



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:01 PM UTC

PDB ID : 7OI4 / pdb_00007oi4
Title : mPI3Kd in complex with compound 12
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

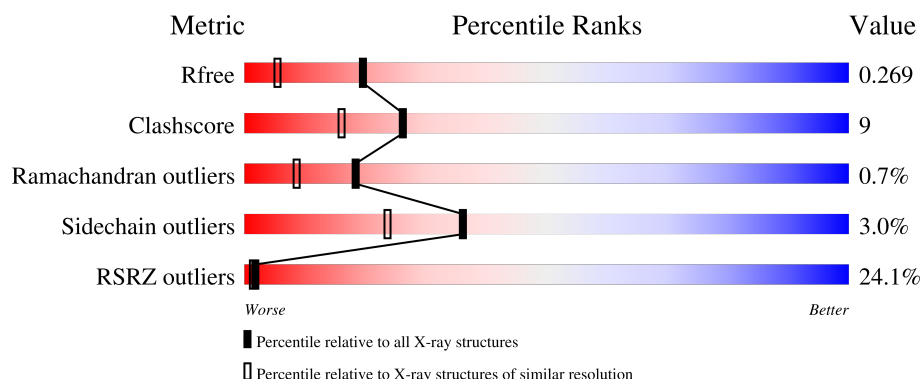
1 Overall quality at a glance

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	18% 63% 12% • 24%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7088 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	3	0
			6684	4285	1131	1212	56			

There are 41 discrepancies between the modelled and reference sequences:

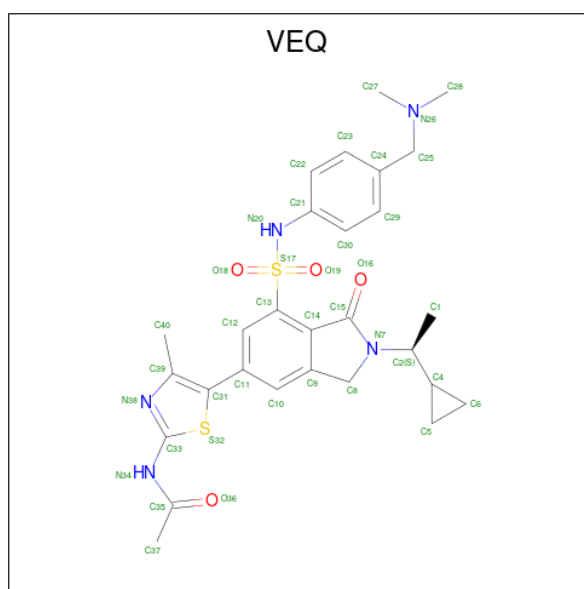
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-39	MET	-	initiating methionine	UNP O35904
AAA	-38	SER	-	expression tag	UNP O35904
AAA	-37	TYR	-	expression tag	UNP O35904
AAA	-36	HIS	-	expression tag	UNP O35904
AAA	-35	ASN	-	expression tag	UNP O35904
AAA	-34	HIS	-	expression tag	UNP O35904
AAA	-33	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 N-[5-[2-[(1S)-1-cyclopropylethyl]-7-[[4-[(dimethylamino)methyl]phenyl]sulfamoyl]-1-oxidanylidene-3H-isindol-5-yl]-4-methyl-1,3-thiazol-2-yl]ethanamide (CCD ID: VEQ) (formula: C₂₈H₃₃N₅O₄S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	S	0	0
			39	28	5	4	2		

