



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:38 AM UTC

PDB ID : 5SWO / pdb_00005swo
Title : Crystal Structure of PI3Kalpha in complex with fragments 4 and 19
Authors : Gabelli, S.B.; Vogelstein, B.; Miller, M.S.; Amzel, L.M.
Deposited on : 2016-08-08
Resolution : 3.50 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

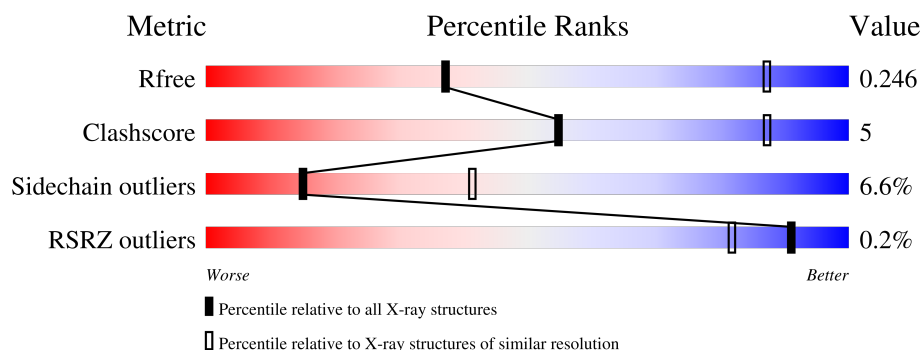
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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)
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	 76% 18% . .
2	B	279	 84% 11% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10899 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	1051	Total	C	N	O	P	S	0	0	0
			8593	5489	1471	1563	1	69			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP P42336
A	-26	SER	-	expression tag	UNP P42336
A	-25	TYR	-	expression tag	UNP P42336
A	-24	TYR	-	expression tag	UNP P42336
A	-23	HIS	-	expression tag	UNP P42336
A	-22	HIS	-	expression tag	UNP P42336
A	-21	HIS	-	expression tag	UNP P42336
A	-20	HIS	-	expression tag	UNP P42336
A	-19	HIS	-	expression tag	UNP P42336
A	-18	HIS	-	expression tag	UNP P42336
A	-17	ASP	-	expression tag	UNP P42336
A	-16	TYR	-	expression tag	UNP P42336
A	-15	ASP	-	expression tag	UNP P42336
A	-14	ILE	-	expression tag	UNP P42336
A	-13	PRO	-	expression tag	UNP P42336
A	-12	THR	-	expression tag	UNP P42336
A	-11	THR	-	expression tag	UNP P42336
A	-10	GLU	-	expression tag	UNP P42336
A	-9	ASN	-	expression tag	UNP P42336
A	-8	LEU	-	expression tag	UNP P42336
A	-7	TYR	-	expression tag	UNP P42336
A	-6	PHE	-	expression tag	UNP P42336
A	-5	GLN	-	expression tag	UNP P42336
A	-4	GLY	-	expression tag	UNP P42336
A	-3	ALA	-	expression tag	UNP P42336
A	-2	MET	-	expression tag	UNP P42336

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

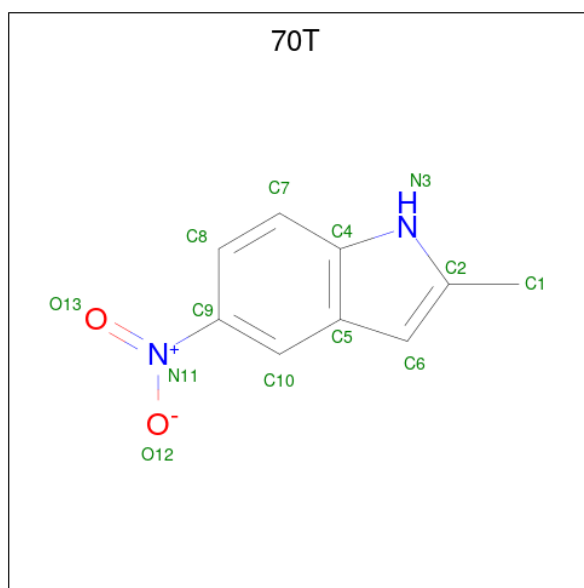
- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	267	Total	C	N	O	S	0	0	0
			2281	1433	407	435	6			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

