



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 09:17 am BST

PDB ID : 5SX8
Title : Crystal Structure of PI3Kalpha in complex with fragments 12 and 15
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Deposited on : 2016-08-09
Resolution : 3.47 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

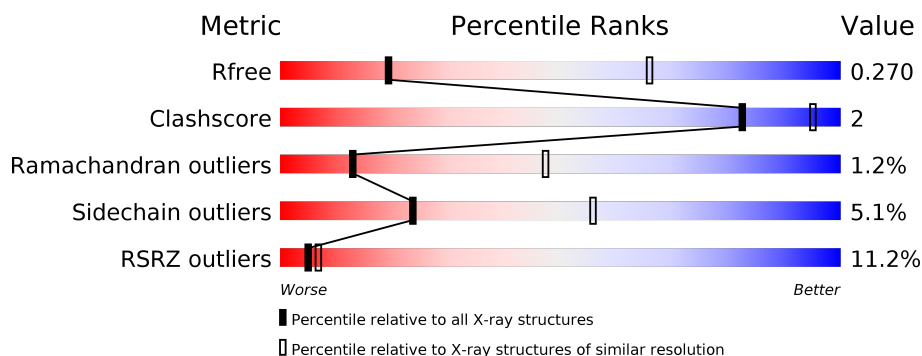
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.47 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	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	1096	<div> <div>9%</div> <div>84%</div> <div>11%</div> <div>• •</div> </div>
2	B	279	<div> <div>15%</div> <div>77%</div> <div>8%</div> <div>• 14%</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	LUZ	A	1102	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10695 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
			8608	5500	1477	1561	1	69			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP P42336
A	-26	SER	-	expression tag	UNP P42336
A	-25	TYR	-	expression tag	UNP P42336
A	-24	TYR	-	expression tag	UNP P42336
A	-23	HIS	-	expression tag	UNP P42336
A	-22	HIS	-	expression tag	UNP P42336
A	-21	HIS	-	expression tag	UNP P42336
A	-20	HIS	-	expression tag	UNP P42336
A	-19	HIS	-	expression tag	UNP P42336
A	-18	HIS	-	expression tag	UNP P42336
A	-17	ASP	-	expression tag	UNP P42336
A	-16	TYR	-	expression tag	UNP P42336
A	-15	ASP	-	expression tag	UNP P42336
A	-14	ILE	-	expression tag	UNP P42336
A	-13	PRO	-	expression tag	UNP P42336
A	-12	THR	-	expression tag	UNP P42336
A	-11	THR	-	expression tag	UNP P42336
A	-10	GLU	-	expression tag	UNP P42336
A	-9	ASN	-	expression tag	UNP P42336
A	-8	LEU	-	expression tag	UNP P42336
A	-7	TYR	-	expression tag	UNP P42336
A	-6	PHE	-	expression tag	UNP P42336
A	-5	GLN	-	expression tag	UNP P42336
A	-4	GLY	-	expression tag	UNP P42336
A	-3	ALA	-	expression tag	UNP P42336
A	-2	MET	-	expression tag	UNP P42336

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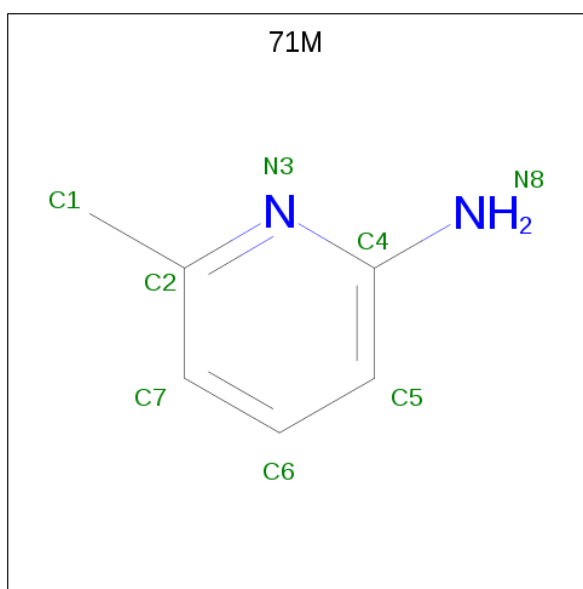
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42336
A	0	SER	-	expression tag	UNP P42336

