



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2017 – 10:12 AM EST

PDB ID : 5SX8  
Title : Crystal Structure of PI3Kalpha in complex with fragments 12 and 15  
Authors : Gabelli, S.B.; Vogelstein, B.; Miller, M.S.; Amzel, L.M.  
Deposited on : 2016-08-09  
Resolution : 3.47 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

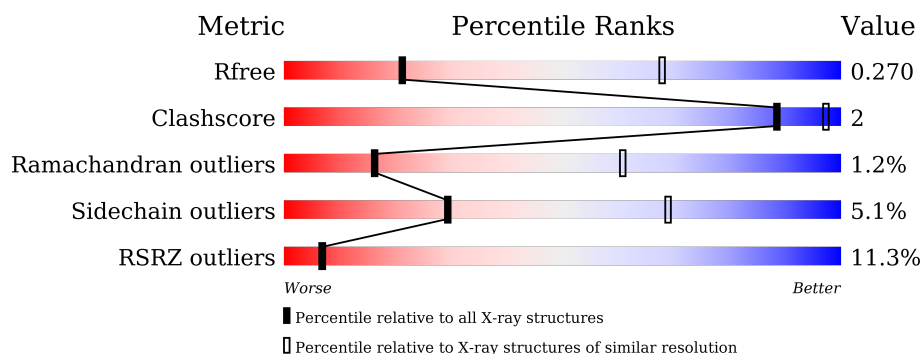
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.47 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	1173 (3.60-3.36)
Clashscore	102246	1010 (3.58-3.38)
Ramachandran outliers	100387	1245 (3.60-3.36)
Sidechain outliers	100360	1246 (3.60-3.36)
RSRZ outliers	91569	1180 (3.60-3.36)

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  $\geq 3$ , 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	1096	<div> <div>10%</div> <div>84%</div> <div>11%</div> <div>• •</div> </div>
2	B	279	<div> <div>15%</div> <div>77%</div> <div>8%</div> <div>• 14%</div> </div>

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
4	LUZ	A	1102	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10695 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 alpha isoform.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1053	Total	C	N	O	P	S	0	0	0
			8608	5500	1477	1561	1	69			

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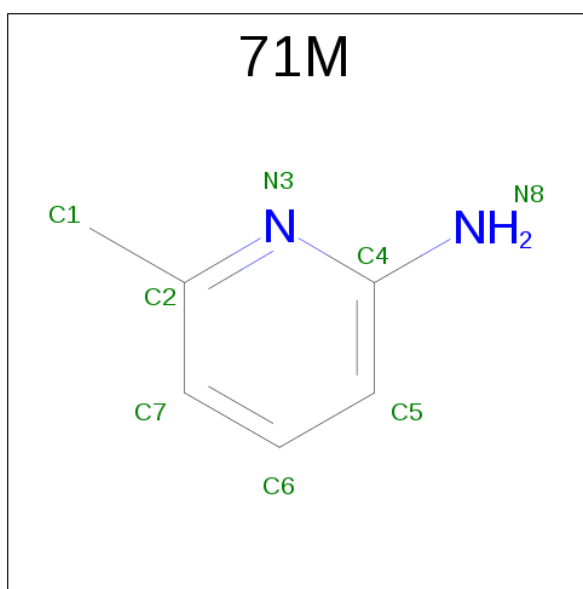
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42336
A	0	SER	-	expression tag	UNP P42336

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

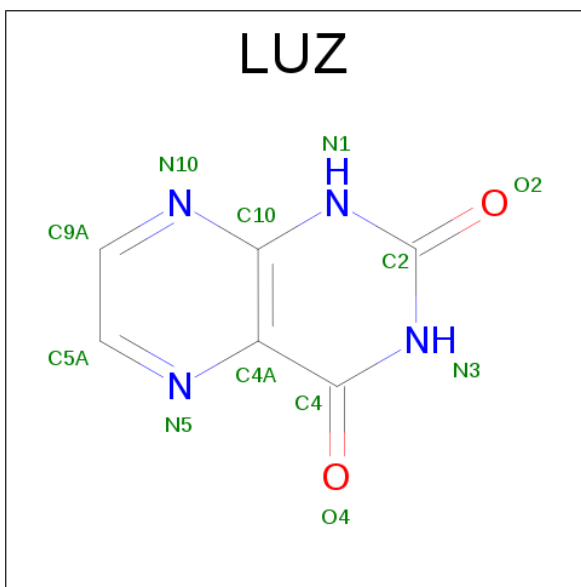
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	240	Total	C	N	O	S	0	0	0
			2059	1294	364	395	6			

