Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 11:04 PM EST

PDB ID	:	4HWR
Title	:	Crystal structure of E. coli Threonyl-tRNA synthetase bound to a novel inhibitor
Authors	:	Hilgers, M.T.
Deposited on	:	2012-11-08
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

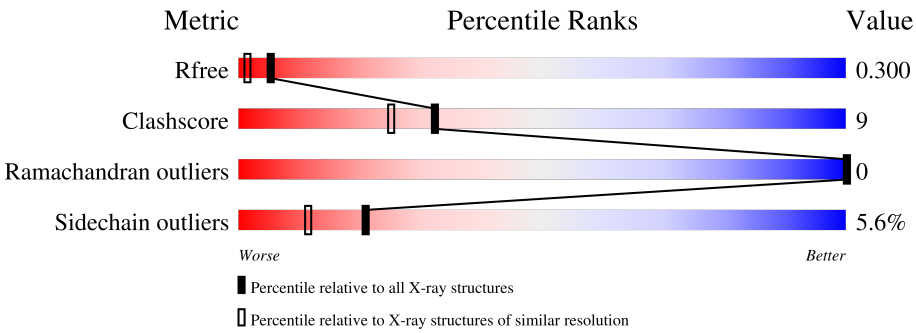
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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%

Mol	Chain	Length	Quality of chain
1	A	411	78% 16% • •
1	B	411	81% 13% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7039 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 Threonine–tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	403	3290	2078	578	611	23	0	0	0
1	B	398	3251	2053	573	602	23	0	0	0

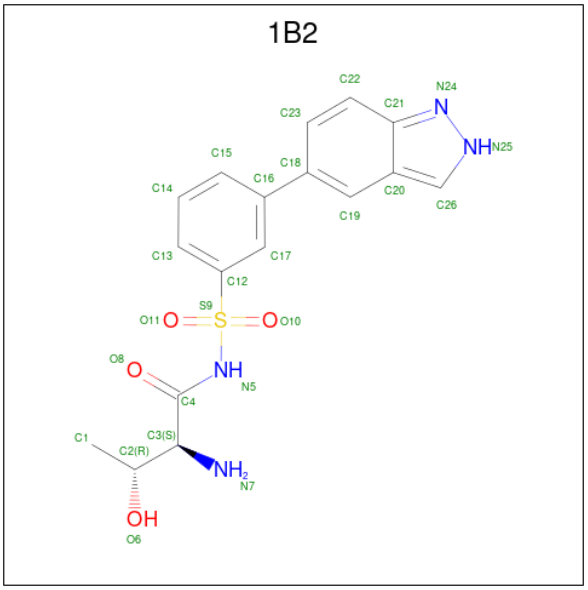
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	MET	-	expression tag	UNP P0A8M3
A	241	ALA	-	expression tag	UNP P0A8M3
A	643	LEU	-	expression tag	UNP P0A8M3
A	644	GLU	-	expression tag	UNP P0A8M3
A	645	HIS	-	expression tag	UNP P0A8M3
A	646	HIS	-	expression tag	UNP P0A8M3
A	647	HIS	-	expression tag	UNP P0A8M3
A	648	HIS	-	expression tag	UNP P0A8M3
A	649	HIS	-	expression tag	UNP P0A8M3
A	650	HIS	-	expression tag	UNP P0A8M3
B	240	MET	-	expression tag	UNP P0A8M3
B	241	ALA	-	expression tag	UNP P0A8M3
B	643	LEU	-	expression tag	UNP P0A8M3
B	644	GLU	-	expression tag	UNP P0A8M3
B	645	HIS	-	expression tag	UNP P0A8M3
B	646	HIS	-	expression tag	UNP P0A8M3
B	647	HIS	-	expression tag	UNP P0A8M3
B	648	HIS	-	expression tag	UNP P0A8M3
B	649	HIS	-	expression tag	UNP P0A8M3
B	650	HIS	-	expression tag	UNP P0A8M3

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0
			Total	Zn		
2	B	1	1	1	0	0

- Molecule 3 is N-{[3-(2H-indazol-5-yl)phenyl]sulfonyl}-L-threoninamide (three-letter code: 1B2) (formula: $C_{17}H_{18}N_4O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	26	17	4	4	1	0	0
			Total	C	N	O	S		
3	B	1	26	17	4	4	1	0	0

- Molecule 4 is water.

