Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2023 – 05:56 PM EDT

PDB ID	:	5SXJ
Title	:	Crystal Structure of PI3Kalpha in complex with fragment 29
Authors	:	Gabelli, S.B.; Vogelstein, B.; Miller, M.S.; Amzel, L.M.
Deposited on	:	2016-08-09
Resolution	:	3.42 Å(reported)

The following versions of software and data (see references ⓘ) 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 3.42 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		0.272
Clashscore		5
Ramachandran outliers		1.3%
Sidechain outliers		7.4%
RSRZ outliers		5.2%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
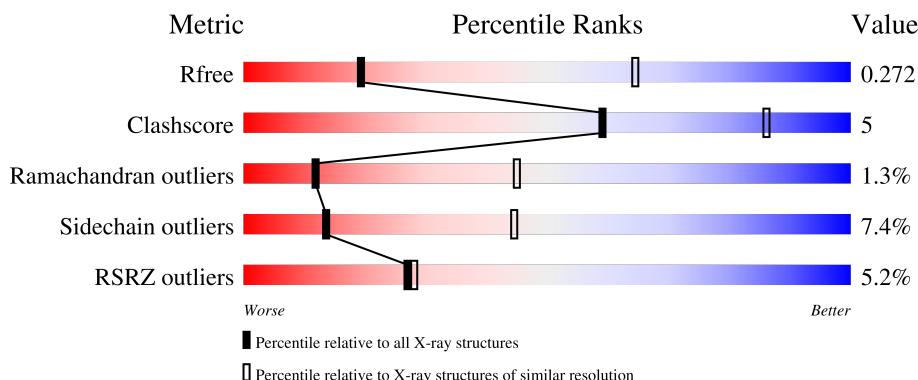
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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% / 15% / • 5%
2	B	279	14% / 62% / 15% / 23%
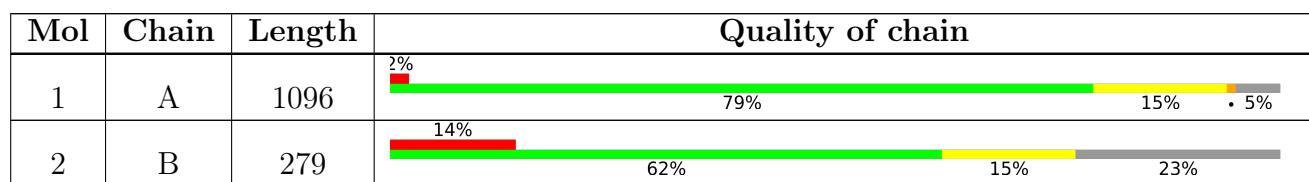
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BHO	A	1101	-	-	-	X
3	BHO	A	1102	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10420 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	8538	5451	1460	1554	3	70	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
			Total	C	N	O	S			
2	B	216	1862	1167	331	358	6	0	0	0

- Molecule 3 is BENZHYDROXAMIC ACID (three-letter code: BHO) (formula: $C_7H_7NO_2$).
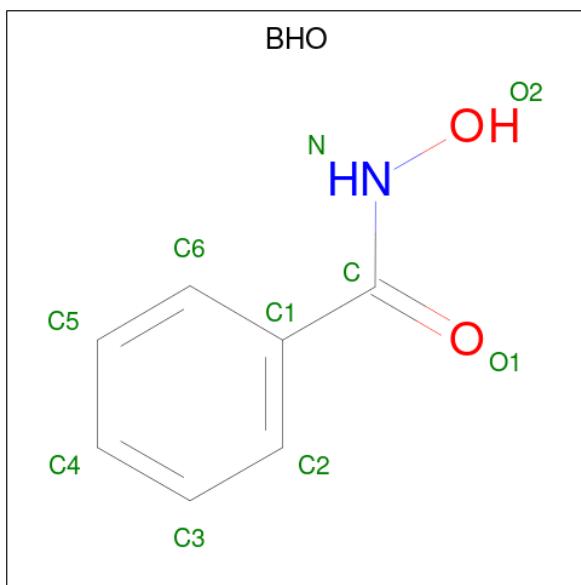
BHO

| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	10	7	1	2	0	0
3	A	1	10	7	1	2	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform
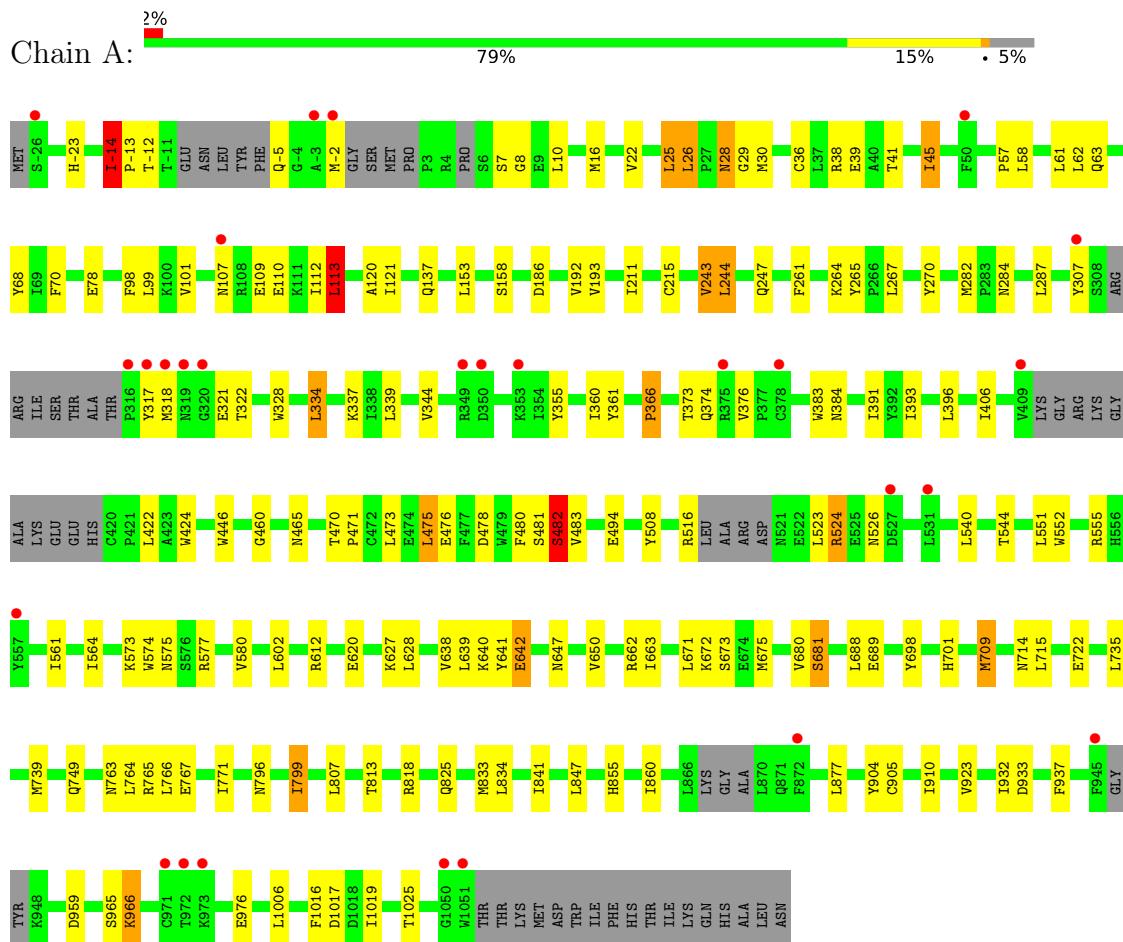
• Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha
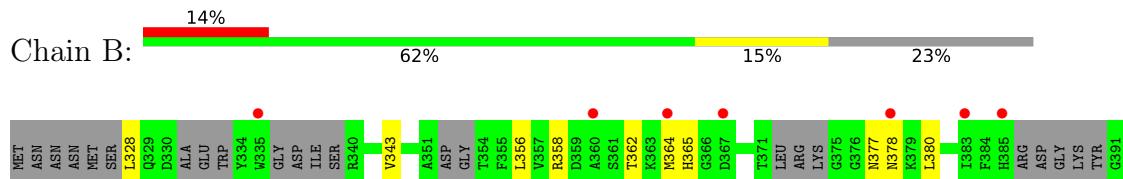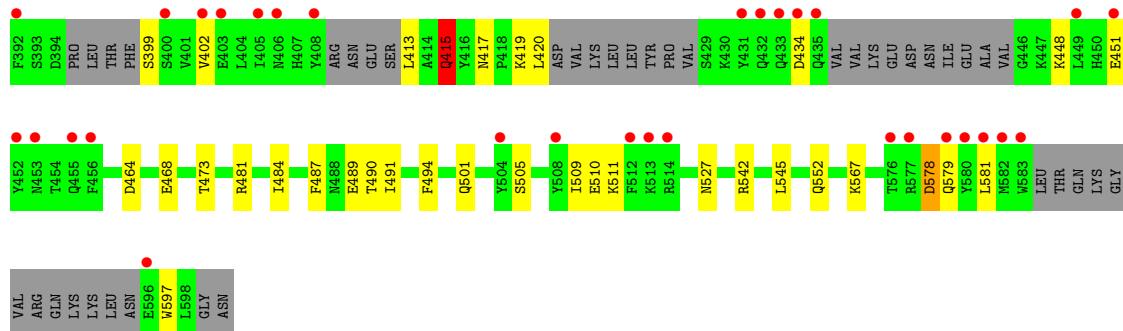
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	114.80Å 117.93Å 150.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.94 – 3.42 36.11 – 3.42	Depositor EDS
% Data completeness (in resolution range)	97.8 (92.94-3.42) 98.0 (36.11-3.42)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 3.39Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.213 , 0.279 0.213 , 0.272	Depositor DCC
R_{free} test set	1410 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	112.1	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 82.8	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.010 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10420	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 3.32% 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: BHO, 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	0.50	0/8699	0.74	1/11745 (0.0%)
2	B	0.48	0/1885	0.68	0/2506
All	All	0.50	0/10584	0.73	1/14251 (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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	113	LEU	CB-CG-CD1	5.09	119.66	111.00