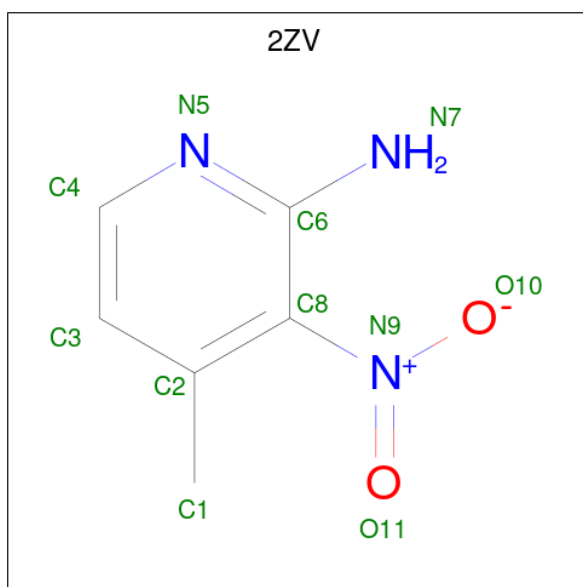
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 2-methyl-5-nitro-1H-indole (CCD ID: 70T) (formula: C₉H₈N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			13	9	2	2		

- Molecule 5 is 4-methyl-3-nitropyridin-2-amine (CCD ID: 2ZV) (formula: C₆H₇N₃O₂).

