



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:45 PM GMT

PDB ID : 4G11
Title : X-ray structure of PI3K-gamma bound to a 4-(morpholin-4-yl)- (6-oxo-1,6-dihydropyrimidin-2-yl)amide inhibitor
Authors : Morales, R.
Deposited on : 2012-07-10
Resolution : 3.40 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

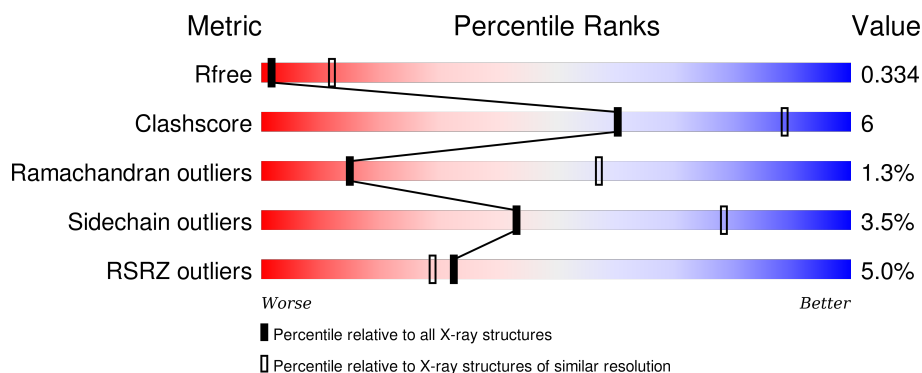
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	A	966	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	0W7	A	1201	-	-	-	X

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6801 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.

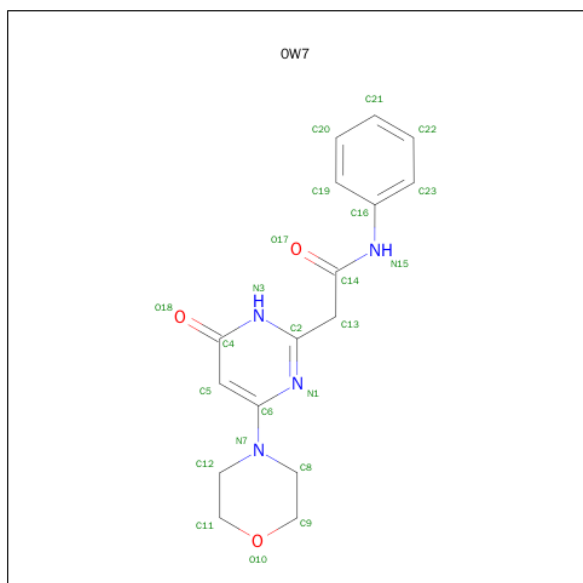
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	836	Total	C	N	O	S	4	0	0
			6778	4349	1157	1237	35			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	EXPRESSION TAG	UNP P48736
A	1103	HIS	-	EXPRESSION TAG	UNP P48736
A	1104	HIS	-	EXPRESSION TAG	UNP P48736
A	1105	HIS	-	EXPRESSION TAG	UNP P48736
A	1106	HIS	-	EXPRESSION TAG	UNP P48736
A	1107	HIS	-	EXPRESSION TAG	UNP P48736
A	1108	HIS	-	EXPRESSION TAG	UNP P48736

- Molecule 2 is 2-[4-(MORPHOLIN-4-YL)-6-OXO-1,6-DIHYDROPYRIMIDIN-2-YL]-N-PHENYLACETAMIDE (three-letter code: 0W7) (formula: C₁₆H₁₈N₄O₃).

