wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 11, 2024 – 09:59 PM EDT

PDB ID	:	2GK9
Title	:	Human Phosphatidylinositol-4-phosphate 5-kinase, type II, gamma
Authors	:	Uppenberg, J.; Hogbom, M.; Ogg, D.; Arrowsmith, C.; Berglund, H.; Collins, R.; Ehn, M.; Flodin, S.; Flores, A.; Graslund, S.; Holmberg-Schiavone, L.; Edwards, A.; Hammarstrom, M.; Kotenyova, T.; Nilsson-Ehle, P.; Nordlund, P.; Nyman, T.; Persson, C.; Sagemark, J.; Stenmark, P.; Sundstrom, M.; Thorsell, A.G.; Van Den Berg, S.; Weigelt, J.; Hallberg, B.M.; Structural Genomics Consortium (SGC)
Deposited on	:	2006-03-31
Resolution	:	2.80 Å(reported)

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

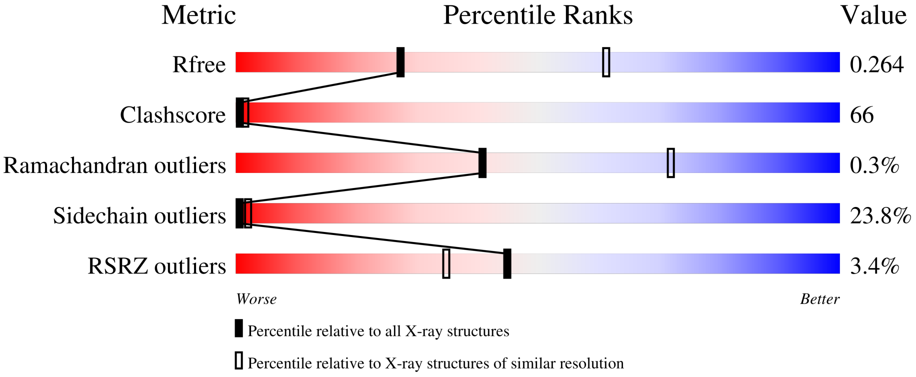
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

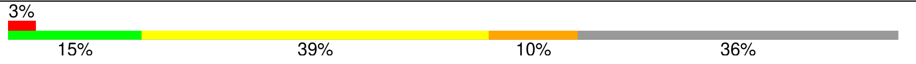
The reported resolution of this entry is 2.80 Å.

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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) : 2.36.2

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 2023 1307 343 362 11	0	0	0
1	B	250	Total C N O S 2084 1345 353 375 11	0	0	0
1	C	245	Total C N O S 2042 1317 347 367 11	0	0	0
1	D	250	Total C N O S 2084 1345 353 375 11	0	0	0

