



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2017 – 09:16 PM EDT

PDB ID : 5SWT  
Title : Crystal Structure of PI3Kalpha in complex with fragments 17 and 27  
Authors : Gabelli, S.B.; Vogelstein, B.; Miller, M.S.; Amzel, L.M.  
Deposited on : unknown  
Resolution : 3.49 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20029824

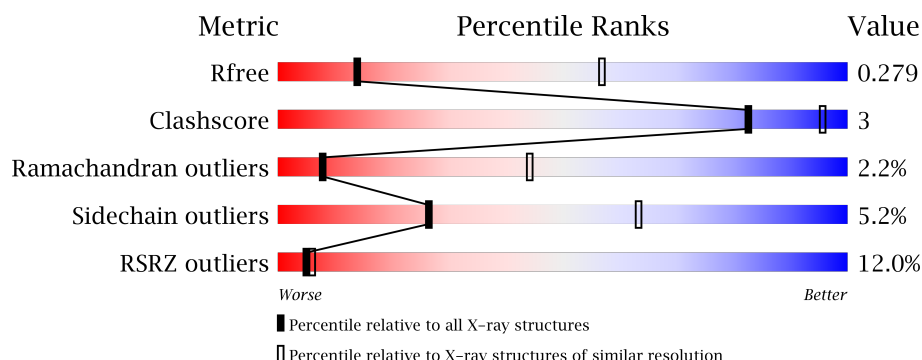
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.49 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))
$R_{free}$	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

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>9%</div> <div>82%</div> <div>13%</div> <div>• •</div> </div>
2	B	279	<div> <div>22%</div> <div>78%</div> <div>10%</div> <div>• 11%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10818 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	1059	Total	C	N	O	P	S	0	0	0
			8655	5524	1483	1575	2	71			

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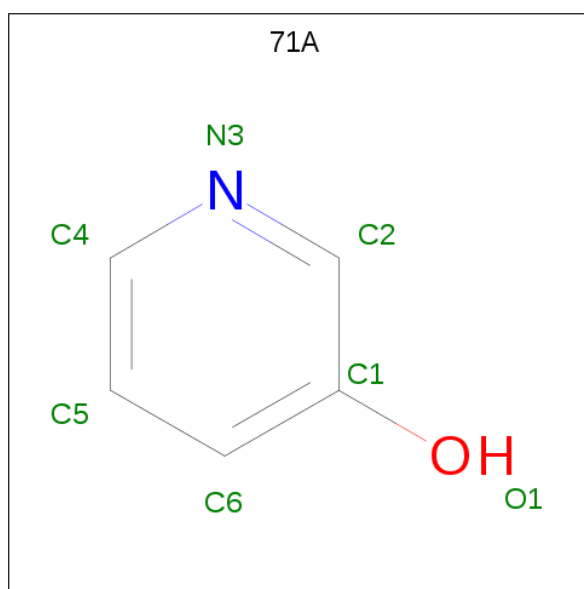
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42336
A	0	SER	-	expression tag	UNP P42336

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

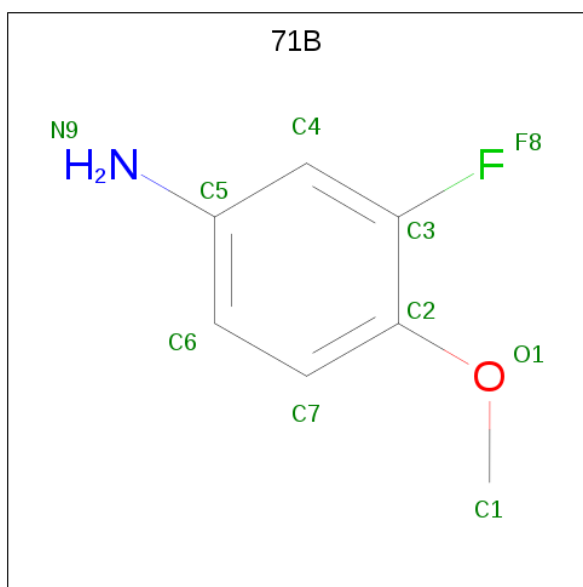
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	249	Total	C	N	O	S	0	0	0
			2146	1348	385	407	6			

- Molecule 3 is pyridin-3-ol (three-letter code: 71A) (formula: C<sub>5</sub>H<sub>5</sub>NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 4 is 3-fluoro-4-methoxyaniline (three-letter code: 71B) (formula: C<sub>7</sub>H<sub>8</sub>FNO).