- Molecule 3 is 6-methylpyridin-2-amine (three-letter code: 71M) (formula: C<sub>6</sub>H<sub>8</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			8	6	2		
3	B	1	Total	C	N	0	0
			8	6	2		

- Molecule 4 is pteridine-2,4(1H,3H)-dione (three-letter code: LUZ) (formula: C<sub>6</sub>H<sub>4</sub>N<sub>4</sub>O<sub>2</sub>).

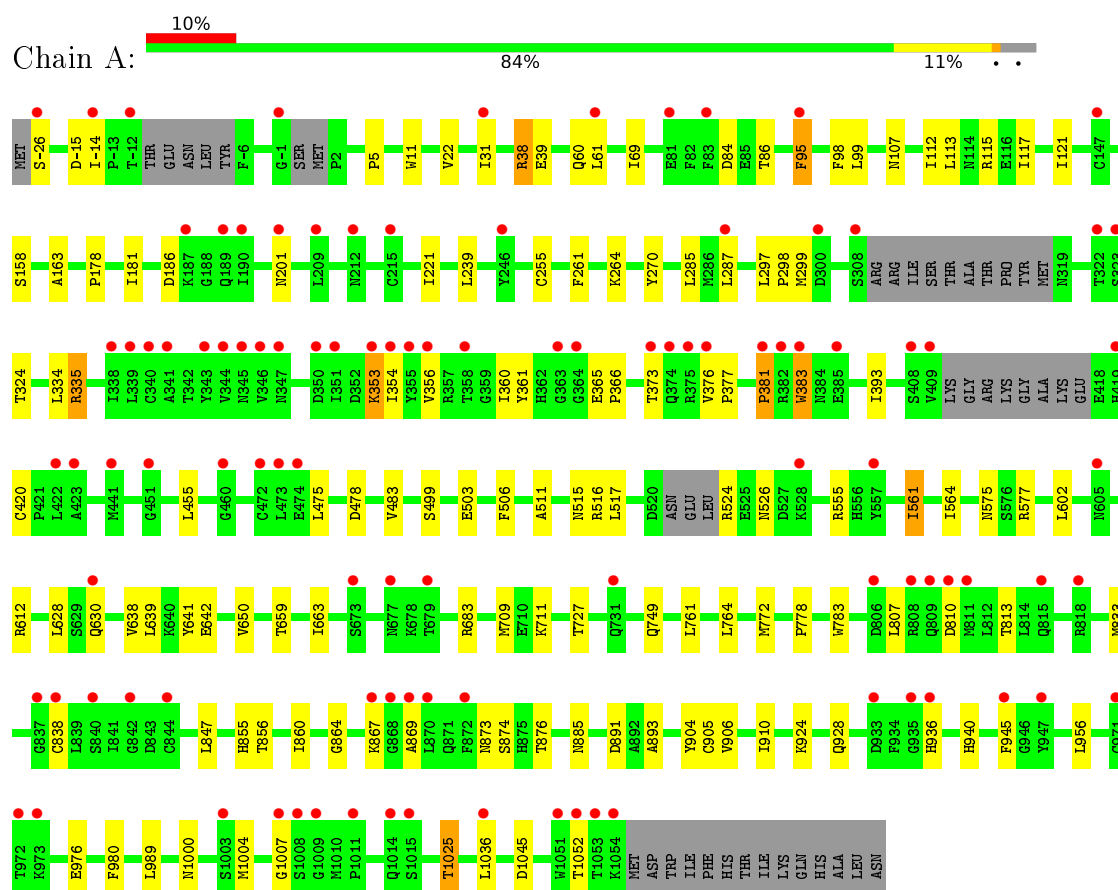


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	6	4	2		

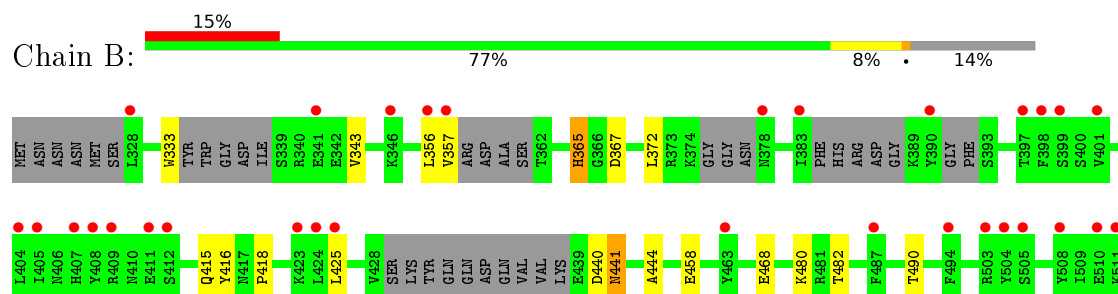
### 3 Residue-property plots

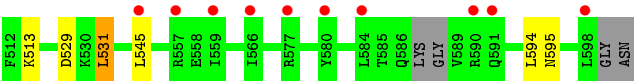
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 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, $\alpha$ , $\beta$ , $\gamma$	113.89Å 116.33Å 148.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.49 – 3.47 48.90 – 3.47	Depositor EDS
% Data completeness (in resolution range)	99.1 (91.49-3.47) 99.2 (48.90-3.47)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 3.48Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.207 , 0.276 0.208 , 0.270	Depositor DCC
$R_{free}$ test set	1324 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	122.1	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 106.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10695	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LUZ, 71M, 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	0.45	0/8797	0.68	0/11886
2	B	0.44	0/2085	0.62	0/2783
All	All	0.45	0/10882	0.67	0/14669

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

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	8608	0	8578	48	0
2	B	2059	0	2056	7	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
4	A	12	0	4	0	0
All	All	10695	0	10638	53	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 2.

All (53) 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:873:ASN:HB3	1:A:876:THR:HG23	1.73	0.70
1:A:628:LEU:HD23	1:A:663:ILE:HD13	1.78	0.65
2:B:333:TRP:HB3	2:B:357:VAL:HB	1.79	0.64
1:A:503:GLU:HA	1:A:506:PHE:CE1	2.34	0.63
1:A:503:GLU:HA	1:A:506:PHE:HE1	1.65	0.61
1:A:989:LEU:HD11	1:A:1036:LEU:HD11	1.85	0.56