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	8538	0	8497	84	0
2	B	1862	0	1819	19	0
3	A	20	0	14	0	0
All	All	10420	0	10330	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)
2:B:328:LEU:HD13	2:B:402:VAL:HG23	1.51	0.93
1:A:8:GLY:HA2	1:A:714:ASN:HD21	1.35	0.91
1:A:639:LEU:HD22	1:A:650:VAL:HG22	1.64	0.79
2:B:343:VAL:HG13	2:B:356:LEU:HD11	1.77	0.67
1:A:715:LEU:HD21	1:A:735:LEU:HD12	1.80	0.64
1:A:612:ARG:NH1	1:A:642:GLU:OE1	2.32	0.62
1:A:735:LEU:HD22	1:A:771:ILE:HG13	1.80	0.62
1:A:749:GLN:HE21	1:A:763:ASN:HA	1.66	0.60
1:A:552:TRP:CZ3	1:A:555:ARG:HD3	2.39	0.58
1:A:540:LEU:HD21	1:A:1016:PHE:CD1	2.39	0.57
1:A:192:VAL:HG12	1:A:193:VAL:N	2.20	0.57
2:B:501:GLN:O	2:B:505:SER:N	2.36	0.56
1:A:799:ILE:CD1	1:A:847:LEU:HD22	2.35	0.56
1:A:602:LEU:HB3	1:A:638:VAL:HG11	1.87	0.55
1:A:26:LEU:HD12	1:A:30:MET:O	2.07	0.55
1:A:640:LYS:HE2	1:A:680:VAL:HG11	1.89	0.54
1:A:45:ILE:HD11	1:A:70:PHE:CZ	2.43	0.53
1:A:10:LEU:HD13	1:A:16:MET:CE	2.38	0.53
1:A:120:ALA:O	1:A:672:LYS:CE	2.57	0.53
1:A:41:THR:O	1:A:45:ILE:HG23	2.09	0.53
1:A:28:ASN:HD22	1:A:62:LEU:HD21	1.74	0.53
1:A:98:PHE:CE2	2:B:490:THR:HG23	2.44	0.52
1:A:282:MET:O	1:A:284:ASN:ND2	2.42	0.52
1:A:120:ALA:O	1:A:672:LYS:HE2	2.10	0.51
1:A:551:LEU:HD21	1:A:564:ILE:HD11	1.92	0.51
1:A:339:LEU:HD12	1:A:475:LEU:HA	1.93	0.51
1:A:265:TYR:HB2	1:A:270:TYR:CE1	2.46	0.51
2:B:328:LEU:HD13	2:B:402:VAL:CG2	2.32	0.51
1:A:524:ARG:NH1	1:A:526:ASN:HD22	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:VAL:HG12	1:A:247:GLN:HE21	1.76	0.50
1:A:339:LEU:CD1	1:A:475:LEU:HA	2.41	0.50
1:A:113:LEU:HD13	1:A:113:LEU:N	2.27	0.49
1:A:628:LEU:HD23	1:A:663:ILE:HD13	1.94	0.49
2:B:487:PHE:HE2	2:B:545:LEU:HD22	1.77	0.49
1:A:121:ILE:HD11	1:A:689:GLU:HA	1.94	0.49
1:A:57:PRO:HB2	1:A:58:LEU:HD12	1.94	0.49
1:A:540:LEU:HD21	1:A:1016:PHE:HD1	1.78	0.49
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.33	0.49
1:A:910:ILE:O	1:A:1025:THR:HG21	2.13	0.49
1:A:739:MET:CE	1:A:764:LEU:HD21	2.43	0.48
1:A:446:TRP:CZ2	1:A:465:ASN:HA	2.49	0.48
1:A:833:MET:HE1	1:A:904:TYR:HA	1.95	0.48
2:B:484:ILE:HG13	2:B:545:LEU:HD23	1.96	0.48
1:A:675:MET:HE1	1:A:681:SER:O	2.14	0.47
1:A:1019:ILE:HG22	1:A:1019:ILE:O	2.14	0.47
1:A:344:VAL:HG11	1:A:422:LEU:HD13	1.96	0.47
1:A:355:TYR:HA	1:A:383:TRP:HZ2	1.79	0.46
1:A:391:ILE:HD13	1:A:396:LEU:HD23	1.97	0.46
1:A:764:LEU:HD23	1:A:766:LEU:CD2	2.45	0.46