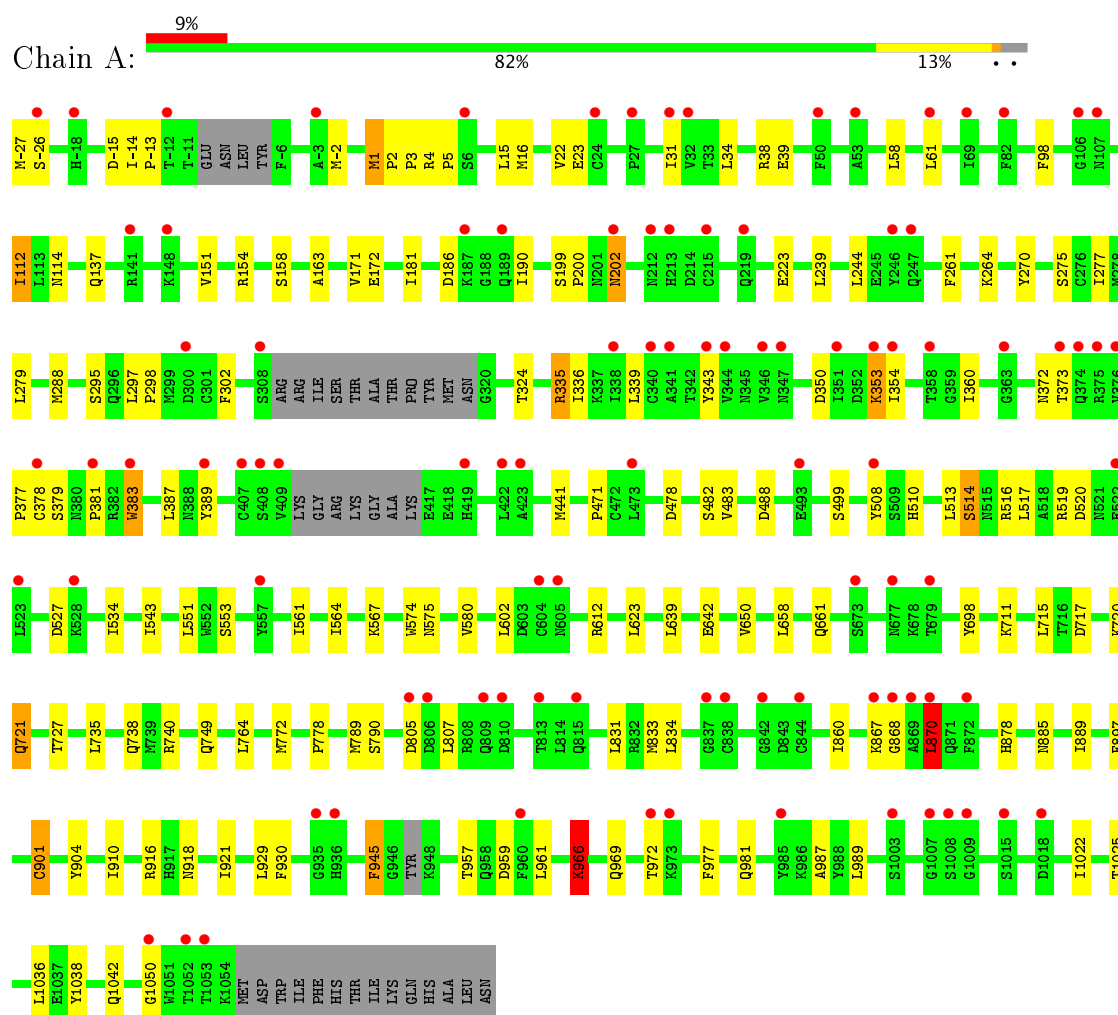


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
4	A	1	10	7	1	1	1	0	0

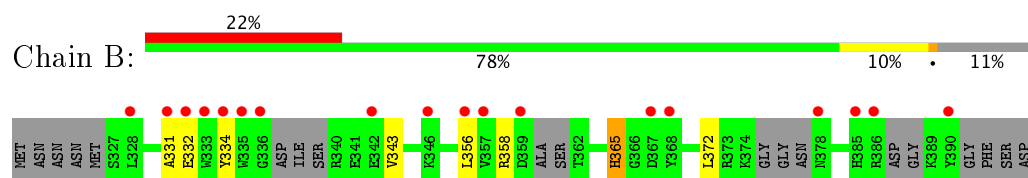
### 3 Residue-property plots

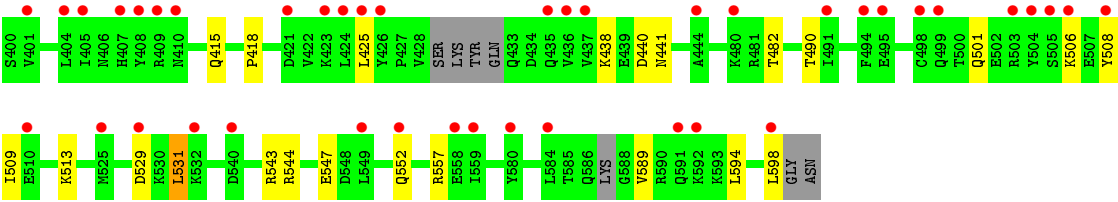
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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, $\alpha$ , $\beta$ , $\gamma$	114.45Å 115.94Å 149.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.57 – 3.49 48.87 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.2 (91.57-3.49) 99.3 (48.87-3.49)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.208 , 0.285 0.210 , 0.279	Depositor DCC
$R_{free}$ test set	1324 reflections (5.42%)	DCC
Wilson B-factor (Å <sup>2</sup> )	116.6	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 104.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10818	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: 71B, 71A, 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	0/8833	0.69	1/11934 (0.0%)
2	B	0.43	0/2175	0.64	0/2902
All	All	0.45	0/11008	0.68	1/14836 (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	870	LEU	CA-CB-CG	6.85	131.05	115.30

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	8655	0	8620	58	0
2	B	2146	0	2135	10	0
3	A	7	0	0	0	0
4	A	10	0	0	0	0
All	All	10818	0	10755	62	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 3.

