



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:55 AM UTC

PDB ID : 8V5G / pdb_00008v5g
Title : Crystal Structure of Acetyl-CoA synthetase from *Cryptococcus neoformans* H99 in complex with an ethylsulfamide AMP inhibitor
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2023-11-30
Resolution : 2.50 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:

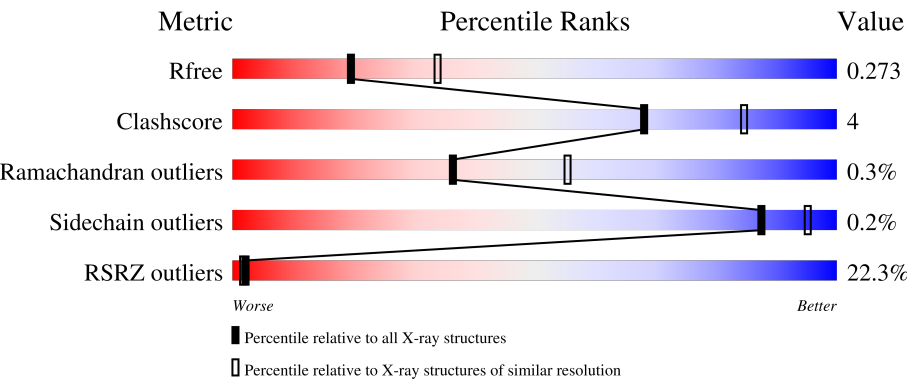
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	694	8% 88% 6% 6%
1	B	694	24% 84% 7% 9%
1	C	694	25% 60% 10% 30%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13931 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 Acetyl-coenzyme A synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	655	Total	C	N	O	S	0	0	0
			5072	3236	867	943	26			
1	B	634	Total	C	N	O	S	0	0	0
			4907	3133	831	917	26			
1	C	483	Total	C	N	O	S	0	0	0
			3790	2427	633	708	22			

There are 45 discrepancies between the modelled and reference sequences:

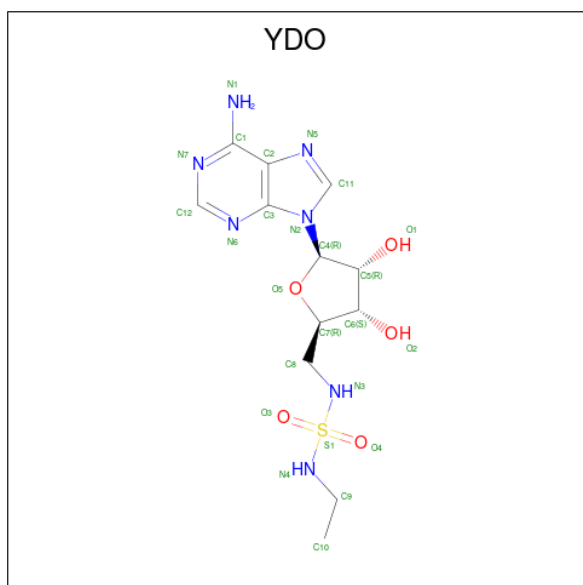
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP J9VFT1
A	-12	HIS	-	expression tag	UNP J9VFT1
A	-11	HIS	-	expression tag	UNP J9VFT1
A	-10	HIS	-	expression tag	UNP J9VFT1
A	-9	HIS	-	expression tag	UNP J9VFT1
A	-8	HIS	-	expression tag	UNP J9VFT1
A	-7	HIS	-	expression tag	UNP J9VFT1
A	-6	HIS	-	expression tag	UNP J9VFT1
A	-5	HIS	-	expression tag	UNP J9VFT1
A	-4	GLU	-	expression tag	UNP J9VFT1
A	-3	ASN	-	expression tag	UNP J9VFT1
A	-2	LEU	-	expression tag	UNP J9VFT1
A	-1	TYR	-	expression tag	UNP J9VFT1
A	0	PHE	-	expression tag	UNP J9VFT1
A	1	GLN	-	expression tag	UNP J9VFT1
B	-13	MET	-	initiating methionine	UNP J9VFT1
B	-12	HIS	-	expression tag	UNP J9VFT1
B	-11	HIS	-	expression tag	UNP J9VFT1
B	-10	HIS	-	expression tag	UNP J9VFT1
B	-9	HIS	-	expression tag	UNP J9VFT1
B	-8	HIS	-	expression tag	UNP J9VFT1
B	-7	HIS	-	expression tag	UNP J9VFT1
B	-6	HIS	-	expression tag	UNP J9VFT1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP J9VFT1
B	-4	GLU	-	expression tag	UNP J9VFT1
B	-3	ASN	-	expression tag	UNP J9VFT1
B	-2	LEU	-	expression tag	UNP J9VFT1
B	-1	TYR	-	expression tag	UNP J9VFT1
B	0	PHE	-	expression tag	UNP J9VFT1
B	1	GLN	-	expression tag	UNP J9VFT1
C	-13	MET	-	initiating methionine	UNP J9VFT1
C	-12	HIS	-	expression tag	UNP J9VFT1
C	-11	HIS	-	expression tag	UNP J9VFT1
C	-10	HIS	-	expression tag	UNP J9VFT1
C	-9	HIS	-	expression tag	UNP J9VFT1
C	-8	HIS	-	expression tag	UNP J9VFT1
C	-7	HIS	-	expression tag	UNP J9VFT1
C	-6	HIS	-	expression tag	UNP J9VFT1
C	-5	HIS	-	expression tag	UNP J9VFT1
C	-4	GLU	-	expression tag	UNP J9VFT1
C	-3	ASN	-	expression tag	UNP J9VFT1
C	-2	LEU	-	expression tag	UNP J9VFT1
C	-1	TYR	-	expression tag	UNP J9VFT1
C	0	PHE	-	expression tag	UNP J9VFT1
C	1	GLN	-	expression tag	UNP J9VFT1

- Molecule 2 is 5'-deoxy-5'-(ethylsulfamamido)adenosine (CCD ID: YDO) (formula: $C_{12}H_{19}N_7O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			25	12	7	5	1		
2	B	1	Total	C	N	O	S	0	0
			25	12	7	5	1		