1:A:544:THR:HG22	2:B:380:LEU:HB3	1.97	0.46
2:B:417:ASN:HB3	2:B:420:LEU:HD12	1.97	0.46
1:A:709:MET:HG3	1:A:841:ILE:HD13	1.98	0.45
1:A:765:ARG:HD3	1:A:796:ASN:HD21	1.80	0.45
1:A:561:ILE:O	1:A:564:ILE:HG22	2.16	0.45
1:A:374:GLN:N	1:A:374:GLN:OE1	2.50	0.45
1:A:-14:ILE:N	1:A:-13:PRO:CD	2.80	0.45
1:A:334:LEU:HA	1:A:393:ILE:HD11	1.98	0.45
1:A:25:LEU:HD21	2:B:494:PHE:CE1	2.52	0.44
1:A:68:TYR:CD1	1:A:101:VAL:HG12	2.52	0.44
1:A:480:PHE:O	1:A:482:SER:N	2.50	0.44
1:A:261:PHE:HA	1:A:270:TYR:CE2	2.53	0.44
2:B:413:LEU:HB3	2:B:420:LEU:HD13	1.98	0.44
2:B:343:VAL:HG21	2:B:358:ARG:HD3	1.99	0.43
2:B:473:THR:HG23	2:B:552:GLN:NE2	2.33	0.43
1:A:698:TYR:CD1	1:A:701:HIS:HB2	2.53	0.43
1:A:120:ALA:O	1:A:672:LYS:HE3	2.18	0.43
1:A:739:MET:HE1	1:A:764:LEU:HD21	2.01	0.43
1:A:965:SER:HA	1:A:976:GLU:HG3	2.01	0.43
1:A:932:ILE:HD12	1:A:933:ASP:CB	2.49	0.43
1:A:764:LEU:HD23	1:A:766:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:VAL:HG21	2:B:358:ARG:CD	2.49	0.42
1:A:243:VAL:HG12	1:A:244:LEU:N	2.35	0.42
1:A:321:GLU:HG3	1:A:322:THR:HG23	2.01	0.42
1:A:328:TRP:CD1	1:A:577:ARG:HD2	2.54	0.42
1:A:29:GLY:HA3	2:B:501:GLN:HB3	2.01	0.42
1:A:406:ILE:HG22	1:A:422:LEU:HD12	2.01	0.42
1:A:709:MET:HE3	1:A:847:LEU:HD21	2.00	0.42
2:B:578:ASP:HA	2:B:581:LEU:HB2	2.02	0.42
1:A:641:TYR:OH	1:A:1006:LEU:HB2	2.19	0.42
1:A:709:MET:CE	1:A:847:LEU:HD21	2.49	0.42
1:A:860:ILE:HG21	1:A:877:LEU:HD12	2.00	0.42
1:A:360:ILE:O	1:A:366:PRO:HD2	2.19	0.42
2:B:413:LEU:HA	2:B:415:GLN:HE21	1.84	0.42
1:A:192:VAL:HG21	1:A:211:ILE:HD11	2.02	0.42
1:A:799:ILE:HD12	1:A:847:LEU:HD22	2.00	0.42
1:A:28:ASN:ND2	1:A:62:LEU:HD21	2.35	0.41
1:A:192:VAL:HG12	1:A:193:VAL:H	1.85	0.41
1:A:671:LEU:HB2	1:A:688:LEU:HD21	2.01	0.41
1:A:361:TYR:HA	1:A:366:PRO:HD3	2.01	0.41
1:A:284:ASN:HD22	1:A:284:ASN:N	2.19	0.41
2:B:491:ILE:CD1	2:B:542:ARG:HE	2.32	0.41
1:A:574:TRP:HA	1:A:580:VAL:CG2	2.51	0.41
1:A:709:MET:CE	1:A:847:LEU:HD11	2.51	0.41
1:A:10:LEU:HD13	1:A:16:MET:HE2	2.02	0.41
1:A:337:LYS:HB3	1:A:476:GLU:HB3	2.02	0.40
1:A:424:TRP:CH2	1:A:460:GLY:HA3	2.56	0.40
1:A:30:MET:SD	2:B:527:ASN:ND2	2.95	0.40
1:A:446:TRP:CH2	1:A:465:ASN:HA	2.57	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	1021/1096 (93%)	916 (90%)	92 (9%)	13 (1%)	12	45
2	B	194/279 (70%)	175 (90%)	16 (8%)	3 (2%)	10	42
All	All	1215/1375 (88%)	1091 (90%)	108 (9%)	16 (1%)	12	45