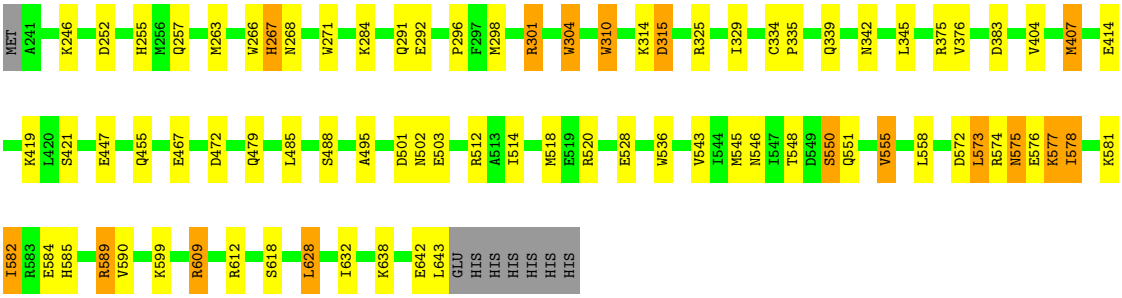
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	220	220	220	0	0
			Total	O		
4	B	224	224	224	0	0

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. 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. 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.

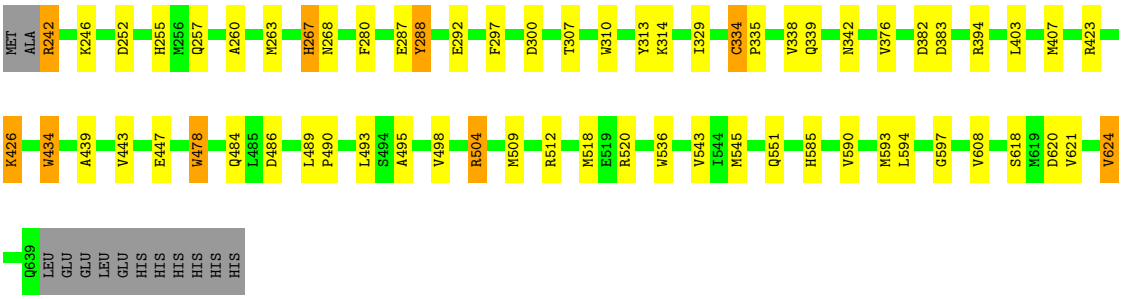
• Molecule 1: Threonine–tRNA ligase

Chain A:



• Molecule 1: Threonine–tRNA ligase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	156.90Å 109.78Å 87.00Å 90.00° 123.76° 90.00°	Depositor
Resolution (Å)	43.50 – 1.90 43.50 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.50-1.90) 99.3 (43.50-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.266 , 0.303 0.261 , 0.300	Depositor DCC
R_{free} test set	4806 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 19.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.348 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7039	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 1B2

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	0.79	6/3361 (0.2%)	0.81	7/4526 (0.2%)
1	B	0.77	4/3322 (0.1%)	0.81	1/4473 (0.0%)
All	All	0.78	10/6683 (0.1%)	0.81	8/8999 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	550	SER	CB-OG	7.54	1.52	1.42
1	A	304	TRP	CD2-CE2	5.89	1.48	1.41
1	A	271	TRP	CD2-CE2	5.82	1.48	1.41
1	A	536	TRP	CD2-CE2	5.61	1.48	1.41
1	B	310	TRP	CD2-CE2	5.45	1.47	1.41
1	B	536	TRP	CD2-CE2	5.31	1.47	1.41
1	B	434	TRP	CD2-CE2	5.25	1.47	1.41
1	A	266	TRP	CD2-CE2	5.24	1.47	1.41
1	A	310	TRP	CD2-CE2	5.22	1.47	1.41
1	B	478	TRP	CD2-CE2	5.21	1.47	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	407	MET	CG-SD-CE	6.70	110.92	100.20
1	A	383	ASP	CB-CG-OD1	5.97	123.67	118.30
1	B	300	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	485	LEU	CB-CG-CD2	-5.67	101.36	111.00
1	A	589	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	A	301	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	A	589	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	A	383	ASP	CB-CG-OD2	-5.08	113.72	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	3290	0	3224	74	0
1	B	3251	0	3185	58	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	26	0	16	1	0
3	B	26	0	16	3	0
4	A	220	0	0	8	1
4	B	224	0	0	7	0
All	All	7039	0	6441	115	1

