



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:42 PM UTC

PDB ID : 5SXC / pdb_00005sxc
Title : Crystal Structure of PI3Kalpha in complex with fragment 8
Authors : Gabelli, S.B.; Vogelstein, B.; Miller, M.S.; Amzel, L.M.
Deposited on : 2016-08-09
Resolution : 3.55 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

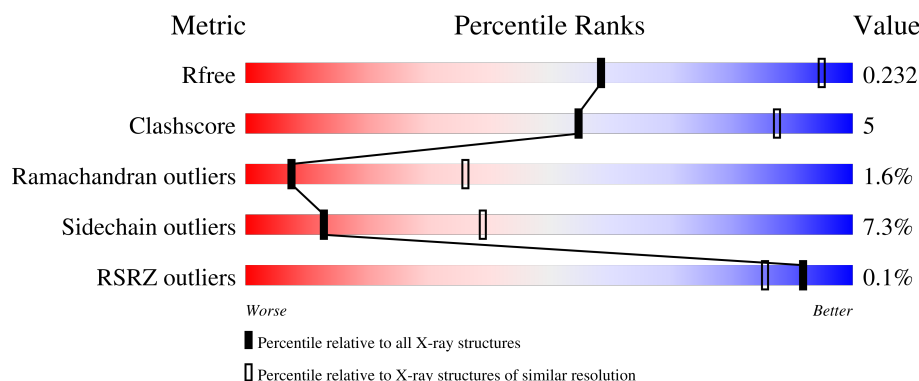
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

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	 77% 16% • 5%
2	B	279	 63% 11% • 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	URF	A	1101	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10334 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	1040	Total	C	N	O	P	S	0	0	0
			8518	5442	1461	1545	2	68			

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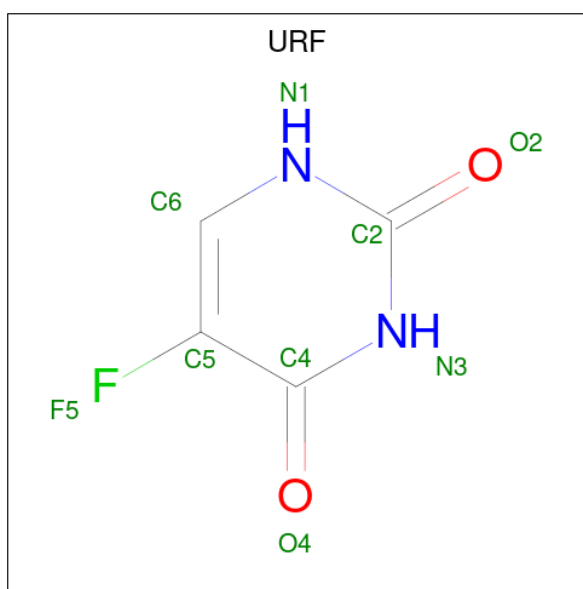
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42336
A	0	SER	-	expression tag	UNP P42336

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	208	Total	C	N	O	S	0	0	0
			1807	1138	321	343	5			

- Molecule 3 is 5-FLUOROURACIL (CCD ID: URF) (formula: $C_4H_3FN_2O_2$).

