



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:02 AM UTC

PDB ID : 7OIJ / pdb_00007oij
Title : mPI3Kd in complex with an inhibitor
Authors : Petersen, J.
Deposited on : 2021-05-11
Resolution : 1.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

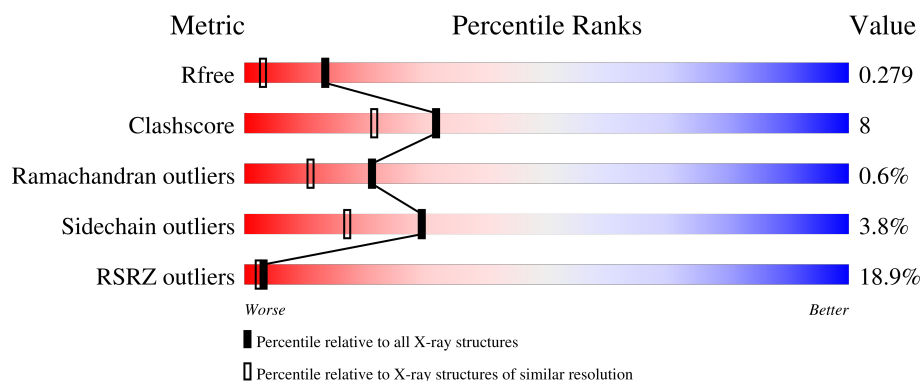
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	1084	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6982 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 sub-unit delta isoform.

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

There are 41 discrepancies between the modelled and reference sequences:

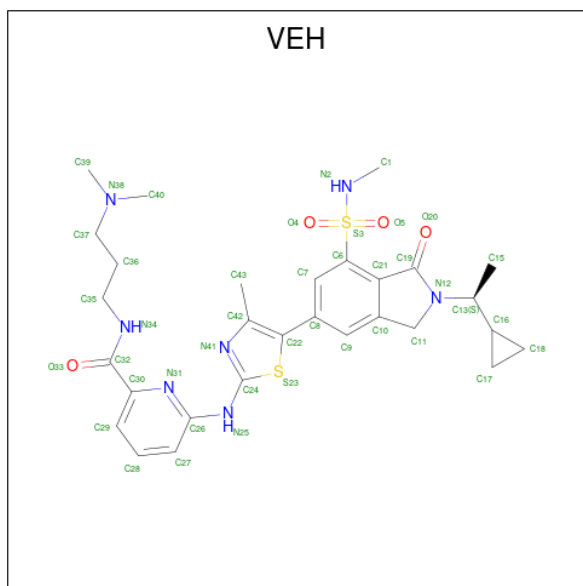
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-39	MET	-	initiating methionine	UNP O35904
AAA	-38	SER	-	expression tag	UNP O35904
AAA	-37	TYR	-	expression tag	UNP O35904
AAA	-36	HIS	-	expression tag	UNP O35904
AAA	-35	ASN	-	expression tag	UNP O35904
AAA	-34	HIS	-	expression tag	UNP O35904
AAA	-33	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 O35904

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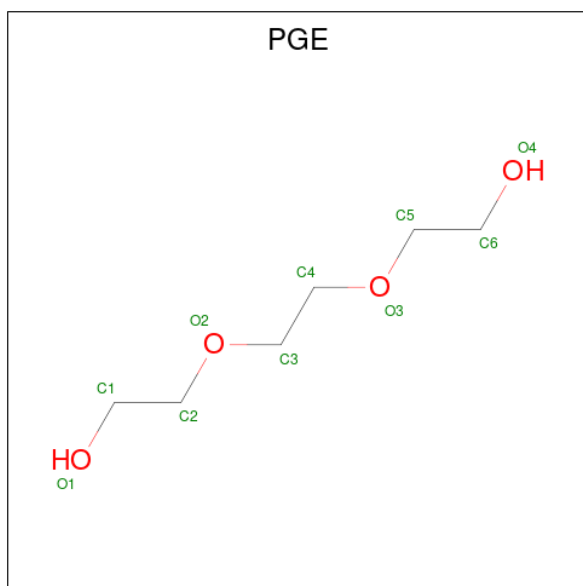
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-13	PHE	-	expression tag	UNP O35904
AAA	-12	GLN	-	expression tag	UNP O35904
AAA	-11	GLY	-	expression tag	UNP O35904
AAA	-10	ALA	-	expression tag	UNP O35904
AAA	-9	MET	-	expression tag	UNP O35904
AAA	-8	ASP	-	expression tag	UNP O35904
AAA	-7	LEU	-	expression 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 O35904
AAA	510A	GLN	-	insertion	UNP O35904

