Full wwPDB X-ray Structure Validation Report ⓘ

Dec 4, 2023 – 10:42 AM EST

PDB ID	:	8V5G
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:

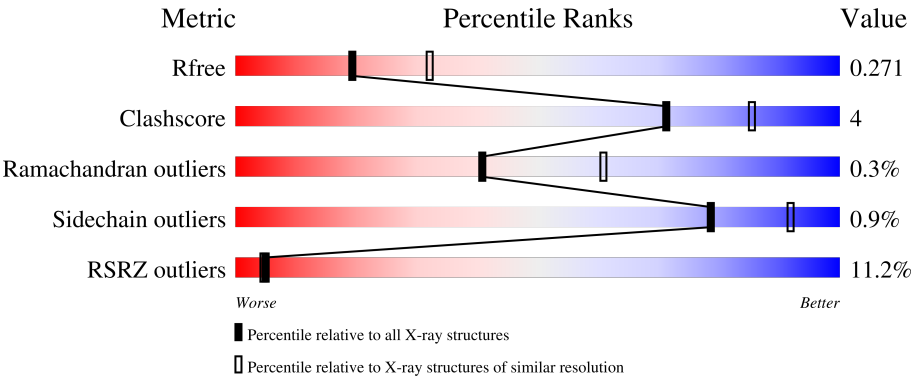
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	3% 88% 6% 6%
1	B	694	10% 84% 7% 9%
1	C	694	15% 60% 10% 30%

2 Entry composition (i)

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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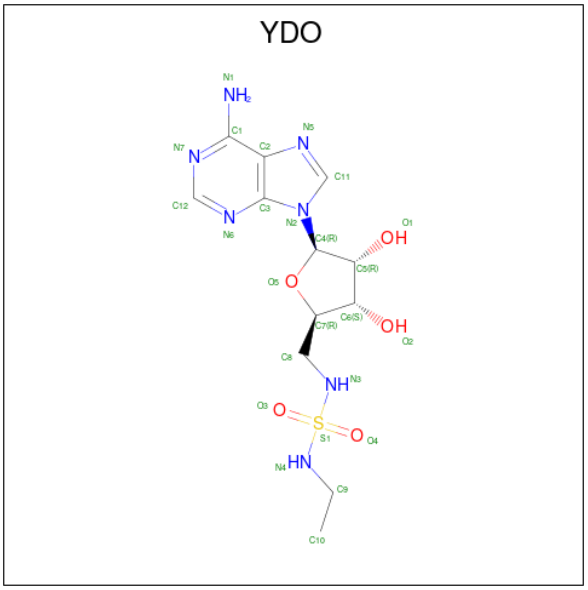
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP J9VFT1
B	-4	GLU	-	expression tag	UNP J9VFT1
B	-3	ASN	-	expression tag	UNP J9VFT1
B	-2	LEU	-	expression tag	UNP J9VFT1
B	-1	TYR	-	expression tag	UNP J9VFT1
B	0	PHE	-	expression tag	UNP J9VFT1
B	1	GLN	-	expression tag	UNP J9VFT1
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 (three-letter code: 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 (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is water.

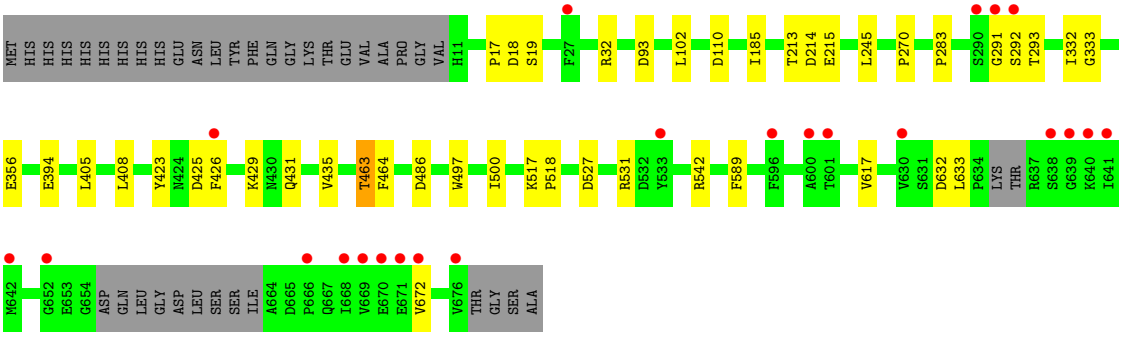
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total	O	0	0
			39	39		
4	B	58	Total	O	0	0
			58	58		
4	C	14	Total	O	0	0
			14	14		

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.

