



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:12 AM UTC

PDB ID : 5SXA / pdb_00005sxa
Title : Crystal Structure of PI3Kalpha in complex with fragment 10
Authors : Gabelli, S.B.; Vogelstein, B.; Miller, M.S.; Amzel, L.M.
Deposited on : 2016-08-09
Resolution : 3.35 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

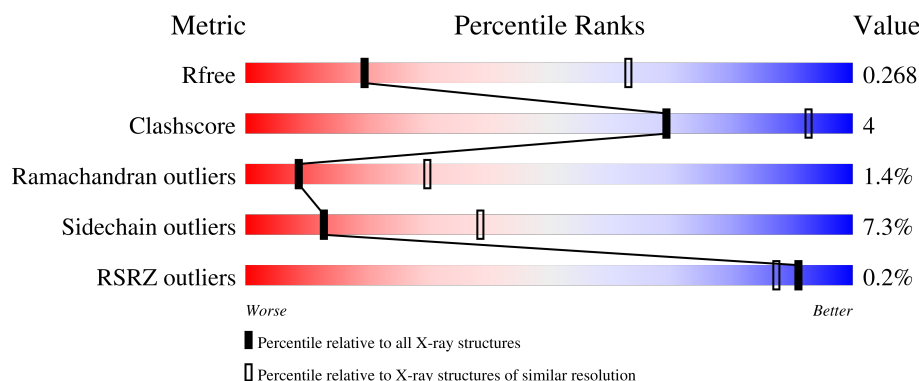
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	 80% 14% . .
2	B	279	 65% 13% 22%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10520 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	1052	Total	C	N	O	P	S	0	0	0
			8629	5510	1474	1572	3	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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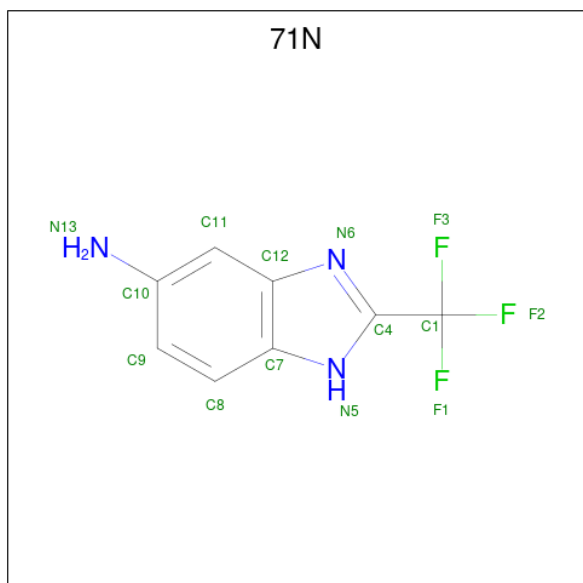
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42336
A	0	SER	-	expression tag	UNP P42336

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1877	1182	329	361	5			

- Molecule 3 is 2-(trifluoromethyl)-1H-benzimidazol-5-amine (CCD ID: 71N) (formula: C₈H₆F₃N₃).