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

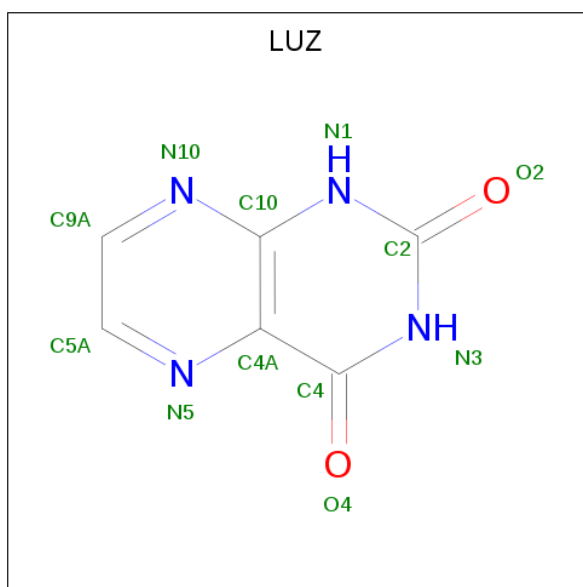
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	240	Total	C	N	O	S	0	0	0
			2059	1294	364	395	6			

- Molecule 3 is 6-methylpyridin-2-amine (three-letter code: 71M) (formula: C₆H₈N₂).



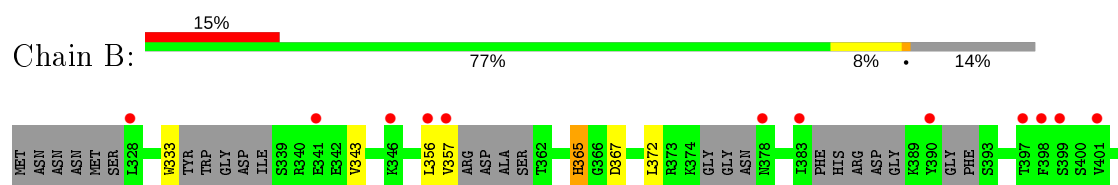
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			8	6	2		
3	B	1	Total	C	N	0	0
			8	6	2		

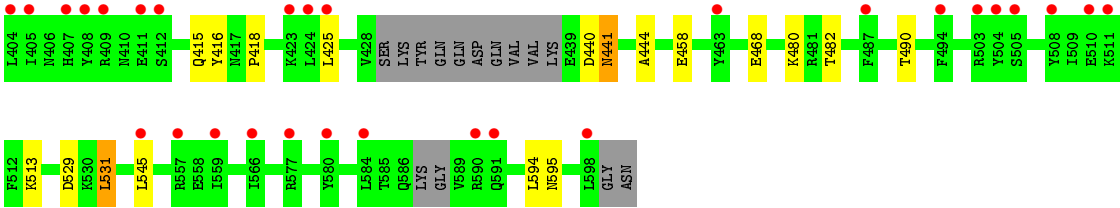
- Molecule 4 is pteridine-2,4(1H,3H)-dione (three-letter code: LUZ) (formula: C₆H₄N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	6	4	2		

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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.89Å 116.33Å 148.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.49 – 3.47 48.90 – 3.47	Depositor EDS
% Data completeness (in resolution range)	99.1 (91.49-3.47) 99.2 (48.90-3.47)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.207 , 0.276 0.208 , 0.270	Depositor DCC
R_{free} test set	1324 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	122.1	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 106.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10695	wwPDB-VP
Average B, all atoms (Å ²)	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: LUZ, 71M, 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	0.45	0/8797	0.68	0/11886
2	B	0.44	0/2085	0.62	0/2783
All	All	0.45	0/10882	0.67	0/14669

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	8608	0	8578	48	0
2	B	2059	0	2056	7	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
4	A	12	0	4	0	0
All	All	10695	0	10638	53	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 2.