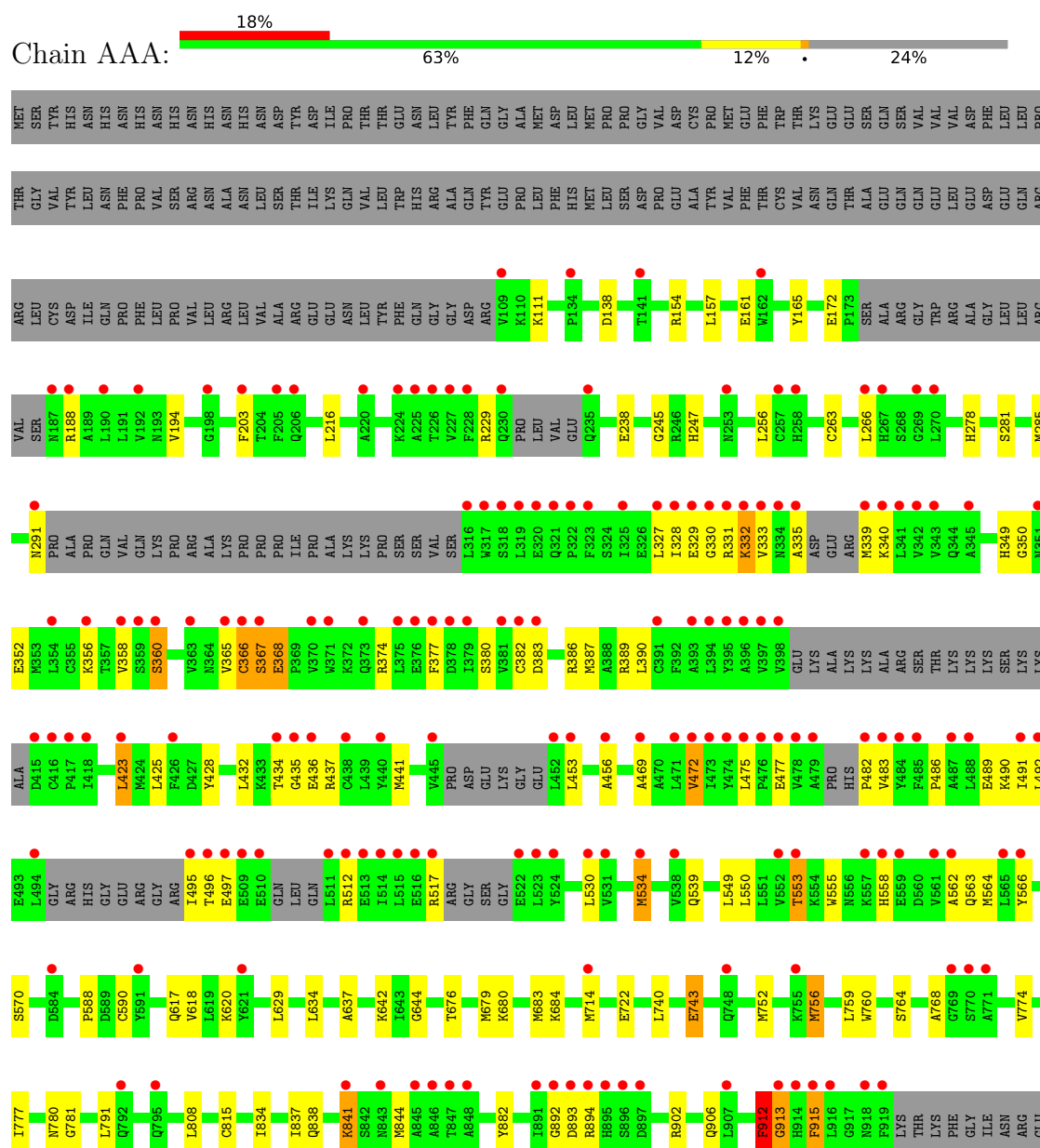
- Molecule 3 is water.

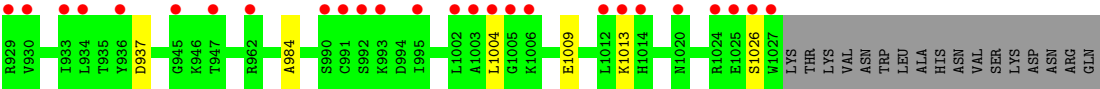
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	365	Total 365	O 365	0	0

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.85Å 65.16Å 116.43Å 90.00° 103.75° 90.00°	Depositor
Resolution (Å)	113.09 – 1.80 113.09 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (113.09-1.80) 97.4 (113.09-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.227 , 0.263 0.231 , 0.269	Depositor DCC
R_{free} test set	4789 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7088	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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: VEQ

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	1.09	1/6836 (0.0%)	1.37	10/9223 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	808	LEU	N-CA	5.11	1.52	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	774	VAL	CA-C-N	5.57	126.02	122.18
1	AAA	774	VAL	C-N-CA	5.57	126.02	122.18
1	AAA	834	ILE	N-CA-C	-5.56	104.95	110.62
1	AAA	912	PHE	CB-CA-C	5.55	121.47	110.42
1	AAA	1013	LYS	CA-C-N	5.53	127.69	120.28
1	AAA	1013	LYS	C-N-CA	5.53	127.69	120.28
1	AAA	915	PHE	CA-CB-CG	5.26	119.06	113.80
1	AAA	837	ILE	CA-C-O	-5.24	115.30	120.85
1	AAA	882	TYR	CA-C-O	-5.01	115.11	120.42
1	AAA	837	ILE	O-C-N	5.00	126.98	121.83

