Full wwPDB X-ray Structure Validation Report (i)

May 23, 2024 – 03:29 PM EDT

PDB ID	:	4K7Q
Title	:	Crystal Structure of AcrB Complexed with Linezolid at 3.5 Resolution
Authors	:	Hung, L.W.; Kim, H.B.; Murakami, S.; Gupta, G.; Kim, C.Y.; Terwilliger, T.C.
Deposited on	:	2013-04-17
Resolution	:	3.50 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 (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 (1)) were used in the production of this report:

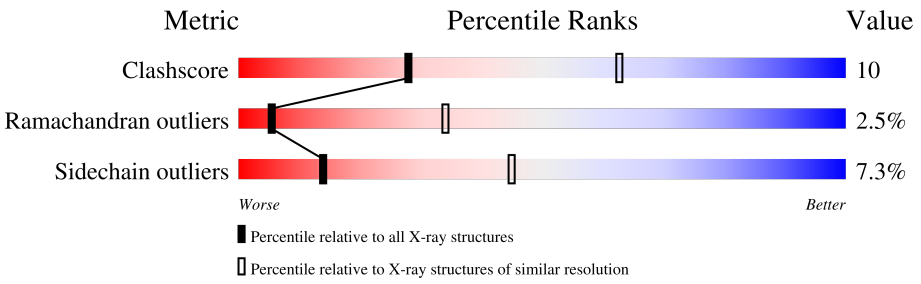
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.50 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))
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	1053	71% 21% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7700 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.

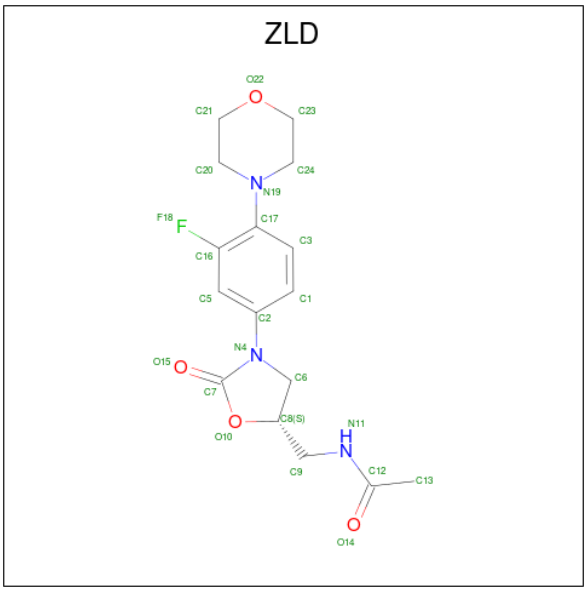
- Molecule 1 is a protein called Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1011	7676	4939	1267	1427	43	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	HIS	-	expression tag	UNP P31224
A	1051	HIS	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224

- Molecule 2 is N-{[(5S)-3-(3-fluoro-4-morpholin-4-ylphenyl)-2-oxo-1,3-oxazolidin-5-yl]methyl }acetamide (three-letter code: ZLD) (formula: $C_{16}H_{20}FN_3O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	24	16	1	3	4	0	0

