



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:22 AM UTC

PDB ID : 5SXE / pdb_00005sxe
Title : Crystal Structure of PI3Kalpha in complex with fragments 19 and 28
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Deposited on : 2016-08-09
Resolution : 3.51 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

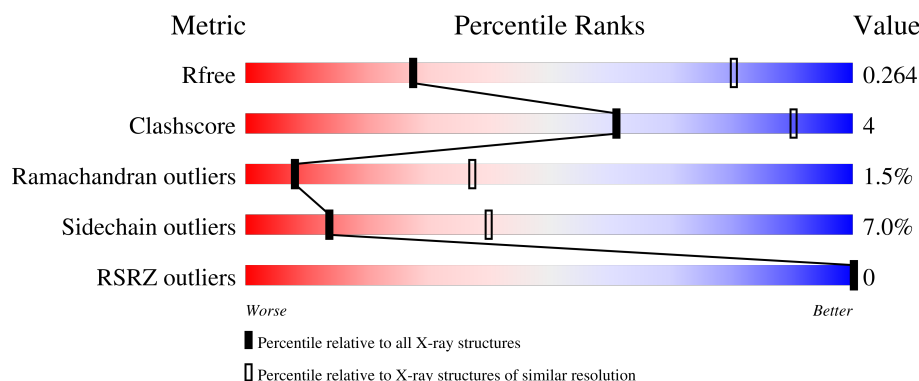
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.51 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	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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	
2	B	279	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10518 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	1048	Total	C	N	O	P	S	0	0	0
			8567	5468	1471	1556	2	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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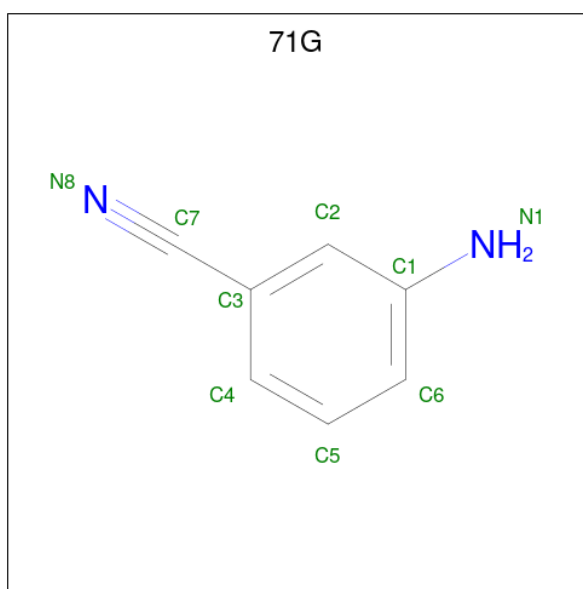
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42336
A	0	SER	-	expression tag	UNP P42336

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

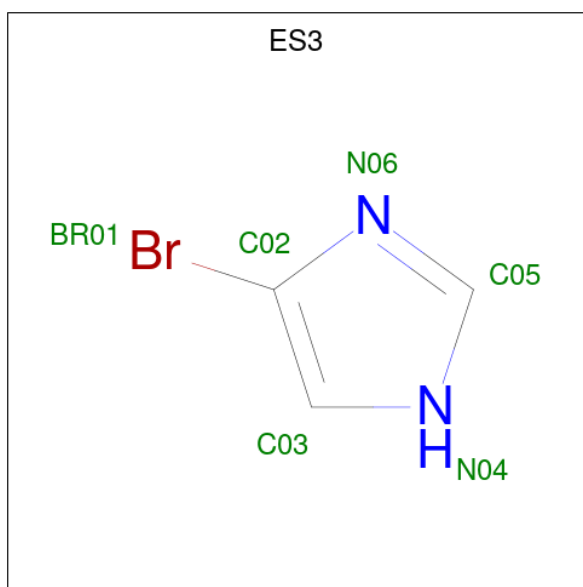
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	225	Total	C	N	O	S	0	0	0
			1936	1215	342	373	6			

- Molecule 3 is 3-aminobenzonitrile (CCD ID: 71G) (formula: $C_7H_6N_2$).