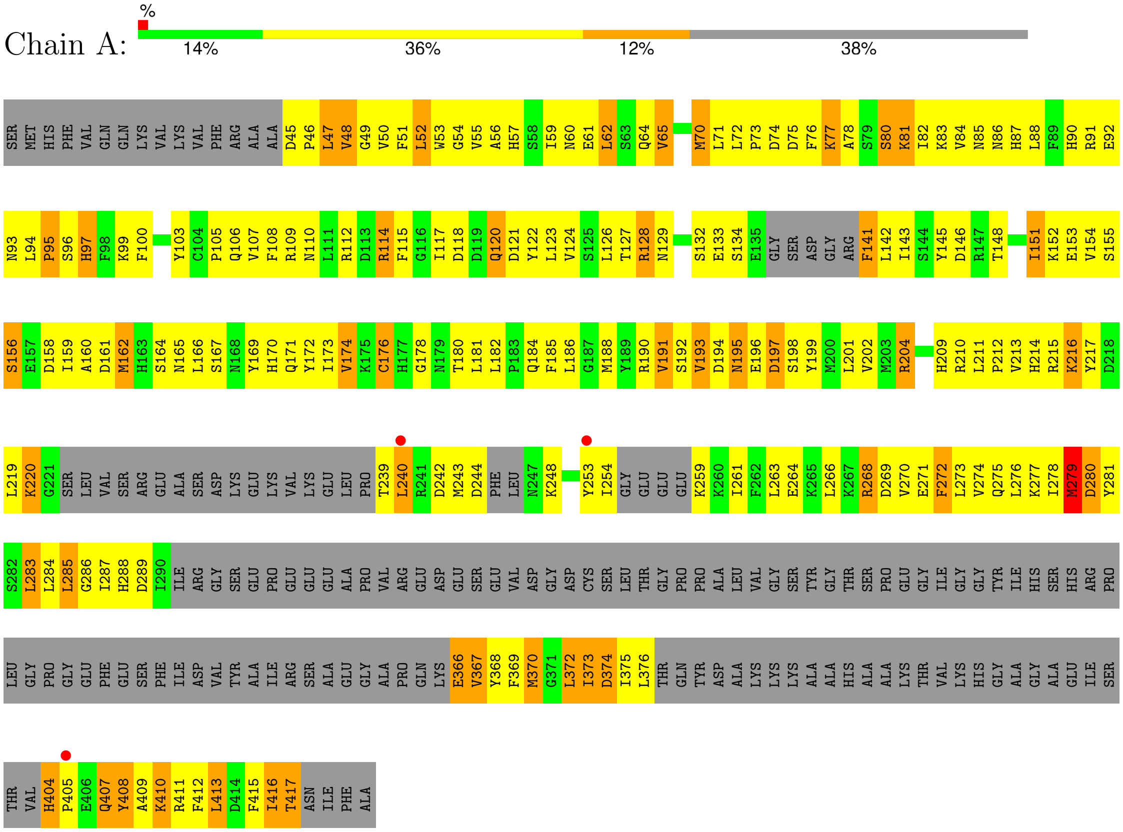
There are 8 discrepancies between the modelled and reference sequences:

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

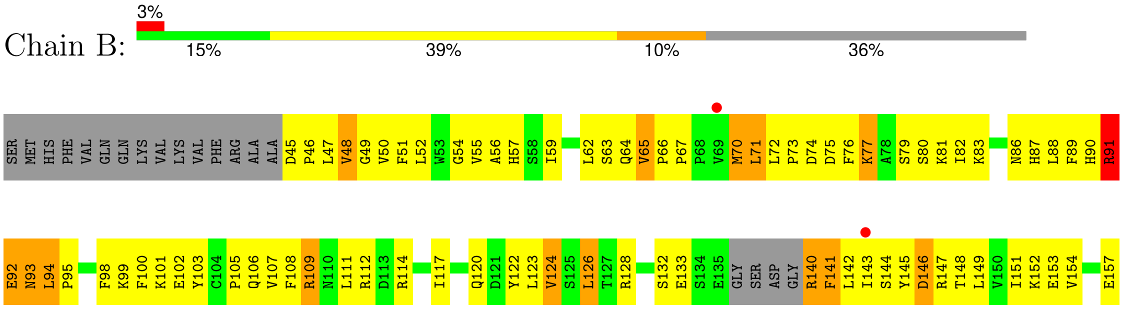
3 Residue-property plots ⓘ

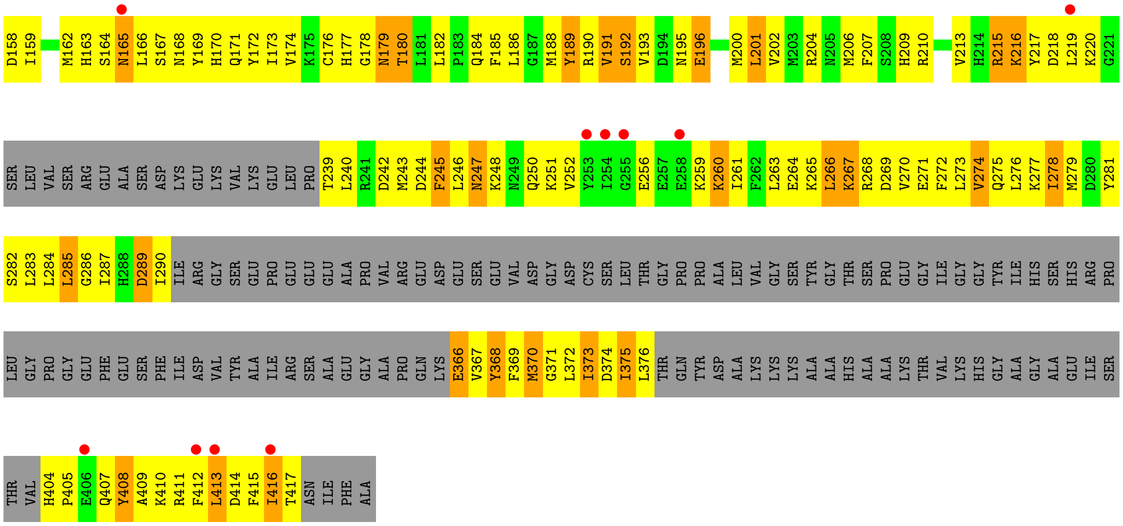
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