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 9.

All (115) 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:A:546:ASN:ND2	1:A:573:LEU:HD12	1.60	1.16
1:B:394:ARG:HG3	4:B:959:HOH:O	1.48	1.11
1:A:575:ASN:OD1	1:A:576:GLU:HA	1.62	0.97
1:A:255:HIS:HD1	1:A:267:HIS:CE1	1.82	0.97
1:A:609:ARG:HD3	4:A:927:HOH:O	1.67	0.93
1:A:255:HIS:HD1	1:A:267:HIS:HE1	0.92	0.90
1:A:419:LYS:HD2	1:A:455:GLN:NE2	1.88	0.89
1:A:546:ASN:HD22	1:A:573:LEU:HD12	1.42	0.84
1:A:255:HIS:ND1	1:A:267:HIS:HE1	1.77	0.81
1:A:329:ILE:HD11	1:B:329:ILE:HD11	1.62	0.79
1:A:546:ASN:HD21	1:A:573:LEU:HD12	1.47	0.79
1:A:546:ASN:ND2	1:A:573:LEU:CD1	2.45	0.77
1:A:551:GLN:O	1:A:555:VAL:HG12	1.85	0.77
1:A:263:MET:HE1	1:B:297:PHE:HB3	1.68	0.76
1:A:575:ASN:OD1	1:A:576:GLU:CA	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:ILE:O	1:A:578:ILE:HD13	1.87	0.74
1:B:551:GLN:NE2	1:B:597:GLY:HA2	2.03	0.74
1:A:585:HIS:HD2	4:A:945:HOH:O	1.72	0.72
1:B:447:GLU:OE1	4:B:1019:HOH:O	2.08	0.71
1:B:498:VAL:HG22	1:B:504:ARG:NH2	2.05	0.71
1:B:594:LEU:HD22	1:B:608:VAL:HG22	1.74	0.70
1:A:575:ASN:OD1	1:A:575:ASN:C	2.30	0.70
1:A:638:LYS:HD2	1:A:642:GLU:HG3	1.72	0.70
1:A:284:LYS:CB	1:A:407:MET:HE2	2.24	0.67
1:A:292:GLU:H	1:B:268:ASN:ND2	1.93	0.67
1:A:292:GLU:H	1:B:268:ASN:HD22	1.42	0.67
1:A:546:ASN:HD21	1:A:573:LEU:HA	1.59	0.67
1:A:298:MET:HG2	1:B:263:MET:CE	2.24	0.66
1:A:575:ASN:OD1	1:A:576:GLU:N	2.29	0.66
1:A:419:LYS:HD2	1:A:455:GLN:HE21	1.60	0.66
1:A:246:LYS:NZ	4:A:996:HOH:O	2.28	0.66
1:A:257:GLN:HE22	1:B:339:GLN:HB3	1.60	0.66
1:A:263:MET:CE	1:B:297:PHE:HB3	2.25	0.65
1:A:284:LYS:HB3	1:A:407:MET:HE2	1.78	0.64
1:A:263:MET:HE2	1:B:297:PHE:H	1.63	0.64
1:B:484:GLN:HE22	3:B:702:1B2:H10	1.44	0.63
1:B:620:ASP:HB2	4:B:882:HOH:O	1.99	0.61