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

- Molecule 4 is 4-bromo-1H-imidazole (CCD ID: ES3) (formula: $C_3H_3BrN_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Br	C	N		
4	B	1	6	1	3	2	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.83Å 116.26Å 148.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.65 – 3.51 91.65 – 3.51	Depositor EDS
% Data completeness (in resolution range)	99.6 (91.65-3.51) 99.8 (91.65-3.51)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.191 , 0.271 0.193 , 0.264	Depositor DCC
R_{free} test set	1306 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	118.7	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 115.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.029 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10518	wwPDB-VP
Average B, all atoms (Å ²)	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: SEP, 71G, ES3

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	0.75	2/8743 (0.0%)	1.02	9/11815 (0.1%)
2	B	0.69	0/1957	0.94	1/2603 (0.0%)
All	All	0.74	2/10700 (0.0%)	1.01	10/14418 (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	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	364	GLY	N-CA	6.33	1.51	1.44
1	A	2	PRO	CA-C	6.01	1.57	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	THR	N-CA-C	10.26	122.54	111.36
1	A	2	PRO	N-CA-C	9.28	122.02	110.70
1	A	365	GLU	N-CA-C	8.32	120.55	110.07
1	A	513	LEU	N-CA-C	-6.44	104.18	111.07
1	A	325	LYS	N-CA-C	6.27	118.67	108.76
1	A	507	SER	N-CA-C	5.37	118.15	109.40
1	A	96	GLN	N-CA-C	-5.32	102.29	110.32
1	A	14	HIS	N-CA-C	5.19	117.84	111.82
2	B	595	ASN	N-CA-C	5.13	117.61	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	SER	N-CA-C	5.11	114.89	108.45