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	264	LYS
1	A	481	SER
1	A	681	SER
1	A	-23	HIS
1	A	186	ASP
2	B	415	GLN
1	A	482	SER
1	A	966	LYS
2	B	377	ASN
1	A	471	PRO
1	A	307	TYR
2	B	567	LYS
1	A	366	PRO
1	A	243	VAL
1	A	-14	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	952/996 (96%)	886 (93%)	66 (7%)	15	48
2	B	203/259 (78%)	183 (90%)	20 (10%)	8	32
All	All	1155/1255 (92%)	1069 (93%)	86 (7%)	13	44

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-14	ILE
1	A	-12	THR
1	A	-5	GLN
1	A	-2	MET
1	A	22	VAL
1	A	25	LEU
1	A	26	LEU
1	A	36	CYS
1	A	38	ARG
1	A	39	GLU
1	A	45	ILE
1	A	61	LEU
1	A	63	GLN
1	A	78	GLU
1	A	99	LEU
1	A	107	ASN
1	A	109	GLU
1	A	110	GLU
1	A	112	ILE
1	A	113	LEU
1	A	137	GLN
1	A	153	LEU
1	A	215	CYS
1	A	244	LEU
1	A	267	LEU
1	A	287	LEU
1	A	317	TYR
1	A	318	MET
1	A	334	LEU
1	A	373	THR
1	A	376	VAL
1	A	384	ASN
1	A	470	THR
1	A	473	LEU
1	A	475	LEU
1	A	478	ASP
1	A	482	SER
1	A	483	VAL
1	A	494	GLU
1	A	508	TYR
1	A	516	ARG
1	A	523	LEU
1	A	524	ARG

