



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2017 – 09:12 PM EDT

PDB ID : 5SXI
Title : Crystal Structure of PI3Kalpha in complex with fragment 13
Authors : Gabelli, S.B.; Vogelstein, B.; Miller, M.S.; Amzel, L.M.
Deposited on : unknown
Resolution : 3.40 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 : 1.7.2 (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

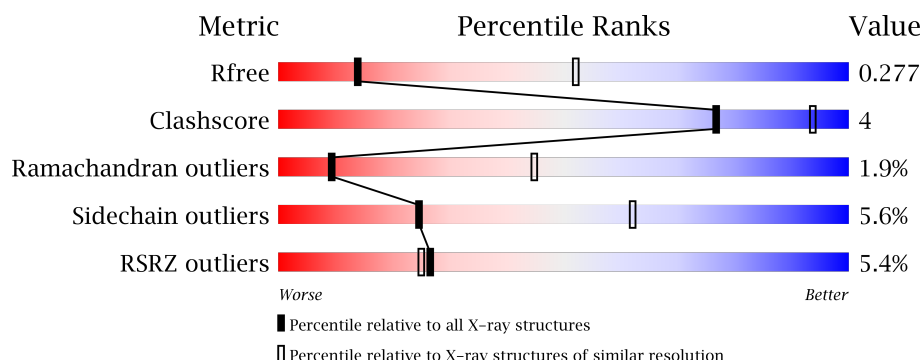
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

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	
2	B	279	

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	71J	B	701	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10360 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	1042	Total	C	N	O	P	S	0	0	0
			8534	5448	1462	1553	2	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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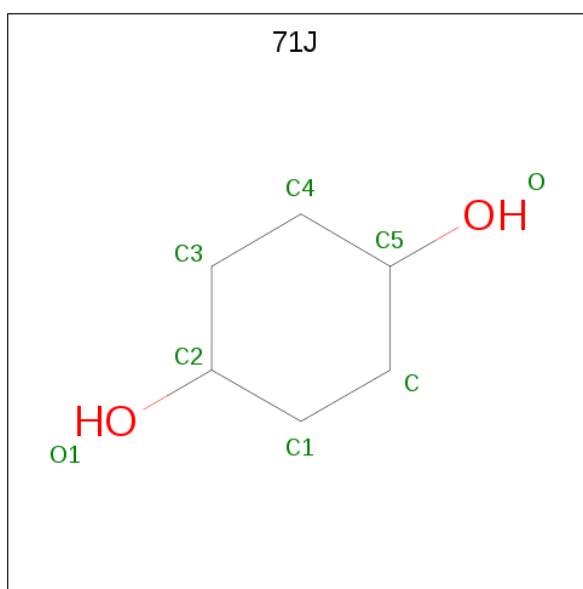
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42336
A	0	SER	-	expression tag	UNP P42336

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	209	Total	C	N	O	S	0	0	0
			1818	1142	324	346	6			

- Molecule 3 is trans-cyclohexane-1,4-diol (three-letter code: 71J) (formula: C₆H₁₂O₂).