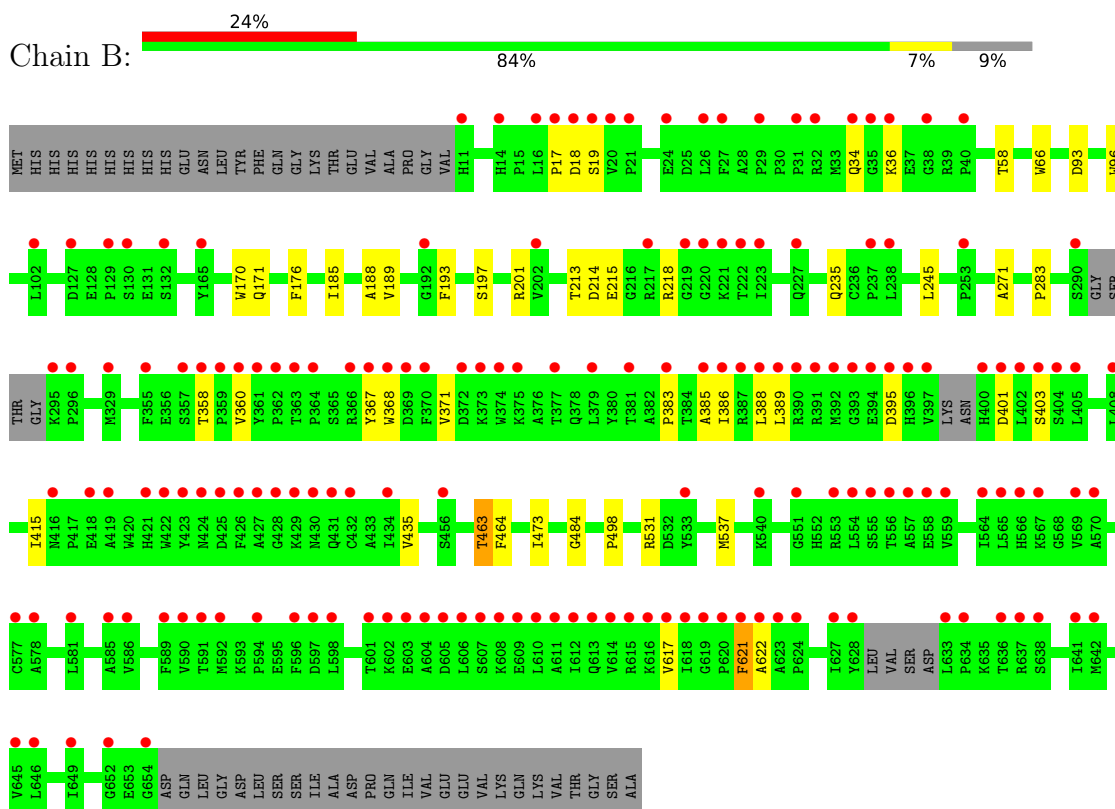
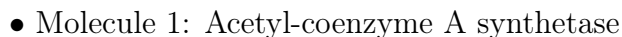
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total	O	0	0
			39	39		
4	B	58	Total	O	0	0
			58	58		
4	C	14	Total	O	0	0
			14	14		

- Molecule 1: Acetyl-coenzyme A synthetase



Chain C:

25% 60% 10% 30%

MET HIS HIS HIS HIS HIS HIS HIS HIS GLU ASN LEU TYR PHE GLN GLY LYS THR
 GLU VAL ALA PRO GLY VAL HIS HIS VAL VAL HIS THR LEU PRO ASP SER VAL
 VAL GLU SER LEU PHE ALA PRO THR LEU LEU MET GLN LYS GLY R39 P40
 K41 P42 H43 I44 G45 P46

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.01Å 183.85Å 84.72Å 90.00° 93.40° 90.00°	Depositor
Resolution (Å)	76.84 – 2.50 76.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (76.84-2.50) 99.5 (76.84-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5162	Depositor
R, R_{free}	0.232 , 0.274 0.236 , 0.273	Depositor DCC
R_{free} test set	3717 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13931	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% 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: YDO, CL

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	0.29	0/5211	0.45	0/7102
1	B	0.31	0/5044	0.46	1/6880 (0.0%)
1	C	0.29	0/3903	0.44	0/5322
All	All	0.30	0/14158	0.45	1/19304 (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	B	395	ASP	N-CA-C	-6.26	104.56	111.82

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	5072	0	4879	24	0
1	B	4907	0	4682	33	0
1	C	3790	0	3587	43	0
2	A	25	0	0	0	0
2	B	25	0	0	0	0
3	B	1	0	0	0	0
4	A	39	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	58	0	0	0	0
4	C	14	0	0	0	0
All	All	13931	0	13148	97	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 4.