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Mol	Chain	Res	Type
1	A	573	LYS
1	A	575	ASN
1	A	620	GLU
1	A	627	LYS
1	A	642	GLU
1	A	662	ARG
1	A	673	SER
1	A	709	MET
1	A	722	GLU
1	A	767	GLU
1	A	799	ILE
1	A	807	LEU
1	A	813	THR
1	A	818	ARG
1	A	825	GLN
1	A	834	LEU
1	A	855	HIS
1	A	905	CYS
1	A	923	VAL
1	A	937	PHE
1	A	959	ASP
1	A	966	LYS
1	A	1017	ASP
2	B	362	THR
2	B	364	MET
2	B	365	HIS
2	B	378	ASN
2	B	399	SER
2	B	415	GLN
2	B	419	LYS
2	B	434	ASP
2	B	448	LYS
2	B	451	GLU
2	B	464	ASP
2	B	468	GLU
2	B	481	ARG
2	B	489	GLU
2	B	509	ILE
2	B	510	GLU
2	B	511	LYS
2	B	578	ASP
2	B	579	GLN

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Mol	Chain	Res	Type
2	B	597	TRP

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	247	GLN
1	A	370	ASN
1	A	526	ASN
1	A	575	ASN
1	A	605	ASN
1	A	661	GLN
1	A	714	ASN
1	A	749	GLN
1	A	763	ASN
1	A	782	ASN
1	A	785	ASN
1	A	796	ASN
1	A	855	HIS
1	A	875	HIS
1	A	931	HIS
1	A	996	ASN
1	A	1014	GLN
1	A	1047	HIS
2	B	415	GLN
2	B	455	GLN
2	B	457	GLN
2	B	527	ASN
2	B	564	ASN
2	B	579	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	158	1	8,9,10	0.58	0	8,12,14	1.37	1 (12%)
1	SEP	A	790	1	8,9,10	0.60	0	8,12,14	1.27	0
1	SEP	A	7	1	8,9,10	0.79	0	8,12,14	1.69	2 (25%)

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	158	1	-	1/5/8/10	-
1	SEP	A	790	1	-	4/5/8/10	-
1	SEP	A	7	1	-	5/5/8/10	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	7	SEP	OG-CB-CA	3.08	111.14	108.14
1	A	7	SEP	P-OG-CB	2.50	125.19	118.30
1	A	158	SEP	OG-CB-CA	2.43	110.51	108.14

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	7	SEP	N-CA-CB-OG
1	A	7	SEP	CB-OG-P-O2P
1	A	158	SEP	N-CA-CB-OG
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	CB-OG-P-O3P
1	A	7	SEP	CA-CB-OG-P

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Mol	Chain	Res	Type	Atoms
1	A	7	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands 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	#$|Z| > 2$
3	BHO	A	1101	-	10,10,10	0.90	0	12,12,12	1.16	1 (8%)
3	BHO	A	1102	-	10,10,10	0.71	0	12,12,12	1.40	1 (8%)