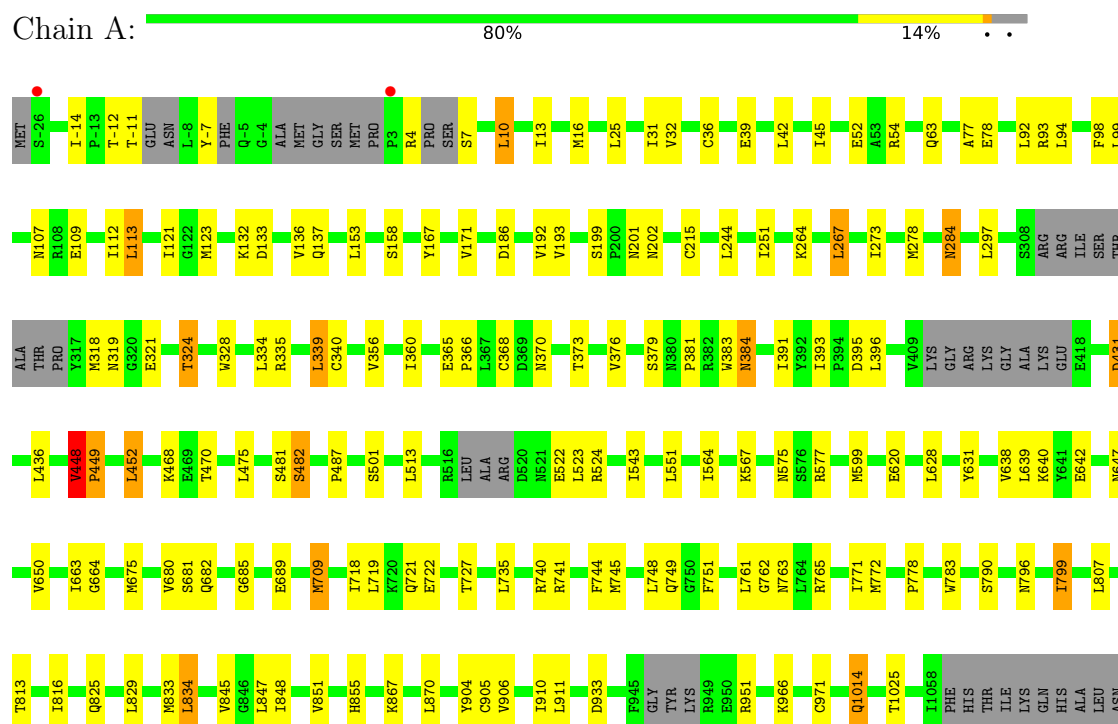


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	N	0	0
			14	8	3	3		

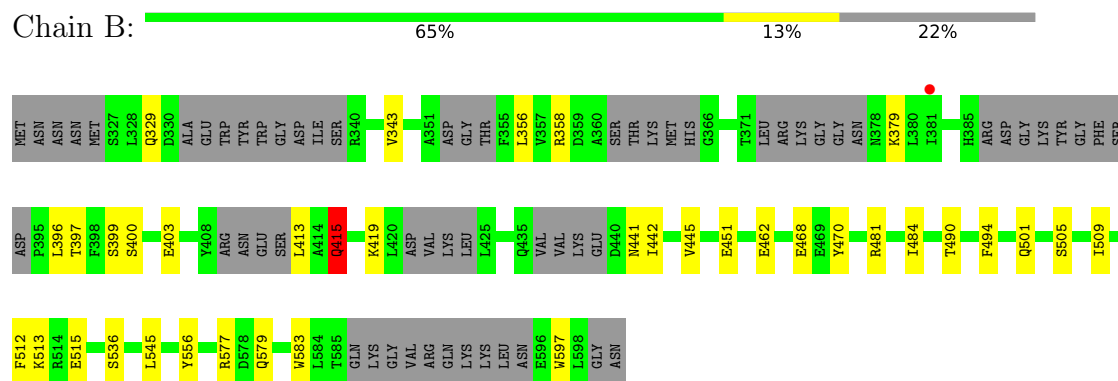
3 Residue-property plots

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	115.22Å 117.37Å 152.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.91 – 3.35 92.91 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (92.91-3.35) 99.9 (92.91-3.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.222 , 0.275 0.220 , 0.268	Depositor DCC
R_{free} test set	1559 reflections (3.69%)	wwPDB-VP
Wilson B-factor (Å ²)	106.0	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 98.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10520	wwPDB-VP
Average B, all atoms (Å ²)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: 71N, 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	0.63	0/8794	0.89	4/11877 (0.0%)
2	B	0.65	0/1900	0.88	1/2533 (0.0%)
All	All	0.63	0/10694	0.89	5/14410 (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	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	365	GLU	N-CA-C	6.28	117.72	109.93
1	A	751	PHE	N-CA-C	5.93	117.26	108.60
2	B	415	GLN	N-CA-C	5.43	119.40	112.34
1	A	448	VAL	N-CA-C	5.42	120.59	108.88
1	A	340	CYS	N-CA-C	5.33	117.01	107.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	LEU	Peptide
1	A	448	VAL	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	8629	0	8581	65	0
2	B	1877	0	1855	11	0
3	A	14	0	0	0	0
All	All	10520	0	10436	74	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 (74) 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:816:ILE:HG21	1:A:911:LEU:HD21	1.74	0.69
1:A:599:MET:HE1	1:A:631:TYR:CD2	2.30	0.67
1:A:765:ARG:HD3	1:A:796:ASN:HD21	1.62	0.64
2:B:343:VAL:HG13	2:B:356:LEU:HD11	1.81	0.63
1:A:121:ILE:HD11	1:A:689:GLU:HA	1.82	0.62
1:A:675:MET:HE1	1:A:685:GLY:CA	2.32	0.58
1:A:910:ILE:O	1:A:1025:THR:HG21	2.07	0.54
1:A:10:LEU:HD13	1:A:16:MET:CE	2.37	0.54
1:A:639:LEU:HD22	1:A:650:VAL:HG22	1.90	0.53
1:A:10:LEU:HD13	1:A:16:MET:HE2	1.89	0.53
1:A:543:ILE:HD11	1:A:567:LYS:HD3	1.91	0.53
1:A:334:LEU:HA	1:A:393:ILE:HD11	1.92	0.52
1:A:123:MET:HE3	1:A:675:MET:HE2	1.92	0.51
1:A:639:LEU:HD22	1:A:650:VAL:CG2	2.40	0.51
2:B:343:VAL:HG21	2:B:358:ARG:CD	2.41	0.51
1:A:370:ASN:N	1:A:370:ASN:HD22	2.08	0.51
1:A:376:VAL:HB	1:A:381:PRO:HA	1.94	0.50
1:A:799:ILE:CD1	1:A:847:LEU:HD22	2.41	0.49
1:A:136:VAL:HG21	1:A:682:GLN:HE22	1.77	0.49
1:A:628:LEU:HD23	1:A:663:ILE:HD13	1.94	0.49
1:A:1014:GLN:HE21	1:A:1014:GLN:HA	1.78	0.49
1:A:735:LEU:HD22	1:A:771:ILE:HG13	1.94	0.48
