



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 03:54 AM EDT

PDB ID : 5SXC  
Title : Crystal Structure of PI3Kalpha in complex with fragment 8  
Authors : Gabelli, S.B.; Vogelstein, B.; Miller, M.S.; Amzel, L.M.  
Deposited on : 2016-08-09  
Resolution : 3.55 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

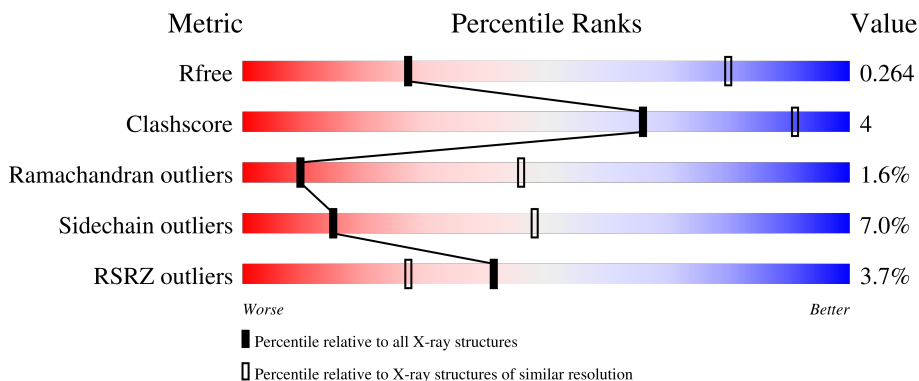
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.55 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	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)

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	 6% 61% 13% • 25%

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
3	URF	A	1101	-	X	-	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10334 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	1040	8518	5442	1461	1545	2	68	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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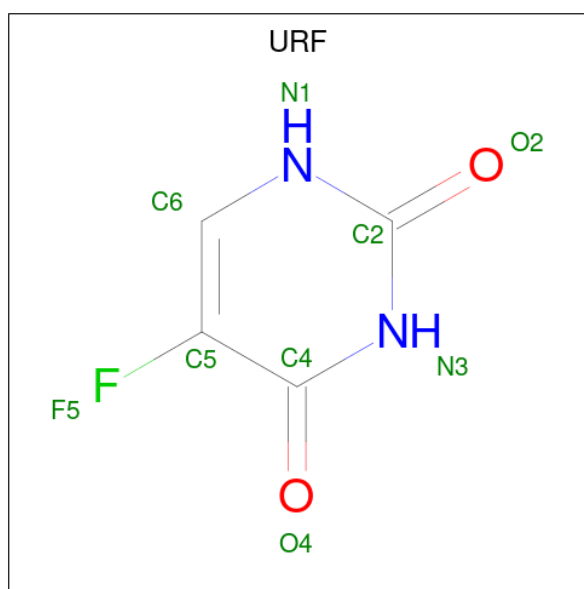
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42336
A	0	SER	-	expression tag	UNP P42336

- 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	208	1807	1138	321	343	5	0	0	0

- Molecule 3 is 5-FLUOROURACIL (three-letter code: URF) (formula: C<sub>4</sub>H<sub>3</sub>FN<sub>2</sub>O<sub>2</sub>).

