



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:17 AM UTC

PDB ID : 5SXF / pdb_00005sxf
Title : Crystal Structure of PI3Kalpha in complex with fragment 9
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Deposited on : 2016-08-09
Resolution : 3.46 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

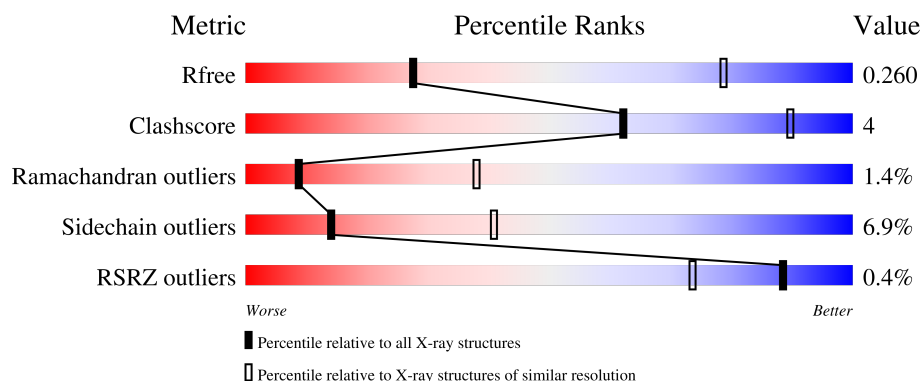
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.46 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	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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	
2	B	279	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9982 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	1024	Total	C	N	O	P	S	0	0	0
			8389	5367	1436	1516	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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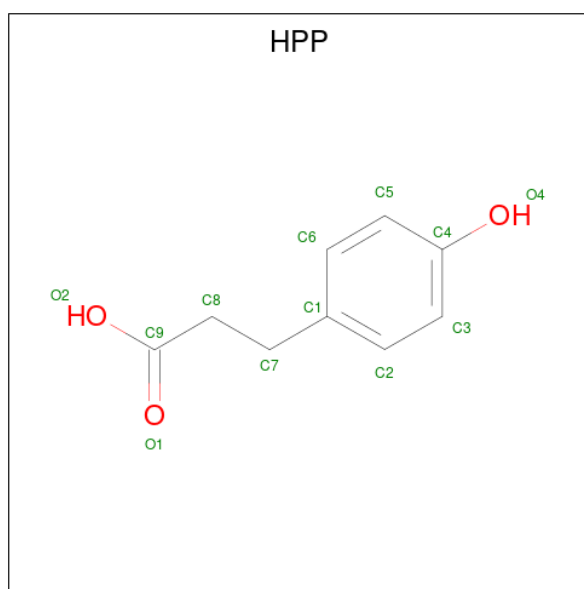
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42336
A	0	SER	-	expression tag	UNP P42336

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	183	Total	C	N	O	S	0	0	0
			1581	982	287	307	5			

- Molecule 3 is HYDROXYPHENYL PROPIONIC ACID (CCD ID: HPP) (formula: C₉H₁₀O₃).