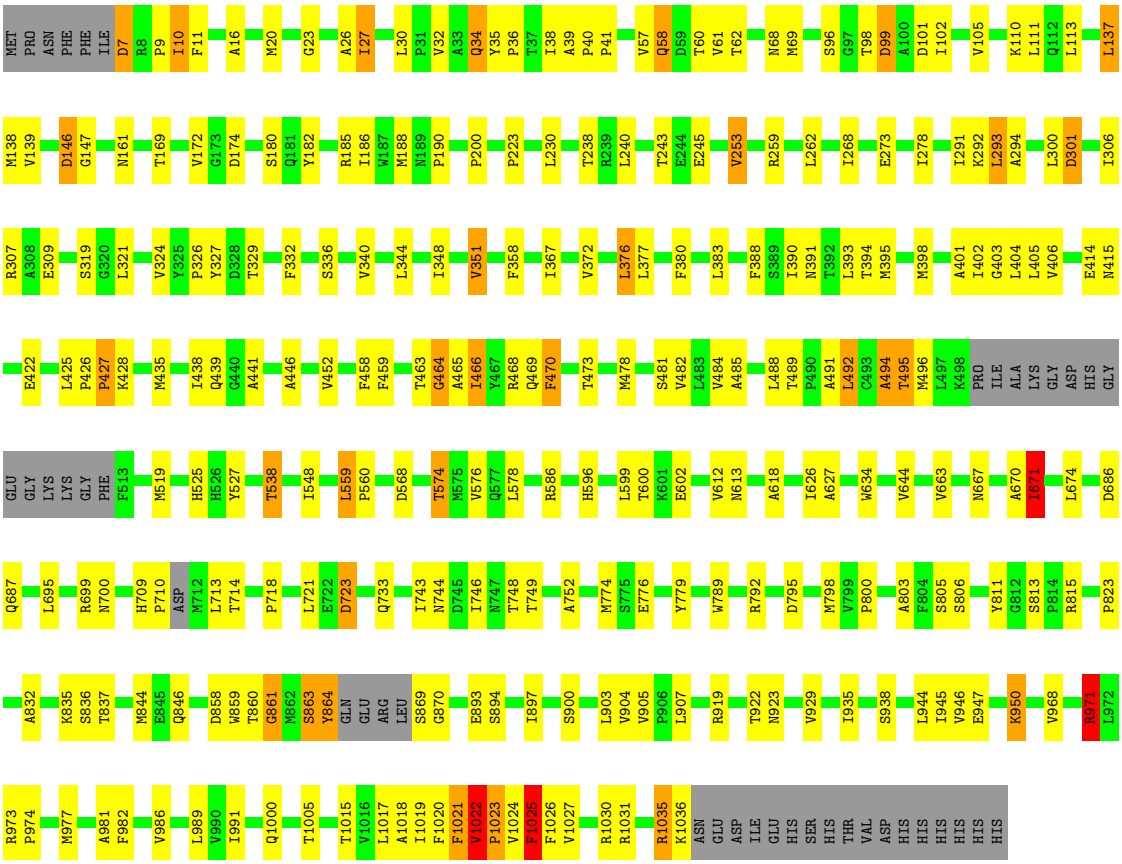
3 Residue-property plots (i)

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.

Note EDS failed to run properly.

- Molecule 1: Acriflavine resistance protein B

Chain A: 71% 21%



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	144.69Å 144.69Å 519.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.59 – 3.50	Depositor
% Data completeness (in resolution range)	99.9 (46.59-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.251 , 0.304	Depositor
Wilson B-factor (Å^2)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
L-test for twinning[1]	$< \|L\| >$ = (Not available), $< L^2 >$ = (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7700	wwPDB-VP
Average B, all atoms (Å^2)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

[1]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: ZLD

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	0.25	0/7817	0.43	1/10614 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1022	VAL	C-N-CD	5.91	140.81	128.40

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	7676	0	7833	154	0
2	A	24	0	20	0	0
All	All	7700	0	7853	154	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 10.

