Full wwPDB X-ray Structure Validation Report (i)

Sep 23, 2023 – 07:06 PM EDT

PDB ID	:	5SWT
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 (i) 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 (1)) were used in the production of this report:

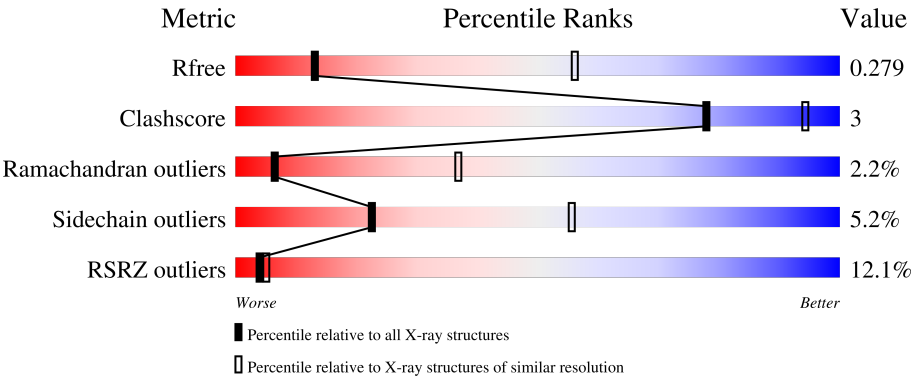
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	8% 82% 13%
2	B	279	23% 78% 10% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	71B	A	1102	-	-	-	X

2 Entry composition (i)

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 subunit alpha isoform.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	1059	8655	5524	1483	1575	2	71	0	0	0

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

Continued on next page...

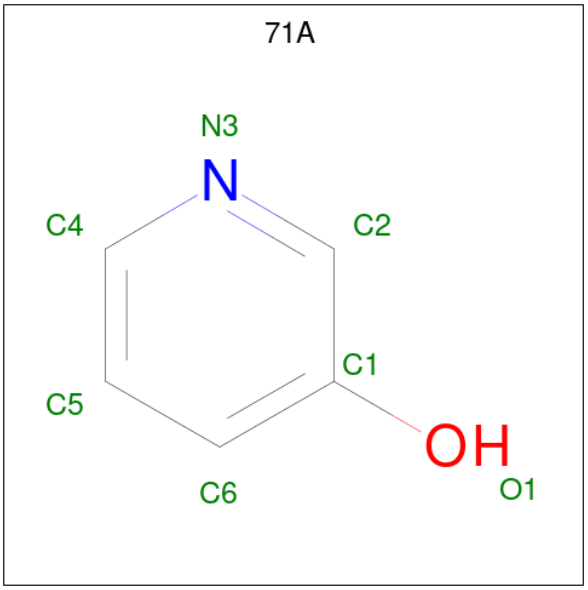
Continued from previous page...

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.

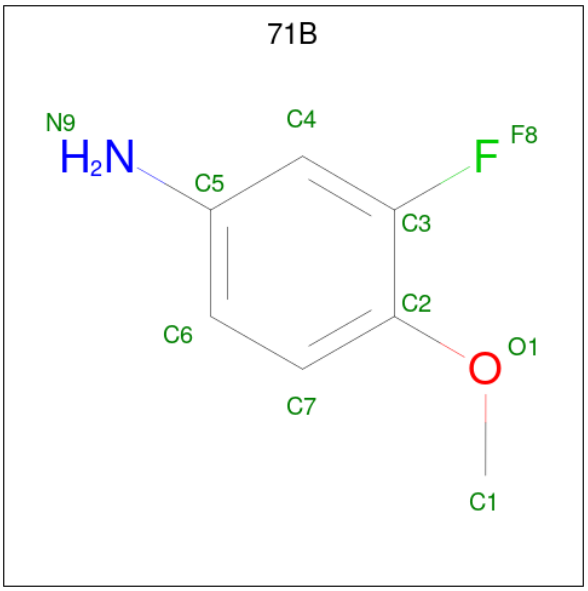
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	249	Total	C	N	O	S	0	0	0
			2146	1348	385	407	6			

- Molecule 3 is pyridin-3-ol (three-letter code: 71A) (formula: C_5H_5NO).