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	LEU	Peptide
1	A	323	SER	Peptide
1	A	511	ALA	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8567	0	8543	84	0
2	B	1936	0	1913	8	0
3	A	9	0	0	0	0
4	B	6	0	3	0	0
All	All	10518	0	10459	87	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 (87) 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:962:ILE:O	1:A:965:SER:O	1.99	0.80
1:A:709:MET:HE1	1:A:847:LEU:HD21	1.75	0.69
1:A:610:MET:HA	1:A:610:MET:HE2	1.76	0.67
1:A:739:MET:O	1:A:745:MET:HE3	2.00	0.62
1:A:910:ILE:O	1:A:1025:THR:HG21	1.99	0.62
1:A:190:ILE:HD11	1:A:213:HIS:HA	1.80	0.61
1:A:261:PHE:HA	1:A:270:TYR:CE2	2.37	0.59
1:A:278:MET:HA	1:A:278:MET:HE2	1.85	0.57
1:A:31:ILE:HD11	2:B:531:LEU:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:MET:HA	1:A:745:MET:HE2	1.86	0.57
1:A:833:MET:HE1	1:A:904:TYR:HA	1.87	0.56
1:A:602:LEU:O	1:A:612:ARG:NH2	2.39	0.56
1:A:1022:ILE:HA	1:A:1025:THR:HG22	1.88	0.56
1:A:372:ASN:HB3	1:A:387:LEU:HD21	1.89	0.55
1:A:671:LEU:HB2	1:A:688:LEU:HD21	1.89	0.54
1:A:772:MET:HB2	1:A:778:PRO:HG2	1.90	0.53
1:A:353:LYS:HA	1:A:377:PRO:HB3	1.90	0.53
1:A:717:ASP:O	1:A:721:GLN:HG2	2.09	0.53
1:A:885:ASN:HB3	1:A:889:ILE:HG22	1.91	0.53
1:A:866:LEU:HD23	1:A:866:LEU:C	2.34	0.53
1:A:561:ILE:O	1:A:564:ILE:HG22	2.08	0.53
1:A:286:MET:HE3	1:A:288:MET:HE3	1.92	0.52
1:A:899:ARG:HG2	1:A:983:MET:HE1	1.92	0.51
1:A:749:GLN:O	1:A:762:GLY:HA2	2.11	0.51
1:A:544:THR:HG22	2:B:380:LEU:HB3	1.92	0.50
1:A:58:LEU:HB3	1:A:61:LEU:HD13	1.93	0.50
2:B:517:ASN:HD22	2:B:518:GLU:H	1.60	0.50
1:A:634:GLN:HB3	1:A:1004:MET:HE2	1.93	0.49
1:A:360:ILE:N	1:A:360:ILE:HD12	2.28	0.48
1:A:866:LEU:HD21	1:A:870:LEU:HB2	1.95	0.48
1:A:866:LEU:HD21	1:A:870:LEU:HD13	1.95	0.48
1:A:446:TRP:CZ2	1:A:465:ASN:HA	2.48	0.48
1:A:1:MET:HB2	1:A:720:LYS:CE	2.43	0.48
1:A:61:LEU:HD11	2:B:508:TYR:CZ	2.49	0.48
1:A:367:LEU:HD12	1:A:368:CYS:O	2.13	0.48
1:A:856:THR:O	1:A:857:ILE:C	2.56	0.48
1:A:361:TYR:HA	1:A:366:PRO:HD3	1.95	0.48
1:A:171:VAL:HG12	1:A:172:GLU:O	2.13	0.47
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.40	0.47
1:A:1023:ARG:O	1:A:1027:ALA:N	2.46	0.47
1:A:612:ARG:NH1	1:A:642:GLU:OE1	2.47	0.46
1:A:0:SER:O	1:A:1:MET:HG2	2.14	0.46
1:A:640:LYS:HE2	1:A:680:VAL:HG11	1.97	0.46
1:A:517:LEU:HD21	1:A:554:HIS:HA	1.97	0.46
1:A:181:ILE:HG23	1:A:277:ILE:HG21	1.97	0.46
1:A:639:LEU:HD23	1:A:649:LEU:HD23	1.98	0.45
1:A:727:THR:O	1:A:728:GLN:C	2.58	0.45
2:B:334:TYR:HH	2:B:368:TYR:HE1	1.61	0.45
1:A:403:CYS:O	1:A:456:LEU:HD21	2.16	0.45
1:A:807:LEU:HD12	1:A:838:CYS:SG	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:LEU:O	1:A:739:MET:HG3	2.17	0.45
1:A:193:VAL:HG22	1:A:208:THR:HG22	1.99	0.45
1:A:543:ILE:HD11	1:A:567:LYS:HD3	1.99	0.45
1:A:147:CYS:O	1:A:151:VAL:HG23	2.17	0.44
1:A:299:MET:HE3	1:A:299:MET:HA	1.99	0.44
1:A:28:ASN:ND2	1:A:62:LEU:HD21	2.32	0.44
1:A:61:LEU:HD11	2:B:508:TYR:CE2	2.53	0.44
1:A:830:ASP:OD2	1:A:832:ARG:NH2	2.51	0.43
1:A:83:PHE:HZ	1:A:112:ILE:HD12	1.83	0.43
1:A:660:ASN:OD1	1:A:660:ASN:C	2.61	0.43
1:A:728:GLN:NE2	1:A:771:ILE:O	2.51	0.43
1:A:194:ILE:N	1:A:194:ILE:HD12	2.34	0.43
1:A:0:SER:HB2	1:A:775:ALA:HB3	1.99	0.43
1:A:181:ILE:HG12	1:A:278:MET:HE3	2.01	0.43
1:A:537:ARG:NH1	1:A:547:GLU:OE1	2.41	0.43
1:A:164:MET:HE3	1:A:169:PRO:HD3	2.01	0.42
1:A:163:ALA:HB2	1:A:297:LEU:HD11	2.00	0.42
1:A:354:ILE:HD11	1:A:381:PRO:CB	2.49	0.42
1:A:424:TRP:CE2	1:A:446:TRP:HB2	2.54	0.42
1:A:763:ASN:HD22	1:A:763:ASN:N	2.18	0.42
1:A:31:ILE:HD12	2:B:531:LEU:HB2	2.01	0.42
1:A:253:LYS:HB3	1:A:286:MET:HB3	2.02	0.42
1:A:92:LEU:HB2	1:A:94:LEU:HD13	2.01	0.42
1:A:374:GLN:O	1:A:377:PRO:HG3	2.20	0.42
1:A:904:TYR:CE2	1:A:930:PHE:HA	2.55	0.42
1:A:897:PHE:O	1:A:901:CYS:HB2	2.20	0.41
1:A:164:MET:HE1	1:A:263:GLU:HB3	2.02	0.41
1:A:958:GLN:O	1:A:959:ASP:C	2.63	0.41
1:A:709:MET:HE2	1:A:841:ILE:HD13	2.01	0.41
1:A:908:THR:HG21	1:A:954:PHE:HB2	2.03	0.41
1:A:148:LYS:HG2	1:A:304:MET:HE2	2.02	0.41
1:A:863:LYS:O	1:A:865:GLY:N	2.54	0.41
1:A:873:ASN:OD1	1:A:875:HIS:HB2	2.20	0.41
2:B:374:LYS:HD2	2:B:422:VAL:HG21	2.03	0.41
1:A:908:THR:HG22	1:A:953:PRO:HD2	2.03	0.40
1:A:70:PHE:CD1	1:A:99:LEU:HB3	2.56	0.40
1:A:762:GLY:O	1:A:763:ASN:O	2.39	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	1036/1096 (94%)	918 (89%)	101 (10%)	17 (2%)	7	36
2	B	200/279 (72%)	185 (92%)	13 (6%)	2 (1%)	12	45
All	All	1236/1375 (90%)	1103 (89%)	114 (9%)	19 (2%)	8	37

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	PRO
1	A	378	CYS
1	A	514	SER
1	A	763	ASN
1	A	107	ASN
1	A	508	TYR
1	A	972	THR
2	B	332	GLU
1	A	555	ARG
2	B	513	LYS
1	A	5	PRO
1	A	186	ASP
1	A	264	LYS
1	A	520	ASP
1	A	864	GLY
1	A	1051	TRP
1	A	112	ILE
1	A	471	PRO
1	A	913	ILE

