%</div></div>

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 16300 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.

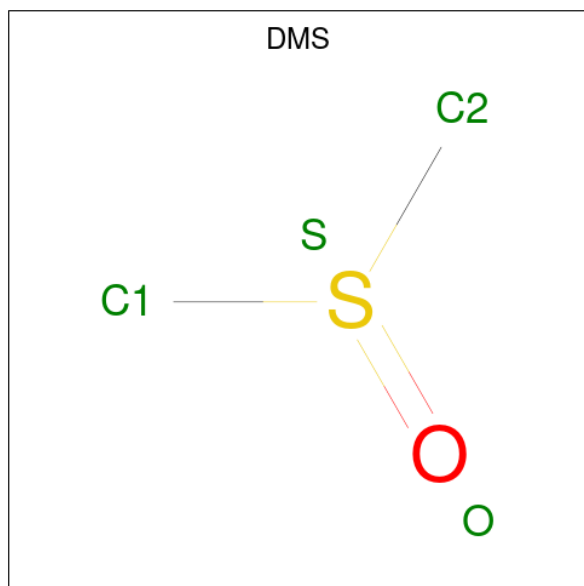
- Molecule 1 is a protein called Tryptophanase (with internal aldimine).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	P	S	0	10	0
			3773	2411	641	700	1	20			
1	C	466	Total	C	N	O	P	S	0	8	0
			3759	2402	638	700	1	18			

- Molecule 2 is a protein called Tryptophanase.

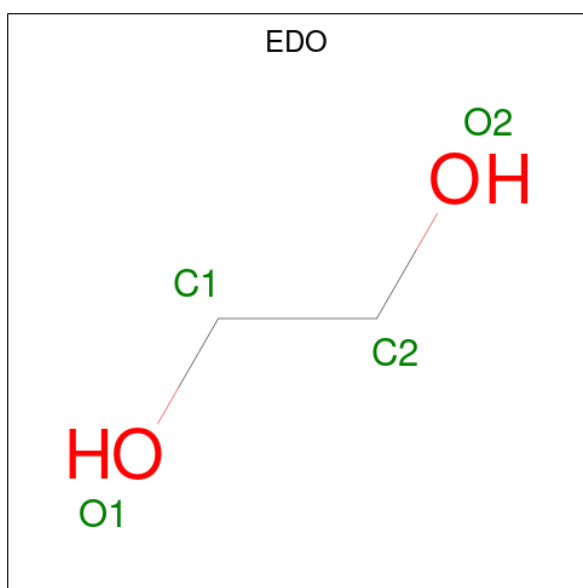
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	466	Total	C	N	O	S	0	5	0
			3731	2386	635	692	18			
2	D	466	Total	C	N	O	S	0	5	0
			3725	2380	636	691	18			

- Molecule 3 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



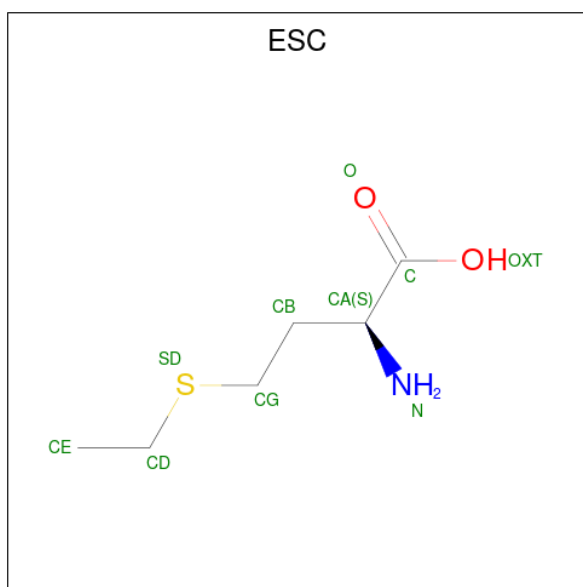
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O S 4 2 1 1	0	0
3	A	1	Total C O S 4 2 1 1	0	0
3	C	1	Total C O S 4 2 1 1	0	0
3	C	1	Total C O S 4 2 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is 2-AMINO-4-ETHYL SULFANYL BUTYRIC ACID (CCD ID: ESC) (formula: C₆H₁₃NO₂S).

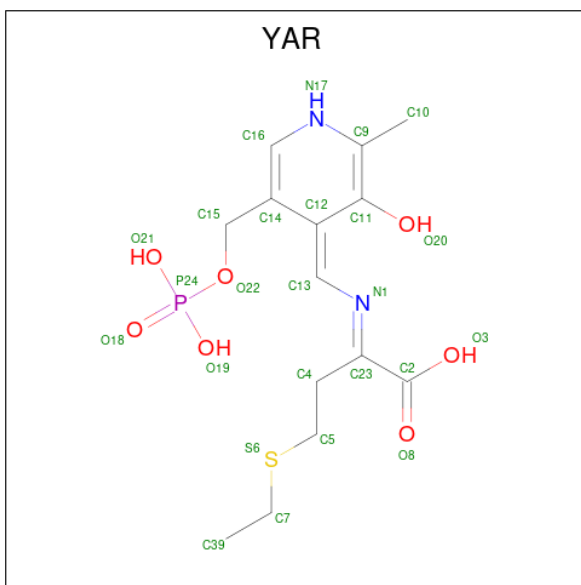


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			10	6	1	2	1		
5	C	1	Total	C	N	O	S	0	0
			10	6	1	2	1		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