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 (three-letter code: 71B) (formula: C_7H_8FNO).



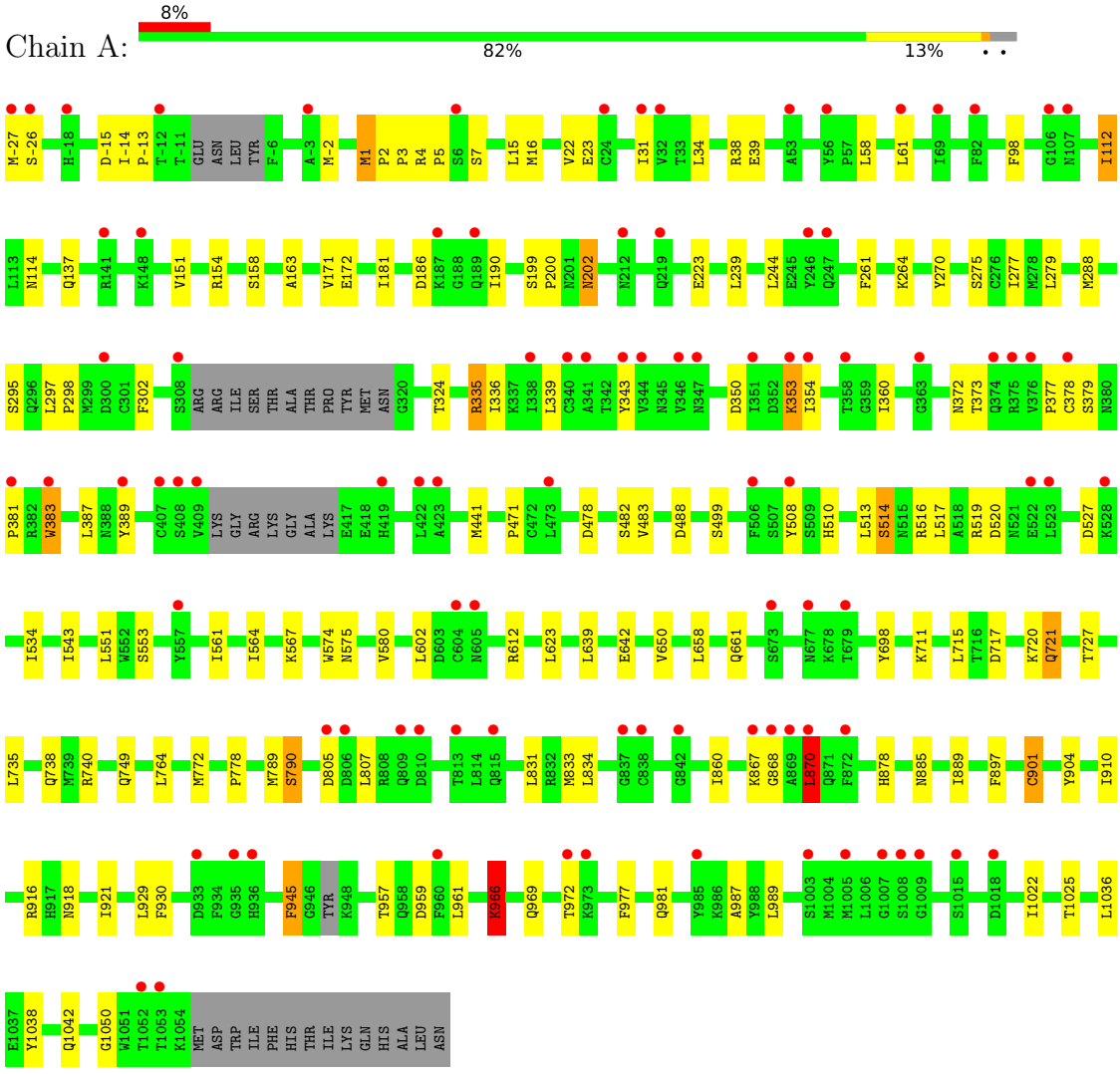
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
4	A	1	10	7	1	1	1	0	0

3 Residue-property plots (i)

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.

