



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:55 AM UTC

PDB ID : 5SWT / pdb_00005swt
Title : Crystal Structure of PI3Kalpha in complex with fragments 17 and 27
Authors : Gabelli, S.B.; Vogelstein, B.; Miller, M.S.; Amzel, L.M.
Deposited on : 2016-08-08
Resolution : 3.49 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

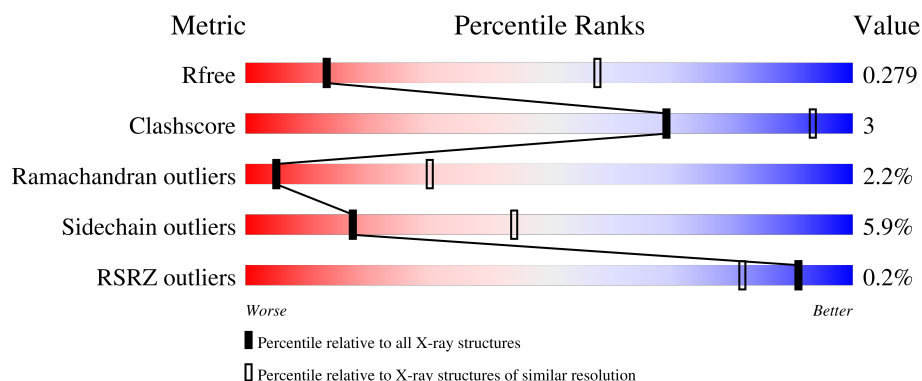
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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% 15% . .
2	B	279	 78% 11% . 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10818 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	1059	Total	C	N	O	P	S	0	0	0
			8655	5524	1483	1575	2	71			

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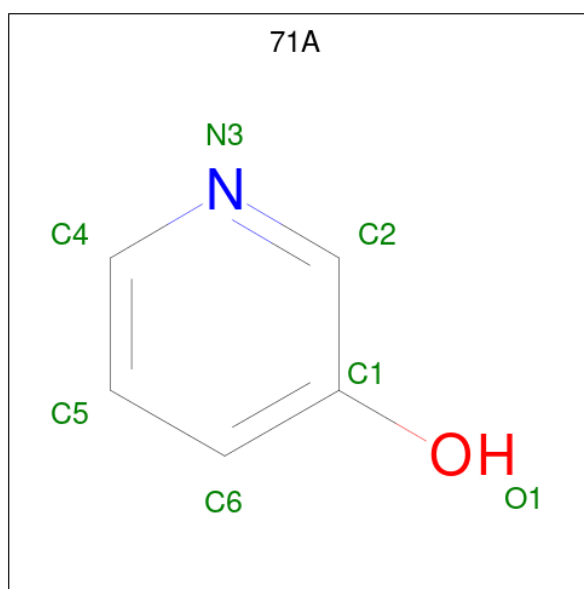
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42336
A	0	SER	-	expression tag	UNP P42336

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

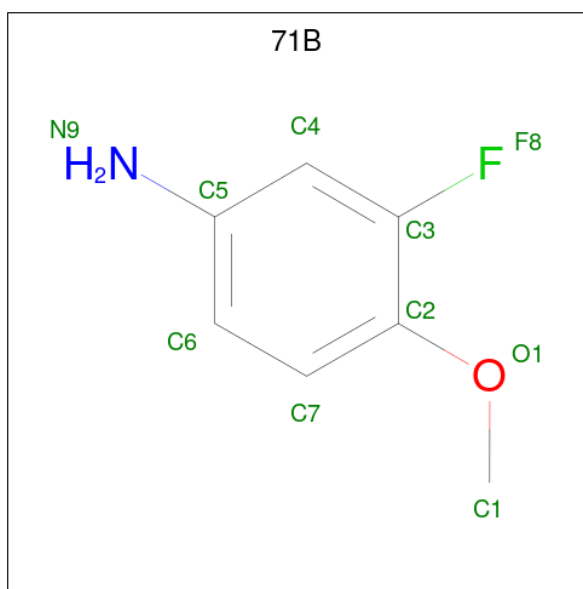
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	249	Total	C	N	O	S	0	0	0
			2146	1348	385	407	6			

- Molecule 3 is pyridin-3-ol (CCD ID: 71A) (formula: C₅H₅NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 4 is 3-fluoro-4-methoxyaniline (CCD ID: 71B) (formula: C₇H₈FNO).