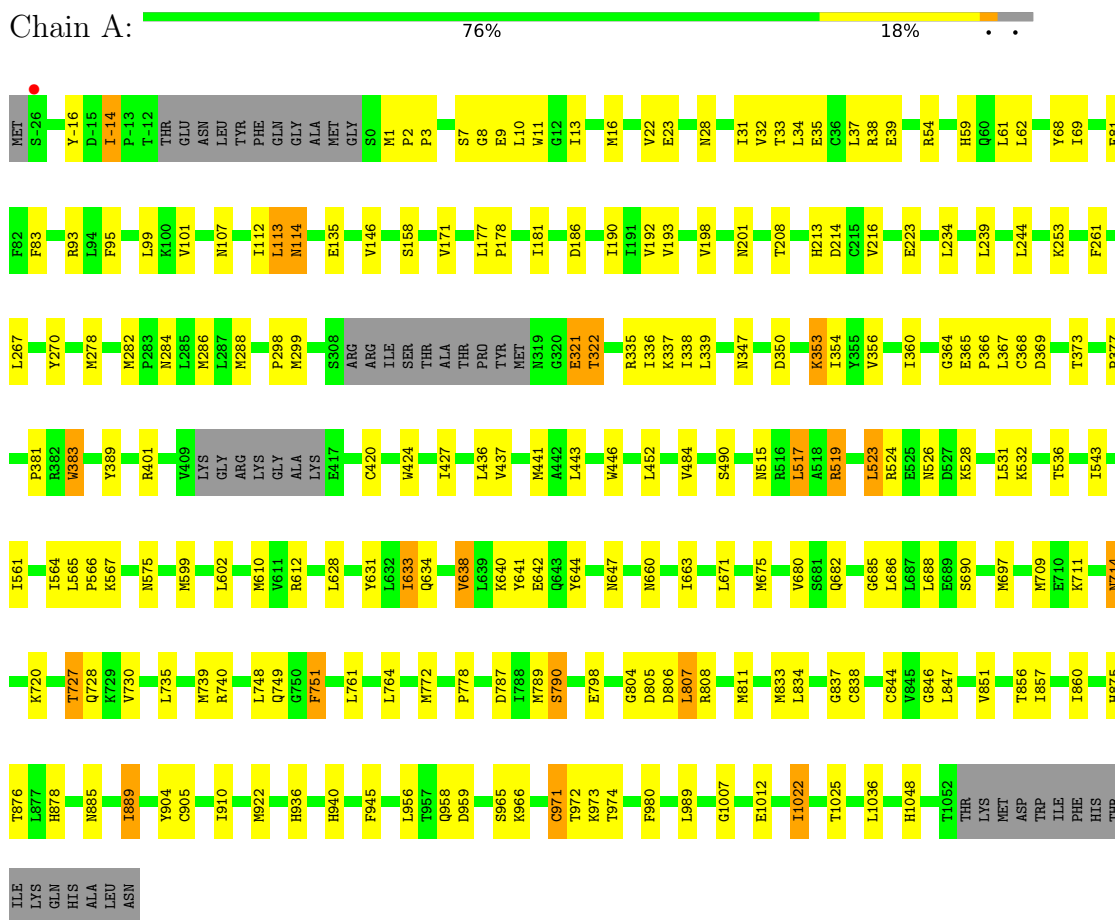


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	11	6	3	2	0	0

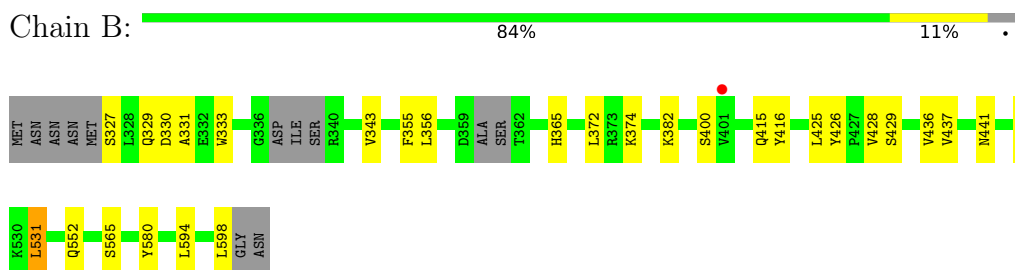
3 Residue-property plots

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	114.83Å 116.36Å 149.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.81 – 3.50 91.81 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (91.81-3.50) 99.4 (91.81-3.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.189 , 0.274 (Not available) , 0.246	Depositor DCC
R_{free} test set	1322 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å ²)	99.6	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 91.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10899	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: CL, 70T, SEP, 2ZV

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	1/8783 (0.0%)	1.02	16/11874 (0.1%)
2	B	0.69	0/2319	0.96	1/3103 (0.0%)
All	All	0.74	1/11102 (0.0%)	1.01	17/14977 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	364	GLY	N-CA	7.16	1.52	1.44

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	GLU	N-CA-C	9.10	121.10	109.72
1	A	198	VAL	N-CA-C	6.90	117.07	111.62
1	A	633	ILE	N-CA-CB	6.44	118.08	110.55
1	A	633	ILE	CB-CA-C	-6.30	103.91	111.97
1	A	751	PHE	N-CA-C	6.25	116.82	108.38
1	A	805	ASP	N-CA-C	6.17	123.94	110.80
1	A	515	ASN	N-CA-C	6.13	117.55	108.60
1	A	114	ASN	N-CA-C	-5.83	106.21	113.38
2	B	355	PHE	N-CA-C	5.82	117.10	108.60
1	A	846	GLY	N-CA-C	5.78	118.95	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	PRO	N-CA-C	5.72	117.67	110.70
1	A	808	ARG	N-CA-C	5.43	119.39	112.87
1	A	146	VAL	CB-CA-C	-5.38	105.09	111.97
1	A	837	GLY	N-CA-C	5.34	117.61	111.36
1	A	366	PRO	N-CA-C	5.33	120.59	114.20
1	A	517	LEU	CA-C-N	5.01	127.30	120.54
1	A	517	LEU	C-N-CA	5.01	127.30	120.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8593	0	8554	97	0
2	B	2281	0	2262	11	0
3	A	1	0	0	0	0
4	A	13	0	0	0	0
5	B	11	0	7	1	0
All	All	10899	0	10823	104	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 5.