1:A:324:THR:HG21	1:A:483:VAL:CG2	2.36	0.55
1:A:1000:ASN:O	1:A:1004:MET:HG3	2.06	0.54
1:A:602:LEU:O	1:A:612:ARG:NH2	2.41	0.53
1:A:261:PHE:HA	1:A:270:TYR:CE2	2.43	0.53
1:A:334:LEU:HA	1:A:393:ILE:HD11	1.89	0.53
1:A:255:CYS:SG	1:A:285:LEU:O	2.67	0.53
1:A:98:PHE:CE1	2:B:490:THR:HG23	2.45	0.52
1:A:772:MET:HB2	1:A:778:PRO:HG2	1.93	0.51
1:A:31:ILE:HD11	2:B:531:LEU:HD13	1.93	0.50
1:A:639:LEU:HD22	1:A:650:VAL:HG22	1.93	0.50
2:B:480:LYS:HG2	2:B:545:LEU:HD11	1.93	0.49
1:A:749:GLN:HE21	1:A:764:LEU:H	1.59	0.49
1:A:354:ILE:HD11	1:A:381:PRO:HB3	1.95	0.48
2:B:441:ASN:OD1	2:B:441:ASN:N	2.47	0.48
1:A:335:ARG:NE	1:A:478:ASP:OD2	2.43	0.47
1:A:561:ILE:O	1:A:564:ILE:HG22	2.14	0.47
1:A:163:ALA:HB2	1:A:297:LEU:HD11	1.97	0.47
1:A:833:MET:HE1	1:A:904:TYR:HA	1.97	0.46
1:A:60:GLN:HG2	1:A:61:LEU:HD12	1.96	0.46
1:A:353:LYS:HA	1:A:377:PRO:HB3	1.97	0.46
1:A:910:ILE:O	1:A:1025:THR:HG21	2.16	0.46
1:A:361:TYR:CE2	1:A:365:GLU:HB3	2.50	0.46
1:A:885:ASN:ND2	1:A:893:ALA:HB2	2.30	0.46
1:A:864:GLY:O	1:A:876:THR:HG21	2.16	0.45
2:B:441:ASN:HB2	2:B:444:ALA:HB3	1.97	0.45
1:A:84:ASP:OD1	1:A:86:THR:OG1	2.29	0.45
1:A:639:LEU:HD22	1:A:650:VAL:CG2	2.47	0.44
1:A:924:LYS:HE3	1:A:928:GLN:HB3	2.00	0.44
1:A:524:ARG:HD3	1:A:526:ASN:HD22	1.82	0.43
1:A:936:HIS:HB3	1:A:940:HIS:HB3	2.01	0.43
1:A:641:TYR:OH	1:A:1007:GLY:N	2.52	0.43
1:A:906:VAL:HG12	1:A:910:ILE:HD12	2.01	0.43
1:A:709:MET:CE	1:A:847:LEU:HD21	2.49	0.42
1:A:360:ILE:N	1:A:360:ILE:HD12	2.34	0.42
1:A:324:THR:HG21	1:A:483:VAL:HG23	2.01	0.42
1:A:356:VAL:HG23	1:A:383:TRP:CH2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:LEU:HD22	1:A:783:TRP:CE3	2.55	0.41
1:A:11:TRP:HB2	1:A:95:PHE:CD1	2.55	0.41
1:A:956:LEU:HD11	1:A:980:PHE:CZ	2.55	0.41
2:B:343:VAL:HG13	2:B:356:LEU:HD11	2.02	0.41
1:A:221:ILE:HG23	1:A:287:LEU:HD21	2.02	0.41
1:A:855:HIS:HB2	1:A:860:ILE:CD1	2.51	0.41
1:A:117:ILE:HG22	1:A:121:ILE:CD1	2.51	0.41
1:A:178:PRO:HD2	1:A:181:ILE:HD12	2.02	0.41
1:A:810:ASP:HA	1:A:813:THR:HG22	2.03	0.41
1:A:602:LEU:HB3	1:A:638:VAL:HG11	2.03	0.41
1:A:807:LEU:HD12	1:A:838:CYS:SG	2.61	0.41

