



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:48 PM UTC

PDB ID : 5SW8 / pdb_00005sw8
Title : Crystal structure of PI3Kalpha in complex with fragments 7 and 11
Authors : Gabelli, S.B.; Vogelstein, B.; Miller, M.S.; Amzel, L.M.
Deposited on : 2016-08-08
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

<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

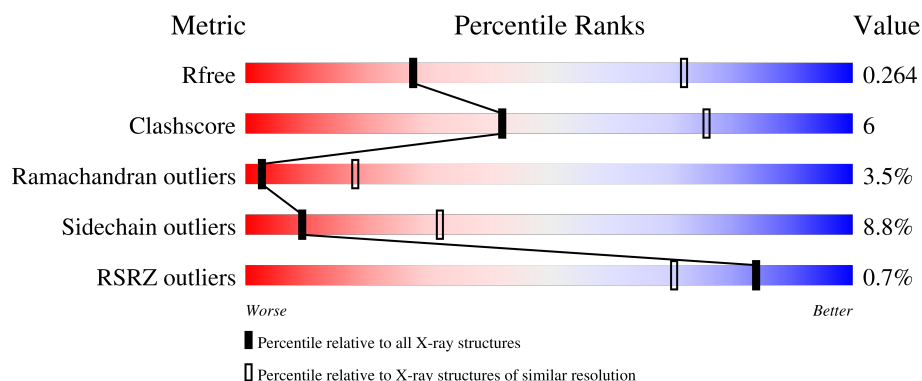
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 5 unique types of molecules in this entry. The entry contains 10223 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	1031	Total	C	N	O	P	S	0	0	0
			8437	5394	1442	1531	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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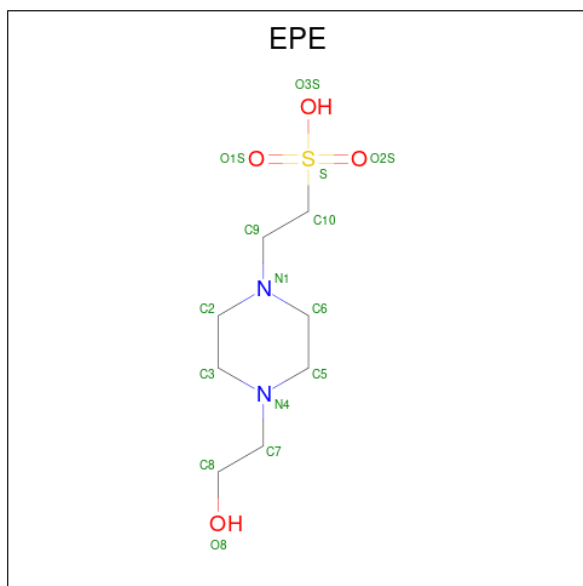
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42336
A	0	SER	-	expression tag	UNP P42336

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

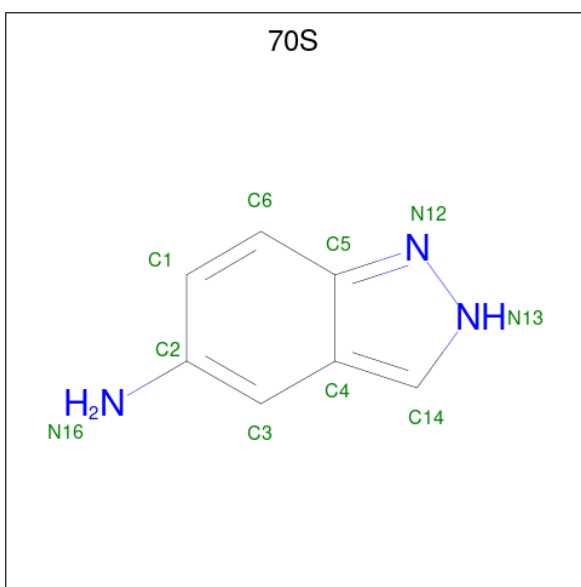
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	201	Total	C	N	O	S	0	0	0
			1739	1085	312	337	5			