All (154) 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:1022:VAL:HG22	1:A:1023:PRO:HD3	1.19	1.09
1:A:1021:PHE:O	1:A:1022:VAL:O	1.83	0.96
1:A:907:LEU:HD21	1:A:1022:VAL:CG1	1.99	0.92
1:A:907:LEU:HD21	1:A:1022:VAL:HG11	1.52	0.90
1:A:1022:VAL:HG13	1:A:1023:PRO:CD	2.08	0.83
1:A:1022:VAL:CG2	1:A:1023:PRO:HD3	2.07	0.80
1:A:907:LEU:CD2	1:A:1022:VAL:HG11	2.11	0.80
1:A:1022:VAL:HG22	1:A:1023:PRO:CD	2.08	0.77
1:A:945:ILE:HD12	1:A:1024:VAL:HG12	1.70	0.74
1:A:1023:PRO:HB3	1:A:1027:VAL:HG13	1.72	0.72
1:A:1022:VAL:HG13	1:A:1023:PRO:HD2	1.69	0.72
1:A:240:LEU:HD12	1:A:245:GLU:HB3	1.71	0.71
1:A:351:VAL:HG23	1:A:981:ALA:HB1	1.74	0.68
1:A:686:ASP:HB3	1:A:823:PRO:HG2	1.75	0.68
1:A:1022:VAL:HG13	1:A:1023:PRO:N	2.08	0.68
1:A:618:ALA:O	1:A:815:ARG:NH1	2.27	0.68
1:A:612:VAL:HB	1:A:626:ILE:HG22	1.75	0.67
1:A:596:HIS:HA	1:A:599:LEU:HB2	1.78	0.66
1:A:351:VAL:HG21	1:A:406:VAL:HG11	1.77	0.66
1:A:485:ALA:HA	1:A:489:THR:HB	1.78	0.65
1:A:459:PHE:HB2	1:A:464:GLY:HA2	1.78	0.65
1:A:860:THR:OG1	1:A:861:GLY:N	2.27	0.65
1:A:574:THR:HG23	1:A:627:ALA:HB3	1.80	0.63
1:A:32:VAL:HG12	1:A:390:ILE:HD12	1.81	0.62
1:A:60:THR:HG23	1:A:61:VAL:HG23	1.82	0.62
1:A:372:VAL:HG11	1:A:406:VAL:HG22	1.81	0.62
1:A:1035:ARG:HD3	1:A:1035:ARG:H	1.66	0.61
1:A:32:VAL:HG23	1:A:300:LEU:HD23	1.82	0.60
1:A:34:GLN:O	1:A:391:ASN:ND2	2.32	0.59
1:A:428:LYS:HZ3	1:A:495:THR:H	1.49	0.59
1:A:709:HIS:O	1:A:709:HIS:ND1	2.35	0.59
1:A:110:LYS:HD3	1:A:113:LEU:HD12	1.84	0.58
1:A:30:LEU:HD23	1:A:390:ILE:HG13	1.85	0.58
1:A:26:ALA:O	1:A:30:LEU:HB2	2.04	0.58
1:A:907:LEU:HD21	1:A:1022:VAL:HG13	1.83	0.58
1:A:186:ILE:HD13	1:A:262:LEU:HD21	1.85	0.58
1:A:559:LEU:HD13	1:A:923:ASN:HB2	1.86	0.57
1:A:393:LEU:HD13	1:A:466:ILE:HA	1.87	0.56
1:A:20:MET:HA	1:A:377:LEU:HD13	1.88	0.56
1:A:903:LEU:HD11	1:A:1031:ARG:HH21	1.70	0.56
1:A:968:VAL:HB	1:A:1025:PHE:HZ	1.70	0.56
1:A:1018:ALA:HB1	1:A:1024:VAL:HG21	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PRO:HA	1:A:491:ALA:HB1	1.88	0.55
1:A:57:VAL:HA	1:A:60:THR:HG22	1.89	0.55
1:A:465:ALA:HA	1:A:468:ARG:HB3	1.88	0.55
1:A:484:VAL:HG13	1:A:488:LEU:HB3	1.88	0.55
1:A:723:ASP:HA	1:A:813:SER:HA	1.89	0.54
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.88	0.54
1:A:435:MET:HA	1:A:438:ILE:HB	1.90	0.53
1:A:904:VAL:HG12	1:A:938:SER:HB3	1.91	0.52
