



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 06:57 pm BST

PDB ID : 5SWO  
Title : Crystal Structure of PI3Kalpha in complex with fragments 4 and 19  
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Deposited on : 2016-08-08  
Resolution : 3.50 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.

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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 : 2.11  
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) : 2.11

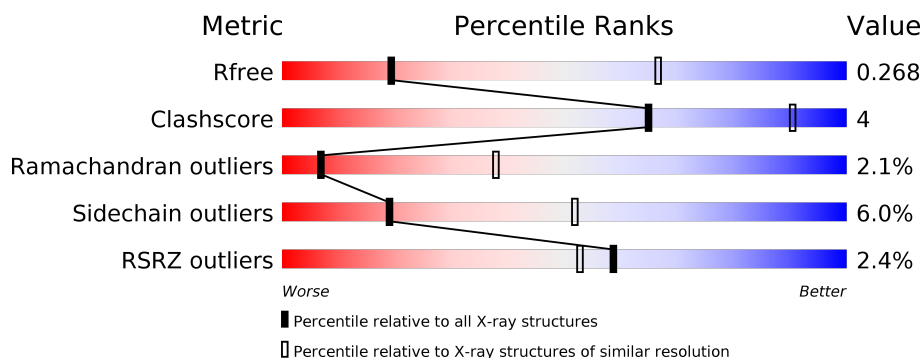
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (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 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	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• •</div> </div> </div>
2	B	279	<div> <div>7%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>• •</div> </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
5	2ZV	B	701	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10899 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	1051	Total	C	N	O	P	S	0	0	0
			8593	5489	1471	1563	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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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42336
A	0	SER	-	expression tag	UNP P42336

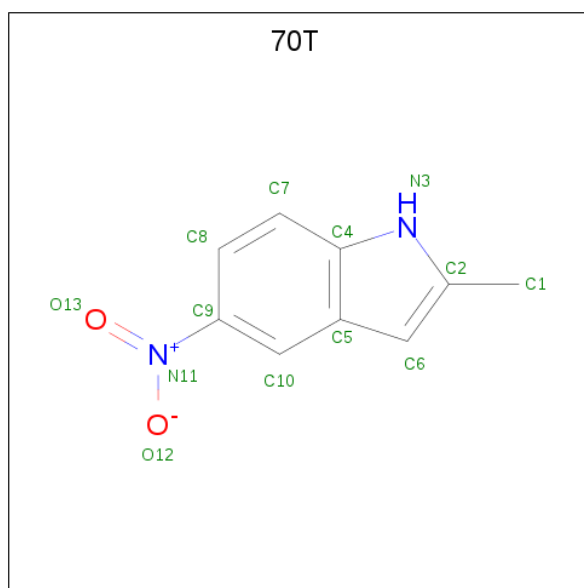
- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	267	Total	C	N	O	S	0	0	0
			2281	1433	407	435	6			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

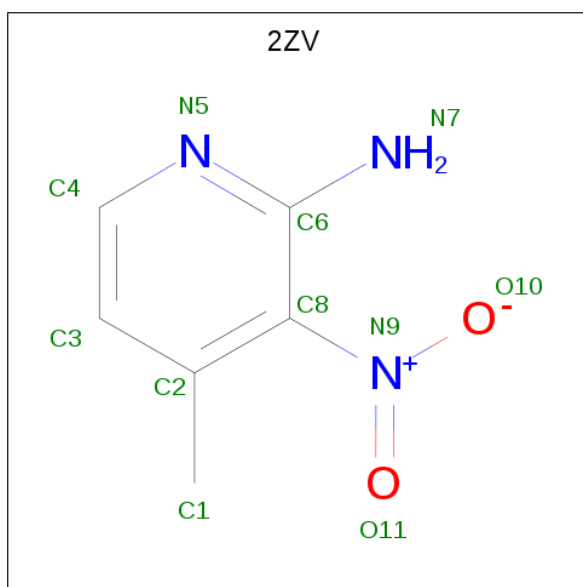
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 2-methyl-5-nitro-1H-indole (three-letter code: 70T) (formula: C<sub>9</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			13	9	2	2		

- Molecule 5 is 4-methyl-3-nitropyridin-2-amine (three-letter code: 2ZV) (formula: C<sub>6</sub>H<sub>7</sub>N<sub>3</sub>O<sub>2</sub>).

