



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 03:08 AM EDT

PDB ID : 5SX9  
Title : Crystal Structure of PI3Kalpha in complex with fragment 14  
Authors : Gabelli, S.B.; Vogelstein, B.; Miller, M.S.; Amzel, L.M.  
Deposited on : 2016-08-09  
Resolution : 3.52 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

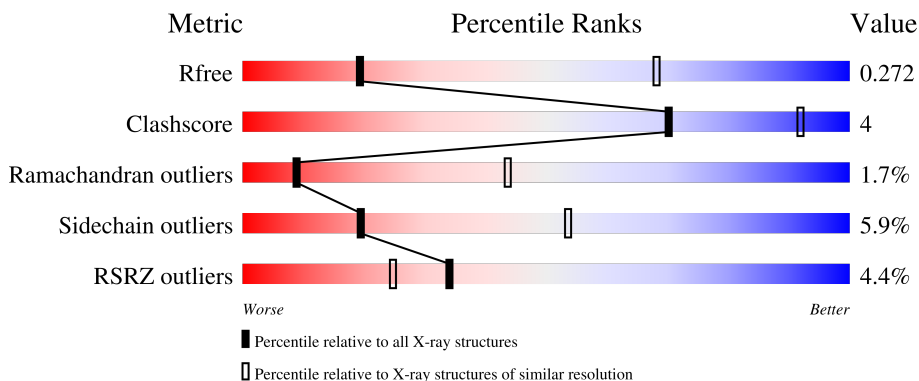
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.52 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))
$R_{free}$	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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  $\geq 3$ , 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	A	1096	 3% 79% 15% • 5%
2	B	279	 7% 73% 11% • 14%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10602 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 alpha isoform.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	1045	8540	5454	1467	1548	1	70	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP P42336
A	-26	SER	-	expression tag	UNP P42336
A	-25	TYR	-	expression tag	UNP P42336
A	-24	TYR	-	expression tag	UNP P42336
A	-23	HIS	-	expression tag	UNP P42336
A	-22	HIS	-	expression tag	UNP P42336
A	-21	HIS	-	expression tag	UNP P42336
A	-20	HIS	-	expression tag	UNP P42336
A	-19	HIS	-	expression tag	UNP P42336
A	-18	HIS	-	expression tag	UNP P42336
A	-17	ASP	-	expression tag	UNP P42336
A	-16	TYR	-	expression tag	UNP P42336
A	-15	ASP	-	expression tag	UNP P42336
A	-14	ILE	-	expression tag	UNP P42336
A	-13	PRO	-	expression tag	UNP P42336
A	-12	THR	-	expression tag	UNP P42336
A	-11	THR	-	expression tag	UNP P42336
A	-10	GLU	-	expression tag	UNP P42336
A	-9	ASN	-	expression tag	UNP P42336
A	-8	LEU	-	expression tag	UNP P42336
A	-7	TYR	-	expression tag	UNP P42336
A	-6	PHE	-	expression tag	UNP P42336
A	-5	GLN	-	expression tag	UNP P42336
A	-4	GLY	-	expression tag	UNP P42336
A	-3	ALA	-	expression tag	UNP P42336
A	-2	MET	-	expression tag	UNP P42336

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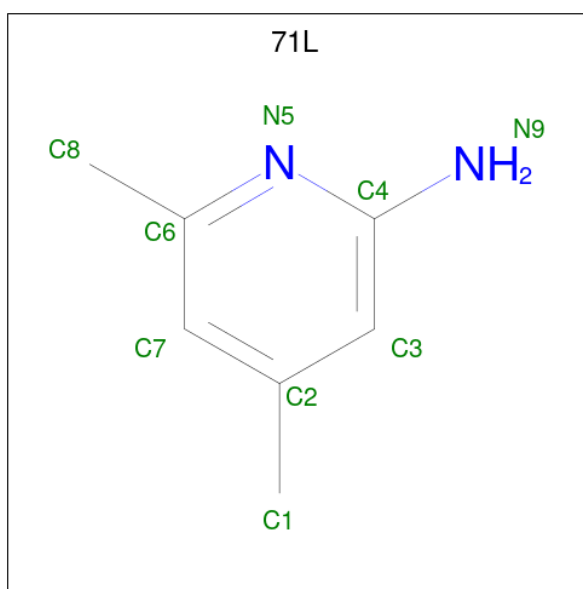
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42336
A	0	SER	-	expression tag	UNP P42336

- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	239	2053	1289	366	392	6	0	0	0

- Molecule 3 is 4,6-dimethylpyridin-2-amine (three-letter code: 71L) (formula: C<sub>7</sub>H<sub>10</sub>N<sub>2</sub>).

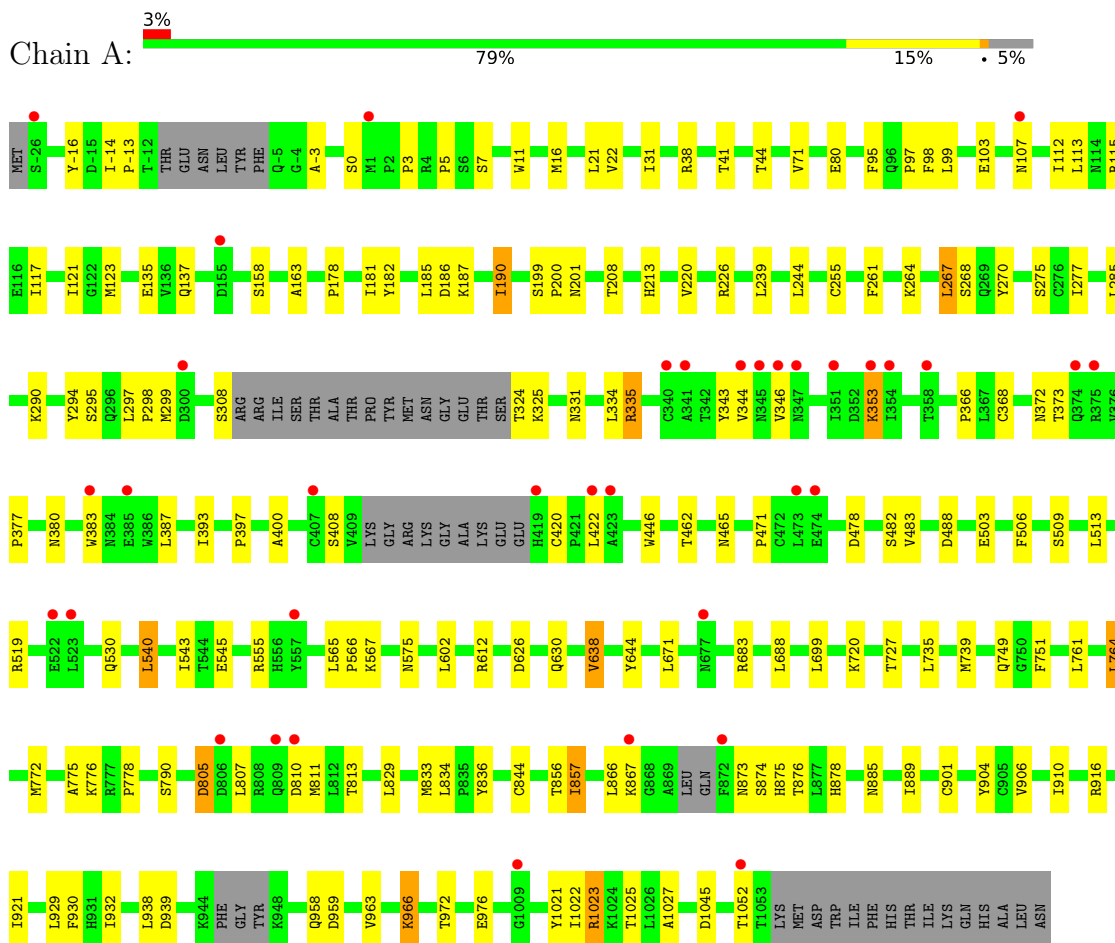


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
3	A	1	9	7	2	0	0

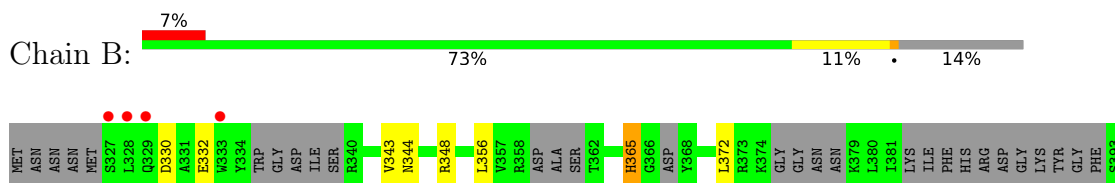
### 3 Residue-property plots [i](#)

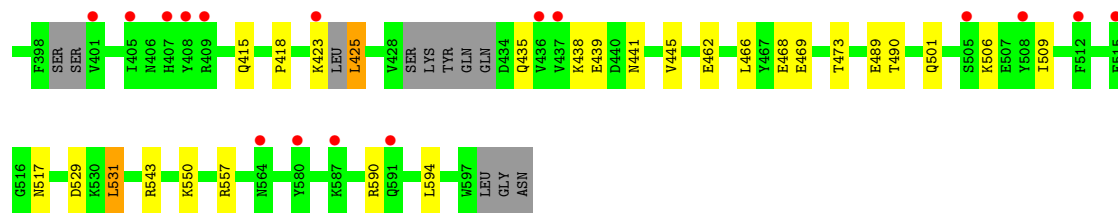
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 alpha isoform



- Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.45Å 116.10Å 147.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.34 – 3.52 48.79 – 3.52	Depositor EDS
% Data completeness (in resolution range)	98.4 (91.34-3.52) 98.6 (48.79-3.52)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.79 (at 3.48Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.192 , 0.277 0.196 , 0.272	Depositor DCC
$R_{free}$ test set	1246 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	110.7	Xtrriage
Anisotropy	0.276	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 97.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10602	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	134.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 71L, SEP

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	0.56	0/8726	0.80	1/11792 (0.0%)
2	B	0.53	0/2078	0.73	0/2771
All	All	0.56	0/10804	0.79	1/14563 (0.0%)

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	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	1023	ARG	NE-CZ-NH1	5.93	123.27	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	ASN	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	A	8540	0	8519	68	0
2	B	2053	0	2048	11	0
3	A	9	0	0	0	0
All	All	10602	0	10567	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 4.