1:A:263:MET:HE3	4:B:1009:HOH:O	2.01	0.61
1:A:578:ILE:O	1:A:582:ILE:HG23	2.01	0.61
1:B:382:ASP:HB3	1:B:518:MET:CE	2.31	0.61
1:A:257:GLN:NE2	1:B:339:GLN:HB3	2.17	0.60
1:B:280:PHE:CE2	1:B:407:MET:HG2	2.37	0.59
1:A:252:ASP:OD1	1:A:267:HIS:HD2	1.86	0.59
1:A:298:MET:HG2	1:B:263:MET:HE2	1.85	0.58
1:A:546:ASN:HD21	1:A:573:LEU:CD1	2.15	0.57
1:B:342:ASN:HD21	1:B:495:ALA:HA	1.70	0.56
1:B:376:VAL:H	3:B:702:1B2:H17	1.54	0.56
1:B:394:ARG:CG	4:B:959:HOH:O	2.27	0.55
1:A:298:MET:HG2	1:B:263:MET:HE1	1.88	0.55
1:A:609:ARG:CD	4:A:927:HOH:O	2.38	0.55
1:A:268:ASN:HD22	1:B:292:GLU:H	1.54	0.55
1:A:376:VAL:H	3:A:702:1B2:H17	1.52	0.55
1:B:334:CYS:HB2	1:B:335:PRO:HD3	1.88	0.54
1:A:546:ASN:ND2	1:A:573:LEU:HA	2.23	0.53
1:B:621:VAL:HA	1:B:624:VAL:HG13	1.90	0.52
1:A:335:PRO:O	1:A:339:GLN:HG2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:VAL:HG11	1:A:585:HIS:CE1	2.44	0.52
1:B:382:ASP:HB3	1:B:518:MET:HE3	1.90	0.52
1:A:545:MET:HG2	1:A:581:LYS:HD3	1.92	0.52
1:A:342:ASN:HD21	1:A:495:ALA:HA	1.75	0.52
1:A:263:MET:CE	4:B:1009:HOH:O	2.58	0.51
1:B:585:HIS:HD2	4:B:921:HOH:O	1.92	0.51
1:B:307:THR:HG22	1:B:493:LEU:HD21	1.92	0.51
1:B:252:ASP:OD1	1:B:267:HIS:HD2	1.93	0.51
1:A:543:VAL:HG23	1:A:590:VAL:HG11	1.92	0.51
1:B:255:HIS:ND1	1:B:267:HIS:HE1	2.09	0.51
1:B:382:ASP:HB3	1:B:518:MET:HE1	1.94	0.50
1:B:490:PRO:HG3	1:B:509:MET:CE	2.41	0.50
1:B:242:ARG:NH2	1:B:246:LYS:HD3	2.26	0.50
1:B:334:CYS:CB	1:B:335:PRO:HD3	2.42	0.50
1:A:578:ILE:HD13	1:A:578:ILE:C	2.33	0.49
1:A:577:LYS:HG2	1:A:577:LYS:O	2.12	0.49
1:A:638:LYS:HD2	1:A:642:GLU:CG	2.41	0.49
1:A:296:PRO:HB3	1:B:263:MET:HB3	1.95	0.49
1:A:325:ARG:NH2	4:A:828:HOH:O	2.39	0.49
1:A:310:TRP:O	1:A:314:LYS:HB2	2.13	0.49
1:B:486:ASP:OD2	1:B:489:LEU:HD12	2.12	0.48
