



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2017 – 09:57 AM EST

PDB ID : 5S XK
Title : Crystal Structure of PI3Kalpha in complex with fragment 18
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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

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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

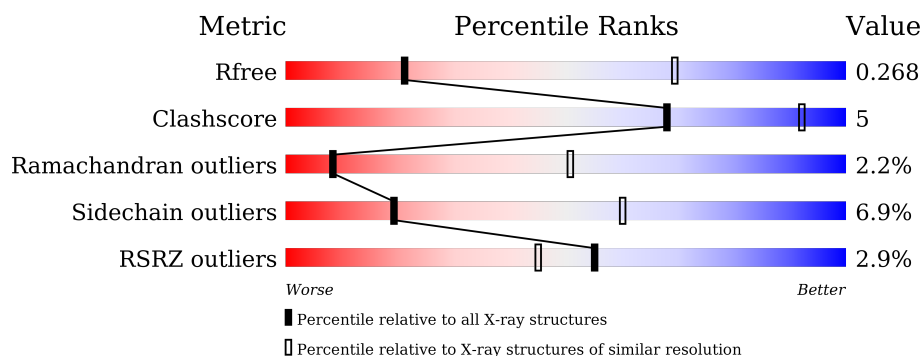
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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}	91344	1240 (3.72-3.40)
Clashscore	102246	1057 (3.70-3.42)
Ramachandran outliers	100387	1017 (3.70-3.42)
Sidechain outliers	100360	1017 (3.70-3.42)
RSRZ outliers	91569	1247 (3.72-3.40)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1096	<div> <div>10%</div> <div>77%</div> <div>18%</div> <div>• •</div> </div>
2	B	279	<div> <div>10%</div> <div>77%</div> <div>14%</div> <div>• 8%</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
3	71K	B	701	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10810 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	1054	Total	C	N	O	P	S	0	0	0
			8615	5503	1474	1567	1	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

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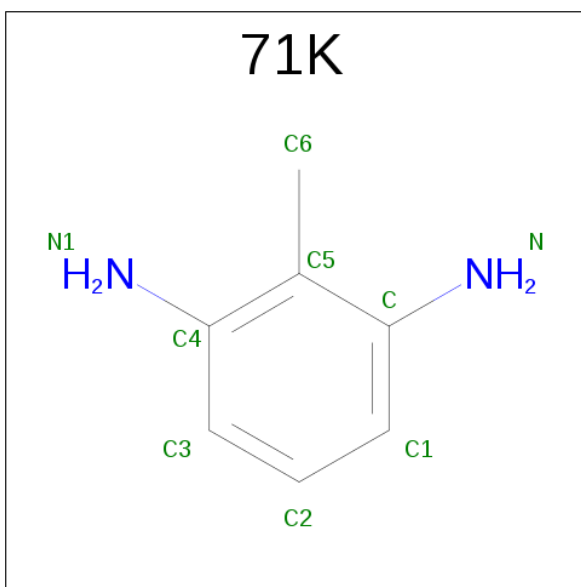
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42336
A	0	SER	-	expression tag	UNP P42336

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	257	Total	C	N	O	S	0	0	0
			2186	1371	389	420	6			

- Molecule 3 is 2-methylbenzene-1,3-diamine (three-letter code: 71K) (formula: C₇H₁₀N₂).