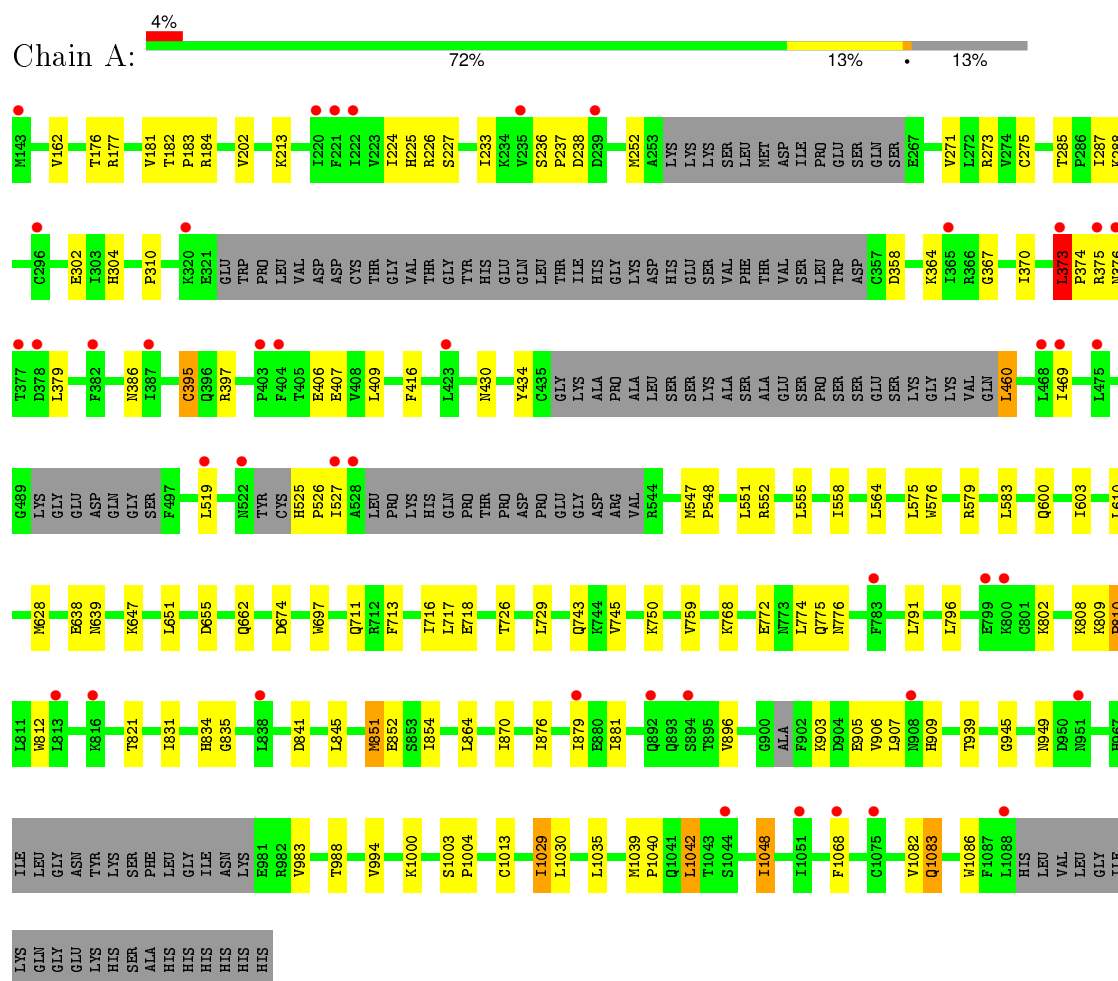


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	16	4	3		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 gamma isoform



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.63Å 67.38Å 105.89Å 90.00° 96.14° 90.00°	Depositor
Resolution (Å)	61.30 – 3.40 61.34 – 3.40	Depositor EDS
% Data completeness (in resolution range)	89.4 (61.30-3.40) 89.4 (61.34-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.282 , 0.349 0.275 , 0.334	Depositor DCC
R_{free} test set	688 reflections (5.88%)	DCC
Wilson B-factor (Å ²)	86.0	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 22.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 12318 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6801	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 0W7

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	0.31	0/6922	0.46	0/9361

There are no bond length outliers.

There are no bond angle outliers.

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	6778	0	6809	75	0
2	A	23	0	18	5	0
All	All	6801	0	6827	76	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 6.