1:A:546:ASN:HD22	1:A:573:LEU:CD1	2.18	0.48
1:B:260:ALA:HB1	1:B:263:MET:HG3	1.95	0.48
1:B:439:ALA:O	1:B:443:VAL:HG23	2.14	0.47
1:A:546:ASN:HD21	1:A:573:LEU:CG	2.28	0.47
1:A:301:ARG:HD2	1:A:310:TRP:CH2	2.49	0.47
1:B:426:LYS:HD3	1:B:426:LYS:HA	1.71	0.47
1:B:498:VAL:HG22	1:B:504:ARG:HH22	1.77	0.47
1:B:490:PRO:HG3	1:B:509:MET:HE3	1.96	0.47
1:B:288:TYR:CZ	1:B:403:LEU:HD13	2.51	0.46
1:B:242:ARG:HH22	1:B:246:LYS:HD3	1.80	0.46
1:B:478:TRP:HB3	1:B:520:ARG:HD3	1.98	0.46
1:B:545:MET:HE1	1:B:593:MET:HB3	1.97	0.46
1:A:572:ASP:OD2	1:A:585:HIS:HE1	1.99	0.46
1:B:338:VAL:HG22	1:B:509:MET:HE1	1.97	0.46
1:B:543:VAL:HG11	1:B:585:HIS:CE1	2.51	0.45
1:A:291:GLN:NE2	4:A:810:HOH:O	2.44	0.45
1:A:268:ASN:ND2	1:B:292:GLU:H	2.15	0.45
1:A:339:GLN:HB3	1:B:257:GLN:OE1	2.17	0.45
1:A:479:GLN:O	1:A:520:ARG:NH1	2.45	0.45
1:A:404:VAL:HA	1:A:514:ILE:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ASP:N	1:A:315:ASP:OD1	2.49	0.44
1:A:421:SER:OG	1:A:467:GLU:OE2	2.27	0.44
1:A:263:MET:HE2	1:B:297:PHE:N	2.29	0.44
1:B:551:GLN:HE21	1:B:597:GLY:HA2	1.81	0.44
1:A:375:ARG:HD2	1:A:375:ARG:HA	1.84	0.44
1:B:307:THR:CG2	1:B:493:LEU:HD21	2.47	0.43
1:A:479:GLN:HG3	4:A:849:HOH:O	2.19	0.43
1:B:338:VAL:CG2	1:B:509:MET:HE1	2.49	0.42
1:B:543:VAL:HG23	1:B:590:VAL:HG11	2.01	0.42
1:A:284:LYS:CB	1:A:407:MET:CE	2.95	0.42
1:B:423:ARG:HB3	1:B:434:TRP:CE3	2.55	0.42
1:B:383:ASP:OD1	3:B:702:1B2:O6	2.37	0.42
1:A:304:TRP:CZ3	1:A:335:PRO:HG2	2.55	0.41
1:A:472:ASP:HB2	1:A:528:GLU:OE1	2.21	0.41
1:A:292:GLU:N	1:B:268:ASN:HD22	2.13	0.41
1:A:574:ARG:NH2	1:A:584:GLU:OE2	2.49	0.41
1:A:628:LEU:O	1:A:632:ILE:HG13	2.21	0.40
1:A:342:ASN:ND2	4:A:948:HOH:O	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:955:HOH:O	4:A:1001:HOH:O[2_656]	1.26	0.94

