



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:46 AM UTC

PDB ID : 5SXI / pdb_00005sxi
Title : Crystal Structure of PI3Kalpha in complex with fragment 13
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Deposited on : 2016-08-09
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

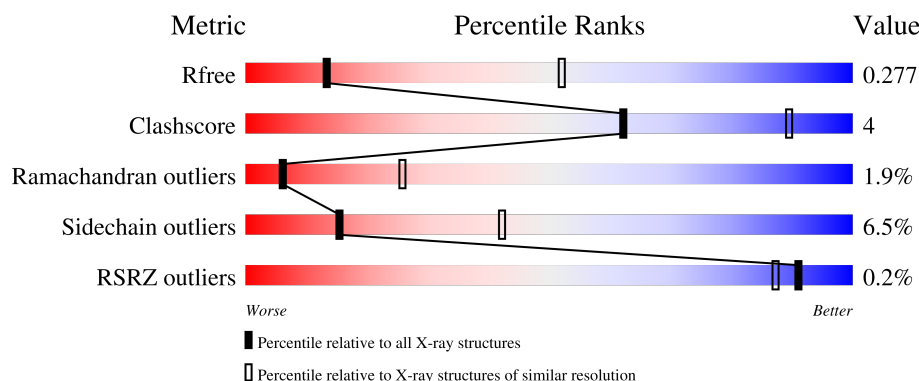
1 Overall quality at a glance

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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	 76% 17% • 5%
2	B	279	 68% 6% 25%

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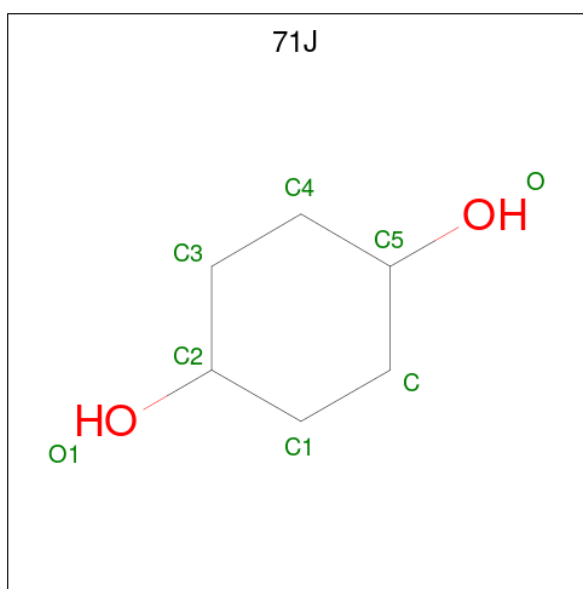
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42336
A	0	SER	-	expression tag	UNP P42336

- 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 (CCD ID: 71J) (formula: C₆H₁₂O₂).