All (62) 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:989:LEU:HD11	1:A:1036:LEU:HD11	1.74	0.70
1:A:163:ALA:HB2	1:A:297:LEU:HD11	1.79	0.65
1:A:639:LEU:HD22	1:A:650:VAL:HG22	1.83	0.61
1:A:910:ILE:O	1:A:1025:THR:HG21	2.04	0.58
1:A:717:ASP:O	1:A:721:GLN:NE2	2.37	0.57
1:A:957:THR:O	1:A:961:LEU:HD12	2.05	0.56
1:A:945:PHE:HB2	2:B:598:LEU:HD13	1.87	0.56
1:A:31:ILE:HD11	2:B:531:LEU:HD13	1.86	0.56
1:A:261:PHE:HA	1:A:270:TYR:CE2	2.41	0.56
1:A:1:MET:HB2	1:A:720:LYS:CE	2.37	0.55
1:A:324:THR:HG22	1:A:483:VAL:HG23	1.90	0.54
1:A:98:PHE:CE1	2:B:490:THR:HG23	2.44	0.53
1:A:602:LEU:O	1:A:612:ARG:NH2	2.43	0.52
1:A:561:ILE:O	1:A:564:ILE:HG22	2.10	0.52
2:B:331:ALA:HB3	2:B:334:TYR:HB3	1.92	0.52
2:B:343:VAL:HG13	2:B:356:LEU:HD11	1.91	0.52
1:A:749:GLN:HE21	1:A:764:LEU:H	1.58	0.51
1:A:981:GLN:NE2	1:A:1050:GLY:O	2.44	0.51
1:A:805:ASP:O	1:A:807:LEU:HD22	2.09	0.50
1:A:833:MET:HE1	1:A:904:TYR:HA	1.94	0.49
1:A:519:ARG:NH2	1:A:527:ASP:OD2	2.45	0.49
1:A:1022:ILE:HA	1:A:1025:THR:HG22	1.94	0.49
1:A:275:SER:O	1:A:279:LEU:HD12	2.14	0.48
1:A:336:ILE:HD12	1:A:389:TYR:CE1	2.49	0.48
1:A:353:LYS:HA	1:A:377:PRO:HB3	1.97	0.47
1:A:58:LEU:HB3	1:A:61:LEU:HD13	1.96	0.47
1:A:61:LEU:HD11	2:B:508:TYR:CZ	2.50	0.47
1:A:961:LEU:HD23	1:A:977:PHE:CE1	2.50	0.47
1:A:517:LEU:HD11	1:A:553:SER:O	2.15	0.47
1:A:181:ILE:HG23	1:A:277:ILE:HG21	1.97	0.46
1:A:885:ASN:HB3	1:A:889:ILE:HG22	1.97	0.46
1:A:151:VAL:HG21	1:A:302:PHE:HB2	1.97	0.46
1:A:360:ILE:N	1:A:360:ILE:HD12	2.31	0.46
1:A:171:VAL:HG12	1:A:172:GLU:O	2.16	0.45
1:A:372:ASN:HB3	1:A:387:LEU:HD21	1.98	0.45
1:A:354:ILE:HD11	1:A:381:PRO:HB3	1.99	0.45
1:A:534:ILE:HG21	1:A:551:LEU:HD11	1.98	0.45
1:A:945:PHE:CG	2:B:598:LEU:HB3	2.51	0.45
1:A:377:PRO:O	1:A:379:SER:N	2.50	0.44
