



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2017 – 09:25 AM EST

PDB ID : 5SXB
Title : Crystal Structure of PI3Kalpha in complex with fragment 23
Authors : Gabelli, S.B.; Vogelstein, B.; Miller, M.S.; Amzel, L.M.
Deposited on : 2016-08-09
Resolution : 3.30 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

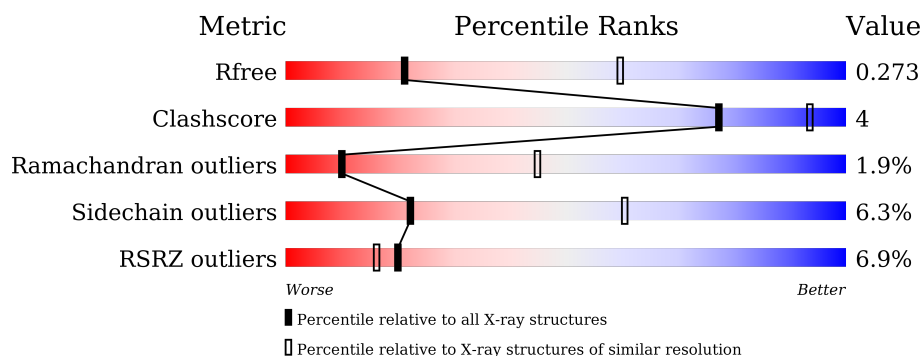
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>4%</div> <div>80%</div> <div>15%</div> <div>••</div> </div>
2	B	279	<div> <div>16%</div> <div>64%</div> <div>10%</div> <div>•</div> <div>24%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10504 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	1058	Total	C	N	O	P	S	0	0	0
			8656	5526	1482	1576	2	70			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP P42336
A	-26	SER	-	expression tag	UNP P42336
A	-25	TYR	-	expression tag	UNP P42336
A	-24	TYR	-	expression tag	UNP P42336
A	-23	HIS	-	expression tag	UNP P42336
A	-22	HIS	-	expression tag	UNP P42336
A	-21	HIS	-	expression tag	UNP P42336
A	-20	HIS	-	expression tag	UNP P42336
A	-19	HIS	-	expression tag	UNP P42336
A	-18	HIS	-	expression tag	UNP P42336
A	-17	ASP	-	expression tag	UNP P42336
A	-16	TYR	-	expression tag	UNP P42336
A	-15	ASP	-	expression tag	UNP P42336
A	-14	ILE	-	expression tag	UNP P42336
A	-13	PRO	-	expression tag	UNP P42336
A	-12	THR	-	expression tag	UNP P42336
A	-11	THR	-	expression tag	UNP P42336
A	-10	GLU	-	expression tag	UNP P42336
A	-9	ASN	-	expression tag	UNP P42336
A	-8	LEU	-	expression tag	UNP P42336
A	-7	TYR	-	expression tag	UNP P42336
A	-6	PHE	-	expression tag	UNP P42336
A	-5	GLN	-	expression tag	UNP P42336
A	-4	GLY	-	expression tag	UNP P42336
A	-3	ALA	-	expression tag	UNP P42336
A	-2	MET	-	expression tag	UNP P42336

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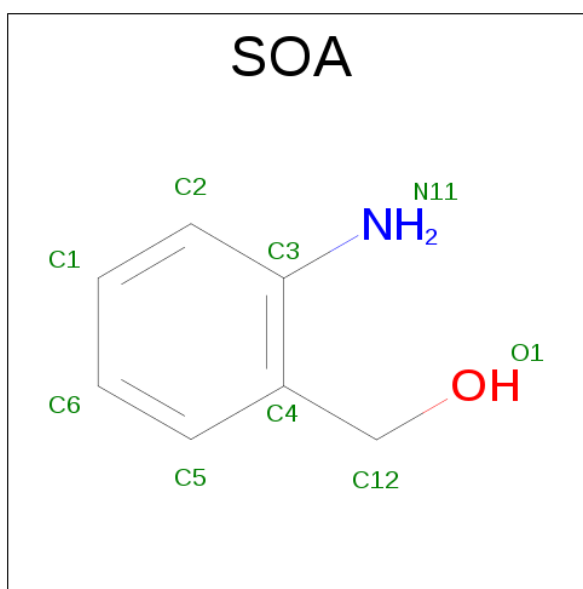
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42336
A	0	SER	-	expression tag	UNP P42336

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1839	1156	327	350	6			

- Molecule 3 is ISATOIC ANHYDRIDE (three-letter code: SOA) (formula: C₇H₉NO).