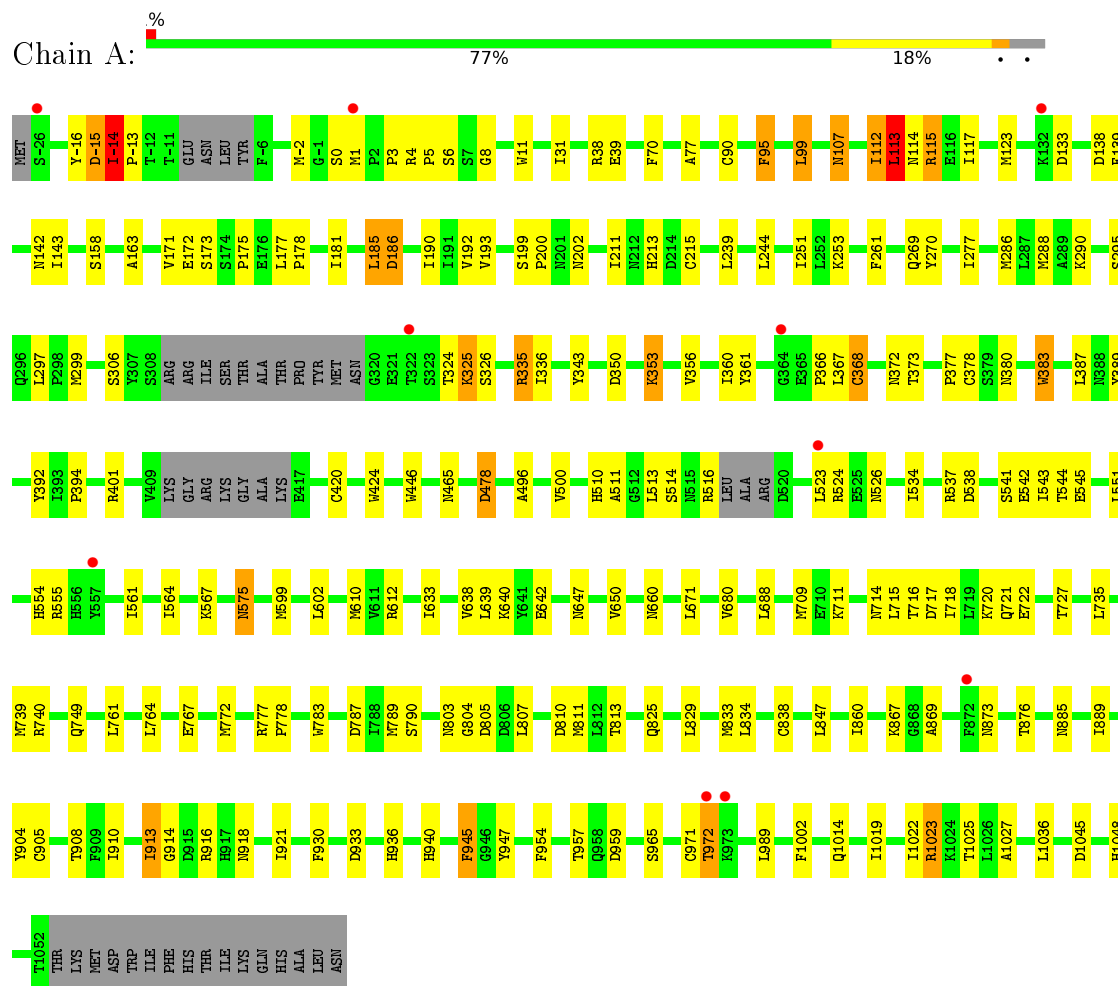


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	N	0	0
			9	7	2		

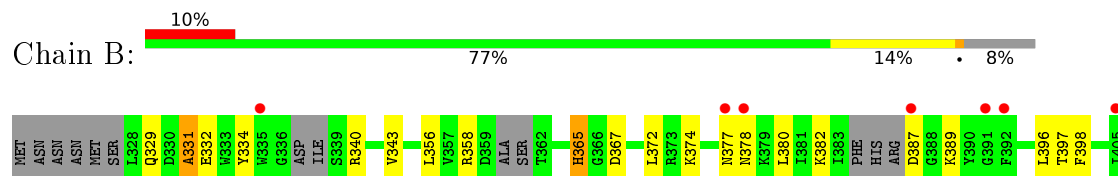
3 Residue-property plots

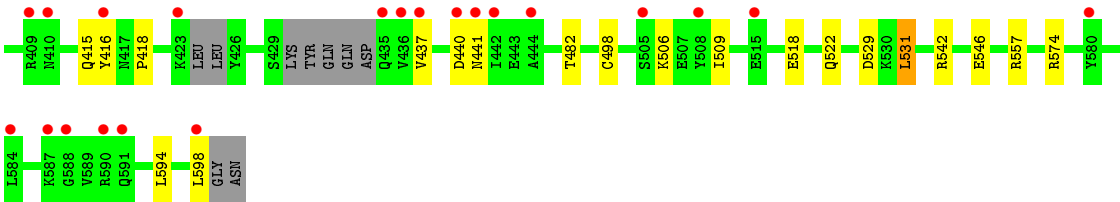
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform



- Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.28Å 115.84Å 149.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.45 – 3.55 36.55 – 3.55	Depositor EDS
% Data completeness (in resolution range)	99.3 (91.45-3.55) 99.5 (36.55-3.55)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 3.56Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.193 , 0.278 0.195 , 0.268	Depositor DCC
R_{free} test set	1238 reflections (5.41%)	DCC
Wilson B-factor (Å ²)	119.4	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 91.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10810	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 71K, 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	0/8805	0.79	6/11900 (0.1%)
2	B	0.51	0/2218	0.74	0/2963
All	All	0.53	0/11023	0.78	6/14863 (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	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	LEU	CA-CB-CG	5.48	127.91	115.30
1	A	1023	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	599	MET	CG-SD-CE	-5.23	91.83	100.20
1	A	555	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	777	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	115	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	ILE	Peptide
1	A	113	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	A	511	ALA	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	8615	0	8573	93	0
2	B	2186	0	2166	14	0
3	B	9	0	0	0	0
All	All	10810	0	10739	101	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 5.

All (101) 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:602:LEU:O	1:A:612:ARG:NH2	2.16	0.78
1:A:367:LEU:HD12	1:A:368:CYS:O	1.93	0.69
2:B:343:VAL:HG13	2:B:356:LEU:HD11	1.78	0.65
1:A:261:PHE:HA	1:A:270:TYR:CE2	2.32	0.65
1:A:735:LEU:O	1:A:739:MET:HG3	1.98	0.64
1:A:873:ASN:HB3	1:A:876:THR:HG23	1.81	0.63
1:A:936:HIS:HB3	1:A:940:HIS:HB3	1.83	0.60
1:A:163:ALA:HB2	1:A:297:LEU:HD11	1.84	0.60
1:A:336:ILE:HD12	1:A:389:TYR:CE2	2.37	0.60
2:B:331:ALA:HB3	2:B:334:TYR:HB3	1.84	0.60
1:A:561:ILE:O	1:A:564:ILE:HG22	2.01	0.59
1:A:192:VAL:HG21	1:A:211:ILE:HD11	1.84	0.59
1:A:772:MET:HB2	1:A:778:PRO:HG2	1.85	0.59
1:A:178:PRO:HD2	1:A:181:ILE:HD12	1.86	0.57
1:A:749:GLN:HE21	1:A:764:LEU:H	1.52	0.56
1:A:31:ILE:HD11	2:B:531:LEU:HD13	1.87	0.56
1:A:1022:ILE:HA	1:A:1025:THR:HG22	1.88	0.55
1:A:1:MET:HB2	1:A:720:LYS:CE	2.38	0.54
1:A:761:LEU:CD2	1:A:783:TRP:CD2	2.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:THR:HG21	2:B:382:LYS:HG2	1.90	0.54
1:A:8:GLY:CA	1:A:714:ASN:HD21	2.21	0.53
1:A:945:PHE:HB2	2:B:598:LEU:HD13	1.91	0.53
1:A:718:ILE:O	1:A:721:GLN:O	2.26	0.53
2:B:506:LYS:HA	2:B:509:ILE:HG22	1.90	0.52
1:A:833:MET:HE1	1:A:904:TYR:HA	1.91	0.52
1:A:671:LEU:HB2	1:A:688:LEU:HD21	1.91	0.52
1:A:789:MET:O	1:A:790:SEP:C	2.57	0.52
2:B:372:LEU:HD13	2:B:374:LYS:HE3	1.91	0.51
1:A:343:TYR:OH	2:B:557:ARG:NH1	2.43	0.51
1:A:181:ILE:HG23	1:A:277:ILE:HG21	1.92	0.51
1:A:805:ASP:O	1:A:807:LEU:HD22	2.10	0.51
1:A:446:TRP:CZ2	1:A:465:ASN:HA	2.47	0.50
1:A:761:LEU:CD2	1:A:783:TRP:CE3	2.95	0.49
1:A:114:ASN:HA	1:A:117:ILE:HD12	1.94	0.49
