

Full wwPDB X-ray Structure Validation Report (i)

Apr 20, 2024 – 10:58 pm BST

PDB ID	:	70IL
Title	:	mPI3Kd in complex with compound 58
Authors	:	Petersen, J.
Deposited on	:	2021-05-11
Resolution	:	1.95 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 1.95 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678(1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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					
			6%					
1	AAA	1084	63%	12%	•	24%		



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6958 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 Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit delta isoform.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	AAA	827	Total 6678	C 4281	N 1131	0 1211	S 55	3	1	0

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-39	MET	-	initiating methionine	UNP O35904
AAA	-38	SER	- expression tag		UNP O35904
AAA	-37	TYR	-	expression tag	UNP O35904
AAA	-36	HIS	-	expression tag	UNP O35904
AAA	-35	ASN	-	expression tag	UNP O35904
AAA	-34	HIS	-	expression tag	UNP O35904
AAA	-33	ASN	-	expression tag	UNP O35904
AAA	-32	HIS	-	expression tag	UNP O35904
AAA	-31	ASN	-	expression tag	UNP O35904
AAA	-30	HIS	-	expression tag	UNP O35904
AAA	-29	ASN	-	expression tag	UNP O35904
AAA	-28	HIS	-	expression tag	UNP O35904
AAA	-27	ASN	-	expression tag	UNP O35904
AAA	-26	HIS	-	expression tag	UNP O35904
AAA	-25	ASN	-	expression tag	UNP O35904
AAA	-24	ASP	-	expression tag	UNP O35904
AAA	-23	TYR	-	expression tag	UNP O35904
AAA	-22	ASP	-	expression tag	UNP O35904
AAA	-21	ILE	-	expression tag	UNP O35904
AAA	-20	PRO	-	expression tag	UNP O35904
AAA	-19	THR	-	expression tag	UNP O35904
AAA	-18	THR	-	expression tag	UNP O35904
AAA	-17	GLU	-	expression tag	UNP O35904
AAA	-16	ASN	-	expression tag	UNP O35904
AAA	-15	LEU	-	expression tag	UNP O35904
AAA	-14	TYR	-	expression tag	UNP 035904

There are 41 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual Comment		Reference
AAA	-13	PHE	-	expression tag	UNP O35904
AAA	-12	GLN	-	expression tag	UNP O35904
AAA	-11	GLY	-	expression tag	UNP O35904
AAA	-10	ALA	-	expression tag	UNP O35904
AAA	-9	MET	-	expression tag	UNP O35904
AAA	-8	ASP	-	expression tag	UNP O35904
AAA	-7	LEU	-	expression tag	UNP O35904
AAA	99	GLU	-	insertion	UNP O35904
AAA	100	ASN	-	insertion	UNP O35904
AAA	101	LEU	-	insertion	UNP O35904
AAA	102	TYR	-	insertion	UNP O35904
AAA	103	PHE	-	insertion	UNP O35904
AAA	104	GLN	-	insertion	UNP O35904
AAA	105	GLY	- insertion		UNP 035904
AAA	510A	GLN	-	insertion	UNP O35904

• Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total Na 1 1	0	0

• Molecule 3 is 2-[(1S)-1-cyclopropylethyl]-5-[4-methyl-2-[[6-(2-oxidanylidenepyrrolidin-1-yl) pyridin-2-yl]amino]-1,3-thiazol-5-yl]-7-methylsulfonyl-3H-isoindol-1-one (three-letter code: VEN) (formula: $C_{27}H_{29}N_5O_4S_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	С	N	0	S	0	0
Ŭ		_	38	27	5	4	2	Ŭ	

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	241	Total O 241 241	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 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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit delta isoform





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	142.01Å 64.75Å 116.38Å	Depositor
a, b, c, α , β , γ	90.00° 103.39° 90.00°	Depositor
Bosolution(A)	31.13 - 1.95	Depositor
Resolution (A)	31.13 - 1.95	EDS
% Data completeness	99.3 (31.13-1.95)	Depositor
(in resolution range)	99.3 (31.13 - 1.95)	EDS
R_{merge}	0.14	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.10 (at 1.95 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
B B.	0.239 , 0.289	Depositor
II, II free	0.244 , 0.293	DCC
R_{free} test set	3750 reflections $(5.03%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	30.8	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , 41.0	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6958	wwPDB-VP
Average B, all atoms $(Å^2)$	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.84% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: NA, VEN

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).