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:910:ILE:O	1:A:1025:THR:HG21	1.90	0.71
1:A:1022:ILE:HA	1:A:1025:THR:HG22	1.84	0.60
1:A:602:LEU:O	1:A:612:ARG:NH2	2.35	0.59
2:B:343:VAL:HG13	2:B:356:LEU:HD11	1.84	0.59
1:A:353:LYS:HA	1:A:377:PRO:HB3	1.84	0.58
1:A:885:ASN:HB3	1:A:889:ILE:HG22	1.86	0.58
1:A:290:LYS:HB3	1:A:294:TYR:CE2	2.40	0.57
1:A:543:ILE:HD11	1:A:567:LYS:HD3	1.87	0.57
1:A:3:PRO:HG2	1:A:844:CYS:CB	2.36	0.55
1:A:343:TYR:OH	2:B:557:ARG:NH1	2.37	0.55
1:A:261:PHE:HA	1:A:270:TYR:CE2	2.43	0.54
1:A:906:VAL:HG12	1:A:910:ILE:HD12	1.90	0.53
1:A:220:VAL:HG21	1:A:267:LEU:CD1	2.40	0.52
1:A:16:MET:HG3	1:A:38:ARG:HB2	1.92	0.52
1:A:805:ASP:O	1:A:807:LEU:HD22	2.08	0.52
1:A:372:ASN:HB3	1:A:387:LEU:HD21	1.91	0.51
1:A:408:SER:OG	1:A:422:LEU:HD21	2.10	0.51
1:A:31:ILE:HD11	2:B:531:LEU:HD13	1.93	0.51
1:A:117:ILE:HG13	1:A:699:LEU:HD21	1.92	0.51
1:A:749:GLN:HE21	1:A:764:LEU:H	1.58	0.51
1:A:135:GLU:OE2	1:A:644:TYR:HB3	2.11	0.50
1:A:22:VAL:HG12	1:A:97:PRO:HB2	1.93	0.50
1:A:873:ASN:HB3	1:A:876:THR:HG23	1.93	0.50
1:A:163:ALA:HB2	1:A:297:LEU:HD11	1.94	0.50
1:A:833:MET:HE1	1:A:904:TYR:HA	1.94	0.49
1:A:836:TYR:CE2	1:A:932:ILE:HG22	2.47	0.49
1:A:-14:ILE:HG13	1:A:-13:PRO:CD	2.43	0.48
1:A:366:PRO:HB3	1:A:575:ASN:HB3	1.95	0.48
1:A:772:MET:HB2	1:A:778:PRO:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:PRO:HG2	1:A:844:CYS:HB3	1.94	0.48
1:A:255:CYS:SG	1:A:285:LEU:O	2.72	0.48
1:A:335:ARG:NE	1:A:478:ASP:OD2	2.46	0.47
2:B:343:VAL:CG1	2:B:356:LEU:HD11	2.44	0.47
1:A:178:PRO:HD2	1:A:181:ILE:HD12	1.96	0.47
1:A:113:LEU:HD12	1:A:113:LEU:N	2.30	0.47
1:A:71:VAL:HG23	1:A:80:GLU:O	2.15	0.47
1:A:-14:ILE:HG13	1:A:-13:PRO:HD2	1.97	0.47
1:A:117:ILE:HG22	1:A:121:ILE:HD11	1.98	0.46
1:A:98:PHE:CE1	2:B:490:THR:HG23	2.51	0.46
