



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:50 PM UTC

PDB ID : 5SXD / pdb_00005sxd
Title : Crystal Structure of PI3Kalpha in complex with fragment 22
Authors : Gabelli, S.B.; Vogelstein, B.; Miller, M.S.; Amzel, L.M.
Deposited on : 2016-08-09
Resolution : 3.50 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

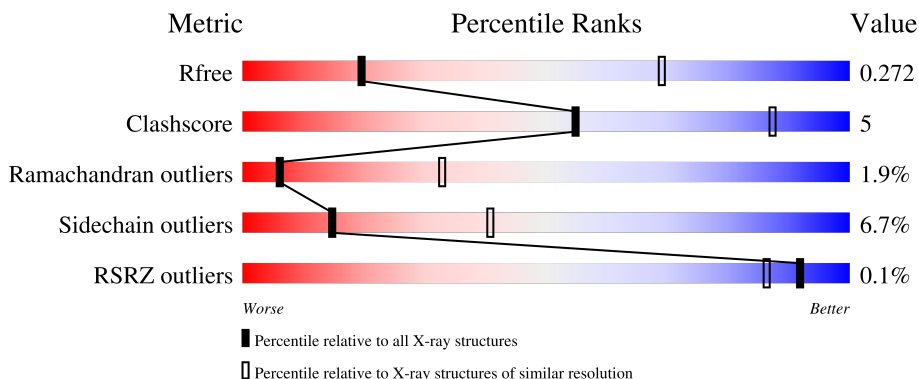
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	 76% 18% . .
2	B	279	 75% 12% 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10694 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	1051	Total	C	N	O	P	S	0	0	0
			8593	5486	1475	1561	2	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

Continued on next page...

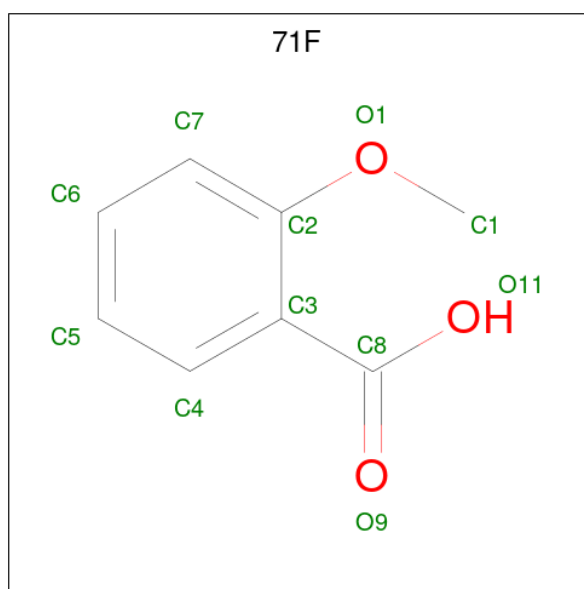
Continued from previous page...

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	244	Total	C	N	O	S	0	0	0
			2090	1315	371	398	6			

- Molecule 3 is 2-methoxybenzoic acid (CCD ID: 71F) (formula: C₈H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			11	8	3		