2:B:506:LYS:HA	2:B:509:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:LEU:O	1:A:383:TRP:O	2.35	0.43
1:A:916:ARG:HB3	1:A:921:ILE:HD11	2.00	0.43
1:A:543:ILE:HD11	1:A:567:LYS:HD3	2.01	0.43
1:A:1038:TYR:O	1:A:1042:GLN:HG2	2.17	0.43
1:A:878:HIS:NE2	1:A:966:LYS:O	2.52	0.42
1:A:16:MET:HG3	1:A:38:ARG:HB2	2.01	0.42
1:A:324:THR:CG2	1:A:483:VAL:HG23	2.50	0.42
1:A:343:TYR:OH	2:B:557:ARG:NH1	2.50	0.42
1:A:831:LEU:HD11	1:A:987:ALA:HB2	2.01	0.42
1:A:772:MET:HB2	1:A:778:PRO:HG2	2.01	0.42
1:A:868:GLY:O	1:A:870:LEU:HD13	2.20	0.42
2:B:544:ARG:O	2:B:547:GLU:HG2	2.20	0.41
1:A:335:ARG:NE	1:A:478:ASP:OD2	2.53	0.41
1:A:904:TYR:CE2	1:A:930:PHE:HA	2.56	0.41
1:A:715:LEU:HD21	1:A:735:LEU:HD12	2.01	0.41
1:A:789:MET:O	1:A:790:SEP:C	2.68	0.41
1:A:15:LEU:HD21	1:A:738:GLN:OE1	2.20	0.41
1:A:661:GLN:OE1	1:A:698:TYR:HB2	2.21	0.41
1:A:154:ARG:HD2	1:A:658:LEU:O	2.21	0.40
1:A:897:PHE:O	1:A:901:CYS:HB2	2.22	0.40
1:A:574:TRP:HA	1:A:580:VAL:CG2	2.51	0.40
1:A:639:LEU:HD22	1:A:650:VAL:CG2	2.50	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	1047/1096 (96%)	946 (90%)	79 (8%)	22 (2%)	8	45
2	B	233/279 (84%)	215 (92%)	12 (5%)	6 (3%)	6	40
All	All	1280/1375 (93%)	1161 (91%)	91 (7%)	28 (2%)	8	44

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	CYS
1	A	508	TYR
1	A	514	SER
1	A	945	PHE
1	A	2	PRO
1	A	264	LYS
1	A	966	LYS
2	B	365	HIS
2	B	513	LYS
1	A	3	PRO
1	A	202	ASN
1	A	482	SER
1	A	867	LYS
1	A	918	ASN
1	A	972	THR
2	B	332	GLU
2	B	438	LYS
1	A	186	ASP
1	A	200	PRO
1	A	-13	PRO
1	A	520	ASP
1	A	623	LEU
2	B	589	VAL
1	A	112	ILE
1	A	298	PRO
1	A	471	PRO
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	965/997 (97%)	916 (95%)	49 (5%)	28	64
2	B	235/259 (91%)	221 (94%)	14 (6%)	22	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1200/1256 (96%)	1137 (95%)	63 (5%)	26	63