- Molecule 2 is 6-[[5-[2-[(1S)-1-cyclopropylethyl]-7-(methanesulfonyl)-1-oxo-1H-indol-5-yl]-4-methyl-1,3-thiazol-2-yl]amino]-N-[3-(dimethylamino)propyl]pyridine-2-carboxamide (CCD ID: VEH) (formula: C₂₉H₃₇N₇O₄S₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	257	Total	O	0	0
			257	257		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.81Å 64.84Å 116.58Å 90.00° 103.66° 90.00°	Depositor
Resolution (Å)	42.97 – 1.80 42.97 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (42.97-1.80) 99.2 (42.97-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.236 , 0.276 0.241 , 0.279	Depositor DCC
R_{free} test set	4709 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6982	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: VEH, NA, PGE

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	AAA	1.06	2/6824 (0.0%)	1.36	3/9207 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	693	LYS	C-O	5.61	1.30	1.24
1	AAA	774	VAL	C-O	5.09	1.29	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	915	PHE	CA-CB-CG	5.89	119.69	113.80
1	AAA	970	HIS	CA-C-N	5.11	125.77	119.99
1	AAA	970	HIS	C-N-CA	5.11	125.77	119.99

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	AAA	6678	0	6656	107	1
2	AAA	42	0	0	1	0
3	AAA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AAA	4	0	5	1	0
5	AAA	257	0	0	3	0
All	All	6982	0	6661	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 distance (Å)	Clash overlap (Å)
1:AAA:495:ILE:HG23	1:AAA:563:GLN:HA	1.38	1.05
1:AAA:549:LEU:HG	1:AAA:564:MET:HE1	1.51	0.92
1:AAA:495:ILE:CG2	1:AAA:563:GLN:HA	2.02	0.90
1:AAA:387:MET:HE3	1:AAA:590:CYS:HB3	1.54	0.87
1:AAA:386:ARG:HG3	1:AAA:387:MET:HE2	1.57	0.87
1:AAA:495:ILE:HD13	1:AAA:562:ALA:O	1.78	0.84
1:AAA:367:SER:HB3	1:AAA:368:GLU:C	2.05	0.82
1:AAA:495:ILE:CD1	1:AAA:562:ALA:O	2.28	0.81
1:AAA:495:ILE:HG12	1:AAA:562:ALA:C	2.08	0.79
1:AAA:912:PHE:CB	1:AAA:913:GLY:HA3	2.15	0.77
1:AAA:642:LYS:HE3	4:AAA:1103:PGE:O4	1.86	0.76
1:AAA:387:MET:HE3	1:AAA:590:CYS:CB	2.16	0.76
1:AAA:549:LEU:CG	1:AAA:564:MET:HE1	2.17	0.74
1:AAA:495:ILE:HG21	1:AAA:566:TYR:CB	2.17	0.73
1:AAA:387:MET:HE3	1:AAA:590:CYS:SG	2.29	0.73
1:AAA:534:MET:HA	1:AAA:534:MET:HE2	1.70	0.72