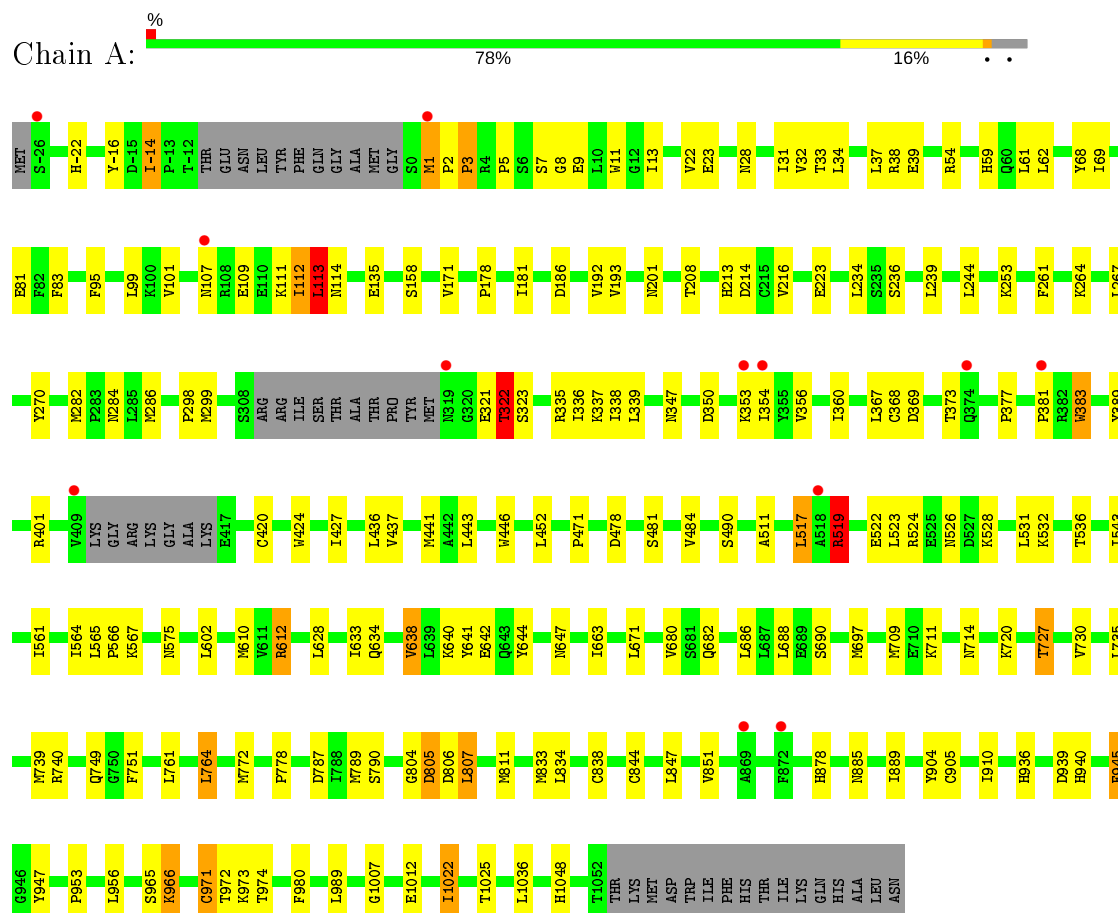


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			11	6	3	2		

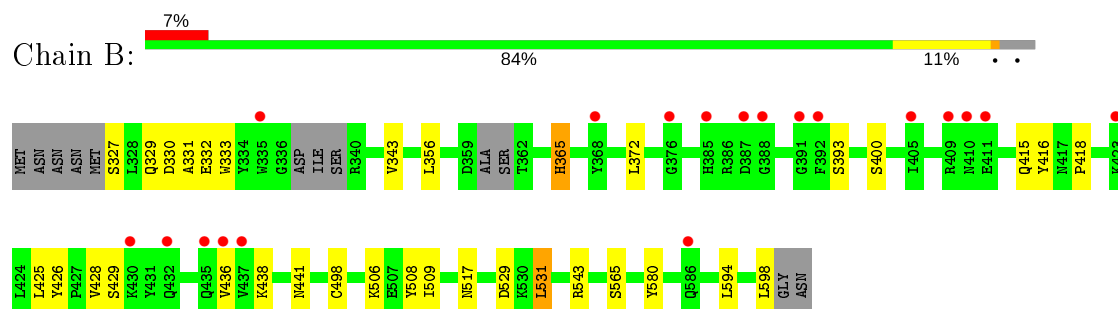
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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, $\alpha$ , $\beta$ , $\gamma$	114.83Å 116.36Å 149.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.81 – 3.50 48.68 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (91.81-3.50) 99.5 (48.68-3.50)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.91 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.189 , 0.274 0.190 , 0.268	Depositor DCC
$R_{free}$ test set	1322 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	99.6	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 76.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10899	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: 70T, 2ZV, CL, 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	0.54	0/8783	0.78	3/11874 (0.0%)
2	B	0.49	0/2319	0.71	0/3103
All	All	0.53	0/11102	0.77	3/14977 (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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	612	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	764	LEU	CA-CB-CG	5.55	128.06	115.30
1	A	113	LEU	CB-CG-CD1	5.05	119.59	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	LEU	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8593	0	8554	82	0
2	B	2281	0	2262	11	0
3	A	1	0	0	0	0
4	A	13	0	0	0	0
5	B	11	0	7	1	0
All	All	10899	0	10823	89	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 (89) 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)
5:B:701:2ZV:O11	5:B:701:2ZV:N9	1.58	1.37
1:A:31:ILE:HD11	2:B:531:LEU:HD13	1.73	0.68
1:A:543:ILE:HD11	1:A:567:LYS:HD3	1.79	0.64
1:A:519:ARG:HB2	1:A:523:LEU:HA	1.81	0.63
1:A:640:LYS:HE2	1:A:680:VAL:HG11	1.81	0.63
1:A:336:ILE:HD12	1:A:389:TYR:CE2	2.34	0.62