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	401/411 (98%)	389 (97%)	12 (3%)	0	100	100
1	B	396/411 (96%)	388 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	797/822 (97%)	777 (98%)	20 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	357/365 (98%)	329 (92%)	28 (8%)	12 5
1	B	353/365 (97%)	341 (97%)	12 (3%)	37 28
All	All	710/730 (97%)	670 (94%)	40 (6%)	21 11

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	267	HIS
1	A	315	ASP
1	A	334	CYS
1	A	345	LEU
1	A	414	GLU
1	A	447	GLU
1	A	488	SER
1	A	501	ASP
1	A	502	ASN
1	A	503	GLU
1	A	512	ARG
1	A	518	MET
1	A	548	THR
1	A	550	SER
1	A	555	VAL
1	A	558	LEU
1	A	573	LEU
1	A	575	ASN
1	A	577	LYS
1	A	578	ILE

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Mol	Chain	Res	Type
1	A	582	ILE
1	A	589	ARG
1	A	599	LYS
1	A	609	ARG
1	A	612	ARG
1	A	618	SER
1	A	628	LEU
1	A	643	LEU
1	B	242	ARG
1	B	267	HIS
1	B	287	GLU
1	B	288	TYR
1	B	313	TYR
1	B	314	LYS
1	B	334	CYS
1	B	426	LYS
1	B	504	ARG
1	B	512	ARG
1	B	618	SER
1	B	624	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	GLN
1	A	267	HIS
1	A	268	ASN
1	A	291	GLN
1	A	342	ASN
1	A	455	GLN
1	A	546	ASN
1	A	556	ASN
1	A	585	HIS
1	B	267	HIS
1	B	268	ASN
1	B	291	GLN
1	B	312	ASN
1	B	342	ASN
1	B	556	ASN
1	B	575	ASN
1	B	585	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are 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	$\#\|Z\| > 2$
3	1B2	A	702	2	26,28,28	1.72	4 (15%)	35,41,41	2.48	8 (22%)
3	1B2	B	702	2	26,28,28	2.17	4 (15%)	35,41,41	2.44	9 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1B2	A	702	2	-	5/23/23/23	0/3/3/3
3	1B2	B	702	2	-	7/23/23/23	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	1B2	C12-S9	-9.18	1.62	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	1B2	C12-S9	-6.42	1.66	1.76
3	A	702	1B2	N25-N24	2.75	1.43	1.37
3	B	702	1B2	N25-N24	2.57	1.42	1.37
3	A	702	1B2	S9-N5	-2.36	1.59	1.64
3	A	702	1B2	C26-C20	2.33	1.45	1.40
3	B	702	1B2	C13-C12	2.24	1.42	1.38
3	B	702	1B2	S9-N5	-2.02	1.60	1.64

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	702	1B2	O11-S9-O10	-10.93	106.12	119.55
3	A	702	1B2	O11-S9-O10	-9.93	107.34	119.55
3	A	702	1B2	C12-S9-N5	4.95	113.46	105.97
3	B	702	1B2	C12-S9-N5	3.95	111.95	105.97
3	A	702	1B2	C20-C26-N25	-3.81	101.55	111.30
3	A	702	1B2	C22-C21-N24	3.56	135.98	130.19
3	A	702	1B2	C26-C20-C21	3.48	112.04	104.66
3	A	702	1B2	C14-C13-C12	3.16	122.23	118.95
3	B	702	1B2	C22-C21-N24	2.96	135.01	130.19
3	B	702	1B2	C13-C12-S9	2.64	122.64	119.77
3	B	702	1B2	C20-C26-N25	-2.62	104.60	111.30
3	B	702	1B2	C13-C12-C17	-2.53	117.52	120.62
3	B	702	1B2	C26-C20-C21	2.47	109.89	104.66
3	A	702	1B2	C23-C22-C21	-2.34	117.89	120.84
3	A	702	1B2	O10-S9-C12	-2.15	105.32	107.97
3	B	702	1B2	C15-C16-C17	2.15	121.20	118.16
3	B	702	1B2	C14-C13-C12	2.05	121.08	118.95

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	702	1B2	C1-C2-C3-C4
3	B	702	1B2	O6-C2-C3-N7
3	B	702	1B2	C17-C12-S9-O10
3	B	702	1B2	C13-C12-S9-O10
3	A	702	1B2	C13-C12-S9-O10
3	A	702	1B2	C17-C12-S9-O10
3	B	702	1B2	O6-C2-C3-C4
3	B	702	1B2	C17-C12-S9-N5
3	B	702	1B2	C13-C12-S9-N5

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Mol	Chain	Res	Type	Atoms
3	A	702	1B2	C17-C12-S9-N5
3	A	702	1B2	C13-C12-S9-N5
3	A	702	1B2	O6-C2-C3-C4