1:AAA:756:MET:CE	1:AAA:781:GLY:HA3	2.21	0.69
1:AAA:495:ILE:HG21	1:AAA:566:TYR:HB3	1.76	0.68
1:AAA:495:ILE:HG12	1:AAA:562:ALA:O	1.98	0.64
1:AAA:495:ILE:HG21	1:AAA:566:TYR:HB2	1.79	0.64
1:AAA:756:MET:HE2	1:AAA:781:GLY:HA3	1.78	0.64
1:AAA:495:ILE:CG1	1:AAA:562:ALA:O	2.45	0.64
1:AAA:549:LEU:HG	1:AAA:564:MET:CE	2.26	0.62
1:AAA:912:PHE:HB2	1:AAA:913:GLY:HA3	1.82	0.61
1:AAA:912:PHE:HB3	1:AAA:913:GLY:HA3	1.82	0.61
1:AAA:386:ARG:CG	1:AAA:387:MET:HE2	2.28	0.61
1:AAA:332:LYS:HE3	1:AAA:333:VAL:N	2.17	0.60
1:AAA:532:TRP:HZ3	1:AAA:564:MET:HE2	1.67	0.60
1:AAA:367:SER:CB	1:AAA:368:GLU:C	2.75	0.60
1:AAA:495:ILE:CG2	1:AAA:566:TYR:HB2	2.32	0.60
1:AAA:154:ARG:HD2	1:AAA:165:TYR:CE2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:330:GLY:C	1:AAA:331:ARG:HG3	2.27	0.59
2:AAA:1101:VEH:N31	2:AAA:1101:VEH:S23	2.76	0.58
1:AAA:833:THR:OG1	1:AAA:836:ASN:HB2	2.02	0.58
1:AAA:194:VAL:HG21	1:AAA:216:LEU:HD21	1.86	0.58
1:AAA:332:LYS:HE3	1:AAA:332:LYS:C	2.29	0.57
1:AAA:495:ILE:O	1:AAA:497:GLU:N	2.37	0.56
1:AAA:534:MET:HA	1:AAA:534:MET:CE	2.35	0.56
1:AAA:841:LYS:HG2	1:AAA:844:MET:HG3	1.88	0.56
1:AAA:549:LEU:CD1	1:AAA:564:MET:HE1	2.35	0.56
1:AAA:394:LEU:HD23	1:AAA:441:MET:HE1	1.86	0.55
1:AAA:601:ARG:HD2	5:AAA:1407:HOH:O	2.05	0.55
1:AAA:495:ILE:HB	1:AAA:566:TYR:HB2	1.88	0.55
1:AAA:495:ILE:CG2	1:AAA:566:TYR:CB	2.84	0.55
1:AAA:1006:LYS:HB3	1:AAA:1010:GLU:HB2	1.89	0.55
1:AAA:495:ILE:HG12	1:AAA:562:ALA:HB1	1.88	0.54
1:AAA:495:ILE:CB	1:AAA:566:TYR:HB2	2.37	0.54
1:AAA:491:ILE:HG22	1:AAA:495:ILE:HD11	1.89	0.54
1:AAA:491:ILE:O	1:AAA:495:ILE:HG13	2.07	0.54
1:AAA:496:THR:HG22	1:AAA:566:TYR:CE1	2.43	0.54
1:AAA:892:GLY:O	1:AAA:894:ARG:HG2	2.09	0.53
1:AAA:495:ILE:HG23	1:AAA:563:GLN:CA	2.27	0.52
1:AAA:756:MET:HE3	1:AAA:781:GLY:HA3	1.92	0.51
1:AAA:434:THR:HG21	1:AAA:477:GLU:HA	1.93	0.51
1:AAA:154:ARG:HD2	1:AAA:165:TYR:CZ	2.45	0.51
1:AAA:331:ARG:O	1:AAA:469:ALA:HA	2.10	0.51
1:AAA:495:ILE:CG1	1:AAA:562:ALA:HB1	2.41	0.51
1:AAA:358:VAL:HG22	1:AAA:377:PHE:CE2	2.46	0.51
1:AAA:366:CYS:O	1:AAA:367:SER:CB	2.59	0.51
1:AAA:492:LEU:HA	1:AAA:495:ILE:HD12	1.93	0.50
1:AAA:188:ARG:HD2	1:AAA:189:ALA:N	2.26	0.50
1:AAA:495:ILE:C	1:AAA:497:GLU:N	2.68	0.50
