



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2017 – 09:31 PM EDT

PDB ID : 5SWR  
Title : Crystal Structure of PI3Kalpha in complex with fragments 20 and 26  
Authors : Gabelli, S.B.; Vogelstein, B.; Miller, M.S.; Amzel, L.M.  
Deposited on : unknown  
Resolution : 3.31 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.

---

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

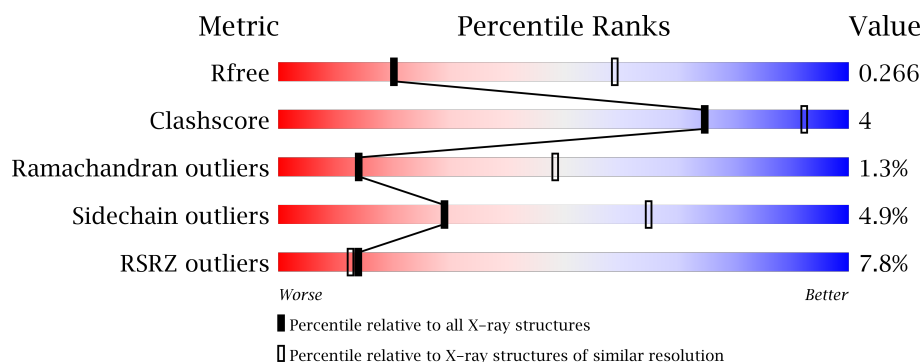
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.31 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	1002 (3.38-3.26)
Clashscore	112137	1066 (3.38-3.26)
Ramachandran outliers	110173	1048 (3.38-3.26)
Sidechain outliers	110143	1047 (3.38-3.26)
RSRZ outliers	101464	1007 (3.38-3.26)

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>5%</div> <div>80%</div> <div>15%</div> <div>• •</div> </div>
2	B	279	<div> <div>16%</div> <div>80%</div> <div>9%</div> <div>• 10%</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	CL	A	1102	-	-	-	X
5	SAL	B	701	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10792 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
			8614	5499	1476	1567	2	70			

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

*Continued on next page...*

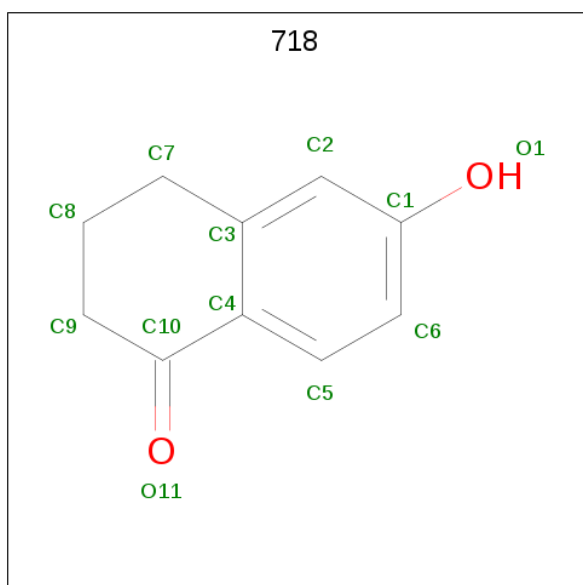
Continued from previous page...

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	252	Total	C	N	O	S	0	0	0
			2154	1349	385	414	6			

- Molecule 3 is 6-hydroxy-3,4-dihydronaphthalen-1(2H)-one (three-letter code: 718) (formula:  $C_{10}H_{10}O_2$ ).

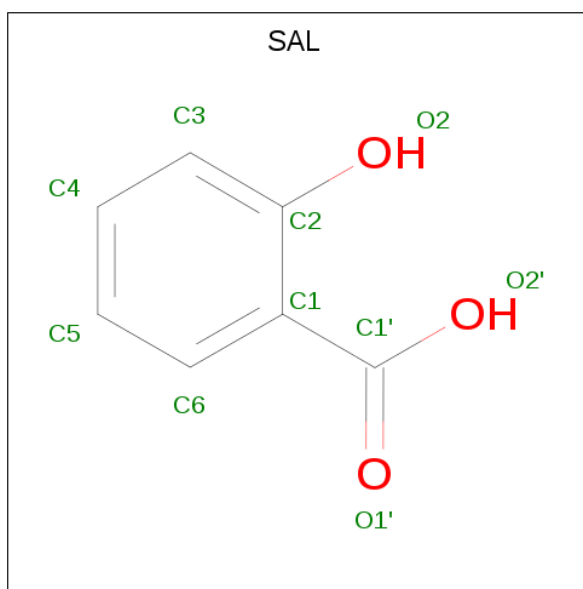


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	10	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		

- Molecule 5 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula:  $C_7H_6O_3$ ).