All (53) 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:873:ASN:HB3	1:A:876:THR:HG23	1.73	0.70
1:A:628:LEU:HD23	1:A:663:ILE:HD13	1.78	0.65
2:B:333:TRP:HB3	2:B:357:VAL:HB	1.79	0.64
1:A:503:GLU:HA	1:A:506:PHE:CE1	2.34	0.63
1:A:503:GLU:HA	1:A:506:PHE:HE1	1.65	0.61
1:A:989:LEU:HD11	1:A:1036:LEU:HD11	1.85	0.56
1:A:324:THR:HG21	1:A:483:VAL:CG2	2.36	0.55
1:A:1000:ASN:O	1:A:1004:MET:HG3	2.06	0.54
1:A:602:LEU:O	1:A:612:ARG:NH2	2.41	0.53
1:A:261:PHE:HA	1:A:270:TYR:CE2	2.43	0.53
1:A:334:LEU:HA	1:A:393:ILE:HD11	1.89	0.53
1:A:255:CYS:SG	1:A:285:LEU:O	2.67	0.53
1:A:98:PHE:CE1	2:B:490:THR:HG23	2.45	0.52
1:A:772:MET:HB2	1:A:778:PRO:HG2	1.93	0.51
1:A:31:ILE:HD11	2:B:531:LEU:HD13	1.93	0.50
1:A:639:LEU:HD22	1:A:650:VAL:HG22	1.93	0.50
2:B:480:LYS:HG2	2:B:545:LEU:HD11	1.93	0.49
1:A:749:GLN:HE21	1:A:764:LEU:H	1.59	0.49
1:A:354:ILE:HD11	1:A:381:PRO:HB3	1.95	0.48
2:B:441:ASN:OD1	2:B:441:ASN:N	2.47	0.48
1:A:335:ARG:NE	1:A:478:ASP:OD2	2.43	0.47
1:A:561:ILE:O	1:A:564:ILE:HG22	2.14	0.47
1:A:163:ALA:HB2	1:A:297:LEU:HD11	1.97	0.47
1:A:833:MET:HE1	1:A:904:TYR:HA	1.97	0.46
1:A:60:GLN:HG2	1:A:61:LEU:HD12	1.96	0.46
1:A:353:LYS:HA	1:A:377:PRO:HB3	1.97	0.46
1:A:910:ILE:O	1:A:1025:THR:HG21	2.16	0.46
1:A:361:TYR:CE2	1:A:365:GLU:HB3	2.50	0.46
1:A:885:ASN:ND2	1:A:893:ALA:HB2	2.30	0.46
1:A:864:GLY:O	1:A:876:THR:HG21	2.16	0.45
2:B:441:ASN:HB2	2:B:444:ALA:HB3	1.97	0.45
1:A:84:ASP:OD1	1:A:86:THR:OG1	2.29	0.45
1:A:639:LEU:HD22	1:A:650:VAL:CG2	2.47	0.44
1:A:924:LYS:HE3	1:A:928:GLN:HB3	2.00	0.44
1:A:524:ARG:HD3	1:A:526:ASN:HD22	1.82	0.43
1:A:936:HIS:HB3	1:A:940:HIS:HB3	2.01	0.43
1:A:641:TYR:OH	1:A:1007:GLY:N	2.52	0.43
1:A:906:VAL:HG12	1:A:910:ILE:HD12	2.01	0.43
1:A:709:MET:CE	1:A:847:LEU:HD21	2.49	0.42
1:A:360:ILE:N	1:A:360:ILE:HD12	2.34	0.42
1:A:324:THR:HG21	1:A:483:VAL:HG23	2.01	0.42
1:A:356:VAL:HG23	1:A:383:TRP:CH2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:LEU:HD22	1:A:783:TRP:CE3	2.55	0.41
1:A:11:TRP:HB2	1:A:95:PHE:CD1	2.55	0.41
1:A:956:LEU:HD11	1:A:980:PHE:CZ	2.55	0.41
2:B:343:VAL:HG13	2:B:356:LEU:HD11	2.02	0.41
1:A:221:ILE:HG23	1:A:287:LEU:HD21	2.02	0.41
1:A:855:HIS:HB2	1:A:860:ILE:CD1	2.51	0.41
1:A:117:ILE:HG22	1:A:121:ILE:CD1	2.51	0.41
1:A:178:PRO:HD2	1:A:181:ILE:HD12	2.02	0.41
1:A:810:ASP:HA	1:A:813:THR:HG22	2.03	0.41
1:A:602:LEU:HB3	1:A:638:VAL:HG11	2.03	0.41
1:A:807:LEU:HD12	1:A:838:CYS:SG	2.61	0.41