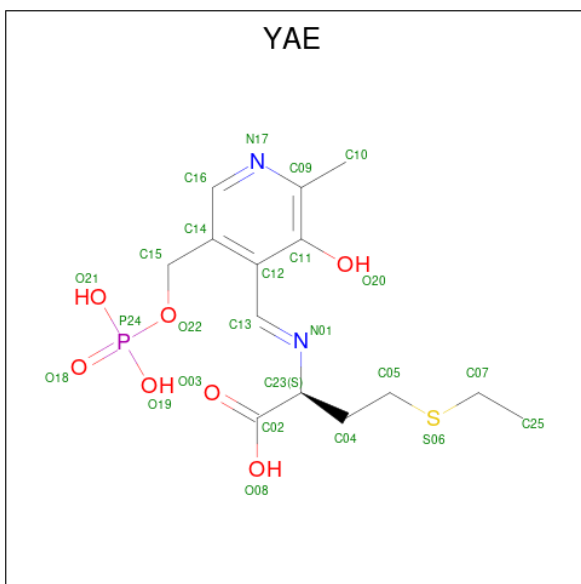
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Na	0	2
			4	4		
6	D	2	Total	Na	0	2
			4	4		

- Molecule 7 is (2E)-4-(ethylsulfanyl)-2-{[(Z)-{3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4(1H)-ylidene}methyl]imino}butanoic acid (CCD ID: YAR) (formula: C₁₄H₂₁N₂O₇PS).



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

- Molecule 8 is (E)-S-ethyl-N-({3-hydroxy-2-methyl-5-[(phosphonomethoxy)methyl]pyridin-4-yl}methylidene)-L-homocysteine (CCD ID: YAE) (formula: C₁₄H₂₁N₂O₇PS).



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

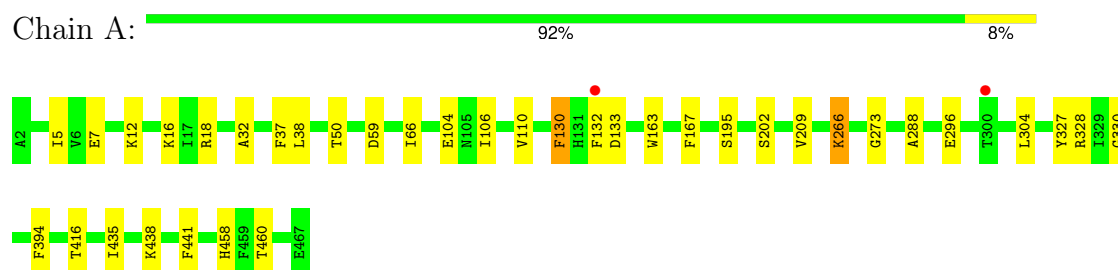
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	340	Total 340	O 340	0	10
9	B	248	Total 248	O 248	0	6
9	C	362	Total 362	O 362	0	8
9	D	260	Total 260	O 260	0	6

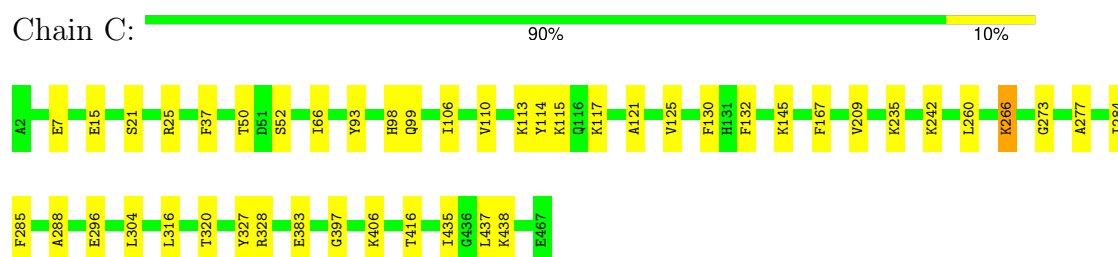
3 Residue-property plots

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.

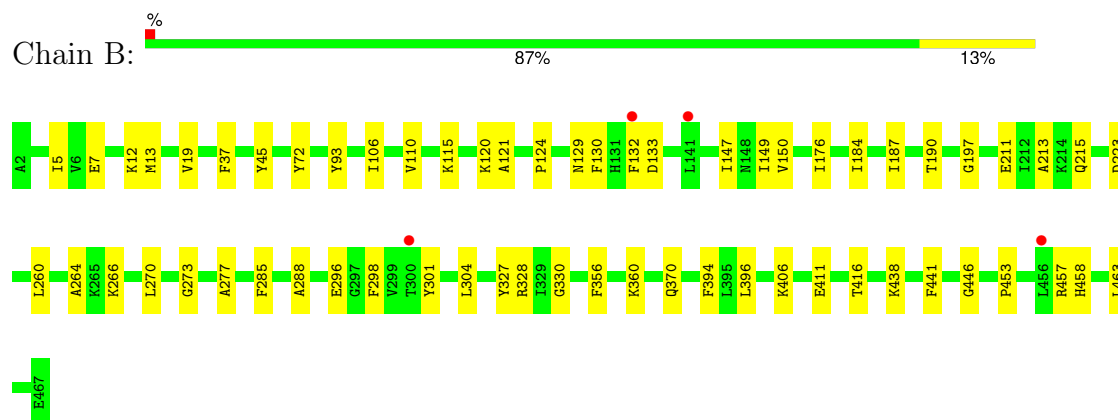
- Molecule 1: Tryptophanase (with internal aldimine)



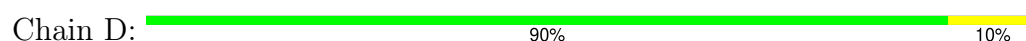
- Molecule 1: Tryptophanase (with internal aldimine)