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



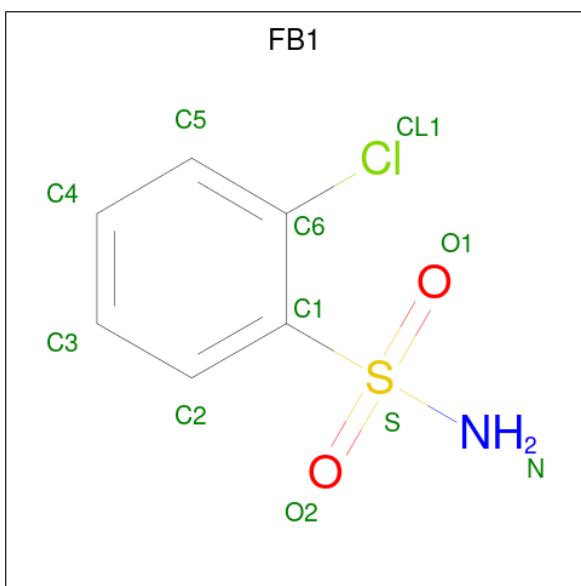
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is 2H-indazol-5-amine (CCD ID: 70S) (formula: $C_7H_7N_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			10	7	3		

- Molecule 5 is 2-CHLOROBENZENESULFONAMIDE (CCD ID: FB1) (formula: $C_6H_5ClNO_2S$).