All (97) 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:411:VAL:HG21	1:C:439:TRP:HE1	1.54	0.72
1:C:473:ILE:HD11	1:C:487:VAL:HG23	1.75	0.69
1:B:368:TRP:CZ2	1:B:389:LEU:HD13	2.29	0.68
1:C:367:TYR:O	1:C:371:VAL:HG23	1.96	0.65
1:C:448:ILE:HG22	1:C:462:ALA:CB	2.26	0.65
1:C:411:VAL:HG23	1:C:437:THR:O	1.98	0.63
1:C:199:ARG:NH1	1:C:235:GLN:OE1	2.33	0.62
1:B:368:TRP:HZ2	1:B:389:LEU:HD13	1.64	0.61
1:B:360:VAL:HG13	1:B:388:LEU:HD21	1.82	0.60
1:C:382:ALA:HB1	1:C:383:PRO:CD	2.30	0.60
1:C:49:GLU:HA	1:C:52:VAL:HG12	1.84	0.58
1:C:411:VAL:HG21	1:C:439:TRP:NE1	2.18	0.58
1:B:484:GLY:O	1:B:531:ARG:NH2	2.25	0.58
1:B:367:TYR:O	1:B:371:VAL:HG23	2.04	0.58
1:A:17:PRO:HB3	1:A:617:VAL:HG11	1.86	0.56
1:A:632:ASP:OD1	1:A:633:LEU:N	2.38	0.56
1:B:473:ILE:HD11	1:B:537:MET:HE1	1.87	0.55
1:C:473:ILE:HD11	1:C:487:VAL:CG2	2.36	0.55
1:B:214:ASP:OD1	1:B:215:GLU:N	2.40	0.55
1:C:306:TYR:O	1:C:310:THR:HG23	2.07	0.55
1:A:214:ASP:OD1	1:A:215:GLU:N	2.40	0.54
1:A:463:THR:OG1	1:A:464:PHE:N	2.37	0.53
1:B:435:VAL:HG23	1:B:435:VAL:O	2.08	0.53
1:A:213:THR:HG22	1:A:245:LEU:HB3	1.92	0.52
1:C:119:LYS:NZ	1:C:322:PRO:O	2.38	0.52
1:C:215:GLU:OE1	1:C:250:ASN:ND2	2.32	0.52
1:B:213:THR:HG22	1:B:245:LEU:HB3	1.92	0.51
1:B:360:VAL:HG13	1:B:388:LEU:CD2	2.41	0.51
1:C:462:ALA:O	1:C:464:PHE:N	2.44	0.50
1:A:32:ARG:NH2	1:A:431:GLN:OE1	2.44	0.50
1:B:218:ARG:HG2	1:B:358:THR:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:ILE:HG22	1:C:462:ALA:HB3	1.93	0.50
1:A:270:PRO:HG3	1:C:503:THR:HG21	1.92	0.50
1:A:93:ASP:HB3	1:B:271:ALA:HB3	1.93	0.50
1:C:500:ILE:O	1:C:502:ARG:NH1	2.44	0.49
1:B:93:ASP:HB3	1:C:271:ALA:HB3	1.94	0.48
1:A:332:ILE:C	1:A:332:ILE:HD12	2.39	0.48
1:C:83:THR:O	1:C:98:PRO:HD2	2.14	0.47
1:C:475:ASP:HB2	1:C:482:LEU:HD21	1.96	0.47
1:C:437:THR:HG21	1:C:446:ILE:HD13	1.96	0.47
1:C:383:PRO:O	1:C:384:THR:C	2.58	0.46
1:C:517:LYS:N	1:C:518:PRO:CD	2.78	0.46
1:C:503:THR:OG1	1:C:504:VAL:N	2.48	0.46
1:B:58:THR:HG22	1:B:66:TRP:CD2	2.51	0.46
1:A:405:LEU:HD13	1:A:408:LEU:HD21	1.96	0.46
1:B:401:ASP:OD1	1:B:403:SER:HB2	2.16	0.46
1:C:332:ILE:C	1:C:332:ILE:HD12	2.41	0.45
1:C:435:VAL:O	1:C:435:VAL:HG23	2.16	0.45
1:A:332:ILE:HD12	1:A:333:GLY:N	2.30	0.45
1:C:469:MET:HE2	1:C:497:TRP:CD1	2.52	0.45
1:C:89:PHE:N	1:C:89:PHE:CD1	2.84	0.45
1:B:360:VAL:CG1	1:B:388:LEU:HD21	2.45	0.45
1:B:385:ALA:O	1:B:388:LEU:HB3	2.15	0.45
1:A:394:GLU:HG2	1:A:426:PHE:CZ	2.52	0.45
1:A:486:ASP:N	1:A:531:ARG:O	2.50	0.45
1:A:527:ASP:OD1	1:A:542:ARG:HD2	2.17	0.45
1:A:291:GLY:O	1:A:293:THR:N	2.50	0.45
1:A:589:PHE:HE2	1:A:672:VAL:HG13	1.82	0.45
1:B:189:VAL:HG22	1:B:201:ARG:HD3	1.98	0.45
1:C:381:THR:O	1:C:410:SER:HA	2.17	0.45
1:A:435:VAL:HG23	1:A:435:VAL:O	2.17	0.44
1:B:193:PHE:HB3	1:B:197:SER:HB2	1.98	0.44
1:C:408:LEU:HB3	1:C:423:TYR:CZ	2.52	0.44
1:B:360:VAL:CG1	1:B:388:LEU:HD11	2.47	0.44
1:B:360:VAL:HG12	1:B:388:LEU:HD11	1.99	0.44
1:A:517:LYS:N	1:A:518:PRO:CD	2.81	0.44
1:A:185:ILE:HD11	1:A:283:PRO:HG2	1.99	0.43
1:C:51:TYR:HB3	1:C:455:ILE:HD11	2.00	0.43
1:B:34:GLN:C	1:B:36:LYS:H	2.27	0.43
1:C:101:THR:HA	1:C:278:MET:O	2.19	0.43
1:B:17:PRO:HB3	1:B:617:VAL:HG11	2.01	0.43
1:B:621:PHE:N	1:B:621:PHE:CD1	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:LYS:HE3	1:C:536:TYR:HD2	1.84	0.43
1:C:58:THR:HG22	1:C:66:TRP:CZ3	2.54	0.43
1:B:96:TRP:CD1	1:B:498:PRO:HA	2.54	0.42
1:C:418:GLU:OE1	1:C:418:GLU:N	2.47	0.42
1:C:416:ASN:HB3	1:C:418:GLU:OE1	2.19	0.42
1:B:383:PRO:HA	1:B:386:ILE:HB	2.01	0.42
1:C:45:GLY:HA2	1:C:454:ALA:HB2	2.01	0.42
1:C:463:THR:OG1	1:C:464:PHE:N	2.53	0.42
1:B:176:PHE:CZ	1:B:188:ALA:HB2	2.55	0.41
1:A:18:ASP:OD1	1:A:19:SER:N	2.53	0.41
1:B:621:PHE:HD1	1:B:622:ALA:N	2.18	0.41
1:A:425:ASP:O	1:A:429:LYS:HA	2.19	0.41
1:A:497:TRP:CH2	1:A:500:ILE:HD12	2.55	0.41
1:B:185:ILE:HD11	1:B:283:PRO:HG2	2.02	0.41
1:B:170:TRP:CE2	1:B:171:GLN:NE2	2.89	0.41
1:B:463:THR:OG1	1:B:464:PHE:N	2.52	0.41
1:A:356:GLU:HG2	1:A:356:GLU:O	2.21	0.41
1:A:634:PRO:HB2	1:A:642:MET:HE3	2.02	0.41
1:C:370:PHE:CD1	1:C:374:TRP:HD1	2.39	0.41
1:C:214:ASP:OD1	1:C:215:GLU:N	2.54	0.41
1:C:450:PRO:HB3	1:C:463:THR:CG2	2.51	0.41
1:C:243:LEU:HD11	1:C:262:TRP:HA	2.03	0.41
1:B:415:ILE:O	1:B:415:ILE:HG23	2.20	0.40
1:B:18:ASP:OD1	1:B:19:SER:N	2.53	0.40
1:C:281:GLU:HA	1:C:302:SER:HB2	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	649/694 (94%)	625 (96%)	22 (3%)	2 (0%)	36 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	626/694 (90%)	607 (97%)	18 (3%)	1 (0%)	43	63
1	C	473/694 (68%)	436 (92%)	34 (7%)	3 (1%)	21	38
All	All	1748/2082 (84%)	1668 (95%)	74 (4%)	6 (0%)	36	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	SER
1	A	463	THR
1	C	463	THR
1	B	463	THR
1	C	452	PRO
1	C	364	PRO