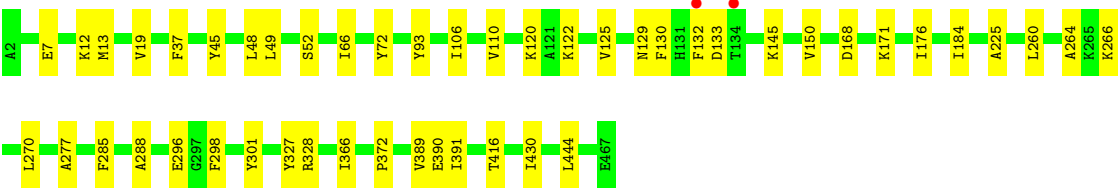


- Molecule 2: Tryptophanase



- Molecule 2: Tryptophanase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.33Å 113.68Å 149.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.16 – 1.87 52.16 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.9 (52.16-1.87) 99.9 (52.16-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.87Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.156 , 0.185 0.157 , 0.186	Depositor DCC
R_{free} test set	154588 reflections (1.27%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16300	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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: LLP, ESC, DMS, YAR, YAE, NA, EDO

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	0.36	0/3852	0.58	1/5194 (0.0%)
1	C	0.35	0/3835	0.57	0/5176
2	B	0.31	0/3824	0.53	0/5161
2	D	0.32	0/3820	0.54	0/5156
All	All	0.34	0/15331	0.56	1/20687 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ASP	CB-CG-OD1	5.96	123.67	118.30

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	3773	0	3765	20	0
1	C	3759	0	3741	22	0
2	B	3731	0	3719	32	0
2	D	3725	0	3718	26	0
3	A	8	0	12	0	0
3	C	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	8	0	12	0	0
5	A	10	0	12	0	0
5	C	10	0	13	2	0
6	B	4	0	0	0	0
6	D	4	0	0	0	0
7	B	25	0	0	1	0
8	D	25	0	0	0	0
9	A	340	0	0	0	0
9	B	248	0	0	0	0
9	C	362	0	0	0	0
9	D	260	0	0	0	0
All	All	16300	0	15004	95	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 3.

