



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:53 PM UTC

PDB ID : 5SWP / pdb_00005swp
Title : Crystal Structure of PI3Kalpha in complex with fragments 6 and 24
Authors : Gabelli, S.B.; Vogelstein, B.; Miller, M.S.; Amzel, L.M.
Deposited on : 2016-08-08
Resolution : 3.41 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

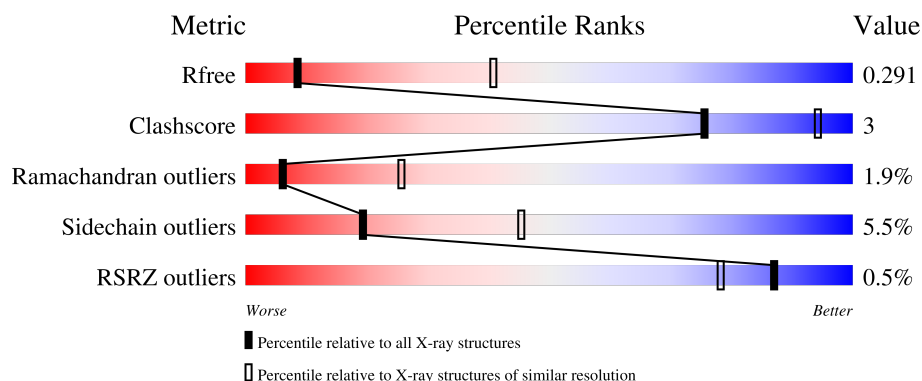
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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	 82% 14% . .
2	B	279	 79% 13% • 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10919 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	1060	Total	C	N	O	P	S	0	0	0
			8667	5532	1485	1578	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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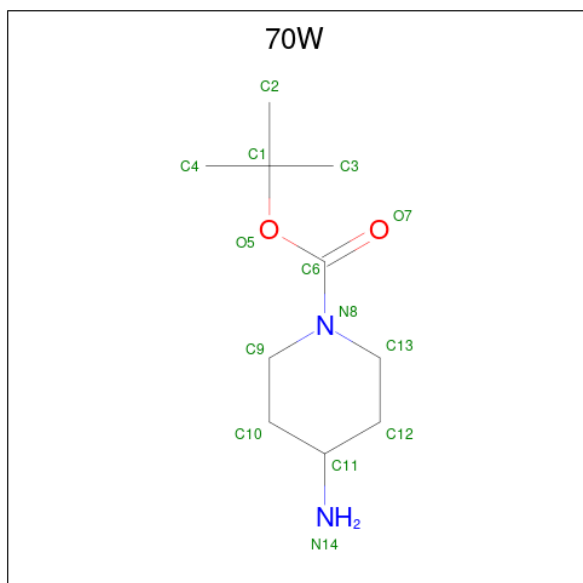
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42336
A	0	SER	-	expression tag	UNP P42336

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

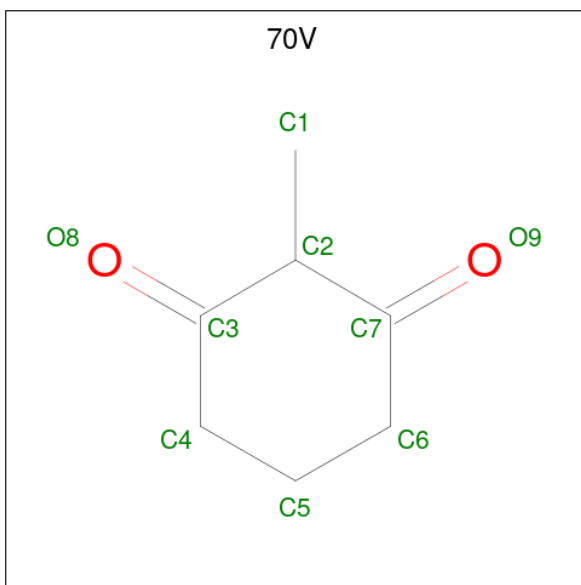
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2205	1383	396	420	6			

- Molecule 3 is tert-butyl 4-aminopiperidine-1-carboxylate (CCD ID: 70W) (formula: $C_{10}H_{20}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	10	2	2		
3	A	1	Total	C	N	O	0	0
			14	10	2	2		

- Molecule 4 is 2-methylcyclohexane-1,3-dione (CCD ID: 70V) (formula: $C_7H_{10}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			9	7	2		
4	B	1	Total	C	O	0	0
			9	7	2		