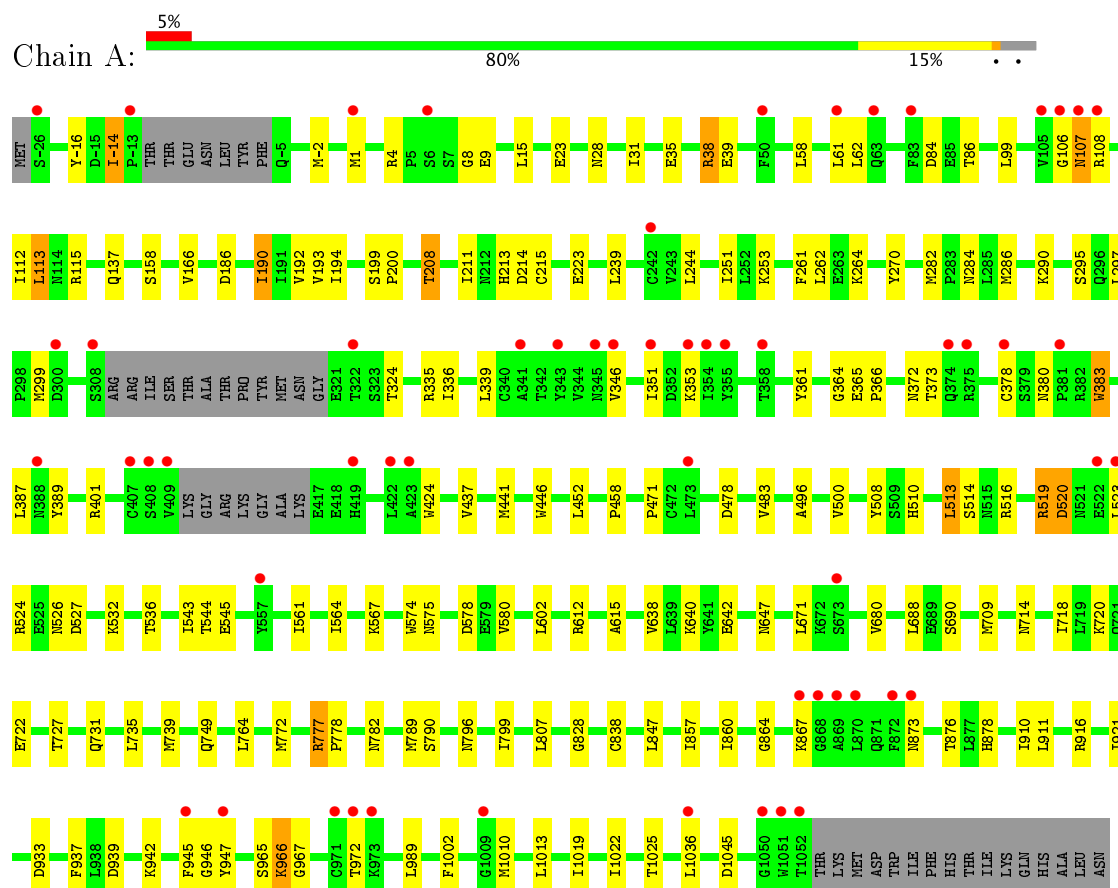


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	7	3		

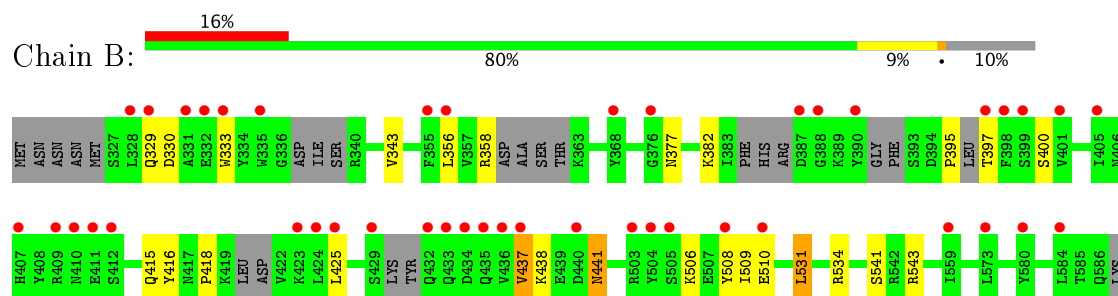
### 3 Residue-property plots [i](#)

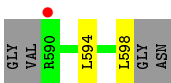
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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, $\alpha$ , $\beta$ , $\gamma$	114.24Å 116.33Å 149.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.76 – 3.31 48.49 – 3.31	Depositor EDS
% Data completeness (in resolution range)	99.3 (91.76-3.31) 99.4 (48.49-3.31)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.198 , 0.273 0.196 , 0.266	Depositor DCC
$R_{free}$ test set	1545 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	104.4	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 82.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10792	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: 718, SAL, 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	0.51	0/8793	0.75	2/11883 (0.0%)
2	B	0.47	0/2182	0.69	0/2910
All	All	0.50	0/10975	0.74	2/14793 (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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	777	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	A	513	LEU	CA-CB-CG	5.56	128.09	115.30