All (95) 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:383:GLU:HG3	1:C:437:LEU:HD21	1.63	0.79
1:C:273:GLY:HA2	1:C:304:LEU:HD21	1.79	0.64
2:B:110:VAL:HG21	2:B:288:ALA:HA	1.80	0.63
2:B:453:PRO:HG2	2:B:457:ARG:HA	1.81	0.62
2:D:225:ALA:HB1	2:D:266:LYS:HG3	1.83	0.60
2:B:273:GLY:HA2	2:B:304:LEU:HD21	1.83	0.59
1:A:273:GLY:HA2	1:A:304:LEU:HD21	1.84	0.58
2:B:7:GLU:HG3	2:B:327[A]:TYR:CZ	2.40	0.57
1:C:113:LYS:HE3	1:C:117:LYS:HG3	1.85	0.56
1:C:110:VAL:HG21	1:C:288:ALA:HA	1.87	0.56
1:A:110:VAL:HG21	1:A:288:ALA:HA	1.87	0.55
1:A:106:ILE:HD11	1:A:296:GLU:HG3	1.88	0.55
2:D:7:GLU:HG3	2:D:327[A]:TYR:CZ	2.41	0.55
1:C:132:PHE:HZ	5:C:503:ESC:HB2	1.72	0.54
1:A:7:GLU:HG3	1:A:327[A]:TYR:CZ	2.44	0.53
2:D:93:TYR:HB3	2:D:285:PHE:CD1	2.43	0.53
2:D:120:LYS:HD3	2:D:122:LYS:HE2	1.89	0.53
1:A:163:TRP:CD2	1:A:202:SER:HB3	2.46	0.51
1:C:98:HIS:CD2	1:C:99:GLN:HG2	2.45	0.51
2:D:52:SER:HB2	2:D:266:LYS:HE3	1.93	0.51
2:B:298:PHE:HB3	2:B:301:TYR:CE2	2.46	0.51
1:C:7:GLU:HG3	1:C:327[A]:TYR:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:TYR:HB3	2:B:285:PHE:CD1	2.47	0.50
2:D:366:ILE:HB	2:D:372:PRO:HB3	1.93	0.50
1:A:5:ILE:HD12	1:A:330:GLY:HA3	1.94	0.50
2:B:12:LYS:HB3	2:D:13:MET:HE3	1.95	0.49
2:B:197:GLY:HA2	2:B:356:PHE:CE1	2.47	0.49
1:A:104:GLU:OE2	1:A:266:LLP:H6	2.13	0.49
2:D:19:VAL:HG22	2:D:45:TYR:CG	2.47	0.49
2:D:110:VAL:HG21	2:D:288:ALA:HA	1.93	0.49
2:B:301:TYR:O	2:B:304:LEU:HB2	2.13	0.49
1:A:132:PHE:HB2	1:A:266:LLP:H2'3	1.94	0.49
2:D:120:LYS:HB3	2:D:122:LYS:HG2	1.95	0.48
1:A:130:PHE:CG	1:A:195:SER:HB2	2.47	0.48
2:B:13:MET:HE3	2:D:12:LYS:HD3	1.95	0.48
1:C:114:TYR:CG	1:C:284[A]:ILE:HD11	2.49	0.47
1:C:93:TYR:HB3	1:C:285:PHE:CD1	2.49	0.47
1:A:438:LYS:HA	1:A:441:PHE:CD2	2.50	0.47
1:A:16:LYS:HE2	1:A:18:ARG:HD3	1.97	0.47
2:D:168:ASP:HB3	2:D:171:LYS:HB2	1.97	0.47
1:A:435:ILE:HG23	1:A:438:LYS:HE2	1.96	0.46
1:C:435:ILE:O	1:C:438:LYS:HG3	2.15	0.46
2:B:5:ILE:HD12	2:B:330:GLY:HA3	1.96	0.46
1:C:260:LEU:HG	1:C:277:ALA:HB3	1.97	0.46
2:B:147:ILE:HG22	2:B:149:ILE:HG23	1.97	0.46
2:B:176:ILE:HA	2:B:184:ILE:HD11	1.97	0.46
2:D:49:LEU:HD12	2:D:389:VAL:HB	1.98	0.46
1:A:167:PHE:CD1	1:A:209:VAL:HG21	2.52	0.45
2:B:438:LYS:HA	2:B:441:PHE:CD2	2.51	0.45
2:B:370:GLN:HB3	2:B:446:GLY:HA3	1.97	0.45
1:C:316:LEU:O	1:C:320:THR:HG23	2.17	0.45
2:B:121:ALA:HB1	2:B:124:PRO:HB3	1.98	0.45
2:B:260:LEU:HG	2:B:277:ALA:HB3	1.98	0.44
2:B:264:ALA:HB1	2:B:270:LEU:HD12	1.99	0.44
2:B:394:PHE:CE2	2:B:458:HIS:HA	2.53	0.44
2:D:106:ILE:HD11	2:D:296:GLU:HG3	1.97	0.44
2:D:132:PHE:CG	2:D:133:ASP:N	2.85	0.44
2:B:129:ASN:O	2:B:150:VAL:HB	2.18	0.43
1:A:32:ALA:HB1	1:A:38:LEU:HB2	2.00	0.43
2:B:187:ILE:HD12	2:B:213:ALA:HB2	2.00	0.43
2:B:396:LEU:HG	2:B:406[A]:LYS:HD3	2.00	0.43
1:C:106:ILE:HD11	1:C:296:GLU:HG3	2.01	0.43
2:D:176:ILE:HA	2:D:184:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:260:LEU:HG	2:D:277:ALA:HB3	2.00	0.43
1:A:132:PHE:CG	1:A:133:ASP:N	2.87	0.43
2:B:106:ILE:HD11	2:B:296:GLU:HG3	2.01	0.43
2:B:132:PHE:CG	2:B:133:ASP:N	2.87	0.43
1:A:12:LYS:HD2	1:C:15:GLU:HB2	2.00	0.43
1:A:38:LEU:HD21	1:A:460:THR:HA	1.99	0.43
2:D:125:VAL:HG12	2:D:145:LYS:HB2	2.00	0.43
1:A:66:ILE:CD1	2:D:66:ILE:HG13	2.49	0.43
2:B:115:LYS:O	2:B:120:LYS:HB2	2.18	0.43
1:A:394:PHE:CZ	1:A:458:HIS:HA	2.54	0.42
1:C:235:LYS:O	1:C:242:LYS:HG2	2.19	0.42
2:B:360:LYS:HG3	2:B:411:GLU:HG3	2.00	0.42
1:C:99:GLN:HB2	1:C:266:LLP:OP3	2.20	0.42
1:C:21:SER:O	1:C:25:ARG:HG3	2.19	0.42
1:C:115:LYS:HG2	1:C:121:ALA:HB2	2.02	0.42
2:B:266:LYS:HZ1	7:B:503[B]:YAR:C13	2.32	0.42
1:A:50:THR:HG21	2:B:72[A]:TYR:CD1	2.54	0.42
2:D:129:ASN:O	2:D:150:VAL:HB	2.19	0.42
2:D:264:ALA:HB1	2:D:270:LEU:HD12	2.02	0.42
2:D:390:GLU:O	2:D:391:ILE:HD13	2.20	0.42
2:B:19:VAL:HG22	2:B:45:TYR:CG	2.55	0.41
1:C:125:VAL:HG12	1:C:145[A]:LYS:HB3	2.03	0.41
1:C:50:THR:HG23	1:C:52:SER:H	1.85	0.41
5:C:503:ESC:HCA1	2:D:72:TYR:OH	2.21	0.41
2:B:190:THR:HA	2:B:223:ASP:HB3	2.03	0.41
2:B:394:PHE:CE1	2:B:463:LEU:HD21	2.54	0.41
1:C:397:GLY:O	1:C:406:LYS:HB2	2.21	0.41
2:D:48:LEU:HD11	2:D:430:ILE:HD13	2.02	0.41
2:D:444:LEU:HD23	2:D:444:LEU:HA	1.85	0.40
2:B:211:GLU:O	2:B:215:GLN:HG2	2.22	0.40
1:C:167:PHE:CD1	1:C:209:VAL:HG21	2.56	0.40
2:D:298:PHE:HB3	2:D:301:TYR:CE2	2.57	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	473/466 (102%)	456 (96%)	17 (4%)	0	100	100
1	C	471/466 (101%)	455 (97%)	16 (3%)	0	100	100
2	B	469/466 (101%)	453 (97%)	16 (3%)	0	100	100
2	D	469/466 (101%)	450 (96%)	19 (4%)	0	100	100
All	All	1882/1864 (101%)	1814 (96%)	68 (4%)	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	394/384 (103%)	390 (99%)	4 (1%)	73	65
1	C	392/384 (102%)	387 (99%)	5 (1%)	65	55
2	B	390/385 (101%)	386 (99%)	4 (1%)	73	65
2	D	390/385 (101%)	386 (99%)	4 (1%)	73	65
All	All	1566/1538 (102%)	1549 (99%)	17 (1%)	70	62

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

Mol	Chain	Res	Type
1	A	37	PHE
1	A	130	PHE
1	A	328	ARG
1	A	416	THR
2	B	37	PHE
2	B	130	PHE
2	B	328	ARG
2	B	416	THR