1:A:293:LEU:HD22	1:A:294:ALA:H	1.73	0.52
1:A:538:THR:HG23	1:A:1030:ARG:HH21	1.74	0.52
1:A:973:ARG:O	1:A:977:MET:HB2	2.09	0.52
1:A:441:ALA:HB2	1:A:947:GLU:HG2	1.93	0.51
1:A:800:PRO:HG2	1:A:803:ALA:HB2	1.93	0.51
1:A:190:PRO:HG3	1:A:789:TRP:CZ2	2.44	0.51
1:A:403:GLY:HA3	1:A:982:PHE:CD2	2.45	0.51
1:A:291:ILE:HG21	1:A:306:ILE:HD11	1.92	0.51
1:A:1023:PRO:CB	1:A:1027:VAL:HG13	2.39	0.51
1:A:405:LEU:HD22	1:A:481:SER:HB3	1.93	0.51
1:A:897:ILE:HG23	1:A:946:VAL:HG11	1.93	0.50
1:A:945:ILE:HD11	1:A:1019:ILE:HD12	1.92	0.50
1:A:670:ALA:O	1:A:671:ILE:HG12	2.12	0.50
1:A:907:LEU:CG	1:A:1022:VAL:HG11	2.40	0.50
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.93	0.50
1:A:16:ALA:O	1:A:20:MET:HG2	2.11	0.50
1:A:560:PRO:O	1:A:922:THR:OG1	2.27	0.50
1:A:919:ARG:NH2	1:A:1005:THR:OG1	2.44	0.50
1:A:1015:THR:O	1:A:1019:ILE:HG22	2.12	0.49
1:A:945:ILE:HA	1:A:971:ARG:CZ	2.42	0.49
1:A:36:PRO:HB3	1:A:469:GLN:HE22	1.78	0.49
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.94	0.49
1:A:402:ILE:O	1:A:406:VAL:HG23	2.12	0.49
1:A:832:ALA:HB3	1:A:835:LYS:HB2	1.95	0.49
1:A:169:THR:HG21	1:A:309:GLU:HB2	1.95	0.48
1:A:401:ALA:O	1:A:405:LEU:HG	2.13	0.48
1:A:971:ARG:O	1:A:974:PRO:HD2	2.13	0.48
1:A:1022:VAL:CG1	1:A:1023:PRO:CD	2.85	0.48
1:A:527:TYR:OH	1:A:1019:ILE:O	2.23	0.48
1:A:973:ARG:HB3	1:A:974:PRO:HD3	1.96	0.48
1:A:968:VAL:HB	1:A:1025:PHE:CZ	2.48	0.48
1:A:858:ASP:OD1	1:A:859:TRP:N	2.45	0.48
1:A:23:GLY:HA3	1:A:377:LEU:HB3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:MET:HE2	1:A:774:MET:O	2.14	0.48
1:A:391:ASN:H	1:A:394:THR:HG1	1.61	0.48
1:A:710:PRO:C	1:A:713:LEU:HA	2.33	0.47
1:A:253:VAL:HG12	1:A:259:ARG:HG2	1.95	0.47
1:A:667:ASN:OD1	1:A:667:ASN:N	2.47	0.47
1:A:744:ASN:O	1:A:748:THR:HG22	2.14	0.47
1:A:1022:VAL:O	1:A:1026:PHE:CD1	2.68	0.47
1:A:859:TRP:HE3	1:A:863:SER:HG	1.62	0.47
1:A:1021:PHE:O	1:A:1022:VAL:C	2.51	0.47
1:A:146:ASP:OD2	1:A:319:SER:OG	2.33	0.46
1:A:869:SER:OG	1:A:870:GLY:N	2.48	0.46
1:A:101:ASP:O	1:A:105:VAL:HG23	2.16	0.46
1:A:180:SER:OG	1:A:273:GLU:HB3	2.16	0.46
1:A:278:ILE:HG13	1:A:613:ASN:HB3	1.98	0.46
1:A:721:LEU:H	1:A:721:LEU:HD12	1.81	0.46
1:A:1035:ARG:HE	1:A:1036:LYS:HZ3	1.64	0.46
1:A:200:PRO:HD2	1:A:749:THR:HG22	1.98	0.45
1:A:1023:PRO:HB2	1:A:1024:VAL:H	1.65	0.45
1:A:301:ASP:N	1:A:301:ASP:OD1	2.48	0.45
1:A:559:LEU:HD23	1:A:560:PRO:HD2	1.98	0.45
