



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 06:19 PM UTC

PDB ID : 2GK9 / pdb_00002gk9
Title : Human Phosphatidylinositol-4-phosphate 5-kinase, type II, gamma
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Deposited on : 2006-03-31
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
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)

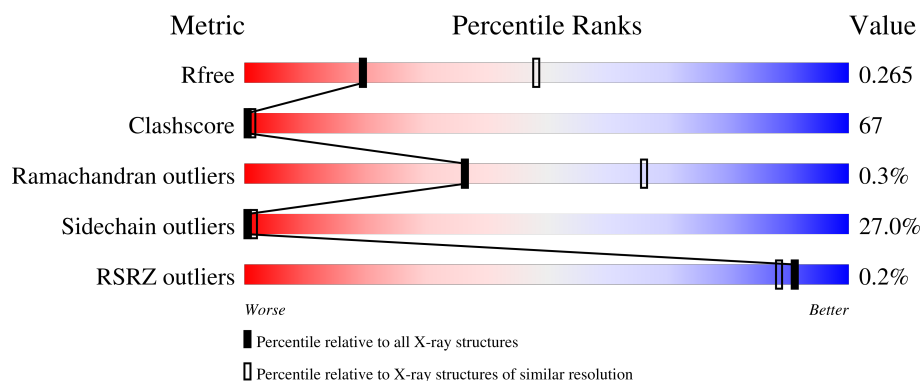
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	392	
1	B	392	
1	C	392	
1	D	392	

Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8233 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-phosphate 5-kinase, type II, gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			2023	1307	343	362	11			
1	B	250	Total	C	N	O	S	0	0	0
			2084	1345	353	375	11			
1	C	245	Total	C	N	O	S	0	0	0
			2042	1317	347	367	11			
1	D	250	Total	C	N	O	S	0	0	0
			2084	1345	353	375	11			

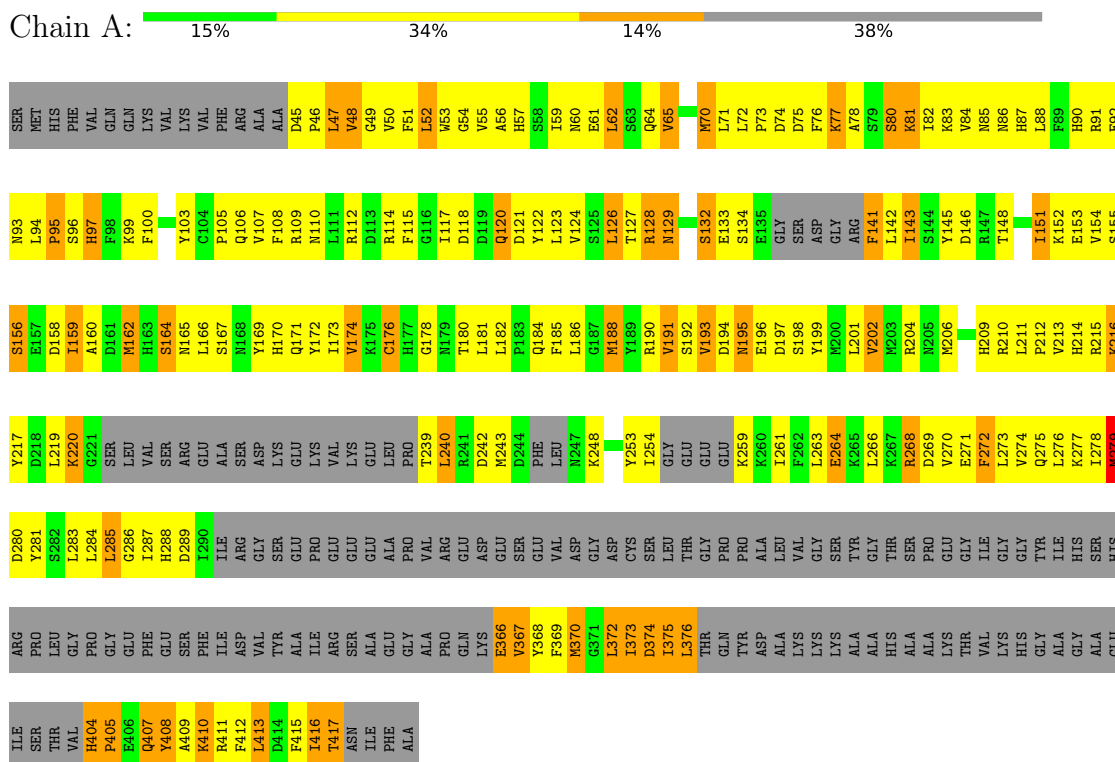
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	SER	-	cloning artifact	UNP Q8TBX8
A	31	MET	-	cloning artifact	UNP Q8TBX8
B	30	SER	-	cloning artifact	UNP Q8TBX8
B	31	MET	-	cloning artifact	UNP Q8TBX8
C	30	SER	-	cloning artifact	UNP Q8TBX8
C	31	MET	-	cloning artifact	UNP Q8TBX8
D	30	SER	-	cloning artifact	UNP Q8TBX8
D	31	MET	-	cloning artifact	UNP Q8TBX8