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Mol	Chain	Res	Type
1	C	37	PHE
1	C	66	ILE
1	C	130	PHE
1	C	328	ARG
1	C	416	THR
2	D	37	PHE
2	D	130	PHE
2	D	328	ARG
2	D	416	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	216	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	LLP	A	266	1	23,24,25	1.13	1 (4%)	25,32,34	1.58	7 (28%)
1	LLP	C	266	1	23,24,25	1.09	1 (4%)	25,32,34	1.46	5 (20%)

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
1	LLP	A	266	1	-	5/16/17/19	0/1/1/1
1	LLP	C	266	1	-	4/16/17/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	LLP	P-OP4	4.07	1.73	1.60
1	C	266	LLP	P-OP4	3.98	1.72	1.60

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	LLP	OP2-P-OP4	-3.26	98.17	106.67
1	C	266	LLP	OP4-P-OP1	-2.72	99.08	106.44
1	A	266	LLP	C4-C4'-NZ	-2.48	112.60	124.04
1	C	266	LLP	C4-C4'-NZ	-2.45	112.76	124.04
1	A	266	LLP	C2'-C2-C3	-2.31	118.10	120.80
1	A	266	LLP	CE-NZ-C4'	2.30	126.10	118.72
1	C	266	LLP	OP3-P-OP2	2.30	116.44	107.80
1	A	266	LLP	OP3-P-OP2	2.14	115.82	107.80
1	C	266	LLP	CE-NZ-C4'	2.09	125.40	118.72
1	C	266	LLP	OP3-P-OP4	-2.08	101.25	106.67
1	A	266	LLP	C2'-C2-N1	2.07	121.55	117.64
1	A	266	LLP	OP4-P-OP1	-2.05	100.89	106.44

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	266	LLP	O-C-CA-CB
1	A	266	LLP	CG-CD-CE-NZ
1	C	266	LLP	O-C-CA-CB
1	C	266	LLP	CG-CD-CE-NZ
1	C	266	LLP	C3-C4-C4'-NZ
1	A	266	LLP	C6-C5-C5'-OP4
1	A	266	LLP	C3-C4-C4'-NZ
1	A	266	LLP	C5-C4-C4'-NZ
1	C	266	LLP	C5-C4-C4'-NZ

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	266	LLP	2	0
1	C	266	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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
8	YAE	D	503	-	25,25,25	1.57	4 (16%)	31,34,34	1.51	6 (19%)
4	EDO	A	502	-	3,3,3	0.19	0	2,2,2	0.36	0
7	YAR	B	503[B]	-	23,25,25	1.83	6 (26%)	26,34,34	3.24	9 (34%)
5	ESC	A	505	-	8,9,9	0.89	0	6,10,10	1.96	2 (33%)
5	ESC	C	503	-	8,9,9	0.91	0	6,10,10	1.99	2 (33%)
3	DMS	A	504	-	3,3,3	0.60	0	3,3,3	0.09	0
3	DMS	C	501	-	3,3,3	0.59	0	3,3,3	0.07	0
3	DMS	C	502	-	3,3,3	0.61	0	3,3,3	0.15	0
4	EDO	A	503	-	3,3,3	0.23	0	2,2,2	0.37	0
3	DMS	A	501	-	3,3,3	0.61	0	3,3,3	0.17	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
8	YAE	D	503	-	-	9/20/20/20	0/1/1/1
4	EDO	A	502	-	-	1/1/1/1	-
7	YAR	B	503[B]	-	-	3/18/20/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ESC	A	505	-	-	3/9/9/9	-
5	ESC	C	503	-	-	1/9/9/9	-
4	EDO	A	503	-	-	1/1/1/1	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	503[B]	YAR	C9-N17	5.01	1.39	1.34
8	D	503	YAE	C12-C14	-4.08	1.36	1.42
8	D	503	YAE	C12-C13	3.35	1.53	1.46
8	D	503	YAE	C12-C11	-2.87	1.36	1.41
7	B	503[B]	YAR	P24-O18	-2.74	1.41	1.50
7	B	503[B]	YAR	O3-C2	2.51	1.37	1.30
7	B	503[B]	YAR	C11-C9	-2.29	1.34	1.37
8	D	503	YAE	C11-C09	-2.20	1.38	1.41
7	B	503[B]	YAR	C15-C14	2.16	1.53	1.50
7	B	503[B]	YAR	C10-C9	2.05	1.53	1.49

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	503[B]	YAR	C11-C12-C14	-11.15	113.39	119.28
7	B	503[B]	YAR	C15-C14-C12	-6.85	117.60	122.19
7	B	503[B]	YAR	C16-N17-C9	-4.46	120.50	124.20
8	D	503	YAE	C23-N01-C13	3.99	122.70	116.77
7	B	503[B]	YAR	O22-P24-O18	3.98	117.20	106.44
7	B	503[B]	YAR	C12-C11-C9	3.83	121.70	118.34
7	B	503[B]	YAR	C16-C14-C12	3.74	121.91	119.00
5	A	505	ESC	OXT-C-O	-3.72	115.65	124.08
8	D	503	YAE	C04-C23-C02	3.39	115.12	109.48
5	C	503	ESC	OXT-C-O	-3.22	116.77	124.08
5	C	503	ESC	CB-CG-SD	-3.02	106.71	113.45
8	D	503	YAE	C05-S06-C07	3.00	110.36	101.05
7	B	503[B]	YAR	O20-C11-C9	2.61	120.81	118.40
8	D	503	YAE	C04-C05-S06	-2.49	107.90	113.45
7	B	503[B]	YAR	O19-P24-O22	-2.42	100.36	106.67
5	A	505	ESC	CB-CG-SD	-2.41	108.07	113.45
8	D	503	YAE	C14-C16-N17	-2.40	119.93	123.83
8	D	503	YAE	O08-C02-O03	-2.31	118.85	124.08
7	B	503[B]	YAR	O21-P24-O22	-2.12	101.14	106.67