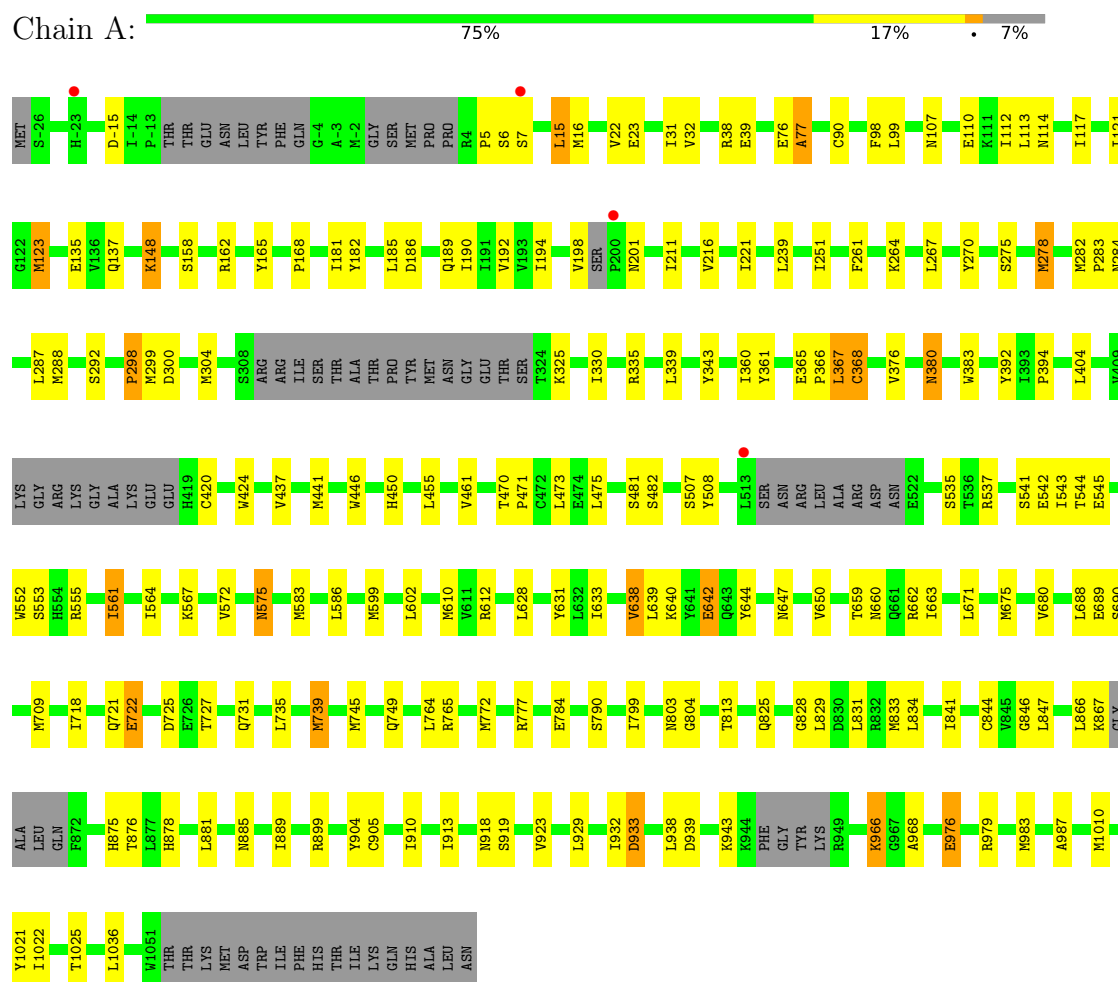


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	9	3		

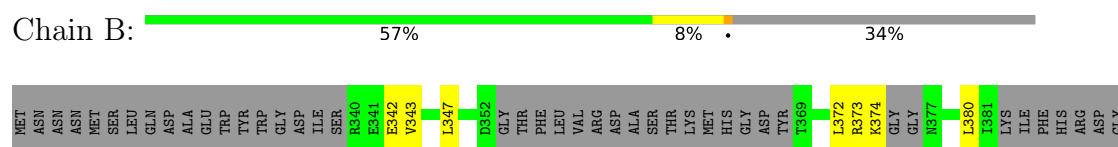
3 Residue-property plots

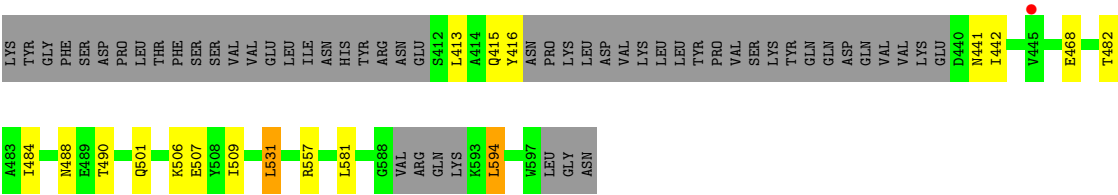
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	112.35Å 115.92Å 147.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.07 – 3.46 91.07 – 3.46	Depositor EDS
% Data completeness (in resolution range)	98.8 (91.07-3.46) 99.0 (91.07-3.46)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.195 , 0.267 0.197 , 0.260	Depositor DCC
R_{free} test set	1314 reflections (3.11%)	wwPDB-VP
Wilson B-factor (Å ²)	109.5	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 98.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9982	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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: HPP, 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	0.73	0/8570	1.00	11/11575 (0.1%)
2	B	0.64	0/1596	0.95	0/2121
All	All	0.71	0/10166	0.99	11/13696 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	846	GLY	N-CA-C	6.98	120.83	110.42
1	A	804	GLY	N-CA-C	6.84	120.77	112.49
1	A	455	LEU	N-CA-C	6.47	118.41	111.36
1	A	1010	MET	N-CA-C	-6.20	100.64	109.62
1	A	828	GLY	N-CA-C	5.87	122.06	113.48
1	A	189	GLN	N-CA-C	5.50	118.43	108.69
1	A	918	ASN	N-CA-C	5.43	118.70	111.75
1	A	461	VAL	N-CA-C	5.38	116.03	109.30
1	A	365	GLU	N-CA-C	5.35	116.56	109.93
1	A	662	ARG	N-CA-C	-5.27	105.45	111.14
1	A	507	SER	N-CA-C	5.05	117.84	107.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8389	0	8368	75	0
2	B	1581	0	1578	13	0
3	A	12	0	8	0	0
All	All	9982	0	9954	82	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 (82) 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:709:MET:HE1	1:A:847:LEU:HD21	1.67	0.76
1:A:599:MET:HE1	1:A:631:TYR:CD2	2.26	0.70