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	523/576 (91%)	523 (100%)	0	100	100
1	B	504/576 (88%)	502 (100%)	2 (0%)	84	93
1	C	390/576 (68%)	389 (100%)	1 (0%)	86	94
All	All	1417/1728 (82%)	1414 (100%)	3 (0%)	87	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	235	GLN
1	B	621	PHE
1	C	39	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	613	GLN
1	B	11	HIS
1	B	91	HIS
1	B	227	GLN
1	C	241	ASN
1	C	421	HIS
1	C	430	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
2	YDO	A	701	-	27,27,27	0.35	0	35,40,40	0.92	2 (5%)
2	YDO	B	702	-	27,27,27	0.34	0	35,40,40	0.91	2 (5%)

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
2	YDO	A	701	-	-	6/14/30/30	0/3/3/3
2	YDO	B	702	-	-	5/14/30/30	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	YDO	N7-C12-N6	-3.81	122.82	128.58
2	A	701	YDO	N7-C12-N6	-3.77	122.88	128.58
2	B	702	YDO	C12-N6-C3	2.03	116.79	111.83
2	A	701	YDO	C12-N6-C3	2.02	116.76	111.83

There are no chirality outliers.

All (11) torsion outliers are listed below:

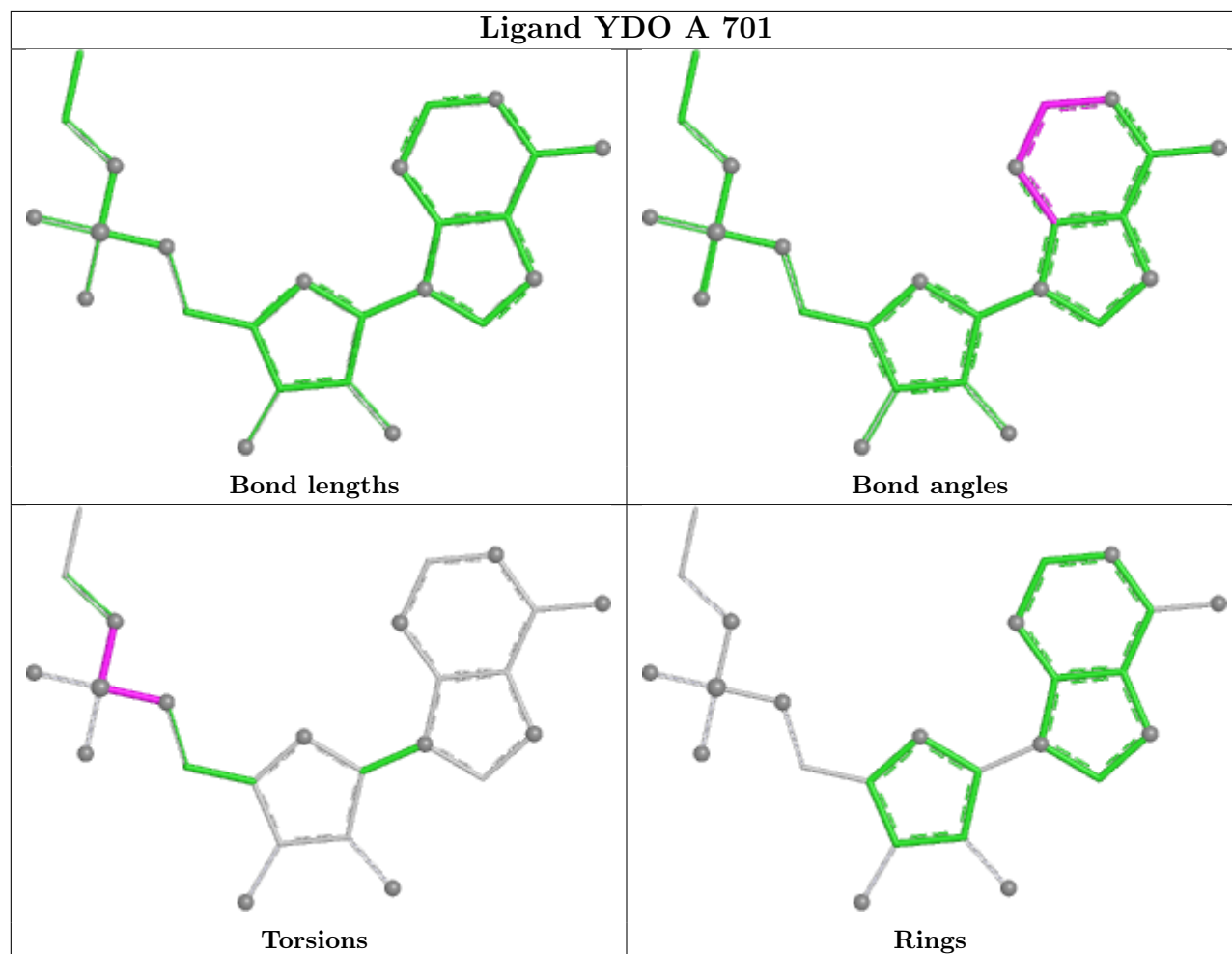
Mol	Chain	Res	Type	Atoms
2	A	701	YDO	C8-N3-S1-N4
2	A	701	YDO	C8-N3-S1-O3
2	A	701	YDO	C8-N3-S1-O4
2	A	701	YDO	C9-N4-S1-N3
2	A	701	YDO	C9-N4-S1-O3
2	B	702	YDO	C8-N3-S1-N4
2	B	702	YDO	C8-N3-S1-O3
2	B	702	YDO	C8-N3-S1-O4
2	A	701	YDO	C9-N4-S1-O4
2	B	702	YDO	C9-N4-S1-O3
2	B	702	YDO	C9-N4-S1-O4