Mal	Chain	Bond	lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	AAA	0.76	0/6824	0.90	5/9207~(0.1%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AAA	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	AAA	902	ARG	NE-CZ-NH2	-9.27	115.66	120.30
1	AAA	912	PHE	CB-CA-C	7.48	125.36	110.40
1	AAA	652	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	AAA	962	ARG	CG-CD-NE	5.67	123.71	111.80
1	AAA	652	ARG	NE-CZ-NH1	5.40	123.00	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	912	PHE	Peptide



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	AAA	6678	0	6656	107	1
2	AAA	1	0	0	0	0
3	AAA	38	0	0	1	0
4	AAA	241	0	0	15	0
All	All	6958	0	6656	108	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 8.

All (108) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:AAA:495:ILE:O	1:AAA:497:GLU:N	2.10	0.85
1:AAA:235:GLN:N	4:AAA:1202:HOH:O	2.13	0.81
1:AAA:495:ILE:CG2	1:AAA:563:GLN:HA	2.12	0.79
1:AAA:495:ILE:HG23	1:AAA:563:GLN:HA	1.64	0.77
1:AAA:756:MET:HE1	1:AAA:781:GLY:HA3	1.67	0.77
1:AAA:367:SER:HB3	1:AAA:368:GLU:HB3	1.66	0.75
1:AAA:383:ASP:OD1	1:AAA:558:HIS:ND1	2.17	0.74
1:AAA:495:ILE:HG12	1:AAA:562:ALA:C	2.08	0.73
1:AAA:271:THR:O	1:AAA:273:HIS:HD2	1.72	0.73
1:AAA:330:GLY:O	1:AAA:331:ARG:HG3	1.88	0.72
1:AAA:328:ILE:HB	1:AAA:472:VAL:HG23	1.73	0.70
1:AAA:756:MET:CE	1:AAA:781:GLY:HA3	2.23	0.69
1:AAA:817:PRO:HD2	4:AAA:1235:HOH:O	1.92	0.69
1:AAA:687:GLU:OE2	4:AAA:1201:HOH:O	2.12	0.66
1:AAA:332:LYS:HE3	1:AAA:333:VAL:N	2.10	0.66
1:AAA:432:LEU:HB3	1:AAA:483:VAL:HG23	1.78	0.66
1:AAA:495:ILE:C	1:AAA:497:GLU:N	2.48	0.66
1:AAA:549:LEU:HG	1:AAA:564:MET:CE	2.25	0.66
3:AAA:1102:VEN:N30	3:AAA:1102:VEN:S22	2.70	0.64
1:AAA:367:SER:HB2	1:AAA:368:GLU:C	2.19	0.63
1:AAA:435:GLY:O	1:AAA:475:LEU:N	2.25	0.62
1:AAA:495:ILE:O	1:AAA:496:THR:C	2.37	0.62
1:AAA:495:ILE:CD1	1:AAA:562:ALA:O	2.48	0.61