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

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	6684	0	6666	126	1
2	AAA	39	0	0	0	0
3	AAA	365	0	0	11	0
All	All	7088	0	6666	126	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 (126) 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:387:MET:HE3	1:AAA:590:CYS:HB3	1.30	1.11
1:AAA:549:LEU:HG	1:AAA:564:MET:HE1	1.16	1.09
1:AAA:495:ILE:HG23	1:AAA:563:GLN:HA	1.36	1.04
1:AAA:549:LEU:CG	1:AAA:564:MET:HE1	1.96	0.95
1:AAA:367:SER:HB3	1:AAA:368:GLU:C	1.96	0.91
1:AAA:491:ILE:O	1:AAA:495:ILE:HG13	1.71	0.90
1:AAA:495:ILE:HD13	1:AAA:562:ALA:O	1.72	0.90
1:AAA:495:ILE:CG2	1:AAA:563:GLN:HA	2.04	0.88
1:AAA:534:MET:HA	1:AAA:534:MET:HE2	1.58	0.85
1:AAA:756:MET:CE	1:AAA:781:GLY:HA3	2.08	0.83
1:AAA:549:LEU:HG	1:AAA:564:MET:CE	2.03	0.83
1:AAA:387:MET:HE3	1:AAA:590:CYS:CB	2.06	0.83
1:AAA:642:LYS:HE2	3:AAA:1460:HOH:O	1.78	0.82
1:AAA:642:LYS:CE	3:AAA:1460:HOH:O	2.26	0.82
1:AAA:495:ILE:CD1	1:AAA:562:ALA:O	2.31	0.79
1:AAA:495:ILE:HB	1:AAA:566:TYR:HB2	1.64	0.78
1:AAA:491:ILE:HG22	1:AAA:495:ILE:HD11	1.66	0.77
1:AAA:756:MET:HE3	1:AAA:781:GLY:HA3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:495:ILE:HG21	1:AAA:566:TYR:HB3	1.68	0.75
1:AAA:892:GLY:O	1:AAA:894:ARG:HG2	1.87	0.74
1:AAA:495:ILE:HG23	1:AAA:563:GLN:CA	2.16	0.73
1:AAA:332:LYS:HE3	1:AAA:333:VAL:N	2.06	0.71
1:AAA:386:ARG:HG3	1:AAA:387:MET:HE2	1.72	0.70
1:AAA:330:GLY:C	1:AAA:331:ARG:HG3	2.15	0.70
1:AAA:495:ILE:CG1	1:AAA:562:ALA:O	2.40	0.69
1:AAA:495:ILE:HG12	1:AAA:562:ALA:C	2.18	0.69
1:AAA:495:ILE:HG12	1:AAA:562:ALA:HB1	1.73	0.69
1:AAA:841:LYS:HG2	1:AAA:844:MET:HG3	1.76	0.68
1:AAA:1004:LEU:HD11	3:AAA:1499:HOH:O	1.93	0.68
1:AAA:495:ILE:HG21	1:AAA:566:TYR:CB	2.24	0.67
1:AAA:912:PHE:CB	1:AAA:913:GLY:HA3	2.25	0.67
1:AAA:367:SER:CB	1:AAA:368:GLU:C	2.70	0.65
1:AAA:495:ILE:CG2	1:AAA:566:TYR:CB	2.75	0.64
1:AAA:330:GLY:O	1:AAA:331:ARG:HG3	1.98	0.64
1:AAA:550:LEU:O	1:AAA:553:THR:HG22	1.97	0.64
1:AAA:495:ILE:CB	1:AAA:566:TYR:HB2	2.27	0.63
1:AAA:495:ILE:CG2	1:AAA:566:TYR:HB3	2.29	0.61
1:AAA:491:ILE:O	1:AAA:495:ILE:CG1	2.47	0.61
1:AAA:756:MET:HE2	1:AAA:781:GLY:HA3	1.82	0.61
1:AAA:642:LYS:HE3	3:AAA:1460:HOH:O	1.97	0.61
1:AAA:495:ILE:HG12	1:AAA:562:ALA:O	2.00	0.61
1:AAA:383:ASP:OD1	1:AAA:558:HIS:ND1	2.29	0.61
1:AAA:172:GLU:HG3	1:AAA:263:CYS:SG	2.41	0.60
1:AAA:194:VAL:HG21	1:AAA:216:LEU:HD21	1.83	0.59
1:AAA:534:MET:HA	1:AAA:534:MET:CE	2.31	0.59
1:AAA:331:ARG:O	1:AAA:469:ALA:HA	2.02	0.59
1:AAA:374:ARG:HD3	3:AAA:1407:HOH:O	2.01	0.59
1:AAA:332:LYS:HE3	1:AAA:332:LYS:C	2.30	0.56
1:AAA:495:ILE:CG2	1:AAA:566:TYR:HB2	2.35	0.56
1:AAA:841:LYS:HD3	1:AAA:841:LYS:H	1.70	0.55
1:AAA:496:THR:HG22	1:AAA:566:TYR:CE1	2.42	0.55
1:AAA:495:ILE:CG2	1:AAA:562:ALA:O	2.55	0.55
1:AAA:912:PHE:HB3	1:AAA:913:GLY:HA3	1.89	0.55
1:AAA:617:GLN:HE22	1:AAA:620:LYS:NZ	2.06	0.54
1:AAA:329:GLU:HG3	1:AAA:472:VAL:CG2	2.38	0.54
1:AAA:495:ILE:HG21	1:AAA:562:ALA:O	2.08	0.54
1:AAA:838:GLN:NE2	1:AAA:937:ASP:OD2	2.41	0.53
1:AAA:841:LYS:H	1:AAA:841:LYS:CD	2.21	0.53
1:AAA:339:MET:O	1:AAA:365:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:423:LEU:N	1:AAA:423:LEU:HD12	2.24	0.53