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	1040/1096 (95%)	935 (90%)	93 (9%)	12 (1%)	13	47
2	B	224/279 (80%)	210 (94%)	11 (5%)	3 (1%)	12	45
All	All	1264/1375 (92%)	1145 (91%)	104 (8%)	15 (1%)	13	47

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	LYS
1	A	555	ARG
2	B	365	HIS
1	A	38	ARG
1	A	186	ASP
1	A	511	ALA
1	A	869	ALA

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Mol	Chain	Res	Type
1	A	945	PHE
1	A	95	PHE
1	A	381	PRO
2	B	513	LYS
1	A	298	PRO
1	A	107	ASN
2	B	418	PRO
1	A	5	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	960/998 (96%)	914 (95%)	46 (5%)	25	58
2	B	228/259 (88%)	213 (93%)	15 (7%)	16	48
All	All	1188/1257 (94%)	1127 (95%)	61 (5%)	24	56

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-26	SER
1	A	-15	ASP
1	A	-14	ILE
1	A	22	VAL
1	A	38	ARG
1	A	39	GLU
1	A	69	ILE
1	A	99	LEU
1	A	112	ILE
1	A	113	LEU
1	A	115	ARG
1	A	158	SER
1	A	201	ASN
1	A	239	LEU
1	A	299	MET

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Mol	Chain	Res	Type
1	A	335	ARG
1	A	353	LYS
1	A	366	PRO
1	A	373	THR
1	A	376	VAL
1	A	383	TRP
1	A	420	CYS
1	A	455	LEU
1	A	475	LEU
1	A	499	SER
1	A	515	ASN
1	A	516	ARG
1	A	517	LEU
1	A	561	ILE
1	A	575	ASN
1	A	577	ARG
1	A	630	GLN
1	A	642	GLU
1	A	659	THR
1	A	683	ARG
1	A	711	LYS
1	A	727	THR
1	A	856	THR
1	A	867	LYS
1	A	874	SER
1	A	891	ASP
1	A	905	CYS
1	A	976	GLU
1	A	1025	THR
1	A	1045	ASP
1	A	1052	THR
2	B	365	HIS
2	B	367	ASP
2	B	372	LEU
2	B	415	GLN
2	B	416	TYR
2	B	425	LEU
2	B	440	ASP
2	B	441	ASN
2	B	458	GLU
2	B	468	GLU
2	B	482	THR