ASN

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.87Å 116.44Å 149.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.97 – 3.50 91.97 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (91.97-3.50) 99.6 (91.97-3.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.194 , 0.276 0.195 , 0.272	Depositor DCC
R_{free} test set	1331 reflections (3.15%)	wwPDB-VP
Wilson B-factor (Å ²)	113.3	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 113.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10694	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 3.10% 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: 71F, 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	0.75	4/8769 (0.0%)	1.02	10/11849 (0.1%)
2	B	0.70	0/2118	0.96	1/2826 (0.0%)
All	All	0.74	4/10887 (0.0%)	1.01	11/14675 (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	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	113	LEU	CA-C	6.54	1.60	1.53
1	A	339	LEU	CA-C	6.51	1.55	1.52
1	A	2	PRO	CA-C	6.19	1.57	1.52
1	A	365	GLU	C-N	5.40	1.38	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	PRO	N-CA-C	11.78	125.07	110.70
1	A	513	LEU	N-CA-C	-6.63	103.98	111.07
1	A	365	GLU	N-CA-C	6.11	117.35	109.72
1	A	456	LEU	N-CA-C	6.07	121.26	113.18
2	B	595	ASN	N-CA-C	5.79	119.87	112.34
1	A	1016	PHE	N-CA-C	5.76	119.12	111.75
1	A	970	GLU	CA-C-N	5.56	127.73	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	970	GLU	C-N-CA	5.56	127.73	120.28
1	A	808	ARG	N-CA-C	5.09	118.98	112.87
1	A	864	GLY	N-CA-C	5.05	120.23	114.67
1	A	114	ASN	N-CA-C	-5.01	107.02	113.23