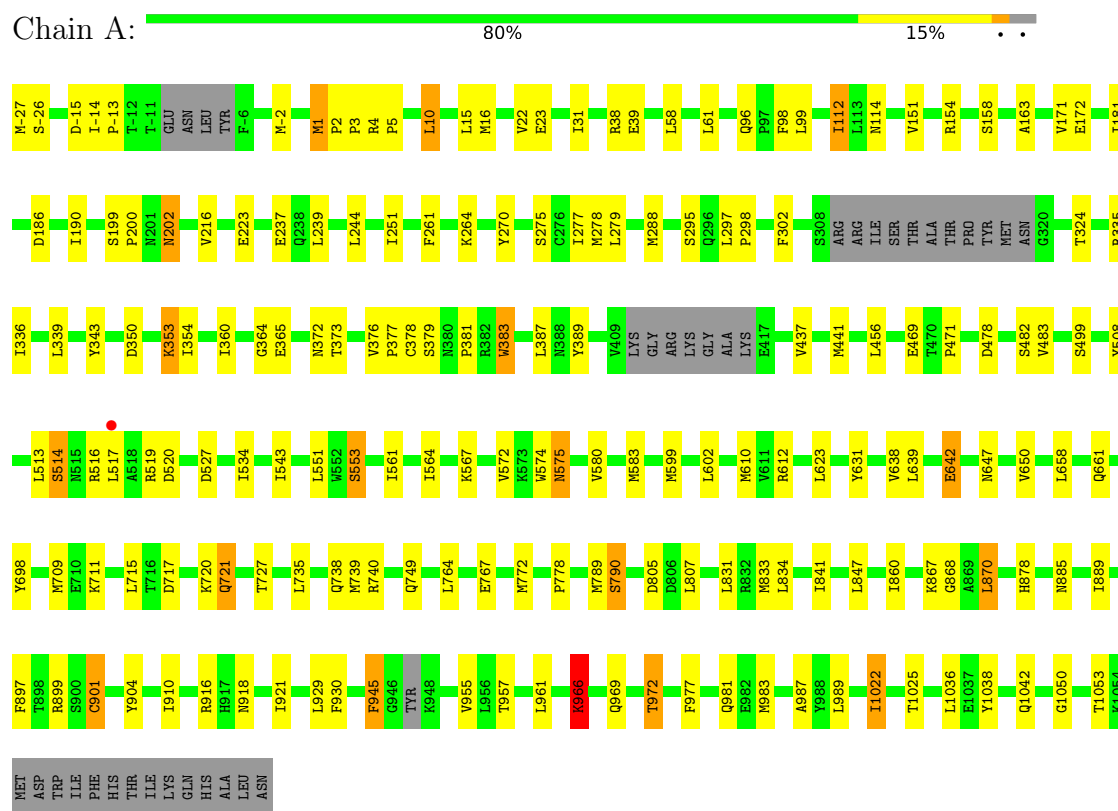


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
4	A	1	10	7	1	1	1	0	0

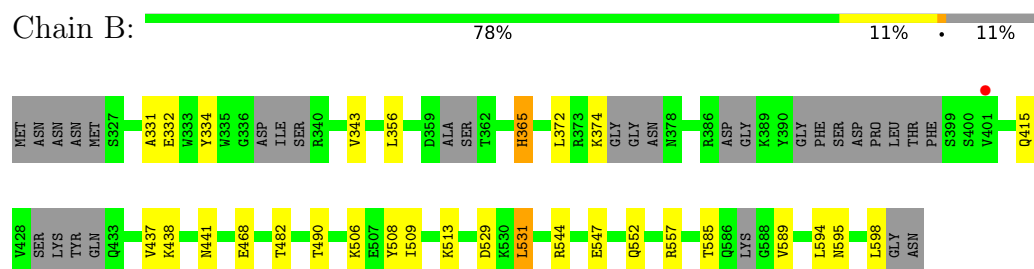
3 Residue-property plots

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	114.45Å 115.94Å 149.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.57 – 3.49 91.57 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.2 (91.57-3.49) 99.5 (91.57-3.49)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.208 , 0.285 0.210 , 0.279	Depositor DCC
R_{free} test set	1329 reflections (3.15%)	wwPDB-VP
Wilson B-factor (Å ²)	116.6	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 117.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10818	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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, 71A, 71B