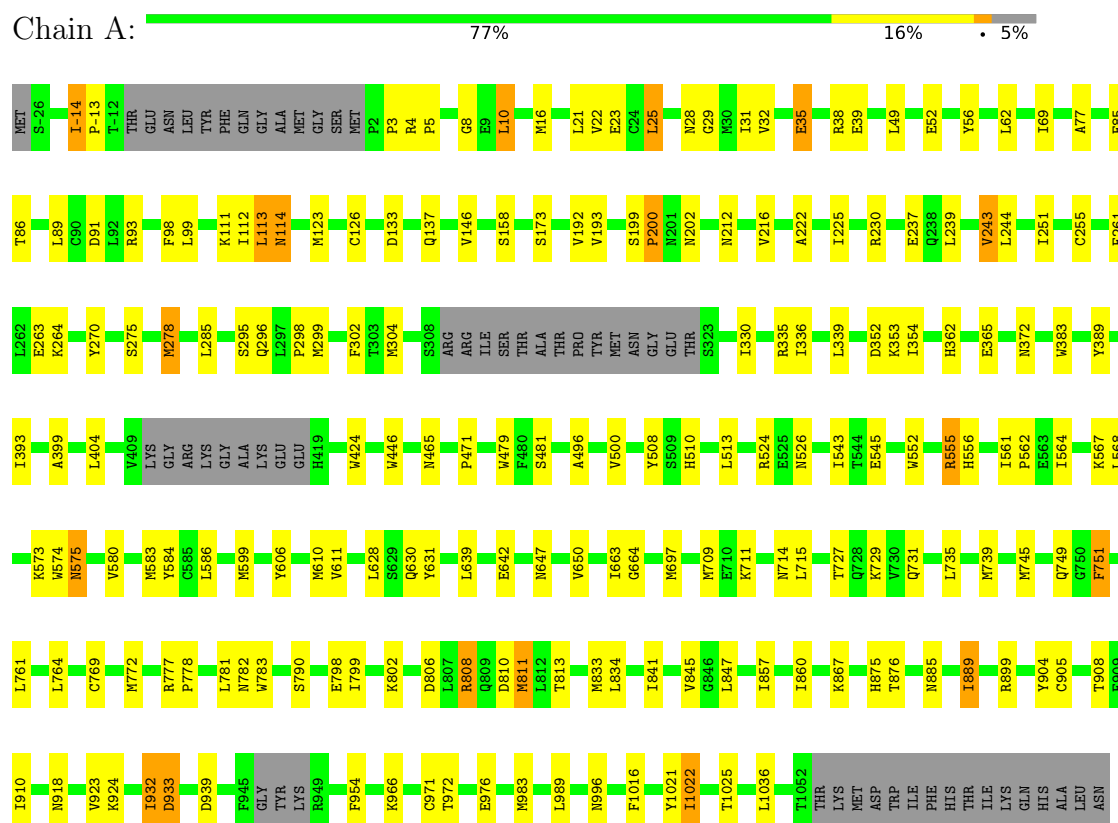


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			9	4	1	2	2		

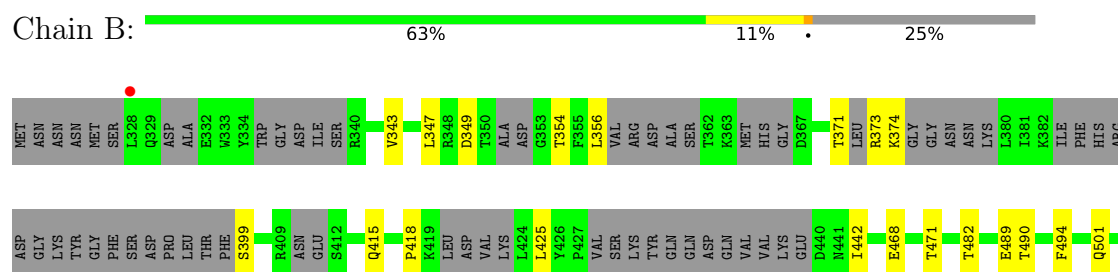
3 Residue-property plots

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



I509	E510	K513	ARG	GLU	G516	N517	E518	D529	K530	L531	R534	R544	E547	L581	T585	GLN	LYS	GLY	V589	R590	L594	N595	E596	N597	LEU	GLY	ASN
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.73Å 117.27Å 150.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.46 – 3.55 92.46 – 3.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (92.46-3.55) 99.9 (92.46-3.55)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.194 , 0.268 (Not available) , 0.232	Depositor DCC
R_{free} test set	1305 reflections (3.09%)	wwPDB-VP
Wilson B-factor (Å ²)	112.4	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 120.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10334	wwPDB-VP