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 [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	8593	0	8572	95	0
2	B	2090	0	2078	13	0
3	B	11	0	0	0	0
All	All	10694	0	10650	102	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 (102) 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:108:ARG:HH12	1:A:111:LYS:HD2	1.51	0.75
1:A:166:VAL:HG21	1:A:297:LEU:HD22	1.74	0.70
1:A:761:LEU:HD22	1:A:783:TRP:CD2	2.26	0.69
1:A:15:LEU:HD13	1:A:718:ILE:HD11	1.75	0.69
2:B:343:VAL:HG13	2:B:356:LEU:HD11	1.78	0.66
1:A:749:GLN:O	1:A:762:GLY:HA2	1.97	0.65
1:A:761:LEU:HD22	1:A:783:TRP:CE3	2.32	0.64
1:A:610:MET:HA	1:A:610:MET:HE2	1.80	0.64
1:A:709:MET:HE1	1:A:847:LEU:HD21	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.23	0.63
1:A:10:LEU:HD13	1:A:16:MET:HE2	1.81	0.62
1:A:278:MET:HA	1:A:278:MET:HE2	1.81	0.62
1:A:261:PHE:HA	1:A:270:TYR:CE2	2.35	0.61
1:A:513:LEU:O	1:A:515:ASN:N	2.35	0.60
1:A:561:ILE:O	1:A:564:ILE:HG22	2.01	0.60
1:A:336:ILE:HD12	1:A:389:TYR:CE2	2.37	0.60
1:A:181:ILE:HG12	1:A:278:MET:HE3	1.82	0.59
1:A:772:MET:HB2	1:A:778:PRO:HG2	1.82	0.59
1:A:8:GLY:HA2	1:A:714:ASN:HD21	1.67	0.59
1:A:106:GLY:O	1:A:108:ARG:N	2.34	0.59
1:A:8:GLY:CA	1:A:714:ASN:HD21	2.16	0.59
1:A:873:ASN:HB3	1:A:876:THR:HG23	1.85	0.58
1:A:452:LEU:HD21	1:A:457:ASN:HD21	1.69	0.58
1:A:543:ILE:HD11	1:A:567:LYS:HD3	1.85	0.58
1:A:111:LYS:O	1:A:114:ASN:ND2	2.38	0.56
1:A:324:THR:HG22	1:A:483:VAL:HG23	1.86	0.56
1:A:31:ILE:HD11	2:B:531:LEU:HD13	1.88	0.56
1:A:745:MET:HA	1:A:745:MET:HE2	1.88	0.56
1:A:98:PHE:CE2	2:B:490:THR:HG23	2.41	0.56
2:B:347:LEU:HD22	2:B:373:ARG:HB2	1.89	0.55
1:A:9:GLU:OE1	1:A:38:ARG:NH1	2.41	0.53
1:A:989:LEU:HD11	1:A:1036:LEU:HD11	1.91	0.53
1:A:178:PRO:HD2	1:A:181:ILE:HD12	1.90	0.53
1:A:671:LEU:HB2	1:A:688:LEU:HD21	1.90	0.53
1:A:164:MET:HE1	1:A:263:GLU:HB3	1.91	0.52
1:A:0:SER:O	1:A:1:MET:HG2	2.09	0.52
1:A:552:TRP:CZ3	1:A:555:ARG:HD3	2.45	0.52
1:A:599:MET:HE1	1:A:631:TYR:CD2	2.44	0.52
1:A:446:TRP:CZ2	1:A:465:ASN:HA	2.46	0.51
1:A:286:MET:HE3	1:A:288:MET:HE3	1.92	0.51
1:A:452:LEU:CD2	1:A:457:ASN:HD21	2.23	0.50
1:A:572:VAL:CG2	1:A:583:MET:HE3	2.41	0.50
1:A:135:GLU:OE2	1:A:644:TYR:HB3	2.12	0.50
1:A:1022:ILE:HA	1:A:1025:THR:HG22	1.94	0.49
2:B:343:VAL:HG21	2:B:358:ARG:HD3	1.94	0.49
1:A:949:ARG:O	1:A:950:GLU:C	2.56	0.48
1:A:759:HIS:HB3	1:A:797:ASN:HD21	1.78	0.48
1:A:524:ARG:HD2	1:A:526:ASN:HD22	1.79	0.47
2:B:488:ASN:HA	2:B:491:ILE:HD12	1.96	0.47