1:AAA:743:GLU:HG2	1:AAA:764:SER:O	2.12	0.49
1:AAA:271:THR:O	1:AAA:273:HIS:HD2	1.95	0.48
1:AAA:581:GLU:HB2	1:AAA:976:HIS:CE1	2.48	0.48
1:AAA:489:GLU:HG3	1:AAA:490:LYS:N	2.28	0.48
1:AAA:859:LEU:HD21	1:AAA:905:GLY:HA2	1.94	0.48
1:AAA:1012:LEU:O	1:AAA:1016:ARG:HG3	2.13	0.48
1:AAA:832:ASP:C	1:AAA:900:MET:HE3	2.38	0.48
1:AAA:356:LYS:HE3	1:AAA:378:ASP:HB2	1.96	0.47
1:AAA:515:LEU:HD12	1:AAA:515:LEU:C	2.39	0.47
1:AAA:491:ILE:O	1:AAA:495:ILE:CD1	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:495:ILE:O	1:AAA:496:THR:C	2.58	0.47
1:AAA:172:GLU:HG3	1:AAA:263:CYS:SG	2.55	0.47
1:AAA:841:LYS:HD3	1:AAA:841:LYS:H	1.79	0.46
1:AAA:435:GLY:O	1:AAA:475:LEU:N	2.25	0.46
1:AAA:617:GLN:HE21	1:AAA:984:ALA:HA	1.80	0.46
1:AAA:349:HIS:HE1	5:AAA:1241:HOH:O	1.99	0.46
1:AAA:617:GLN:HE22	1:AAA:620:LYS:NZ	2.14	0.45
1:AAA:247:HIS:HB2	1:AAA:738:SER:HA	1.98	0.45
1:AAA:157:LEU:HD22	1:AAA:161:GLU:HB3	1.97	0.45
1:AAA:915:PHE:C	1:AAA:915:PHE:CD1	2.94	0.45
1:AAA:188:ARG:NH2	1:AAA:266:LEU:HD22	2.31	0.45
1:AAA:367:SER:HA	1:AAA:368:GLU:HB3	1.99	0.45
1:AAA:192:VAL:HG13	1:AAA:272:PRO:HB2	1.99	0.45
1:AAA:912:PHE:CB	1:AAA:913:GLY:CA	2.91	0.44
1:AAA:368:GLU:N	1:AAA:369:PRO:CD	2.81	0.44
1:AAA:784:LEU:O	1:AAA:788:MET:HG2	2.17	0.44
1:AAA:365:VAL:O	1:AAA:366:CYS:C	2.61	0.44
1:AAA:423:LEU:H	1:AAA:423:LEU:HD12	1.82	0.44
1:AAA:423:LEU:HD12	1:AAA:423:LEU:N	2.33	0.44
1:AAA:495:ILE:HG12	1:AAA:562:ALA:CB	2.47	0.44
1:AAA:587:PHE:HB3	1:AAA:592:VAL:HG11	1.99	0.43
1:AAA:579:ALA:HB1	1:AAA:600:LEU:HG	2.00	0.43
1:AAA:238:GLU:HB3	1:AAA:278:HIS:CE1	2.53	0.43
1:AAA:281:SER:O	1:AAA:285:MET:HG3	2.18	0.43
1:AAA:329:GLU:O	1:AAA:472:VAL:HG22	2.18	0.43
1:AAA:930:VAL:HG22	1:AAA:997:TYR:OH	2.18	0.43
1:AAA:496:THR:HG22	1:AAA:566:TYR:CZ	2.54	0.43
1:AAA:913:GLY:CA	1:AAA:914:HIS:HB2	2.49	0.43
1:AAA:316:LEU:HA	5:AAA:1424:HOH:O	2.18	0.43
1:AAA:367:SER:HB2	1:AAA:369:PRO:N	2.35	0.42
1:AAA:637:ALA:HB1	1:AAA:644:GLY:HA2	2.02	0.42
1:AAA:617:GLN:NE2	1:AAA:984:ALA:HA	2.35	0.42
1:AAA:913:GLY:N	1:AAA:914:HIS:HB2	2.35	0.42
1:AAA:523:LEU:O	1:AAA:528:LYS:HE3	2.21	0.41
1:AAA:550:LEU:O	1:AAA:553:THR:CG2	2.68	0.41
1:AAA:511:LEU:O	1:AAA:514:ILE:HG22	2.21	0.41