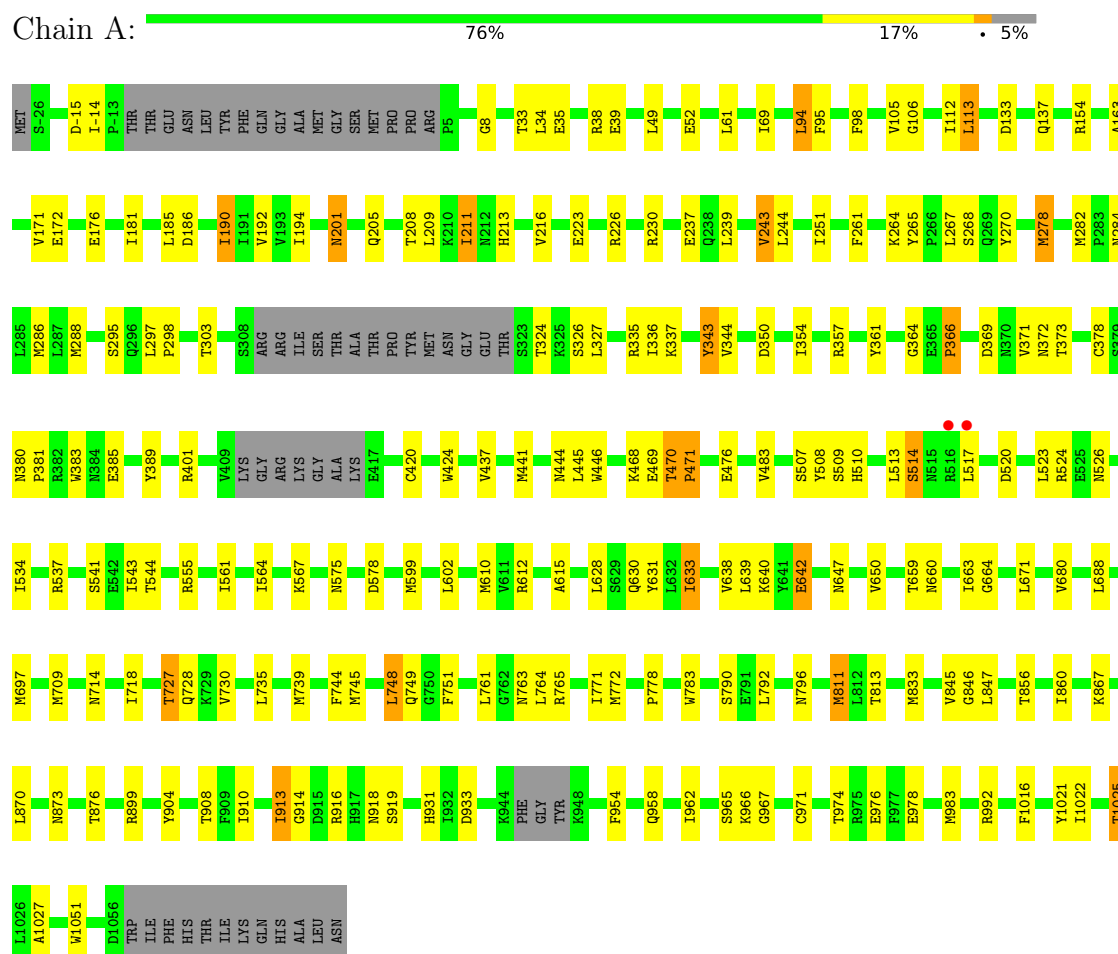


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			8	6	2		

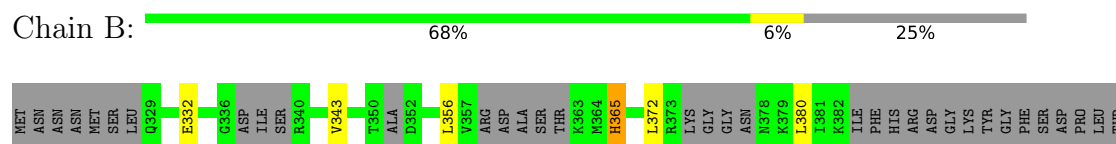
3 Residue-property plots

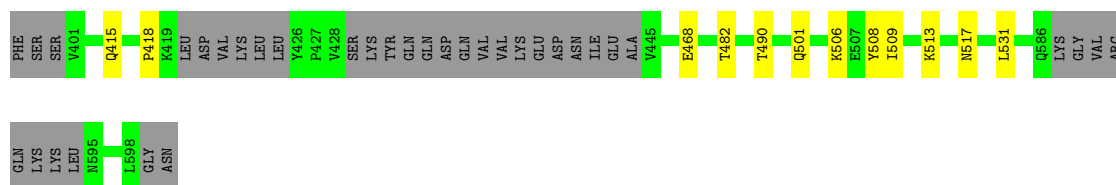
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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



- Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha





4 Data and refinement statistics

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 92.27 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.4 (92.27-3.40) 98.4 (92.27-3.40)	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	1445 reflections (3.42%)	wwPDB-VP
Wilson B-factor (Å ²)	110.8	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 88.4	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	0.95	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

5.1 Standard geometry

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	0.74	1/8708 (0.0%)	1.00	9/11765 (0.1%)
2	B	0.69	0/1843	0.92	0/2457
All	All	0.73	1/10551 (0.0%)	0.99	9/14222 (0.1%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	364	GLY	N-CA	5.12	1.50	1.44

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	751	PHE	N-CA-C	7.99	119.76	108.74
1	A	846	GLY	N-CA-C	6.39	120.45	111.19
1	A	154	ARG	N-CA-C	5.61	117.48	111.36
1	A	1051	TRP	N-CA-C	5.38	119.90	113.23
1	A	1016	PHE	N-CA-C	5.36	119.31	112.34
1	A	230	ARG	N-CA-C	-5.31	101.87	110.32
1	A	918	ASN	N-CA-C	5.25	117.74	111.71
1	A	94	LEU	N-CA-C	5.20	119.62	113.28
1	A	205	GLN	N-CA-C	5.20	117.07	108.13

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 ⓘ

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	82	0
2	B	1818	0	1786	5	0
3	B	8	0	0	0	0
All	All	10360	0	10289	84	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 (84) 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:709:MET:HE1	1:A:847:LEU:HD21	1.49	0.95
1:A:639:LEU:HD22	1:A:650:VAL:HG22	1.74	0.70
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.17	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:610:MET:HA	1:A:610:MET:HE2	1.80	0.64
1:A:561:ILE:O	1:A:564:ILE:HG22	2.01	0.60
1:A:633:ILE:HD11	1:A:811:MET:HE3	1.83	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:599:MET:HE1	1:A:631:TYR:CB	2.37	0.54
1:A:354:ILE:HD11	1:A:381:PRO:CB	2.37	0.54
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: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:372:ASN:HB2	1:A:385:GLU:CD	2.34	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
1:A:190:ILE:HD11	1:A:213:HIS:HA	1.93	0.50
1:A:278:MET:HA	1:A:278:MET:HE2	1.93	0.50
1:A:194:ILE:N	1:A:194:ILE:HD12	2.26	0.49
1:A:98:PHE:CE1	2:B:490:THR:HG23	2.47	0.48
1:A:727:THR:O	1:A:728:GLN:C	2.56	0.48
1:A:663:ILE:O	1:A:664:GLY:C	2.56	0.48
1:A:543:ILE:HD11	1:A:567:LYS:HD3	1.94	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:772:MET:HA	1:A:772:MET:HE2	1.96	0.46
1:A:361:TYR:HA	1:A:366:PRO:HD3	1.97	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: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:181:ILE:HG12	1:A:278:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:992:ARG:NH2	1:A:1027:ALA:O	2.44	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:326:SER:O	1:A:327:LEU:C	2.60	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:1021:TYR:CD1	1:A:1021:TYR:C	2.98	0.41
1:A:833:MET:HE1	1:A:904:TYR:CD1	2.54	0.41
1:A:628:LEU:HD23	1:A:663:ILE:HD13	2.01	0.41
1:A:286:MET:HE3	1:A:288:MET:HE3	2.02	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
1:A:899:ARG:HG2	1:A:983:MET:HE1	2.03	0.41
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:185:LEU:O	1:A:186:ASP:C	2.64	0.40
1:A:517:LEU:HD22	1:A:523:LEU:HD22	2.04	0.40
1:A:739:MET:O	1:A:745:MET:HE3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	7	28
2	B	191/279 (68%)	176 (92%)	10 (5%)	5 (3%)	4	21
All	All	1221/1375 (89%)	1088 (89%)	110 (9%)	23 (2%)	6	26