Average B, all atoms (Å ²)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: URF, 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	0.79	1/8695 (0.0%)	1.05	12/11752 (0.1%)
2	B	0.71	0/1824	0.95	1/2421 (0.0%)
All	All	0.77	1/10519 (0.0%)	1.03	13/14173 (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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	339	LEU	CA-C	6.09	1.58	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	GLU	N-CA-C	7.86	119.97	110.07
1	A	808	ARG	N-CA-C	6.89	121.14	112.87
1	A	199	SER	N-CA-C	6.67	114.22	108.22
1	A	751	PHE	N-CA-C	6.15	116.68	108.38
1	A	146	VAL	CB-CA-C	-5.72	104.65	111.97
1	A	354	ILE	N-CA-C	5.52	116.62	108.45
1	A	230	ARG	N-CA-C	-5.31	103.39	110.55
1	A	263	GLU	N-CA-C	5.27	116.81	108.96
1	A	114	ASN	N-CA-C	-5.18	106.47	112.89
1	A	383	TRP	N-CA-C	-5.11	102.59	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	GLN	N-CA-C	5.08	116.90	111.36
1	A	89	LEU	N-CA-C	5.04	116.77	111.28
2	B	349	ASP	N-CA-C	5.01	121.33	113.72

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	LEU	Peptide
1	A	200	PRO	Peptide