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	1040/1096 (95%)	935 (90%)	93 (9%)	12 (1%)	16	61
2	B	224/279 (80%)	210 (94%)	11 (5%)	3 (1%)	15	59
All	All	1264/1375 (92%)	1145 (91%)	104 (8%)	15 (1%)	16	61

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	LYS
1	A	555	ARG
2	B	365	HIS
1	A	38	ARG
1	A	186	ASP
1	A	511	ALA
1	A	869	ALA

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Mol	Chain	Res	Type
1	A	945	PHE
1	A	95	PHE
1	A	381	PRO
2	B	513	LYS
1	A	298	PRO
1	A	107	ASN
2	B	418	PRO
1	A	5	PRO

### 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	A	960/998 (96%)	914 (95%)	46 (5%)	31	71
2	B	228/259 (88%)	213 (93%)	15 (7%)	21	61
All	All	1188/1257 (94%)	1127 (95%)	61 (5%)	29	69

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-26	SER
1	A	-15	ASP
1	A	-14	ILE
1	A	22	VAL
1	A	38	ARG
1	A	39	GLU
1	A	69	ILE
1	A	99	LEU
1	A	112	ILE
1	A	113	LEU
1	A	115	ARG
1	A	158	SER
1	A	201	ASN
1	A	239	LEU
1	A	299	MET

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Mol	Chain	Res	Type
1	A	335	ARG
1	A	353	LYS
1	A	366	PRO
1	A	373	THR
1	A	376	VAL
1	A	383	TRP
1	A	420	CYS
1	A	455	LEU
1	A	475	LEU
1	A	499	SER
1	A	515	ASN
1	A	516	ARG
1	A	517	LEU
1	A	561	ILE
1	A	575	ASN
1	A	577	ARG
1	A	630	GLN
1	A	642	GLU
1	A	659	THR
1	A	683	ARG
1	A	711	LYS
1	A	727	THR
1	A	856	THR
1	A	867	LYS
1	A	874	SER
1	A	891	ASP
1	A	905	CYS
1	A	976	GLU
1	A	1025	THR
1	A	1045	ASP
1	A	1052	THR
2	B	365	HIS
2	B	367	ASP
2	B	372	LEU
2	B	415	GLN
2	B	416	TYR
2	B	425	LEU
2	B	440	ASP
2	B	441	ASN
2	B	458	GLU
2	B	468	GLU
2	B	482	THR