1:A:834:LEU:HD21	1:A:851:VAL:HG11	1.93	0.48
1:A:709:MET:CE	1:A:847:LEU:HD21	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:MET:HE2	1:A:847:LEU:HD11	1.96	0.48
1:A:772:MET:HB2	1:A:778:PRO:HG2	1.96	0.48
1:A:599:MET:HE1	1:A:631:TYR:HD2	1.76	0.47
1:A:284:ASN:HD22	1:A:284:ASN:N	2.12	0.47
2:B:501:GLN:O	2:B:505:SER:N	2.39	0.46
1:A:718:ILE:O	1:A:721:GLN:O	2.34	0.46
1:A:-11:THR:HB	1:A:-7:TYR:HB2	1.98	0.46
1:A:368:CYS:O	1:A:370:ASN:ND2	2.49	0.46
1:A:675:MET:HE1	1:A:685:GLY:N	2.30	0.46
1:A:121:ILE:HD11	1:A:689:GLU:CA	2.45	0.45
1:A:719:LEU:HD13	1:A:771:ILE:HD13	1.97	0.45
1:A:376:VAL:HG12	1:A:379:SER:O	2.17	0.45
2:B:399:SER:HB2	2:B:403:GLU:HB3	1.97	0.45
1:A:324:THR:CG2	1:A:482:SER:HB3	2.47	0.45
1:A:740:ARG:HA	1:A:745:MET:HE2	1.98	0.45
1:A:749:GLN:O	1:A:762:GLY:O	2.35	0.45
1:A:356:VAL:HG23	1:A:383:TRP:CH2	2.52	0.45
1:A:25:LEU:HD21	2:B:494:PHE:CE1	2.53	0.44
1:A:448:VAL:N	1:A:449:PRO:HA	2.32	0.44
1:A:807:LEU:HD11	1:A:848:ILE:HD11	1.99	0.44
2:B:445:VAL:HG11	2:B:583:TRP:CE3	2.53	0.44
1:A:192:VAL:HG12	1:A:193:VAL:N	2.33	0.44
1:A:663:ILE:O	1:A:664:GLY:C	2.60	0.43
1:A:391:ILE:HD13	1:A:396:LEU:HD23	2.00	0.43
1:A:431:ASP:C	1:A:431:ASP:OD1	2.61	0.43
1:A:324:THR:HG21	1:A:482:SER:HB3	2.01	0.43
1:A:761:LEU:HD22	1:A:783:TRP:CE3	2.54	0.43
2:B:343:VAL:HG21	2:B:358:ARG:HD3	2.00	0.43
1:A:167:TYR:CE2	1:A:297:LEU:HD21	2.54	0.43
1:A:640:LYS:HE2	1:A:680:VAL:HG11	2.01	0.42
1:A:833:MET:HE1	1:A:904:TYR:HA	2.01	0.42
1:A:551:LEU:HD21	1:A:564:ILE:HD11	2.02	0.42
1:A:395:ASP:HA	1:A:577:ARG:HB2	2.00	0.42
1:A:749:GLN:HG2	1:A:763:ASN:HA	2.01	0.42
1:A:328:TRP:CE2	1:A:487:PRO:HG3	2.55	0.41
2:B:470:TYR:CE1	2:B:556:TYR:CE1	3.08	0.41
1:A:383:TRP:O	1:A:384:ASN:ND2	2.52	0.41
1:A:136:VAL:HG21	1:A:682:GLN:NE2	2.34	0.41
1:A:98:PHE:CE2	2:B:490:THR:HG23	2.56	0.41
1:A:10:LEU:HB2	1:A:13:ILE:HD11	2.02	0.41
1:A:339:LEU:N	1:A:339:LEU:HD13	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ILE:O	1:A:366:PRO:HD2	2.21	0.41
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.45	0.41
1:A:92:LEU:HB2	1:A:94:LEU:HG	2.03	0.40
1:A:267:LEU:HD22	1:A:273:ILE:HG13	2.02	0.40
1:A:906:VAL:HG12	1:A:910:ILE:HD12	2.03	0.40
2:B:413:LEU:HA	2:B:415:GLN:HE21	1.85	0.40
2:B:484:ILE:HG13	2:B:545:LEU:HD23	2.04	0.40
1:A:744:PHE:HD2	1:A:748:LEU:HD12	1.86	0.40
1:A:132:LYS:O	1:A:133:ASP:C	2.65	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	1032/1096 (94%)	923 (89%)	96 (9%)	13 (1%)	9	32
2	B	198/279 (71%)	177 (89%)	17 (9%)	4 (2%)	6	24
All	All	1230/1375 (90%)	1100 (89%)	113 (9%)	17 (1%)	9	30