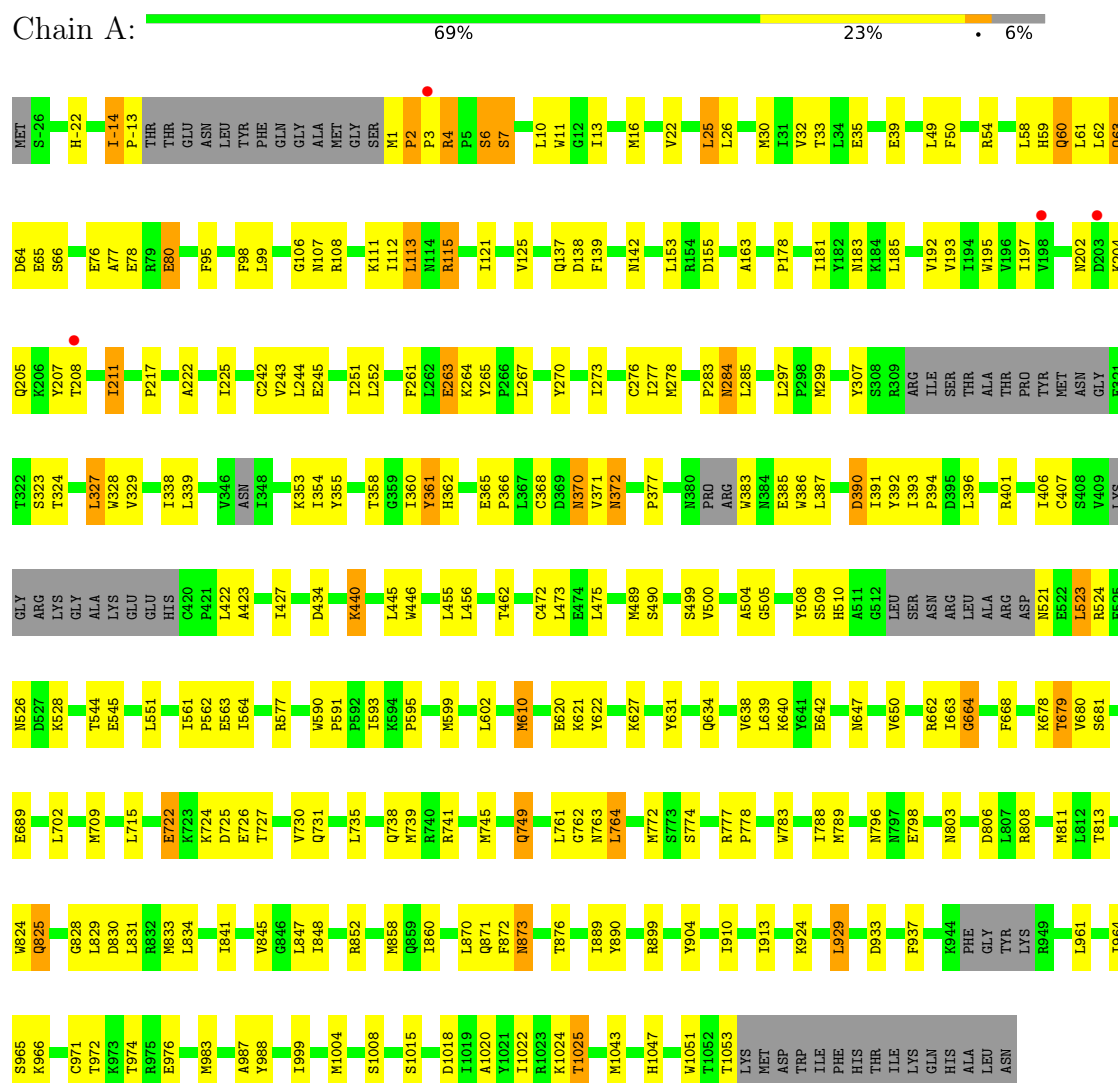


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	S	0	0
			11	6	1	1	2	1		
5	A	1	Total	C	Cl	N	O	S	0	0
			11	6	1	1	2	1		

3 Residue-property plots

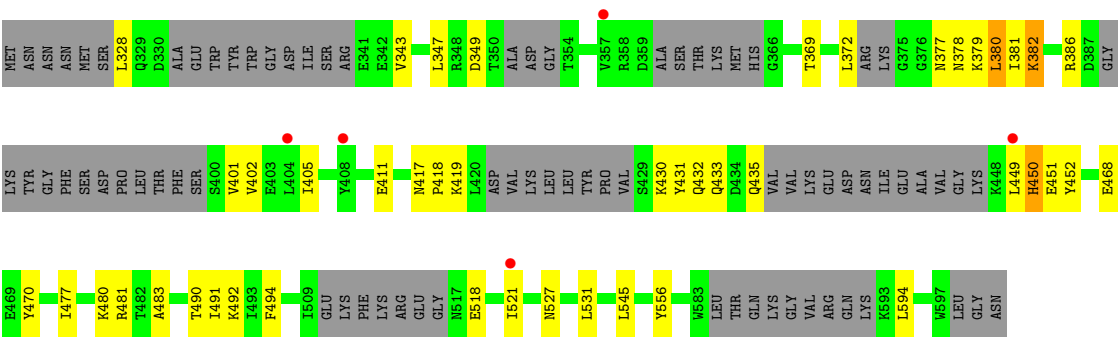
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	115.65Å 117.82Å 152.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.24 – 3.30 93.24 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (93.24-3.30) 98.9 (93.24-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.226 , 0.298 (Not available) , 0.264	Depositor DCC
R_{free} test set	1574 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	98.9	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 95.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10223	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: 70S, SEP, EPE, FB1

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.79	2/8619 (0.0%)	1.05	16/11646 (0.1%)
2	B	0.78	0/1757	1.03	1/2338 (0.0%)
All	All	0.79	2/10376 (0.0%)	1.04	17/13984 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	362	HIS	CA-C	8.76	1.63	1.52
1	A	-14	ILE	CA-C	5.28	1.57	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	LEU	N-CA-C	6.83	121.58	112.30
1	A	4	ARG	N-CA-C	6.41	113.78	108.07
2	B	382	LYS	N-CA-C	6.19	117.80	108.46
1	A	509	SER	N-CA-C	6.01	117.83	111.28
1	A	2	PRO	C-N-CD	-5.92	107.59	120.60
1	A	-14	ILE	CB-CA-C	-5.70	108.31	114.35
1	A	371	VAL	N-CA-C	5.52	121.39	113.16
1	A	263	GLU	N-CA-C	5.51	117.45	109.07
1	A	-14	ILE	N-CA-C	5.48	120.55	112.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	TYR	N-CA-C	5.46	117.37	109.07
1	A	510	HIS	N-CA-C	5.25	117.29	108.73
1	A	845	VAL	CB-CA-C	-5.22	103.76	111.80
1	A	142	ASN	N-CA-C	5.12	116.95	111.36
1	A	370	ASN	N-CA-C	5.11	117.58	109.50
1	A	937	PHE	N-CA-CB	5.09	117.55	110.07
1	A	245	GLU	N-CA-C	5.05	116.48	111.07
1	A	749	GLN	N-CA-C	5.03	119.87	113.18