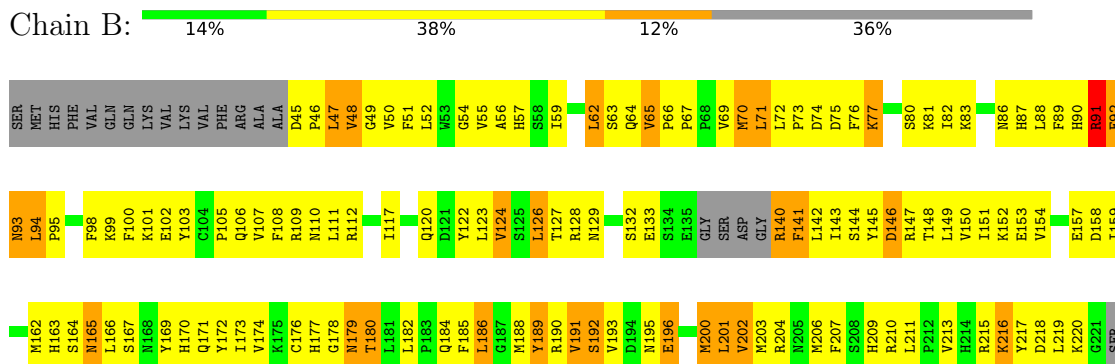
3 Residue-property plots

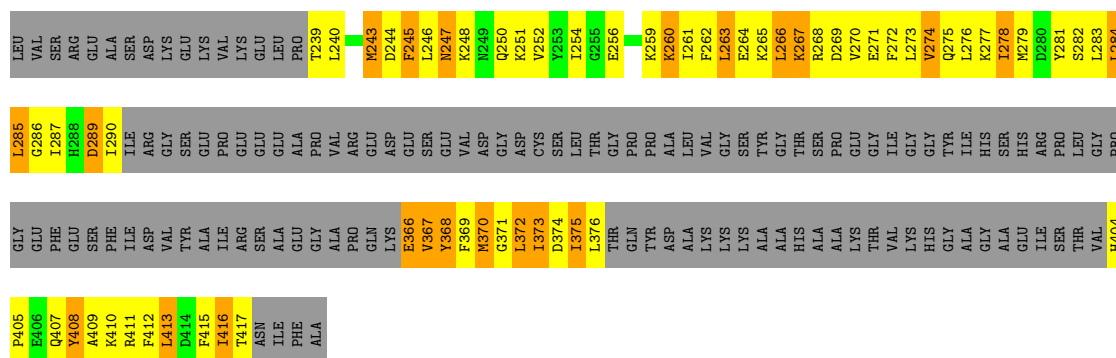
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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-phosphate 5-kinase, type II, gamma



