WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 01:06 AM EDT

PDB ID	:	5SXI
Title	:	Crystal Structure of PI3Kalpha in complex with fragment 13
Authors	:	Gabelli, S.B.; Vogelstein, B.; Miller, M.S.; Amzel, L.M.
Deposited on	:	2016-08-09
Resolution	:	3.40 Å(reported)

The following versions of software and data (see references (i)) 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 ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	Percentile Ranks	Value
Rfree		0.277
Clashscore		4
Ramachandran outliers		1.9%
Sidechain outliers		5.6%
RSRZ outliers		5.7%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
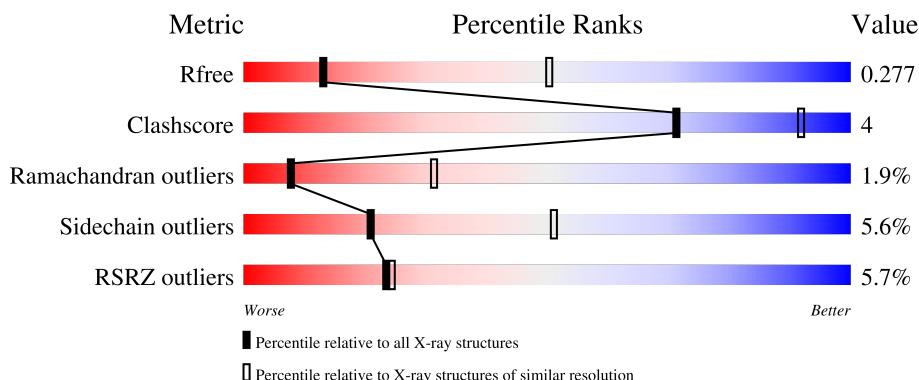
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	2% 79% 16% · 5%
2	B	279	18% 67% 8% 25%
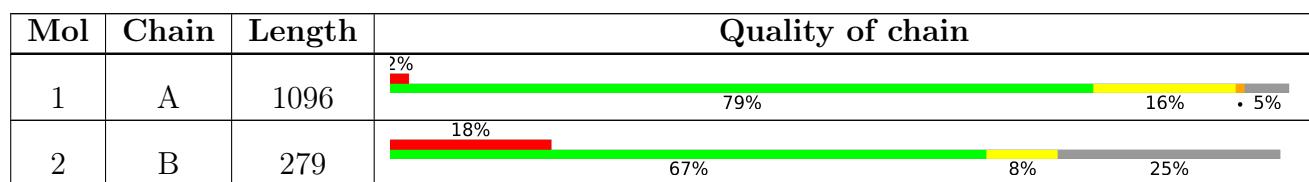
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	71J	B	701	-	-	-	X

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 10360 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	1042	8534	5448	1462	1553	2	69	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

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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	209	Total 1818	C 1142	N 324	O 346	S 6	0	0	0

- Molecule 3 is trans-cyclohexane-1,4-diol (three-letter code: 71J) (formula: $C_6H_{12}O_2$).
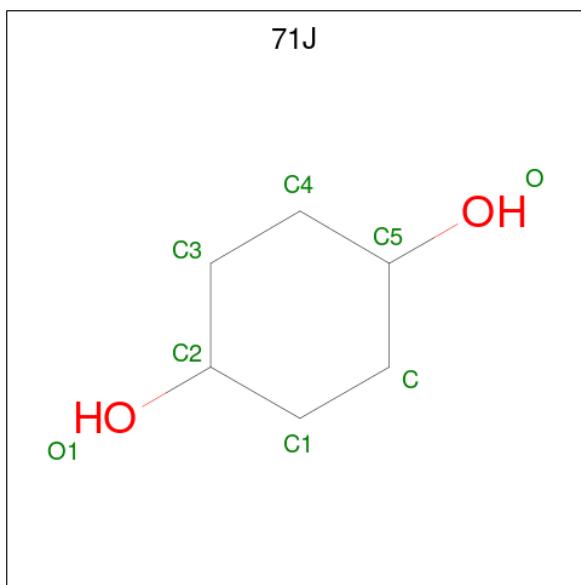
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 8	C 6	O 2	0	0