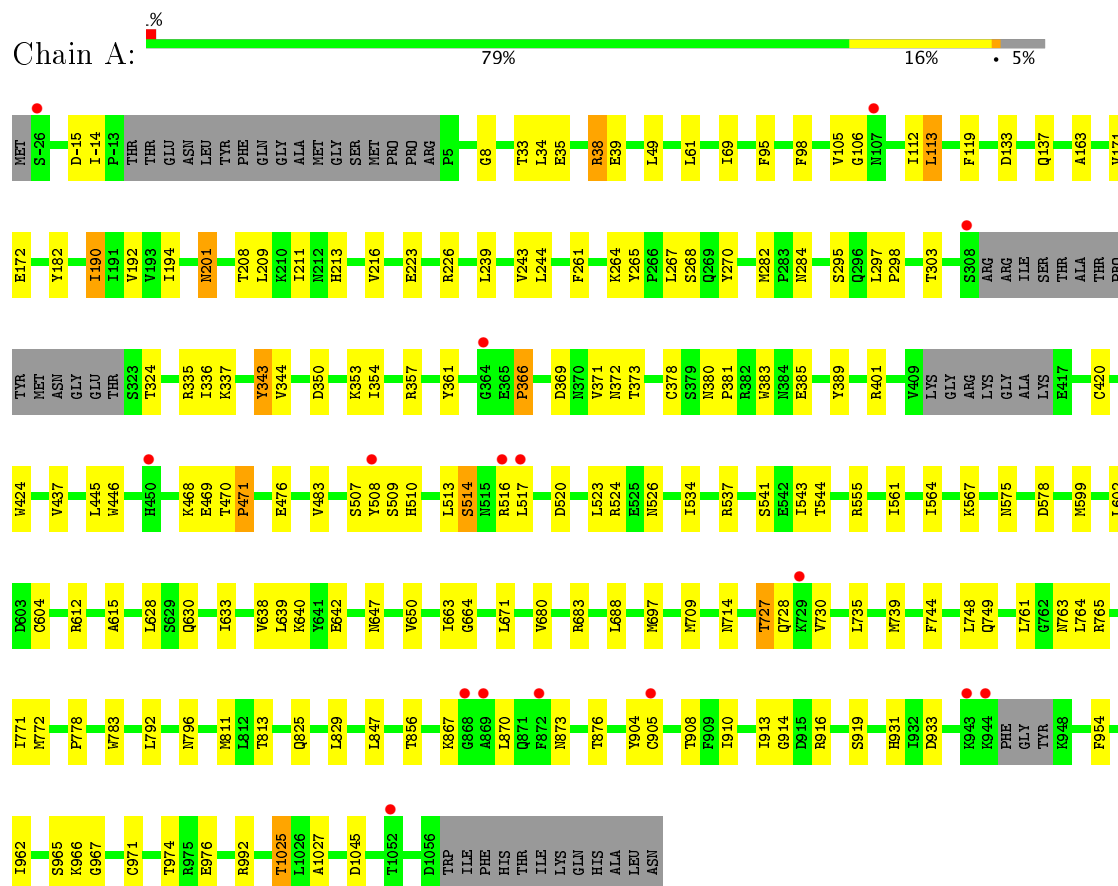


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			8	6	2		

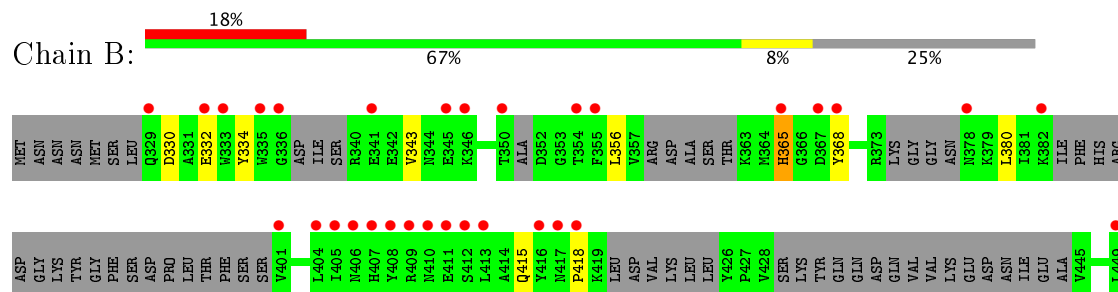
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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, α , β , γ	114.16Å 116.77Å 150.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.27 – 3.40 34.57 – 3.38	Depositor EDS
% Data completeness (in resolution range)	98.4 (92.27-3.40) 97.9 (34.57-3.38)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.39Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.201 , 0.279 0.202 , 0.277	Depositor DCC
R_{free} test set	1428 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	110.8	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 81.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10360	wwPDB-VP
Average B, all atoms (Å ²)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 71J, 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	0.53	0/8708	0.77	2/11765 (0.0%)
2	B	0.50	0/1843	0.67	0/2457
All	All	0.53	0/10551	0.76	2/14222 (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	829	LEU	CA-CB-CG	5.47	127.88	115.30
1	A	599	MET	CG-SD-CE	-5.12	92.01	100.20