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 [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	8614	0	8575	72	0
2	B	2154	0	2131	13	0
3	A	12	0	0	0	0
4	A	2	0	0	0	0
5	B	10	0	5	0	0
All	All	10792	0	10711	79	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 (79) 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:640:LYS:HE2	1:A:680:VAL:HG11	1.75	0.68
1:A:519:ARG:NH2	1:A:527:ASP:OD2	2.30	0.65
1:A:372:ASN:HB3	1:A:387:LEU:HD21	1.82	0.62
1:A:23:GLU:OE1	2:B:534:ARG:NE	2.33	0.61
1:A:31:ILE:HD11	2:B:531:LEU:HD13	1.83	0.61
1:A:911:LEU:O	1:A:937:PHE:O	2.19	0.61
1:A:190:ILE:HD11	1:A:213:HIS:HA	1.82	0.61
1:A:15:LEU:HD13	1:A:718:ILE:HD11	1.84	0.58
1:A:8:GLY:HA2	1:A:714:ASN:HD21	1.67	0.58
1:A:84:ASP:OD1	1:A:86:THR:OG1	2.22	0.57
1:A:873:ASN:HB3	1:A:876:THR:HG23	1.88	0.55
1:A:519:ARG:HD2	1:A:523:LEU:HA	1.87	0.55
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.28	0.54
1:A:28:ASN:ND2	1:A:62:LEU:HD21	2.23	0.54
1:A:336:ILE:HD12	1:A:389:TYR:CE2	2.43	0.53
1:A:709:MET:HE1	1:A:847:LEU:HD21	1.90	0.53
1:A:-16:TYR:CE2	1:A:-14:ILE:HG23	2.45	0.52
1:A:671:LEU:HB2	1:A:688:LEU:HD21	1.92	0.51
1:A:989:LEU:HD11	1:A:1036:LEU:HD11	1.92	0.51
2:B:441:ASN:OD1	2:B:441:ASN:N	2.44	0.51
1:A:1022:ILE:HA	1:A:1025:THR:HG22	1.92	0.51
1:A:282:MET:O	1:A:284:ASN:ND2	2.44	0.50
1:A:401:ARG:NH2	1:A:458:PRO:O	2.40	0.50
2:B:343:VAL:HG21	2:B:358:ARG:HD3	1.94	0.50
2:B:343:VAL:HG13	2:B:356:LEU:HD11	1.94	0.50
1:A:261:PHE:HA	1:A:270:TYR:CE2	2.48	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:ILE:HD11	1:A:567:LYS:HD3	1.95	0.49
1:A:910:ILE:O	1:A:1025:THR:HG21	2.13	0.49
1:A:193:VAL:HG22	1:A:208:THR:HG22	1.93	0.48
1:A:772:MET:HB2	1:A:778:PRO:HG2	1.95	0.48
1:A:799:ILE:CD1	1:A:847:LEU:HD22	2.44	0.48
1:A:749:GLN:HE21	1:A:764:LEU:H	1.60	0.48
1:A:561:ILE:O	1:A:564:ILE:HG22	2.14	0.47
2:B:437:VAL:HG12	2:B:437:VAL:O	2.13	0.47
2:B:506:LYS:HA	2:B:509:ILE:HG22	1.96	0.47
1:A:864:GLY:O	1:A:876:THR:HG21	2.15	0.47
1:A:709:MET:CE	1:A:847:LEU:HD21	2.46	0.46