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	0.64	1/8833 (0.0%)	0.91	2/11934 (0.0%)
2	B	0.63	0/2175	0.87	1/2902 (0.0%)
All	All	0.64	1/11008 (0.0%)	0.90	3/14836 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	364	GLY	N-CA	5.74	1.50	1.44

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	GLU	N-CA-C	5.99	117.56	109.24
1	A	1053	THR	N-CA-C	5.92	118.21	111.11
2	B	595	ASN	N-CA-C	5.50	118.04	111.71

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	8655	0	8621	71	0
2	B	2146	0	2135	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	7	0	0	0	0
4	A	10	0	0	0	0
All	All	10818	0	10756	75	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 3.

All (75) 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:989:LEU:HD11	1:A:1036:LEU:HD11	1.74	0.70
1:A:899:ARG:HG2	1:A:983:MET:HE1	1.75	0.68
1:A:163:ALA:HB2	1:A:297:LEU:HD11	1.79	0.65
1:A:610:MET:HA	1:A:610:MET:HE2	1.79	0.62
1:A:639:LEU:HD22	1:A:650:VAL:HG22	1.83	0.61
1:A:910:ILE:O	1:A:1025:THR:HG21	2.04	0.58
1:A:717:ASP:O	1:A:721:GLN:NE2	2.37	0.57
1:A:599:MET:HE1	1:A:631:TYR:CB	2.34	0.57
1:A:957:THR:O	1:A:961:LEU:HD12	2.05	0.56
1:A:945:PHE:HB2	2:B:598:LEU:HD13	1.87	0.56
1:A:31:ILE:HD11	2:B:531:LEU:HD13	1.86	0.56
1:A:261:PHE:HA	1:A:270:TYR:CE2	2.41	0.56
1:A:1:MET:HB2	1:A:720:LYS:CE	2.37	0.55
1:A:709:MET:HE1	1:A:847:LEU:HD21	1.88	0.54
1:A:324:THR:HG22	1:A:483:VAL:HG23	1.90	0.54
1:A:98:PHE:CE1	2:B:490:THR:HG23	2.44	0.53
1:A:278:MET:HA	1:A:278:MET:HE2	1.91	0.53
1:A:602:LEU:O	1:A:612:ARG:NH2	2.43	0.52
1:A:561:ILE:O	1:A:564:ILE:HG22	2.10	0.52
2:B:331:ALA:HB3	2:B:334:TYR:HB3	1.92	0.52
2:B:343:VAL:HG13	2:B:356:LEU:HD11	1.91	0.52
1:A:749:GLN:HE21	1:A:764:LEU:H	1.58	0.51
1:A:981:GLN:NE2	1:A:1050:GLY:O	2.44	0.51
1:A:805:ASP:O	1:A:807:LEU:HD22	2.09	0.50
1:A:833:MET:HE1	1:A:904:TYR:HA	1.94	0.49
1:A:519:ARG:NH2	1:A:527:ASP:OD2	2.45	0.49
1:A:1022:ILE:HA	1:A:1025:THR:HG22	1.94	0.49
1:A:181:ILE:HG12	1:A:278:MET:HE3	1.94	0.48
1:A:275:SER:O	1:A:279:LEU:HD12	2.14	0.48
1:A:336:ILE:HD12	1:A:389:TYR:CE1	2.49	0.48
1:A:10:LEU:HD13	1:A:16:MET:HE2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:LYS:HA	1:A:377:PRO:HB3	1.97	0.47
1:A:58:LEU:HB3	1:A:61:LEU:HD13	1.96	0.47
1:A:61:LEU:HD11	2:B:508:TYR:CZ	2.50	0.47
1:A:961:LEU:HD23	1:A:977:PHE:CE1	2.50	0.47
1:A:517:LEU:HD11	1:A:553:SER:O	2.15	0.47
1:A:181:ILE:HG23	1:A:277:ILE:HG21	1.97	0.46
1:A:885:ASN:HB3	1:A:889:ILE:HG22	1.97	0.46
1:A:151:VAL:HG21	1:A:302:PHE:HB2	1.97	0.46