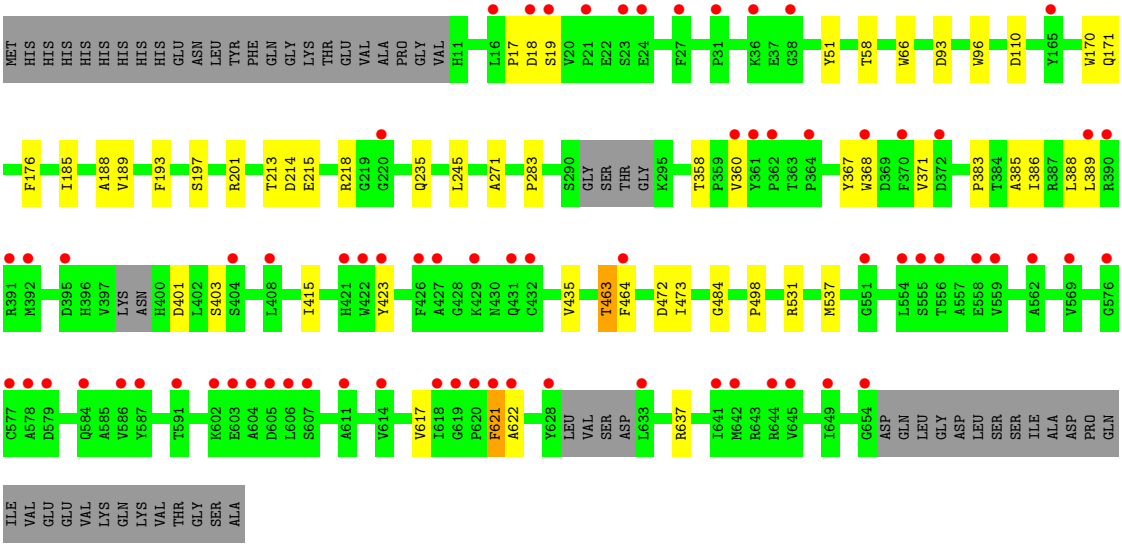
• Molecule 1: Acetyl-coenzyme A synthetase

Chain A:



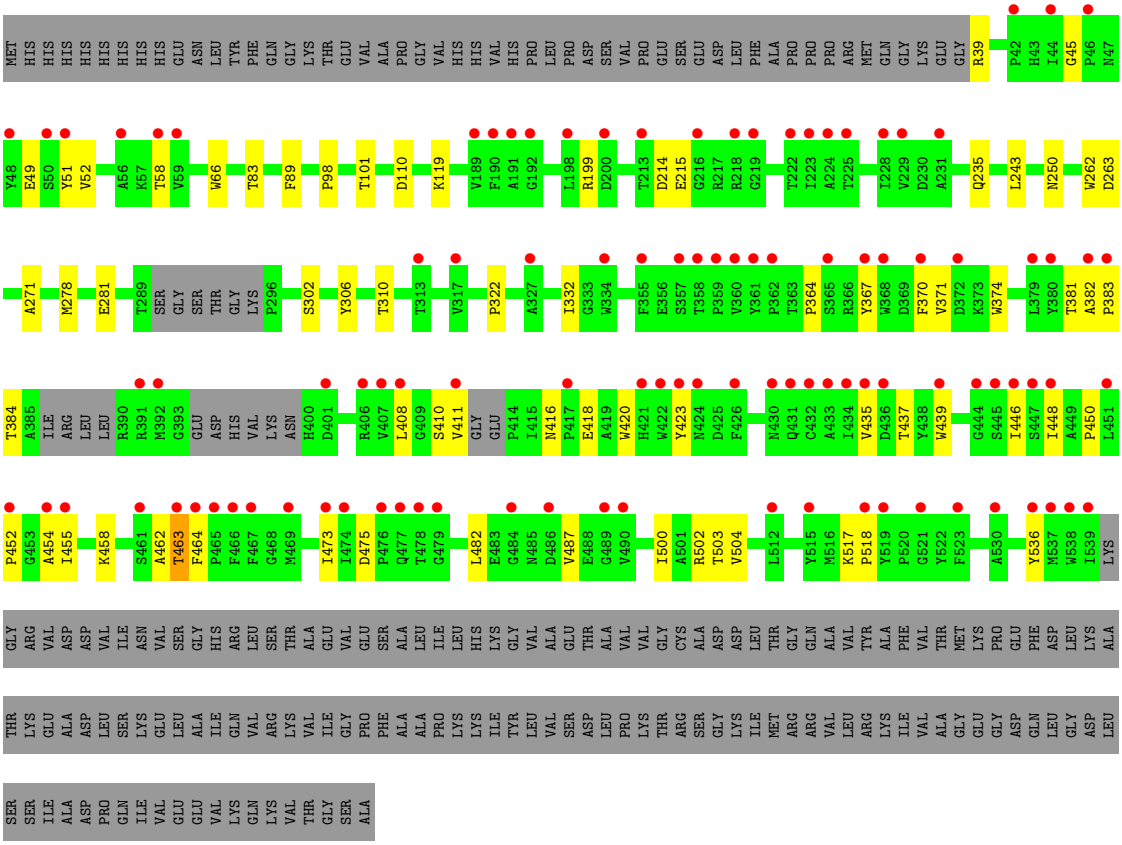
• Molecule 1: Acetyl-coenzyme A synthetase