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Mol	Chain	Res	Type
2	B	529	ASP
2	B	531	LEU
2	B	594	LEU
2	B	595	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
1	A	202	ASN
1	A	331	ASN
1	A	347	ASN
1	A	374	GLN
1	A	467	ASN
1	A	526	ASN
1	A	575	ASN
1	A	643	GLN
1	A	749	GLN
1	A	759	HIS
1	A	861	GLN
2	B	344	ASN
2	B	378	ASN
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 ⓘ

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	7,9,10	0.68	0	8,12,14	2.02	1 (12%)

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	-	0/5/8/10	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	790	SEP	OG-CB-CA	4.41	112.10	108.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands are 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	71M	A	1101	-	8,8,8	1.85	1 (12%)	10,10,10	1.39	2 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	LUZ	A	1102	-	11,13,13	1.84	2 (18%)	12,18,18	3.09	6 (50%)
3	71M	B	701	-	8,8,8	1.90	1 (12%)	10,10,10	1.37	2 (20%)

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	71M	A	1101	-	-	0/0/0/0	0/1/1/1
4	LUZ	A	1102	-	-	0/0/0/0	0/2/2/2
3	71M	B	701	-	-	0/0/0/0	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1102	LUZ	C4A-N5	2.10	1.36	1.33
4	A	1102	LUZ	O4-C4	4.84	1.36	1.24
3	A	1101	71M	C4-N8	4.95	1.49	1.35
3	B	701	71M	C4-N8	5.10	1.49	1.35

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1102	LUZ	N3-C2-N1	-4.28	120.48	127.69
4	A	1102	LUZ	C4A-C4-N3	-3.01	119.59	123.52
3	B	701	71M	C1-C2-N3	2.06	119.84	116.59
3	A	1101	71M	C1-C2-N3	2.08	119.86	116.59
3	B	701	71M	C4-N3-C2	2.81	121.34	118.17
4	A	1102	LUZ	C4-C4A-N5	2.84	121.92	118.28
3	A	1101	71M	C4-N3-C2	2.88	121.42	118.17
4	A	1102	LUZ	C9A-N10-C10	2.96	120.59	116.32
4	A	1102	LUZ	N10-C10-N1	3.31	120.96	115.90
4	A	1102	LUZ	C4-N3-C2	6.76	120.80	115.16