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Mol	Chain	Res	Type
2	B	529	ASP
2	B	531	LEU
2	B	594	LEU
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	202	ASN
1	A	331	ASN
1	A	347	ASN
1	A	374	GLN
1	A	467	ASN
1	A	526	ASN
1	A	575	ASN
1	A	643	GLN
1	A	749	GLN
1	A	759	HIS
1	A	861	GLN
2	B	344	ASN
2	B	378	ASN
2	B	527	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 ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SEP	A	790	1	8,9,10	0.62	0	8,12,14	1.89	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	790	1	-	4/5/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	790	SEP	OG-CB-CA	4.07	112.10	108.14
1	A	790	SEP	P-OG-CB	2.04	123.92	118.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	790	SEP	N-CA-CB-OG
1	A	790	SEP	CB-OG-P-O1P
1	A	790	SEP	CB-OG-P-O2P
1	A	790	SEP	CB-OG-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 ligands 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
3	71M	B	701	-	8,8,8	1.83	1 (12%)	10,10,10	1.22	1 (10%)
4	LUZ	A	1102	-	12,13,13	1.80	2 (16%)	11,18,18	3.20	6 (54%)
3	71M	A	1101	-	8,8,8	1.78	1 (12%)	10,10,10	1.22	1 (10%)

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	71M	B	701	-	-	-	0/1/1/1
4	LUZ	A	1102	-	-	-	0/2/2/2
3	71M	A	1101	-	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	71M	C4-N8	4.90	1.49	1.35
4	A	1102	LUZ	O4-C4	4.89	1.36	1.24
3	A	1101	71M	C4-N8	4.75	1.49	1.35
4	A	1102	LUZ	C4A-N5	2.25	1.36	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1102	LUZ	C4-N3-C2	6.70	120.80	115.14
4	A	1102	LUZ	N10-C10-N1	4.35	120.96	114.93
4	A	1102	LUZ	C9A-N10-C10	3.23	120.59	116.60
4	A	1102	LUZ	C4-C4A-N5	2.96	121.92	118.24
4	A	1102	LUZ	C4A-C4-N3	-2.81	119.59	123.43
4	A	1102	LUZ	C10-C4A-N5	-2.71	119.19	122.32
3	A	1101	71M	C1-C2-N3	2.07	119.86	116.56
3	B	701	71M	C1-C2-N3	2.05	119.84	116.56