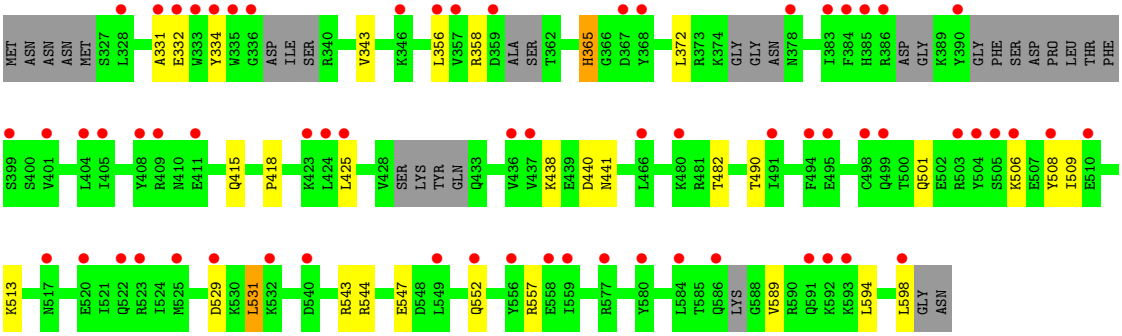
• Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform

Chain A:



• Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha

Chain B:


MET ASN ASN ASN MET S327 L328 A331 E332 W333 Y334 W335 G336 ASP ILE SER R340 V343 K346 L356 V357 R358 D359 ALA SER T362 H365 G366 D367 Y368 L372 R373 K374 GLY GLY ASN N378 I383 F384 H385 R386 ASP GLY K389 Y390 GLY PHE SER ASP PRO LEU THR PHE
S399 S400 V401 L404 I405 Y408 R409 M410 E411 Q415 P418 K423 L424 L425 V428 SER LYS TYR GLN Q433 V436 V437 K438 E439 D440 N441 L466 K480 R481 T482 T490 I491 F494 E495 C498 Q499 T500 Q501 E502 R503 Y504 S505 K506 E507 Y508 I509 E510
K513 M517 E520 I521 Q522 R523 I524 M525 D529 K530 L531 K532 D540 R543 R544 E547 D548 L549 Q552 Y556 R557 E558 I559 R577 Y580 L584 T585 Q586 LYS G588 V589 R590 Q591 K592 K593 L594 L598 GLY ASN

4 Data and refinement statistics (i)

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 48.87 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.2 (91.57-3.49) 99.3 (48.87-3.49)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	1325 reflections (5.14%)	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)	0.32 , 104.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.45	0/8833	0.69	1/11934 (0.0%)
2	B	0.43	0/2175	0.64	0/2902
All	All	0.45	0/11008	0.68	1/14836 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	870	LEU	CA-CB-CG	6.85	131.05	115.30

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	8620	58	0
2	B	2146	0	2135	10	0
3	A	7	0	0	0	0
4	A	10	0	0	0	0
All	All	10818	0	10755	62	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 (62) 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:163:ALA:HB2	1:A:297:LEU:HD11	1.79	0.65
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: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: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: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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:897:PHE:O	1:A:901:CYS:HB2	2.22	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%)	7	38
2	B	233/279 (84%)	215 (92%)	12 (5%)	6 (3%)	5	33
All	All	1280/1375 (93%)	1161 (91%)	91 (7%)	28 (2%)	6	37

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
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 (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	965/997 (97%)	916 (95%)	49 (5%)	24 57
2	B	235/259 (91%)	221 (94%)	14 (6%)	19 52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1200/1256 (96%)	1137 (95%)	63 (5%)	22 55