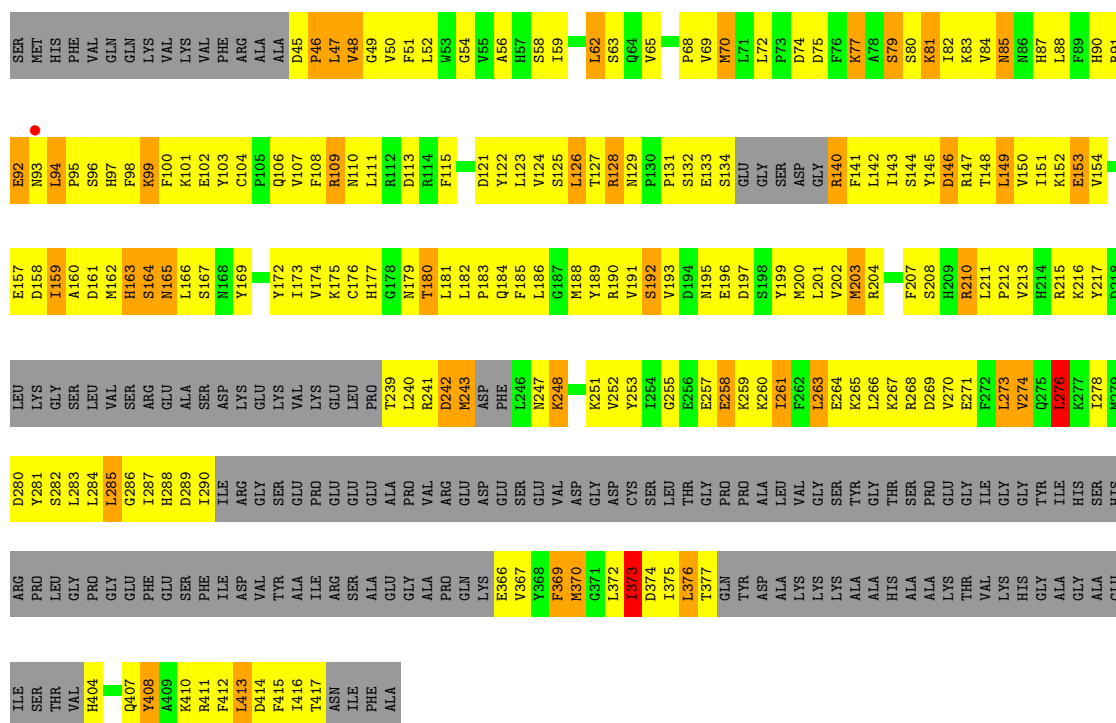
- Molecule 1: phosphatidylinositol-4-phosphate 5-kinase, type II, gamma





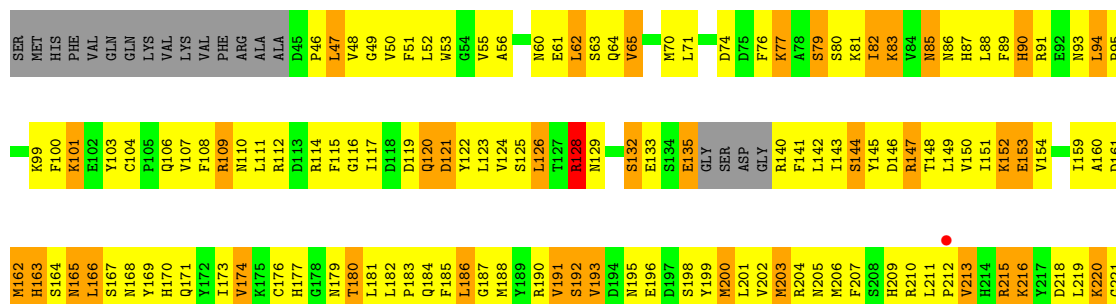
- Molecule 1: phosphatidylinositol-4-phosphate 5-kinase, type II, gamma

Chain C: 13% 38% 10% 38%



- Molecule 1: phosphatidylinositol-4-phosphate 5-kinase, type II, gamma

Chain D: 14% 35% 15% 36%



Y408	A409	GLU	PHE	T287	SER
	K410	GLU	H288	LEU	VAL
	R411	SER	D289	SER	ARG
	F412	PHE	T290	ILE	GLU
	L413	ASP	ARG	ARG	LYS
	F414	VAL	GLY	GLU	VAL
	F415	TYR	SER	SER	LYS
	I416	ALA	GLU	ALA	GLU
	T417	ILE	PRO	VAL	LEU
	ASN	ARG	GLU	ARG	PRO
PHE	ILE	SER	GLU	T239	
	PHE	ALA	ASP	D242	
	ALA	GLU	SER	F245	
		GLU	VAL	L246	
		ASP	ASP	Q250	
		GLY	ASP	K251	
		GLY	CYS	V252	
		SER	SER	G255	
		LEU	LEU	E256	
		THR	GLY	E257	
GLN	GLN	PRO	PRO	E258	
		TYR	PRO	K259	
		ASP	ALA	K260	
		ALA	LEU	I261	
		LYS	VAL	F262	
		LYS	GLY	L263	
		LYS	SER	E264	
		ALA	TYR	K265	
		ALA	GLY	L266	
		HIS	THR	K267	
HIS	ALA	SER	R268		
	ALA	PRO	D269		
	LYS	GLU	V270		
	THR	GLY	E271		
	VAL	ILE	F272		
	LYS	GLY	L273		
	HIS	GLY	V274		
	GLY	TYR	Q275		
	ALA	ILE	L276		
	GLY	HIS	K277		
GLU	GLU	SER	I278		
	ALA	HIS	M279		
	ILE	ARG	D280		
	THR	PRO	Y281		
	SER	LEU	S282		
	VAL	GLY	L283		
		PRO	L284		
		GLY	L285		
		GLY	CYS		