Chain B:



• Molecule 1: Acetyl-coenzyme A synthetase

Chain C:


MET HIS HIS HIS HIS HIS HIS GLU ASN LEU TYR PHE GLN GLY LYS THR GLU VAL ALA PRO GLY VAL HIS HIS VAL HIS PRO LEU PRO ASP SER VAL PRO GLU SER GLU ASP LEU PHE ALA PRO PRO PRO ARG MET GLN GLY LYS GLU GLY
R39 P42 H43 I44 G45 P46 N47
Y48 E49 S50 Y51 V52 A56 K57 T58 V59 W66 T83 F89 P98 T101 D110 K119 V189 F190 A191 G192 L198 R199 D200 T213 D214 E215 G216 R217 R218 G219 T222 I223 A224 T225 I228 V229 D230 A231 Q235 L243 N250 W262 D263
A271 M278 E281 T289 SER GLY SER THR GLY LYS P296 S302 Y306 T310 T313 V317 P322 A327 I332 G333 W334 F355 E356 S357 T358 P359 V360 Y361 P362 T363 P364 S365 R366 Y367 W368 D369 F370 V371 D372 K373 W374 L379 Y380 T381 A382 P383
T384 A385 ILE ARG LEU LEU R390 R391 M392 G393 GLU ASP HIS VAL LYS ASN H400 D401 R406 V407 L408 G409 S410 V411 GLY GLU P414 I415 N416 P417 E418 A419 W420 H421 W422 Y423 N424 D425 F426 N430 Q431 C432 A433 I434 V435 D436 T437 Y438 W439 G444 S445 I446 S447 I448 A449 P450 L451
P452 G453 A454 I455 K458 S461 A462 T463 F464 P465 F466 F467 G468 M469 I473 I474 D475 P476 Q477 T478 G479 L482 E483 G484 N485 D486 V487 E488 G489 V490 I500 A501 R502 T503 V504 L512 Y515 M516 K517 P518 Y519 P520 G521 Y522 F523 A530 Y536 M537 W538 I539 LYS
GLY ARG VAL ASP ASP VAL ILE ASN VAL SER GLY HIS ARG LEU SER THR ALA GLU VAL GLU SER ALA LEU ILE LEU HIS LYS GLY VAL VAL ALA GLU THR ALA VAL VAL GLY CYS ALA ASP ASP LEU THR GLY GLN ALA VAL TYR ALA PHE VAL THR MET LYS PRO GLU PHE ASP LEU LYS ASP
THR LYS GLU ALA ASP LEU SER LYS GLU LEU ALA ILE GLN VAL ARG LYS VAL ILE GLY PRO PHE ALA ALA PRO LYS LYS ILE TYR LEU VAL SER ASP LEU PRO VAL LYS THR ARG SER GLY LYS ILE MET ARG ARG VAL LEU ARG LYS ILE VAL ALA GLY GLU GLY ASP GLN LEU GLY ASP LEU
SER SER ILE ALA ASP PRO GLN ILE VAL GLU GLU VAL LYS GLN LYS VAL THR GLY SER ALA

4 Data and refinement statistics (i)

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 84.58 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (76.84-2.50) 99.5 (84.58-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5162	Depositor
R, R_{free}	0.232 , 0.274 0.234 , 0.271	Depositor DCC
R_{free} test set	3713 reflections (4.92%)	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)	0.30 , 43.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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.*

[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: CL, YDO

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	0/5211	0.58	0/7102
1	B	0.39	0/5044	0.58	0/6880
1	C	0.36	0/3903	0.55	0/5322
All	All	0.38	0/14158	0.57	0/19304

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	23	0
1	B	4907	0	4682	32	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
4	B	58	0	0	0	0
4	C	14	0	0	0	0
All	All	13931	0	13148	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 4.

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: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:463:THR:OG1	1:A:464:PHE:N	2.37	0.56
1:A:632:ASP:OD1	1:A:633:LEU:N	2.38	0.56
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:THR:HG21	1:C:446:ILE:HD13	1.96	0.47
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:473:ILE:HD11	1:B:537:MET:HE1	1.97	0.46
1:B:401:ASP:OD1	1:B:403:SER:HB2	2.16	0.46
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: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:A:332:ILE:HD12	1:A:332:ILE:C	2.39	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
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:383:PRO:O	1:C:384:THR:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:332:ILE:C	1:C:332:ILE:HD12	2.41	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
1:C:263:ASP:N	1:C:263:ASP:OD1	2.54	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	649/694 (94%)	625 (96%)	22 (3%)	2 (0%)	41	61
1	B	626/694 (90%)	607 (97%)	18 (3%)	1 (0%)	47	68
1	C	473/694 (68%)	436 (92%)	34 (7%)	3 (1%)	25	43
All	All	1748/2082 (84%)	1668 (95%)	74 (4%)	6 (0%)	41	61