All (63) 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	22	VAL
1	A	23	GLU
1	A	34	LEU
1	A	39	GLU
1	A	112	ILE
1	A	114	ASN
1	A	137	GLN
1	A	158	SER
1	A	190	ILE
1	A	199	SER
1	A	202	ASN
1	A	223	GLU
1	A	239	LEU
1	A	244	LEU
1	A	288	MET
1	A	295	SER
1	A	335	ARG
1	A	350	ASP
1	A	353	LYS
1	A	373	THR
1	A	383	TRP
1	A	441	MET
1	A	488	ASP
1	A	499	SER
1	A	510	HIS
1	A	513	LEU
1	A	514	SER
1	A	516	ARG
1	A	575	ASN
1	A	642	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	711	LYS
1	A	721	GLN
1	A	727	THR
1	A	740	ARG
1	A	834	LEU
1	A	860	ILE
1	A	870	LEU
1	A	901	CYS
1	A	929	LEU
1	A	959	ASP
1	A	966	LYS
1	A	969	GLN
2	B	358	ARG
2	B	365	HIS
2	B	372	LEU
2	B	415	GLN
2	B	425	LEU
2	B	440	ASP
2	B	441	ASN
2	B	482	THR
2	B	501	GLN
2	B	529	ASP
2	B	531	LEU
2	B	543	ARG
2	B	552	GLN
2	B	594	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	331	ASN
1	A	347	ASN
1	A	374	GLN
1	A	526	ASN
1	A	575	ASN
1	A	670	HIS
1	A	721	GLN
1	A	749	GLN
1	A	782	ASN
1	A	796	ASN
1	A	885	ASN
1	A	1047	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	0.79	0	8,12,14	1.34	1 (12%)
1	SEP	A	790	1	8,9,10	0.64	0	8,12,14	2.41	1 (12%)

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	-	5/5/8/10	-
1	SEP	A	790	1	-	4/5/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	790	SEP	OG-CB-CA	5.93	113.92	108.14
1	A	7	SEP	P-OG-CB	2.63	125.53	118.30

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	7	SEP	N-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	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 monosaccharides 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	71B	A	1102	-	10,10,10	1.04	1 (10%)	12,13,13	1.66	2 (16%)
3	71A	A	1101	-	6,7,7	0.63	0	8,8,8	1.21	1 (12%)

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	71B	A	1102	-	-	2/2/2/2	0/1/1/1
3	71A	A	1101	-	-	-	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	3.04	1.49	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1102	71B	O1-C2-C3	4.11	119.11	116.26
3	A	1101	71A	C4-N3-C2	2.90	121.87	116.85
4	A	1102	71B	O1-C2-C7	-2.18	120.64	124.37