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]	1.48	0.72

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%)	778 (96%)	23 (3%)	5 (1%)	21 11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	367	SER
1	AAA	893	ASP
1	AAA	1026	SER
1	AAA	368	GLU
1	AAA	496	THR

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	AAA	734/962 (76%)	706 (96%)	28 (4%)	29 17

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	111	LYS

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Mol	Chain	Res	Type
1	AAA	190	LEU
1	AAA	203	PHE
1	AAA	212	MET
1	AAA	291	ASN
1	AAA	316	LEU
1	AAA	332	LYS
1	AAA	340	LYS
1	AAA	352	GLU
1	AAA	356	LYS
1	AAA	360	SER
1	AAA	423	LEU
1	AAA	453	LEU
1	AAA	517	ARG
1	AAA	530	LEU
1	AAA	534	MET
1	AAA	553	THR
1	AAA	634	LEU
1	AAA	743	GLU
1	AAA	752	MET
1	AAA	756	MET
1	AAA	779	LYS
1	AAA	795	GLN
1	AAA	836	ASN
1	AAA	841	LYS
1	AAA	898	ASN
1	AAA	915	PHE
1	AAA	1026	SER

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

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	VEH	AAA	1101	-	44,46,46	1.26	4 (9%)	60,68,68	2.62	21 (35%)
4	PGE	AAA	1103	-	3,3,9	0.55	0	2,2,8	0.18	0

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	VEH	AAA	1101	-	-	2/36/50/50	0/5/5/5
4	PGE	AAA	1103	-	-	0/1/1/7	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	1101	VEH	C9-C10	-3.71	1.33	1.39
2	AAA	1101	VEH	C29-C30	2.63	1.44	1.39
2	AAA	1101	VEH	C24-N25	2.45	1.40	1.36
2	AAA	1101	VEH	S3-N2	2.10	1.64	1.61

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	1101	VEH	C11-N12-C19	-8.16	109.71	113.15
2	AAA	1101	VEH	C24-N41-C42	8.04	115.28	110.38
2	AAA	1101	VEH	S23-C24-N41	-6.70	109.79	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	1101	VEH	C10-C11-N12	6.51	105.77	102.31
2	AAA	1101	VEH	C24-S23-C22	4.14	90.93	88.35
2	AAA	1101	VEH	C11-C10-C21	-4.06	107.00	109.96
2	AAA	1101	VEH	C30-C32-N34	4.04	121.18	115.56
2	AAA	1101	VEH	C1-N2-S3	3.52	123.83	119.16
2	AAA	1101	VEH	C29-C28-C27	-3.32	115.98	120.24
2	AAA	1101	VEH	C42-C22-S23	-3.11	108.02	109.91
2	AAA	1101	VEH	C26-N25-C24	-2.98	122.97	126.67
2	AAA	1101	VEH	C29-C30-N31	-2.97	119.45	122.92
2	AAA	1101	VEH	C35-N34-C32	2.88	128.63	122.11
2	AAA	1101	VEH	C30-N31-C26	2.70	119.78	117.80
2	AAA	1101	VEH	C28-C29-C30	2.45	121.55	118.63
2	AAA	1101	VEH	O20-C19-C21	-2.38	125.53	129.15
2	AAA	1101	VEH	O5-S3-O4	2.36	122.38	119.52
2	AAA	1101	VEH	C29-C30-C32	2.21	123.15	119.57
2	AAA	1101	VEH	S23-C24-N25	2.19	130.44	122.19
2	AAA	1101	VEH	C8-C22-C42	2.09	133.65	130.81
2	AAA	1101	VEH	C17-C16-C13	-2.04	114.90	119.25