5.2 Too-close contacts [i](#)

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	8518	0	8488	91	0
2	B	1807	0	1800	12	0
3	A	9	0	3	0	0
All	All	10334	0	10291	98	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 (98) 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:8:GLY:HA2	1:A:714:ASN:HD21	1.51	0.76
1:A:628:LEU:HD23	1:A:663:ILE:HD13	1.71	0.72
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.17	0.69
1:A:561:ILE:O	1:A:564:ILE:HG22	1.96	0.66
1:A:8:GLY:CA	1:A:714:ASN:HD21	2.09	0.65
1:A:642:GLU:HG2	1:A:647:ASN:ND2	2.11	0.64
1:A:610:MET:HA	1:A:610:MET:HE2	1.80	0.63
1:A:261:PHE:HA	1:A:270:TYR:CE2	2.36	0.60
1:A:806:ASP:OD2	1:A:808:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:932:ILE:HD12	1:A:933:ASP:HB2	1.83	0.60
1:A:749:GLN:O	1:A:761:LEU:O	2.20	0.59
1:A:715:LEU:HD21	1:A:735:LEU:HD12	1.85	0.59
1:A:772:MET:HA	1:A:772:MET:HE2	1.84	0.58
1:A:98:PHE:CE1	2:B:490:THR:HG23	2.39	0.57
2:B:347:LEU:CD1	2:B:371:THR:HG21	2.36	0.56
1:A:10:LEU:HD13	1:A:16:MET:HE2	1.88	0.56
2:B:343:VAL:HG13	2:B:356:LEU:HD11	1.88	0.55
1:A:745:MET:HA	1:A:745:MET:HE2	1.89	0.55
1:A:772:MET:HB2	1:A:778:PRO:HG2	1.88	0.55
1:A:552:TRP:CZ3	1:A:555:ARG:HD3	2.42	0.55
1:A:25:LEU:HD21	2:B:494:PHE:CE2	2.42	0.54
1:A:731:GLN:HE22	1:A:777:ARG:HE	1.56	0.53
1:A:10:LEU:HD13	1:A:16:MET:CE	2.39	0.53
1:A:192:VAL:HG12	1:A:193:VAL:N	2.24	0.52
1:A:222:ALA:O	1:A:225:ILE:N	2.42	0.52
1:A:910:ILE:O	1:A:1025:THR:HG21	2.10	0.52
2:B:347:LEU:HD11	2:B:371:THR:HG21	1.92	0.52
1:A:261:PHE:CD2	1:A:270:TYR:CD2	2.99	0.51
1:A:31:ILE:HD11	2:B:531:LEU:HD13	1.93	0.50
2:B:347:LEU:HD22	2:B:373:ARG:HB2	1.94	0.49
1:A:32:VAL:HG21	1:A:49:LEU:CD1	2.43	0.49
1:A:524:ARG:HD2	1:A:526:ASN:HD22	1.78	0.49
1:A:1021:TYR:C	1:A:1021:TYR:CD1	2.90	0.49
1:A:899:ARG:HG2	1:A:983:MET:HE1	1.95	0.49
1:A:989:LEU:HD21	1:A:1036:LEU:HG	1.95	0.49
1:A:543:ILE:HD11	1:A:567:LYS:CD	2.43	0.48
1:A:496:ALA:O	1:A:500:VAL:HG23	2.13	0.48
1:A:735:LEU:O	1:A:739:MET:HG3	2.13	0.48
1:A:875:HIS:O	1:A:876:THR:C	2.57	0.48
1:A:302:PHE:HE2	1:A:304:MET:HE2	1.79	0.47
1:A:446:TRP:CZ2	1:A:465:ASN:HA	2.50	0.47
1:A:709:MET:HG3	1:A:841:ILE:HD13	1.95	0.47
1:A:584:TYR:CD2	1:A:610:MET:HG3	2.49	0.47
1:A:330:ILE:HG21	1:A:393:ILE:HG21	1.97	0.47
1:A:524:ARG:CD	1:A:526:ASN:HD22	2.28	0.47
1:A:255:CYS:SG	1:A:285:LEU:O	2.73	0.46
1:A:749:GLN:HE21	1:A:764:LEU:H	1.61	0.46
1:A:336:ILE:HD12	1:A:389:TYR:CE2	2.49	0.46