4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	95.39Å 95.39Å 189.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.80) 95.9 (20.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.80Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.254 , 0.297 0.256 , 0.265	Depositor DCC
R_{free} test set	1933 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 124.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.469 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8233	wwPDB-VP
Average B, all atoms (Å ²)	66.0	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.*

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

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	0.51	0/2068	0.83	2/2784 (0.1%)
1	B	0.48	0/2132	0.80	4/2872 (0.1%)
1	C	0.56	1/2088 (0.0%)	0.84	5/2813 (0.2%)
1	D	0.50	0/2132	0.88	5/2872 (0.2%)
All	All	0.51	1/8420 (0.0%)	0.84	16/11341 (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
1	B	0	1
1	D	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	261	ILE	CG1-CD1	5.73	1.74	1.51

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	250	GLN	OE1-CD-NE2	-10.23	112.37	122.60
1	A	164	SER	N-CA-C	-7.48	101.59	111.24
1	D	162	MET	N-CA-C	-7.10	103.47	111.14
1	B	410	LYS	CA-C-N	7.10	130.50	120.28
1	B	410	LYS	C-N-CA	7.10	130.50	120.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	279	MET	Peptide
1	B	91	ARG	Peptide
1	D	128	ARG	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	2023	0	2012	308	0
1	B	2084	0	2068	286	0
1	C	2042	0	2028	285	0
1	D	2084	0	2068	272	0
All	All	8233	0	8176	1106	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 67.

The worst 5 of 1106 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:C:266:LEU:CD2	1:C:413:LEU:HD23	1.52	1.39
1:C:176:CYS:SG	1:C:180:THR:HG22	1.65	1.34
1:A:72:LEU:HD21	1:B:95:PRO:CA	1.64	1.25
1:A:72:LEU:CD2	1:B:95:PRO:HA	1.67	1.24
1:D:285:LEU:CD2	1:D:370:MET:HG2	1.66	1.24

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	229/392 (58%)	189 (82%)	39 (17%)	1 (0%)	30	60
1	B	240/392 (61%)	203 (85%)	37 (15%)	0	100	100
1	C	233/392 (59%)	197 (84%)	35 (15%)	1 (0%)	30	60
1	D	240/392 (61%)	194 (81%)	45 (19%)	1 (0%)	30	60
All	All	942/1568 (60%)	783 (83%)	156 (17%)	3 (0%)	36	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	375	ILE
1	C	241	ARG
1	A	95	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	231/348 (66%)	168 (73%)	63 (27%)	0	1
1	B	237/348 (68%)	174 (73%)	63 (27%)	0	2
1	C	233/348 (67%)	176 (76%)	57 (24%)	1	2
1	D	237/348 (68%)	167 (70%)	70 (30%)	0	1
All	All	938/1392 (67%)	685 (73%)	253 (27%)	0	1

5 of 253 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	366	GLU
1	D	203	MET
1	C	128	ARG
1	D	193	VAL
1	D	279	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	86	ASN
1	D	288	HIS
1	C	129	ASN
1	D	195	ASN
1	C	97	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	243/392 (61%)	-1.28	0 100 100	24, 58, 114, 158	0
1	B	250/392 (63%)	-1.20	0 100 100	24, 58, 138, 152	0
1	C	245/392 (62%)	-1.25	1 (0%) 88 84	25, 59, 128, 158	0
1	D	250/392 (63%)	-1.25	1 (0%) 88 84	24, 60, 144, 158	0
All	All	988/1568 (63%)	-1.25	2 (0%) 91 88	24, 59, 136, 158	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	93	ASN	3.3
1	D	212	PRO	2.8

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.