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

Chain A:
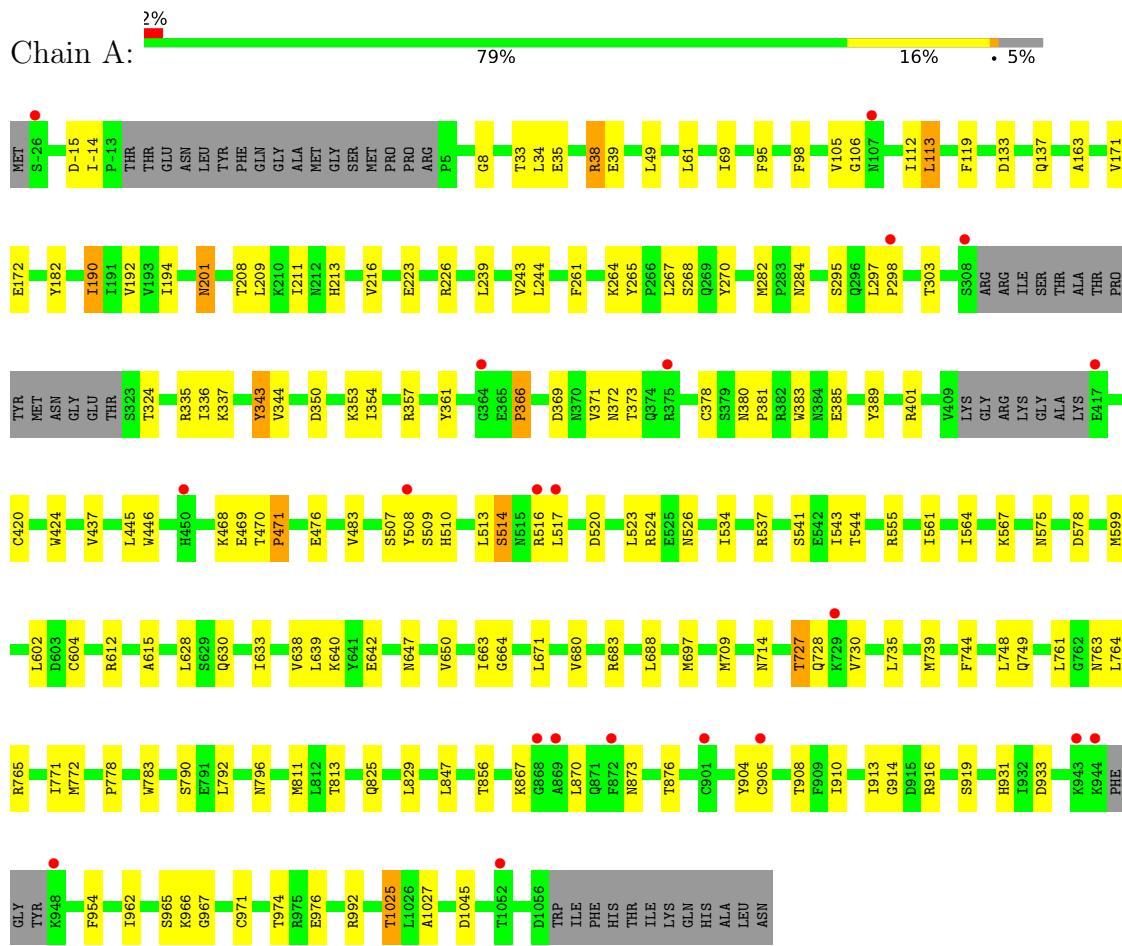
• Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha

Chain B:

ASP GLY LYS TYR GLY PHE SER ASP PRO LEU THR PHE SER SER V401 L404 I405 N406 H407 Y408 R409 N410 E411 S412 L413 A414 Q415 Y416 N417 P418 K419 LEU ASP VAL LYS LEU Y426 P427 V428 SER LYS TYR GLN GLN ASP GLN VAL VAL LYS GLU ASP ASN ILE GLU ALA V445 L449

H450 N453 T454 Q457 R461 R472 T482 T490 Q501 K506 E507 Y508 I509 E510 K511 F512 K513 R514 E515 G516 N517 L531 S536 R543 R577 Y580 L581 M582 W583 L584 T585 Q586 LYS GLY VAL ARG GLN LYS LYS LEU N595 E596 W597 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	114.16Å 116.77Å 150.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.27 – 3.40 34.57 – 3.38	Depositor EDS
% Data completeness (in resolution range)	98.4 (92.27-3.40) 97.9 (34.57-3.38)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 3.39Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.201 , 0.279 0.202 , 0.277	Depositor DCC
R_{free} test set	1443 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	110.8	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 81.6	EDS
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10360	wwPDB-VP
Average B, all atoms (Å^2)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: 71J, SEP