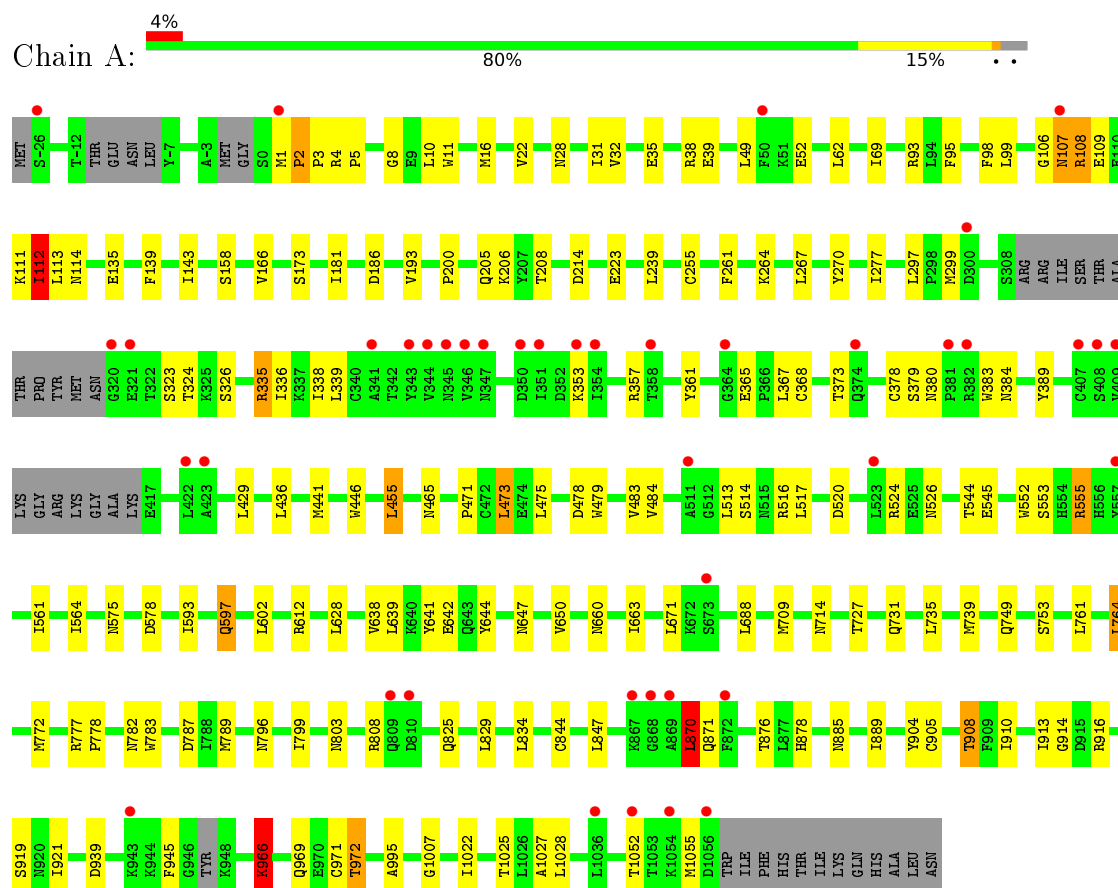


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			9	7	1	1		

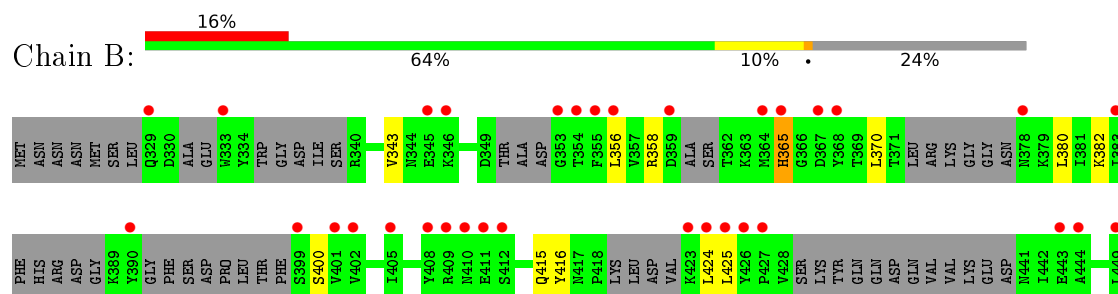
3 Residue-property plots

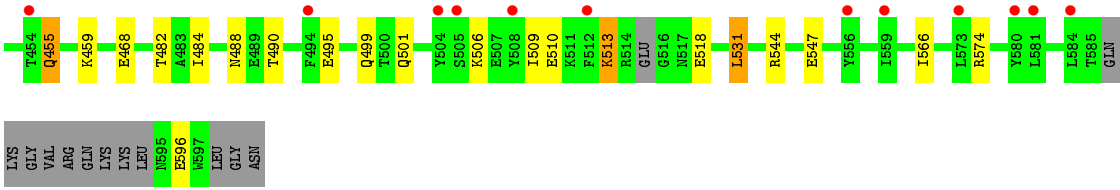
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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