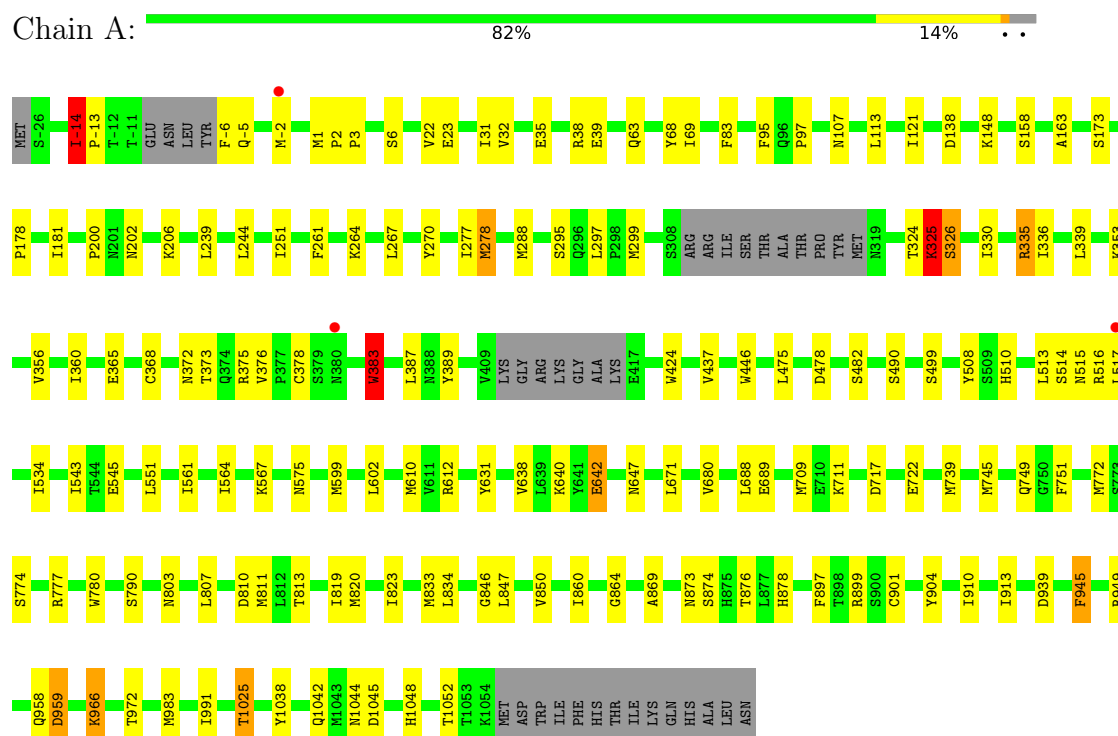
- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

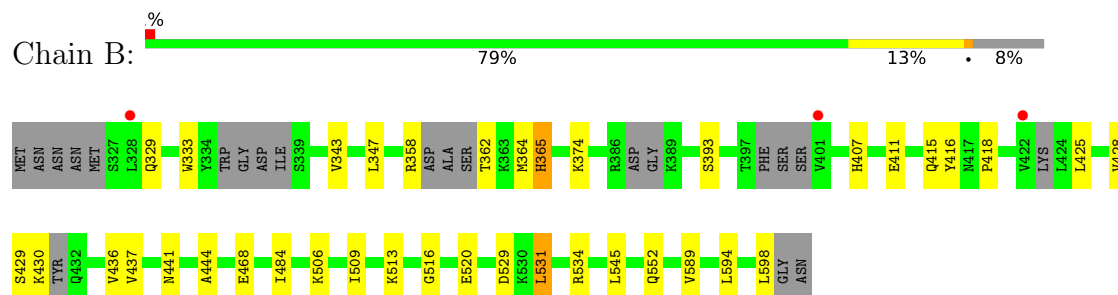
3 Residue-property plots

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	114.12Å 116.13Å 148.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.41 50.00 – 3.41	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-3.41) 99.2 (50.00-3.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.216 , 0.296 0.216 , 0.291	Depositor DCC
R_{free} test set	1397 reflections (3.31%)	wwPDB-VP
Wilson B-factor (Å ²)	99.2	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 88.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10919	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: 70W, CL, SEP, 70V

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.63	0/8847	0.92	7/11956 (0.1%)
2	B	0.63	0/2235	0.92	0/2983
All	All	0.63	0/11082	0.92	7/14939 (0.0%)