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	LEU	Peptide
1	A	526	ASN	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	8437	0	8413	118	0
2	B	1739	0	1706	17	0
3	A	15	0	18	0	0
4	A	10	0	0	0	0
5	A	22	0	12	0	0
All	All	10223	0	10149	129	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 6.

All (129) 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:1:MET:H2	1:A:2:PRO:HA	1.50	0.74
1:A:192:VAL:HG12	1:A:193:VAL:N	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:GLN:O	1:A:762:GLY:HA2	1.91	0.70
1:A:599:MET:HE1	1:A:631:TYR:CD2	2.27	0.70
1:A:731:GLN:HE22	1:A:777:ARG:HE	1.39	0.68
1:A:709:MET:HE1	1:A:847:LEU:HD21	1.77	0.65
1:A:361:TYR:HA	1:A:366:PRO:HD3	1.78	0.65
1:A:25:LEU:HD21	2:B:494:PHE:CE1	2.32	0.64
1:A:106:GLY:O	1:A:108:ARG:N	2.30	0.64
1:A:640:LYS:HE2	1:A:680:VAL:HG11	1.81	0.62
1:A:108:ARG:HG3	1:A:111:LYS:HB2	1.82	0.62
1:A:6:SER:OG	1:A:7:SER:N	2.34	0.58
1:A:639:LEU:HD22	1:A:650:VAL:HG22	1.85	0.58
1:A:391:ILE:HD13	1:A:396:LEU:HD23	1.87	0.57
1:A:961:LEU:HA	1:A:964:ILE:HD12	1.86	0.57
1:A:283:PRO:C	1:A:284:ASN:HD22	2.12	0.57
1:A:610:MET:HA	1:A:610:MET:HE2	1.85	0.56
1:A:739:MET:HE2	1:A:764:LEU:HD21	1.87	0.56
1:A:98:PHE:CE2	2:B:490:THR:HG23	2.40	0.56
1:A:328:TRP:CE2	1:A:577:ARG:HD2	2.42	0.55
1:A:551:LEU:HD21	1:A:564:ILE:HD11	1.90	0.53
2:B:477:ILE:HD11	2:B:556:TYR:HB2	1.91	0.53
1:A:192:VAL:CG1	1:A:193:VAL:N	2.71	0.53
1:A:663:ILE:O	1:A:664:GLY:C	2.51	0.53
1:A:749:GLN:HE21	1:A:763:ASN:HA	1.72	0.53
1:A:285:LEU:HD23	1:A:285:LEU:N	2.24	0.53
1:A:217:PRO:HB3	1:A:252:LEU:HD12	1.90	0.53
1:A:446:TRP:CZ3	1:A:679:THR:HG22	2.45	0.52
1:A:634:GLN:HB3	1:A:1004:MET:HE2	1.91	0.52
1:A:25:LEU:HD12	1:A:25:LEU:N	2.24	0.52
1:A:32:VAL:HG21	1:A:49:LEU:CD1	2.40	0.52
1:A:205:GLN:NE2	1:A:207:TYR:OH	2.43	0.52
1:A:323:SER:O	1:A:324:THR:HG23	2.10	0.52
1:A:726:GLU:O	1:A:730:VAL:HB	2.09	0.52
1:A:965:SER:HB2	1:A:974:THR:HG21	1.92	0.52
1:A:181:ILE:HG23	1:A:277:ILE:HG21	1.91	0.52
1:A:899:ARG:HG2	1:A:983:MET:HE1	1.92	0.52
1:A:338:ILE:HD11	1:A:358:THR:HG21	1.92	0.51