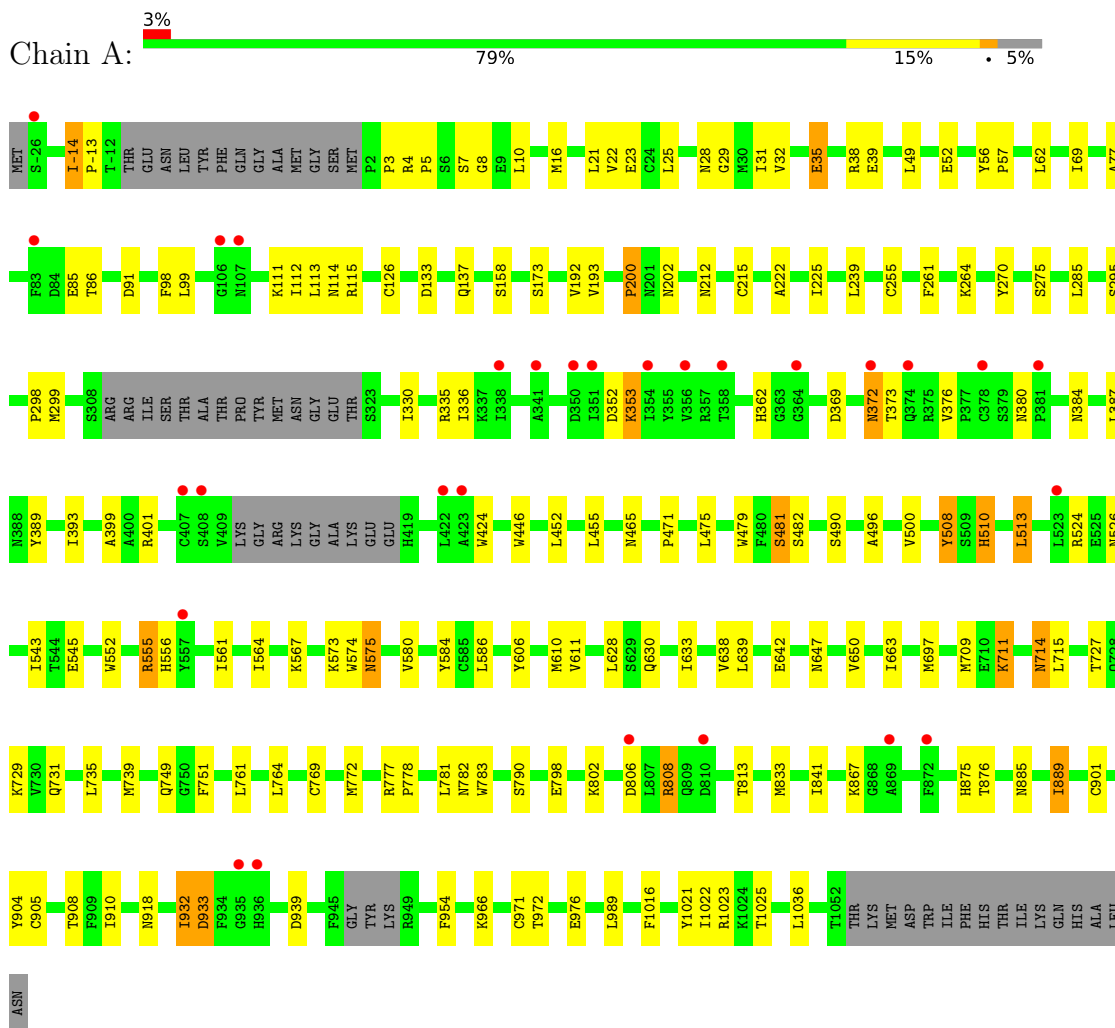


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	A	1	9	4	1	2	2	0	0

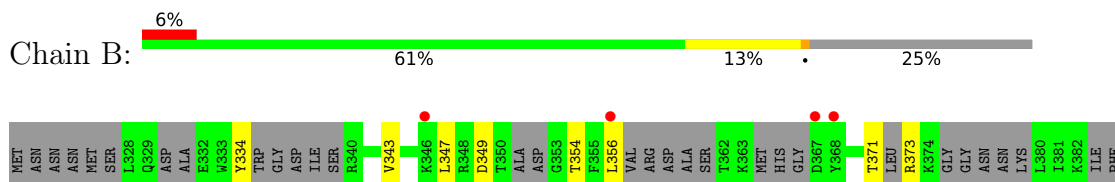
### 3 Residue-property plots [i](#)