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	503[B]	YAR	C23-C4-C5-S6
7	B	503[B]	YAR	O3-C2-C23-C4
8	D	503	YAE	C05-C04-C23-C02
8	D	503	YAE	C05-C04-C23-N01
8	D	503	YAE	C02-C23-N01-C13
8	D	503	YAE	C04-C23-N01-C13
5	C	503	ESC	CA-CB-CG-SD
8	D	503	YAE	C23-C04-C05-S06
7	B	503[B]	YAR	C39-C7-S6-C5
8	D	503	YAE	C12-C14-C15-O22
5	A	505	ESC	CB-CG-SD-CD
5	A	505	ESC	OXT-C-CA-CB
5	A	505	ESC	O-C-CA-CB
8	D	503	YAE	C04-C05-S06-C07
4	A	503	EDO	O1-C1-C2-O2
8	D	503	YAE	O03-C02-C23-C04
8	D	503	YAE	O08-C02-C23-C04
4	A	502	EDO	O1-C1-C2-O2

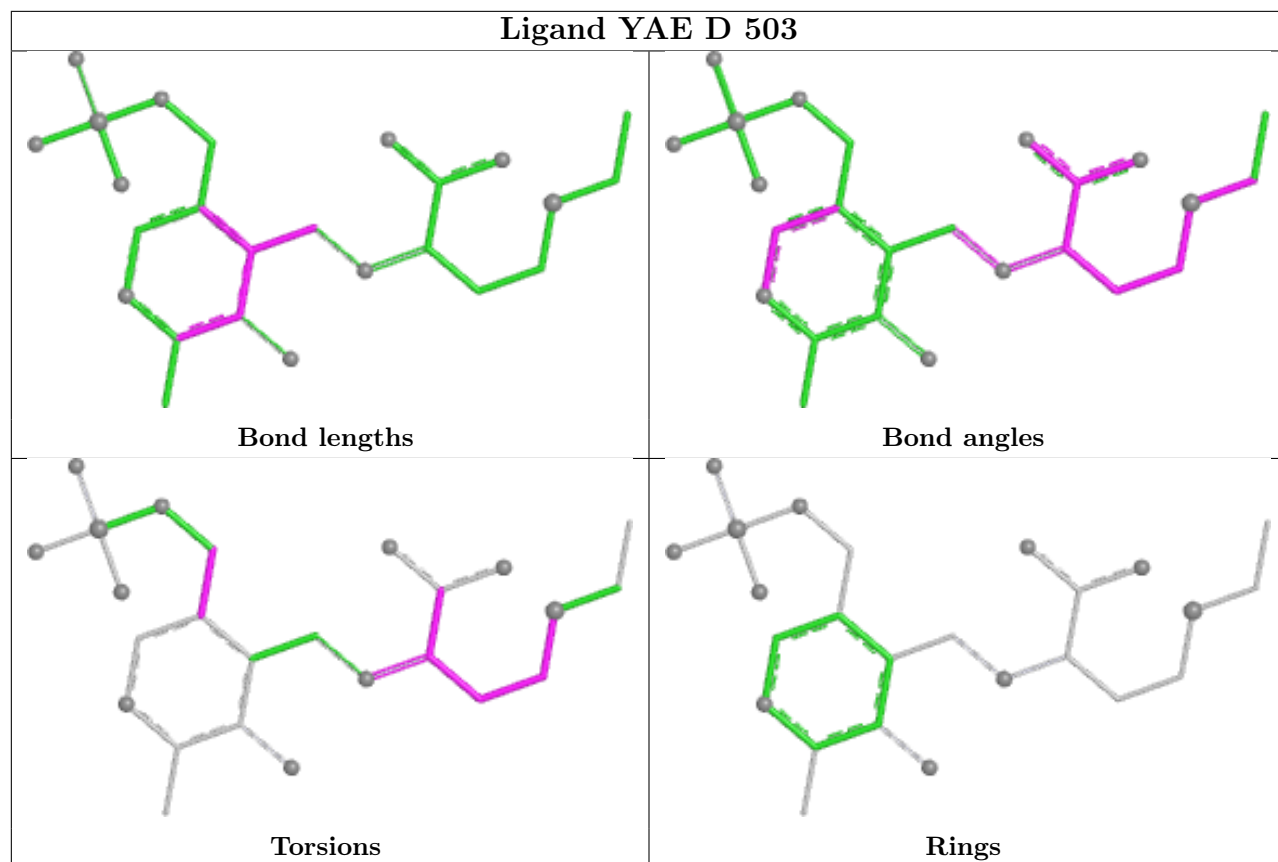
There are no ring outliers.