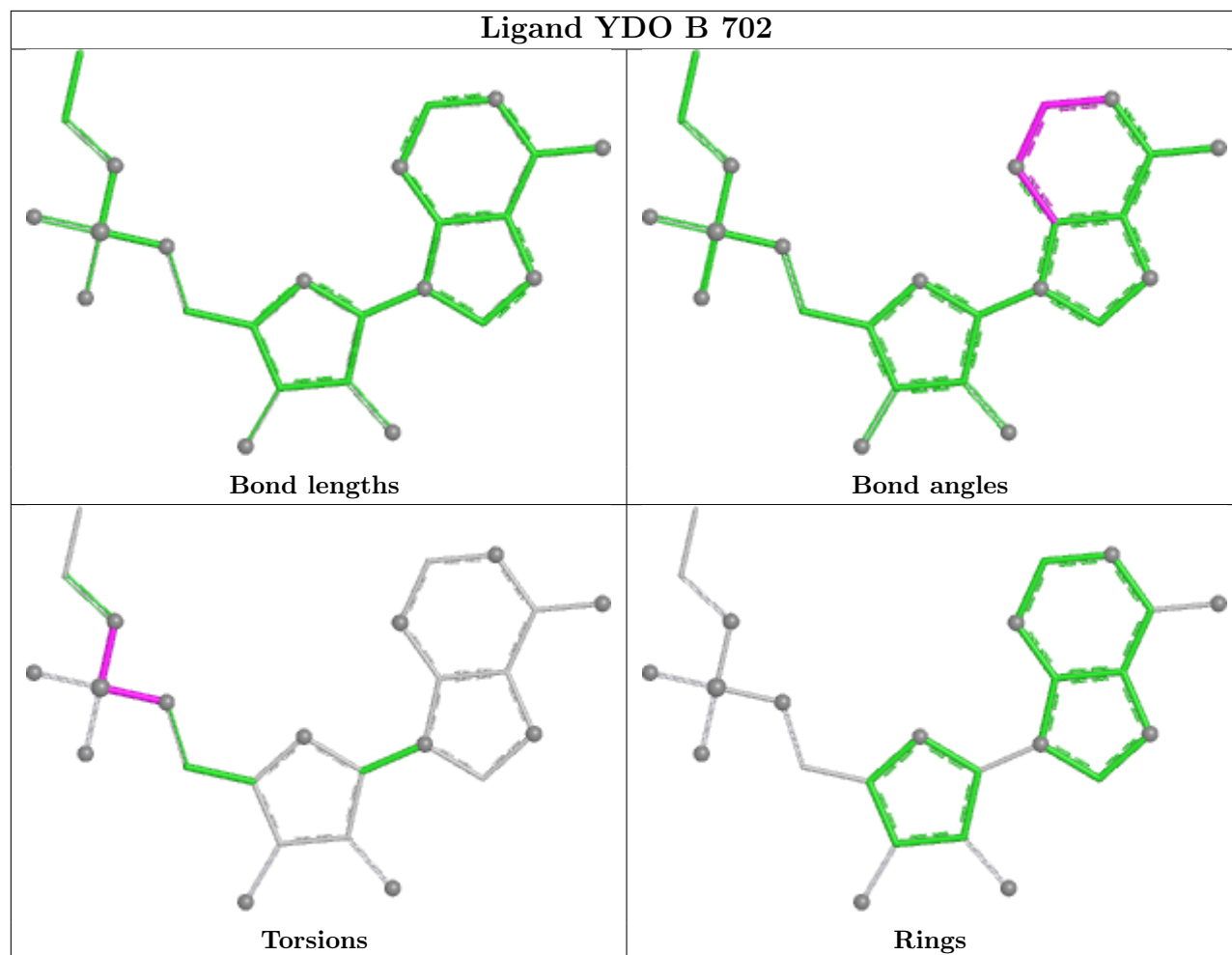
There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	655/694 (94%)	0.62	53 (8%) 18 15	28, 54, 97, 148	0
1	B	634/694 (91%)	1.19	167 (26%) 1 1	26, 68, 133, 187	0
1	C	483/694 (69%)	1.61	176 (36%) 1 1	31, 87, 132, 165	0
All	All	1772/2082 (85%)	1.09	396 (22%) 2 2	26, 65, 128, 187	0