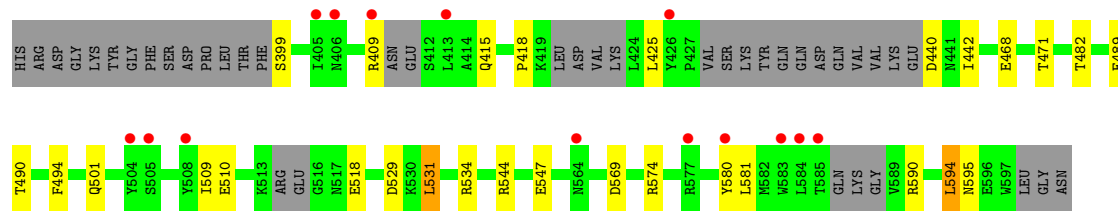
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.73Å 117.27Å 150.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.46 – 3.55 49.32 – 3.54	Depositor EDS
% Data completeness (in resolution range)	99.9 (92.46-3.55) 99.9 (49.32-3.54)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 3.57Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.194 , 0.268 0.195 , 0.264	Depositor DCC
$R_{free}$ test set	1305 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	112.4	Xtrriage
Anisotropy	0.281	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 102.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.013 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10334	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	138.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: URF, 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	0.57	0/8695	0.78	1/11752 (0.0%)
2	B	0.52	0/1824	0.70	0/2421
All	All	0.56	0/10519	0.77	1/14173 (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	2