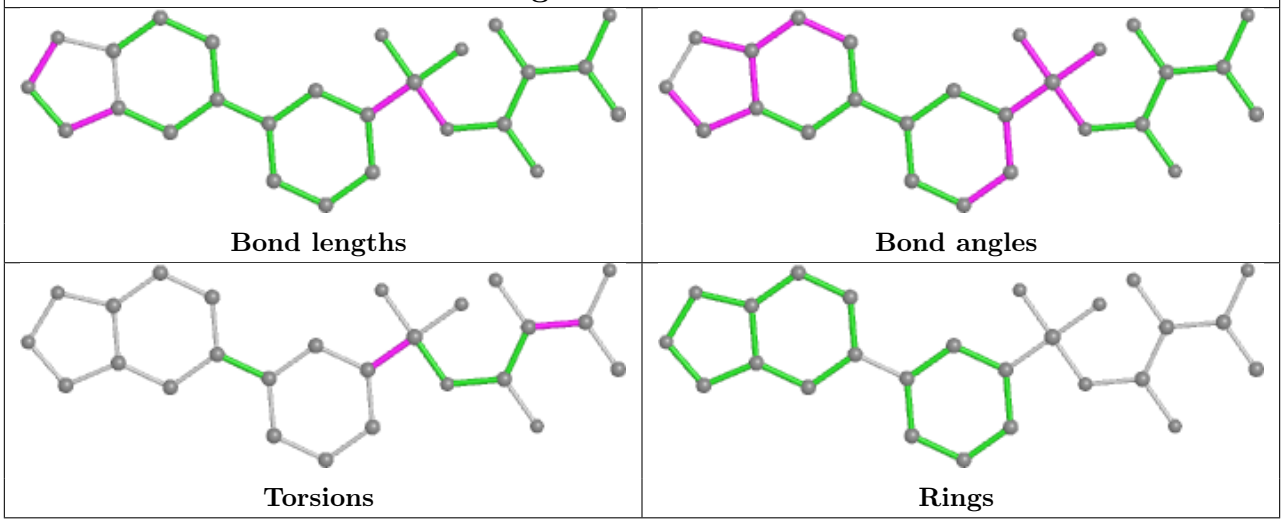
There are no ring outliers.

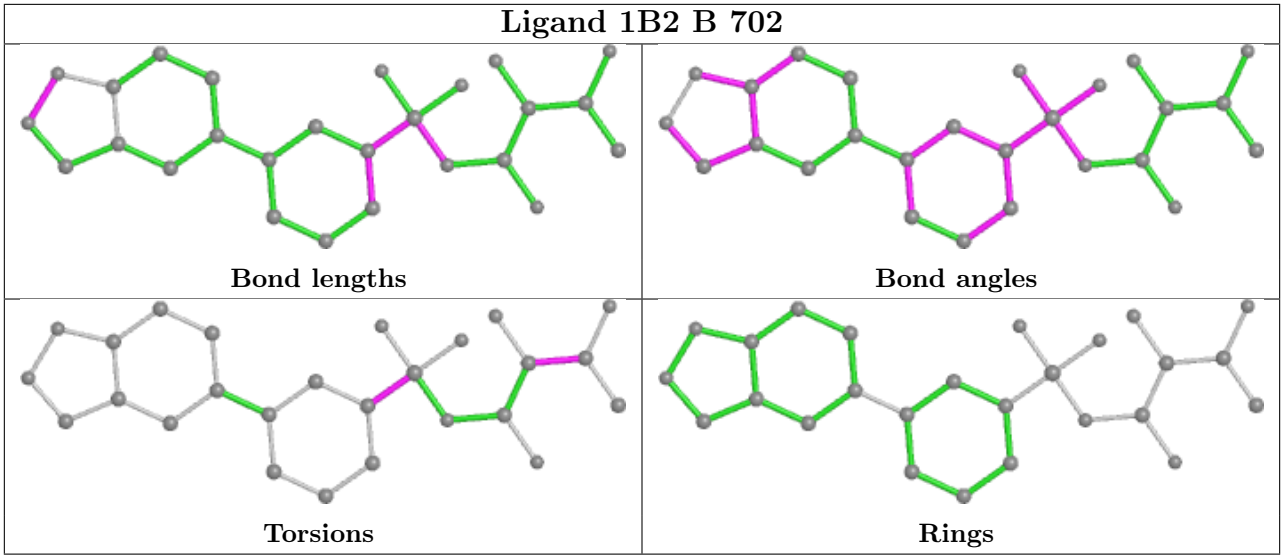
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	1B2	1	0
3	B	702	1B2	3	0

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

Ligand 1B2 A 702





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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