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

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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	365	GLU	N-CA-C	5.61	117.57	109.04
1	A	383	TRP	N-CA-C	-5.43	101.03	109.72
1	A	-14	ILE	N-CA-C	5.25	120.22	108.88
1	A	850	VAL	CB-CA-C	-5.21	104.99	111.08
1	A	846	GLY	N-CA-C	5.19	119.06	110.55
1	A	751	PHE	N-CA-C	5.15	115.33	108.38
1	A	326	SER	N-CA-C	-5.01	101.14	109.46

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	325	LYS	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	8667	0	8627	54	0
2	B	2205	0	2198	15	0
3	A	28	0	0	0	0
4	A	9	0	0	0	0
4	B	9	0	0	0	0
5	A	1	0	0	0	0
All	All	10919	0	10825	66	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 (66) 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)
2:B:407:HIS:HE1	2:B:411:GLU:OE1	1.47	0.97
2:B:407:HIS:CE1	2:B:411:GLU:OE1	2.19	0.94
1:A:745:MET:SD	1:A:749:GLN:NE2	2.68	0.66
1:A:709:MET:HE1	1:A:847:LEU:HD21	1.77	0.65
1:A:163:ALA:HB2	1:A:297:LEU:HD11	1.81	0.61
2:B:429:SER:O	2:B:430:LYS:C	2.43	0.61
2:B:333:TRP:HA	2:B:429:SER:HB2	1.86	0.56
1:A:31:ILE:HD11	2:B:531:LEU:HD13	1.87	0.56
1:A:372:ASN:HB3	1:A:387:LEU:HD21	1.88	0.56
1:A:339:LEU:O	1:A:383:TRP:O	2.26	0.54
1:A:325:LYS:HG2	1:A:330:ILE:HD11	1.90	0.53
1:A:602:LEU:O	1:A:612:ARG:NH2	2.41	0.53
1:A:640:LYS:HE2	1:A:680:VAL:HG11	1.91	0.53
1:A:261:PHE:HA	1:A:270:TYR:CE2	2.45	0.52
1:A:910:ILE:O	1:A:1025:THR:HG21	2.10	0.51
1:A:873:ASN:HB3	1:A:876:THR:HG23	1.93	0.51
1:A:278:MET:HA	1:A:278:MET:HE2	1.93	0.50
1:A:599:MET:HE1	1:A:631:TYR:CB	2.42	0.49
1:A:945:PHE:CG	2:B:598:LEU:HB3	2.47	0.49
1:A:717:ASP:OD1	1:A:803:ASN:ND2	2.46	0.49
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:506:LYS:HA	2:B:509:ILE:HG22	1.96	0.48
2:B:362:THR:HG22	2:B:364:MET:N	2.29	0.47
1:A:819:ILE:HG22	1:A:823:ILE:HD12	1.96	0.47
2:B:516:GLY:O	2:B:520:GLU:N	2.48	0.47
1:A:534:ILE:HG21	1:A:551:LEU:HD11	1.97	0.46
1:A:774:SER:O	1:A:777:ARG:NH1	2.47	0.46
1:A:335:ARG:NE	1:A:478:ASP:OD2	2.48	0.45
1:A:864:GLY:O	1:A:876:THR:HG21	2.16	0.45
1:A:878:HIS:CE1	1:A:966:LYS:O	2.70	0.45
1:A:739:MET:O	1:A:745:MET:HE3	2.16	0.45
1:A:-14:ILE:HD13	1:A:-13:PRO:HD3	1.98	0.45
1:A:1038:TYR:O	1:A:1042:GLN:HG2	2.17	0.45
1:A:424:TRP:CE2	1:A:446:TRP:HB2	2.51	0.45
1:A:878:HIS:NE2	1:A:966:LYS:O	2.49	0.45
1:A:63:GLN:HB2	1:A:68:TYR:CE2	2.51	0.45
1:A:23:GLU:OE1	2:B:534:ARG:NE	2.48	0.44
1:A:121:ILE:HD11	1:A:689:GLU:HA	2.00	0.44
1:A:939:ASP:OD1	1:A:949:ARG:NH2	2.51	0.43
1:A:610:MET:HA	1:A:610:MET:HE2	1.99	0.43
1:A:897:PHE:O	1:A:901:CYS:HB2	2.18	0.43
1:A:336:ILE:HD12	1:A:389:TYR:CE1	2.53	0.43
1:A:899:ARG:NH1	1:A:983:MET:HE1	2.34	0.43
1:A:181:ILE:HG23	1:A:277:ILE:HG21	1.99	0.43
2:B:407:HIS:ND1	2:B:407:HIS:C	2.76	0.43
1:A:561:ILE:O	1:A:564:ILE:HG22	2.18	0.43
2:B:343:VAL:HG12	2:B:347:LEU:HD12	2.01	0.43
1:A:772:MET:HE3	1:A:780:TRP:HB2	2.01	0.43
1:A:810:ASP:HA	1:A:813:THR:HG22	2.01	0.43
2:B:484:ILE:HG13	2:B:545:LEU:HD23	2.01	0.42
1:A:833:MET:HE1	1:A:904:TYR:HA	2.01	0.42
1:A:22:VAL:HG12	1:A:97:PRO:HB2	2.01	0.42
1:A:958:GLN:O	1:A:959:ASP:C	2.62	0.41
1:A:820:MET:HG2	1:A:991:ILE:HD12	2.03	0.41
1:A:69:ILE:HD11	1:A:83:PHE:HA	2.03	0.41
1:A:356:VAL:HG23	1:A:383:TRP:CH2	2.55	0.41
1:A:745:MET:HA	1:A:745:MET:HE2	2.03	0.41
1:A:360:ILE:HD12	1:A:360:ILE:N	2.36	0.41
1:A:671:LEU:HB2	1:A:688:LEU:HD21	2.03	0.40
1:A:375:ARG:O	1:A:376:VAL:C	2.64	0.40
1:A:899:ARG:HG2	1:A:983:MET:HE1	2.04	0.40
1:A:178:PRO:HD2	1:A:181:ILE:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:362:THR:HG22	2:B:364:MET:H	1.86	0.40
2:B:441:ASN:HB3	2:B:444:ALA:HB3	2.03	0.40
1:A:543:ILE:HD11	1:A:567:LYS:HD3	2.04	0.40
1:A:1044:ASN:O	1:A:1048:HIS:N	2.53	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	1050/1096 (96%)	937 (89%)	95 (9%)	18 (2%)	7	27
2	B	244/279 (88%)	220 (90%)	17 (7%)	7 (3%)	3	19
All	All	1294/1375 (94%)	1157 (89%)	112 (9%)	25 (2%)	6	26