LYS
GLY
VAL
ARG
GLN
LYS
LYS
LEU
W595
E596
W597
LEU
GLY
ASN

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.46Å 116.77Å 150.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.16 – 3.30 49.14 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (92.16-3.30) 99.6 (49.14-3.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 3.33Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.204 , 0.278 0.203 , 0.273	Depositor DCC
R_{free} test set	1578 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	100.0	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 79.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10504	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: SOA, 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	0.54	0/8834	0.77	2/11935 (0.0%)
2	B	0.48	0/1860	0.67	0/2474
All	All	0.53	0/10694	0.75	2/14409 (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	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	870	LEU	CA-CB-CG	6.16	129.46	115.30
1	A	764	LEU	CA-CB-CG	5.61	128.20	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	ILE	Peptide
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	8656	0	8617	67	0
2	B	1839	0	1816	14	0
3	B	9	0	9	0	0
All	All	10504	0	10442	77	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 (77) 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	1.66	0.76
1:A:561:ILE:O	1:A:564:ILE:HG22	1.96	0.65
1:A:28:ASN:ND2	1:A:62:LEU:HD21	2.14	0.63
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.20	0.61
1:A:98:PHE:CE1	2:B:490:THR:HG23	2.35	0.61
1:A:166:VAL:HG21	1:A:297:LEU:HD22	1.81	0.61
1:A:8:GLY:HA2	1:A:714:ASN:HD21	1.66	0.60
1:A:642:GLU:HG2	1:A:647:ASN:ND2	2.17	0.60
1:A:111:LYS:O	1:A:114:ASN:ND2	2.35	0.60
1:A:2:PRO:HB2	1:A:3:PRO:HD3	1.84	0.58
1:A:593:ILE:HD12	1:A:597:GLN:HB3	1.86	0.58
1:A:772:MET:HB2	1:A:778:PRO:HG2	1.84	0.58
2:B:343:VAL:HG13	2:B:356:LEU:HD11	1.87	0.56
1:A:735:LEU:O	1:A:739:MET:HG3	2.06	0.56
1:A:324:THR:HG22	1:A:483:VAL:HG23	1.88	0.55
1:A:31:ILE:HD11	2:B:531:LEU:HD13	1.88	0.55
1:A:139:PHE:CE1	1:A:143:ILE:HD13	2.43	0.54
1:A:799:ILE:CD1	1:A:847:LEU:HD22	2.39	0.53
1:A:916:ARG:HB3	1:A:921:ILE:HD11	1.91	0.53
1:A:336:ILE:HD12	1:A:389:TYR:CE2	2.45	0.52
1:A:261:PHE:HA	1:A:270:TYR:CE2	2.46	0.51
1:A:641:TYR:OH	1:A:1007:GLY:N	2.45	0.50
1:A:1022:ILE:HA	1:A:1025:THR:HG22	1.93	0.50
1:A:552:TRP:CZ3	1:A:555:ARG:HD3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:LEU:HD22	1:A:650:VAL:HG22	1.94	0.49