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	0.53	0/8708	0.77	2/11765 (0.0%)
2	B	0.50	0/1843	0.67	0/2457
All	All	0.53	0/10551	0.76	2/14222 (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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	829	LEU	CA-CB-CG	5.47	127.88	115.30
1	A	599	MET	CG-SD-CE	-5.12	92.01	100.20

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	8534	0	8503	70	0
2	B	1818	0	1786	6	0
3	B	8	0	0	0	0
All	All	10360	0	10289	73	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (73) 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:639:LEU:HD22	1:A:650:VAL:HG22	1.74	0.70
1:A:8:GLY:HA2	1:A:714:ASN:HD21	1.58	0.68
1:A:908:THR:OG1	1:A:916:ARG:NH2	2.25	0.68
2:B:343:VAL:HG13	2:B:356:LEU:HD11	1.75	0.67
1:A:544:THR:HG22	2:B:380:LEU:HB3	1.78	0.66
1:A:192:VAL:HG21	1:A:211:ILE:HD11	1.79	0.65
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.17	0.64
1:A:561:ILE:O	1:A:564:ILE:HG22	2.01	0.60
1:A:735:LEU:O	1:A:739:MET:HG3	2.04	0.58
1:A:749:GLN:HE21	1:A:764:LEU:H	1.50	0.58
1:A:910:ILE:O	1:A:1025:THR:HG21	2.05	0.57
1:A:962:ILE:O	1:A:965:SER:O	2.23	0.55
1:A:772:MET:HB2	1:A:778:PRO:HG2	1.88	0.55
1:A:354:ILE:HD11	1:A:381:PRO:HB3	1.89	0.54
1:A:873:ASN:HB3	1:A:876:THR:HG23	1.88	0.54
1:A:424:TRP:CE2	1:A:446:TRP:HB2	2.42	0.54
1:A:354:ILE:HD11	1:A:381:PRO:CB	2.37	0.54
1:A:709:MET:CE	1:A:847:LEU:HD21	2.38	0.53
1:A:61:LEU:HD11	2:B:508:TYR:CZ	2.43	0.53
1:A:640:LYS:HE2	1:A:680:VAL:HG11	1.89	0.53
1:A:709:MET:HE1	1:A:847:LEU:HD21	1.91	0.53
1:A:468:LYS:O	1:A:470:THR:N	2.43	0.52
1:A:8:GLY:CA	1:A:714:ASN:HD21	2.22	0.52
1:A:916:ARG:NH2	1:A:931:HIS:CD2	2.78	0.51
1:A:534:ILE:HA	1:A:537:ARG:HD3	1.92	0.51
1:A:744:PHE:HD2	1:A:748:LEU:HD12	1.76	0.51
1:A:357:ARG:HA	1:A:371:VAL:HG12	1.93	0.51
1:A:324:THR:HG22	1:A:483:VAL:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ILE:HD11	1:A:213:HIS:HA	1.93	0.50
1:A:194:ILE:N	1:A:194:ILE:HD12	2.26	0.49
1:A:98:PHE:CE1	2:B:490:THR:HG23	2.47	0.48
1:A:543:ILE:HD11	1:A:567:LYS:HD3	1.94	0.47
1:A:372:ASN:HB2	1:A:385:GLU:CD	2.34	0.47
1:A:209:LEU:HD13	1:A:223:GLU:HB3	1.97	0.47
1:A:343:TYR:O	1:A:344:VAL:HG23	2.13	0.47
1:A:771:ILE:HG22	1:A:772:MET:O	2.14	0.47
1:A:445:LEU:HG	1:A:471:PRO:O	2.16	0.46
1:A:361:TYR:HA	1:A:366:PRO:HD3	1.97	0.46
2:B:334:TYR:HH	2:B:368:TYR:HE1	1.61	0.46
1:A:171:VAL:HG12	1:A:172:GLU:O	2.16	0.46
1:A:913:ILE:HD12	1:A:914:GLY:N	2.31	0.45
1:A:749:GLN:O	1:A:761:LEU:O	2.36	0.44
1:A:765:ARG:HD3	1:A:796:ASN:HD21	1.81	0.44
2:B:506:LYS:HA	2:B:509:ILE:HG22	2.00	0.44
1:A:727:THR:O	1:A:728:GLN:C	2.56	0.43
1:A:663:ILE:O	1:A:664:GLY:C	2.56	0.43
1:A:764:LEU:HD23	1:A:783:TRP:CD1	2.52	0.43
1:A:282:MET:O	1:A:284:ASN:ND2	2.51	0.43
1:A:163:ALA:HA	1:A:297:LEU:HD11	2.00	0.43
1:A:171:VAL:HG11	1:A:265:TYR:CE1	2.54	0.43
1:A:965:SER:O	1:A:967:GLY:N	2.52	0.43
1:A:908:THR:HG21	1:A:954:PHE:HB2	2.00	0.42
1:A:34:LEU:HD11	1:A:49:LEU:HA	2.00	0.42
1:A:336:ILE:HD12	1:A:389:TYR:CE2	2.54	0.42
1:A:261:PHE:HA	1:A:270:TYR:CE1	2.54	0.42
1:A:602:LEU:O	1:A:612:ARG:NH2	2.53	0.42
1:A:992:ARG:NH2	1:A:1027:ALA:O	2.44	0.42
1:A:243:VAL:HG12	1:A:244:LEU:HD12	2.02	0.42
1:A:727:THR:O	1:A:730:VAL:N	2.53	0.42
1:A:105:VAL:HG13	1:A:106:GLY:N	2.34	0.42
1:A:602:LEU:HD21	1:A:615:ALA:HB3	2.00	0.42
1:A:965:SER:HB2	1:A:974:THR:HG21	2.01	0.42
1:A:337:LYS:HB3	1:A:476:GLU:HB3	2.02	0.41
1:A:524:ARG:HD3	1:A:526:ASN:HD22	1.85	0.41
1:A:628:LEU:HD23	1:A:663:ILE:HD13	2.01	0.41
1:A:671:LEU:HB2	1:A:688:LEU:HD21	2.01	0.41
1:A:904:TYR:CD1	1:A:931:HIS:CD2	3.08	0.41
1:A:749:GLN:HG2	1:A:763:ASN:HA	2.01	0.41
1:A:507:SER:O	1:A:509:SER:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:744:PHE:CD2	1:A:748:LEU:HD12	2.55	0.41
1:A:261:PHE:CD1	1:A:270:TYR:CD1	3.09	0.40
1:A:298:PRO:CG	1:A:697:MET:HG3	2.52	0.40
1:A:517:LEU:HD22	1:A:523:LEU:HD22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1030/1096 (94%)	912 (88%)	100 (10%)	18 (2%)	9	34
2	B	191/279 (68%)	176 (92%)	10 (5%)	5 (3%)	5	26
All	All	1221/1375 (89%)	1088 (89%)	110 (9%)	23 (2%)	8	31