All (104) 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)
5:B:701:2ZV:O11	5:B:701:2ZV:N9	1.58	1.37
1:A:610:MET:HA	1:A:610:MET:HE2	1.66	0.78
1:A:709:MET:HE1	1:A:847:LEU:HD21	1.67	0.75
1:A:31:ILE:HD11	2:B:531:LEU:HD13	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:ILE:HD11	1:A:567:LYS:HD3	1.79	0.64
1:A:519:ARG:HB2	1:A:523:LEU:HA	1.81	0.63
1:A:640:LYS:HE2	1:A:680:VAL:HG11	1.81	0.63
1:A:336:ILE:HD12	1:A:389:TYR:CE2	2.34	0.62
1:A:10:LEU:HD13	1:A:16:MET:HE2	1.82	0.62
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.26	0.60
1:A:278:MET:HA	1:A:278:MET:HE2	1.83	0.60
1:A:602:LEU:O	1:A:612:ARG:NH2	2.34	0.60
1:A:178:PRO:HD2	1:A:181:ILE:HD12	1.82	0.59
1:A:806:ASP:HB2	1:A:844:CYS:SG	2.42	0.59
1:A:675:MET:HE1	1:A:685:GLY:N	2.19	0.58
1:A:261:PHE:HA	1:A:270:TYR:CE2	2.39	0.58
1:A:171:VAL:HG12	1:A:270:TYR:HA	1.87	0.57
1:A:807:LEU:HD12	1:A:838:CYS:SG	2.45	0.57
1:A:789:MET:O	1:A:790:SEP:C	2.52	0.56
1:A:599:MET:HE1	1:A:631:TYR:CB	2.35	0.56
1:A:61:LEU:HD11	2:B:508:TYR:CZ	2.41	0.56
1:A:367:LEU:HD12	1:A:368:CYS:O	2.05	0.56
1:A:321:GLU:O	1:A:322:THR:HG23	2.07	0.55
2:B:333:TRP:HA	2:B:429:SER:HB2	1.89	0.54
1:A:23:GLU:CG	1:A:33:THR:HG22	2.37	0.54
1:A:965:SER:HB2	1:A:974:THR:HG21	1.90	0.54
1:A:-16:TYR:HE1	1:A:-14:ILE:HG23	1.73	0.54
1:A:834:LEU:HD21	1:A:851:VAL:HG21	1.90	0.54
1:A:8:GLY:HA3	1:A:714:ASN:HD21	1.73	0.53
1:A:628:LEU:HD23	1:A:663:ILE:HD13	1.90	0.52
1:A:561:ILE:O	1:A:564:ILE:HG22	2.09	0.52
1:A:28:ASN:ND2	1:A:62:LEU:HD21	2.25	0.52
1:A:936:HIS:HB3	1:A:940:HIS:HB3	1.92	0.52
1:A:519:ARG:NH1	1:A:523:LEU:HD22	2.25	0.51
1:A:772:MET:HB2	1:A:778:PRO:HG2	1.93	0.51
1:A:424:TRP:CE2	1:A:446:TRP:HB2	2.46	0.51
1:A:3:PRO:HG3	1:A:804:GLY:HA2	1.92	0.51
1:A:32:VAL:O	1:A:32:VAL:HG23	2.11	0.51
1:A:856:THR:HG23	1:A:922:MET:HE3	1.93	0.51
2:B:343:VAL:HG13	2:B:356:LEU:HD11	1.93	0.51
1:A:298:PRO:HG2	1:A:697:MET:HG3	1.92	0.50
1:A:1022:ILE:HA	1:A:1025:THR:HG22	1.93	0.50
1:A:23:GLU:HG2	1:A:33:THR:HG22	1.93	0.50
1:A:599:MET:HE1	1:A:631:TYR:HB3	1.95	0.48
1:A:360:ILE:N	1:A:360:ILE:HD12	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:878:HIS:NE2	1:A:966:LYS:O	2.46	0.48
1:A:885:ASN:HB3	1:A:889:ILE:HG22	1.95	0.48
1:A:524:ARG:HD3	1:A:526:ASN:HD22	1.78	0.48
1:A:945:PHE:HB2	2:B:598:LEU:HD13	1.96	0.47
1:A:956:LEU:HD11	1:A:980:PHE:CZ	2.50	0.47
1:A:8:GLY:CA	1:A:714:ASN:HD21	2.27	0.47
1:A:337:LYS:HD3	1:A:339:LEU:HD11	1.95	0.47