2:B:469:GLU:O	2:B:473:THR:OG1	2.26	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:ILE:O	1:A:1025:THR:HG21	2.14	0.47
1:A:660:ASN:OD1	1:A:660:ASN:C	2.58	0.47
1:A:789:MET:O	1:A:790:SEP:C	2.63	0.47
1:A:833:MET:HE1	1:A:904:TYR:HA	1.97	0.47
1:A:513:LEU:O	1:A:516:ARG:N	2.42	0.47
1:A:807:LEU:HD12	1:A:838:CYS:SG	2.55	0.47
1:A:568:LEU:HG	1:A:583:MET:HE1	1.96	0.46
1:A:718:ILE:O	1:A:721:GLN:O	2.32	0.46
1:A:457:ASN:N	1:A:457:ASN:HD22	2.13	0.46
1:A:885:ASN:HB3	1:A:889:ILE:HG22	1.96	0.46
1:A:324:THR:HG22	1:A:483:VAL:CG2	2.45	0.46
1:A:79:ARG:HD2	2:B:489:GLU:OE1	2.16	0.45
2:B:506:LYS:HA	2:B:509:ILE:HG22	1.99	0.45
1:A:286:MET:HE1	1:A:788:ILE:HD13	1.99	0.44
1:A:519:ARG:NE	1:A:527:ASP:OD2	2.50	0.44
1:A:899:ARG:HG2	1:A:983:MET:HE1	1.99	0.44
1:A:524:ARG:CD	1:A:526:ASN:HD22	2.31	0.43
1:A:739:MET:O	1:A:745:MET:HE3	2.18	0.43
2:B:362:THR:HB	2:B:365:HIS:HB2	1.99	0.43
1:A:1002:PHE:HB3	1:A:1019:ILE:HG12	2.01	0.43
1:A:111:LYS:HE2	1:A:305:PRO:HA	2.00	0.43
1:A:213:HIS:CE1	1:A:214:ASP:HB3	2.54	0.43
1:A:639:LEU:HD22	1:A:650:VAL:HG22	2.00	0.43
1:A:360:ILE:N	1:A:360:ILE:HD12	2.34	0.42
1:A:31:ILE:CD1	2:B:531:LEU:HD13	2.48	0.42
1:A:544:THR:HG22	2:B:380:LEU:HB3	2.02	0.42
1:A:856:THR:O	1:A:857:ILE:C	2.62	0.42
1:A:192:VAL:HG12	1:A:193:VAL:H	1.84	0.42
1:A:347:ASN:ND2	2:B:565:SER:OG	2.52	0.42
1:A:114:ASN:HA	1:A:117:ILE:HD12	2.01	0.42
1:A:171:VAL:HG12	1:A:269:GLN:HG2	2.02	0.42
1:A:628:LEU:HD23	1:A:663:ILE:HD13	2.00	0.42
1:A:727:THR:O	1:A:730:VAL:N	2.53	0.41
1:A:10:LEU:HD13	1:A:16:MET:CE	2.49	0.41
1:A:192:VAL:HG12	1:A:193:VAL:N	2.34	0.41
1:A:908:THR:HG21	1:A:954:PHE:HB2	2.01	0.41
1:A:856:THR:HG23	1:A:922:MET:HE3	2.02	0.41
1:A:735:LEU:O	1:A:739:MET:HG3	2.20	0.41
1:A:932:ILE:O	1:A:933:ASP:C	2.64	0.41
1:A:353:LYS:HA	1:A:377:PRO:HB2	2.02	0.41
1:A:819:ILE:HG22	1:A:823:ILE:HD12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-14:ILE:N	1:A:-13:PRO:CD	2.84	0.41
1:A:731:GLN:OE1	1:A:777:ARG:NH2	2.49	0.41
1:A:338:ILE:O	1:A:339:LEU:HD12	2.21	0.41
1:A:965:SER:OG	1:A:971:CYS:HB3	2.22	0.40
1:A:193:VAL:HG22	1:A:208:THR:HG22	2.03	0.40
1:A:936:HIS:HB3	1:A:940:HIS:HB3	2.03	0.40
1:A:-16:TYR:CD1	1:A:-16:TYR:C	2.99	0.40
1:A:599:MET:HB3	1:A:1004:MET:SD	2.62	0.40
1:A:253:LYS:HD3	1:A:286:MET:HE2	2.02	0.40
1:A:555:ARG:HG3	1:A:556:HIS:CD2	2.56	0.40
1:A:727:THR:O	1:A:728:GLN:C	2.64	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	1037/1096 (95%)	906 (87%)	111 (11%)	20 (2%)	6	33
2	B	228/279 (82%)	210 (92%)	14 (6%)	4 (2%)	6	34
All	All	1265/1375 (92%)	1116 (88%)	125 (10%)	24 (2%)	6	33