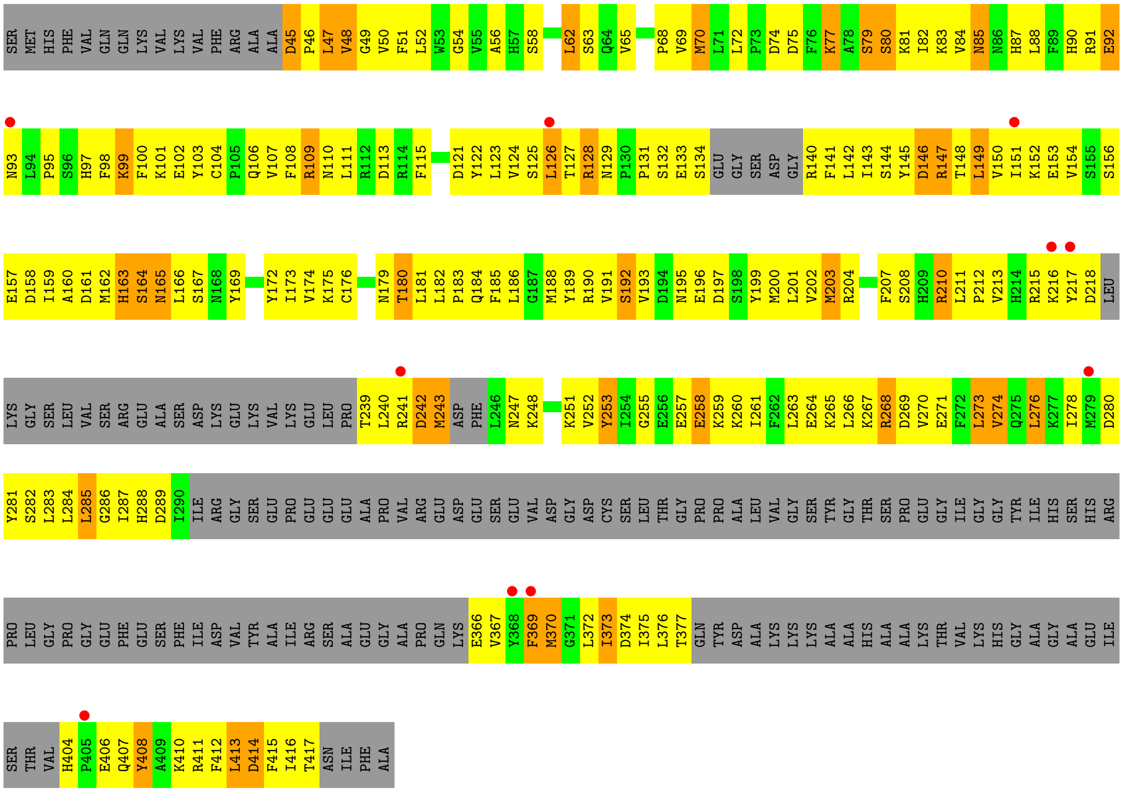
- Molecule 1: phosphatidylinositol-4-phosphate 5-kinase, type II, gamma