1:A:904:TYR:O	1:A:908:THR:HB	2.13	0.49
1:A:628:LEU:HD23	1:A:663:ILE:HD13	1.95	0.48
1:A:255:CYS:SG	1:A:789:MET:HE3	2.53	0.48
1:A:870:LEU:HD22	1:A:871:GLN:HB2	1.95	0.48
1:A:602:LEU:O	1:A:612:ARG:NH2	2.47	0.47
1:A:106:GLY:O	1:A:108:ARG:N	2.47	0.47
1:A:612:ARG:NH1	1:A:642:GLU:OE1	2.47	0.47
1:A:803:ASN:O	1:A:844:CYS:O	2.32	0.47
1:A:338:ILE:HD12	1:A:338:ILE:N	2.29	0.47
1:A:552:TRP:O	1:A:555:ARG:NH1	2.48	0.46
1:A:731:GLN:HE22	1:A:777:ARG:HE	1.62	0.46
1:A:255:CYS:SG	1:A:789:MET:CE	3.04	0.46
1:A:193:VAL:HG22	1:A:208:THR:HG22	1.97	0.46
1:A:446:TRP:CZ2	1:A:465:ASN:HA	2.51	0.45
2:B:343:VAL:HG21	2:B:358:ARG:HD3	1.98	0.45
1:A:436:LEU:HB3	1:A:484:VAL:HB	1.98	0.45
1:A:10:LEU:HD13	1:A:16:MET:CE	2.48	0.44
2:B:495:GLU:O	2:B:499:GLN:HG2	2.18	0.44
1:A:367:LEU:HD12	1:A:368:CYS:O	2.18	0.44
2:B:455:GLN:HB2	2:B:455:GLN:HE21	1.60	0.44
2:B:484:ILE:O	2:B:488:ASN:ND2	2.51	0.44
1:A:671:LEU:HB2	1:A:688:LEU:HD21	1.98	0.44
1:A:910:ILE:O	1:A:1025:THR:HG21	2.18	0.43
1:A:878:HIS:NE2	1:A:966:LYS:O	2.51	0.43
2:B:370:LEU:HD21	2:B:424:LEU:HD11	2.01	0.43
2:B:544:ARG:O	2:B:547:GLU:HG2	2.19	0.43
1:A:181:ILE:HG23	1:A:277:ILE:HG21	2.01	0.43
2:B:506:LYS:HA	2:B:509:ILE:HG22	2.01	0.42
1:A:524:ARG:HD3	1:A:526:ASN:HD22	1.84	0.42
1:A:335:ARG:NE	1:A:478:ASP:OD2	2.49	0.42
1:A:885:ASN:HB3	1:A:889:ILE:HG22	2.01	0.42
2:B:509:ILE:HG23	2:B:510:GLU:HG3	2.01	0.42
1:A:473:LEU:C	1:A:473:LEU:HD12	2.40	0.42
1:A:383:TRP:O	1:A:384:ASN:ND2	2.53	0.42
1:A:8:GLY:CA	1:A:714:ASN:HD21	2.31	0.42
1:A:544:THR:HG22	2:B:380:LEU:HB3	2.02	0.41
1:A:552:TRP:CE2	1:A:555:ARG:NH1	2.88	0.41
1:A:357:ARG:HD3	1:A:455:LEU:HD13	2.01	0.41
1:A:870:LEU:HD22	1:A:871:GLN:N	2.35	0.41
1:A:782:ASN:OD1	1:A:796:ASN:ND2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:ASN:C	1:A:660:ASN:OD1	2.59	0.41
1:A:135:GLU:OE2	1:A:644:TYR:HB3	2.21	0.41
1:A:749:GLN:O	1:A:761:LEU:O	2.38	0.41
1:A:361:TYR:CD1	1:A:365:GLU:HB3	2.56	0.40
1:A:32:VAL:CG2	1:A:49:LEU:CD1	3.00	0.40
1:A:913:ILE:HD12	1:A:914:GLY:O	2.21	0.40
1:A:11:TRP:HB2	1:A:95:PHE:CD1	2.56	0.40
2:B:459:LYS:HE3	2:B:566:ILE:HG23	2.03	0.40
1:A:544:THR:HG21	2:B:382:LYS:HG2	2.03	0.40
1:A:429:LEU:HD23	1:A:429:LEU:HA	1.93	0.40
1:A:761:LEU:HD22	1:A:783:TRP:CE3	2.56	0.40
1:A:995:ALA:CB	1:A:1028:LEU:HD21	2.51	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	1044/1096 (95%)	927 (89%)	96 (9%)	21 (2%)	9	43
2	B	188/279 (67%)	179 (95%)	7 (4%)	2 (1%)	17	57
All	All	1232/1375 (90%)	1106 (90%)	103 (8%)	23 (2%)	10	45