1:A:602:LEU:O	1:A:612:ARG:NH2	2.34	0.60
1:A:178:PRO:HD2	1:A:181:ILE:HD12	1.82	0.59
1:A:709:MET:HE1	1:A:847:LEU:HD21	1.84	0.59
1:A:806:ASP:HB2	1:A:844:CYS:SG	2.42	0.59
1:A:261:PHE:HA	1:A:270:TYR:CE2	2.39	0.58
1:A:171:VAL:HG12	1:A:270:TYR:HA	1.87	0.57
1:A:807:LEU:HD12	1:A:838:CYS:SG	2.45	0.57
1:A:789:MET:O	1:A:790:SEP:C	2.52	0.56
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.26	0.56
1:A:367:LEU:HD12	1:A:368:CYS:O	2.05	0.56
1:A:61:LEU:HD11	2:B:508:TYR:CZ	2.41	0.56
1:A:321:GLU:O	1:A:322:THR:HG23	2.07	0.55
2:B:333:TRP:HA	2:B:429:SER:HB2	1.89	0.54
1:A:23:GLU:CG	1:A:33:THR:HG22	2.37	0.54
1:A:965:SER:HB2	1:A:974:THR:HG21	1.90	0.54
1:A:-16:TYR:HE1	1:A:-14:ILE:HG23	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:LEU:HD21	1:A:851:VAL:HG21	1.90	0.54
1:A:8:GLY:HA3	1:A:714:ASN:HD21	1.73	0.53
1:A:628:LEU:HD23	1:A:663:ILE:HD13	1.90	0.52
1:A:561:ILE:O	1:A:564:ILE:HG22	2.09	0.52
1:A:28:ASN:ND2	1:A:62:LEU:HD21	2.25	0.52
1:A:936:HIS:HB3	1:A:940:HIS:HB3	1.92	0.52
1:A:519:ARG:NH1	1:A:523:LEU:HD22	2.25	0.51
1:A:772:MET:HB2	1:A:778:PRO:HG2	1.93	0.51
1:A:424:TRP:CE2	1:A:446:TRP:HB2	2.46	0.51
1:A:3:PRO:HG3	1:A:804:GLY:HA2	1.92	0.51
1:A:32:VAL:O	1:A:32:VAL:HG23	2.11	0.51
2:B:343:VAL:HG13	2:B:356:LEU:HD11	1.93	0.51
1:A:298:PRO:HG2	1:A:697:MET:HG3	1.92	0.50
1:A:1022:ILE:HA	1:A:1025:THR:HG22	1.93	0.50
1:A:23:GLU:HG2	1:A:33:THR:HG22	1.93	0.50
1:A:610:MET:CE	1:A:610:MET:HA	2.42	0.49
1:A:360:ILE:N	1:A:360:ILE:HD12	2.29	0.48
1:A:885:ASN:HB3	1:A:889:ILE:HG22	1.95	0.48
1:A:878:HIS:NE2	1:A:966:LYS:O	2.46	0.48
1:A:524:ARG:HD3	1:A:526:ASN:HD22	1.78	0.48
1:A:945:PHE:HB2	2:B:598:LEU:HD13	1.96	0.47
1:A:956:LEU:HD11	1:A:980:PHE:CZ	2.50	0.47
1:A:337:LYS:HD3	1:A:339:LEU:HD11	1.95	0.47
1:A:8:GLY:CA	1:A:714:ASN:HD21	2.27	0.47
1:A:735:LEU:O	1:A:739:MET:HG3	2.15	0.46
1:A:910:ILE:O	1:A:1025:THR:HG21	2.15	0.46
1:A:671:LEU:HB2	1:A:688:LEU:HD21	1.98	0.45
1:A:213:HIS:CE1	1:A:214:ASP:HB3	2.52	0.45