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 (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	523/576 (91%)	520 (99%)	3 (1%)	86 95
1	B	504/576 (88%)	497 (99%)	7 (1%)	67 86
1	C	390/576 (68%)	387 (99%)	3 (1%)	81 93
All	All	1417/1728 (82%)	1404 (99%)	13 (1%)	78 92

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	LEU
1	A	110	ASP
1	A	423	TYR
1	B	51	TYR
1	B	110	ASP
1	B	235	GLN
1	B	423	TYR
1	B	472	ASP
1	B	621	PHE
1	B	637	ARG
1	C	39	ARG
1	C	110	ASP
1	C	420	TRP

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

Mol	Chain	Res	Type
1	B	430	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	B	702	-	24,27,27	0.64	0	22,40,40	1.09	1 (4%)
2	YDO	A	701	-	24,27,27	0.68	0	22,40,40	1.08	1 (4%)

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	B	702	-	-	5/10/30/30	0/3/3/3
2	YDO	A	701	-	-	6/10/30/30	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	702	YDO	N6-C12-N7	-3.75	122.82	128.68
2	A	701	YDO	N6-C12-N7	-3.71	122.88	128.68

There are no chirality outliers.

All (11) torsion outliers are listed below:

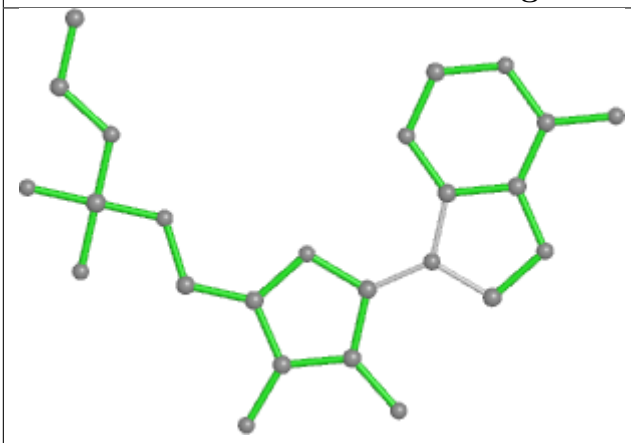
Mol	Chain	Res	Type	Atoms
2	A	701	YDO	C8-N3-S1-N4
2	A	701	YDO	C8-N3-S1-O3
2	A	701	YDO	C8-N3-S1-O4
2	A	701	YDO	C9-N4-S1-N3
2	A	701	YDO	C9-N4-S1-O3
2	B	702	YDO	C8-N3-S1-N4
2	B	702	YDO	C8-N3-S1-O3
2	B	702	YDO	C8-N3-S1-O4
2	A	701	YDO	C9-N4-S1-O4
2	B	702	YDO	C9-N4-S1-O3
2	B	702	YDO	C9-N4-S1-O4

There are no ring outliers.

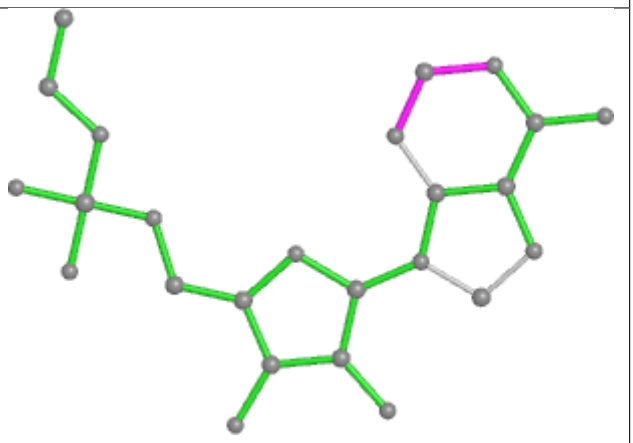
No monomer is involved in short contacts.

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 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.