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	1101	VEH	C21-C6-S3-O4
2	AAA	1101	VEH	C36-C37-N38-C40

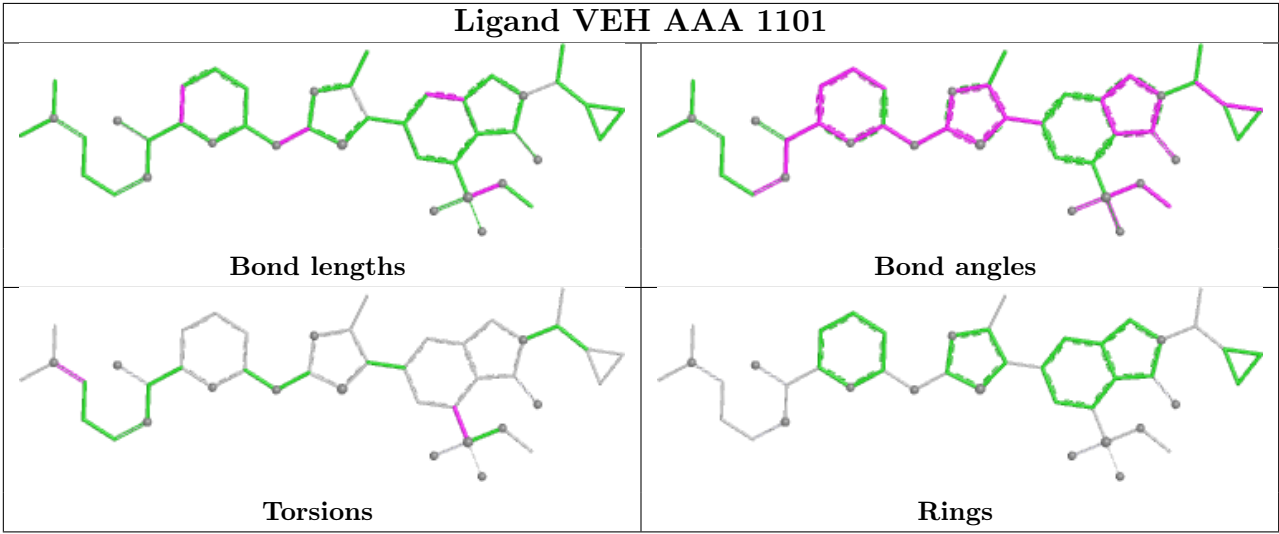
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	1101	VEH	1	0
4	AAA	1103	PGE	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	C	509:GLU	N	21.77

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	827/1084 (76%)	1.07	156 (18%) 3 2	11, 34, 64, 99	2 (0%)