2 monomers are involved in 3 short contacts:

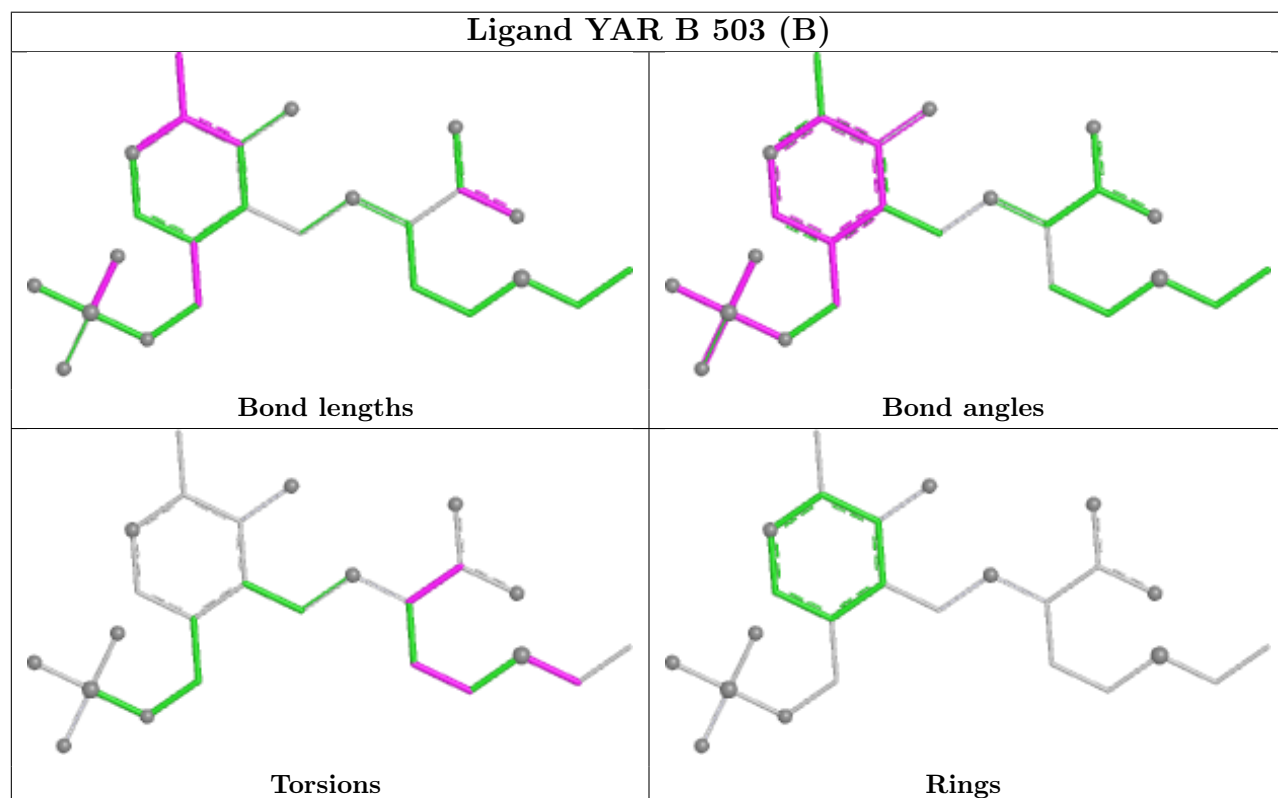
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	503[B]	YAR	1	0
5	C	503	ESC	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand YAE D 503



Ligand YAR B 503 (B)



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	465/466 (99%)	-0.45	2 (0%) 89 92	14, 39, 88, 138	10 (2%)
1	C	465/466 (99%)	-0.55	0 100 100	14, 36, 75, 151	8 (1%)
2	B	466/466 (100%)	-0.06	4 (0%) 81 85	21, 54, 102, 154	5 (1%)
2	D	466/466 (100%)	-0.20	2 (0%) 89 92	18, 53, 98, 166	5 (1%)
All	All	1862/1864 (99%)	-0.31	8 (0%) 89 92	14, 46, 94, 166	28 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	132	PHE	3.3
1	A	132	PHE	2.7
2	B	141	LEU	2.4
2	D	132	PHE	2.4
2	B	300	THR	2.3
2	D	134	THR	2.3
2	B	456	LEU	2.1
1	A	300	THR	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	LLP	A	266	24/25	0.97	0.09	20,40,59,70	0
1	LLP	C	266	24/25	0.97	0.08	18,35,45,55	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

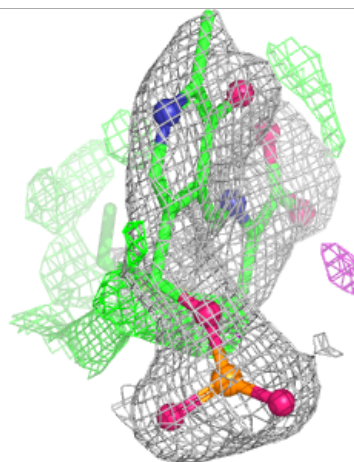
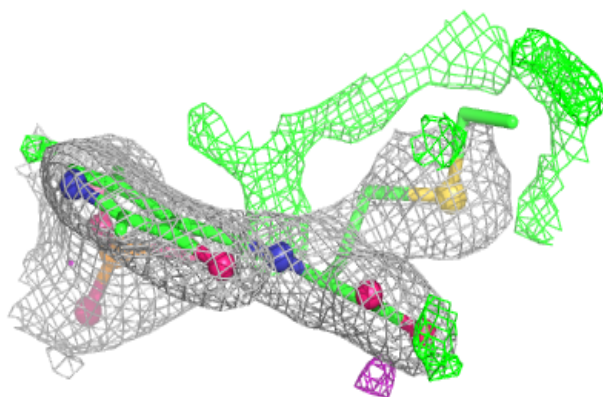
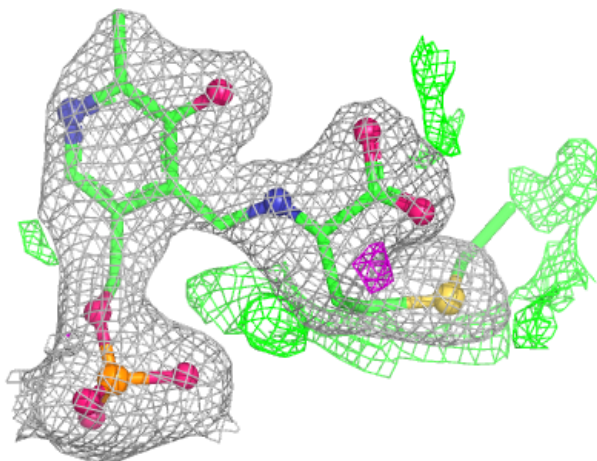
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