1:A:360:ILE:N	1:A:360:ILE:HD12	2.31	0.46
1:A:171:VAL:HG12	1:A:172:GLU:O	2.16	0.45
1:A:372:ASN:HB3	1:A:387:LEU:HD21	1.98	0.45
1:A:354:ILE:HD11	1:A:381:PRO:HB3	1.99	0.45
1:A:534:ILE:HG21	1:A:551:LEU:HD11	1.98	0.45
1:A:945:PHE:CG	2:B:598:LEU:HB3	2.51	0.45
1:A:377:PRO:O	1:A:379:SER:N	2.50	0.44
2:B:506:LYS:HA	2:B:509:ILE:HG22	2.00	0.43
1:A:339:LEU:O	1:A:383:TRP:O	2.35	0.43
1:A:916:ARG:HB3	1:A:921:ILE:HD11	2.00	0.43
1:A:543:ILE:HD11	1:A:567:LYS:HD3	2.01	0.43
1:A:1038:TYR:O	1:A:1042:GLN:HG2	2.17	0.43
1:A:878:HIS:NE2	1:A:966:LYS:O	2.52	0.42
1:A:16:MET:HG3	1:A:38:ARG:HB2	2.01	0.42
1:A:324:THR:CG2	1:A:483:VAL:HG23	2.50	0.42
1:A:343:TYR:OH	2:B:557:ARG:NH1	2.50	0.42
1:A:831:LEU:HD11	1:A:987:ALA:HB2	2.01	0.42
1:A:772:MET:HB2	1:A:778:PRO:HG2	2.01	0.42
1:A:868:GLY:O	1:A:870:LEU:HD13	2.20	0.42
2:B:544:ARG:O	2:B:547:GLU:HG2	2.20	0.41
1:A:335:ARG:NE	1:A:478:ASP:OD2	2.53	0.41
1:A:904:TYR:CE2	1:A:930:PHE:HA	2.56	0.41
1:A:715:LEU:HD21	1:A:735:LEU:HD12	2.01	0.41
1:A:437:VAL:CG2	1:A:441:MET:HE3	2.51	0.41
1:A:739:MET:HE2	1:A:764:LEU:HD11	2.02	0.41
1:A:709:MET:HE2	1:A:841:ILE:HD13	2.02	0.41
1:A:789:MET:O	1:A:790:SEP:C	2.68	0.41
1:A:15:LEU:HD21	1:A:738:GLN:OE1	2.20	0.41
1:A:575:ASN:HD22	1:A:575:ASN:C	2.28	0.41
1:A:661:GLN:OE1	1:A:698:TYR:HB2	2.21	0.41
1:A:154:ARG:HD2	1:A:658:LEU:O	2.21	0.40
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.46	0.40
1:A:897:PHE:O	1:A:901:CYS:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:VAL:CG2	1:A:583:MET:HE3	2.51	0.40
1:A:574:TRP:HA	1:A:580:VAL:CG2	2.51	0.40
1:A:639:LEU:HD22	1:A:650:VAL:CG2	2.50	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	1047/1096 (96%)	946 (90%)	79 (8%)	22 (2%)	5	31
2	B	233/279 (84%)	215 (92%)	12 (5%)	6 (3%)	4	27
All	All	1280/1375 (93%)	1161 (91%)	91 (7%)	28 (2%)	5	30

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	CYS
1	A	508	TYR
1	A	514	SER
1	A	945	PHE
1	A	2	PRO
1	A	264	LYS
1	A	966	LYS
2	B	365	HIS
2	B	513	LYS
1	A	3	PRO
1	A	202	ASN
1	A	482	SER
1	A	867	LYS
1	A	918	ASN
1	A	972	THR

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Mol	Chain	Res	Type
2	B	332	GLU
2	B	438	LYS
1	A	186	ASP
1	A	200	PRO
1	A	-13	PRO
1	A	520	ASP
1	A	623	LEU
2	B	589	VAL
1	A	112	ILE
1	A	298	PRO
1	A	471	PRO
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	965/997 (97%)	908 (94%)	57 (6%)	18	44
2	B	235/259 (91%)	221 (94%)	14 (6%)	17	44
All	All	1200/1256 (96%)	1129 (94%)	71 (6%)	18	44