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		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:AAA:833:THR:OG1	1:AAA:836:ASN:HB2	2.01	0.59
1:AAA:238:GLU:HG3	4:AAA:1386:HOH:O	2.02	0.59
1:AAA:358:VAL:HG22	1:AAA:377:PHE:CE1	2.36	0.59
1:AAA:495:ILE:HB	1:AAA:566:TYR:HB2	1.85	0.59
1:AAA:367:SER:CB	1:AAA:368:GLU:C	2.72	0.59
1:AAA:495:ILE:HD13	1:AAA:562:ALA:O	2.03	0.59
1:AAA:278:HIS:HE1	4:AAA:1386:HOH:O	1.85	0.58
1:AAA:892:GLY:O	1:AAA:894:ARG:NE	2.38	0.57
1:AAA:387:MET:HE3	1:AAA:590:CYS:HB3	1.86	0.57
1:AAA:1004:LEU:HD11	4:AAA:1424:HOH:O	2.04	0.57
1:AAA:495:ILE:HG21	1:AAA:563:GLN:HA	1.86	0.57
1:AAA:394:LEU:HD23	1:AAA:441:MET:HE1	1.88	0.56
1:AAA:700:LYS:HE2	1:AAA:756:MET:HE3	1.88	0.56
1:AAA:912:PHE:CB	1:AAA:913:GLY:HA3	2.36	0.55
1:AAA:954:GLU:OE1	1:AAA:957:ARG:NE	2.36	0.55
1:AAA:756:MET:HE2	1:AAA:780:ASN:O	2.06	0.55
1:AAA:495:ILE:HD13	1:AAA:566:TYR:HB2	1.89	0.54
1:AAA:495:ILE:HG12	1:AAA:562:ALA:O	2.06	0.53
1:AAA:245:GLY:HA3	1:AAA:768:ALA:HB2	1.90	0.52
1:AAA:662:LEU:O	1:AAA:666:LEU:HG	2.09	0.52
1:AAA:349:HIS:HE1	4:AAA:1265:HOH:O	1.92	0.52
1:AAA:331:ARG:O	1:AAA:469:ALA:HA	2.10	0.52
1:AAA:495:ILE:O	1:AAA:497:GLU:C	2.47	0.52
1:AAA:912:PHE:HB3	1:AAA:913:GLY:HA3	1.90	0.52
1:AAA:549:LEU:HG	1:AAA:564:MET:HE3	1.91	0.52
1:AAA:617:GLN:NE2	1:AAA:984:ALA:HA	2.26	0.51
1:AAA:340:LYS:HG3	1:AAA:364:ASN:HA	1.92	0.51
1:AAA:194:VAL:HG21	1:AAA:216:LEU:HD21	1.92	0.51
1:AAA:492:LEU:HA	1:AAA:495:ILE:HD12	1.93	0.51
1:AAA:367:SER:HB3	1:AAA:368:GLU:CB	2.37	0.50
1:AAA:579:ALA:HB1	1:AAA:600:LEU:HG	1.93	0.50
1:AAA:289:GLN:HG2	1:AAA:677:HIS:CD2	2.46	0.50
1:AAA:329:GLU:HG2	1:AAA:472:VAL:CG2	2.42	0.50
1:AAA:329:GLU:O	1:AAA:472:VAL:HG22	2.11	0.50
1:AAA:792:GLN:HB3	4:AAA:1419:HOH:O	2.11	0.50
1:AAA:902:ARG:HD2	4:AAA:1305:HOH:O	2.10	0.49
1:AAA:162:TRP:NE1	4:AAA:1216:HOH:O	2.44	0.49
1:AAA:278:HIS:CE1	4:AAA:1386:HOH:O	2.63	0.49
1:AAA:550:LEU:O	1:AAA:553:THR:HG23	2.13	0.49
1:AAA:419:ALA:HB3	1:AAA:441:MET:HE1	1.96	0.48
1:AAA:247:HIS:O	1:AAA:738:SER:HB2	2.12	0.48



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:AAA:962:ARG:HH11	1:AAA:962:ARG:HG2	1.79	0.48
1:AAA:170:GLN:HG3	4:AAA:1396:HOH:O	2.13	0.48
1:AAA:330:GLY:C	1:AAA:331:ARG:HG3	2.33	0.48
1:AAA:495:ILE:CG1	1:AAA:562:ALA:O	2.62	0.48
1:AAA:423:LEU:N	1:AAA:423:LEU:CD1	2.78	0.47
1:AAA:271:THR:O	1:AAA:273:HIS:CD2	2.60	0.47
1:AAA:495:ILE:CB	1:AAA:566:TYR:HB2	2.44	0.47
1:AAA:617:GLN:HE22	1:AAA:620:LYS:NZ	2.11	0.47
1:AAA:617:GLN:HE21	1:AAA:984:ALA:HA	1.80	0.47
1:AAA:970:HIS:HD2	4:AAA:1437:HOH:O	1.98	0.47
1:AAA:238:GLU:CG	4:AAA:1386:HOH:O	2.61	0.46
1:AAA:154:ARG:HD2	1:AAA:165:TYR:CE2	2.51	0.46
1:AAA:329:GLU:HB2	1:AAA:369:PRO:O	2.15	0.46
1:AAA:549:LEU:O	1:AAA:552:VAL:HG22	2.16	0.46
1:AAA:828:VAL:CG1	1:AAA:902:ARG:HD3	2.46	0.46
1:AAA:808:LEU:HA	1:AAA:877:LEU:HB3	1.98	0.45
1:AAA:235:GLN:HG3	1:AAA:237:GLU:OE1	2.17	0.45
1:AAA:700:LYS:HE2	1:AAA:756:MET:CE	2.47	0.45
1:AAA:859:LEU:HD21	1:AAA:905:GLY:HA2	1.98	0.45
1:AAA:138:ASP:OD2	1:AAA:428:TYR:OH	2.24	0.45
1:AAA:489:GLU:HG3	1:AAA:490:LYS:N	2.32	0.44
1:AAA:976:HIS:O	1:AAA:980:LEU:HG	2.17	0.44
1:AAA:433:LYS:O	1:AAA:475:LEU:HD22	2.17	0.44
1:AAA:860:LYS:HG2	1:AAA:868:LEU:HD22	2.00	0.44
1:AAA:700:LYS:HE3	1:AAA:756:MET:O	2.17	0.44
1:AAA:419:ALA:HB1	1:AAA:441:MET:HB3	1.99	0.43
1:AAA:495:ILE:CG1	1:AAA:562:ALA:HB1	2.48	0.43
1:AAA:494:LEU:O	1:AAA:494:LEU:HG	2.18	0.43
1:AAA:329:GLU:HG2	1:AAA:472:VAL:HG22	2.00	0.43
1:AAA:495:ILE:HG21	1:AAA:566:TYR:CB	2.49	0.43
1:AAA:386:ARG:HG3	1:AAA:387:MET:HE2	2.01	0.43
1:AAA:366:CYS:O	1:AAA:367:SER:CB	2.66	0.42
1:AAA:332:LYS:HE3	1:AAA:332:LYS:C	2.39	0.42
1:AAA:394:LEU:HD23	1:AAA:441:MET:CE	2.50	0.42
1:AAA:684:LYS:CE	4:AAA:1257:HOH:O	2.68	0.42
1:AAA:367:SER:CB	1:AAA:368:GLU:CA	2.98	0.42
1:AAA:898:ASN:HB3	1:AAA:911:ASP:OD2	2.20	0.41
1:AAA:155:GLN:NE2	1:AAA:290:SER:HB3	2.36	0.41
1:AAA:429:LYS:O	1:AAA:430:ASP:HB2	2.21	0.41
1:AAA:340:LYS:O	1:AAA:396:ALA:HA	2.20	0.41
1:AAA:587:PHE:HB3	1:AAA:592:VAL:HG11	2.02	0.41