1:A:8:GLY:CA	1:A:714:ASN:HD21	2.28	0.46
1:A:106:GLY:O	1:A:108:ARG:N	2.48	0.46
1:A:602:LEU:HD21	1:A:615:ALA:HB3	1.98	0.46
1:A:731:GLN:OE1	1:A:777:ARG:NH2	2.47	0.46
1:A:253:LYS:HB3	1:A:286:MET:HB3	1.98	0.46
1:A:361:TYR:HA	1:A:366:PRO:HD3	1.98	0.46
1:A:878:HIS:NE2	1:A:966:LYS:O	2.48	0.46
1:A:1010:MET:CE	1:A:1013:LEU:HD12	2.46	0.45
1:A:483:VAL:HG23	1:A:483:VAL:O	2.15	0.45
1:A:789:MET:O	1:A:790:SEP:C	2.64	0.45
1:A:602:LEU:O	1:A:612:ARG:NH2	2.49	0.45
1:A:166:VAL:HG21	1:A:297:LEU:HD22	1.99	0.45
1:A:496:ALA:O	1:A:500:VAL:HG23	2.17	0.45
1:A:965:SER:O	1:A:967:GLY:N	2.50	0.45
1:A:324:THR:HB	1:A:483:VAL:O	2.18	0.44
1:A:942:LYS:HB2	1:A:946:GLY:HA2	1.99	0.44
1:A:945:PHE:HB2	2:B:598:LEU:HD13	1.99	0.44
1:A:807:LEU:HD12	1:A:838:CYS:SG	2.58	0.44
2:B:509:ILE:HG23	2:B:510:GLU:HG3	2.00	0.43
1:A:361:TYR:CE2	1:A:365:GLU:HB3	2.53	0.43
1:A:424:TRP:CE2	1:A:446:TRP:HB2	2.54	0.43
1:A:574:TRP:HA	1:A:580:VAL:CG2	2.49	0.43
1:A:213:HIS:CE1	1:A:214:ASP:HB3	2.54	0.43
1:A:194:ILE:HD12	1:A:194:ILE:N	2.33	0.43
1:A:857:ILE:O	1:A:860:ILE:HB	2.19	0.43
1:A:1002:PHE:HB3	1:A:1019:ILE:HG12	2.01	0.42
1:A:251:ILE:HG23	1:A:290:LYS:HE2	2.00	0.42
1:A:1:MET:HB2	1:A:720:LYS:CE	2.49	0.42
1:A:782:ASN:OD1	1:A:796:ASN:ND2	2.52	0.42
1:A:735:LEU:O	1:A:739:MET:HG3	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:ARG:HD3	1:A:526:ASN:HD22	1.85	0.42
2:B:395:PRO:O	2:B:397:THR:N	2.53	0.42
1:A:9:GLU:OE1	1:A:38:ARG:NH1	2.53	0.42
1:A:192:VAL:HG21	1:A:211:ILE:HD11	2.01	0.42
1:A:532:LYS:O	1:A:536:THR:HG23	2.20	0.42
1:A:61:LEU:HD11	2:B:508:TYR:CZ	2.55	0.41
1:A:544:THR:HG21	2:B:382:LYS:HG2	2.02	0.41
1:A:916:ARG:HB3	1:A:921:ILE:HD11	2.01	0.41
1:A:58:LEU:HB3	1:A:61:LEU:HD13	2.02	0.41
1:A:339:LEU:O	1:A:383:TRP:O	2.39	0.41
1:A:346:VAL:HG13	1:A:351:ILE:HG13	2.04	0.40
1:A:364:GLY:HA2	2:B:377:ASN:HD21	1.86	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	1043/1096 (95%)	934 (90%)	96 (9%)	13 (1%)	15	50
2	B	234/279 (84%)	217 (93%)	13 (6%)	4 (2%)	11	43
All	All	1277/1375 (93%)	1151 (90%)	109 (8%)	17 (1%)	14	48