1:A:23:GLU:HG3	1:A:33:THR:HG22	1.99	0.45
2:B:436:VAL:HG12	2:B:580:TYR:CD1	2.52	0.45
1:A:353:LYS:HG3	1:A:377:PRO:HB3	1.98	0.45
2:B:327:SER:O	2:B:331:ALA:N	2.50	0.45
1:A:68:TYR:CD1	1:A:101:VAL:HG12	2.52	0.44
1:A:833:MET:HE1	1:A:904:TYR:HA	1.99	0.44
1:A:532:LYS:O	1:A:536:THR:HG23	2.18	0.44
1:A:427:ILE:HG12	1:A:443:LEU:HD13	1.98	0.44
1:A:192:VAL:HG12	1:A:193:VAL:N	2.33	0.44
1:A:528:LYS:HA	1:A:531:LEU:HD12	2.00	0.43
1:A:81:GLU:HB2	1:A:83:PHE:CZ	2.53	0.43
1:A:54:ARG:HG2	1:A:59:HIS:CE1	2.53	0.43
1:A:749:GLN:HE21	1:A:764:LEU:H	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:VAL:HG23	1:A:383:TRP:CH2	2.54	0.43
1:A:354:ILE:HD11	1:A:381:PRO:HB3	2.01	0.43
1:A:11:TRP:HB2	1:A:95:PHE:CD1	2.54	0.42
1:A:135:GLU:OE2	1:A:644:TYR:HB3	2.18	0.42
1:A:9:GLU:OE1	1:A:38:ARG:NH1	2.51	0.42
1:A:971:CYS:C	1:A:973:LYS:H	2.23	0.42
1:A:1:MET:HB2	1:A:720:LYS:HE3	2.01	0.42
1:A:634:GLN:O	1:A:638:VAL:HB	2.20	0.42
1:A:751:PHE:CE2	1:A:761:LEU:HD12	2.55	0.42
1:A:282:MET:O	1:A:284:ASN:ND2	2.53	0.41
2:B:506:LYS:HA	2:B:509:ILE:HG22	2.01	0.41
1:A:338:ILE:O	1:A:339:LEU:HD12	2.21	0.41
1:A:347:ASN:ND2	2:B:565:SER:OG	2.51	0.41
1:A:267:LEU:HA	1:A:267:LEU:HD23	1.97	0.41
1:A:945:PHE:CB	2:B:598:LEU:HD13	2.49	0.41
1:A:13:ILE:HD12	1:A:13:ILE:O	2.20	0.41
1:A:253:LYS:HB3	1:A:286:MET:HB3	2.02	0.41
1:A:709:MET:CE	1:A:847:LEU:HD21	2.51	0.41
2:B:426:TYR:HB3	2:B:428:VAL:HG23	2.02	0.41
1:A:436:LEU:HB3	1:A:484:VAL:HB	2.03	0.40
1:A:641:TYR:OH	1:A:1007:GLY:N	2.55	0.40
1:A:936:HIS:ND1	1:A:1012:GLU:OE2	2.55	0.40
1:A:989:LEU:HD11	1:A:1036:LEU:HD11	2.04	0.40
1:A:565:LEU:HB3	1:A:566:PRO:HD3	2.03	0.40
1:A:-14:ILE:N	1:A:-14:ILE:HD13	2.36	0.40
1:A:727:THR:O	1:A:730:VAL:N	2.55	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	1042/1096 (95%)	918 (88%)	103 (10%)	21 (2%)	7	39
2	B	261/279 (94%)	228 (87%)	27 (10%)	6 (2%)	6	36
All	All	1303/1375 (95%)	1146 (88%)	130 (10%)	27 (2%)	7	38