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	A	452	LEU
2	B	400	SER
1	A	77	ALA
1	A	186	ASP
1	A	681	SER
1	A	264	LYS
1	A	522	GLU
1	A	966	LYS

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Mol	Chain	Res	Type
2	B	442	ILE
2	B	515	GLU
1	A	201	ASN
1	A	481	SER
1	A	933	ASP
1	A	324	THR
2	B	512	PHE
1	A	449	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	961/996 (96%)	893 (93%)	68 (7%)	13	39
2	B	207/259 (80%)	190 (92%)	17 (8%)	10	35
All	All	1168/1255 (93%)	1083 (93%)	85 (7%)	13	39

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-14	ILE
1	A	-12	THR
1	A	4	ARG
1	A	10	LEU
1	A	31	ILE
1	A	32	VAL
1	A	36	CYS
1	A	39	GLU
1	A	42	LEU
1	A	45	ILE
1	A	52	GLU
1	A	54	ARG
1	A	63	GLN
1	A	78	GLU
1	A	93	ARG

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Mol	Chain	Res	Type
1	A	99	LEU
1	A	107	ASN
1	A	109	GLU
1	A	112	ILE
1	A	113	LEU
1	A	137	GLN
1	A	153	LEU
1	A	171	VAL
1	A	199	SER
1	A	215	CYS
1	A	244	LEU
1	A	251	ILE
1	A	267	LEU
1	A	278	MET
1	A	284	ASN
1	A	318	MET
1	A	319	ASN
1	A	321	GLU
1	A	335	ARG
1	A	339	LEU
1	A	373	THR
1	A	384	ASN
1	A	431	ASP
1	A	436	LEU
1	A	452	LEU
1	A	468	LYS
1	A	470	THR
1	A	475	LEU
1	A	482	SER
1	A	501	SER
1	A	513	LEU
1	A	523	LEU
1	A	524	ARG
1	A	575	ASN
1	A	620	GLU
1	A	638	VAL
1	A	709	MET
1	A	722	GLU
1	A	727	THR
1	A	741	ARG
1	A	799	ILE
1	A	813	THR