1:A:910:ILE:O	1:A:1025:THR:HG21	2.11	0.51
1:A:163:ALA:HB2	1:A:297:LEU:HD11	1.91	0.51
1:A:871:GLN:HE21	1:A:872:PHE:H	1.59	0.51
1:A:98:PHE:HE2	2:B:490:THR:HG23	1.76	0.51
1:A:353:LYS:HA	1:A:377:PRO:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:HIS:O	1:A:60:GLN:HB3	2.11	0.50
1:A:10:LEU:HD13	1:A:16:MET:CE	2.42	0.50
1:A:738:GLN:HE22	1:A:741:ARG:HH21	1.58	0.50
2:B:518:GLU:HA	2:B:521:ILE:HD12	1.94	0.50
1:A:273:ILE:O	1:A:276:CYS:N	2.45	0.50
1:A:390:ASP:N	1:A:390:ASP:OD1	2.44	0.49
1:A:803:ASN:OD1	1:A:803:ASN:C	2.56	0.49
1:A:192:VAL:HG12	1:A:193:VAL:H	1.74	0.49
2:B:491:ILE:O	2:B:494:PHE:N	2.45	0.49
1:A:138:ASP:O	1:A:139:PHE:C	2.56	0.49
1:A:1043:MET:O	1:A:1047:HIS:ND1	2.42	0.49
1:A:599:MET:HE1	1:A:631:TYR:HD2	1.73	0.48
1:A:261:PHE:HA	1:A:270:TYR:CE2	2.48	0.48
1:A:353:LYS:HA	1:A:377:PRO:CB	2.44	0.48
1:A:715:LEU:HD21	1:A:735:LEU:HD12	1.94	0.48
1:A:26:LEU:CD1	1:A:30:MET:O	2.62	0.47
1:A:1015:SER:OG	1:A:1018:ASP:N	2.48	0.47
1:A:-14:ILE:HD12	1:A:-13:PRO:N	2.30	0.47
1:A:327:LEU:HD13	1:A:394:PRO:HA	1.96	0.47
1:A:545:GLU:CG	2:B:379:LYS:HG2	2.45	0.47
1:A:735:LEU:O	1:A:739:MET:HG3	2.15	0.47
1:A:521:ASN:HD22	1:A:523:LEU:HD21	1.79	0.47
1:A:621:LYS:HB3	1:A:622:TYR:CE1	2.50	0.47
1:A:407:CYS:SG	1:A:455:LEU:HD22	2.55	0.46
1:A:561:ILE:O	1:A:564:ILE:HG22	2.14	0.46
2:B:450:HIS:O	2:B:452:TYR:N	2.48	0.46
1:A:889:ILE:O	1:A:890:TYR:C	2.58	0.46
1:A:872:PHE:O	1:A:873:ASN:CB	2.64	0.46
1:A:824:TRP:O	1:A:825:GLN:C	2.58	0.46
1:A:929:LEU:C	1:A:929:LEU:HD23	2.41	0.46
1:A:709:MET:HE2	1:A:841:ILE:HD13	1.98	0.46
1:A:192:VAL:HG21	1:A:211:ILE:HD11	1.98	0.46
1:A:50:PHE:CD2	1:A:65:GLU:HB3	2.52	0.45
1:A:11:TRP:HB2	1:A:95:PHE:CD1	2.51	0.45
1:A:749:GLN:NE2	1:A:763:ASN:HA	2.32	0.45
2:B:480:LYS:HG2	2:B:545:LEU:HD11	1.97	0.45
2:B:402:VAL:HA	2:B:405:ILE:HD12	1.98	0.45
1:A:121:ILE:HD11	1:A:689:GLU:HA	1.98	0.45
1:A:80:GLU:OE2	1:A:115:ARG:NH1	2.51	0.44
1:A:833:MET:HE1	1:A:904:TYR:HA	1.99	0.44
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:798:GLU:OE1	1:A:852:ARG:NH1	2.51	0.44
1:A:988:TYR:CD1	1:A:988:TYR:C	2.95	0.44