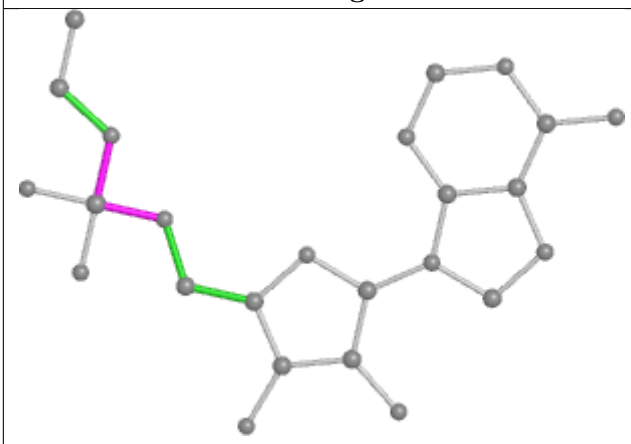
Ligand YDO B 702



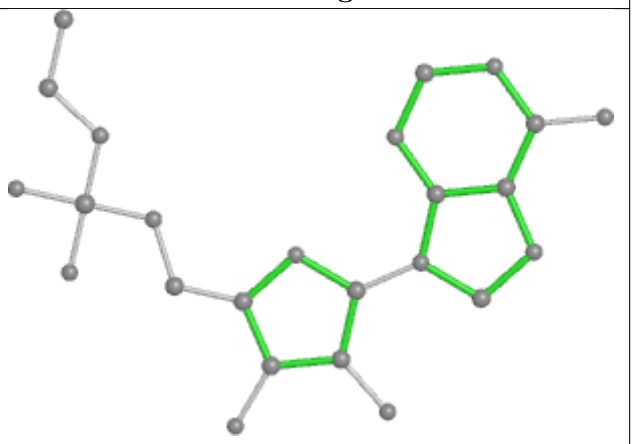
Bond lengths



Bond angles

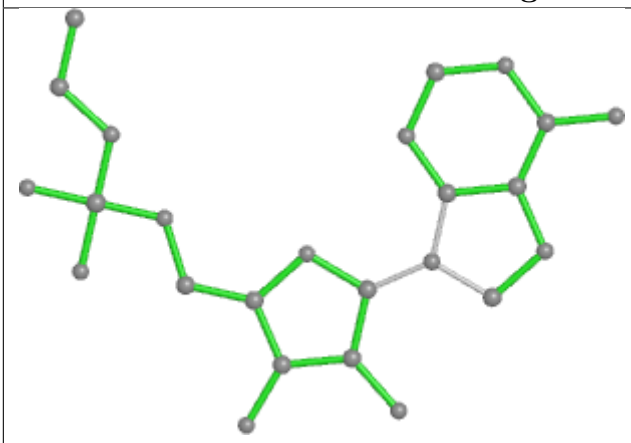


Torsions

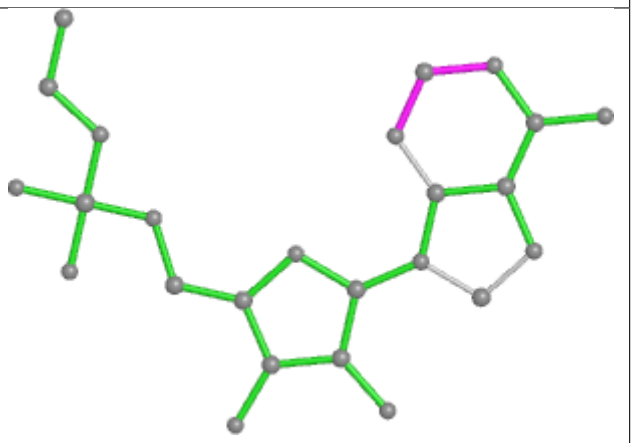


Rings

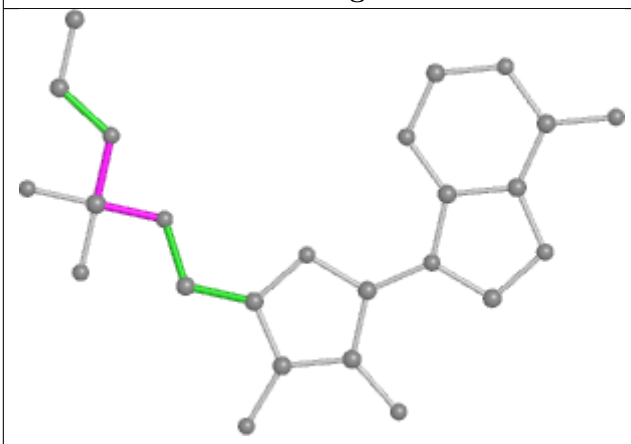
Ligand YDO A 701



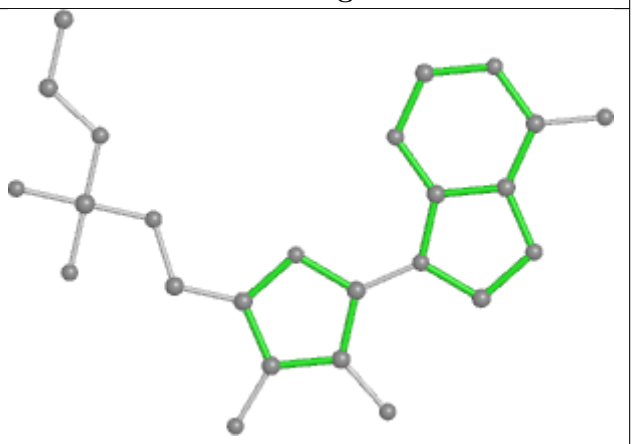
Bond lengths



Bond angles



Torsions



Rings

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, 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	655/694 (94%)	0.20	23 (3%) 44 47	28, 54, 97, 148	0
1	B	634/694 (91%)	0.70	72 (11%) 5 4	26, 68, 133, 187	0
1	C	483/694 (69%)	1.10	104 (21%) 0 0	31, 87, 132, 165	0
All	All	1772/2082 (85%)	0.62	199 (11%) 5 4	26, 65, 128, 187	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	423	TYR	7.1
1	A	672	VAL	7.0
1	C	382	ALA	6.8
1	B	622	ALA	6.7
1	C	426	PHE	6.5
1	B	577	CYS	6.4
1	B	555	SER	5.9
1	C	355	PHE	5.9
1	B	602	LYS	5.7
1	C	435	VAL	5.6
1	B	389	LEU	5.6
1	A	639	GLY	5.5
1	A	669	VAL	5.4
1	C	408	LEU	5.3
1	C	422	TRP	5.1
1	C	358	THR	4.9
1	C	455	ILE	4.9
1	B	603	GLU	4.8
1	C	417	PRO	4.8
1	B	606	LEU	4.7
1	B	554	LEU	4.7
1	C	359	PRO	4.7
1	C	490	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	368	TRP	4.5
1	C	434	ILE	4.5
1	A	642	MET	4.4
1	C	380	TYR	4.4
1	C	474	ILE	4.4
1	A	600	ALA	4.4
1	C	466	PHE	4.4
1	B	586	VAL	4.2
1	B	392	MET	4.2
1	C	477	GLN	4.2
1	C	44	ILE	4.2
1	C	46	PRO	4.2
1	B	361	TYR	4.1
1	B	576	GLY	4.1
1	B	16	LEU	4.0
1	A	601	THR	4.0
1	C	489	GLY	4.0
1	C	372	ASP	4.0
1	C	370	PHE	3.9
1	C	448	ILE	3.9
1	C	465	PRO	3.9
1	B	641	ILE	3.9
1	B	390	ARG	3.9
1	B	36	LYS	3.8
1	C	467	PHE	3.8
1	C	469	MET	3.8
1	C	189	VAL	3.8
1	C	327	ALA	3.7
1	B	607	SER	3.7
1	C	367	TYR	3.7
1	A	676	VAL	3.7
1	C	191	ALA	3.7
1	C	536	TYR	3.7
1	A	638	SER	3.6
1	C	383	PRO	3.6
1	B	628	TYR	3.6
1	C	464	PHE	3.6
1	C	537	MET	3.6
1	B	426	PHE	3.5
1	A	668	ILE	3.4
1	C	198	LEU	3.4
1	B	604	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	357	SER	3.4
1	C	479	GLY	3.4
1	C	362	PRO	3.4
1	B	621	PHE	3.4
1	B	551	GLY	3.4
1	C	463	THR	3.4
1	C	424	ASN	3.3
1	C	222	THR	3.3
1	C	518	PRO	3.3
1	B	614	VAL	3.3
1	B	619	GLY	3.3
1	B	569	VAL	3.3
1	C	192	GLY	3.2