1:A:735:LEU:O	1:A:739:MET:HG3	2.15	0.46
1:A:610:MET:HA	1:A:610:MET:CE	2.42	0.46
1:A:971:CYS:C	1:A:973:LYS:H	2.23	0.46
1:A:833:MET:HE1	1:A:904:TYR:HA	1.98	0.46
1:A:910:ILE:O	1:A:1025:THR:HG21	2.15	0.46
1:A:671:LEU:HB2	1:A:688:LEU:HD21	1.98	0.45
1:A:23:GLU:HG3	1:A:33:THR:HG22	1.99	0.45
1:A:213:HIS:CE1	1:A:214:ASP:HB3	2.52	0.45
2:B:436:VAL:HG12	2:B:580:TYR:CD1	2.52	0.45
1:A:353:LYS:HG3	1:A:377:PRO:HB3	1.98	0.45
2:B:327:SER:O	2:B:331:ALA:N	2.50	0.45
1:A:68:TYR:CD1	1:A:101:VAL:HG12	2.52	0.44
1:A:532:LYS:O	1:A:536:THR:HG23	2.18	0.44
1:A:427:ILE:HG12	1:A:443:LEU:HD13	1.98	0.44
1:A:856:THR:O	1:A:857:ILE:C	2.60	0.44
1:A:192:VAL:HG12	1:A:193:VAL:N	2.33	0.44
1:A:81:GLU:HB2	1:A:83:PHE:CZ	2.53	0.43
1:A:528:LYS:HA	1:A:531:LEU:HD12	2.00	0.43
1:A:772:MET:HA	1:A:772:MET:HE2	1.99	0.43
1:A:958:GLN:O	1:A:959:ASP:C	2.61	0.43
1:A:54:ARG:HG2	1:A:59:HIS:CE1	2.53	0.43
1:A:749:GLN:HE21	1:A:764:LEU:H	1.66	0.43
1:A:354:ILE:HD11	1:A:381:PRO:HB3	2.01	0.43
1:A:356:VAL:HG23	1:A:383:TRP:CH2	2.54	0.43
1:A:9:GLU:OE1	1:A:38:ARG:NH1	2.51	0.42
1:A:11:TRP:HB2	1:A:95:PHE:CD1	2.54	0.42
1:A:135:GLU:OE2	1:A:644:TYR:HB3	2.18	0.42
1:A:727:THR:O	1:A:728:GLN:C	2.62	0.42
1:A:660:ASN:OD1	1:A:660:ASN:C	2.63	0.42
1:A:1:MET:HB2	1:A:720:LYS:HE3	2.01	0.42
1:A:634:GLN:O	1:A:638:VAL:HB	2.20	0.42
1:A:739:MET:HE2	1:A:748:LEU:HD13	2.02	0.42
1:A:751:PHE:CE2	1:A:761:LEU:HD12	2.55	0.42
1:A:282:MET:O	1:A:284:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:506:LYS:HA	2:B:509:ILE:HG22	2.01	0.41
1:A:338:ILE:O	1:A:339:LEU:HD12	2.21	0.41
1:A:347:ASN:ND2	2:B:565:SER:OG	2.51	0.41
1:A:875:HIS:O	1:A:876:THR:C	2.64	0.41
1:A:267:LEU:HD23	1:A:267:LEU:HA	1.97	0.41
1:A:945:PHE:CB	2:B:598:LEU:HD13	2.49	0.41
1:A:13:ILE:HD12	1:A:13:ILE:O	2.20	0.41
1:A:253:LYS:HB3	1:A:286:MET:HB3	2.02	0.41
1:A:286:MET:HE3	1:A:288:MET:HE3	2.03	0.41
2:B:426:TYR:HB3	2:B:428:VAL:HG23	2.02	0.41
1:A:436:LEU:HB3	1:A:484:VAL:HB	2.03	0.40
1:A:565:LEU:HB3	1:A:566:PRO:HD3	2.03	0.40
1:A:641:TYR:OH	1:A:1007:GLY:N	2.55	0.40
1:A:936:HIS:ND1	1:A:1012:GLU:OE2	2.55	0.40
1:A:989:LEU:HD11	1:A:1036:LEU:HD11	2.04	0.40
1:A:-16:TYR:CD1	1:A:-16:TYR:C	2.99	0.40
1:A:-14:ILE:HD13	1:A:-14:ILE:N	2.36	0.40
1:A:727:THR:O	1:A:730:VAL:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	960/998 (96%)	896 (93%)	64 (7%)	15	41
2	B	249/259 (96%)	233 (94%)	16 (6%)	16	42
All	All	1209/1257 (96%)	1129 (93%)	80 (7%)	15	41