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	5.30	122.95	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	LEU	Peptide
1	A	200	PRO	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	8518	0	8488	76	0
2	B	1807	0	1800	12	0
3	A	9	0	3	0	0
All	All	10334	0	10291	83	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 (83) 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:8:GLY:HA2	1:A:714:ASN:HD21	1.51	0.76
1:A:628:LEU:HD23	1:A:663:ILE:HD13	1.71	0.72
1:A:561:ILE:O	1:A:564:ILE:HG22	1.96	0.66
1:A:8:GLY:CA	1:A:714:ASN:HD21	2.09	0.65
1:A:642:GLU:HG2	1:A:647:ASN:ND2	2.11	0.64
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.17	0.64
1:A:261:PHE:HA	1:A:270:TYR:CE2	2.36	0.60
1:A:806:ASP:OD2	1:A:808:ARG:NH1	2.34	0.60
1:A:932:ILE:HD12	1:A:933:ASP:HB2	1.83	0.60
1:A:749:GLN:O	1:A:761:LEU:O	2.20	0.59
1:A:715:LEU:HD21	1:A:735:LEU:HD12	1.85	0.59
1:A:98:PHE:CE1	2:B:490:THR:HG23	2.39	0.57
2:B:347:LEU:CD1	2:B:371:THR:HG21	2.36	0.56
2:B:343:VAL:HG13	2:B:356:LEU:HD11	1.88	0.55
1:A:772:MET:HB2	1:A:778:PRO:HG2	1.88	0.55
1:A:552:TRP:CZ3	1:A:555:ARG:HD3	2.42	0.55
1:A:25:LEU:HD21	2:B:494:PHE:CE2	2.42	0.54
1:A:731:GLN:HE22	1:A:777:ARG:HE	1.56	0.53
1:A:10:LEU:HD13	1:A:16:MET:CE	2.39	0.53
1:A:192:VAL:HG12	1:A:193:VAL:N	2.24	0.52
1:A:222:ALA:O	1:A:225:ILE:N	2.42	0.52
1:A:910:ILE:O	1:A:1025:THR:HG21	2.10	0.52
2:B:347:LEU:HD11	2:B:371:THR:HG21	1.92	0.52
1:A:261:PHE:CD2	1:A:270:TYR:CD2	2.99	0.51
1:A:31:ILE:HD11	2:B:531:LEU:HD13	1.93	0.50
2:B:347:LEU:HD22	2:B:373:ARG:HB2	1.94	0.49
1:A:32:VAL:HG21	1:A:49:LEU:CD1	2.43	0.49
1:A:524:ARG:HD2	1:A:526:ASN:HD22	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:989:LEU:HD21	1:A:1036:LEU:HG	1.95	0.49
1:A:543:ILE:HD11	1:A:567:LYS:CD	2.43	0.48
1:A:496:ALA:O	1:A:500:VAL:HG23	2.13	0.48
1:A:735:LEU:O	1:A:739:MET:HG3	2.13	0.48
1:A:446:TRP:CZ2	1:A:465:ASN:HA	2.50	0.47
1:A:709:MET:HG3	1:A:841:ILE:HD13	1.95	0.47
1:A:584:TYR:CD2	1:A:610:MET:HG3	2.49	0.47
1:A:330:ILE:HG21	1:A:393:ILE:HG21	1.97	0.47
1:A:524:ARG:CD	1:A:526:ASN:HD22	2.28	0.47
1:A:255:CYS:SG	1:A:285:LEU:O	2.73	0.46
1:A:749:GLN:HE21	1:A:764:LEU:H	1.61	0.46
1:A:336:ILE:HD12	1:A:389:TYR:CE2	2.49	0.46
1:A:192:VAL:HG12	1:A:193:VAL:H	1.81	0.46
1:A:10:LEU:HD13	1:A:16:MET:HE2	1.97	0.46
1:A:628:LEU:HD23	1:A:663:ILE:CD1	2.43	0.45
1:A:362:HIS:CD2	1:A:399:ALA:HB3	2.51	0.45
1:A:939:ASP:HB2	1:A:1021:TYR:CE2	2.52	0.45
1:A:751:PHE:CE2	1:A:761:LEU:HD12	2.52	0.45
1:A:639:LEU:HD22	1:A:650:VAL:HG22	1.99	0.45
1:A:573:LYS:HB3	1:A:575:ASN:ND2	2.32	0.45
1:A:989:LEU:HD11	1:A:1036:LEU:HD11	1.99	0.44
1:A:1021:TYR:C	1:A:1021:TYR:CD1	2.90	0.44
1:A:510:HIS:N	1:A:513:LEU:HD12	2.33	0.44
1:A:510:HIS:HB2	1:A:513:LEU:HD12	2.00	0.44
1:A:885:ASN:HB3	1:A:889:ILE:HG22	2.00	0.43
1:A:372:ASN:OD1	1:A:372:ASN:N	2.51	0.43
1:A:261:PHE:CD2	1:A:270:TYR:CG	3.07	0.43
1:A:574:TRP:HA	1:A:580:VAL:CG2	2.48	0.43
1:A:769:CYS:SG	1:A:781:LEU:HA	2.58	0.43
1:A:875:HIS:O	1:A:876:THR:C	2.57	0.43
1:A:23:GLU:OE1	2:B:534:ARG:NE	2.39	0.42
1:A:606:TYR:HB3	1:A:611:VAL:HG11	1.99	0.42
2:B:581:LEU:HD11	2:B:594:LEU:HD23	2.02	0.42
1:A:298:PRO:HG2	1:A:697:MET:HG3	2.01	0.42
1:A:28:ASN:ND2	1:A:62:LEU:HD21	2.34	0.42
1:A:833:MET:HE1	1:A:904:TYR:HA	2.01	0.42
1:A:479:TRP:CZ2	1:A:481:SER:HA	2.55	0.42
2:B:544:ARG:O	2:B:547:GLU:HG2	2.18	0.42
1:A:32:VAL:HG12	1:A:56:TYR:CD1	2.55	0.42
1:A:778:PRO:HB3	1:A:802:LYS:HG3	2.02	0.42
1:A:91:ASP:OD1	1:A:711:LYS:NZ	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LYS:O	1:A:114:ASN:ND2	2.53	0.41
1:A:1022:ILE:HA	1:A:1025:THR:HG22	2.03	0.41
1:A:352:ASP:HB3	1:A:353:LYS:HD2	2.02	0.41
1:A:543:ILE:HD11	1:A:567:LYS:HD2	2.01	0.41
1:A:556:HIS:CE1	1:A:586:LEU:HD21	2.54	0.41
1:A:543:ILE:HD11	1:A:567:LYS:HD3	2.01	0.41
1:A:764:LEU:HD21	1:A:783:TRP:CE2	2.55	0.41
2:B:509:ILE:HG23	2:B:510:GLU:HG3	2.02	0.41
1:A:21:LEU:HD23	1:A:35:GLU:HA	2.03	0.41
1:A:424:TRP:CE2	1:A:446:TRP:HB2	2.56	0.41
1:A:908:THR:HG21	1:A:954:PHE:HB2	2.03	0.40
1:A:29:GLY:HA3	2:B:501:GLN:HB3	2.03	0.40
1:A:782:ASN:HD22	1:A:798:GLU:HB3	1.85	0.40
1:A:-14:ILE:HD13	1:A:-13:PRO:HD2	2.02	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	1028/1096 (94%)	882 (86%)	130 (13%)	16 (2%)	9	46
2	B	180/279 (64%)	168 (93%)	9 (5%)	3 (2%)	9	45
All	All	1208/1375 (88%)	1050 (87%)	139 (12%)	19 (2%)	9	46