1:A:885:ASN:HB3	1:A:889:ILE:HG22	1.93	0.49
1:A:715:LEU:HD21	1:A:735:LEU:HD12	1.94	0.49
1:A:335:ARG:NE	1:A:478:ASP:OD2	2.44	0.49
1:A:-16:TYR:CE1	1:A:-14:ILE:HG23	2.47	0.48
1:A:761:LEU:HD22	1:A:783:TRP:CD2	2.49	0.48
1:A:496:ALA:O	1:A:500:VAL:HG23	2.13	0.48
1:A:639:LEU:HD22	1:A:650:VAL:HG22	1.95	0.48
1:A:575:ASN:C	1:A:575:ASN:HD22	2.17	0.48
1:A:251:ILE:HG23	1:A:290:LYS:HE3	1.94	0.48
1:A:908:THR:HG21	1:A:954:PHE:HB2	1.94	0.48
1:A:523:LEU:HD13	1:A:554:HIS:HD2	1.80	0.47
1:A:709:MET:CE	1:A:847:LEU:HD21	2.44	0.47
1:A:640:LYS:HE2	1:A:680:VAL:HG11	1.96	0.47
1:A:910:ILE:O	1:A:1025:THR:HG21	2.15	0.47
1:A:807:LEU:HD12	1:A:838:CYS:SG	2.55	0.47
1:A:372:ASN:HB3	1:A:387:LEU:HD21	1.96	0.46
1:A:660:ASN:OD1	1:A:660:ASN:C	2.53	0.46
1:A:1002:PHE:HB3	1:A:1019:ILE:HG12	1.97	0.46
1:A:356:VAL:HG23	1:A:383:TRP:CH2	2.51	0.46
1:A:171:VAL:HG12	1:A:172:GLU:O	2.16	0.45
1:A:717:ASP:OD1	1:A:803:ASN:ND2	2.49	0.45
1:A:945:PHE:CB	2:B:598:LEU:HD13	2.45	0.45
1:A:761:LEU:HD23	1:A:783:TRP:CD2	2.52	0.45
1:A:353:LYS:HA	1:A:377:PRO:HB2	1.99	0.45
1:A:171:VAL:HG13	1:A:269:GLN:HG2	2.00	0.44
1:A:186:ASP:OD1	1:A:186:ASP:O	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ILE:N	1:A:360:ILE:HD12	2.32	0.44
1:A:113:LEU:HD13	1:A:113:LEU:N	2.32	0.44
1:A:543:ILE:HD11	1:A:567:LYS:HD3	1.98	0.44
1:A:424:TRP:CE2	1:A:446:TRP:HB2	2.53	0.44
1:A:8:GLY:HA2	1:A:714:ASN:HD21	1.82	0.44
1:A:537:ARG:HB3	1:A:541:SER:OG	2.18	0.43
1:A:70:PHE:CE1	1:A:99:LEU:HD23	2.53	0.43
1:A:251:ILE:HG23	1:A:290:LYS:CE	2.49	0.43
1:A:392:TYR:HB3	1:A:394:PRO:HD2	2.00	0.43
1:A:709:MET:HE1	1:A:847:LEU:HD21	2.00	0.43
1:A:716:THR:O	1:A:717:ASP:C	2.56	0.43
2:B:542:ARG:NH1	2:B:546:GLU:OE2	2.51	0.43
1:A:138:ASP:O	1:A:142:ASN:ND2	2.51	0.43
1:A:913:ILE:HD12	1:A:914:GLY:O	2.19	0.43
1:A:524:ARG:HD3	1:A:526:ASN:HD22	1.83	0.43
1:A:324:THR:O	1:A:325:LYS:HB2	2.19	0.43
1:A:361:TYR:HA	1:A:366:PRO:HD3	2.00	0.43
1:A:8:GLY:HA3	1:A:714:ASN:HD21	1.84	0.42
1:A:916:ARG:HB3	1:A:921:ILE:HD11	2.01	0.42
1:A:610:MET:CE	1:A:610:MET:HA	2.50	0.42
1:A:-15:ASP:HB3	1:A:-13:PRO:HD2	2.01	0.42
1:A:715:LEU:HA	1:A:718:ILE:HD12	2.01	0.42
1:A:1023:ARG:O	1:A:1027:ALA:N	2.53	0.42
2:B:396:LEU:O	2:B:398:PHE:N	2.51	0.42
1:A:904:TYR:CE2	1:A:930:PHE:HA	2.55	0.42
1:A:192:VAL:HG12	1:A:193:VAL:N	2.34	0.41
1:A:253:LYS:HB3	1:A:286:MET:HB3	2.02	0.41
1:A:0:SER:O	1:A:1:MET:HG2	2.20	0.41
1:A:810:ASP:HA	1:A:813:THR:HG22	2.03	0.41
2:B:389:LYS:HB3	2:B:396:LEU:O	2.20	0.41
2:B:518:GLU:O	2:B:522:GLN:HB3	2.21	0.41
1:A:139:PHE:CE1	1:A:143:ILE:HD13	2.56	0.41
1:A:523:LEU:HD22	1:A:554:HIS:CD2	2.55	0.41
1:A:534:ILE:HG21	1:A:551:LEU:HD11	2.03	0.41
1:A:1048:HIS:CG	1:A:1048:HIS:O	2.74	0.41
1:A:3:PRO:CG	1:A:804:GLY:HA2	2.51	0.41
1:A:542:GLU:HG3	2:B:380:LEU:HD13	2.02	0.40
1:A:11:TRP:HB2	1:A:95:PHE:CD1	2.57	0.40
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.41	0.40
1:A:989:LEU:HD11	1:A:1036:LEU:HD11	2.02	0.40
1:A:-14:ILE:N	1:A:-13:PRO:CD	2.85	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%)	909 (87%)	113 (11%)	21 (2%)	9	53
2	B	245/279 (88%)	216 (88%)	22 (9%)	7 (3%)	6	44
All	All	1288/1375 (94%)	1125 (87%)	135 (10%)	28 (2%)	8	51