All (76) 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:373:LEU:H	1:A:374:PRO:HD3	1.50	0.77
1:A:525:HIS:HB3	1:A:526:PRO:HD3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:LEU:HD22	1:A:406:GLU:HG3	1.69	0.73
1:A:225:HIS:HE1	1:A:304:HIS:HD2	1.40	0.69
1:A:202:VAL:HG11	1:A:285:THR:HG21	1.73	0.69
1:A:373:LEU:H	1:A:374:PRO:CD	2.07	0.67
1:A:1042:LEU:HD13	1:A:1042:LEU:H	1.60	0.65
1:A:225:HIS:HE1	1:A:304:HIS:CD2	2.17	0.62
1:A:182:THR:HB	1:A:183:PRO:HD3	1.82	0.62
1:A:881:ILE:HA	2:A:1201:OW7:H17	1.83	0.60
2:A:1201:OW7:H4	2:A:1201:OW7:O17	2.00	0.60
1:A:905:GLU:HB3	1:A:909:HIS:HE1	1.67	0.59
1:A:988:THR:HG21	1:A:1083:GLN:HG3	1.84	0.59
1:A:373:LEU:N	1:A:374:PRO:CD	2.66	0.58
1:A:662:GLN:HG2	1:A:1030:LEU:HD22	1.86	0.58
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.39	0.57
1:A:905:GLU:HB3	1:A:909:HIS:CE1	2.39	0.57
1:A:397:ARG:HE	1:A:416:PHE:HA	1.71	0.55
1:A:903:LYS:HB2	1:A:906:VAL:HG23	1.89	0.54
1:A:469:ILE:HD13	1:A:527:ILE:HD11	1.88	0.54
1:A:638:GLU:HG3	1:A:639:ASN:HD22	1.73	0.54
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.44	0.53
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.90	0.53
1:A:810:PRO:HG2	2:A:1201:OW7:H5	1.90	0.52
1:A:271:VAL:HB	1:A:310:PRO:HG3	1.91	0.52
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.90	0.52
1:A:768:LYS:O	1:A:772:GLU:HG2	2.11	0.51
1:A:1083:GLN:HA	1:A:1083:GLN:HE21	1.76	0.51
1:A:983:VAL:HB	1:A:1082:VAL:HG21	1.93	0.51
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.75	0.50
1:A:583:LEU:HD12	1:A:610:LEU:HG	1.92	0.50
1:A:852:GLU:HG3	1:A:864:LEU:HD12	1.95	0.49
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.94	0.49
1:A:831:ILE:HB	1:A:879:ILE:HB	1.94	0.49
1:A:812:TRP:HE3	2:A:1201:OW7:C20	2.26	0.48
1:A:743:GLN:HE21	1:A:876:ILE:HG12	1.79	0.48
1:A:939:THR:HG23	1:A:945:GLY:HA2	1.97	0.47
1:A:386:ASN:HB2	1:A:430:ASN:HB3	1.95	0.47
1:A:548:PRO:HG2	1:A:551:LEU:HD12	1.97	0.47
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.97	0.47
1:A:547:MET:HB2	1:A:552:ARG:HH11	1.80	0.46
1:A:745:VAL:HG21	1:A:774:LEU:HD11	1.98	0.46
1:A:181:VAL:HG22	1:A:184:ARG:HH22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1035:LEU:HD23	1:A:1039:MET:HG3	1.97	0.46
1:A:809:LYS:HA	1:A:810:PRO:HD3	1.78	0.45
1:A:697:TRP:HB3	1:A:870:ILE:HG21	1.99	0.45
1:A:628:MET:HB3	1:A:1029:ILE:HD12	1.97	0.45
1:A:1042:LEU:CD1	1:A:1042:LEU:H	2.28	0.44
1:A:275:CYS:HB3	1:A:821:THR:O	2.18	0.44
1:A:949:ASN:N	1:A:1083:GLN:HE22	2.15	0.44
1:A:395:CYS:HB3	1:A:416:PHE:HD2	1.83	0.44
1:A:576:TRP:O	1:A:579:ARG:HG3	2.17	0.43
1:A:600:GLN:HG3	1:A:603:ILE:HD12	2.00	0.43
1:A:224:ILE:HD13	1:A:233:ILE:HD13	1.99	0.43
1:A:851:MET:HA	1:A:854:ILE:HD12	2.01	0.43
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.99	0.43
1:A:907:LEU:HD22	1:A:994:VAL:HG21	2.00	0.43
1:A:812:TRP:CE3	2:A:1201:OW7:H3	2.53	0.43
1:A:558:ILE:HG21	1:A:575:LEU:HD21	2.00	0.43
1:A:775:GLN:HE22	1:A:796:LEU:H	1.67	0.43
1:A:555:LEU:HA	1:A:558:ILE:HD12	2.00	0.42
1:A:713:PHE:HA	1:A:716:ILE:HD12	2.02	0.42
1:A:600:GLN:HB2	1:A:603:ILE:HB	2.02	0.42
1:A:177:ARG:HD2	1:A:718:GLU:OE1	2.19	0.42
1:A:525:HIS:HB3	1:A:526:PRO:CD	2.45	0.42
1:A:364:LYS:HB3	1:A:519:LEU:HB3	2.02	0.41
1:A:1003:SER:HB2	1:A:1004:PRO:HD2	2.02	0.41
1:A:434:TYR:HA	1:A:460:LEU:HA	2.02	0.41
1:A:579:ARG:HB3	1:A:610:LEU:HD12	2.01	0.41
1:A:287:ILE:HG13	1:A:287:ILE:H	1.69	0.41
1:A:750:LYS:HG3	1:A:809:LYS:HB2	2.02	0.41
1:A:373:LEU:HD23	1:A:374:PRO:HD3	2.02	0.41
1:A:808:LYS:HD3	1:A:835:GLY:HA3	2.03	0.41
1:A:236:SER:C	1:A:238:ASP:H	2.25	0.40
1:A:726:THR:HA	1:A:729:LEU:HB2	2.03	0.40
1:A:367:GLY:HA3	1:A:409:LEU:HD23	2.03	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	818/966 (85%)	755 (92%)	52 (6%)	11 (1%)	15	57