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	A	508	TYR
1	A	555	ARG
1	A	38	ARG

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Mol	Chain	Res	Type
1	A	77	ALA
1	A	264	LYS
1	A	471	PRO
1	A	867	LYS
1	A	918	ASN
2	B	418	PRO
2	B	590	ARG
1	A	5	PRO
1	A	1016	PHE
1	A	133	ASP
1	A	200	PRO
2	B	442	ILE
1	A	3	PRO
1	A	889	ILE
1	A	4	ARG

### 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	951/997 (95%)	891 (94%)	60 (6%)	18	52
2	B	199/259 (77%)	179 (90%)	20 (10%)	7	34
All	All	1150/1256 (92%)	1070 (93%)	80 (7%)	15	48

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-14	ILE
1	A	22	VAL
1	A	35	GLU
1	A	39	GLU
1	A	52	GLU
1	A	57	PRO
1	A	69	ILE
1	A	85	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	86	THR
1	A	99	LEU
1	A	112	ILE
1	A	115	ARG
1	A	126	CYS
1	A	137	GLN
1	A	158	SER
1	A	173	SER
1	A	212	ASN
1	A	215	CYS
1	A	239	LEU
1	A	275	SER
1	A	295	SER
1	A	299	MET
1	A	335	ARG
1	A	353	LYS
1	A	369	ASP
1	A	372	ASN
1	A	373	THR
1	A	376	VAL
1	A	380	ASN
1	A	384	ASN
1	A	387	LEU
1	A	401	ARG
1	A	452	LEU
1	A	455	LEU
1	A	475	LEU
1	A	481	SER
1	A	482	SER
1	A	490	SER
1	A	508	TYR
1	A	510	HIS
1	A	513	LEU
1	A	545	GLU
1	A	575	ASN
1	A	630	GLN
1	A	633	ILE
1	A	638	VAL
1	A	711	LYS
1	A	714	ASN
1	A	727	THR
1	A	729	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	808	ARG
1	A	813	THR
1	A	901	CYS
1	A	905	CYS
1	A	932	ILE
1	A	933	ASP
1	A	966	LYS
1	A	971	CYS
1	A	972	THR
1	A	976	GLU
2	B	334	TYR
2	B	349	ASP
2	B	354	THR
2	B	399	SER
2	B	409	ARG
2	B	415	GLN
2	B	425	LEU
2	B	440	ASP
2	B	468	GLU
2	B	471	THR
2	B	482	THR
2	B	489	GLU
2	B	518	GLU
2	B	529	ASP
2	B	531	LEU
2	B	569	ASP
2	B	574	ARG
2	B	580	TYR
2	B	594	LEU
2	B	595	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	114	ASN
1	A	284	ASN
1	A	419	HIS
1	A	526	ASN
1	A	554	HIS
1	A	556	HIS
1	A	605	ASN
1	A	643	GLN