All (396) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	423	TYR	6.4
1	A	639	GLY	6.3
1	B	426	PHE	5.7
1	B	389	LEU	5.6
1	A	664	ALA	5.6
1	B	392	MET	5.5
1	C	424	ASN	5.4
1	C	414	PRO	5.4
1	B	220	GLY	5.3
1	A	654	GLY	5.3
1	B	622	ALA	5.1
1	B	555	SER	5.1
1	C	415	ILE	5.0
1	B	395	ASP	5.0
1	C	426	PHE	5.0
1	C	435	VAL	5.0
1	C	448	ILE	4.9
1	C	464	PHE	4.8
1	B	620	PRO	4.8
1	C	419	ALA	4.7
1	C	434	ILE	4.7
1	B	362	PRO	4.7
1	C	383	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	637	ARG	4.6
1	A	676	VAL	4.6
1	C	489	GLY	4.6
1	B	393	GLY	4.5
1	B	427	ALA	4.5
1	C	385	ALA	4.5
1	C	461	SER	4.5
1	B	390	ARG	4.5
1	B	567	LYS	4.5
1	A	672	VAL	4.4
1	B	612	ILE	4.4
1	B	617	VAL	4.4
1	B	394	GLU	4.4
1	C	474	ILE	4.4
1	B	31	PRO	4.4
1	C	444	GLY	4.4
1	B	397	VAL	4.4
1	B	290	SER	4.4
1	C	422	TRP	4.4
1	B	423	TYR	4.4
1	B	628	TYR	4.4
1	C	382	ALA	4.4
1	C	462	ALA	4.3
1	B	604	ALA	4.3
1	C	478	THR	4.3
1	B	614	VAL	4.3
1	C	411	VAL	4.3
1	B	606	LEU	4.3
1	C	533	TYR	4.3
1	C	467	PHE	4.2
1	C	56	ALA	4.2
1	A	638	SER	4.2
1	B	641	ILE	4.2
1	A	642	MET	4.2
1	C	431	GLN	4.2
1	B	645	VAL	4.2
1	B	361	TYR	4.1
1	B	364	PRO	4.1
1	C	438	TYR	4.1
1	C	479	GLY	4.1
1	B	621	PHE	4.1
1	C	536	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	231	ALA	4.0
1	C	427	ALA	4.0
1	B	419	ALA	3.9
1	C	530	ALA	3.9
1	B	422	TRP	3.9
1	C	296	PRO	3.9
1	B	554	LEU	3.8
1	C	408	LEU	3.8
1	B	404	SER	3.8
1	B	432	CYS	3.8
1	C	463	THR	3.8
1	C	471	VAL	3.8
1	C	522	TYR	3.8
1	B	602	LYS	3.8
1	B	564	ILE	3.8
1	A	292	SER	3.8
1	B	192	GLY	3.8
1	C	465	PRO	3.8
1	A	640	LYS	3.8
1	A	641	ILE	3.8
1	C	417	PRO	3.7
1	C	519	TYR	3.7
1	C	61	PRO	3.7
1	A	669	VAL	3.7
1	C	421	HIS	3.7
1	C	539	ILE	3.7
1	C	48	TYR	3.7
1	C	51	TYR	3.7
1	B	360	VAL	3.7
1	B	559	VAL	3.7
1	C	44	ILE	3.7
1	A	634	PRO	3.7
1	C	495	ARG	3.7
1	B	585	ALA	3.6
1	B	429	LYS	3.6
1	C	390	ARG	3.6
1	C	327	ALA	3.6
1	C	317	VAL	3.6
1	B	607	SER	3.6
1	C	460	GLY	3.6
1	C	367	TYR	3.5
1	B	598	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	488	GLU	3.5
1	C	469	MET	3.5
1	B	611	ALA	3.5
1	B	359	PRO	3.5
1	C	520	PRO	3.5
1	C	538	TRP	3.5
1	B	36	LYS	3.5
1	C	447	SER	3.5
1	B	618	ILE	3.5
1	C	368	TRP	3.5
1	C	407	VAL	3.4
1	B	388	LEU	3.4
1	A	675	LYS	3.4
1	C	359	PRO	3.4
1	C	466	PHE	3.4
1	B	408	LEU	3.4
1	C	392	MET	3.4
1	C	420	TRP	3.4
1	C	457	THR	3.4
1	C	490	VAL	3.4
1	B	27	PHE	3.3
1	C	380	TYR	3.3
1	B	569	VAL	3.3
1	A	600	ALA	3.3
1	B	368	TRP	3.3
1	A	291	GLY	3.3
1	B	219	GLY	3.3
1	B	566	HIS	3.3
1	C	517	LYS	3.3
1	C	355	PHE	3.3
1	C	46	PRO	3.3
1	B	642	MET	3.3
1	C	393	GLY	3.3
1	C	537	MET	3.3
1	A	290	SER	3.2
1	C	482	LEU	3.2
1	C	455	ILE	3.2
1	C	89	PHE	3.2
1	C	436	ASP	3.2
1	B	646	LEU	3.2
1	C	439	TRP	3.2
1	B	589	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	421	HIS	3.2
1	B	558	GLU	3.2
1	C	362	PRO	3.2
1	A	668	ILE	3.2
1	B	556	THR	3.2
1	B	634	PRO	3.1
1	A	670	GLU	3.1
1	C	459	PRO	3.1
1	C	521	GLY	3.1
1	B	603	GLU	3.1
1	C	512	LEU	3.1
1	C	535	GLY	3.1
1	C	481	VAL	3.1
1	B	357	SER	3.1
1	C	222	THR	3.0
1	C	451	LEU	3.0
1	C	523	PHE	3.0
1	B	19	SER	3.0
1	B	615	ARG	3.0
1	B	608	LYS	3.0
1	B	431	GLN	3.0
1	B	649	ILE	3.0
1	C	473	ILE	3.0
1	C	62	ASN	3.0
1	B	586	VAL	3.0
1	C	360	VAL	3.0
1	B	402	LEU	3.0
1	B	551	GLY	3.0
1	A	643	ARG	3.0
1	C	518	PRO	2.9
1	B	610	LEU	2.9
1	B	130	SER	2.9
1	C	526	GLY	2.9
1	B	223	ILE	2.9
1	C	384	THR	2.9
1	B	391	ARG	2.9
1	C	364	PRO	2.9
1	C	491	LEU	2.9
1	B	425	ASP	2.9
1	B	613	GLN	2.9
1	B	638	SER	2.9
1	B	416	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	293	THR	2.9
1	C	437	THR	2.9
1	B	132	SER	2.9
1	B	418	GLU	2.9
1	B	654	GLY	2.9
1	B	296	PRO	2.9
1	C	477	GLN	2.9
1	A	648	LYS	2.8
1	B	636	THR	2.8
1	C	391	ARG	2.8
1	B	20	VAL	2.8
1	B	590	VAL	2.8
1	B	129	PRO	2.8
1	A	601	THR	2.8
1	B	605	ASP	2.8
1	A	652	GLY	2.8
1	A	666	PRO	2.8
1	B	557	ALA	2.8
1	C	443	THR	2.8
1	B	18	ASP	2.8
1	B	227	GLN	2.8
1	C	445	SER	2.7
1	C	452	PRO	2.7
1	C	458	LYS	2.7
1	B	14	HIS	2.7
1	B	16	LEU	2.7
1	B	385	ALA	2.7
1	B	601	THR	2.7
1	C	470	ASP	2.7
1	A	393	GLY	2.7
1	B	370	PHE	2.7
1	B	21	PRO	2.7
1	C	476	PRO	2.7
1	C	191	ALA	2.7
1	C	449	ALA	2.7
1	C	309	GLY	2.6
1	B	217	ARG	2.6
1	C	430	ASN	2.6
1	B	202	VAL	2.6
1	A	674	GLN	2.6
1	B	570	ALA	2.6
1	C	433	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	616	LYS	2.6
1	C	528	GLY	2.6
1	B	424	ASN	2.6
1	C	410	SER	2.6
1	B	400	HIS	2.6
1	B	533	TYR	2.6
1	B	35	GLY	2.6
1	B	38	GLY	2.6
1	B	17	PRO	2.6
1	C	40	PRO	2.6
1	C	446	ILE	2.6
1	B	633	LEU	2.6
1	B	366	ARG	2.6
1	B	637	ARG	2.6
1	A	671	GLU	2.6
1	B	609	GLU	2.6
1	C	59	VAL	2.6
1	C	492	VAL	2.6
1	C	432	CYS	2.6
1	C	58	THR	2.6
1	C	527	ASP	2.5
1	A	27	PHE	2.5
1	C	483	GLU	2.5
1	B	565	LEU	2.5
1	B	577	CYS	2.5
1	B	358	THR	2.5
1	C	441	THR	2.5
1	A	479	GLY	2.5
1	B	619	GLY	2.5
1	B	363	THR	2.5
1	B	434	ILE	2.5
1	B	238	LEU	2.5
1	C	405	LEU	2.5
1	C	289	THR	2.5
1	B	624	PRO	2.5
1	C	450	PRO	2.5
1	C	468	GLY	2.5
1	C	515	TYR	2.5
1	C	524	PHE	2.5
1	B	11	HIS	2.5
1	A	630	VAL	2.5
1	C	494	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	592	MET	2.5
1	B	24	GLU	2.4
1	C	60	GLY	2.4
1	A	605	ASP	2.4
1	B	405	LEU	2.4
1	B	387	ARG	2.4
1	C	440	MET	2.4
1	C	381	THR	2.4
1	A	476	PRO	2.4
1	B	295	LYS	2.4
1	B	367	TYR	2.4
1	C	55	TRP	2.4
1	C	370	PHE	2.4
1	B	430	ASN	2.4
1	B	375	LYS	2.4
1	C	358	THR	2.4
1	B	627	ILE	2.4
1	C	234	GLN	2.4
1	C	480	GLN	2.4
1	C	534	ASP	2.4
1	A	12	HIS	2.4
1	C	377	THR	2.3
1	A	667	GLN	2.3
1	C	486	ASP	2.3
1	B	355	PHE	2.3
1	C	318	PHE	2.3
1	C	487	VAL	2.3
1	C	454	ALA	2.3
1	C	39	ARG	2.3
1	C	50	SER	2.3
1	C	456	SER	2.3
1	B	396	HIS	2.3
1	C	509	LYS	2.3
1	A	481	VAL	2.3
1	C	189	VAL	2.3
1	B	40	PRO	2.3
1	B	383	PRO	2.3
1	C	42	PRO	2.3
1	C	195	ALA	2.3
1	C	496	PRO	2.3
1	A	294	GLY	2.3
1	B	379	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	386	ILE	2.3
1	C	372	ASP	2.3
1	C	425	ASP	2.3
1	B	540	LYS	2.3
1	B	596	PHE	2.3
1	B	594	PRO	2.3
1	B	591	THR	2.3
1	A	646	LEU	2.3
1	A	632	ASP	2.3
1	B	372	ASP	2.3
1	B	401	ASP	2.3
1	A	645	VAL	2.3
1	B	237	PRO	2.3
1	B	578	ALA	2.2
1	B	623	ALA	2.2
1	C	232	ALA	2.2
1	B	403	SER	2.2
1	B	456	SER	2.2
1	A	596	PHE	2.2
1	B	253	PRO	2.2
1	C	299	VAL	2.2
1	C	235	GLN	2.2
1	C	379	LEU	2.2
1	B	127	ASP	2.2
1	B	374	TRP	2.2
1	A	116	ASN	2.2
1	C	511	TYR	2.2
1	C	525	PHE	2.2
1	C	529	ALA	2.2
1	B	222	THR	2.2
1	B	377	THR	2.2
1	A	633	LEU	2.2
1	B	652	GLY	2.2
1	C	409	GLY	2.2
1	C	223	ILE	2.2
1	C	52	VAL	2.1
1	A	267	ALA	2.1
1	A	581	LEU	2.1
1	B	428	GLY	2.1
1	B	581	LEU	2.1
1	B	165	TYR	2.1
1	C	406	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	323	ASP	2.1
1	B	369	ASP	2.1
1	B	373	LYS	2.1
1	C	326	PHE	2.1
1	C	43	HIS	2.1
1	B	34	GLN	2.1
1	A	482	LEU	2.1
1	B	381	THR	2.1
1	C	484	GLY	2.1
1	C	196	GLU	2.1
1	A	602	LYS	2.1
1	B	329	MET	2.1
1	A	487	VAL	2.1
1	A	402	LEU	2.1
1	B	553	ARG	2.1
1	C	316	TYR	2.1
1	B	221	LYS	2.1
1	C	53	LYS	2.1
1	C	57	LYS	2.1
1	C	311	ALA	2.1
1	C	501	ALA	2.1
1	B	32	ARG	2.1
1	B	102	LEU	2.1
1	C	287	LEU	2.1
1	C	500	ILE	2.1
1	A	665	ASP	2.1
1	B	597	ASP	2.1
1	C	532	ASP	2.1
1	B	29	PRO	2.1
1	A	271	ALA	2.0
1	A	651	ALA	2.0
1	C	218	ARG	2.0
1	C	312	LEU	2.0
1	C	416	ASN	2.0
1	B	26	LEU	2.0
1	C	313	THR	2.0
1	C	369	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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](#)