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.58	93 (8%) 10 10	81, 126, 192, 262	0
2	B	249/279 (89%)	1.27	65 (26%) 0 0	113, 186, 229, 264	0
All	All	1306/1375 (94%)	0.71	158 (12%) 4 5	81, 134, 211, 264	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	335	TRP	9.1
2	B	505	SER	5.6
1	A	869	ALA	4.8
2	B	409	ARG	4.4
2	B	580	TYR	4.4
1	A	107	ASN	4.4
2	B	333	TRP	4.4
1	A	523	LEU	4.4
1	A	872	PHE	4.3
2	B	357	VAL	4.2
2	B	359	ASP	4.1
1	A	-12	THR	4.1
1	A	1052	THR	4.1
2	B	504	TYR	4.0
1	A	-26	SER	4.0
1	A	810	ASP	3.9
1	A	374	GLN	3.9
2	B	424	LEU	3.8
1	A	1009	GLY	3.8
2	B	378	ASN	3.8
1	A	522	GLU	3.7
2	B	405	ILE	3.7
1	A	24	CYS	3.7
1	A	61	LEU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	423	LYS	3.7
1	A	347	ASN	3.6
2	B	390	TYR	3.6
1	A	557	TYR	3.6
1	A	354	ILE	3.6
1	A	868	GLY	3.6
2	B	508	TYR	3.6
1	A	673	SER	3.6
1	A	346	VAL	3.5
1	A	375	ARG	3.5
2	B	332	GLU	3.4
2	B	368	TYR	3.4
2	B	503	ARG	3.4
1	A	341	ALA	3.4
1	A	338	ILE	3.4
2	B	559	ILE	3.4
2	B	385	HIS	3.4
2	B	437	VAL	3.3
1	A	605	ASN	3.3
2	B	584	LEU	3.3
2	B	408	TYR	3.3
1	A	340	CYS	3.3
2	B	506	LYS	3.3
1	A	31	ILE	3.3
1	A	422	LEU	3.2
1	A	423	ALA	3.1
2	B	331	ALA	3.1
1	A	936	HIS	3.1
1	A	32	VAL	3.1
2	B	510	GLU	3.1
1	A	1008	SER	3.1
2	B	549	LEU	3.1
1	A	806	ASP	3.0
2	B	498	CYS	3.0
1	A	419	HIS	3.0
1	A	383	TRP	3.0
2	B	356	LEU	3.0
2	B	399	SER	3.0
2	B	336	GLY	2.9
1	A	381	PRO	2.9
1	A	1053	THR	2.9
2	B	367	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	480	LYS	2.9
2	B	552	GLN	2.9
1	A	677	ASN	2.9
1	A	344	VAL	2.9
2	B	436	VAL	2.9
1	A	679	THR	2.9
1	A	870	LEU	2.9
2	B	532	LYS	2.9
1	A	867	LYS	2.9
1	A	358	THR	2.8
1	A	187	LYS	2.8
1	A	247	GLN	2.8
1	A	389	TYR	2.8
1	A	409	VAL	2.8
1	A	1007	GLY	2.8
1	A	219	GLN	2.8
1	A	1003	SER	2.8
1	A	1015	SER	2.8
1	A	300	ASP	2.8
1	A	106	GLY	2.7
1	A	935	GLY	2.7
1	A	809	GLN	2.7
1	A	837	GLY	2.7
1	A	353	LYS	2.7
2	B	540	ASP	2.7
2	B	499	GLN	2.7
1	A	6	SER	2.6
2	B	346	LYS	2.6
2	B	591	GLN	2.6
1	A	351	ILE	2.6
1	A	408	SER	2.6
2	B	328	LEU	2.5
2	B	495	GLU	2.5
1	A	141	ARG	2.5
1	A	838	CYS	2.5
1	A	308	SER	2.5
1	A	246	TYR	2.5
1	A	805	ASP	2.5
1	A	473	LEU	2.5
2	B	522	GLN	2.5
2	B	384	PHE	2.5
1	A	508	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	604	CYS	2.5
1	A	212	ASN	2.5
2	B	383	ILE	2.5
2	B	529	ASP	2.4
2	B	334	TYR	2.4
1	A	363	GLY	2.4
2	B	386	ARG	2.4
2	B	494	PHE	2.4
2	B	525	MET	2.4
1	A	376	VAL	2.4
1	A	842	GLY	2.3
2	B	598	LEU	2.3
1	A	-27	MET	2.3
1	A	1018	ASP	2.3
2	B	425	LEU	2.3
1	A	-18	HIS	2.3
1	A	69	ILE	2.2
1	A	528	LYS	2.2
1	A	973	LYS	2.2
2	B	491	ILE	2.2
1	A	82	PHE	2.2
2	B	558	GLU	2.2
1	A	985	TYR	2.2
2	B	404	LEU	2.2
2	B	577	ARG	2.2
1	A	813	THR	2.1
2	B	520	GLU	2.1
1	A	148	LYS	2.1
2	B	523	ARG	2.1
1	A	407	CYS	2.1
1	A	972	THR	2.1
1	A	506	PHE	2.1
1	A	933	ASP	2.1
2	B	592	LYS	2.1
1	A	189	GLN	2.1
1	A	343	TYR	2.1
1	A	815	GLN	2.1
1	A	-3	ALA	2.1
2	B	411	GLU	2.1
1	A	53	ALA	2.1
2	B	556	TYR	2.1
2	B	466	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	56	TYR	2.0
2	B	517	ASN	2.0
1	A	960	PHE	2.0
1	A	1005	MET	2.0
2	B	401	VAL	2.0
2	B	586	GLN	2.0
1	A	378	CYS	2.0
2	B	593	LYS	2.0

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, 95^{th} 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	0.52	0.30	173,201,218,220	0
1	SEP	A	790	10/11	0.91	0.16	115,132,186,190	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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
4	71B	A	1102	10/10	0.61	0.67	90,110,118,124	10
3	71A	A	1101	7/7	0.90	1.53	146,162,167,169	0

6.5 Other polymers (i)

There are no such residues in this entry.