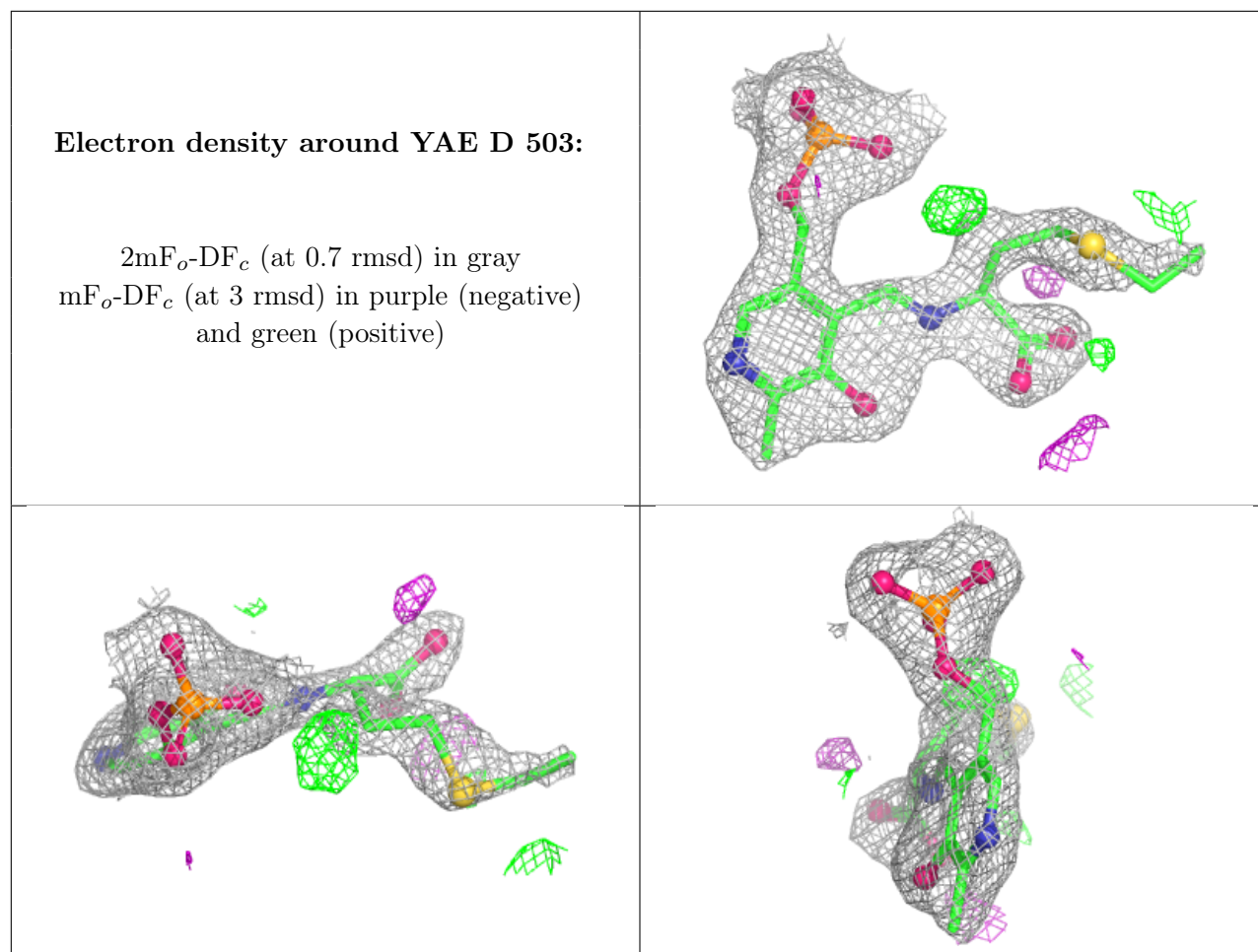
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	DMS	C	501	4/4	0.77	0.21	57,61,66,83	4
5	ESC	C	503	10/10	0.78	0.19	59,73,80,124	0
5	ESC	A	505	10/10	0.79	0.19	57,73,88,110	0
3	DMS	A	501	4/4	0.82	0.17	72,75,81,111	0
3	DMS	A	504	4/4	0.83	0.17	56,57,79,95	4
3	DMS	C	502	4/4	0.83	0.15	73,81,81,104	0
6	NA	D	501[A]	1/1	0.84	0.18	17,17,17,17	1
6	NA	D	501[B]	1/1	0.84	0.18	20,20,20,20	1
4	EDO	A	502	4/4	0.85	0.11	46,47,57,74	0
4	EDO	A	503	4/4	0.88	0.11	48,52,60,62	0
7	YAR	B	503[B]	25/25	0.92	0.12	33,53,71,85	25
8	YAE	D	503	25/25	0.95	0.10	29,52,71,94	25
6	NA	D	502[A]	1/1	0.97	0.09	21,21,21,21	1
6	NA	D	502[B]	1/1	0.97	0.09	20,20,20,20	1
6	NA	B	502[A]	1/1	0.98	0.04	26,26,26,26	1
6	NA	B	502[B]	1/1	0.98	0.04	27,27,27,27	1
6	NA	B	501[A]	1/1	0.99	0.07	19,19,19,19	1
6	NA	B	501[B]	1/1	0.99	0.07	20,20,20,20	1

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

Electron density around YAR B 503 (B):

$2mF_o-DF_c$ (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.