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	1052/1096 (95%)	0.62	104 (9%) 7 9	79, 134, 198, 254	0
2	B	240/279 (86%)	1.00	41 (17%) 1 2	121, 192, 242, 264	0
All	All	1292/1375 (93%)	0.69	145 (11%) 5 7	79, 142, 217, 264	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	390	TYR	6.5
1	A	1054	LYS	6.2
1	A	947	TYR	5.9
1	A	374	GLN	5.4
1	A	419	HIS	5.2
1	A	346	VAL	5.2
2	B	378	ASN	5.1
1	A	-26	SER	5.0
2	B	401	VAL	4.9
1	A	347	ASN	4.9
2	B	357	VAL	4.8
1	A	1009	GLY	4.7
1	A	351	ILE	4.5
1	A	945	PHE	4.5
2	B	405	ILE	4.4
1	A	423	ALA	4.4
1	A	557	TYR	4.4
1	A	872	PHE	4.3
1	A	323	SER	4.3
2	B	508	TYR	4.2
1	A	345	ASN	4.2
1	A	806	ASP	4.1
1	A	810	ASP	4.1
2	B	424	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	322	THR	4.0
1	A	473	LEU	3.9
1	A	344	VAL	3.9
1	A	869	ALA	3.9
1	A	867	LYS	3.8
1	A	300	ASP	3.8
2	B	584	LEU	3.8
1	A	381	PRO	3.8
2	B	510	GLU	3.7
1	A	61	LEU	3.7
1	A	933	ASP	3.7
2	B	409	ARG	3.6
1	A	339	LEU	3.6
2	B	346	LYS	3.6
1	A	343	TYR	3.6
1	A	338	ILE	3.6
2	B	425	LEU	3.5
2	B	505	SER	3.5
1	A	809	GLN	3.5
2	B	504	TYR	3.4
2	B	580	TYR	3.4
1	A	353	LYS	3.4
2	B	399	SER	3.3
1	A	870	LEU	3.3
1	A	341	ALA	3.3
2	B	412	SER	3.3
1	A	358	THR	3.2
1	A	375	ARG	3.2
1	A	673	SER	3.2
1	A	441	MET	3.2
1	A	355	TYR	3.2
1	A	971	CYS	3.2
1	A	364	GLY	3.1
2	B	463	TYR	3.1
1	A	190	ILE	3.1
2	B	407	HIS	3.1
2	B	423	LYS	3.1
1	A	936	HIS	3.1
1	A	354	ILE	3.0
1	A	409	VAL	3.0
2	B	383	ILE	3.0
2	B	408	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	356	LEU	3.0
2	B	598	LEU	2.9
1	A	1014	GLN	2.9
1	A	1051	TRP	2.9
1	A	189	GLN	2.9
1	A	-1	GLY	2.9
1	A	-12	THR	2.8
1	A	209	LEU	2.8
1	A	837	GLY	2.8
1	A	408	SER	2.8
1	A	935	GLY	2.8
2	B	590	ARG	2.8
1	A	422	LEU	2.8
2	B	559	ILE	2.8
1	A	31	ILE	2.8
2	B	328	LEU	2.8
2	B	398	PHE	2.7
1	A	605	ASN	2.7
2	B	404	LEU	2.7
1	A	808	ARG	2.7
1	A	246	TYR	2.7
1	A	287	LEU	2.7
1	A	838	CYS	2.7
1	A	1053	THR	2.6
2	B	494	PHE	2.6
1	A	1007	GLY	2.6
2	B	397	THR	2.6
1	A	460	GLY	2.6
1	A	811	MET	2.6
2	B	577	ARG	2.6
1	A	677	ASN	2.6
1	A	868	GLY	2.6
1	A	363	GLY	2.5
1	A	1008	SER	2.5
2	B	411	GLU	2.5
2	B	503	ARG	2.5
1	A	350	ASP	2.5
1	A	679	THR	2.4
1	A	1015	SER	2.4
1	A	356	VAL	2.4
1	A	844	CYS	2.4
1	A	382	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	528	LYS	2.4
1	A	201	ASN	2.4
1	A	340	CYS	2.3
1	A	731	GLN	2.3
1	A	83	PHE	2.3
1	A	373	THR	2.3
1	A	630	GLN	2.3
1	A	81	GLU	2.3
1	A	187	LYS	2.3
1	A	147	CYS	2.2
1	A	383	TRP	2.2
1	A	972	THR	2.2
1	A	1011	PRO	2.2
1	A	212	ASN	2.2
1	A	215	CYS	2.2
1	A	1036	LEU	2.2
1	A	973	LYS	2.2
1	A	1052	THR	2.2
2	B	591	GLN	2.1
1	A	818	ARG	2.1
2	B	566	ILE	2.1
1	A	474	GLU	2.1
1	A	815	GLN	2.1
1	A	308	SER	2.1
1	A	842	GLY	2.1
2	B	557	ARG	2.1
2	B	487	PHE	2.1
1	A	840	SER	2.1
2	B	545	LEU	2.1
1	A	-14	ILE	2.0
1	A	1003	SER	2.0
2	B	341	GLU	2.0
1	A	376	VAL	2.0
2	B	511	LYS	2.0
1	A	472	CYS	2.0
1	A	385	GLU	2.0
1	A	462	THR	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. 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	B-factors(Å ²)	Q<0.9
1	SEP	A	790	10/11	0.95	0.14	113,134,169,176	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å ²)	Q<0.9
3	71M	B	701	8/8	0.67	0.29	169,182,187,187	0
4	LUZ	A	1102	12/12	0.69	0.55	193,217,224,224	0
3	71M	A	1101	8/8	0.81	1.46	164,173,179,181	0

6.5 Other polymers [i](#)

There are no such residues in this entry.