1:A:406:ILE:HG22	1:A:422:LEU:HD12	2.00	0.44
2:B:480:LYS:O	2:B:481:ARG:C	2.61	0.44
1:A:98:PHE:O	1:A:99:LEU:HD23	2.17	0.44
1:A:284:ASN:HD22	1:A:284:ASN:N	2.15	0.44
1:A:739:MET:O	1:A:745:MET:HE3	2.17	0.43
1:A:195:TRP:HB3	1:A:789:MET:HE1	2.00	0.43
1:A:590:TRP:CD1	1:A:591:PRO:HD2	2.53	0.43
2:B:480:LYS:O	2:B:483:ALA:N	2.51	0.43
1:A:423:ALA:O	1:A:445:LEU:HD13	2.18	0.43
1:A:265:TYR:HB2	1:A:270:TYR:CE1	2.54	0.43
1:A:745:MET:HA	1:A:745:MET:HE2	2.01	0.43
1:A:602:LEU:HB3	1:A:638:VAL:HG11	2.01	0.43
1:A:59:HIS:CD2	1:A:62:LEU:HD12	2.53	0.42
1:A:32:VAL:HG21	1:A:49:LEU:HD11	2.01	0.42
1:A:544:THR:HG22	2:B:380:LEU:HD13	2.02	0.42
1:A:745:MET:O	1:A:749:GLN:HB2	2.19	0.42
1:A:761:LEU:HD23	1:A:783:TRP:CE2	2.55	0.42
1:A:354:ILE:HD12	1:A:354:ILE:O	2.19	0.42
1:A:360:ILE:O	1:A:366:PRO:HD2	2.19	0.42
1:A:668:PHE:CD2	1:A:702:LEU:HD13	2.54	0.42
2:B:433:GLN:N	2:B:433:GLN:OE1	2.53	0.42
1:A:806:ASP:OD1	1:A:808:ARG:HG2	2.20	0.42
1:A:339:LEU:HD12	1:A:339:LEU:N	2.35	0.42
1:A:777:ARG:N	1:A:778:PRO:CD	2.83	0.42
1:A:440:LYS:HA	1:A:475:LEU:O	2.20	0.42
1:A:806:ASP:OD1	1:A:806:ASP:C	2.61	0.42
1:A:489:MET:O	1:A:490:SER:C	2.63	0.41
1:A:178:PRO:HB2	1:A:181:ILE:HD12	2.01	0.41
1:A:222:ALA:O	1:A:225:ILE:N	2.53	0.41
1:A:125:VAL:HG13	1:A:689:GLU:OE2	2.20	0.41
1:A:831:LEU:HD11	1:A:987:ALA:HB2	2.02	0.41
1:A:355:TYR:HA	1:A:383:TRP:HZ2	1.85	0.41
2:B:417:ASN:HB3	2:B:418:PRO:HD3	2.03	0.41
1:A:197:ILE:HG22	1:A:204:LYS:HG2	2.03	0.41
1:A:76:GLU:O	1:A:78:GLU:N	2.52	0.41
1:A:472:CYS:SG	1:A:473:LEU:N	2.94	0.41
1:A:562:PRO:HB2	1:A:593:ILE:HG22	2.02	0.41
1:A:392:TYR:O	1:A:393:ILE:C	2.63	0.40
2:B:470:TYR:CE1	2:B:556:TYR:CE1	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:ILE:HA	1:A:1025:THR:CG2	2.52	0.40
1:A:-14:ILE:N	1:A:-13:PRO:HD2	2.36	0.40
1:A:30:MET:HE1	2:B:527:ASN:HB3	2.03	0.40
1:A:725:ASP:O	1:A:726:GLU:C	2.64	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	1014/1096 (92%)	862 (85%)	118 (12%)	34 (3%)	3	18
2	B	181/279 (65%)	145 (80%)	28 (16%)	8 (4%)	2	13
All	All	1195/1375 (87%)	1007 (84%)	146 (12%)	42 (4%)	3	18