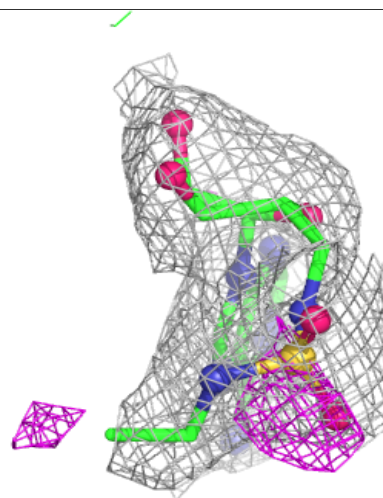
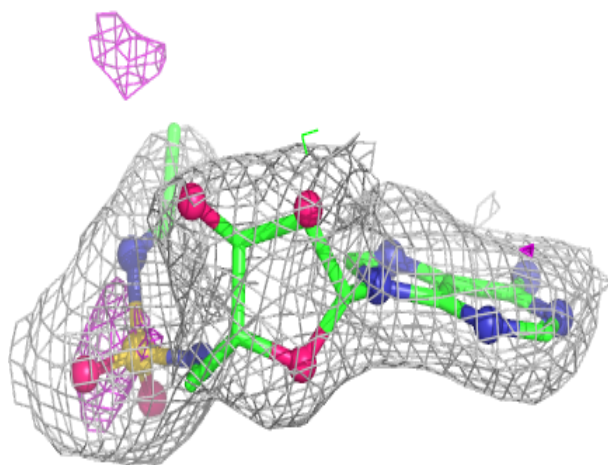
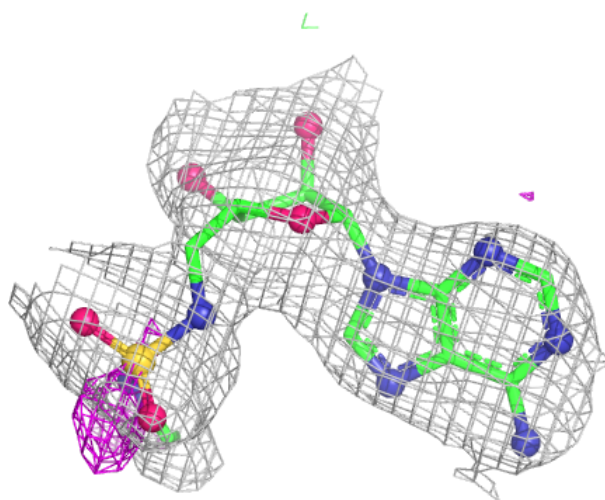
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