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	508	TYR
2	B	332	GLU
1	A	264	LYS
1	A	378	CYS
1	A	555	ARG
2	B	365	HIS
1	A	514	SER
1	A	966	LYS
1	A	38	ARG
1	A	95	PHE
1	A	201	ASN
1	A	469	GLU
1	A	471	PRO
1	A	520	ASP

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Mol	Chain	Res	Type
1	A	541	SER
1	A	867	LYS
1	A	933	ASP
1	A	133	ASP
1	A	226	ARG
2	B	513	LYS
2	B	517	ASN
2	B	418	PRO
1	A	366	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	953/997 (96%)	897 (94%)	56 (6%)	19	49
2	B	198/259 (76%)	189 (96%)	9 (4%)	27	58
All	All	1151/1256 (92%)	1086 (94%)	65 (6%)	21	51

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-15	ASP
1	A	-14	ILE
1	A	33	THR
1	A	35	GLU
1	A	38	ARG
1	A	39	GLU
1	A	69	ILE
1	A	112	ILE
1	A	113	LEU
1	A	119	PHE
1	A	137	GLN
1	A	182	TYR
1	A	190	ILE
1	A	201	ASN

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Mol	Chain	Res	Type
1	A	208	THR
1	A	216	VAL
1	A	239	LEU
1	A	267	LEU
1	A	268	SER
1	A	295	SER
1	A	303	THR
1	A	335	ARG
1	A	343	TYR
1	A	350	ASP
1	A	353	LYS
1	A	369	ASP
1	A	373	THR
1	A	380	ASN
1	A	383	TRP
1	A	401	ARG
1	A	420	CYS
1	A	437	VAL
1	A	510	HIS
1	A	513	LEU
1	A	514	SER
1	A	516	ARG
1	A	575	ASN
1	A	578	ASP
1	A	604	CYS
1	A	630	GLN
1	A	633	ILE
1	A	638	VAL
1	A	683	ARG
1	A	727	THR
1	A	792	LEU
1	A	811	MET
1	A	813	THR
1	A	825	GLN
1	A	856	THR
1	A	870	LEU
1	A	905	CYS
1	A	919	SER
1	A	971	CYS
1	A	976	GLU
1	A	1025	THR
1	A	1045	ASP