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	PRO
1	A	945	PHE
1	A	966	LYS
1	A	1	MET
1	A	322	THR
1	A	972	THR
2	B	332	GLU
2	B	365	HIS
2	B	438	LYS
1	A	-22	HIS
1	A	2	PRO
1	A	264	LYS
1	A	517	LEU
1	A	805	ASP
1	A	939	ASP
1	A	5	PRO
1	A	481	SER
1	A	519	ARG
1	A	947	TYR
2	B	393	SER
2	B	418	PRO
2	B	517	ASN
1	A	323	SER
1	A	471	PRO
1	A	511	ALA
1	A	953	PRO
1	A	112	ILE

### 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%)	902 (94%)	58 (6%)	19	52
2	B	249/259 (96%)	235 (94%)	14 (6%)	21	54
All	All	1209/1257 (96%)	1137 (94%)	72 (6%)	19	52

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-14	ILE
1	A	7	SER
1	A	22	VAL
1	A	34	LEU
1	A	37	LEU
1	A	39	GLU
1	A	69	ILE
1	A	99	LEU
1	A	107	ASN
1	A	109	GLU
1	A	111	LYS
1	A	112	ILE
1	A	113	LEU
1	A	114	ASN
1	A	158	SER
1	A	186	ASP
1	A	201	ASN
1	A	208	THR
1	A	216	VAL
1	A	223	GLU
1	A	234	LEU
1	A	236	SER
1	A	239	LEU
1	A	244	LEU
1	A	299	MET
1	A	322	THR
1	A	335	ARG
1	A	350	ASP
1	A	369	ASP
1	A	373	THR
1	A	383	TRP
1	A	401	ARG
1	A	420	CYS
1	A	437	VAL

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Mol	Chain	Res	Type
1	A	441	MET
1	A	452	LEU
1	A	478	ASP
1	A	490	SER
1	A	517	LEU
1	A	519	ARG
1	A	522	GLU
1	A	575	ASN
1	A	633	ILE
1	A	638	VAL
1	A	682	GLN
1	A	686	LEU
1	A	690	SER
1	A	711	LYS
1	A	727	THR
1	A	740	ARG
1	A	787	ASP
1	A	805	ASP
1	A	807	LEU
1	A	811	MET
1	A	905	CYS
1	A	971	CYS
1	A	1022	ILE
1	A	1048	HIS
2	B	329	GLN
2	B	330	ASP
2	B	365	HIS
2	B	372	LEU
2	B	400	SER
2	B	415	GLN
2	B	416	TYR
2	B	425	LEU
2	B	441	ASN
2	B	498	CYS
2	B	529	ASP
2	B	531	LEU
2	B	543	ARG
2	B	594	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-21	HIS
1	A	137	GLN
1	A	374	GLN
1	A	467	ASN
1	A	526	ASN
1	A	575	ASN
1	A	597	GLN
1	A	682	GLN
1	A	714	ASN
1	A	749	GLN
1	A	996	ASN
2	B	457	GLN