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	BHO	A	1101	-	-	6/6/6/6	0/1/1/1
3	BHO	A	1102	-	-	6/6/6/6	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1102	BHO	C1-C-N	3.90	122.42	116.16
3	A	1101	BHO	C1-C-N	3.23	121.34	116.16

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	BHO	N-C-C1-C2
3	A	1101	BHO	N-C-C1-C6
3	A	1101	BHO	C1-C-N-O2
3	A	1101	BHO	O1-C-N-O2
3	A	1102	BHO	C1-C-N-O2
3	A	1102	BHO	O1-C-N-O2
3	A	1101	BHO	O1-C-C1-C6
3	A	1101	BHO	O1-C-C1-C2
3	A	1102	BHO	N-C-C1-C2
3	A	1102	BHO	N-C-C1-C6
3	A	1102	BHO	O1-C-C1-C2
3	A	1102	BHO	O1-C-C1-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	1039/1096 (94%)	-0.11	27 (2%)	56	54	67, 120, 191, 244	0
2	B	216/279 (77%)	0.85	38 (17%)	1	2	108, 194, 250, 295	0
All	All	1255/1375 (91%)	0.06	65 (5%)	27	28	67, 129, 216, 295	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	406	ASN	5.4
2	B	360	ALA	5.4
1	A	316	PRO	4.8
2	B	580	TYR	4.7
2	B	385	HIS	4.6
2	B	367	ASP	4.6
2	B	432	GLN	4.4
1	A	945	PHE	4.3
2	B	449	LEU	4.1
1	A	409	VAL	4.1
1	A	1050	GLY	4.0
2	B	405	ILE	4.0
2	B	435	GLN	3.9
1	A	350	ASP	3.9
1	A	557	TYR	3.9
2	B	583	TRP	3.9
2	B	512	PHE	3.8
1	A	378	CYS	3.8
2	B	514	ARG	3.8
2	B	582	MET	3.8
2	B	335	TRP	3.8
2	B	453	ASN	3.7
2	B	433	GLN	3.6
1	A	353	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	504	TYR	3.5
1	A	-26	SER	3.5
2	B	364	MET	3.5
2	B	431	TYR	3.4
1	A	971	CYS	3.2
2	B	576	THR	3.2
2	B	577	ARG	3.2
2	B	579	GLN	3.2
2	B	451	GLU	3.2
2	B	508	TYR	3.2
1	A	872	PHE	2.9
1	A	972	THR	2.9
1	A	317	TYR	2.8
2	B	383	ILE	2.8
1	A	531	LEU	2.7
1	A	-3	ALA	2.7
2	B	596	GLU	2.7
2	B	402	VAL	2.7
2	B	513	LYS	2.6
1	A	318	MET	2.6
1	A	1051	TRP	2.6
1	A	319	ASN	2.6
2	B	400	SER	2.4
2	B	408	TYR	2.4
1	A	-2	MET	2.4
2	B	452	TYR	2.4
2	B	434	ASP	2.3
1	A	973	LYS	2.3
1	A	527	ASP	2.3
2	B	581	LEU	2.2
1	A	375	ARG	2.2
1	A	107	ASN	2.2
1	A	307	TYR	2.2
1	A	349	ARG	2.2
1	A	320	GLY	2.2
2	B	456	PHE	2.1
2	B	455	GLN	2.1
2	B	392	PHE	2.1
1	A	50	PHE	2.1
2	B	403	GLU	2.0
2	B	378	ASN	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	0.75	0.24	155,180,211,218	0
1	SEP	A	158	10/11	0.93	0.11	144,178,229,232	0
1	SEP	A	790	10/11	0.94	0.15	108,120,186,200	0

6.3 Carbohydrates (i)

There are no monosaccharides 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($Å^2$)	Q<0.9
3	BHO	A	1102	10/10	0.48	0.72	213,221,233,233	0
3	BHO	A	1101	10/10	0.62	0.68	170,194,203,205	0

6.5 Other polymers (i)

There are no such residues in this entry.