1	C	530	ALA	3.2
1	A	666	PRO	3.2
1	B	559	VAL	3.2
1	B	423	TYR	3.1
1	B	558	GLU	3.1
1	B	645	VAL	3.1
1	C	223	ILE	3.1
1	B	578	ALA	3.1
1	C	379	LEU	3.1
1	A	640	LYS	3.1
1	A	290	SER	3.1
1	C	478	THR	3.1
1	C	486	ASP	3.0
1	C	51	TYR	3.0
1	B	432	CYS	3.0
1	A	292	SER	3.0
1	B	362	PRO	3.0
1	C	432	CYS	3.0
1	B	19	SER	2.9
1	C	190	PHE	2.9
1	B	605	ASP	2.9
1	B	21	PRO	2.9
1	B	31	PRO	2.9
1	C	48	TYR	2.9
1	B	611	ALA	2.8
1	C	231	ALA	2.8
1	B	562	ALA	2.8
1	B	38	GLY	2.8
1	C	452	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	364	PRO	2.7
1	B	360	VAL	2.7
1	C	461	SER	2.7
1	C	515	TYR	2.7
1	C	439	TRP	2.7
1	B	618	ILE	2.7
1	C	421	HIS	2.7
1	C	219	GLY	2.7
1	A	641	ILE	2.6
1	B	579	ASP	2.6
1	B	591	THR	2.6
1	C	360	VAL	2.6
1	C	436	ASP	2.6
1	A	670	GLU	2.6
1	B	620	PRO	2.6
1	C	431	GLN	2.6
1	C	538	TRP	2.6
1	C	200	ASP	2.6
1	C	444	GLY	2.6
1	B	587	TYR	2.6
1	C	56	ALA	2.5
1	A	426	PHE	2.5
1	C	224	ALA	2.5
1	C	451	LEU	2.5
1	C	446	ILE	2.5
1	B	372	ASP	2.5
1	C	407	VAL	2.5
1	C	484	GLY	2.5
1	B	649	ILE	2.5
1	C	523	PHE	2.5
1	B	633	LEU	2.5
1	C	519	TYR	2.5
1	A	671	GLU	2.4
1	C	473	ILE	2.4
1	C	476	PRO	2.4
1	B	27	PHE	2.4
1	C	454	ALA	2.4
1	B	408	LEU	2.4
1	A	596	PHE	2.4
1	B	421	HIS	2.4
1	C	42	PRO	2.4
1	B	431	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	430	ASN	2.3
1	C	50	SER	2.3
1	C	411	VAL	2.3
1	B	644	ARG	2.3
1	B	422	TRP	2.3
1	C	317	VAL	2.3
1	C	445	SER	2.3
1	C	512	LEU	2.3
1	A	27	PHE	2.3
1	B	654	GLY	2.3
1	C	521	GLY	2.3
1	B	24	GLU	2.2
1	B	23	SER	2.2
1	B	584	GLN	2.2
1	C	216	GLY	2.2
1	C	213	THR	2.2
1	C	59	VAL	2.2
1	B	427	ALA	2.2
1	C	313	THR	2.2
1	B	18	ASP	2.2
1	B	429	LYS	2.2
1	B	165	TYR	2.2
1	C	391	ARG	2.2
1	A	630	VAL	2.2
1	C	229	VAL	2.2
1	B	556	THR	2.2
1	A	291	GLY	2.2
1	C	365	SER	2.2
1	C	447	SER	2.2
1	B	642	MET	2.1
1	C	392	MET	2.1
1	B	395	ASP	2.1
1	C	406	ARG	2.1
1	B	370	PHE	2.1
1	B	220	GLY	2.1
1	C	401	ASP	2.1
1	C	361	TYR	2.1
1	C	433	ALA	2.1
1	C	539	ILE	2.1
1	B	464	PHE	2.1
1	C	218	ARG	2.1
1	C	58	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	225	THR	2.1
1	A	533	TYR	2.1
1	C	228	ILE	2.1
1	B	391	ARG	2.1
1	A	652	GLY	2.0
1	B	404	SER	2.0
1	B	368	TRP	2.0
1	C	334	TRP	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)