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-27	MET
1	A	-26	SER
1	A	-15	ASP
1	A	-14	ILE
1	A	-2	MET
1	A	1	MET
1	A	4	ARG
1	A	10	LEU
1	A	22	VAL
1	A	23	GLU

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Mol	Chain	Res	Type
1	A	39	GLU
1	A	96	GLN
1	A	99	LEU
1	A	112	ILE
1	A	114	ASN
1	A	158	SER
1	A	190	ILE
1	A	199	SER
1	A	202	ASN
1	A	216	VAL
1	A	223	GLU
1	A	237	GLU
1	A	239	LEU
1	A	244	LEU
1	A	251	ILE
1	A	288	MET
1	A	295	SER
1	A	350	ASP
1	A	353	LYS
1	A	373	THR
1	A	376	VAL
1	A	383	TRP
1	A	456	LEU
1	A	469	GLU
1	A	499	SER
1	A	513	LEU
1	A	514	SER
1	A	516	ARG
1	A	553	SER
1	A	575	ASN
1	A	638	VAL
1	A	642	GLU
1	A	711	LYS
1	A	721	GLN
1	A	727	THR
1	A	740	ARG
1	A	767	GLU
1	A	834	LEU
1	A	860	ILE
1	A	870	LEU
1	A	901	CYS
1	A	929	LEU

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Mol	Chain	Res	Type
1	A	955	VAL
1	A	966	LYS
1	A	969	GLN
1	A	972	THR
1	A	1022	ILE
2	B	365	HIS
2	B	372	LEU
2	B	374	LYS
2	B	415	GLN
2	B	425	LEU
2	B	437	VAL
2	B	441	ASN
2	B	468	GLU
2	B	482	THR
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 (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	ASN
1	A	331	ASN
1	A	345	ASN
1	A	526	ASN
1	A	554	HIS
1	A	575	ASN
1	A	597	GLN
1	A	637	GLN
1	A	643	GLN
1	A	670	HIS
1	A	738	GLN
1	A	749	GLN
1	A	827	GLN
1	A	885	ASN
1	A	917	HIS
1	A	994	HIS
1	A	1047	HIS
2	B	415	GLN
2	B	564	ASN

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Mol	Chain	Res	Type
2	B	591	GLN
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	1.02	0
1	SEP	A	790	1	8,9,10	0.65	0	7,12,14	2.51	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	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	5.93	113.92	108.14

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
1	A	7	SEP	C-CA-CB-OG
1	A	7	SEP	CA-CB-OG-P
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
1	A	7	SEP	CB-OG-P-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	790	SEP	1	0

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	$\# Z > 2$
3	71A	A	1101	-	7,7,7	0.64	0	7,8,8	1.41	2 (28%)
4	71B	A	1102	-	10,10,10	1.04	1 (10%)	13,13,13	1.60	3 (23%)

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	71A	A	1101	-	-	-	0/1/1/1
4	71B	A	1102	-	-	2/2/2/2	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1102	71B	C5-N9	3.03	1.49	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1102	71B	O1-C2-C3	3.96	119.11	116.27
3	A	1101	71A	C4-N3-C2	2.86	121.87	116.85
4	A	1102	71B	O1-C2-C7	-2.17	120.64	124.30
4	A	1102	71B	C4-C3-C2	-2.17	119.93	122.86
3	A	1101	71A	C1-C2-N3	-2.10	119.96	122.50

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1102	71B	C3-C2-O1-C1
4	A	1102	71B	C7-C2-O1-C1

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	1057/1096 (96%)	-0.57	1 (0%) 92 86	81, 126, 192, 262	0
2	B	249/279 (89%)	-0.46	1 (0%) 88 72	113, 186, 229, 264	0
All	All	1306/1375 (94%)	-0.55	2 (0%) 91 82	81, 134, 211, 264	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	401	VAL	2.9
1	A	517	LEU	2.5

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	0.43	0.13	173,201,218,220	0
1	SEP	A	790	10/11	0.90	0.06	115,132,186,190	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	71A	A	1101	7/7	0.79	0.10	146,162,167,169	0
4	71B	A	1102	10/10	0.93	0.18	90,110,118,124	10

6.5 Other polymers [i](#)

There are no such residues in this entry.