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
1	A	3	PRO
1	A	514	SER
2	B	365	HIS
1	A	202	ASN
1	A	264	LYS
1	A	378	CYS
1	A	869	ALA
1	A	945	PHE
1	A	966	LYS
1	A	972	THR
2	B	513	LYS
1	A	95	PHE
1	A	517	LEU

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Mol	Chain	Res	Type
1	A	508	TYR
2	B	393	SER
1	A	959	ASP
1	A	1052	THR
2	B	418	PRO
1	A	38	ARG
1	A	913	ILE
2	B	589	VAL
2	B	436	VAL
2	B	428	VAL
1	A	200	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	966/997 (97%)	912 (94%)	54 (6%)	19	45
2	B	242/259 (93%)	229 (95%)	13 (5%)	20	46
All	All	1208/1256 (96%)	1141 (94%)	67 (6%)	19	45

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-14	ILE
1	A	-6	PHE
1	A	-5	GLN
1	A	-2	MET
1	A	1	MET
1	A	6	SER
1	A	32	VAL
1	A	35	GLU
1	A	39	GLU
1	A	107	ASN
1	A	113	LEU
1	A	138	ASP

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Mol	Chain	Res	Type
1	A	148	LYS
1	A	158	SER
1	A	173	SER
1	A	206	LYS
1	A	239	LEU
1	A	244	LEU
1	A	251	ILE
1	A	267	LEU
1	A	278	MET
1	A	288	MET
1	A	295	SER
1	A	299	MET
1	A	324	THR
1	A	325	LYS
1	A	326	SER
1	A	335	ARG
1	A	353	LYS
1	A	368	CYS
1	A	373	THR
1	A	383	TRP
1	A	437	VAL
1	A	475	LEU
1	A	482	SER
1	A	490	SER
1	A	499	SER
1	A	510	HIS
1	A	513	LEU
1	A	515	ASN
1	A	516	ARG
1	A	545	GLU
1	A	575	ASN
1	A	638	VAL
1	A	642	GLU
1	A	711	LYS
1	A	722	GLU
1	A	807	LEU
1	A	811	MET
1	A	834	LEU
1	A	860	ILE
1	A	874	SER
1	A	1025	THR
1	A	1045	ASP