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	A	514	SER
1	A	945	PHE
1	A	77	ALA
1	A	325	LYS
1	A	869	ALA
1	A	918	ASN
1	A	972	THR
2	B	331	ALA
2	B	332	GLU
2	B	365	HIS
1	A	947	TYR
2	B	397	THR
2	B	418	PRO
1	A	95	PHE
1	A	186	ASP
1	A	378	CYS
1	A	933	ASP
2	B	340	ARG
1	A	107	ASN
1	A	133	ASP
1	A	957	THR

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Mol	Chain	Res	Type
1	A	913	ILE
1	A	-14	ILE
1	A	175	PRO
2	B	437	VAL
1	A	5	PRO
1	A	200	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	962/998 (96%)	896 (93%)	66 (7%)	19	60
2	B	239/259 (92%)	222 (93%)	17 (7%)	18	59
All	All	1201/1257 (96%)	1118 (93%)	83 (7%)	19	60

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-15	ASP
1	A	-14	ILE
1	A	-2	MET
1	A	4	ARG
1	A	6	SER
1	A	38	ARG
1	A	39	GLU
1	A	90	CYS
1	A	99	LEU
1	A	107	ASN
1	A	112	ILE
1	A	113	LEU
1	A	115	ARG
1	A	123	MET
1	A	158	SER
1	A	173	SER
1	A	177	LEU

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Mol	Chain	Res	Type
1	A	185	LEU
1	A	190	ILE
1	A	199	SER
1	A	213	HIS
1	A	215	CYS
1	A	239	LEU
1	A	244	LEU
1	A	288	MET
1	A	295	SER
1	A	299	MET
1	A	306	SER
1	A	326	SER
1	A	335	ARG
1	A	350	ASP
1	A	353	LYS
1	A	368	CYS
1	A	373	THR
1	A	380	ASN
1	A	383	TRP
1	A	401	ARG
1	A	420	CYS
1	A	478	ASP
1	A	510	HIS
1	A	513	LEU
1	A	516	ARG
1	A	538	ASP
1	A	545	GLU
1	A	575	ASN
1	A	633	ILE
1	A	638	VAL
1	A	711	LYS
1	A	722	GLU
1	A	727	THR
1	A	740	ARG
1	A	767	GLU
1	A	787	ASP
1	A	811	MET
1	A	825	GLN
1	A	829	LEU
1	A	834	LEU
1	A	860	ILE
1	A	867	LYS