1:A:190:ILE:HD11	1:A:213:HIS:HA	1.99	0.45
1:A:41:THR:OG1	1:A:44:THR:OG1	2.20	0.45
1:A:335:ARG:HA	1:A:387:LEU:O	2.17	0.45
1:A:958:GLN:O	1:A:959:ASP:C	2.56	0.44
2:B:506:LYS:HA	2:B:509:ILE:HG22	2.00	0.44
1:A:344:VAL:HG12	1:A:346:VAL:HG23	2.00	0.44
1:A:671:LEU:HB2	1:A:688:LEU:HD21	1.99	0.44
1:A:181:ILE:HG23	1:A:277:ILE:HG21	2.00	0.43
1:A:720:LYS:HE3	1:A:776:LYS:O	2.18	0.43
2:B:469:GLU:O	2:B:473:THR:OG1	2.26	0.43
1:A:334:LEU:HA	1:A:393:ILE:HD11	1.99	0.43
2:B:423:LYS:O	2:B:425:LEU:N	2.52	0.43
1:A:11:TRP:HB2	1:A:95:PHE:CD1	2.54	0.43
1:A:751:PHE:CE2	1:A:761:LEU:HD12	2.54	0.43
1:A:916:ARG:HB3	1:A:921:ILE:HD11	2.00	0.43
1:A:875:HIS:O	1:A:878:HIS:N	2.52	0.43
1:A:1023:ARG:O	1:A:1027:ALA:N	2.53	0.42
1:A:324:THR:HA	1:A:483:VAL:HG23	2.02	0.42
2:B:439:GLU:HB2	2:B:445:VAL:HG22	2.00	0.42
1:A:397:PRO:HD2	1:A:400:ALA:HB2	2.02	0.42
1:A:810:ASP:HA	1:A:813:THR:HG22	2.02	0.42
1:A:602:LEU:HB3	1:A:638:VAL:HG11	2.01	0.41
2:B:344:ASN:O	2:B:348:ARG:N	2.53	0.41
2:B:462:GLU:O	2:B:466:LEU:HD12	2.21	0.41
1:A:540:LEU:HB3	1:A:1023:ARG:HD2	2.02	0.41
1:A:834:LEU:HD23	1:A:930:PHE:CD1	2.56	0.41
1:A:878:HIS:HB2	1:A:963:VAL:HG22	2.02	0.41
1:A:446:TRP:CZ2	1:A:465:ASN:HA	2.56	0.41
1:A:503:GLU:HA	1:A:506:PHE:CE2	2.56	0.41
1:A:735:LEU:O	1:A:739:MET:HG3	2.22	0.41
1:A:938:LEU:HD22	1:A:1021:TYR:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:LEU:HD23	1:A:735:LEU:C	2.41	0.40
1:A:0:SER:OG	1:A:775:ALA:HB3	2.21	0.40
1:A:565:LEU:HB3	1:A:566:PRO:HD3	2.03	0.40
1:A:856:THR:O	1:A:857:ILE:C	2.59	0.40
1:A:182:TYR:O	1:A:185:LEU:HB2	2.22	0.40
1:A:901:CYS:HA	1:A:929:LEU:HD22	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	1032/1096 (94%)	907 (88%)	112 (11%)	13 (1%)	12	49
2	B	221/279 (79%)	189 (86%)	24 (11%)	8 (4%)	3	28
All	All	1253/1375 (91%)	1096 (88%)	136 (11%)	21 (2%)	9	44