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Mol	Chain	Res	Type
2	B	329	GLN
2	B	358	ARG
2	B	365	HIS
2	B	374	LYS
2	B	415	GLN
2	B	416	TYR
2	B	425	LEU
2	B	437	VAL
2	B	468	GLU
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	114	ASN
1	A	137	GLN
1	A	219	GLN
1	A	331	ASN
1	A	384	ASN
1	A	467	ASN
1	A	497	ASN
1	A	526	ASN
1	A	554	HIS
1	A	575	ASN
1	A	643	GLN
1	A	738	GLN
1	A	760	GLN
1	A	785	ASN
1	A	827	GLN
1	A	917	HIS
2	B	365	HIS
2	B	407	HIS
2	B	432	GLN
2	B	441	ASN
2	B	457	GLN
2	B	527	ASN
2	B	564	ASN
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	790	1	8,9,10	0.63	0	7,12,14	2.08	1 (14%)
1	SEP	A	7	1	8,9,10	0.73	0	7,12,14	1.21	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
1	SEP	A	790	1	-	5/6/8/10	-
1	SEP	A	7	1	-	1/6/8/10	-

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	4.67	112.69	108.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
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.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
3	70W	A	1101	-	14,14,14	2.30	1 (7%)	20,20,20	2.90	6 (30%)
3	70W	A	1102	-	14,14,14	2.17	2 (14%)	20,20,20	1.92	4 (20%)
4	70V	A	1103	-	9,9,9	0.63	0	9,12,12	2.55	2 (22%)
4	70V	B	701	-	9,9,9	0.51	0	9,12,12	2.52	2 (22%)

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	70W	A	1101	-	-	2/9/19/19	0/1/1/1
3	70W	A	1102	-	-	9/9/19/19	0/1/1/1
4	70V	A	1103	-	-	-	0/1/1/1
4	70V	B	701	-	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	70W	O5-C6	7.84	1.48	1.33
3	A	1102	70W	O5-C6	7.26	1.47	1.33
3	A	1102	70W	O5-C1	-2.32	1.44	1.48

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	70W	O5-C6-N8	6.58	120.77	110.78
3	A	1101	70W	C1-O5-C6	6.50	128.08	120.92
3	A	1101	70W	C12-C11-C10	-5.45	104.74	110.29
3	A	1101	70W	O5-C6-O7	-5.34	117.83	126.43
3	A	1102	70W	O5-C6-N8	5.27	118.77	110.78
4	A	1103	70V	C6-C7-C2	5.23	121.06	115.02
4	B	701	70V	C6-C7-C2	5.05	120.84	115.02
4	B	701	70V	C4-C3-C2	4.80	120.56	115.02
4	A	1103	70V	C4-C3-C2	4.72	120.47	115.02
3	A	1102	70W	O5-C6-O7	-4.60	119.02	126.43
3	A	1102	70W	C1-O5-C6	3.61	124.90	120.92
3	A	1101	70W	C13-N8-C9	3.50	119.81	112.68
3	A	1101	70W	C10-C9-N8	2.13	114.84	110.66
3	A	1102	70W	C13-N8-C9	2.13	117.02	112.68

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	70W	O7-C6-O5-C1
3	A	1101	70W	N8-C6-O5-C1
3	A	1102	70W	O5-C6-N8-C9
3	A	1102	70W	O5-C6-N8-C13
3	A	1102	70W	O7-C6-N8-C9
3	A	1102	70W	O7-C6-N8-C13
3	A	1102	70W	N8-C6-O5-C1
3	A	1102	70W	O7-C6-O5-C1
3	A	1102	70W	C2-C1-O5-C6
3	A	1102	70W	C3-C1-O5-C6
3	A	1102	70W	C4-C1-O5-C6

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	1058/1096 (96%)	-0.42	3 (0%)	90 84	56, 102, 166, 228	0
2	B	258/279 (92%)	-0.13	3 (1%)	76 64	100, 154, 197, 223	0
All	All	1316/1375 (95%)	-0.36	6 (0%)	87 78	56, 111, 184, 228	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	401	VAL	4.3
1	A	517	LEU	2.7
1	A	380	ASN	2.3
2	B	422	VAL	2.1
1	A	-2	MET	2.1
2	B	328	LEU	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, 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	0.61	0.14	139,178,197,201	0
1	SEP	A	790	10/11	0.90	0.08	92,107,153,159	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	70V	A	1103	9/9	0.86	0.10	124,139,142,143	0
3	70W	A	1102	14/14	0.88	0.15	144,159,175,176	0
4	70V	B	701	9/9	0.88	0.11	150,156,161,163	0
3	70W	A	1101	14/14	0.89	0.13	100,113,125,126	0
5	CL	A	1104	1/1	0.97	0.09	78,78,78,78	0

6.5 Other polymers

There are no such residues in this entry.