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	1052/1096 (95%)	0.62	105 (9%) <b>9</b> <b>9</b>	79, 134, 198, 254	0
2	B	240/279 (86%)	1.00	41 (17%) <b>2</b> <b>2</b>	121, 192, 242, 264	0
All	All	1292/1375 (93%)	0.69	146 (11%) <b>7</b> <b>7</b>	79, 142, 217, 264	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	390	TYR	6.5
1	A	1054	LYS	6.2
1	A	947	TYR	5.9
1	A	374	GLN	5.4
1	A	419	HIS	5.2
1	A	346	VAL	5.2
2	B	378	ASN	5.0
1	A	-26	SER	5.0
1	A	347	ASN	4.9
2	B	401	VAL	4.9
2	B	357	VAL	4.8
1	A	1009	GLY	4.6
1	A	945	PHE	4.5
1	A	351	ILE	4.5
2	B	405	ILE	4.4
1	A	872	PHE	4.4
1	A	423	ALA	4.4
1	A	323	SER	4.4
1	A	557	TYR	4.3
2	B	508	TYR	4.2
1	A	345	ASN	4.2
2	B	424	LEU	4.1
1	A	810	ASP	4.1
1	A	322	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	806	ASP	4.0
1	A	473	LEU	3.9
1	A	869	ALA	3.9
1	A	344	VAL	3.9
1	A	300	ASP	3.9
2	B	584	LEU	3.9
1	A	867	LYS	3.8
1	A	381	PRO	3.8
2	B	510	GLU	3.7
1	A	61	LEU	3.7
1	A	933	ASP	3.7
2	B	409	ARG	3.6
1	A	339	LEU	3.6
2	B	346	LYS	3.6
1	A	343	TYR	3.6
1	A	338	ILE	3.6
2	B	425	LEU	3.5
1	A	809	GLN	3.5
2	B	505	SER	3.5
2	B	504	TYR	3.4
2	B	580	TYR	3.4
2	B	399	SER	3.4
1	A	353	LYS	3.3
1	A	870	LEU	3.3
1	A	358	THR	3.3
1	A	341	ALA	3.3
1	A	375	ARG	3.2
2	B	412	SER	3.2
1	A	441	MET	3.2
1	A	673	SER	3.2
1	A	971	CYS	3.2
1	A	355	TYR	3.1
1	A	364	GLY	3.1
2	B	463	TYR	3.1
1	A	190	ILE	3.1
2	B	407	HIS	3.1
1	A	936	HIS	3.1
2	B	423	LYS	3.0
1	A	354	ILE	3.0
1	A	409	VAL	3.0
2	B	408	TYR	3.0
2	B	383	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	356	LEU	3.0
2	B	598	LEU	2.9
1	A	1014	GLN	2.9
1	A	-1	GLY	2.9
1	A	189	GLN	2.9
1	A	408	SER	2.8
1	A	837	GLY	2.8
1	A	1051	TRP	2.8
1	A	935	GLY	2.8
2	B	590	ARG	2.8
1	A	422	LEU	2.8
1	A	209	LEU	2.8
2	B	559	ILE	2.8
1	A	31	ILE	2.8
1	A	605	ASN	2.8
2	B	398	PHE	2.7
1	A	-12	THR	2.7
2	B	328	LEU	2.7
1	A	808	ARG	2.7
1	A	246	TYR	2.7
2	B	404	LEU	2.7
1	A	838	CYS	2.7
1	A	287	LEU	2.7
1	A	1053	THR	2.7
1	A	1007	GLY	2.7
2	B	494	PHE	2.6
1	A	460	GLY	2.6
1	A	811	MET	2.6
2	B	397	THR	2.6
2	B	577	ARG	2.6
1	A	868	GLY	2.6
1	A	677	ASN	2.6
1	A	363	GLY	2.5
1	A	1008	SER	2.5
2	B	411	GLU	2.5
2	B	503	ARG	2.5
1	A	350	ASP	2.5
1	A	1015	SER	2.5
1	A	679	THR	2.4
1	A	844	CYS	2.4
1	A	201	ASN	2.4
1	A	356	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	382	ARG	2.4
1	A	528	LYS	2.4
1	A	731	GLN	2.3
1	A	81	GLU	2.3
1	A	340	CYS	2.3
1	A	83	PHE	2.3
1	A	187	LYS	2.3
1	A	373	THR	2.3
1	A	630	GLN	2.2
1	A	383	TRP	2.2
1	A	1011	PRO	2.2
1	A	972	THR	2.2
1	A	215	CYS	2.2
1	A	147	CYS	2.2
1	A	973	LYS	2.2
1	A	212	ASN	2.2
1	A	1036	LEU	2.1
2	B	566	ILE	2.1
1	A	815	GLN	2.1
1	A	818	ARG	2.1
1	A	474	GLU	2.1
2	B	591	GLN	2.1
1	A	842	GLY	2.1
1	A	-14	ILE	2.1
1	A	1052	THR	2.1
1	A	308	SER	2.1
2	B	487	PHE	2.1
1	A	840	SER	2.1
2	B	545	LEU	2.1
1	A	451	GLY	2.1
2	B	511	LYS	2.0
2	B	557	ARG	2.0
1	A	376	VAL	2.0
1	A	1003	SER	2.0
2	B	341	GLU	2.0
1	A	385	GLU	2.0
1	A	95	PHE	2.0
1	A	472	CYS	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. 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEP	A	790	10/11	0.94	0.14	-	113,134,169,176	0

## 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	LUZ	A	1102	12/12	0.69	0.56	1.83	193,217,224,224	0
3	71M	B	701	8/8	0.66	0.29	-	169,182,187,187	0
3	71M	A	1101	8/8	0.80	1.47	-	164,173,179,181	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.