1:A:192:VAL:HG12	1:A:193:VAL:H	1.81	0.46
1:A:278:MET:HA	1:A:278:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:LEU:HD23	1:A:663:ILE:CD1	2.43	0.45
1:A:362:HIS:CD2	1:A:399:ALA:HB3	2.51	0.45
1:A:939:ASP:HB2	1:A:1021:TYR:CE2	2.52	0.45
1:A:751:PHE:CE2	1:A:761:LEU:HD12	2.52	0.45
1:A:639:LEU:HD22	1:A:650:VAL:HG22	1.99	0.45
1:A:573:LYS:HB3	1:A:575:ASN:ND2	2.32	0.45
1:A:575:ASN:C	1:A:575:ASN:HD22	2.24	0.44
1:A:989:LEU:HD11	1:A:1036:LEU:HD11	1.99	0.44
1:A:510:HIS:N	1:A:513:LEU:HD12	2.33	0.44
1:A:510:HIS:HB2	1:A:513:LEU:HD12	2.00	0.44
1:A:663:ILE:O	1:A:664:GLY:C	2.61	0.44
1:A:885:ASN:HB3	1:A:889:ILE:HG22	2.00	0.43
1:A:372:ASN:OD1	1:A:372:ASN:N	2.51	0.43
1:A:261:PHE:CD2	1:A:270:TYR:CG	3.07	0.43
1:A:574:TRP:HA	1:A:580:VAL:CG2	2.48	0.43
1:A:769:CYS:SG	1:A:781:LEU:HA	2.58	0.43
1:A:243:VAL:O	1:A:244:LEU:C	2.62	0.43
1:A:404:LEU:C	1:A:404:LEU:HD12	2.44	0.43
1:A:23:GLU:OE1	2:B:534:ARG:NE	2.39	0.42
1:A:606:TYR:HB3	1:A:611:VAL:HG11	1.99	0.42
2:B:581:LEU:HD11	2:B:594:LEU:HD23	2.02	0.42
1:A:298:PRO:HG2	1:A:697:MET:HG3	2.01	0.42
1:A:28:ASN:ND2	1:A:62:LEU:HD21	2.34	0.42
1:A:479:TRP:CZ2	1:A:481:SER:HA	2.55	0.42
2:B:544:ARG:O	2:B:547:GLU:HG2	2.18	0.42
1:A:833:MET:HE1	1:A:904:TYR:HA	2.01	0.42
1:A:32:VAL:HG12	1:A:56:TYR:CD1	2.55	0.42
1:A:778:PRO:HB3	1:A:802:LYS:HG3	2.02	0.42
1:A:91:ASP:OD1	1:A:711:LYS:NZ	2.52	0.42
1:A:599:MET:HE1	1:A:631:TYR:CB	2.49	0.41
1:A:111:LYS:O	1:A:114:ASN:ND2	2.53	0.41
1:A:568:LEU:HG	1:A:583:MET:HE1	2.02	0.41
1:A:1022:ILE:HA	1:A:1025:THR:HG22	2.03	0.41
1:A:352:ASP:HB3	1:A:353:LYS:HD2	2.02	0.41
1:A:709:MET:HE1	1:A:847:LEU:HD21	2.01	0.41
1:A:543:ILE:HD11	1:A:567:LYS:HD2	2.01	0.41
1:A:556:HIS:CE1	1:A:586:LEU:HD21	2.54	0.41
1:A:543:ILE:HD11	1:A:567:LYS:HD3	2.01	0.41
1:A:764:LEU:HD21	1:A:783:TRP:CE2	2.55	0.41
2:B:509:ILE:HG23	2:B:510:GLU:HG3	2.02	0.41
1:A:21:LEU:HD23	1:A:35:GLU:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:TRP:CE2	1:A:446:TRP:HB2	2.56	0.41
1:A:908:THR:HG21	1:A:954:PHE:HB2	2.03	0.40
1:A:810:ASP:O	1:A:811:MET:C	2.64	0.40
1:A:29:GLY:HA3	2:B:501:GLN:HB3	2.03	0.40
1:A:561:ILE:O	1:A:562:PRO:C	2.64	0.40
1:A:782:ASN:HD22	1:A:798:GLU:HB3	1.85	0.40
1:A:-14:ILE:HD13	1:A:-13:PRO:HD2	2.02	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	1028/1096 (94%)	882 (86%)	130 (13%)	16 (2%)	7	36
2	B	180/279 (64%)	168 (93%)	9 (5%)	3 (2%)	7	35
All	All	1208/1375 (88%)	1050 (87%)	139 (12%)	19 (2%)	7	36