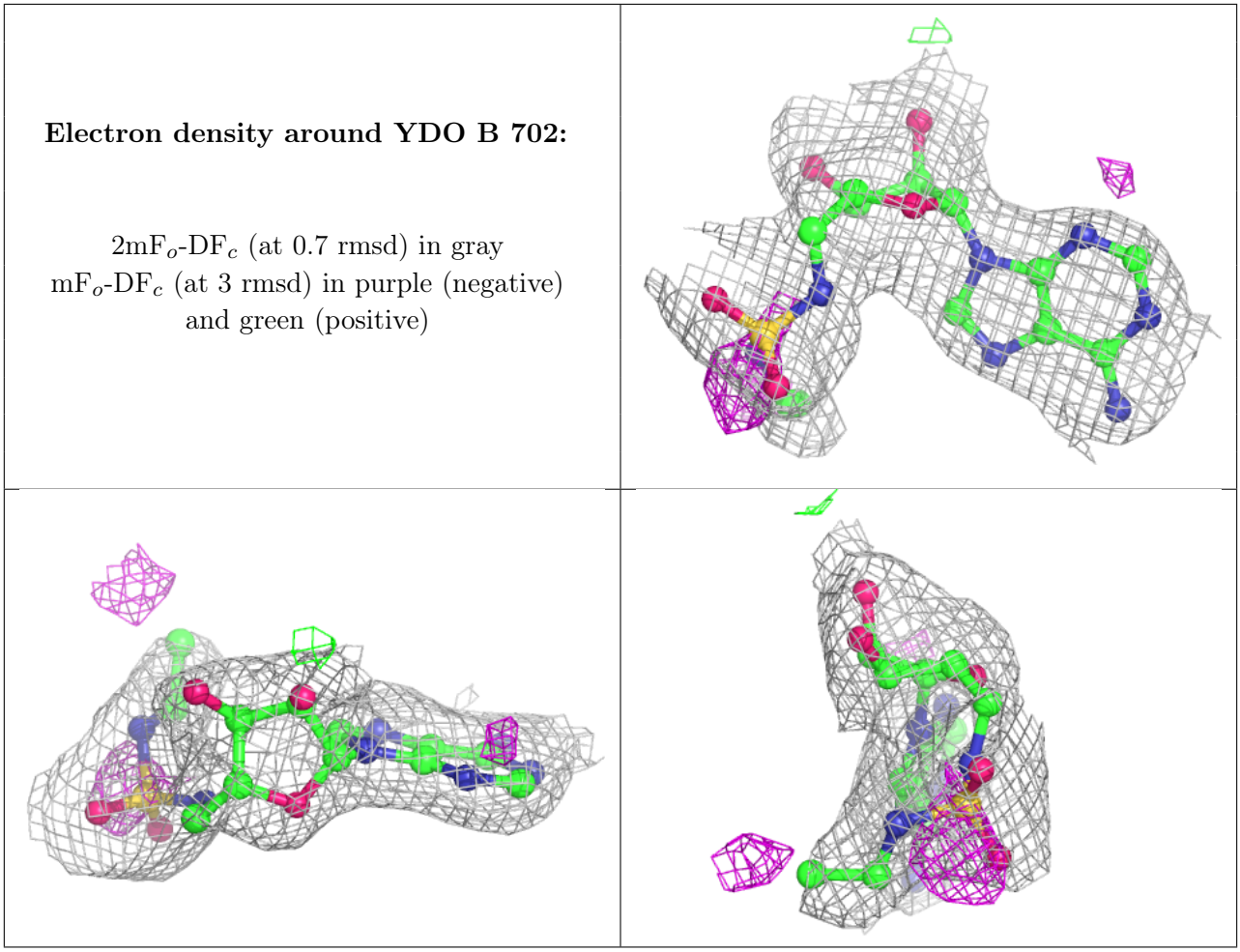
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	CL	B	701	1/1	0.90	0.15	73,73,73,73	0
2	YDO	B	702	25/25	0.91	0.18	47,59,63,70	0
2	YDO	A	701	25/25	0.93	0.17	37,41,50,54	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.