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	514	SER
1	A	945	PHE
1	A	3	PRO
1	A	38	ARG
1	A	201	ASN
1	A	379	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	763	ASN
1	A	869	ALA
1	A	966	LYS
2	B	438	LYS
1	A	520	ASP
1	A	918	ASN
1	A	972	THR
2	B	332	GLU
2	B	365	HIS
1	A	108	ARG
1	A	471	PRO
1	A	950	GLU
1	A	-13	PRO
1	A	202	ASN
1	A	307	TYR
2	B	513	LYS
1	A	933	ASP

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	959/997 (96%)	895 (93%)	64 (7%)	15	41
2	B	229/259 (88%)	213 (93%)	16 (7%)	14	39
All	All	1188/1256 (95%)	1108 (93%)	80 (7%)	15	41

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-26	SER
1	A	-15	ASP
1	A	-14	ILE
1	A	-12	THR
1	A	4	ARG
1	A	15	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	22	VAL
1	A	25	LEU
1	A	32	VAL
1	A	35	GLU
1	A	39	GLU
1	A	52	GLU
1	A	69	ILE
1	A	99	LEU
1	A	107	ASN
1	A	110	GLU
1	A	111	LYS
1	A	112	ILE
1	A	137	GLN
1	A	158	SER
1	A	171	VAL
1	A	190	ILE
1	A	199	SER
1	A	206	LYS
1	A	212	ASN
1	A	216	VAL
1	A	223	GLU
1	A	236	SER
1	A	239	LEU
1	A	244	LEU
1	A	251	ILE
1	A	267	LEU
1	A	275	SER
1	A	299	MET
1	A	323	SER
1	A	350	ASP
1	A	353	LYS
1	A	369	ASP
1	A	373	THR
1	A	380	ASN
1	A	383	TRP
1	A	420	CYS
1	A	437	VAL
1	A	510	HIS
1	A	517	LEU
1	A	545	GLU
1	A	575	ASN
1	A	638	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	714	ASN
1	A	722	GLU
1	A	727	THR
1	A	764	LEU
1	A	791	GLU
1	A	799	ILE
1	A	811	MET
1	A	841	ILE
1	A	845	VAL
1	A	858	MET
1	A	923	VAL
1	A	924	LYS
1	A	972	THR
1	A	1015	SER
1	A	1017	ASP
1	A	1022	ILE
2	B	329	GLN
2	B	365	HIS
2	B	367	ASP
2	B	372	LEU
2	B	374	LYS
2	B	400	SER
2	B	415	GLN
2	B	416	TYR
2	B	425	LEU
2	B	437	VAL
2	B	441	ASN
2	B	482	THR
2	B	529	ASP
2	B	552	GLN
2	B	594	LEU
2	B	595	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	114	ASN
1	A	180	HIS
1	A	212	ASN
1	A	219	GLN
1	A	331	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	370	ASN
1	A	384	ASN
1	A	457	ASN
1	A	526	ASN
1	A	554	HIS
1	A	556	HIS
1	A	575	ASN
1	A	597	GLN
1	A	605	ASN
1	A	670	HIS
1	A	676	HIS
1	A	714	ASN
1	A	749	GLN
1	A	785	ASN
1	A	795	GLN
1	A	797	ASN
1	A	827	GLN
1	A	918	ASN
1	A	1042	GLN
1	A	1048	HIS
2	B	377	ASN
2	B	378	ASN
2	B	415	GLN
2	B	499	GLN
2	B	552	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	0.82	0	7,12,14	1.87	2 (28%)
1	SEP	A	790	1	8,9,10	0.67	0	7,12,14	1.74	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	-	6/6/8/10	-
1	SEP	A	790	1	-	5/6/8/10	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	SEP	OG-CB-CA	3.94	111.98	108.14
1	A	790	SEP	OG-CB-CA	3.37	111.42	108.14
1	A	7	SEP	O3P-P-OG	-2.09	101.21	106.67
1	A	790	SEP	O2P-P-OG	-2.04	101.35	106.67

There are no chirality outliers.

All (11) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	790	SEP	1	0

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	71F	B	701	-	11,11,11	1.02	0	14,14,14	1.64	3 (21%)

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	71F	B	701	-	-	6/6/6/6	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	71F	C1-O1-C2	4.24	123.73	117.51
3	B	701	71F	C2-C3-C8	-2.31	119.56	123.73
3	B	701	71F	O1-C2-C3	2.09	119.58	116.55

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	701	71F	C2-C3-C8-O9
3	B	701	71F	C2-C3-C8-O11
3	B	701	71F	C7-C2-O1-C1
3	B	701	71F	C3-C2-O1-C1
3	B	701	71F	C4-C3-C8-O11
3	B	701	71F	C4-C3-C8-O9

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	1049/1096 (95%)	-0.74	0	100 100	69, 121, 188, 257	0
2	B	244/279 (87%)	-0.62	1 (0%)	88 72	113, 188, 232, 272	0
All	All	1293/1375 (94%)	-0.72	1 (0%)	92 86	69, 129, 210, 272	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	401	VAL	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	0.69	0.10	164,181,187,203	0
1	SEP	A	790	10/11	0.91	0.06	92,113,186,194	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	71F	B	701	11/11	0.87	0.13	153,158,171,172	0

6.5 Other polymers [i](#)

There are no such residues in this entry.