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:214:LEU:HD12	1:AAA:217:MET:HE3	2.03	0.41
1:AAA:387:MET:HE2	1:AAA:590:CYS:SG	2.60	0.40
1:AAA:419:ALA:HB3	1:AAA:441:MET:CE	2.51	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)
1:AAA:714:MET:SD	1:AAA:714:MET:SD[2_555]	1.78	0.42

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	AAA	806/1084~(74%)	766~(95%)	35~(4%)	5(1%)	25 14

All (5) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	AAA	367	SER
1	AAA	496	THR
1	AAA	1026	SER
1	AAA	372	LYS
1	AAA	514	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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, a	and	the	total	number	of	residues.
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	734/962~(76%)	699~(95%)	35~(5%)	25	12

All (35) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	AAA	111	LYS
1	AAA	203	PHE
1	AAA	206	GLN
1	AAA	270	LEU
1	AAA	281	SER
1	AAA	291	ASN
1	AAA	316	LEU
1	AAA	332	LYS
1	AAA	340	LYS
1	AAA	352	GLU
1	AAA	360	SER
1	AAA	366	CYS
1	AAA	374	ARG
1	AAA	389	ARG
1	AAA	423	LEU
1	AAA	475	LEU
1	AAA	483	VAL
1	AAA	495	ILE
1	AAA	517	ARG
1	AAA	523	LEU
1	AAA	530	LEU
1	AAA	553	THR
1	AAA	557	LYS
1	AAA	560	ASP
1	AAA	634	LEU
1	AAA	731	LEU
1	AAA	754	SER
1	AAA	841	LYS
1	AAA	847	THR
1	AAA	898	ASN
1	AAA	915	PHE
1	AAA	947	THR
1	AAA	962	ARG
1	AAA	990	SER
1	AAA	1004	LEU



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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).

Mal	Tuno	Chain	Dog	Link	Bo	ond leng	\mathbf{ths}	В	ond ang	gles
	Type	Ullaili	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	VEN	AAA	1102	-	37,43,43	1.32	6 (16%)	43,66,66	3.98	15 (34%)

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	VEN	AAA	1102	-	-	2/24/50/50	0/6/6/6

All (6) bond length outliers are listed below:



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Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
3	AAA	1102	VEN	C8-N7	3.10	1.49	1.46
3	AAA	1102	VEN	C10-C9	-2.90	1.34	1.39
3	AAA	1102	VEN	C20-S17	2.33	1.84	1.75
3	AAA	1102	VEN	C28-C29	2.27	1.44	1.39
3	AAA	1102	VEN	C32-N31	2.09	1.50	1.47
3	AAA	1102	VEN	C23-N24	2.00	1.40	1.36