1:A:572:VAL:HG21	1:A:583:MET:HG2	1.76	0.68
1:A:123:MET:HE3	1:A:675:MET:HE1	1.76	0.67
1:A:98:PHE:CE1	2:B:490:THR:HG23	2.32	0.65
1:A:749:GLN:HE21	1:A:764:LEU:H	1.44	0.65
1:A:278:MET:HA	1:A:278:MET:HE2	1.80	0.64
1:A:772:MET:HA	1:A:772:MET:HE2	1.80	0.64
1:A:910:ILE:O	1:A:1025:THR:HG21	1.98	0.63
1:A:31:ILE:HD11	2:B:531:LEU:HD13	1.81	0.62
1:A:878:HIS:NE2	1:A:966:LYS:O	2.34	0.60
1:A:640:LYS:HE2	1:A:680:VAL:HG11	1.85	0.59
1:A:544:THR:HG22	2:B:380:LEU:HB3	1.85	0.58
1:A:899:ARG:HG2	1:A:983:MET:HE1	1.84	0.58
1:A:660:ASN:OD1	1:A:660:ASN:C	2.49	0.55
1:A:543:ILE:HD11	1:A:567:LYS:HD3	1.90	0.54
1:A:182:TYR:O	1:A:185:LEU:HB2	2.08	0.54
1:A:803:ASN:O	1:A:844:CYS:O	2.25	0.54
1:A:15:LEU:HB2	1:A:718:ILE:HD11	1.89	0.53
1:A:162:ARG:NH2	1:A:298:PRO:O	2.41	0.53
1:A:361:TYR:HA	1:A:366:PRO:HD3	1.91	0.52
1:A:537:ARG:HB3	1:A:541:SER:OG	2.09	0.52
2:B:372:LEU:HD23	2:B:373:ARG:N	2.24	0.52
1:A:561:ILE:O	1:A:564:ILE:HG22	2.11	0.51
1:A:610:MET:HA	1:A:610:MET:HE2	1.92	0.51
2:B:506:LYS:HA	2:B:509:ILE:HG22	1.91	0.51
1:A:671:LEU:HB2	1:A:688:LEU:HD21	1.92	0.51
1:A:739:MET:O	1:A:745:MET:HE3	2.11	0.50
1:A:575:ASN:C	1:A:575:ASN:HD22	2.19	0.50
1:A:192:VAL:HG21	1:A:211:ILE:HD11	1.93	0.50
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:LEU:O	1:A:612:ARG:NH2	2.45	0.49
1:A:360:ILE:N	1:A:360:ILE:HD12	2.28	0.49
1:A:831:LEU:HD11	1:A:987:ALA:HB2	1.94	0.49
1:A:31:ILE:CD1	2:B:531:LEU:HD13	2.43	0.47
1:A:181:ILE:HG12	1:A:278:MET:HE3	1.95	0.47
1:A:552:TRP:CZ3	1:A:555:ARG:HD3	2.49	0.47
1:A:148:LYS:HG2	1:A:304:MET:HE2	1.97	0.46
2:B:581:LEU:HD11	2:B:594:LEU:HD23	1.98	0.46
1:A:114:ASN:HA	1:A:117:ILE:HD12	1.98	0.46
1:A:424:TRP:CE2	1:A:446:TRP:HB2	2.51	0.46
1:A:1022:ILE:HA	1:A:1025:THR:HG22	1.98	0.46
1:A:639:LEU:HD22	1:A:650:VAL:HG22	1.98	0.46
1:A:367:LEU:HD12	1:A:368:CYS:O	2.17	0.45