1:AAA:752:MET:HE1	1:AAA:760:TRP:HB2	1.89	0.53
1:AAA:435:GLY:O	1:AAA:475:LEU:N	2.34	0.53
1:AAA:386:ARG:CG	1:AAA:387:MET:HE2	2.38	0.52
1:AAA:154:ARG:HD2	1:AAA:165:TYR:CE2	2.43	0.52
1:AAA:550:LEU:O	1:AAA:553:THR:CG2	2.58	0.51
1:AAA:328:ILE:HG22	1:AAA:329:GLU:HG2	1.93	0.50
1:AAA:358:VAL:HG22	1:AAA:377:PHE:CE2	2.47	0.50
1:AAA:432:LEU:HB3	1:AAA:483:VAL:HG22	1.94	0.50
1:AAA:495:ILE:HG12	1:AAA:562:ALA:CB	2.39	0.50
1:AAA:390:LEU:HB2	1:AAA:425:LEU:HD21	1.93	0.49
1:AAA:791:LEU:HD13	1:AAA:815[B]:CYS:SG	2.52	0.49
1:AAA:387:MET:HE3	1:AAA:590:CYS:SG	2.52	0.49
1:AAA:553:THR:HG23	1:AAA:555:TRP:NE1	2.28	0.49
1:AAA:743:GLU:HG2	1:AAA:764:SER:O	2.13	0.48
1:AAA:350:GLY:N	1:AAA:588:PRO:HG3	2.28	0.48
1:AAA:756:MET:HE2	1:AAA:781:GLY:CA	2.44	0.48
1:AAA:327:LEU:HD23	1:AAA:360:SER:OG	2.13	0.48
1:AAA:549:LEU:CD1	1:AAA:564:MET:HE1	2.43	0.48
1:AAA:157:LEU:HD22	1:AAA:161:GLU:HB3	1.96	0.47
1:AAA:637:ALA:HB1	1:AAA:644:GLY:HA2	1.96	0.47
1:AAA:679:MET:O	1:AAA:683:MET:HG3	2.15	0.47
1:AAA:335:ALA:C	1:AAA:365:VAL:HG21	2.39	0.47
1:AAA:684:LYS:HD2	3:AAA:1218:HOH:O	2.15	0.47
1:AAA:912:PHE:HB2	1:AAA:913:GLY:HA3	1.95	0.47
1:AAA:188:ARG:NH2	1:AAA:266:LEU:HD22	2.30	0.46
1:AAA:380:SER:OG	1:AAA:382:CYS:SG	2.66	0.46
1:AAA:366:CYS:O	1:AAA:367:SER:CB	2.62	0.46
1:AAA:245:GLY:HA3	1:AAA:768:ALA:HB2	1.98	0.46
1:AAA:902:ARG:HD3	1:AAA:906:GLN:HB2	1.98	0.46
1:AAA:841:LYS:CG	1:AAA:844:MET:HG3	2.43	0.46
1:AAA:441:MET:HE3	1:AAA:469:ALA:HB3	1.98	0.45
1:AAA:387:MET:CE	1:AAA:590:CYS:SG	3.04	0.45
1:AAA:676:THR:HG22	1:AAA:680:LYS:HE2	1.97	0.45
1:AAA:432:LEU:HB3	1:AAA:483:VAL:CG2	2.47	0.45
1:AAA:482:PRO:HA	3:AAA:1236:HOH:O	2.16	0.45
1:AAA:138:ASP:OD2	1:AAA:428:TYR:OH	2.25	0.45
1:AAA:491:ILE:O	1:AAA:495:ILE:CD1	2.64	0.45
1:AAA:756:MET:HG3	1:AAA:780:ASN:O	2.17	0.44
1:AAA:892:GLY:O	1:AAA:894:ARG:N	2.50	0.44
1:AAA:367:SER:HB3	1:AAA:368:GLU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:456:ALA:HB3	3:AAA:1217:HOH:O	2.18	0.44
1:AAA:365:VAL:O	1:AAA:366:CYS:C	2.62	0.43
1:AAA:492:LEU:HA	1:AAA:495:ILE:HD12	2.00	0.43
1:AAA:489:GLU:HG3	1:AAA:490:LYS:N	2.34	0.43
1:AAA:894:ARG:HA	1:AAA:894:ARG:NE	2.33	0.43
1:AAA:329:GLU:CG	1:AAA:472:VAL:CG2	2.97	0.42
1:AAA:495:ILE:C	1:AAA:497:GLU:N	2.76	0.42
1:AAA:238:GLU:HB3	1:AAA:278:HIS:CE1	2.54	0.42
1:AAA:247:HIS:CD2	1:AAA:740:LEU:HD21	2.55	0.42
1:AAA:229:ARG:NH1	3:AAA:1222:HOH:O	2.52	0.42
1:AAA:281:SER:O	1:AAA:285:MET:HG3	2.19	0.42
1:AAA:486:PRO:HG2	1:AAA:491:ILE:HD11	2.02	0.41
1:AAA:553:THR:HG23	1:AAA:555:TRP:CE2	2.55	0.41
1:AAA:617:GLN:HE21	1:AAA:984:ALA:HA	1.85	0.41
1:AAA:194:VAL:CG2	1:AAA:216:LEU:HD21	2.49	0.41
1:AAA:539:GLN:NE2	1:AAA:570[A]:SER:OG	2.53	0.41
1:AAA:618:VAL:HG12	1:AAA:629:LEU:CD2	2.49	0.41
1:AAA:333:VAL:HA	3:AAA:1462:HOH:O	2.21	0.40
1:AAA:512:ARG:CZ	1:AAA:512:ARG:HB3	2.51	0.40
1:AAA:216:LEU:HD12	1:AAA:256:LEU:HD11	2.03	0.40
1:AAA:349:HIS:CE1	1:AAA:588:PRO:HG2	2.56	0.40
1:AAA:495:ILE:HD13	1:AAA:566:TYR:H	1.87	0.40
1:AAA:722:GLU:HG3	3:AAA:1427:HOH:O	2.22	0.40
1:AAA:434:THR:HG21	1:AAA:477:GLU:HA	2.02	0.40
1:AAA:436:GLU:O	1:AAA:437:ARG:HD2	2.22	0.40
1:AAA:759:LEU:O	1:AAA:777:ILE:HA	2.22	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]	1.48	0.72