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	CYS
1	A	508	TYR
1	A	514	SER
1	A	966	LYS
2	B	333	TRP
1	A	107	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	828	GLY
1	A	947	TYR
1	A	186	ASP
1	A	200	PRO
1	A	933	ASP
1	A	939	ASP
2	B	438	LYS
1	A	520	ASP
2	B	418	PRO
1	A	471	PRO
2	B	437	VAL

### 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	960/997 (96%)	912 (95%)	48 (5%)	28	64
2	B	236/259 (91%)	225 (95%)	11 (5%)	30	66
All	All	1196/1256 (95%)	1137 (95%)	59 (5%)	29	65

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-14	ILE
1	A	-2	MET
1	A	4	ARG
1	A	35	GLU
1	A	38	ARG
1	A	39	GLU
1	A	99	LEU
1	A	107	ASN
1	A	112	ILE
1	A	113	LEU
1	A	115	ARG
1	A	137	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	158	SER
1	A	190	ILE
1	A	199	SER
1	A	208	THR
1	A	215	CYS
1	A	223	GLU
1	A	239	LEU
1	A	244	LEU
1	A	262	LEU
1	A	264	LYS
1	A	295	SER
1	A	299	MET
1	A	335	ARG
1	A	353	LYS
1	A	373	THR
1	A	380	ASN
1	A	383	TRP
1	A	437	VAL
1	A	441	MET
1	A	452	LEU
1	A	478	ASP
1	A	510	HIS
1	A	513	LEU
1	A	516	ARG
1	A	519	ARG
1	A	520	ASP
1	A	545	GLU
1	A	575	ASN
1	A	578	ASP
1	A	638	VAL
1	A	690	SER
1	A	722	GLU
1	A	727	THR
1	A	867	LYS
1	A	972	THR
1	A	1045	ASP
2	B	329	GLN
2	B	330	ASP
2	B	400	SER
2	B	415	GLN
2	B	416	TYR
2	B	425	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	441	ASN
2	B	531	LEU
2	B	541	SER
2	B	543	ARG
2	B	594	LEU

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

Mol	Chain	Res	Type
1	A	331	ASN
1	A	347	ASN
1	A	374	GLN
1	A	444	ASN
1	A	526	ASN
1	A	556	HIS
1	A	575	ASN
1	A	605	ASN
1	A	643	GLN
1	A	670	HIS
1	A	714	ASN
1	A	749	GLN
1	A	782	ASN
1	A	785	ASN
1	A	796	ASN
1	A	861	GLN
1	A	885	ASN
2	B	329	GLN
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	1.25	1 (11%)
1	SEP	A	790	1	9,9,10	0.72	0	9,12,14	1.83	2 (22%)

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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	790	SEP	P-OG-CB	2.08	124.02	118.30
1	A	7	SEP	P-OG-CB	2.50	125.19	118.30
1	A	790	SEP	OG-CB-CA	4.17	112.28	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](#)

Of 4 ligands modelled in this entry, 2 are 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	$\# Z  > 2$
3	718	A	1101	-	13,13,13	0.89	1 (7%)	17,18,18	0.63	0
5	SAL	B	701	-	7,10,10	0.60	0	9,13,13	0.87	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
3	718	A	1101	-	-	0/0/10/10	0/2/2/2
5	SAL	B	701	-	-	0/0/4/4	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	718	C4-C10	2.10	1.51	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	701	SAL	C6-C1-C1'	-2.07	117.05	120.23