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	A	508	TYR
1	A	555	ARG
1	A	38	ARG
1	A	77	ALA
1	A	264	LYS
1	A	471	PRO
1	A	867	LYS
1	A	918	ASN
2	B	418	PRO
2	B	590	ARG

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Mol	Chain	Res	Type
1	A	5	PRO
1	A	1016	PHE
1	A	133	ASP
1	A	200	PRO
2	B	442	ILE
1	A	3	PRO
1	A	889	ILE
1	A	4	ARG

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	717/997 (72%)	664 (93%)	53 (7%)	13	39
2	B	199/259 (77%)	185 (93%)	14 (7%)	14	40
All	All	916/1256 (73%)	849 (93%)	67 (7%)	13	39

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

Mol	Chain	Res	Type
1	A	-14	ILE
1	A	10	LEU
1	A	22	VAL
1	A	25	LEU
1	A	35	GLU
1	A	39	GLU
1	A	52	GLU
1	A	69	ILE
1	A	85	GLU
1	A	86	THR
1	A	93	ARG
1	A	99	LEU
1	A	112	ILE
1	A	113	LEU
1	A	123	MET

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Mol	Chain	Res	Type
1	A	126	CYS
1	A	137	GLN
1	A	158	SER
1	A	173	SER
1	A	212	ASN
1	A	216	VAL
1	A	237	GLU
1	A	239	LEU
1	A	243	VAL
1	A	251	ILE
1	A	275	SER
1	A	278	MET
1	A	295	SER
1	A	299	MET
1	A	335	ARG
1	A	545	GLU
1	A	575	ASN
1	A	630	GLN
1	A	727	THR
1	A	729	LYS
1	A	799	ILE
1	A	811	MET
1	A	813	THR
1	A	834	LEU
1	A	845	VAL
1	A	857	ILE
1	A	860	ILE
1	A	905	CYS
1	A	923	VAL
1	A	924	LYS
1	A	932	ILE
1	A	933	ASP
1	A	966	LYS
1	A	971	CYS
1	A	972	THR
1	A	976	GLU
1	A	996	ASN
1	A	1022	ILE
2	B	354	THR
2	B	374	LYS
2	B	399	SER
2	B	415	GLN

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Mol	Chain	Res	Type
2	B	425	LEU
2	B	468	GLU
2	B	471	THR
2	B	482	THR
2	B	489	GLU
2	B	518	GLU
2	B	529	ASP
2	B	531	LEU
2	B	594	LEU
2	B	595	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	219	GLN
1	A	284	ASN
1	A	526	ASN
1	A	530	GLN
1	A	554	HIS
1	A	556	HIS
1	A	605	ASN
1	A	630	GLN
1	A	731	GLN
1	A	738	GLN
1	A	749	GLN
1	A	759	HIS
1	A	782	ASN
1	A	785	ASN
1	A	796	ASN
1	A	826	ASN
1	A	827	GLN
1	A	853	ASN
1	A	917	HIS
2	B	407	HIS
2	B	417	ASN
2	B	478	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 ⓘ

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	0.80	0	7,12,14	1.08	0
1	SEP	A	790	1	8,9,10	0.58	0	7,12,14	1.32	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	7	1	-	2/6/8/10	-
1	SEP	A	790	1	-	4/6/8/10	-

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	O2P-P-OG	-2.22	100.89	106.67
1	A	790	SEP	O3P-P-O2P	2.13	115.78	107.80

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
1	A	790	SEP	C-CA-CB-OG
1	A	790	SEP	CB-OG-P-O1P
1	A	7	SEP	CA-CB-OG-P
1	A	7	SEP	CB-OG-P-O3P
1	A	790	SEP	CB-OG-P-O2P

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](#)

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	URF	A	1101	-	9,9,9	2.82	2 (22%)	12,12,12	4.45	7 (58%)

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	URF	A	1101	-	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	URF	C6-C5	6.88	1.39	1.33
3	A	1101	URF	C4-C5	4.08	1.49	1.44

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	URF	C5-C4-N3	7.08	119.12	112.64
3	A	1101	URF	O4-C4-C5	-6.57	120.09	125.69
3	A	1101	URF	N1-C2-N3	6.33	121.84	115.17
3	A	1101	URF	F5-C5-C4	5.94	121.67	116.47
3	A	1101	URF	C6-C5-C4	-5.68	117.22	122.11
3	A	1101	URF	C4-N3-C2	-4.44	120.26	126.37
3	A	1101	URF	O2-C2-N1	-3.66	119.01	122.79

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 [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	1038/1096 (94%)	-0.66	0	100 100	58, 121, 192, 248	0
2	B	208/279 (74%)	-0.49	1 (0%)	87 66	114, 194, 241, 283	0
All	All	1246/1375 (90%)	-0.63	1 (0%)	92 85	58, 131, 216, 283	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	328	LEU	2.3

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	0.68	0.10	151,173,195,202	0
1	SEP	A	790	10/11	0.90	0.06	102,115,195,217	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	URF	A	1101	9/9	0.61	0.06	162,178,184,186	0

6.5 Other polymers [i](#)

There are no such residues in this entry.