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	495	ILE	10.2
1	AAA	317	TRP	7.7
1	AAA	1027	TRP	7.6
1	AAA	919	PHE	6.7
1	AAA	445	VAL	6.3
1	AAA	366	CYS	6.1
1	AAA	333	VAL	6.0
1	AAA	514	ILE	5.9
1	AAA	335	ALA	5.8
1	AAA	397	VAL	5.7
1	AAA	515	LEU	5.6
1	AAA	496	THR	5.3
1	AAA	479	ALA	5.3
1	AAA	846	ALA	5.3
1	AAA	478	VAL	5.1
1	AAA	847	THR	5.0
1	AAA	845	ALA	5.0
1	AAA	316	LEU	4.9
1	AAA	367	SER	4.8
1	AAA	523	LEU	4.8
1	AAA	227	VAL	4.7
1	AAA	228	PHE	4.6
1	AAA	511	LEU	4.4
1	AAA	109	VAL	4.1
1	AAA	377	PHE	4.1
1	AAA	205	PHE	4.1
1	AAA	913	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	AAA	363	VAL	3.8
1	AAA	510	GLU	3.8
1	AAA	332	LYS	3.8
1	AAA	482	PRO	3.8
1	AAA	319	LEU	3.7
1	AAA	517	ARG	3.7
1	AAA	512	ARG	3.6
1	AAA	483	VAL	3.5
1	AAA	342	VAL	3.4
1	AAA	472	VAL	3.4
1	AAA	323	PHE	3.4
1	AAA	198	GLY	3.4
1	AAA	318	SER	3.4
1	AAA	471	LEU	3.4
1	AAA	226	THR	3.4
1	AAA	360	SER	3.3
1	AAA	914	HIS	3.3
1	AAA	894	ARG	3.3
1	AAA	398	VAL	3.2
1	AAA	270	LEU	3.2
1	AAA	1004	LEU	3.2
1	AAA	334	ASN	3.2
1	AAA	895	HIS	3.2
1	AAA	491	ILE	3.2
1	AAA	475	LEU	3.2
1	AAA	494	LEU	3.2
1	AAA	896	SER	3.2
1	AAA	893	ASP	3.2
1	AAA	379	ILE	3.1
1	AAA	187	ASN	3.1
1	AAA	374	ARG	3.1
1	AAA	395	TYR	3.1
1	AAA	1023	LEU	3.1
1	AAA	516	GLU	3.1
1	AAA	230	GLN	3.1
1	AAA	917	GLY	3.1
1	AAA	375	LEU	3.0
1	AAA	341	LEU	3.0
1	AAA	553	THR	3.0
1	AAA	897	ASP	3.0
1	AAA	365	VAL	2.9
1	AAA	843	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	AAA	474	TYR	2.9
1	AAA	452	LEU	2.9
1	AAA	848	ALA	2.9
1	AAA	356	LYS	2.9
1	AAA	382	CYS	2.8
1	AAA	394	LEU	2.8
1	AAA	473	ILE	2.8
1	AAA	936	TYR	2.8
1	AAA	1024	ARG	2.8
1	AAA	530	LEU	2.8
1	AAA	370	VAL	2.8
1	AAA	203	PHE	2.7
1	AAA	358	VAL	2.7
1	AAA	188	ARG	2.6
1	AAA	497	GLU	2.6
1	AAA	934	LEU	2.6
1	AAA	930	VAL	2.6
1	AAA	396	ALA	2.6
1	AAA	141	THR	2.6
1	AAA	488	LEU	2.6
1	AAA	351	ASN	2.6
1	AAA	331	ARG	2.5
1	AAA	509	GLU	2.5
1	AAA	415	ASP	2.5
1	AAA	918	ASN	2.5
1	AAA	378	ASP	2.5
1	AAA	162	TRP	2.5
1	AAA	891	ILE	2.5
1	AAA	345	ALA	2.5
1	AAA	1017	VAL	2.5
1	AAA	326	GLU	2.4
1	AAA	1025	GLU	2.4
1	AAA	189	ALA	2.4
1	AAA	841	LYS	2.4
1	AAA	477	GLU	2.4
1	AAA	339	MET	2.4
1	AAA	915	PHE	2.4
1	AAA	995	ILE	2.4
1	AAA	470	ALA	2.4
1	AAA	322	PRO	2.4
1	AAA	381	VAL	2.4
1	AAA	435	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	AAA	562	ALA	2.3
1	AAA	359	SER	2.3
1	AAA	1003	ALA	2.3
1	AAA	493	GLU	2.3
1	AAA	867	ALA	2.3
1	AAA	929	ARG	2.3
1	AAA	985	GLY	2.3
1	AAA	383	ASP	2.3
1	AAA	1006	LYS	2.3
1	AAA	320	GLU	2.2
1	AAA	865	GLY	2.2
1	AAA	1005	GLY	2.2
1	AAA	325	ILE	2.2
1	AAA	898	ASN	2.2
1	AAA	465	THR	2.2
1	AAA	191	LEU	2.2
1	AAA	453	LEU	2.2
1	AAA	492	LEU	2.2
1	AAA	842	SER	2.2
1	AAA	1026	SER	2.2
1	AAA	484	TYR	2.2
1	AAA	522	GLU	2.2
1	AAA	269	GLY	2.2
1	AAA	524	TYR	2.2
1	AAA	563	GLN	2.2
1	AAA	354	LEU	2.2
1	AAA	432	LEU	2.2
1	AAA	468	ALA	2.2
1	AAA	291	ASN	2.1
1	AAA	267	HIS	2.1
1	AAA	767	GLU	2.1
1	AAA	771	ALA	2.1
1	AAA	990	SER	2.1
1	AAA	330	GLY	2.1
1	AAA	417	PRO	2.1
1	AAA	438	CYS	2.1
1	AAA	768	ALA	2.1
1	AAA	132	ARG	2.1
1	AAA	110	LYS	2.0
1	AAA	542	PHE	2.0
1	AAA	992	SER	2.0
1	AAA	548	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	AAA	892	GLY	2.0
1	AAA	566	TYR	2.0
1	AAA	591	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