5.3 Torsion angles

5.3.1 Protein backbone

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	808/1084 (74%)	775 (96%)	27 (3%)	6 (1%)	18	8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	367	SER
1	AAA	893	ASP
1	AAA	366	CYS
1	AAA	913	GLY
1	AAA	1026	SER
1	AAA	368	GLU

5.3.2 Protein sidechains ⓘ

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	736/962 (76%)	714 (97%)	22 (3%)	36	24

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	111	LYS
1	AAA	203	PHE
1	AAA	291	ASN
1	AAA	332	LYS
1	AAA	340	LYS
1	AAA	352	GLU
1	AAA	356	LYS
1	AAA	360	SER
1	AAA	389	ARG
1	AAA	423	LEU
1	AAA	453	LEU
1	AAA	472	VAL
1	AAA	517	ARG

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Mol	Chain	Res	Type
1	AAA	530	LEU
1	AAA	534	MET
1	AAA	553	THR
1	AAA	634	LEU
1	AAA	743	GLU
1	AAA	756	MET
1	AAA	841	LYS
1	AAA	915	PHE
1	AAA	1009	GLU

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 oligosaccharides 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	VEQ	AAA	1101	-	41,43,43	1.37	6 (14%)	58,65,65	2.73	15 (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
2	VEQ	AAA	1101	-	-	1/31/45/45	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	1101	VEQ	C33-N34	3.31	1.43	1.38
2	AAA	1101	VEQ	C40-C39	2.79	1.55	1.49
2	AAA	1101	VEQ	O18-S17	-2.64	1.40	1.43
2	AAA	1101	VEQ	C21-N20	-2.64	1.39	1.43
2	AAA	1101	VEQ	C12-C11	2.28	1.42	1.39
2	AAA	1101	VEQ	S17-N20	-2.23	1.60	1.63

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	1101	VEQ	C8-N7-C15	-11.44	108.33	113.15
2	AAA	1101	VEQ	C33-N38-C39	6.14	114.12	110.38
2	AAA	1101	VEQ	C9-C8-N7	6.07	105.54	102.31
2	AAA	1101	VEQ	S32-C33-N38	-5.45	110.90	115.78
2	AAA	1101	VEQ	C33-S32-C31	5.12	91.53	88.35
2	AAA	1101	VEQ	C39-C31-S32	-5.00	106.87	109.91
2	AAA	1101	VEQ	C6-C4-C2	-4.53	109.58	119.25
2	AAA	1101	VEQ	S32-C33-N34	3.88	128.92	123.72
2	AAA	1101	VEQ	C8-C9-C14	-3.78	107.21	109.96
2	AAA	1101	VEQ	C28-N26-C25	3.74	118.29	110.69
2	AAA	1101	VEQ	O16-C15-C14	-3.35	124.06	129.15
2	AAA	1101	VEQ	C30-C29-C24	-2.18	118.14	121.00
2	AAA	1101	VEQ	C31-C39-N38	2.14	116.50	115.01
2	AAA	1101	VEQ	C11-C10-C9	-2.11	118.31	121.47
2	AAA	1101	VEQ	C13-S17-N20	2.00	109.66	107.30

There are no chirality outliers.