1:A:836:SER:OG	1:A:837:THR:N	2.49	0.45
1:A:1021:PHE:C	1:A:1022:VAL:O	2.55	0.45
1:A:548:ILE:HD13	1:A:1017:LEU:HD21	1.99	0.45
1:A:578:LEU:HD12	1:A:586:ARG:HD2	1.99	0.45
1:A:34:GLN:HB3	1:A:35:TYR:H	1.55	0.44
1:A:746:ILE:O	1:A:749:THR:OG1	2.29	0.44
1:A:699:ARG:NH1	1:A:700:ASN:OD1	2.51	0.44
1:A:805:SER:OG	1:A:806:SER:N	2.50	0.44
1:A:137:LEU:HG	1:A:138:MET:H	1.82	0.44
1:A:494:ALA:O	1:A:496:MET:N	2.50	0.44
1:A:699:ARG:HE	1:A:718:PRO:HB3	1.82	0.44
1:A:415:ASN:HB3	1:A:438:ILE:HD11	2.00	0.44
1:A:172:VAL:HG13	1:A:291:ILE:HG23	2.01	0.43
1:A:425:LEU:C	1:A:427:PRO:HD3	2.38	0.43
1:A:58:GLN:O	1:A:62:THR:HB	2.19	0.43
1:A:576:VAL:HG13	1:A:663:VAL:HG22	2.01	0.43
1:A:41:PRO:HD2	1:A:96:SER:HA	2.01	0.43
1:A:376:LEU:HD22	1:A:398:MET:HE3	2.00	0.43
1:A:174:ASP:HB3	1:A:292:LYS:HD2	2.00	0.43
1:A:348:ILE:O	1:A:351:VAL:HG12	2.18	0.43
1:A:99:ASP:HB3	1:A:102:ILE:HG22	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:THR:O	1:A:864:TYR:HB2	2.19	0.42
1:A:733:GLN:OE1	1:A:743:ILE:HG12	2.20	0.42
1:A:596:HIS:O	1:A:600:THR:HG22	2.19	0.42
1:A:752:ALA:O	1:A:774:MET:HA	2.19	0.42
1:A:383:LEU:HB3	1:A:388:PHE:HB2	2.00	0.42
1:A:367:ILE:HG12	1:A:492:LEU:HD22	2.02	0.42
1:A:559:LEU:HA	1:A:560:PRO:HD2	1.92	0.42
1:A:27:ILE:HA	1:A:27:ILE:HD12	1.75	0.42
1:A:905:VAL:HG22	1:A:935:ILE:HG23	2.02	0.42
1:A:7:ASP:N	1:A:7:ASP:OD1	2.51	0.41
1:A:39:ALA:HA	1:A:40:PRO:HD3	1.95	0.41
1:A:139:VAL:O	1:A:326:PRO:HD2	2.19	0.41
1:A:27:ILE:HD13	1:A:380:PHE:CG	2.55	0.41
1:A:944:LEU:HD23	1:A:944:LEU:HA	1.90	0.41
1:A:1023:PRO:C	1:A:1025:PHE:N	2.73	0.41
1:A:332:PHE:O	1:A:336:SER:OG	2.32	0.41
1:A:900:SER:HA	1:A:1027:VAL:HB	2.03	0.41
1:A:989:LEU:HB3	1:A:1000:GLN:O	2.21	0.41
1:A:10:ILE:HD13	1:A:11:PHE:CE1	2.56	0.40
1:A:36:PRO:O	1:A:38:ILE:HG13	2.21	0.40
1:A:470:PHE:CD2	1:A:929:VAL:HG21	2.56	0.40
1:A:776:GLU:HB2	1:A:779:TYR:HD2	1.87	0.40
1:A:945:ILE:HA	1:A:971:ARG:NH1	2.35	0.40
1:A:414:GLU:OE2	1:A:974:PRO:HG3	2.22	0.40
1:A:568:ASP:OD2	1:A:644:VAL:HG23	2.21	0.40
1:A:903:LEU:HD12	1:A:1027:VAL:HG12	2.03	0.40
1:A:35:TYR:CD1	1:A:671:ILE:HG22	2.57	0.40
1:A:383:LEU:HD11	1:A:473:THR:HG23	2.04	0.40
1:A:907:LEU:HG	1:A:1022:VAL:HG11	2.04	0.40
1:A:950:LYS:HA	1:A:950:LYS:HD3	1.88	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	1003/1053 (95%)	884 (88%)	94 (9%)	25 (2%)	5 34