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-27	MET
1	A	-26	SER
1	A	-15	ASP
1	A	-14	ILE
1	A	-2	MET
1	A	1	MET
1	A	4	ARG
1	A	22	VAL
1	A	23	GLU
1	A	34	LEU
1	A	39	GLU
1	A	112	ILE
1	A	114	ASN
1	A	137	GLN
1	A	158	SER
1	A	190	ILE
1	A	199	SER
1	A	202	ASN
1	A	223	GLU
1	A	239	LEU
1	A	244	LEU
1	A	288	MET
1	A	295	SER
1	A	335	ARG
1	A	350	ASP
1	A	353	LYS
1	A	373	THR
1	A	383	TRP
1	A	441	MET
1	A	488	ASP
1	A	499	SER
1	A	510	HIS
1	A	513	LEU
1	A	514	SER
1	A	516	ARG
1	A	575	ASN
1	A	642	GLU

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Mol	Chain	Res	Type
1	A	711	LYS
1	A	721	GLN
1	A	727	THR
1	A	740	ARG
1	A	834	LEU
1	A	860	ILE
1	A	870	LEU
1	A	901	CYS
1	A	929	LEU
1	A	959	ASP
1	A	966	LYS
1	A	969	GLN
2	B	358	ARG
2	B	365	HIS
2	B	372	LEU
2	B	415	GLN
2	B	425	LEU
2	B	440	ASP
2	B	441	ASN
2	B	482	THR
2	B	501	GLN
2	B	529	ASP
2	B	531	LEU
2	B	543	ARG
2	B	552	GLN
2	B	594	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	331	ASN
1	A	347	ASN
1	A	374	GLN
1	A	526	ASN
1	A	575	ASN
1	A	670	HIS
1	A	721	GLN
1	A	749	GLN
1	A	782	ASN
1	A	796	ASN
1	A	885	ASN
1	A	1047	HIS

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Mol	Chain	Res	Type
2	B	595	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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
1	SEP	A	7	1	9,9,10	0.72	0	9,12,14	1.31	1 (11%)
1	SEP	A	790	1	9,9,10	0.58	0	9,12,14	2.29	1 (11%)

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	7	1	-	0/5/8/10	0/0/0/0
1	SEP	A	790	1	-	0/5/8/10	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	SEP	P-OG-CB	2.63	125.53	118.30
1	A	790	SEP	OG-CB-CA	5.83	113.92	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	790	SEP	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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	71A	A	1101	-	7,7,7	0.76	0	8,8,8	1.28	1 (12%)
4	71B	A	1102	-	10,10,10	1.02	1 (10%)	13,13,13	1.53	2 (15%)

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	71A	A	1101	-	-	0/0/0/0	0/1/1/1
4	71B	A	1102	-	-	0/2/2/2	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1102	71B	C5-N9	2.97	1.49	1.38



All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1102	71B	O1-C2-C7	-2.22	120.64	124.37
3	A	1101	71A	C4-N3-C2	2.88	121.87	116.83
4	A	1102	71B	O1-C2-C3	3.65	119.11	116.28