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	555	ARG
1	A	972	THR
2	B	438	LYS
2	B	590	ARG
1	A	264	LYS
1	A	939	ASP
1	A	966	LYS
1	A	-3	ALA
1	A	5	PRO
1	A	186	ASP
2	B	332	GLU
2	B	365	HIS

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Mol	Chain	Res	Type
2	B	418	PRO
2	B	435	GLN
1	A	-16	TYR
2	B	330	ASP
2	B	517	ASN
1	A	380	ASN
1	A	471	PRO
1	A	857	ILE
1	A	200	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	954/998 (96%)	897 (94%)	57 (6%)	19	53
2	B	226/259 (87%)	213 (94%)	13 (6%)	20	54
All	All	1180/1257 (94%)	1110 (94%)	70 (6%)	19	53

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	21	LEU
1	A	99	LEU
1	A	103	GLU
1	A	107	ASN
1	A	112	ILE
1	A	115	ARG
1	A	123	MET
1	A	137	GLN
1	A	158	SER
1	A	187	LYS
1	A	190	ILE
1	A	199	SER
1	A	208	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	226	ARG
1	A	239	LEU
1	A	244	LEU
1	A	267	LEU
1	A	268	SER
1	A	275	SER
1	A	295	SER
1	A	298	PRO
1	A	299	MET
1	A	308	SER
1	A	325	LYS
1	A	331	ASN
1	A	335	ARG
1	A	353	LYS
1	A	368	CYS
1	A	373	THR
1	A	383	TRP
1	A	420	CYS
1	A	462	THR
1	A	482	SER
1	A	488	ASP
1	A	509	SER
1	A	513	LEU
1	A	519	ARG
1	A	530	GLN
1	A	540	LEU
1	A	545	GLU
1	A	626	ASP
1	A	630	GLN
1	A	638	VAL
1	A	683	ARG
1	A	727	THR
1	A	764	LEU
1	A	805	ASP
1	A	811	MET
1	A	829	LEU
1	A	866	LEU
1	A	867	LYS
1	A	874	SER
1	A	966	LYS
1	A	976	GLU
1	A	1045	ASP

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Mol	Chain	Res	Type
1	A	1052	THR
2	B	365	HIS
2	B	372	LEU
2	B	415	GLN
2	B	425	LEU
2	B	441	ASN
2	B	468	GLU
2	B	489	GLU
2	B	501	GLN
2	B	529	ASP
2	B	531	LEU
2	B	543	ARG
2	B	550	LYS
2	B	594	LEU