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	AAA	1102	VEN	C8-N7-C15	-15.05	106.93	113.12
3	AAA	1102	VEN	C9-C8-N7	14.66	107.06	102.18
3	AAA	1102	VEN	C34-C35-N31	5.94	112.21	108.23
3	AAA	1102	VEN	C32-N31-C29	5.63	126.52	120.53
3	AAA	1102	VEN	C33-C32-N31	5.01	108.80	103.42
3	AAA	1102	VEN	C25-N30-C29	4.87	123.01	117.69
3	AAA	1102	VEN	O19-S17-O18	4.19	125.13	117.92
3	AAA	1102	VEN	O16-C15-N7	-3.87	122.34	125.24
3	AAA	1102	VEN	O19-S17-C13	-3.63	104.04	108.27
3	AAA	1102	VEN	O19-S17-C20	-3.32	103.72	108.49
3	AAA	1102	VEN	C32-N31-C35	-3.30	109.88	112.95
3	AAA	1102	VEN	C12-C13-C14	-3.23	117.29	120.72
3	AAA	1102	VEN	C1-C2-C4	-2.33	108.21	113.36
3	AAA	1102	VEN	O16-C15-C14	-2.15	126.04	129.09
3	AAA	1102	VEN	C28-C29-N30	-2.06	120.17	123.53

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	1102	VEN	C10-C11-C21-C38
3	AAA	1102	VEN	C12-C11-C21-C38

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	1102	VEN	1	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 similar 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AAA	1

All chain breaks are listed below:



Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AAA	497:GLU	С	509:GLU	Ν	21.72



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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		$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	AAA	827/1084 (76%)	0.51	68 (8%) 11	18	17, 39, 74, 115	2~(0%)

All (68) RSRZ outliers are listed below:

Mol	ol Chain Re		Type	RSRZ	
1	AAA	228	PHE	9.2	
1	AAA	847	THR	6.7	
1	AAA	367	SER	6.2	
1	AAA	495	ILE	5.9	
1	AAA	366	CYS	5.9	
1	AAA	846	ALA	5.1	
1	AAA	894	ARG	5.0	
1	AAA	514	ILE	5.0	
1	AAA	445	VAL	5.0	
1	AAA	416	CYS	4.9	
1	AAA	317	TRP	4.7	
1	AAA	522	GLU	4.7	
1	AAA	919	PHE	4.7	
1	AAA	523	LEU	4.3	
1	AAA	913	GLY	4.3	
1	AAA	990	SER	3.9	
1	AAA	398	VAL	3.9	
1	AAA	842	SER	3.8	
1	AAA	843	ASN	3.8	
1	AAA	515	LEU	3.5	
1	AAA	417	PRO	3.4	
1	AAA	512	ARG	3.2	
1	AAA	484	TYR	3.1	
1	AAA	845	ALA	3.1	
1	AAA	467	SER	3.1	
1	AAA	524	TYR	3.1	
1	AAA	397	VAL	3.0	



Continued from previous page								
Mol	Chain	Res	Type	RSRZ				
1	AAA	1024	ARG	3.0				
1	AAA	1025	GLU	3.0				
1	AAA	225	ALA	3.0				
1	AAA	109	VAL	2.9				
1	AAA	792	GLN	2.9				
1	AAA	993	LYS	2.9				
1	AAA	466	GLU	2.9				
1	AAA	841	LYS	2.9				
1	AAA	619	LEU	2.8				
1	AAA	227	VAL	2.8				
1	AAA	1027	TRP	2.8				
1	AAA	510	GLU	2.7				
1	AAA	526	HIS	2.7				
1	AAA	1017	VAL	2.7				
1	AAA	866	GLU	2.7				
1	AAA	200	GLU	2.7				
1	AAA	530	LEU	2.6				
1	AAA	517	ARG	2.6				
1	AAA	334	ASN	2.6				
1	AAA	987	PRO	2.5				
1	AAA	533	LYS	2.5				
1	AAA	893	ASP	2.5				
1	AAA	198	GLY	2.5				
1	AAA	267	HIS	2.5				
1	AAA	478	VAL	2.4				
1	AAA	897	ASP	2.3				
1	AAA	513	GLU	2.3				
1	AAA	885	ALA	2.3				
1	AAA	891	ILE	2.3				
1	AAA	226	THR	2.3				
1	AAA	883	CYS	2.3				
1	AAA	991	CYS	2.3				
1	AAA	496	THR	2.2				
1	AAA	794	ILE	2.2				
1	AAA	395	TYR	2.2				
1	AAA	474	TYR	2.2				
1	AAA	132	ARG	2.1				
1	AAA	914	HIS	2.1				
1	AAA	1014	HIS	2.1				
1	AAA	488	LEU	2.1				
1	AAA	880	ALA	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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	NA	AAA	1101	1/1	0.87	0.30	45,45,45,45	0
3	VEN	AAA	1102	38/38	0.97	0.08	19,21,27,30	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.





6.5 Other polymers (i)

There are no such residues in this entry.