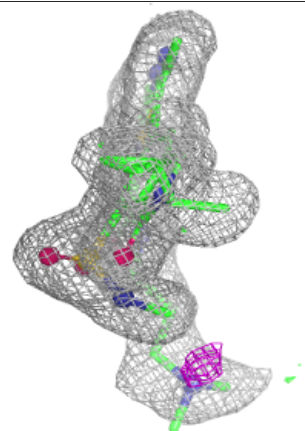
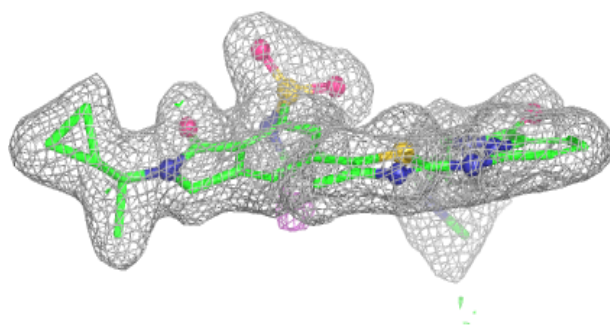
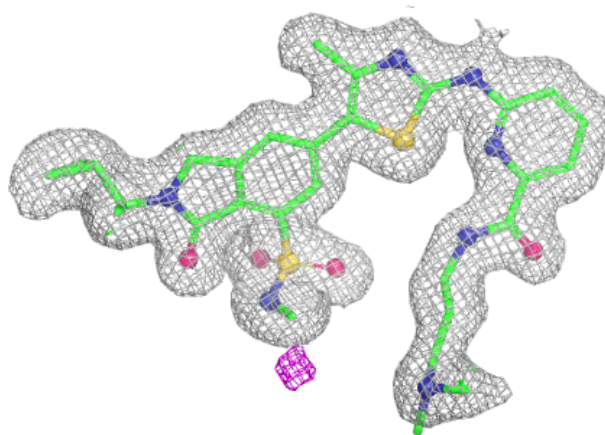
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	AAA	1102	1/1	0.88	0.31	54,54,54,54	0
4	PGE	AAA	1103	4/10	0.96	0.07	26,29,31,33	0
2	VEH	AAA	1101	42/42	0.98	0.07	16,21,44,53	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 VEH AAA 1101:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.