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

Mol	Chain	Res	Type
1	A	-21	HIS
1	A	47	HIS
1	A	247	GLN
1	A	331	ASN
1	A	362	HIS
1	A	374	GLN
1	A	467	ASN
1	A	526	ASN
1	A	556	HIS
1	A	749	GLN
1	A	797	ASN
1	A	855	HIS
1	A	859	GLN
1	A	873	ASN
1	A	1042	GLN
2	B	453	ASN
2	B	475	GLN
2	B	527	ASN
2	B	564	ASN

### 5.3.3 RNA

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue 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
1	SEP	A	790	1	8,9,10	0.67	0	8,12,14	2.74	2 (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
1	SEP	A	790	1	-	4/5/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	790	SEP	OG-CB-CA	6.35	114.32	108.14
1	A	790	SEP	P-OG-CB	2.92	126.33	118.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	790	SEP	N-CA-CB-OG
1	A	790	SEP	CB-OG-P-O2P
1	A	790	SEP	CB-OG-P-O3P
1	A	790	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	71L	A	1101	-	9,9,9	1.68	1 (11%)	12,12,12	1.25	2 (16%)

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	71L	A	1101	-	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	71L	C4-N9	4.57	1.48	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	71L	N9-C4-N5	2.11	119.82	116.49
3	A	1101	71L	C8-C6-N5	2.04	119.82	116.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1044/1096 (95%)	0.11	36 (3%) 45 34	68, 118, 180, 271	0
2	B	239/279 (85%)	0.60	20 (8%) 11 9	106, 175, 219, 241	0
All	All	1283/1375 (93%)	0.20	56 (4%) 34 25	68, 127, 204, 271	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	409	ARG	5.1
1	A	347	ASN	4.2
1	A	346	VAL	3.9
1	A	341	ALA	3.9
1	A	-26	SER	3.6
1	A	300	ASP	3.5
1	A	473	LEU	3.3
2	B	591	GLN	3.2
2	B	329	GLN	3.0
2	B	405	ILE	3.0
2	B	587	LYS	2.9
1	A	422	LEU	2.9
1	A	810	ASP	2.8
2	B	437	VAL	2.8
1	A	867	LYS	2.7
1	A	354	ILE	2.7
2	B	505	SER	2.7
1	A	522	GLU	2.7
2	B	512	PHE	2.7
1	A	1	MET	2.6
1	A	344	VAL	2.6
1	A	374	GLN	2.6
2	B	408	TYR	2.6
1	A	872	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	423	ALA	2.5
1	A	155	ASP	2.5
1	A	523	LEU	2.5
1	A	358	THR	2.5
1	A	1009	GLY	2.5
2	B	508	TYR	2.4
1	A	340	CYS	2.3
2	B	333	TRP	2.3
1	A	809	GLN	2.3
2	B	580	TYR	2.3
1	A	107	ASN	2.3
1	A	351	ILE	2.3
1	A	407	CYS	2.3
1	A	385	GLU	2.2
1	A	353	LYS	2.2
2	B	401	VAL	2.2
1	A	806	ASP	2.2
1	A	375	ARG	2.2
2	B	564	ASN	2.2
1	A	474	GLU	2.2
2	B	423	LYS	2.1
2	B	327	SER	2.1
1	A	1052	THR	2.1
1	A	419	HIS	2.1
2	B	407	HIS	2.1
2	B	328	LEU	2.1
1	A	557	TYR	2.1
2	B	436	VAL	2.1
1	A	345	ASN	2.1
2	B	515	GLU	2.0
1	A	677	ASN	2.0
1	A	383	TRP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
1	SEP	A	790	10/11	0.94	0.15	95,120,180,190	0

### 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<sup>th</sup> 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	71L	A	1101	9/9	0.90	1.14	143,157,165,165	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.