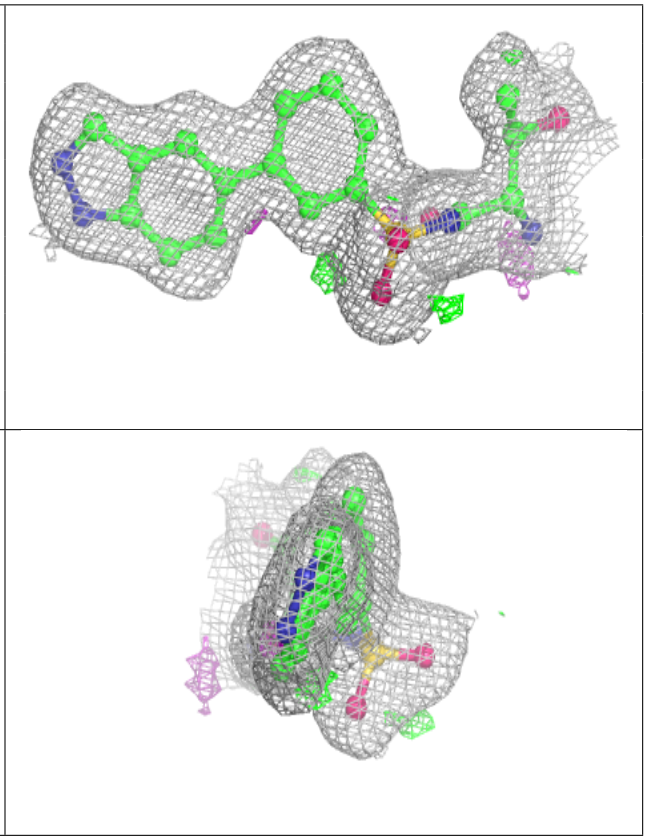
6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

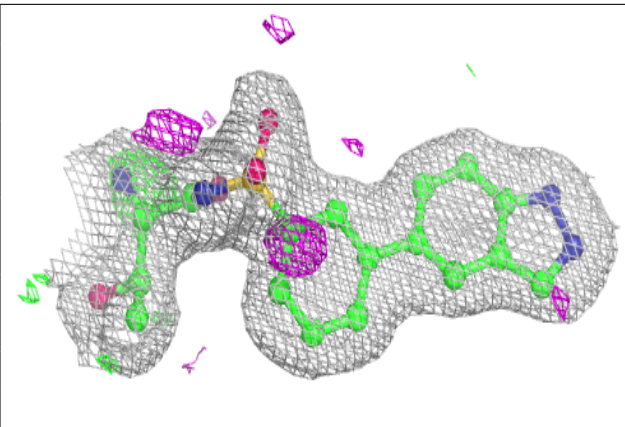
Electron density around 1B2 A 702:

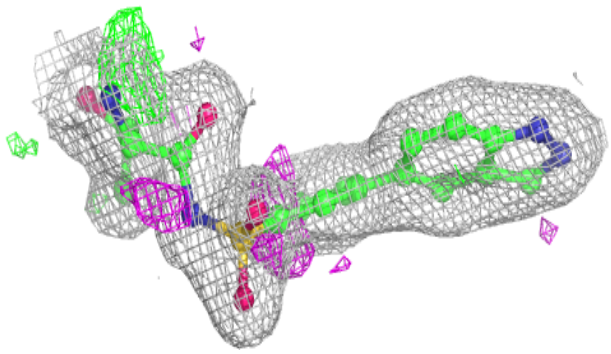
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

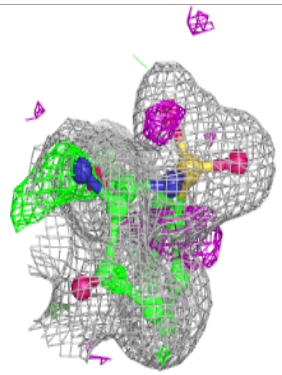


Electron density around 1B2 B 702:

$2mF_o$-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 (i)

Unable to reproduce the depositors R factor - this section is therefore empty.