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	1057/1096 (96%)	0.58	97 (9%) <b>10</b> <b>10</b>	81, 126, 192, 262	0
2	B	249/279 (89%)	1.21	60 (24%) <b>1</b> <b>1</b>	113, 186, 229, 264	0
All	All	1306/1375 (94%)	0.70	157 (12%) <b>5</b> <b>6</b>	81, 134, 211, 264	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	335	TRP	9.0
2	B	505	SER	5.5
2	B	409	ARG	5.0
1	A	872	PHE	4.9
1	A	869	ALA	4.8
1	A	523	LEU	4.7
2	B	333	TRP	4.7
2	B	424	LEU	4.5
1	A	107	ASN	4.4
1	A	374	GLN	4.3
1	A	1052	THR	4.2
2	B	405	ILE	4.2
2	B	580	TYR	4.2
1	A	-12	THR	4.2
2	B	359	ASP	4.1
2	B	504	TYR	4.1
1	A	61	LEU	4.0
2	B	423	LYS	4.0
1	A	-26	SER	3.9
1	A	346	VAL	3.9
2	B	357	VAL	3.9
1	A	347	ASN	3.9
1	A	810	ASP	3.9
2	B	390	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	375	ARG	3.8
1	A	354	ILE	3.8
1	A	1009	GLY	3.8
2	B	408	TYR	3.8
1	A	868	GLY	3.7
1	A	522	GLU	3.6
2	B	378	ASN	3.6
1	A	24	CYS	3.6
1	A	557	TYR	3.6
2	B	385	HIS	3.5
2	B	508	TYR	3.5
1	A	341	ALA	3.5
1	A	673	SER	3.5
1	A	419	HIS	3.5
1	A	340	CYS	3.5
2	B	437	VAL	3.5
2	B	332	GLU	3.5
1	A	1053	THR	3.4
2	B	584	LEU	3.3
1	A	605	ASN	3.3
2	B	356	LEU	3.3
1	A	870	LEU	3.3
1	A	338	ILE	3.2
2	B	559	ILE	3.2
1	A	344	VAL	3.1
2	B	331	ALA	3.1
2	B	436	VAL	3.1
1	A	31	ILE	3.1
2	B	506	LYS	3.1
1	A	806	ASP	3.1
1	A	936	HIS	3.1
2	B	399	SER	3.0
2	B	510	GLU	3.0
1	A	422	LEU	3.0
1	A	32	VAL	3.0
2	B	336	GLY	3.0
1	A	187	LYS	3.0
1	A	867	LYS	3.0
2	B	549	LEU	3.0
1	A	219	GLN	3.0
1	A	409	VAL	3.0
2	B	503	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	368	TYR	3.0
1	A	381	PRO	3.0
1	A	1008	SER	2.9
1	A	353	LYS	2.9
2	B	425	LEU	2.9
1	A	389	TYR	2.8
2	B	328	LEU	2.8
1	A	383	TRP	2.8
1	A	677	ASN	2.8
1	A	106	GLY	2.8
1	A	837	GLY	2.8
1	A	935	GLY	2.8
1	A	423	ALA	2.8
2	B	346	LYS	2.8
1	A	1015	SER	2.8
1	A	1003	SER	2.8
2	B	498	CYS	2.8
1	A	300	ASP	2.7
1	A	351	ILE	2.7
1	A	679	THR	2.7
1	A	473	LEU	2.7
1	A	247	GLN	2.7
1	A	212	ASN	2.7
1	A	1007	GLY	2.7
2	B	334	TYR	2.6
1	A	809	GLN	2.6
1	A	376	VAL	2.6
1	A	805	ASP	2.6
2	B	532	LYS	2.6
1	A	408	SER	2.6
1	A	363	GLY	2.6
1	A	838	CYS	2.6
1	A	973	LYS	2.6
1	A	985	TYR	2.5
2	B	480	LYS	2.5
2	B	386	ARG	2.5
1	A	842	GLY	2.5
1	A	6	SER	2.5
2	B	525	MET	2.4
1	A	343	TYR	2.4
1	A	69	ILE	2.4
1	A	972	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	495	GLU	2.4
2	B	591	GLN	2.4
2	B	421	ASP	2.3
1	A	1018	ASP	2.3
1	A	148	LYS	2.3
1	A	141	ARG	2.3
1	A	960	PHE	2.3
2	B	494	PHE	2.3
1	A	308	SER	2.3
2	B	552	GLN	2.3
1	A	358	THR	2.3
1	A	82	PHE	2.3
1	A	246	TYR	2.3
2	B	540	ASP	2.3
1	A	378	CYS	2.3
1	A	528	LYS	2.3
1	A	604	CYS	2.3
1	A	-18	HIS	2.3
2	B	426	TYR	2.2
2	B	558	GLU	2.2
1	A	-3	ALA	2.2
1	A	202	ASN	2.2
1	A	215	CYS	2.2
2	B	367	ASP	2.2
2	B	404	LEU	2.2
2	B	401	VAL	2.2
2	B	499	GLN	2.2
1	A	508	TYR	2.2
1	A	189	GLN	2.1
2	B	435	GLN	2.1
1	A	813	THR	2.1
2	B	592	LYS	2.1
1	A	53	ALA	2.1
1	A	844	CYS	2.1
2	B	410	ASN	2.1
2	B	444	ALA	2.1
2	B	491	ILE	2.1
1	A	815	GLN	2.1
1	A	27	PRO	2.1
1	A	407	CYS	2.1
1	A	50	PHE	2.1
1	A	213	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	529	ASP	2.1
2	B	598	LEU	2.0
1	A	1050	GLY	2.0
2	B	342	GLU	2.0
2	B	407	HIS	2.0
1	A	373	THR	2.0
1	A	493	GLU	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	0.90	0.16	-	115,132,186,190	0
1	SEP	A	7	10/11	0.53	0.29	-	173,201,218,220	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
3	71A	A	1101	7/7	0.87	1.54	-	146,162,167,169	0
4	71B	A	1102	10/10	0.58	0.67	-	90,110,118,124	10

## 6.5 Other polymers [i](#)

There are no such residues in this entry.