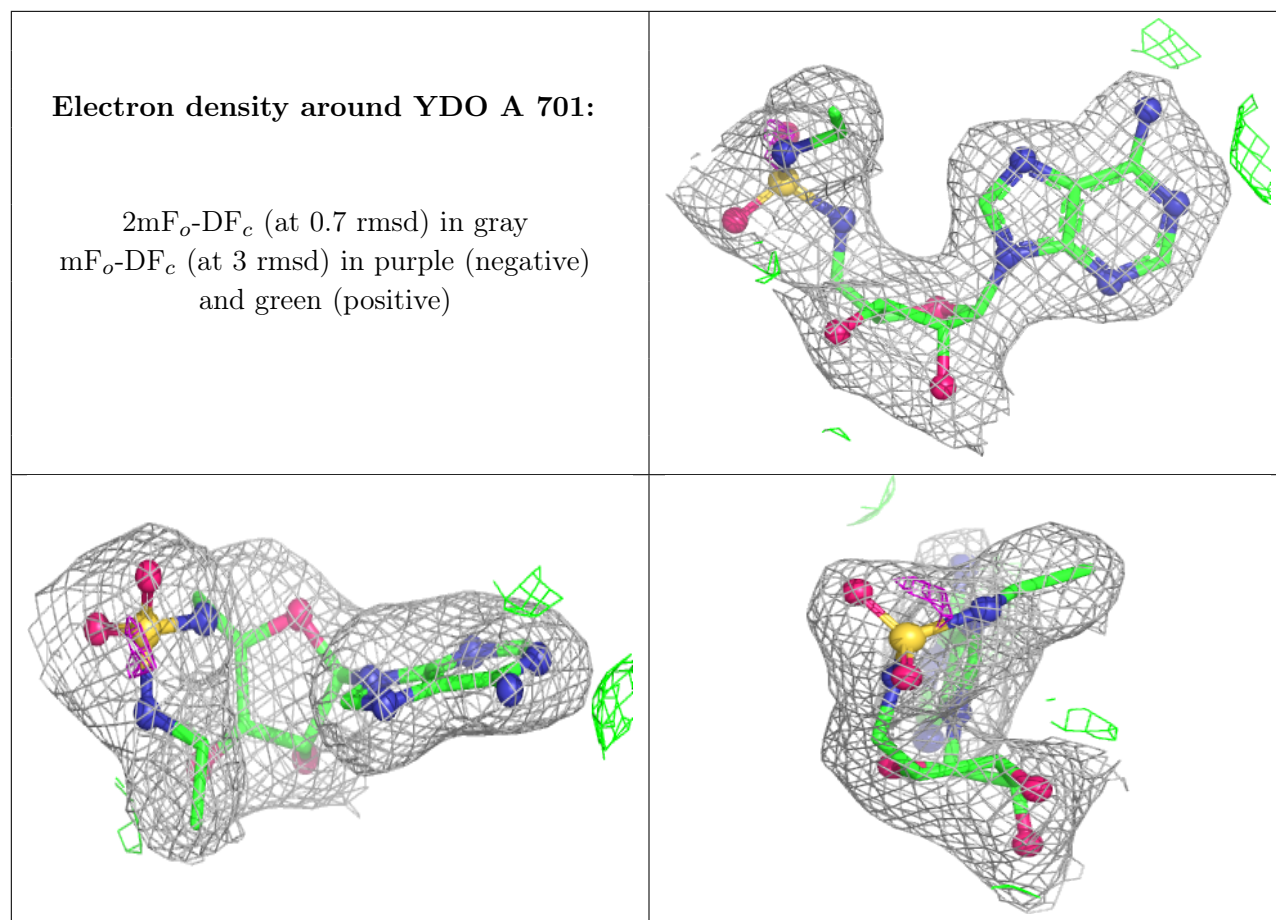
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	YDO	B	702	25/25	0.86	0.13	47,59,63,70	0
2	YDO	A	701	25/25	0.92	0.10	37,41,50,54	0
3	CL	B	701	1/1	0.92	0.22	73,73,73,73	0

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 YDO B 702:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.