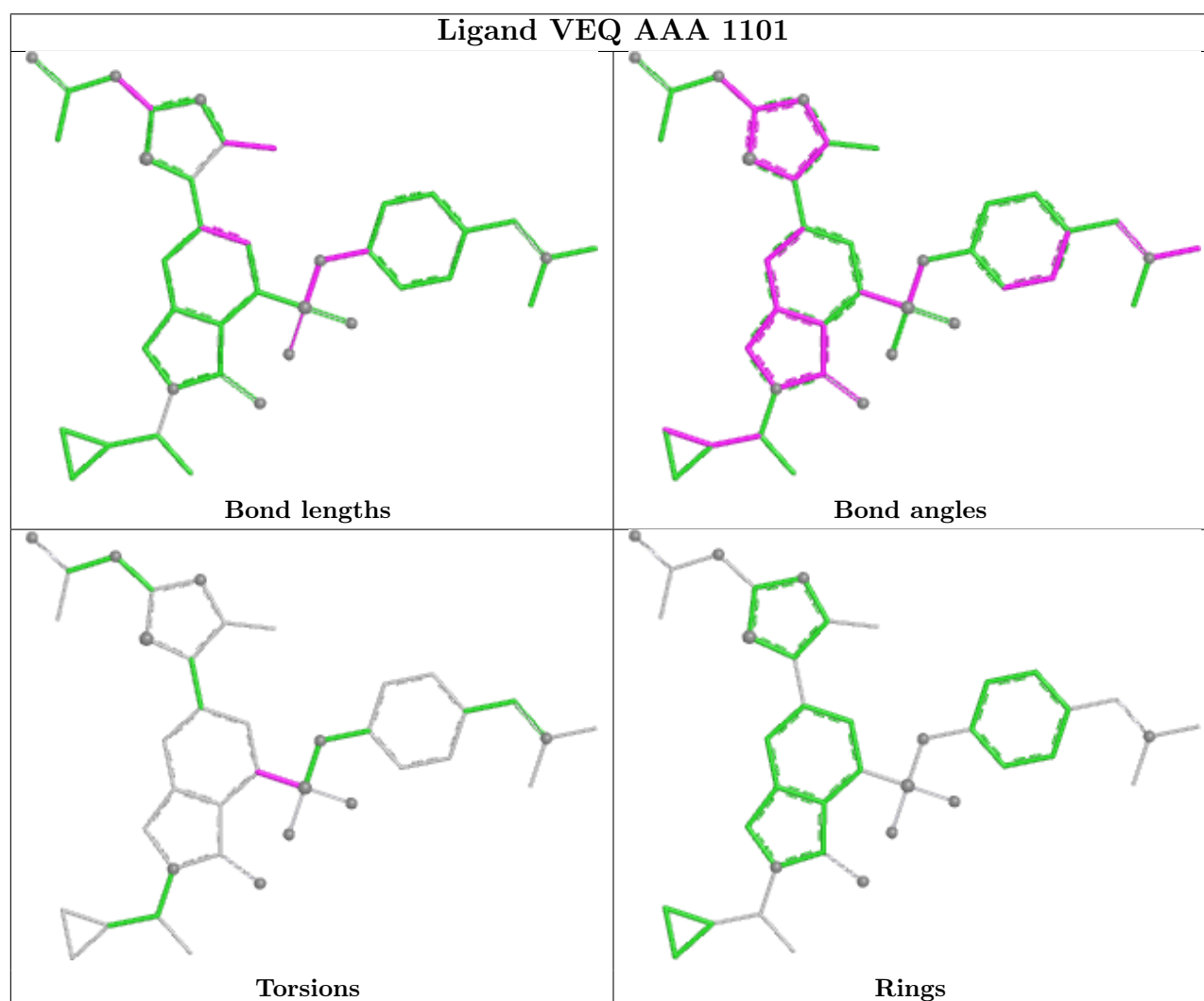
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	1101	VEQ	C14-C13-S17-O18

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 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	21.82

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%)	1.31	199 (24%) 2 1	12, 40, 72, 105	4 (0%)