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Mol	Chain	Res	Type
1	A	905	CYS
1	A	959	ASP
1	A	965	SER
1	A	971	CYS
1	A	972	THR
1	A	1014	GLN
1	A	1045	ASP
2	B	329	GLN
2	B	358	ARG
2	B	365	HIS
2	B	367	ASP
2	B	377	ASN
2	B	378	ASN
2	B	387	ASP
2	B	415	GLN
2	B	416	TYR
2	B	440	ASP
2	B	441	ASN
2	B	482	THR
2	B	498	CYS
2	B	529	ASP
2	B	531	LEU
2	B	574	ARG
2	B	594	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-21	HIS
1	A	142	ASN
1	A	202	ASN
1	A	331	ASN
1	A	374	GLN
1	A	380	ASN
1	A	444	ASN
1	A	521	ASN
1	A	526	ASN
1	A	575	ASN
1	A	647	ASN
1	A	714	ASN
1	A	749	GLN
1	A	878	HIS

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Mol	Chain	Res	Type
1	A	885	ASN
1	A	917	HIS
1	A	996	ASN
1	A	1014	GLN
2	B	329	GLN
2	B	377	ASN
2	B	406	ASN
2	B	517	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SEP	A	790	1	7,9,10	0.61	0	8,12,14	2.01	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	-	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	O2P-P-OG	-2.39	99.75	106.72
1	A	790	SEP	O3P-P-O2P	2.29	115.83	107.44
1	A	790	SEP	OG-CB-CA	4.05	111.79	108.26

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](#)

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	71K	B	701	-	9,9,9	1.64	2 (22%)	7,12,12	0.69	0

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	71K	B	701	-	-	0/0/0/0	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	71K	C-C5	3.30	1.51	1.39
3	B	701	71K	C4-C5	3.37	1.51	1.39

There are no bond angle outliers.

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, 95th 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 ²)	Q<0.9
1	A	1053/1096 (96%)	-0.30	10 (0%) 85 79	74, 126, 190, 251	0
2	B	257/279 (92%)	0.45	28 (10%) 7 7	119, 188, 230, 282	0
All	All	1310/1375 (95%)	-0.15	38 (2%) 55 45	74, 132, 211, 282	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	409	ARG	4.5
2	B	423	LYS	4.4
2	B	378	ASN	4.3
1	A	1	MET	3.6
1	A	322	THR	3.6
1	A	523	LEU	3.5
2	B	587	LYS	3.5
1	A	872	PHE	3.4
2	B	436	VAL	3.4
2	B	437	VAL	3.3
2	B	391	GLY	3.3
2	B	335	TRP	3.1
1	A	132	LYS	3.0
2	B	580	TYR	3.0
2	B	387	ASP	2.9
2	B	590	ARG	2.8
2	B	392	PHE	2.7
2	B	435	GLN	2.7
2	B	377	ASN	2.7
2	B	515	GLU	2.7
1	A	-26	SER	2.5
1	A	557	TYR	2.5
2	B	405	ILE	2.4
2	B	598	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	508	TYR	2.4
1	A	364	GLY	2.3
1	A	972	THR	2.3
2	B	584	LEU	2.3
2	B	440	ASP	2.3
2	B	410	ASN	2.3
2	B	588	GLY	2.3
2	B	505	SER	2.2
2	B	444	ALA	2.2
2	B	416	TYR	2.2
2	B	441	ASN	2.1
1	A	973	LYS	2.1
2	B	442	ILE	2.1
2	B	591	GLN	2.1

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, 95th 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 ²)	Q<0.9
1	SEP	A	790	10/11	0.92	0.12	-	111,129,186,189	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, 95th 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(\AA^2)	Q<0.9
3	71K	B	701	9/9	0.87	1.15	3.50	137,144,156,156	0

6.5 Other polymers ⓘ

There are no such residues in this entry.