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	1051/1096 (95%)	0.31	57 (5%) 26 25	59, 104, 169, 235	0
2	B	252/279 (90%)	0.87	44 (17%) 2 1	95, 162, 206, 231	0
All	All	1303/1375 (94%)	0.42	101 (7%) 14 13	59, 112, 191, 235	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	335	TRP	8.0
1	A	872	PHE	6.7
1	A	523	LEU	5.3
1	A	351	ILE	5.1
1	A	869	ALA	4.7
2	B	409	ARG	4.7
1	A	868	GLY	4.6
1	A	-26	SER	4.6
2	B	432	GLN	4.4
2	B	405	ILE	4.2
2	B	425	LEU	4.1
1	A	947	TYR	4.0
2	B	424	LEU	4.0
2	B	429	SER	4.0
1	A	322	THR	4.0
1	A	341	ALA	3.9
1	A	354	ILE	3.7
2	B	433	GLN	3.7
2	B	580	TYR	3.7
2	B	435	GLN	3.6
2	B	434	ASP	3.6
1	A	300	ASP	3.5
2	B	332	GLU	3.5
2	B	412	SER	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	328	LEU	3.5
1	A	381	PRO	3.4
1	A	358	THR	3.4
2	B	423	LYS	3.4
1	A	1	MET	3.3
1	A	375	ARG	3.3
1	A	409	VAL	3.2
1	A	355	TYR	3.2
1	A	346	VAL	3.1
1	A	1052	THR	3.0
2	B	510	GLU	3.0
1	A	107	ASN	3.0
1	A	1050	GLY	3.0
1	A	353	LYS	3.0
2	B	376	GLY	3.0
1	A	1036	LEU	2.9
2	B	398	PHE	2.9
1	A	407	CYS	2.9
1	A	867	LYS	2.9
1	A	63	GLN	2.8
2	B	355	PHE	2.8
2	B	437	VAL	2.8
2	B	333	TRP	2.7
1	A	374	GLN	2.7
1	A	308	SER	2.7
2	B	508	TYR	2.7
2	B	411	GLU	2.6
1	A	83	PHE	2.6
2	B	390	TYR	2.6
2	B	436	VAL	2.5
1	A	408	SER	2.5
2	B	329	GLN	2.5
1	A	870	LEU	2.5
1	A	973	LYS	2.5
2	B	397	THR	2.5
1	A	106	GLY	2.5
2	B	399	SER	2.5
2	B	505	SER	2.5
2	B	504	TYR	2.4
2	B	503	ARG	2.4
2	B	410	ASN	2.4
2	B	401	VAL	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	343	TYR	2.4
1	A	1051	TRP	2.4
1	A	945	PHE	2.4
1	A	378	CYS	2.4
1	A	345	ASN	2.4
1	A	61	LEU	2.4
2	B	440	ASP	2.3
1	A	673	SER	2.3
1	A	522	GLU	2.3
2	B	331	ALA	2.3
2	B	559	ILE	2.3
2	B	368	TYR	2.3
1	A	873	ASN	2.3
1	A	423	ALA	2.3
1	A	388	ASN	2.2
1	A	557	TYR	2.2
1	A	1009	GLY	2.2
2	B	573	LEU	2.2
1	A	419	HIS	2.2
2	B	590	ARG	2.1
2	B	407	HIS	2.1
1	A	971	CYS	2.1
1	A	105	VAL	2.1
1	A	50	PHE	2.1
1	A	473	LEU	2.1
2	B	356	LEU	2.1
2	B	584	LEU	2.1
2	B	387	ASP	2.1
1	A	422	LEU	2.0
1	A	6	SER	2.0
1	A	972	THR	2.0
2	B	388	GLY	2.0
1	A	108	ARG	2.0
1	A	242	CYS	2.0
1	A	-13	PRO	2.0

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

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( $\text{\AA}^2$ )	Q<0.9
1	SEP	A	7	10/11	0.71	0.24	-	163,180,207,229	0
1	SEP	A	790	10/11	0.93	0.18	-	80,93,164,166	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( $\text{\AA}^2$ )	Q<0.9
4	CL	A	1102	1/1	0.96	0.35	5.63	80,80,80,80	0
5	SAL	B	701	10/10	0.83	0.84	5.19	146,156,166,172	0
4	CL	A	1103	1/1	0.79	0.93	-	93,93,93,93	0
3	718	A	1101	12/12	0.77	0.32	-	135,160,163,163	0

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

There are no such residues in this entry.