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	495	ILE	8.6
1	AAA	919	PHE	8.4
1	AAA	445	VAL	8.0
1	AAA	317	TRP	8.0
1	AAA	335	ALA	7.5
1	AAA	1027	TRP	7.1
1	AAA	316	LEU	6.7
1	AAA	514	ILE	6.3
1	AAA	333	VAL	6.3
1	AAA	515	LEU	6.1
1	AAA	479	ALA	6.0
1	AAA	478	VAL	5.7
1	AAA	397	VAL	5.6
1	AAA	511	LEU	5.6
1	AAA	341	LEU	5.6
1	AAA	319	LEU	5.4
1	AAA	227	VAL	5.3
1	AAA	894	ARG	5.3
1	AAA	366	CYS	5.2
1	AAA	332	LYS	5.1
1	AAA	472	VAL	4.9
1	AAA	367	SER	4.8
1	AAA	205	PHE	4.8
1	AAA	914	HIS	4.7
1	AAA	846	ALA	4.7
1	AAA	523	LEU	4.7
1	AAA	228	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	AAA	342	VAL	4.5
1	AAA	398	VAL	4.5
1	AAA	345	ALA	4.4
1	AAA	936	TYR	4.3
1	AAA	109	VAL	4.3
1	AAA	395	TYR	4.2
1	AAA	377	PHE	4.2
1	AAA	482	PRO	4.1
1	AAA	375	LEU	4.1
1	AAA	363	VAL	4.1
1	AAA	452	LEU	4.1
1	AAA	322	PRO	4.0
1	AAA	318	SER	4.0
1	AAA	517	ARG	4.0
1	AAA	203	PHE	3.9
1	AAA	491	ILE	3.9
1	AAA	474	TYR	3.8
1	AAA	379	ILE	3.8
1	AAA	512	ARG	3.8
1	AAA	381	VAL	3.8
1	AAA	475	LEU	3.7
1	AAA	330	GLY	3.7
1	AAA	483	VAL	3.7
1	AAA	1026	SER	3.7
1	AAA	913	GLY	3.7
1	AAA	621	TYR	3.6
1	AAA	198	GLY	3.6
1	AAA	509	GLU	3.6
1	AAA	331	ARG	3.6
1	AAA	416	CYS	3.6
1	AAA	354	LEU	3.6
1	AAA	494	LEU	3.6
1	AAA	1004	LEU	3.6
1	AAA	530	LEU	3.5
1	AAA	325	ILE	3.5
1	AAA	323	PHE	3.4
1	AAA	382	CYS	3.4
1	AAA	471	LEU	3.4
1	AAA	895	HIS	3.3
1	AAA	893	ASP	3.3
1	AAA	365	VAL	3.3
1	AAA	370	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	AAA	771	ALA	3.3
1	AAA	845	ALA	3.3
1	AAA	492	LEU	3.3
1	AAA	360	SER	3.3
1	AAA	516	GLU	3.2
1	AAA	383	ASP	3.2
1	AAA	553	THR	3.2
1	AAA	371	TRP	3.2
1	AAA	496	THR	3.2
1	AAA	473	ILE	3.1
1	AAA	891	ILE	3.1
1	AAA	1002	LEU	3.1
1	AAA	257	CYS	3.1
1	AAA	192	VAL	3.1
1	AAA	334	ASN	3.1
1	AAA	897	ASP	3.0
1	AAA	453	LEU	3.0
1	AAA	187	ASN	3.0
1	AAA	770	SER	3.0
1	AAA	440	TYR	3.0
1	AAA	1003	ALA	3.0
1	AAA	235	GLN	2.9
1	AAA	945	GLY	2.9
1	AAA	267	HIS	2.9
1	AAA	848	ALA	2.9
1	AAA	438	CYS	2.8
1	AAA	566	TYR	2.8
1	AAA	226	THR	2.8
1	AAA	394	LEU	2.8
1	AAA	418	ILE	2.8
1	AAA	434	THR	2.8
1	AAA	522	GLU	2.8
1	AAA	847	THR	2.8
1	AAA	378	ASP	2.8
1	AAA	393	ALA	2.7
1	AAA	356	LYS	2.7
1	AAA	769	GLY	2.7
1	AAA	339	MET	2.7
1	AAA	488	LEU	2.7
1	AAA	991	CYS	2.7
1	AAA	415	ASP	2.7
1	AAA	559	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	AAA	291	ASN	2.7
1	AAA	358	VAL	2.6
1	AAA	561	VAL	2.6
1	AAA	714	MET	2.6
1	AAA	225	ALA	2.6
1	AAA	510	GLU	2.6
1	AAA	484	TYR	2.6
1	AAA	1013	LYS	2.6
1	AAA	918	ASN	2.6
1	AAA	269	GLY	2.6
1	AAA	230	GLN	2.6
1	AAA	436	GLU	2.6
1	AAA	896	SER	2.6
1	AAA	934	LEU	2.5
1	AAA	531	VAL	2.5
1	AAA	391	CYS	2.5
1	AAA	376	GLU	2.5
1	AAA	513	GLU	2.5
1	AAA	557	LYS	2.4
1	AAA	562	ALA	2.4
1	AAA	188	ARG	2.4
1	AAA	843	ASN	2.4
1	AAA	995	ILE	2.4
1	AAA	929	ARG	2.4
1	AAA	1025	GLU	2.4
1	AAA	321	GLN	2.4
1	AAA	1005	GLY	2.4
1	AAA	206	GLN	2.4
1	AAA	343	VAL	2.4
1	AAA	190	LEU	2.3
1	AAA	565	LEU	2.3
1	AAA	916	LEU	2.3
1	AAA	962	ARG	2.3
1	AAA	524	TYR	2.3
1	AAA	373	GLN	2.3
1	AAA	258	HIS	2.3
1	AAA	396	ALA	2.3
1	AAA	456	ALA	2.3
1	AAA	558	HIS	2.3
1	AAA	328	ILE	2.3
1	AAA	435	GLY	2.3
1	AAA	933	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	AAA	359	SER	2.3
1	AAA	477	GLU	2.3
1	AAA	930	VAL	2.3
1	AAA	253	ASN	2.3
1	AAA	1020	ASN	2.3
1	AAA	426	PHE	2.2
1	AAA	340	LYS	2.2
1	AAA	841	LYS	2.2
1	AAA	1024	ARG	2.2
1	AAA	320	GLU	2.2
1	AAA	1012	LEU	2.2
1	AAA	795	GLN	2.2
1	AAA	915	PHE	2.2
1	AAA	266	LEU	2.2
1	AAA	992	SER	2.2
1	AAA	469	ALA	2.2
1	AAA	487	ALA	2.2
1	AAA	162	TRP	2.2
1	AAA	993	LYS	2.2
1	AAA	497	GLU	2.2
1	AAA	792	GLN	2.2
1	AAA	947	THR	2.2
1	AAA	423	LEU	2.2
1	AAA	907	LEU	2.2
1	AAA	141	THR	2.1
1	AAA	584	ASP	2.1
1	AAA	538	VAL	2.1
1	AAA	990	SER	2.1
1	AAA	134	PRO	2.1
1	AAA	327	LEU	2.1
1	AAA	351	ASN	2.1
1	AAA	591	TYR	2.1
1	AAA	892	GLY	2.1
1	AAA	1014	HIS	2.1
1	AAA	270	LEU	2.1
1	AAA	220	ALA	2.1
1	AAA	485	PHE	2.1
1	AAA	224	LYS	2.1
1	AAA	329	GLU	2.1
1	AAA	1006	LYS	2.1
1	AAA	534	MET	2.1
1	AAA	552	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	AAA	748	GLN	2.1
1	AAA	755	LYS	2.0
1	AAA	417	PRO	2.0
1	AAA	476	PRO	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](#)