1:A:555:ARG:HD2	1:A:586:LEU:HD11	1.99	0.45
1:A:16:MET:HE3	1:A:90:CYS:HA	1.99	0.45
1:A:833:MET:HE1	1:A:904:TYR:HA	1.99	0.44
1:A:866:LEU:HD23	1:A:867:LYS:N	2.31	0.44
1:A:392:TYR:HB3	1:A:394:PRO:HD2	1.99	0.44
1:A:121:ILE:HD11	1:A:689:GLU:HA	2.00	0.44
1:A:194:ILE:N	1:A:194:ILE:HD12	2.33	0.43
1:A:325:LYS:HE2	1:A:330:ILE:HD11	2.01	0.43
1:A:165:TYR:O	1:A:168:PRO:HD3	2.18	0.43
1:A:261:PHE:HA	1:A:270:TYR:CE2	2.54	0.43
1:A:938:LEU:HD22	1:A:1021:TYR:HB3	2.00	0.43
1:A:404:LEU:CD1	1:A:473:LEU:HD23	2.48	0.43
1:A:721:GLN:O	1:A:722:GLU:HB2	2.18	0.43
1:A:765:ARG:HD2	1:A:784:GLU:HG3	2.00	0.43
1:A:5:PRO:HB3	1:A:721:GLN:HE22	1.84	0.43
1:A:343:TYR:OH	2:B:557:ARG:NH1	2.48	0.43
1:A:875:HIS:O	1:A:876:THR:C	2.61	0.43
1:A:628:LEU:HD23	1:A:663:ILE:HD13	2.00	0.42
1:A:535:SER:HA	1:A:564:ILE:HD12	2.00	0.42
1:A:612:ARG:NH1	1:A:642:GLU:OE1	2.52	0.42
1:A:135:GLU:OE2	1:A:644:TYR:HB3	2.20	0.42
1:A:76:GLU:O	1:A:77:ALA:HB3	2.20	0.42
1:A:721:GLN:O	1:A:722:GLU:CB	2.68	0.42
2:B:531:LEU:HD12	2:B:531:LEU:O	2.20	0.41
2:B:343:VAL:HG12	2:B:347:LEU:HD12	2.01	0.41
1:A:885:ASN:HB3	1:A:889:ILE:HG22	2.03	0.41
2:B:413:LEU:HD22	2:B:416:TYR:CD2	2.56	0.41
1:A:282:MET:O	1:A:284:ASN:ND2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:VAL:HG11	1:A:380:ASN:HD22	1.83	0.41
1:A:339:LEU:O	1:A:383:TRP:O	2.39	0.41
1:A:602:LEU:HB3	1:A:638:VAL:HG11	2.02	0.41
1:A:731:GLN:OE1	1:A:777:ARG:NH2	2.51	0.41
1:A:976:GLU:N	1:A:976:GLU:OE2	2.54	0.41
1:A:542:GLU:HG2	2:B:380:LEU:HD13	2.01	0.40
1:A:221:ILE:HG23	1:A:287:LEU:CD2	2.52	0.40
1:A:932:ILE:O	1:A:933:ASP:C	2.64	0.40
2:B:484:ILE:HG22	2:B:488:ASN:ND2	2.36	0.40
1:A:282:MET:O	1:A:283:PRO:C	2.65	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	1005/1096 (92%)	916 (91%)	72 (7%)	17 (2%)	7	35
2	B	171/279 (61%)	160 (94%)	11 (6%)	0	100	100
All	All	1176/1375 (86%)	1076 (92%)	83 (7%)	17 (1%)	9	38