5.3.2 Protein sidechains [i](#)

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	956/997 (96%)	887 (93%)	69 (7%)	13	39
2	B	214/259 (83%)	201 (94%)	13 (6%)	17	44
All	All	1170/1256 (93%)	1088 (93%)	82 (7%)	14	40

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-15	ASP
1	A	-14	ILE
1	A	1	MET
1	A	23	GLU
1	A	39	GLU
1	A	69	ILE
1	A	94	LEU
1	A	99	LEU
1	A	112	ILE
1	A	113	LEU
1	A	114	ASN
1	A	123	MET
1	A	148	LYS
1	A	177	LEU
1	A	190	ILE
1	A	196	VAL
1	A	216	VAL
1	A	236	SER
1	A	239	LEU
1	A	251	ILE
1	A	274	ARG
1	A	295	SER
1	A	299	MET
1	A	308	SER
1	A	323	SER
1	A	350	ASP
1	A	353	LYS
1	A	368	CYS
1	A	373	THR
1	A	376	VAL
1	A	380	ASN
1	A	401	ARG
1	A	420	CYS

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Mol	Chain	Res	Type
1	A	437	VAL
1	A	441	MET
1	A	444	ASN
1	A	452	LEU
1	A	470	THR
1	A	475	LEU
1	A	499	SER
1	A	510	HIS
1	A	513	LEU
1	A	516	ARG
1	A	575	ASN
1	A	595	PRO
1	A	630	GLN
1	A	633	ILE
1	A	638	VAL
1	A	642	GLU
1	A	659	THR
1	A	683	ARG
1	A	711	LYS
1	A	721	GLN
1	A	727	THR
1	A	767	GLU
1	A	791	GLU
1	A	799	ILE
1	A	800	ILE
1	A	825	GLN
1	A	858	MET
1	A	860	ILE
1	A	866	LEU
1	A	867	LYS
1	A	870	LEU
1	A	901	CYS
1	A	919	SER
1	A	923	VAL
1	A	966	LYS
1	A	1022	ILE
2	B	372	LEU
2	B	374	LYS
2	B	415	GLN
2	B	441	ASN
2	B	468	GLU
2	B	515	GLU

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Mol	Chain	Res	Type
2	B	517	ASN
2	B	518	GLU
2	B	529	ASP
2	B	531	LEU
2	B	552	GLN
2	B	585	THR
2	B	594	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	-5	GLN
1	A	107	ASN
1	A	201	ASN
1	A	202	ASN
1	A	331	ASN
1	A	444	ASN
1	A	510	HIS
1	A	526	ASN
1	A	556	HIS
1	A	575	ASN
1	A	597	GLN
1	A	634	GLN
1	A	643	GLN
1	A	677	ASN
1	A	738	GLN
1	A	749	GLN
1	A	760	GLN
1	A	763	ASN
1	A	815	GLN
1	A	827	GLN
1	A	861	GLN
1	A	871	GLN
1	A	878	HIS
1	A	917	HIS
1	A	931	HIS
1	A	1042	GLN
2	B	417	ASN
2	B	455	GLN
2	B	517	ASN
2	B	564	ASN
2	B	595	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	0.81	0	7,12,14	0.78	0
1	SEP	A	790	1	8,9,10	0.69	0	7,12,14	2.01	2 (28%)

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	790	1	-	5/6/8/10	-

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	4.22	112.25	108.14
1	A	790	SEP	O2P-P-OG	-2.23	100.84	106.67

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	7	SEP	N-CA-CB-OG

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

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](#)

2 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	$\# Z > 2$
4	ES3	B	701	-	5,6,6	4.70	1 (20%)	4,7,7	1.71	1 (25%)
3	71G	A	1101	-	9,9,9	2.63	2 (22%)	11,11,11	0.70	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
4	ES3	B	701	-	-	-	0/1/1/1
3	71G	A	1101	-	-	0/2/2/2	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	701	ES3	BR01-C02	10.36	2.00	1.87
3	A	1101	71G	C3-C7	-7.00	1.29	1.44
3	A	1101	71G	C1-N1	3.07	1.49	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	ES3	C02-C03-N04	-2.41	103.13	105.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	1046/1096 (95%)	-0.72	0 100 100	73, 123, 193, 254	0
2	B	225/279 (80%)	-0.56	0 100 100	111, 189, 231, 275	0
All	All	1271/1375 (92%)	-0.69	0 100 100	73, 130, 212, 275	0

There are no RSRZ outliers to report.

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	0.56	0.12	163,190,249,258	0
1	SEP	A	790	10/11	0.93	0.04	94,118,199,203	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
4	ES3	B	701	6/6	0.78	0.09	191,195,207,240	0
3	71G	A	1101	9/9	0.82	0.11	146,183,195,196	0

6.5 Other polymers [i](#)

There are no such residues in this entry.