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-14	ILE
1	A	7	SER
1	A	22	VAL
1	A	34	LEU
1	A	35	GLU
1	A	37	LEU
1	A	39	GLU
1	A	69	ILE
1	A	93	ARG
1	A	99	LEU
1	A	107	ASN
1	A	112	ILE
1	A	113	LEU
1	A	114	ASN
1	A	158	SER
1	A	177	LEU
1	A	186	ASP
1	A	190	ILE
1	A	201	ASN
1	A	208	THR
1	A	216	VAL
1	A	223	GLU
1	A	234	LEU
1	A	239	LEU
1	A	244	LEU
1	A	299	MET
1	A	321	GLU
1	A	322	THR
1	A	335	ARG
1	A	350	ASP
1	A	353	LYS
1	A	369	ASP
1	A	373	THR
1	A	383	TRP
1	A	401	ARG
1	A	420	CYS
1	A	437	VAL
1	A	441	MET
1	A	452	LEU
1	A	490	SER
1	A	517	LEU
1	A	519	ARG

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Mol	Chain	Res	Type
1	A	523	LEU
1	A	575	ASN
1	A	633	ILE
1	A	638	VAL
1	A	682	GLN
1	A	686	LEU
1	A	690	SER
1	A	711	LYS
1	A	714	ASN
1	A	727	THR
1	A	740	ARG
1	A	787	ASP
1	A	798	GLU
1	A	807	LEU
1	A	811	MET
1	A	860	ILE
1	A	889	ILE
1	A	905	CYS
1	A	971	CYS
1	A	972	THR
1	A	1022	ILE
1	A	1048	HIS
2	B	329	GLN
2	B	330	ASP
2	B	365	HIS
2	B	372	LEU
2	B	374	LYS
2	B	382	LYS
2	B	400	SER
2	B	415	GLN
2	B	416	TYR
2	B	425	LEU
2	B	437	VAL
2	B	441	ASN
2	B	529	ASP
2	B	531	LEU
2	B	552	GLN
2	B	594	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	183	ASN
1	A	374	GLN
1	A	380	ASN
1	A	467	ASN
1	A	497	ASN
1	A	510	HIS
1	A	526	ASN
1	A	556	HIS
1	A	575	ASN
1	A	597	GLN
1	A	643	GLN
1	A	670	HIS
1	A	682	GLN
1	A	714	ASN
1	A	721	GLN
1	A	749	GLN
1	A	917	HIS
1	A	918	ASN
1	A	996	ASN
2	B	415	GLN
2	B	457	GLN
2	B	475	GLN
2	B	552	GLN
2	B	564	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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
1	SEP	A	790	1	8,9,10	0.73	0	7,12,14	1.86	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	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	3.74	111.79	108.14
1	A	790	SEP	O2P-P-OG	-2.45	100.28	106.67

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	70T	A	1102	-	14,14,14	1.50	1 (7%)	17,20,20	3.42	6 (35%)
5	2ZV	B	701	-	11,11,11	6.82	5 (45%)	11,15,15	1.41	2 (18%)

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	70T	A	1102	-	-	2/2/4/4	0/2/2/2
5	2ZV	B	701	-	-	0/0/4/4	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	701	2ZV	O11-N9	20.54	1.58	1.22
5	B	701	2ZV	C8-N9	-6.53	1.34	1.45
5	B	701	2ZV	C1-C2	-5.09	1.41	1.51
4	A	1102	70T	C5-C4	4.48	1.48	1.41
5	B	701	2ZV	C4-N5	3.53	1.42	1.34
5	B	701	2ZV	O10-N9	2.37	1.50	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1102	70T	C1-C2-C6	-9.65	116.54	131.95
4	A	1102	70T	C1-C2-N3	6.90	132.65	121.55
4	A	1102	70T	C6-C2-N3	4.15	110.81	107.60
4	A	1102	70T	C7-C4-C5	-3.76	118.73	122.13
4	A	1102	70T	C7-C4-N3	2.81	136.51	130.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1102	70T	C5-C4-N3	-2.77	104.77	107.65
5	B	701	2ZV	C3-C4-N5	-2.57	120.82	123.97
5	B	701	2ZV	C8-C6-N7	-2.30	117.44	123.84

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1102	70T	C8-C9-N11-O13
4	A	1102	70T	C10-C9-N11-O13

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	701	2ZV	1	0

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	1050/1096 (95%)	-0.64	1 (0%) 92 86	53, 100, 162, 231	0
2	B	267/279 (95%)	-0.44	1 (0%) 88 72	97, 162, 206, 228	0
All	All	1317/1375 (95%)	-0.60	2 (0%) 91 82	53, 108, 187, 231	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	401	VAL	2.1
1	A	-26	SER	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	790	10/11	0.91	0.07	82,100,161,174	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
5	2ZV	B	701	11/11	0.84	0.12	153,178,200,201	0
4	70T	A	1102	13/13	0.90	0.14	109,132,144,144	0
3	CL	A	1101	1/1	0.98	0.11	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.