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Mol	Chain	Res	Type
1	A	825	GLN
1	A	829	LEU
1	A	834	LEU
1	A	845	VAL
1	A	855	HIS
1	A	867	LYS
1	A	870	LEU
1	A	905	CYS
1	A	951	ARG
1	A	971	CYS
1	A	1014	GLN
2	B	329	GLN
2	B	379	LYS
2	B	396	LEU
2	B	397	THR
2	B	415	GLN
2	B	419	LYS
2	B	441	ASN
2	B	451	GLU
2	B	462	GLU
2	B	468	GLU
2	B	481	ARG
2	B	509	ILE
2	B	513	LYS
2	B	536	SER
2	B	577	ARG
2	B	579	GLN
2	B	597	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
1	A	180	HIS
1	A	201	ASN
1	A	319	ASN
1	A	345	ASN
1	A	370	ASN
1	A	444	ASN
1	A	515	ASN
1	A	597	GLN
1	A	643	GLN

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Mol	Chain	Res	Type
1	A	670	HIS
1	A	714	ASN
1	A	738	GLN
1	A	749	GLN
1	A	760	GLN
1	A	782	ASN
1	A	785	ASN
1	A	796	ASN
1	A	875	HIS
1	A	878	HIS
1	A	885	ASN
1	A	994	HIS
1	A	1014	GLN
1	A	1042	GLN
1	A	1047	HIS
2	B	415	GLN
2	B	417	ASN
2	B	457	GLN
2	B	499	GLN
2	B	527	ASN
2	B	564	ASN
2	B	579	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	1.22	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SEP	A	158	1	8,9,10	0.62	0	7,12,14	2.02	1 (14%)
1	SEP	A	790	1	8,9,10	0.67	0	7,12,14	2.12	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	-	6/6/8/10	-
1	SEP	A	158	1	-	4/6/8/10	-
1	SEP	A	790	1	-	5/6/8/10	-

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	OG-CB-CA	5.17	113.18	108.14
1	A	158	SEP	OG-CB-CA	4.58	112.60	108.14
1	A	7	SEP	OG-CB-CA	2.13	110.22	108.14

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	7	SEP	N-CA-CB-OG
1	A	7	SEP	C-CA-CB-OG
1	A	7	SEP	CB-OG-P-O2P
1	A	7	SEP	CB-OG-P-O3P
1	A	158	SEP	C-CA-CB-OG
1	A	790	SEP	N-CA-CB-OG
1	A	790	SEP	C-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
1	A	7	SEP	CB-OG-P-O1P
1	A	158	SEP	CB-OG-P-O1P
1	A	158	SEP	N-CA-CB-OG
1	A	158	SEP	CB-OG-P-O2P
1	A	7	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	71N	A	1101	-	15,15,15	1.26	3 (20%)	22,23,23	0.98	1 (4%)

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	71N	A	1101	-	-	0/6/6/6	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	71N	C10-N13	3.02	1.48	1.38
3	A	1101	71N	C7-N5	-2.21	1.34	1.38
3	A	1101	71N	C12-N6	-2.06	1.35	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	71N	C8-C7-C12	-2.06	119.84	122.10

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	1049/1096 (95%)	-0.48	2 (0%) 91 87	66, 117, 189, 248	0
2	B	218/279 (78%)	-0.28	1 (0%) 87 78	110, 192, 249, 273	0
All	All	1267/1375 (92%)	-0.44	3 (0%) 91 87	66, 125, 217, 273	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-26	SER	2.8
1	A	3	PRO	2.6
2	B	381	ILE	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. 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	0.64	0.11	154,178,227,235	0
1	SEP	A	158	10/11	0.83	0.06	133,165,229,235	0
1	SEP	A	790	10/11	0.89	0.07	110,126,204,217	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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	71N	A	1101	14/14	0.62	0.14	202,208,217,221	0

6.5 Other polymers

There are no such residues in this entry.