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	8534	0	8503	70	0
2	B	1818	0	1786	6	0
3	B	8	0	0	0	0
All	All	10360	0	10289	73	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 (73) 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:639:LEU:HD22	1:A:650:VAL:HG22	1.74	0.70
1:A:8:GLY:HA2	1:A:714:ASN:HD21	1.58	0.68
1:A:908:THR:OG1	1:A:916:ARG:NH2	2.25	0.68
2:B:343:VAL:HG13	2:B:356:LEU:HD11	1.75	0.67
1:A:544:THR:HG22	2:B:380:LEU:HB3	1.78	0.66
1:A:192:VAL:HG21	1:A:211:ILE:HD11	1.79	0.65
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.17	0.64
1:A:561:ILE:O	1:A:564:ILE:HG22	2.01	0.60
1:A:735:LEU:O	1:A:739:MET:HG3	2.04	0.58
1:A:749:GLN:HE21	1:A:764:LEU:H	1.50	0.58
1:A:910:ILE:O	1:A:1025:THR:HG21	2.05	0.57
1:A:962:ILE:O	1:A:965:SER:O	2.23	0.55
1:A:772:MET:HB2	1:A:778:PRO:HG2	1.88	0.55
1:A:354:ILE:HD11	1:A:381:PRO:HB3	1.89	0.54
1:A:873:ASN:HB3	1:A:876:THR:HG23	1.88	0.54
1:A:424:TRP:CE2	1:A:446:TRP:HB2	2.42	0.54
1:A:354:ILE:HD11	1:A:381:PRO:CB	2.37	0.54
1:A:709:MET:CE	1:A:847:LEU:HD21	2.38	0.53
1:A:61:LEU:HD11	2:B:508:TYR:CZ	2.43	0.53
1:A:640:LYS:HE2	1:A:680:VAL:HG11	1.89	0.53
1:A:709:MET:HE1	1:A:847:LEU:HD21	1.91	0.53
1:A:468:LYS:O	1:A:470:THR:N	2.43	0.52
1:A:8:GLY:CA	1:A:714:ASN:HD21	2.22	0.52
1:A:916:ARG:NH2	1:A:931:HIS:CD2	2.78	0.51
1:A:534:ILE:HA	1:A:537:ARG:HD3	1.92	0.51
1:A:744:PHE:HD2	1:A:748:LEU:HD12	1.76	0.51
1:A:357:ARG:HA	1:A:371:VAL:HG12	1.93	0.51
1:A:324:THR:HG22	1:A:483:VAL:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ILE:HD11	1:A:213:HIS:HA	1.93	0.50
1:A:194:ILE:HD12	1:A:194:ILE:N	2.26	0.49
1:A:98:PHE:CE1	2:B:490:THR:HG23	2.47	0.48
1:A:543:ILE:HD11	1:A:567:LYS:HD3	1.94	0.47
1:A:372:ASN:HB2	1:A:385:GLU:CD	2.34	0.47
1:A:209:LEU:HD13	1:A:223:GLU:HB3	1.97	0.47
1:A:343:TYR:O	1:A:344:VAL:HG23	2.13	0.47
1:A:771:ILE:HG22	1:A:772:MET:O	2.14	0.47
1:A:445:LEU:HG	1:A:471:PRO:O	2.16	0.46
1:A:361:TYR:HA	1:A:366:PRO:HD3	1.97	0.46
2:B:334:TYR:HH	2:B:368:TYR:HE1	1.61	0.46
1:A:171:VAL:HG12	1:A:172:GLU:O	2.16	0.46
1:A:913:ILE:HD12	1:A:914:GLY:N	2.31	0.45
1:A:749:GLN:O	1:A:761:LEU:O	2.36	0.44
1:A:765:ARG:HD3	1:A:796:ASN:HD21	1.81	0.44
2:B:506:LYS:HA	2:B:509:ILE:HG22	2.00	0.44
1:A:727:THR:O	1:A:728:GLN:C	2.56	0.43
1:A:663:ILE:O	1:A:664:GLY:C	2.56	0.43
1:A:764:LEU:HD23	1:A:783:TRP:CD1	2.52	0.43
1:A:282:MET:O	1:A:284:ASN:ND2	2.51	0.43
1:A:163:ALA:HA	1:A:297:LEU:HD11	2.00	0.43
1:A:171:VAL:HG11	1:A:265:TYR:CE1	2.54	0.43
1:A:965:SER:O	1:A:967:GLY:N	2.52	0.43
1:A:908:THR:HG21	1:A:954:PHE:HB2	2.00	0.42
1:A:34:LEU:HD11	1:A:49:LEU:HA	2.00	0.42
1:A:336:ILE:HD12	1:A:389:TYR:CE2	2.54	0.42
1:A:992:ARG:NH2	1:A:1027:ALA:O	2.44	0.42
1:A:261:PHE:HA	1:A:270:TYR:CE1	2.54	0.42
1:A:602:LEU:O	1:A:612:ARG:NH2	2.53	0.42
1:A:243:VAL:HG12	1:A:244:LEU:HD12	2.02	0.42
1:A:727:THR:O	1:A:730:VAL:N	2.53	0.42
1:A:105:VAL:HG13	1:A:106:GLY:N	2.34	0.42
1:A:602:LEU:HD21	1:A:615:ALA:HB3	2.00	0.42
1:A:965:SER:HB2	1:A:974:THR:HG21	2.01	0.42
1:A:337:LYS:HB3	1:A:476:GLU:HB3	2.02	0.41
1:A:524:ARG:HD3	1:A:526:ASN:HD22	1.85	0.41
1:A:628:LEU:HD23	1:A:663:ILE:HD13	2.01	0.41
1:A:671:LEU:HB2	1:A:688:LEU:HD21	2.01	0.41
1:A:904:TYR:CD1	1:A:931:HIS:CD2	3.08	0.41
1:A:749:GLN:HG2	1:A:763:ASN:HA	2.01	0.41
1:A:507:SER:O	1:A:509:SER:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:744:PHE:CD2	1:A:748:LEU:HD12	2.55	0.41
1:A:261:PHE:CD1	1:A:270:TYR:CD1	3.09	0.40
1:A:298:PRO:CG	1:A:697:MET:HG3	2.52	0.40
1:A:517:LEU:HD22	1:A:523:LEU:HD22	2.04	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	1030/1096 (94%)	912 (88%)	100 (10%)	18 (2%)	11	47
2	B	191/279 (68%)	176 (92%)	10 (5%)	5 (3%)	6	38
All	All	1221/1375 (89%)	1088 (89%)	110 (9%)	23 (2%)	9	45