### 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	8,9,10	0.71	0	8,12,14	1.94	3 (37%)

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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	790	SEP	OG-CB-CA	3.74	111.79	108.14
1	A	790	SEP	P-OG-CB	2.44	125.02	118.30
1	A	790	SEP	O2P-P-OG	-2.42	100.28	106.73

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-O1P
1	A	790	SEP	CB-OG-P-O2P
1	A	790	SEP	CB-OG-P-O3P

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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	$\# Z  > 2$
5	2ZV	B	701	-	10,11,11	7.17	4 (40%)	11,15,15	1.39	2 (18%)
4	70T	A	1102	-	11,14,14	1.12	2 (18%)	13,20,20	2.32	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
5	2ZV	B	701	-	-	0/0/4/4	0/1/1/1
4	70T	A	1102	-	-	2/2/4/4	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	701	2ZV	O11-N9	20.86	1.58	1.22
5	B	701	2ZV	C8-N9	-6.30	1.34	1.45
5	B	701	2ZV	C1-C2	-4.77	1.41	1.51
5	B	701	2ZV	C4-N5	3.51	1.42	1.34
4	A	1102	70T	C10-C9	2.18	1.41	1.36
4	A	1102	70T	C7-C8	2.05	1.40	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1102	70T	C1-C2-N3	5.46	132.65	119.98
4	A	1102	70T	C1-C2-C6	-4.73	116.54	129.06
5	B	701	2ZV	C3-C4-N5	-2.53	120.82	123.96
5	B	701	2ZV	C8-C6-N7	-2.16	117.44	123.82

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1102	70T	C8-C9-N11-O13
4	A	1102	70T	C10-C9-N11-O13

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	701	2ZV	1	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, 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	1050/1096 (95%)	-0.12	12 (1%) 80 75	53, 100, 162, 231	0
2	B	267/279 (95%)	0.32	19 (7%) 16 15	97, 162, 206, 228	0
All	All	1317/1375 (95%)	-0.03	31 (2%) 59 53	53, 108, 187, 231	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	ASN	4.9
2	B	391	GLY	4.5
1	A	872	PHE	4.4
1	A	869	ALA	4.0
1	A	-26	SER	3.7
2	B	335	TRP	3.6
1	A	409	VAL	3.1
1	A	107	ASN	3.0
1	A	374	GLN	2.8
2	B	388	GLY	2.7
2	B	435	GLN	2.7
2	B	409	ARG	2.6
2	B	410	ASN	2.6
2	B	437	VAL	2.6
1	A	353	LYS	2.6
2	B	405	ILE	2.5
2	B	385	HIS	2.5
2	B	586	GLN	2.5
2	B	430	LYS	2.4
1	A	354	ILE	2.4
2	B	436	VAL	2.4
2	B	423	LYS	2.4
2	B	376	GLY	2.4
2	B	387	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	392	PHE	2.3
2	B	411	GLU	2.1
1	A	1	MET	2.1
2	B	432	GLN	2.1
1	A	381	PRO	2.1
2	B	368	TYR	2.0
1	A	518	ALA	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( $\text{\AA}^2$ )	Q<0.9
1	SEP	A	790	10/11	0.93	0.20	82,100,161,174	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. 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
5	2ZV	B	701	11/11	0.66	0.73	153,178,200,201	0
4	70T	A	1102	13/13	0.86	0.50	109,132,144,144	0
3	CL	A	1101	1/1	0.96	0.23	71,71,71,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.