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	426	PRO
1	A	671	ILE
1	A	1022	VAL
1	A	1023	PRO
1	A	146	ASP
1	A	458	PHE
1	A	466	ILE
1	A	495	THR
1	A	861	GLY
1	A	1025	PHE
1	A	525	HIS
1	A	971	ARG
1	A	991	ILE
1	A	161	ASN
1	A	723	ASP
1	A	894	SER
1	A	34	GLN
1	A	427	PRO
1	A	494	ALA
1	A	1021	PHE
1	A	464	GLY
1	A	538	THR
1	A	147	GLY
1	A	223	PRO
1	A	986	VAL

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	822/859 (96%)	762 (93%)	60 (7%)	14 45

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	10	ILE
1	A	27	ILE
1	A	58	GLN
1	A	68	ASN
1	A	69	MET
1	A	98	THR
1	A	99	ASP
1	A	111	LEU
1	A	137	LEU
1	A	182	TYR
1	A	185	ARG
1	A	230	LEU
1	A	238	THR
1	A	243	THR
1	A	253	VAL
1	A	293	LEU
1	A	301	ASP
1	A	307	ARG
1	A	321	LEU
1	A	324	VAL
1	A	327	TYR
1	A	329	THR
1	A	344	LEU
1	A	351	VAL
1	A	358	PHE
1	A	376	LEU
1	A	404	LEU
1	A	422	GLU
1	A	439	GLN
1	A	452	VAL
1	A	463	THR
1	A	470	PHE
1	A	478	MET
1	A	492	LEU
1	A	519	MET
1	A	559	LEU
1	A	574	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	602	GLU
1	A	634	TRP
1	A	671	ILE
1	A	674	LEU
1	A	687	GLN
1	A	695	LEU
1	A	714	THR
1	A	792	ARG
1	A	795	ASP
1	A	798	MET
1	A	811	TYR
1	A	844	MET
1	A	846	GLN
1	A	863	SER
1	A	864	TYR
1	A	893	GLU
1	A	950	LYS
1	A	971	ARG
1	A	1020	PHE
1	A	1022	VAL
1	A	1025	PHE
1	A	1035	ARG

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

Mol	Chain	Res	Type
1	A	605	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
2	ZLD	A	1101	-	26,26,26	2.91	5 (19%)	36,36,36	2.21	15 (41%)