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	508	TYR
2	B	332	GLU
1	A	264	LYS
1	A	378	CYS
1	A	555	ARG
2	B	365	HIS
1	A	514	SER
1	A	966	LYS
1	A	38	ARG
1	A	95	PHE
1	A	201	ASN
1	A	469	GLU
1	A	471	PRO
1	A	520	ASP

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Mol	Chain	Res	Type
1	A	541	SER
1	A	867	LYS
1	A	933	ASP
1	A	133	ASP
1	A	226	ARG
2	B	513	LYS
2	B	517	ASN
2	B	418	PRO
1	A	366	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	953/997 (96%)	897 (94%)	56 (6%)	23	60
2	B	198/259 (76%)	189 (96%)	9 (4%)	32	69
All	All	1151/1256 (92%)	1086 (94%)	65 (6%)	25	62

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-15	ASP
1	A	-14	ILE
1	A	33	THR
1	A	35	GLU
1	A	38	ARG
1	A	39	GLU
1	A	69	ILE
1	A	112	ILE
1	A	113	LEU
1	A	119	PHE
1	A	137	GLN
1	A	182	TYR
1	A	190	ILE
1	A	201	ASN

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Mol	Chain	Res	Type
1	A	208	THR
1	A	216	VAL
1	A	239	LEU
1	A	267	LEU
1	A	268	SER
1	A	295	SER
1	A	303	THR
1	A	335	ARG
1	A	343	TYR
1	A	350	ASP
1	A	353	LYS
1	A	369	ASP
1	A	373	THR
1	A	380	ASN
1	A	383	TRP
1	A	401	ARG
1	A	420	CYS
1	A	437	VAL
1	A	510	HIS
1	A	513	LEU
1	A	514	SER
1	A	516	ARG
1	A	575	ASN
1	A	578	ASP
1	A	604	CYS
1	A	630	GLN
1	A	633	ILE
1	A	638	VAL
1	A	683	ARG
1	A	727	THR
1	A	792	LEU
1	A	811	MET
1	A	813	THR
1	A	825	GLN
1	A	856	THR
1	A	870	LEU
1	A	905	CYS
1	A	919	SER
1	A	971	CYS
1	A	976	GLU
1	A	1025	THR
1	A	1045	ASP