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	776	ASN
1	A	1040	PRO
1	A	1086	TRP
1	A	227	SER
1	A	376	ASN
1	A	373	LEU
1	A	237	PRO
1	A	759	VAL
1	A	896	VAL
1	A	1000	LYS
1	A	810	PRO

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	751/864 (87%)	725 (96%)	26 (4%)	43	78

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	VAL
1	A	213	LYS
1	A	226	ARG
1	A	252	MET
1	A	273	ARG
1	A	288	LYS
1	A	358	ASP
1	A	370	ILE
1	A	373	LEU
1	A	375	ARG
1	A	379	LEU
1	A	395	CYS
1	A	407	GLU
1	A	460	LEU
1	A	647	LYS
1	A	711	GLN
1	A	717	LEU
1	A	791	LEU
1	A	802	LYS
1	A	841	ASP
1	A	845	LEU
1	A	851	MET
1	A	1029	ILE
1	A	1042	LEU
1	A	1048	ILE
1	A	1083	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	225	HIS
1	A	291	GLN
1	A	299	ASN
1	A	304	HIS
1	A	391	GLN
1	A	554	GLN
1	A	601	GLN
1	A	639	ASN
1	A	711	GLN
1	A	734	GLN
1	A	743	GLN
1	A	769	GLN

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Mol	Chain	Res	Type
1	A	773	ASN
1	A	846	GLN
1	A	909	HIS
1	A	948	HIS
1	A	1007	GLN
1	A	1083	GLN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	0W7	A	1201	-	23,25,25	0.87	0	30,33,33	2.22	9 (30%)

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	0W7	A	1201	-	-	0/12/20/20	0/3/3/3

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	0W7	C8-N7-C6	-4.01	110.69	120.22
2	A	1201	0W7	N3-C2-N1	-4.00	120.41	126.18
2	A	1201	0W7	C12-N7-C6	-3.92	110.91	120.22
2	A	1201	0W7	C5-C4-N3	-3.36	119.98	124.05
2	A	1201	0W7	C2-C13-C14	-2.72	106.04	113.71
2	A	1201	0W7	C5-C6-N1	-2.17	119.00	122.53
2	A	1201	0W7	C4-C5-C6	2.22	119.11	116.33
2	A	1201	0W7	N1-C6-N7	3.66	120.78	116.63
2	A	1201	0W7	C2-N1-C6	6.68	121.25	115.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	0W7	5	0

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 ⓘ

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	A	836/966 (86%)	0.53	42 (5%) 32 29	43, 80, 106, 138	1 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	528	ALA	8.4
1	A	377	THR	4.3
1	A	373	LEU	3.8
1	A	892	GLN	3.5
1	A	403	PRO	3.2
1	A	894	SER	3.1
1	A	376	ASN	3.0
1	A	222	ILE	3.0
1	A	527	ILE	3.0
1	A	375	ARG	2.8
1	A	387	ILE	2.8
1	A	468	LEU	2.7
1	A	783	PHE	2.7
1	A	522	ASN	2.7
1	A	382	PHE	2.7
1	A	879	ILE	2.7
1	A	404	PHE	2.6
1	A	296	CYS	2.5
1	A	1068	PHE	2.5
1	A	221	PHE	2.5
1	A	235	VAL	2.5
1	A	519	LEU	2.4
1	A	220	ILE	2.4
1	A	800	LYS	2.4
1	A	378	ASP	2.4
1	A	816	LYS	2.3
1	A	1044	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	951	ASN	2.3
1	A	799	GLU	2.3
1	A	1051	ILE	2.3
1	A	239	ASP	2.3
1	A	469	ILE	2.2
1	A	813	LEU	2.2
1	A	1075	CYS	2.2
1	A	1088	LEU	2.1
1	A	908	ASN	2.1
1	A	423	LEU	2.1
1	A	143	MET	2.1
1	A	320	LYS	2.1
1	A	475	LEU	2.1
1	A	838	LEU	2.1
1	A	365	ILE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	0W7	A	1201	23/23	0.84	0.44	1.40	93,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.