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	ASN
1	A	722	GLU
1	A	77	ALA
1	A	107	ASN
1	A	264	LYS
1	A	939	ASP
1	A	968	ALA
1	A	38	ARG

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Mol	Chain	Res	Type
1	A	471	PRO
1	A	508	TYR
1	A	186	ASP
1	A	298	PRO
1	A	450	HIS
1	A	933	ASP
1	A	368	CYS
1	A	725	ASP
1	A	913	ILE

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	937/998 (94%)	871 (93%)	66 (7%)	14	40
2	B	173/259 (67%)	162 (94%)	11 (6%)	16	43
All	All	1110/1257 (88%)	1033 (93%)	77 (7%)	14	41

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-15	ASP
1	A	6	SER
1	A	7	SER
1	A	15	LEU
1	A	22	VAL
1	A	23	GLU
1	A	32	VAL
1	A	39	GLU
1	A	99	LEU
1	A	110	GLU
1	A	112	ILE
1	A	113	LEU
1	A	123	MET
1	A	137	GLN

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Mol	Chain	Res	Type
1	A	148	LYS
1	A	158	SER
1	A	190	ILE
1	A	198	VAL
1	A	201	ASN
1	A	216	VAL
1	A	239	LEU
1	A	251	ILE
1	A	267	LEU
1	A	275	SER
1	A	278	MET
1	A	288	MET
1	A	292	SER
1	A	299	MET
1	A	300	ASP
1	A	335	ARG
1	A	367	LEU
1	A	420	CYS
1	A	437	VAL
1	A	441	MET
1	A	470	THR
1	A	475	LEU
1	A	481	SER
1	A	482	SER
1	A	545	GLU
1	A	553	SER
1	A	561	ILE
1	A	575	ASN
1	A	633	ILE
1	A	638	VAL
1	A	642	GLU
1	A	659	THR
1	A	690	SER
1	A	727	THR
1	A	735	LEU
1	A	739	MET
1	A	799	ILE
1	A	813	THR
1	A	825	GLN
1	A	829	LEU
1	A	834	LEU
1	A	841	ILE

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Mol	Chain	Res	Type
1	A	881	LEU
1	A	905	CYS
1	A	919	SER
1	A	923	VAL
1	A	929	LEU
1	A	943	LYS
1	A	966	LYS
1	A	976	GLU
1	A	979	ARG
1	A	1036	LEU
2	B	342	GLU
2	B	374	LYS
2	B	415	GLN
2	B	441	ASN
2	B	442	ILE
2	B	468	GLU
2	B	482	THR
2	B	501	GLN
2	B	507	GLU
2	B	531	LEU
2	B	594	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-20	HIS
1	A	14	HIS
1	A	63	GLN
1	A	107	ASN
1	A	157	ASN
1	A	205	GLN
1	A	219	GLN
1	A	238	GLN
1	A	247	GLN
1	A	331	ASN
1	A	362	HIS
1	A	374	GLN
1	A	380	ASN
1	A	384	ASN
1	A	444	ASN
1	A	575	ASN
1	A	721	GLN

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Mol	Chain	Res	Type
1	A	749	GLN
1	A	760	GLN
1	A	763	ASN
1	A	825	GLN
1	A	861	GLN
1	A	931	HIS
1	A	1014	GLN
1	A	1044	ASN
2	B	377	ASN
2	B	450	HIS
2	B	453	ASN
2	B	455	GLN
2	B	475	GLN
2	B	499	GLN
2	B	517	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 ⓘ

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	0.61	0	7,12,14	1.63	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	2.40	110.48	108.14
1	A	790	SEP	OG-P-O1P	-2.17	100.58	106.44

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.

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	HPP	A	1101	-	12,12,12	0.83	0	15,15,15	0.63	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	HPP	A	1101	-	-	2/5/5/5	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	HPP	C7-C8-C9-O1
3	A	1101	HPP	C7-C8-C9-O2

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	1023/1096 (93%)	-0.58	4 (0%)	88 73	68, 114, 176, 235	0
2	B	183/279 (65%)	-0.43	1 (0%)	87 70	105, 177, 216, 242	0
All	All	1206/1375 (87%)	-0.56	5 (0%)	88 73	68, 122, 196, 242	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	PRO	3.8
2	B	445	VAL	2.8
1	A	-23	HIS	2.6
1	A	513	LEU	2.5
1	A	7	SER	2.4

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	0.93	0.05	92,110,175,176	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
3	HPP	A	1101	12/12	0.69	0.10	152,176,190,191	0

6.5 Other polymers

There are no such residues in this entry.