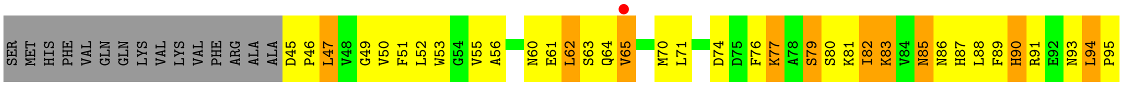
- Molecule 1: phosphatidylinositol-4-phosphate 5-kinase, type II, gamma

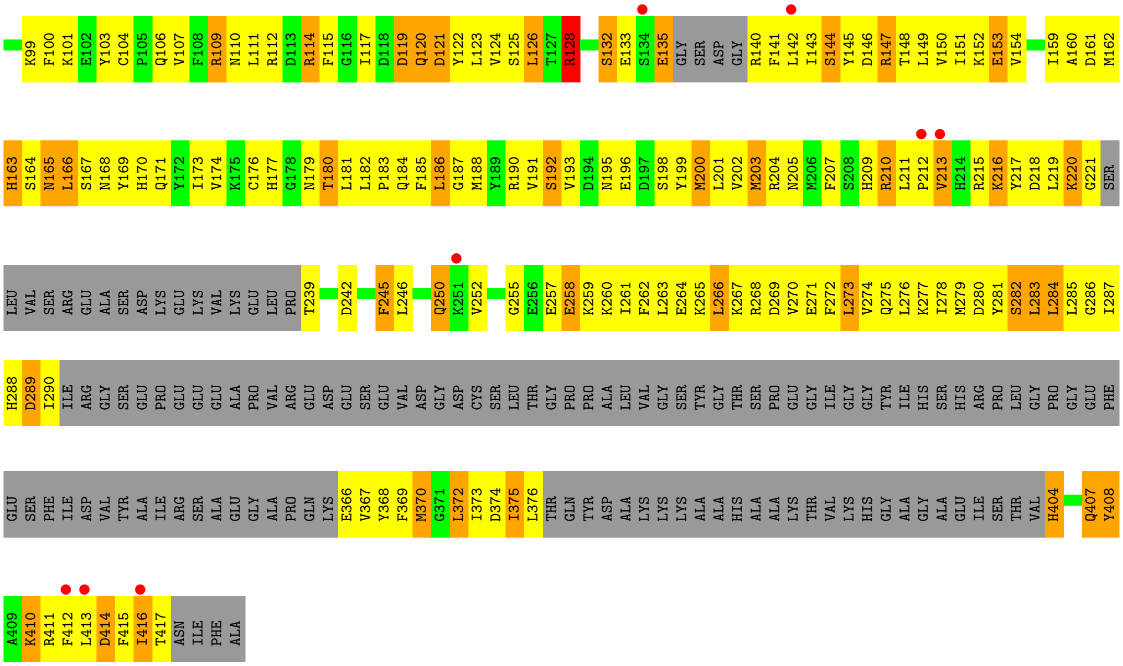
Chain C:



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

Chain D:




K99 F100 K101 E102 Y103 C104 P105 Q106 V107 F108 R109 N110 L111 R112 D113 R114 F115 G116 I117 D118 D119 Q120 D121 Y122 L123 V124 S125 L126 T127 R128 S132 E133 S134 E135 GLY SER ASP GLY R140 F141 L142 I143 S144 Y145 D146 R147 T148 L149 V150 I151 K152 E153 V154 I159 A160 D161 M162
H163 S164 N165 L166 S167 N168 Y169 H170 Q171 Y172 I173 V174 K175 C176 H177 G178 N179 T180 L181 L182 P183 Q184 F185 L186 G187 M188 Y189 R190 V191 S192 V193 D194 N195 E196 D197 S198 Y199 M200 L201 V202 M203 R204 N205 M206 F207 S208 H209 R210 L211 P212 V213 H214 R215 K216 Y217 D218 L219 K220 G221 SER
LEU VAL SER ARG GLU ALA SER ASP LYS GLU LYS VAL LYS GLU LEU PRO T239 D242 F245 L246 Q250 K251 V252 G255 E256 E257 E258 K259 K260 I261 F262 L263 E264 K265 L266 K267 R268 D269 V270 E271 F272 L273 V274 Q275 L276 K277 I278 M279 D280 Y281 S282 L283 L284 L285 G286 I287
H288 D289 I290 ILE ARG GLY SER GLU PRO GLU GLU GLU ALA PRO VAL ARG GLU ASP GLU SER GLU VAL ASP GLY ASP CYS SER LEU THR GLY PRO PRO ALA LEU VAL GLY SER TYR GLY THR SER PRO GLU GLY ILE GLY GLY TYR ILE HIS SER HIS ARG PRO LEU GLY PRO GLY GLU PHE
GLU SER PHE ILE ASP VAL TYR ALA ILE ARG SER ALA GLU GLY ALA PRO GLN LYS E366 V367 Y368 F369 M370 G371 L372 I373 D374 I375 L376 THR GLN TYR ASP ALA LYS LYS LYS ALA ALA HIS ALA ALA LYS THR VAL LYS HIS GLY ALA GLY ALA GLU ILE SER THR VAL H404 Q407 Y408
A409 K410 R411 F412 L413 D414 F415 I416 T417 ASN ILE PHE ALA

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 29.74 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.80) 95.5 (29.74-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 2.80Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.254 , 0.297 0.258 , 0.264	Depositor DCC
R_{free} test set	1932 reflections (4.73%)	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 , 85.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.469 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	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.*

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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 ⓘ

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	0.47	0/2068	0.58	4/2784 (0.1%)
1	B	0.47	0/2132	0.52	2/2872 (0.1%)
1	C	0.50	0/2088	0.58	5/2813 (0.2%)
1	D	0.45	0/2132	0.55	1/2872 (0.0%)
All	All	0.47	0/8420	0.56	12/11341 (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

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	114	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	C	253	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	A	244	ASP	CB-CG-OD2	5.27	123.05	118.30
1	B	242	ASP	CB-CG-OD2	5.26	123.03	118.30
1	C	414	ASP	CB-CG-OD2	5.26	123.03	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	279	MET	Peptide

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Mol	Chain	Res	Type	Group
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	301	0
1	B	2084	0	2068	279	0
1	C	2042	0	2028	277	0
1	D	2084	0	2068	265	0
All	All	8233	0	8176	1077	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 66.

The worst 5 of 1077 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%)	34	66
1	B	240/392 (61%)	203 (85%)	37 (15%)	0	100	100
1	C	233/392 (59%)	197 (84%)	35 (15%)	1 (0%)	34	66
1	D	240/392 (61%)	194 (81%)	45 (19%)	1 (0%)	34	66
All	All	942/1568 (60%)	783 (83%)	156 (17%)	3 (0%)	41	72

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%)	175 (76%)	56 (24%)	0	2
1	B	237/348 (68%)	182 (77%)	55 (23%)	1	2
1	C	233/348 (67%)	181 (78%)	52 (22%)	1	2
1	D	237/348 (68%)	177 (75%)	60 (25%)	0	1
All	All	938/1392 (67%)	715 (76%)	223 (24%)	0	2

5 of 223 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	69	VAL
1	D	410	LYS
1	C	242	ASP
1	D	407	GLN
1	D	213	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	163	HIS
1	D	87	HIS
1	D	85	ASN
1	D	195	ASN
1	B	57	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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(Å^2)	Q<0.9
1	A	243/392 (61%)	-0.10	3 (1%)	79	73	24, 58, 114, 158	0
1	B	250/392 (63%)	0.02	12 (4%)	30	21	24, 58, 138, 152	0
1	C	245/392 (62%)	-0.08	10 (4%)	37	27	25, 59, 128, 158	0
1	D	250/392 (63%)	-0.06	9 (3%)	42	32	24, 60, 144, 158	0
All	All	988/1568 (63%)	-0.05	34 (3%)	45	35	24, 59, 136, 158	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	93	ASN	5.1
1	B	416	ILE	4.7
1	A	405	PRO	4.1
1	A	253	TYR	4.1
1	B	219	LEU	3.6

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.