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Mol	Chain	Res	Type
2	B	330	ASP
2	B	365	HIS
2	B	415	GLN
2	B	482	THR
2	B	501	GLN
2	B	531	LEU
2	B	536	SER
2	B	543	ARG
2	B	595	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
1	A	331	ASN
1	A	374	GLN
1	A	444	ASN
1	A	515	ASN
1	A	526	ASN
1	A	575	ASN
1	A	643	GLN
1	A	714	ASN
1	A	749	GLN
1	A	785	ASN
1	A	917	HIS
1	A	931	HIS
2	B	406	ASN
2	B	417	ASN
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 ⓘ

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	0.62	0	8,12,14	1.92	2 (25%)
1	SEP	A	7	1	8,9,10	0.75	0	8,12,14	1.07	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	-	4/5/8/10	-
1	SEP	A	7	1	-	1/5/8/10	-

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	P-OG-CB	3.39	127.62	118.30
1	A	790	SEP	OG-CB-CA	3.35	111.40	108.14

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	CB-OG-P-O2P
1	A	790	SEP	CB-OG-P-O3P
1	A	790	SEP	CB-OG-P-O1P
1	A	7	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand 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	$\#|Z| > 2$
3	71J	B	701	-	8,8,8	0.69	0	10,10,10	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
3	71J	B	701	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 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	1040/1096 (94%)	-0.14	21 (2%)	65	64	70, 117, 180, 229	0
2	B	209/279 (74%)	0.99	50 (23%)	0	0	110, 182, 227, 296	0
All	All	1249/1375 (90%)	0.05	71 (5%)	23	24	70, 122, 207, 296	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	409	ARG	7.0
2	B	335	TRP	6.3
2	B	405	ILE	6.2
2	B	404	LEU	5.0
2	B	410	ASN	4.9
2	B	350	THR	4.7
2	B	449	LEU	4.5
2	B	412	SER	4.5
1	A	107	ASN	4.3
2	B	584	LEU	4.1
2	B	585	THR	3.9
2	B	416	TYR	3.8
2	B	408	TYR	3.7
2	B	595	ASN	3.7
2	B	333	TRP	3.7
1	A	905	CYS	3.6
2	B	407	HIS	3.6
2	B	406	ASN	3.5
2	B	510	GLU	3.5
1	A	-26	SER	3.4
1	A	450	HIS	3.4
1	A	868	GLY	3.3
2	B	512	PHE	3.3
2	B	332	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	450	HIS	3.2
1	A	1052	THR	3.1
2	B	598	LEU	3.1
2	B	580	TYR	3.1
2	B	417	ASN	3.1
2	B	411	GLU	3.0
2	B	341	GLU	3.0
2	B	345	GLU	2.9
2	B	581	LEU	2.9
1	A	943	LYS	2.9
2	B	401	VAL	2.9
1	A	944	LYS	2.7
1	A	516	ARG	2.7
2	B	378	ASN	2.6
2	B	577	ARG	2.6
2	B	336	GLY	2.5
2	B	346	LYS	2.5
2	B	413	LEU	2.5
1	A	308	SER	2.5
2	B	596	GLU	2.5
1	A	364	GLY	2.4
2	B	368	TYR	2.4
2	B	454	THR	2.4
1	A	517	LEU	2.3
2	B	583	TRP	2.3
2	B	457	GLN	2.3
1	A	869	ALA	2.2
1	A	872	PHE	2.2
2	B	354	THR	2.2
1	A	729	LYS	2.2
2	B	382	LYS	2.2
2	B	355	PHE	2.2
2	B	472	ARG	2.2
1	A	375	ARG	2.1
2	B	418	PRO	2.1
2	B	508	TYR	2.1
2	B	515	GLU	2.1
2	B	586	GLN	2.1
2	B	365	HIS	2.1
2	B	461	ARG	2.1
1	A	417	GLU	2.1
2	B	453	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	901	CYS	2.0
1	A	948	LYS	2.0
1	A	298	PRO	2.0
2	B	367	ASP	2.0
1	A	508	TYR	2.0

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

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	0.75	0.22	140,161,200,217	0
1	SEP	A	790	10/11	0.93	0.12	92,105,192,197	0

6.3 Carbohydrates ⓘ

There are no monosaccharides 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(Å^2)	Q<0.9
3	71J	B	701	8/8	0.67	1.00	156,176,178,178	0

6.5 Other polymers ⓘ

There are no such residues in this entry.