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
1	A	107	ASN
1	A	323	SER
1	A	514	SER
1	A	38	ARG
1	A	264	LYS

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Mol	Chain	Res	Type
1	A	939	ASP
1	A	945	PHE
1	A	966	LYS
2	B	365	HIS
1	A	378	CYS
1	A	471	PRO
1	A	787	ASP
1	A	972	THR
2	B	513	LYS
1	A	186	ASP
1	A	520	ASP
1	A	1027	ALA
1	A	379	SER
1	A	555	ARG
1	A	112	ILE
1	A	5	PRO
1	A	200	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	965/997 (97%)	905 (94%)	60 (6%)	23	61
2	B	202/259 (78%)	188 (93%)	14 (7%)	19	57
All	All	1167/1256 (93%)	1093 (94%)	74 (6%)	22	60

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	ARG
1	A	22	VAL
1	A	35	GLU
1	A	39	GLU
1	A	52	GLU

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Mol	Chain	Res	Type
1	A	69	ILE
1	A	93	ARG
1	A	99	LEU
1	A	107	ASN
1	A	108	ARG
1	A	109	GLU
1	A	112	ILE
1	A	158	SER
1	A	173	SER
1	A	205	GLN
1	A	206	LYS
1	A	214	ASP
1	A	223	GLU
1	A	239	LEU
1	A	267	LEU
1	A	299	MET
1	A	326	SER
1	A	335	ARG
1	A	339	LEU
1	A	353	LYS
1	A	373	THR
1	A	380	ASN
1	A	441	MET
1	A	455	LEU
1	A	473	LEU
1	A	475	LEU
1	A	479	TRP
1	A	513	LEU
1	A	516	ARG
1	A	517	LEU
1	A	545	GLU
1	A	553	SER
1	A	575	ASN
1	A	578	ASP
1	A	597	GLN
1	A	638	VAL
1	A	727	THR
1	A	753	SER
1	A	764	LEU
1	A	808	ARG
1	A	825	GLN
1	A	829	LEU

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Mol	Chain	Res	Type
1	A	834	LEU
1	A	870	LEU
1	A	876	THR
1	A	905	CYS
1	A	908	THR
1	A	919	SER
1	A	966	LYS
1	A	969	GLN
1	A	971	CYS
1	A	972	THR
1	A	1052	THR
1	A	1055	MET
2	B	365	HIS
2	B	400	SER
2	B	415	GLN
2	B	416	TYR
2	B	425	LEU
2	B	455	GLN
2	B	468	GLU
2	B	482	THR
2	B	501	GLN
2	B	513	LYS
2	B	518	GLU
2	B	531	LEU
2	B	574	ARG
2	B	596	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	GLN
1	A	444	ASN
1	A	526	ASN
1	A	554	HIS
1	A	575	ASN
1	A	605	ASN
1	A	643	GLN
1	A	670	HIS
1	A	714	ASN
1	A	721	GLN
1	A	731	GLN
1	A	738	GLN

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Mol	Chain	Res	Type
1	A	782	ASN
1	A	785	ASN
1	A	795	GLN
1	A	796	ASN
1	A	885	ASN
1	A	917	HIS
1	A	1047	HIS
2	B	329	GLN
2	B	455	GLN
2	B	475	GLN
2	B	595	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SEP	A	7	1	7,9,10	0.73	0	8,12,14	1.74	2 (25%)
1	SEP	A	790	1	7,9,10	0.59	0	8,12,14	1.65	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	7	1	-	0/5/8/10	0/0/0/0
1	SEP	A	790	1	-	0/5/8/10	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	7	SEP	OG-CB-CA	-3.16	105.51	108.26
1	A	7	SEP	OG-P-O1P	-2.13	101.72	107.08
1	A	790	SEP	O-C-CA	-2.02	120.31	125.72
1	A	790	SEP	OG-CB-CA	2.41	110.36	108.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	SOA	B	701	-	9,9,9	1.31	1 (11%)	10,11,11	0.55	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	SOA	B	701	-	-	0/2/2/2	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	SOA	C3-N11	3.65	1.49	1.37