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Mol	Chain	Res	Type
2	B	330	ASP
2	B	365	HIS
2	B	415	GLN
2	B	482	THR
2	B	501	GLN
2	B	531	LEU
2	B	536	SER
2	B	543	ARG
2	B	595	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
1	A	331	ASN
1	A	374	GLN
1	A	444	ASN
1	A	515	ASN
1	A	526	ASN
1	A	575	ASN
1	A	643	GLN
1	A	714	ASN
1	A	749	GLN
1	A	785	ASN
1	A	917	HIS
1	A	931	HIS
2	B	406	ASN
2	B	417	ASN
2	B	564	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	0.70	0	9,12,14	1.07	0
1	SEP	A	790	1	9,9,10	0.62	0	9,12,14	1.85	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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	790	SEP	OG-CB-CA	3.28	111.40	108.17
1	A	790	SEP	P-OG-CB	3.39	127.62	118.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	71J	B	701	-	8,8,8	0.67	0	10,10,10	1.20	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	71J	B	701	-	-	0/0/10/10	0/1/1/1

There are no bond length outliers.

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 ⓘ

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, 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	1040/1096 (94%)	-0.15	16 (1%) 74 69	70, 117, 180, 229	0
2	B	209/279 (74%)	0.98	51 (24%) 1 1	111, 182, 227, 296	0
All	All	1249/1375 (90%)	0.04	67 (5%) 26 25	70, 122, 207, 296	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	409	ARG	7.0
2	B	335	TRP	6.4
2	B	405	ILE	6.2
2	B	404	LEU	5.0
2	B	350	THR	4.9
2	B	410	ASN	4.8
2	B	449	LEU	4.7
2	B	412	SER	4.3
1	A	107	ASN	4.2
2	B	584	LEU	4.0
2	B	585	THR	3.8
2	B	333	TRP	3.7
2	B	416	TYR	3.6
1	A	905	CYS	3.6
2	B	595	ASN	3.6
2	B	406	ASN	3.5
2	B	408	TYR	3.5
2	B	407	HIS	3.4
1	A	450	HIS	3.3
2	B	510	GLU	3.3
1	A	-26	SER	3.3
1	A	868	GLY	3.3
2	B	332	GLU	3.3
2	B	450	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	512	PHE	3.2
2	B	580	TYR	3.1
1	A	1052	THR	3.1
2	B	411	GLU	3.1
2	B	598	LEU	3.0
2	B	341	GLU	3.0
2	B	417	ASN	3.0
2	B	401	VAL	3.0
1	A	944	LYS	2.9
2	B	581	LEU	2.8
1	A	943	LYS	2.8
1	A	516	ARG	2.7
2	B	577	ARG	2.6
2	B	378	ASN	2.6
2	B	596	GLU	2.5
2	B	345	GLU	2.5
2	B	413	LEU	2.4
1	A	308	SER	2.4
2	B	336	GLY	2.4
1	A	364	GLY	2.4
2	B	368	TYR	2.4
1	A	872	PHE	2.4
2	B	454	THR	2.4
2	B	355	PHE	2.3
2	B	354	THR	2.3
2	B	457	GLN	2.3
1	A	517	LEU	2.3
2	B	346	LYS	2.3
2	B	583	TRP	2.3
2	B	586	GLN	2.2
1	A	869	ALA	2.2
2	B	508	TYR	2.2
2	B	472	ARG	2.2
2	B	382	LYS	2.2
1	A	729	LYS	2.1
1	A	508	TYR	2.1
2	B	365	HIS	2.1
2	B	418	PRO	2.1
2	B	461	ARG	2.1
2	B	367	ASP	2.1
2	B	453	ASN	2.0
2	B	515	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	329	GLN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	0.93	0.12	-	92,105,192,197	0
1	SEP	A	7	10/11	0.75	0.22	-	140,161,200,217	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(Å ²)	Q<0.9
3	71J	B	701	8/8	0.69	0.99	7.50	156,176,178,178	0

6.5 Other polymers [i](#)

There are no such residues in this entry.