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	PRO
1	A	6	SER
1	A	7	SER
1	A	66	SER
1	A	77	ALA
1	A	107	ASN
1	A	524	ARG
1	A	528	LYS
1	A	681	SER
1	A	873	ASN
1	A	966	LYS
2	B	431	TYR
1	A	54	ARG
1	A	183	ASN

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Mol	Chain	Res	Type
1	A	307	TYR
1	A	722	GLU
1	A	830	ASP
1	A	1051	TRP
2	B	377	ASN
2	B	450	HIS
2	B	451	GLU
1	A	60	GLN
1	A	63	GLN
1	A	202	ASN
1	A	264	LYS
1	A	372	ASN
2	B	401	VAL
2	B	432	GLN
2	B	492	LYS
2	B	594	LEU
1	A	-22	HIS
1	A	504	ALA
1	A	727	THR
1	A	933	ASP
1	A	1020	ALA
1	A	828	GLY
1	A	267	LEU
1	A	368	CYS
1	A	772	MET
1	A	505	GLY
1	A	595	PRO
1	A	664	GLY

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	944/998 (95%)	862 (91%)	82 (9%)	9	32
2	B	192/259 (74%)	174 (91%)	18 (9%)	8	30
All	All	1136/1257 (90%)	1036 (91%)	100 (9%)	9	32

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	13	ILE
1	A	22	VAL
1	A	25	LEU
1	A	33	THR
1	A	35	GLU
1	A	39	GLU
1	A	58	LEU
1	A	61	LEU
1	A	63	GLN
1	A	64	ASP
1	A	80	GLU
1	A	112	ILE
1	A	113	LEU
1	A	115	ARG
1	A	137	GLN
1	A	153	LEU
1	A	155	ASP
1	A	208	THR
1	A	211	ILE
1	A	242	CYS
1	A	243	VAL
1	A	244	LEU
1	A	251	ILE
1	A	263	GLU
1	A	278	MET
1	A	284	ASN
1	A	299	MET
1	A	327	LEU
1	A	329	VAL
1	A	365	GLU
1	A	370	ASN
1	A	372	ASN
1	A	385	GLU
1	A	386	TRP
1	A	387	LEU
1	A	390	ASP
1	A	401	ARG
1	A	427	ILE
1	A	434	ASP
1	A	440	LYS
1	A	456	LEU

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Mol	Chain	Res	Type
1	A	462	THR
1	A	499	SER
1	A	500	VAL
1	A	508	TYR
1	A	523	LEU
1	A	563	GLU
1	A	610	MET
1	A	620	GLU
1	A	627	LYS
1	A	662	ARG
1	A	678	LYS
1	A	679	THR
1	A	722	GLU
1	A	724	LYS
1	A	764	LEU
1	A	774	SER
1	A	788	ILE
1	A	796	ASN
1	A	811	MET
1	A	813	THR
1	A	825	GLN
1	A	829	LEU
1	A	834	LEU
1	A	848	ILE
1	A	858	MET
1	A	860	ILE
1	A	870	LEU
1	A	876	THR
1	A	913	ILE
1	A	924	LYS
1	A	929	LEU
1	A	971	CYS
1	A	972	THR
1	A	976	GLU
1	A	999	ILE
1	A	1008	SER
1	A	1022	ILE
1	A	1024	LYS
1	A	1025	THR
1	A	1053	THR
2	B	328	LEU
2	B	343	VAL

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Mol	Chain	Res	Type
2	B	347	LEU
2	B	349	ASP
2	B	369	THR
2	B	372	LEU
2	B	378	ASN
2	B	380	LEU
2	B	381	ILE
2	B	382	LYS
2	B	386	ARG
2	B	411	GLU
2	B	419	LYS
2	B	430	LYS
2	B	435	GLN
2	B	449	LEU
2	B	468	GLU
2	B	531	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	96	GLN
1	A	137	GLN
1	A	205	GLN
1	A	296	GLN
1	A	388	ASN
1	A	444	ASN
1	A	521	ASN
1	A	630	GLN
1	A	661	GLN
1	A	676	HIS
1	A	721	GLN
1	A	728	GLN
1	A	731	GLN
1	A	738	GLN
1	A	749	GLN
1	A	782	ASN
1	A	826	ASN
1	A	827	GLN
1	A	855	HIS
1	A	871	GLN
1	A	993	GLN

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Mol	Chain	Res	Type
1	A	996	ASN
1	A	1014	GLN
1	A	1042	GLN
2	B	385	HIS
2	B	417	ASN
2	B	450	HIS
2	B	455	GLN
2	B	488	ASN
2	B	499	GLN
2	B	564	ASN
2	B	579	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 ⓘ

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	1.17	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
1	SEP	A	790	1	-	0/6/8/10	-

There are no bond length outliers.