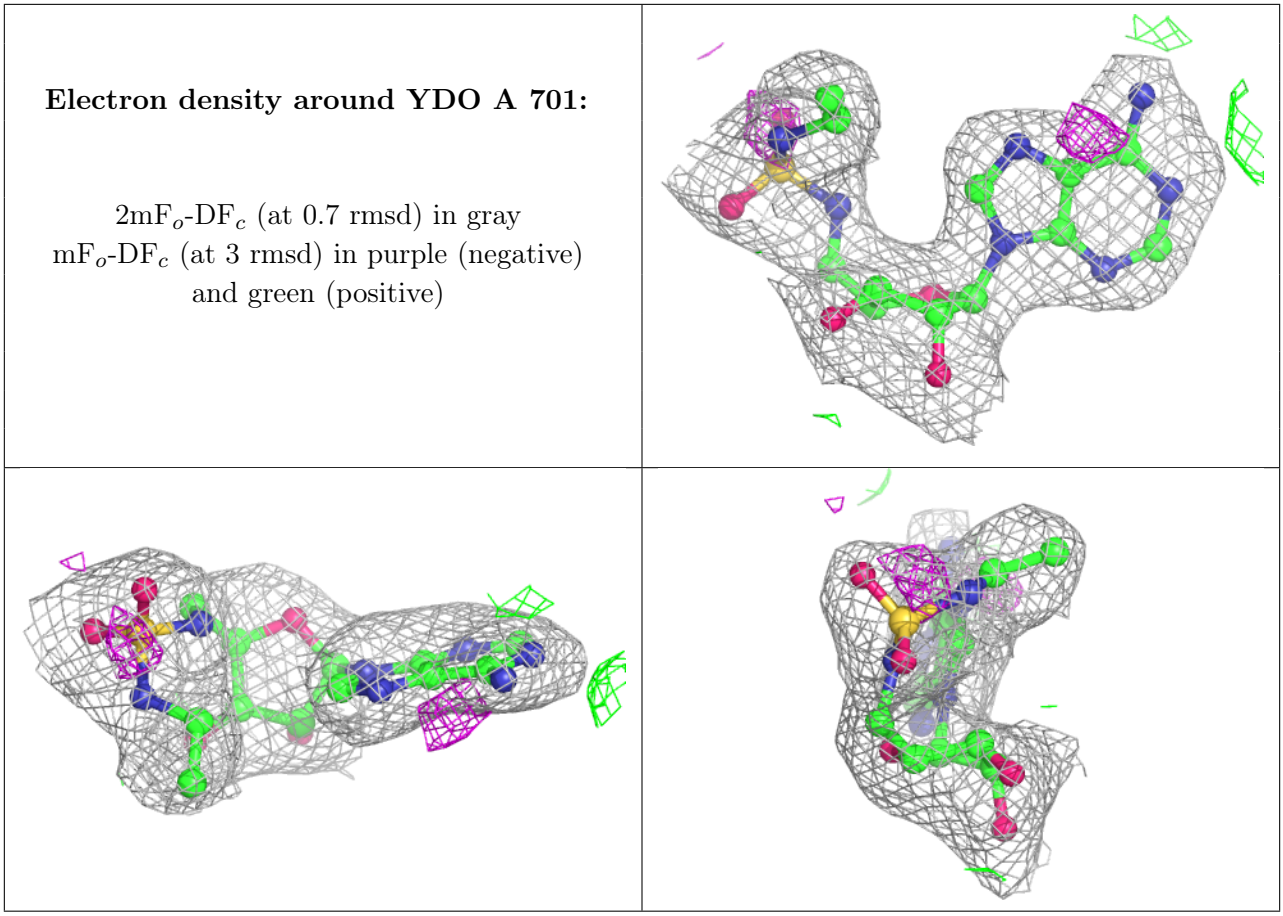
Electron density around YDO B 702:

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



Electron density around YDO A 701:

$2mF_o$-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.