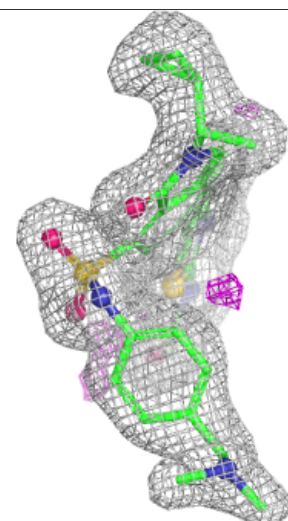
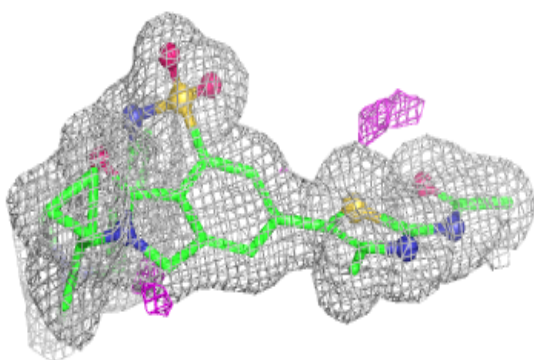
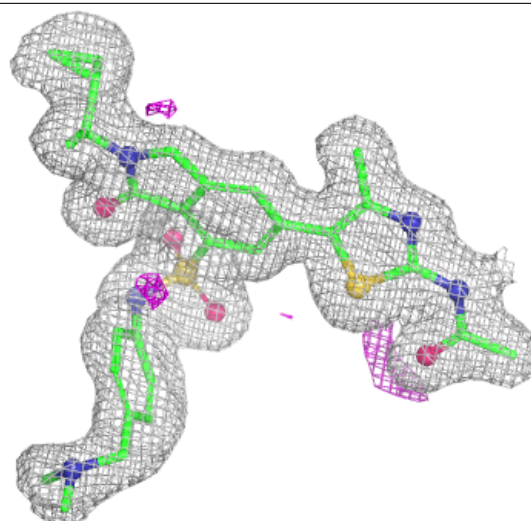
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	VEQ	AAA	1101	39/39	0.98	0.06	19,24,39,40	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 VEQ 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.