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	1056/1096 (96%)	0.22	42 (3%) 42 34	52, 103, 180, 220	0
2	B	212/279 (75%)	0.98	45 (21%) 1 1	91, 178, 226, 259	0
All	All	1268/1375 (92%)	0.35	87 (6%) 20 16	52, 111, 198, 259	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	409	ARG	5.7
2	B	405	ILE	5.5
1	A	381	PRO	5.4
2	B	410	ASN	5.0
1	A	1056	ASP	4.9
1	A	351	ILE	4.7
1	A	-26	SER	4.7
2	B	423	LYS	4.6
1	A	868	GLY	4.4
2	B	367	ASP	4.4
1	A	347	ASN	4.2
2	B	368	TYR	4.1
1	A	350	ASP	4.1
2	B	365	HIS	4.1
2	B	449	LEU	3.9
2	B	401	VAL	3.9
2	B	580	TYR	3.9
2	B	359	ASP	3.9
2	B	425	LEU	3.8
2	B	364	MET	3.8
2	B	512	PHE	3.8
2	B	559	ILE	3.7
2	B	378	ASN	3.6
2	B	505	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	107	ASN	3.5
2	B	581	LEU	3.5
1	A	869	ALA	3.5
2	B	504	TYR	3.4
2	B	408	TYR	3.4
2	B	573	LEU	3.3
2	B	390	TYR	3.2
2	B	424	LEU	3.1
1	A	346	VAL	3.1
1	A	523	LEU	3.0
2	B	427	PRO	3.0
2	B	426	TYR	3.0
1	A	872	PHE	3.0
1	A	358	THR	3.0
1	A	321	GLU	2.9
1	A	354	ILE	2.8
1	A	343	TYR	2.8
1	A	423	ALA	2.8
1	A	382	ARG	2.8
2	B	454	THR	2.7
2	B	383	ILE	2.7
1	A	344	VAL	2.7
1	A	1054	LYS	2.7
1	A	374	GLN	2.7
1	A	943	LYS	2.7
2	B	399	SER	2.6
1	A	1052	THR	2.6
1	A	511	ALA	2.6
2	B	329	GLN	2.6
1	A	867	LYS	2.6
1	A	407	CYS	2.6
1	A	300	ASP	2.6
1	A	1	MET	2.5
2	B	346	LYS	2.5
2	B	411	GLU	2.5
1	A	557	TYR	2.5
2	B	494	PHE	2.4
2	B	444	ALA	2.4
1	A	408	SER	2.4
2	B	355	PHE	2.4
1	A	345	ASN	2.4
1	A	50	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	422	LEU	2.3
1	A	673	SER	2.3
2	B	556	TYR	2.3
2	B	443	GLU	2.3
2	B	508	TYR	2.3
1	A	810	ASP	2.2
2	B	353	GLY	2.2
2	B	356	LEU	2.2
1	A	364	GLY	2.2
1	A	353	LYS	2.2
2	B	584	LEU	2.2
2	B	354	THR	2.2
1	A	341	ALA	2.2
1	A	320	GLY	2.1
2	B	333	TRP	2.1
1	A	1036	LEU	2.1
2	B	402	VAL	2.1
2	B	412	SER	2.0
2	B	345	GLU	2.0
1	A	409	VAL	2.0
1	A	809	GLN	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	SEP	A	790	10/11	0.95	0.15	-	75,94,166,169	0
1	SEP	A	7	10/11	0.80	0.24	-	145,156,183,193	0

6.3 Carbohydrates

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	SOA	B	701	9/9	0.77	0.70	-	141,156,162,165	0

6.5 Other polymers [i](#)

There are no such residues in this entry.