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	ZLD	A	1101	-	-	4/13/33/33	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	ZLD	C7-N4	11.49	1.47	1.36
2	A	1101	ZLD	O10-C7	5.46	1.42	1.35
2	A	1101	ZLD	O10-C8	-4.68	1.39	1.46
2	A	1101	ZLD	C12-N11	3.60	1.44	1.34
2	A	1101	ZLD	C6-C8	-2.07	1.49	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1101	ZLD	C6-N4-C7	-7.36	107.02	111.28
2	A	1101	ZLD	C5-C16-C17	-4.23	119.85	123.34
2	A	1101	ZLD	O10-C7-N4	-3.47	107.44	109.83
2	A	1101	ZLD	O10-C8-C6	3.43	108.03	104.57
2	A	1101	ZLD	O10-C7-O15	2.95	125.64	122.37
2	A	1101	ZLD	C6-C8-C9	-2.72	110.07	113.08
2	A	1101	ZLD	F18-C16-C17	2.63	120.81	118.42
2	A	1101	ZLD	O15-C7-N4	-2.51	126.92	128.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1101	ZLD	C6-N4-C2	2.42	125.55	121.45
2	A	1101	ZLD	C24-N19-C20	2.38	116.76	111.52
2	A	1101	ZLD	C3-C17-N19	-2.34	118.56	122.30
2	A	1101	ZLD	C13-C12-N11	2.21	120.01	116.09
2	A	1101	ZLD	C8-C6-N4	2.20	104.02	101.81
2	A	1101	ZLD	C8-O10-C7	-2.17	108.44	110.15
2	A	1101	ZLD	C23-O22-C21	2.03	116.66	109.89

There are no chirality outliers.

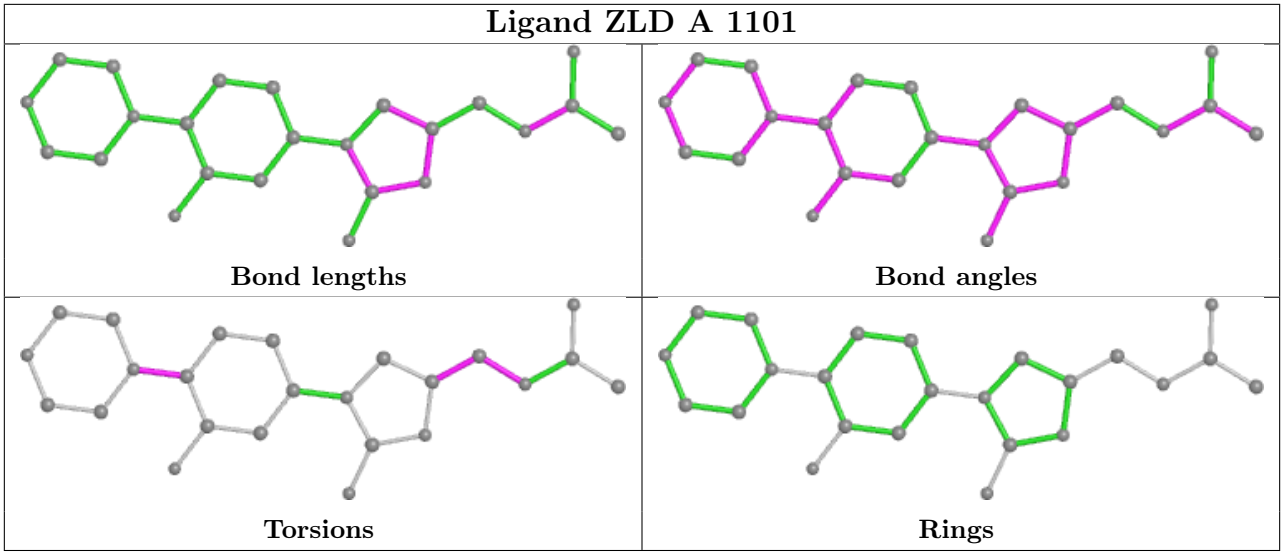
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	ZLD	C6-C8-C9-N11
2	A	1101	ZLD	O10-C8-C9-N11
2	A	1101	ZLD	C16-C17-N19-C24
2	A	1101	ZLD	C8-C9-N11-C12

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.



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)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.