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.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	EPE	A	1101	-	15,15,15	2.08	1 (6%)	19,20,20	1.00	0
4	70S	A	1102	-	9,11,11	1.67	3 (33%)	9,15,15	1.93	4 (44%)
5	FB1	A	1104	-	11,11,11	4.44	5 (45%)	16,16,16	2.05	3 (18%)
5	FB1	A	1103	-	11,11,11	4.21	5 (45%)	16,16,16	2.44	4 (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
3	EPE	A	1101	-	-	1/9/19/19	0/1/1/1
4	70S	A	1102	-	-	-	0/2/2/2
5	FB1	A	1104	-	-	0/6/6/6	0/1/1/1
5	FB1	A	1103	-	-	0/6/6/6	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1104	FB1	C1-S	-12.98	1.61	1.77
5	A	1103	FB1	C1-S	-12.23	1.62	1.77
3	A	1101	EPE	C10-S	-7.70	1.66	1.77
5	A	1103	FB1	S-N	-3.94	1.52	1.60
5	A	1104	FB1	S-N	-3.93	1.52	1.60
5	A	1104	FB1	C6-CL1	3.30	1.81	1.73
4	A	1102	70S	N13-N12	3.28	1.42	1.36
5	A	1103	FB1	O1-S	2.98	1.49	1.43
5	A	1104	FB1	O1-S	2.77	1.48	1.43
5	A	1103	FB1	C6-CL1	2.75	1.80	1.73
5	A	1103	FB1	O2-S	2.72	1.48	1.43
4	A	1102	70S	C5-N12	2.68	1.36	1.33
5	A	1104	FB1	O2-S	2.66	1.48	1.43
4	A	1102	70S	C5-C4	-2.26	1.38	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1103	FB1	O2-S-O1	-7.55	107.18	118.80
5	A	1104	FB1	O2-S-O1	-6.55	108.72	118.80
4	A	1102	70S	C14-N13-N12	-3.61	107.07	112.59
5	A	1103	FB1	C1-C6-CL1	3.07	123.73	121.52
5	A	1103	FB1	O1-S-C1	2.97	111.57	107.26
4	A	1102	70S	C5-N12-N13	2.62	110.83	105.24
5	A	1103	FB1	O2-S-C1	2.47	110.86	107.26
5	A	1104	FB1	O2-S-C1	2.41	110.76	107.26
4	A	1102	70S	C4-C14-N13	-2.23	106.90	108.93
4	A	1102	70S	C2-C3-C4	-2.23	119.31	121.05
5	A	1104	FB1	C1-C6-CL1	2.03	122.98	121.52

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	EPE	N4-C7-C8-O8

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	1030/1096 (93%)	-0.29	4 (0%) 88 79	60, 109, 172, 219	0
2	B	201/279 (72%)	0.07	5 (2%) 58 39	100, 170, 225, 272	0
All	All	1231/1375 (89%)	-0.23	9 (0%) 84 70	60, 116, 196, 272	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	408	TYR	4.2
1	A	198	VAL	2.6
1	A	3	PRO	2.6
2	B	357	VAL	2.6
1	A	208	THR	2.4
2	B	521	ILE	2.3
1	A	203	ASP	2.2
2	B	449	LEU	2.1
2	B	404	LEU	2.1

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	0.85	0.10	104,109,202,208	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	EPE	A	1101	15/15	0.39	0.14	137,173,220,224	0
5	FB1	A	1104	11/11	0.63	0.11	183,213,228,231	0
4	70S	A	1102	10/10	0.70	0.09	164,174,177,178	0
5	FB1	A	1103	11/11	0.76	0.14	196,214,220,220	0

6.5 Other polymers [i](#)

There are no such residues in this entry.