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Mol	Chain	Res	Type
1	A	714	ASN
1	A	731	GLN
1	A	749	GLN
1	A	759	HIS
1	A	782	ASN
1	A	785	ASN
1	A	796	ASN
2	B	407	HIS
2	B	417	ASN
2	B	475	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	790	1	8,9,10	0.57	0	8,12,14	1.52	3 (37%)
1	SEP	A	7	1	8,9,10	0.78	0	8,12,14	1.44	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	-	3/5/8/10	-
1	SEP	A	7	1	-	2/5/8/10	-



There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	7	SEP	P-OG-CB	2.87	126.21	118.30
1	A	790	SEP	P-OG-CB	2.53	125.26	118.30
1	A	790	SEP	O2P-P-OG	-2.20	100.89	106.73
1	A	790	SEP	O3P-P-O2P	2.13	115.78	107.64

There are no chirality outliers.

All (5) 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	7	SEP	CA-CB-OG-P
1	A	7	SEP	CB-OG-P-O3P
1	A	790	SEP	CB-OG-P-O2P

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	URF	A	1101	-	9,9,9	2.76	3 (33%)	12,12,12	4.14	7 (58%)

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	URF	A	1101	-	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	URF	C6-C5	6.61	1.39	1.33
3	A	1101	URF	C4-C5	4.19	1.49	1.44
3	A	1101	URF	C4-N3	-2.00	1.35	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	URF	C5-C4-N3	6.66	119.12	112.56
3	A	1101	URF	O4-C4-C5	-6.23	120.09	125.72
3	A	1101	URF	N1-C2-N3	5.93	121.84	115.13
3	A	1101	URF	F5-C5-C4	5.69	121.67	116.40
3	A	1101	URF	C6-C5-C4	-4.65	117.22	122.12
3	A	1101	URF	C4-N3-C2	-4.22	120.26	126.34
3	A	1101	URF	O2-C2-N1	-3.43	119.01	122.79

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	1038/1096 (94%)	0.03	28 (2%) 54 38	58, 121, 192, 248	0
2	B	208/279 (74%)	0.52	18 (8%) 10 7	114, 194, 241, 283	0
All	All	1246/1375 (90%)	0.11	46 (3%) 41 27	58, 131, 216, 283	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	409	ARG	3.9
2	B	405	ILE	3.8
1	A	-26	SER	3.6
2	B	505	SER	3.5
1	A	381	PRO	3.4
2	B	577	ARG	3.4
2	B	504	TYR	3.3
2	B	580	TYR	3.1
2	B	584	LEU	3.1
2	B	508	TYR	3.1
2	B	368	TYR	3.1
2	B	346	LYS	3.0
1	A	408	SER	3.0
1	A	341	ALA	2.9
2	B	406	ASN	2.9
1	A	358	THR	2.8
1	A	354	ILE	2.8
1	A	423	ALA	2.7
1	A	869	ALA	2.7
1	A	935	GLY	2.6
1	A	407	CYS	2.6
1	A	557	TYR	2.6
1	A	364	GLY	2.6
1	A	372	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	378	CYS	2.5
1	A	107	ASN	2.5
1	A	374	GLN	2.4
2	B	585	THR	2.4
1	A	351	ILE	2.4
2	B	583	TRP	2.4
2	B	426	TYR	2.3
2	B	564	ASN	2.3
2	B	367	ASP	2.3
1	A	806	ASP	2.3
1	A	83	PHE	2.2
1	A	422	LEU	2.2
1	A	810	ASP	2.1
1	A	338	ILE	2.1
1	A	936	HIS	2.1
1	A	356	VAL	2.1
2	B	356	LEU	2.1
1	A	350	ASP	2.0
1	A	523	LEU	2.0
1	A	872	PHE	2.0
2	B	413	LEU	2.0
1	A	106	GLY	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	7	10/11	0.73	0.26	151,173,195,202	0
1	SEP	A	790	10/11	0.93	0.17	102,115,195,217	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

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	URF	A	1101	9/9	0.76	0.23	162,178,184,186	0

## 6.5 Other polymers

There are no such residues in this entry.