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
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%)	885 (93%)	68 (7%)	13	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	198/259 (76%)	191 (96%)	7 (4%)	32 56
All	All	1151/1256 (92%)	1076 (94%)	75 (6%)	15 42

All (75) 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	39	GLU
1	A	52	GLU
1	A	69	ILE
1	A	94	LEU
1	A	112	ILE
1	A	113	LEU
1	A	137	GLN
1	A	176	GLU
1	A	190	ILE
1	A	201	ASN
1	A	208	THR
1	A	211	ILE
1	A	216	VAL
1	A	237	GLU
1	A	239	LEU
1	A	243	VAL
1	A	251	ILE
1	A	267	LEU
1	A	268	SER
1	A	278	MET
1	A	295	SER
1	A	303	THR
1	A	335	ARG
1	A	343	TYR
1	A	350	ASP
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

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Mol	Chain	Res	Type
1	A	441	MET
1	A	444	ASN
1	A	470	THR
1	A	510	HIS
1	A	513	LEU
1	A	514	SER
1	A	575	ASN
1	A	578	ASP
1	A	630	GLN
1	A	633	ILE
1	A	638	VAL
1	A	642	GLU
1	A	659	THR
1	A	660	ASN
1	A	718	ILE
1	A	727	THR
1	A	748	LEU
1	A	792	LEU
1	A	811	MET
1	A	813	THR
1	A	845	VAL
1	A	856	THR
1	A	860	ILE
1	A	870	LEU
1	A	913	ILE
1	A	919	SER
1	A	958	GLN
1	A	971	CYS
1	A	976	GLU
1	A	978	GLU
1	A	1022	ILE
1	A	1025	THR
2	B	365	HIS
2	B	372	LEU
2	B	415	GLN
2	B	468	GLU
2	B	482	THR
2	B	501	GLN
2	B	531	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
1	A	212	ASN
1	A	219	GLN
1	A	331	ASN
1	A	362	HIS
1	A	374	GLN
1	A	384	ASN
1	A	444	ASN
1	A	495	HIS
1	A	515	ASN
1	A	526	ASN
1	A	556	HIS
1	A	575	ASN
1	A	630	GLN
1	A	643	GLN
1	A	714	ASN
1	A	738	GLN
1	A	749	GLN
1	A	760	GLN
1	A	785	ASN
1	A	803	ASN
1	A	827	GLN
1	A	917	HIS
1	A	931	HIS
1	A	958	GLN
1	A	1048	HIS
2	B	406	ASN
2	B	417	ASN
2	B	517	ASN
2	B	552	GLN
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	8,9,10	0.76	0	7,12,14	0.93	0
1	SEP	A	790	1	8,9,10	0.63	0	7,12,14	1.60	1 (14%)

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	-	1/6/8/10	-
1	SEP	A	790	1	-	5/6/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	790	SEP	OG-CB-CA	3.35	111.40	108.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	790	SEP	N-CA-CB-OG
1	A	790	SEP	C-CA-CB-OG
1	A	790	SEP	CB-OG-P-O2P
1	A	790	SEP	CB-OG-P-O3P
1	A	790	SEP	CB-OG-P-O1P
1	A	7	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	0.71	0	10,10,10	1.29	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	71J	B	701	-	-	-	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	B	701	71J	C3-C4-C5	2.12	114.92	111.53

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.63	2 (0%) 91 87	70, 117, 180, 229	0
2	B	209/279 (74%)	-0.42	0 100 100	110, 182, 227, 296	0
All	All	1249/1375 (90%)	-0.59	2 (0%) 91 87	70, 122, 207, 296	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	517	LEU	2.5
1	A	516	ARG	2.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	7	10/11	0.77	0.10	140,161,200,217	0
1	SEP	A	790	10/11	0.93	0.06	92,105,192,197	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	71J	B	701	8/8	0.79	0.12	156,176,178,178	0

6.5 Other polymers [i](#)

There are no such residues in this entry.