



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:58 am BST

PDB ID : 3ZZG
Title : Crystal structure of the amino acid kinase domain from *Saccharomyces cerevisiae* acetylglutamate kinase without ligands
Authors : de Cima, S.; Gil-Ortiz, F.; Crabeel, M.; Fita, I.; Rubio, V.
Deposited on : 2011-09-01
Resolution : 2.95 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)
Validation Pipeline (wwPDB-VP)	:	2.11

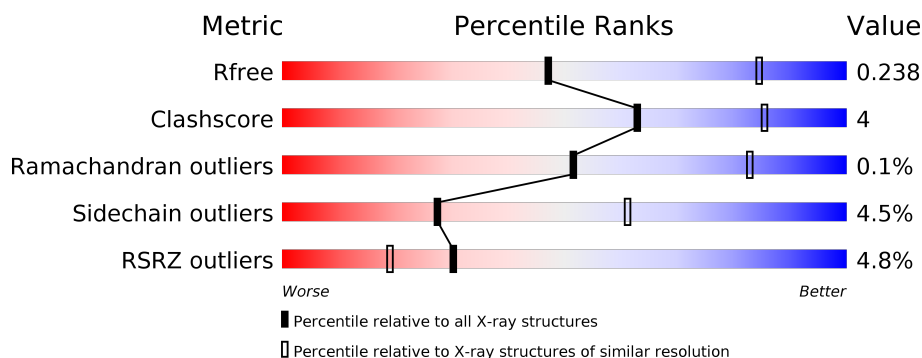
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 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	307	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>• 5%</div> </div> </div>
1	B	307	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>• 6%</div> </div> </div>
1	C	307	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>• 5%</div> </div> </div>
1	D	307	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>• 6%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8978 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 ACETYLGLUTAMATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2252	1431	382	432	7			
1	B	289	Total	C	N	O	S	0	0	0
			2239	1424	379	429	7			
1	C	291	Total	C	N	O	S	0	0	0
			2252	1431	382	432	7			
1	D	289	Total	C	N	O	S	0	0	0
			2235	1421	378	429	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	MET	-	expression tag	UNP Q01217
A	51	GLY	-	expression tag	UNP Q01217
A	52	HIS	-	expression tag	UNP Q01217
A	53	HIS	-	expression tag	UNP Q01217
A	54	HIS	-	expression tag	UNP Q01217
A	55	HIS	-	expression tag	UNP Q01217
A	56	HIS	-	expression tag	UNP Q01217
A	57	HIS	-	expression tag	UNP Q01217
B	50	MET	-	expression tag	UNP Q01217
B	51	GLY	-	expression tag	UNP Q01217
B	52	HIS	-	expression tag	UNP Q01217
B	53	HIS	-	expression tag	UNP Q01217
B	54	HIS	-	expression tag	UNP Q01217
B	55	HIS	-	expression tag	UNP Q01217
B	56	HIS	-	expression tag	UNP Q01217
B	57	HIS	-	expression tag	UNP Q01217
C	50	MET	-	expression tag	UNP Q01217
C	51	GLY	-	expression tag	UNP Q01217
C	52	HIS	-	expression tag	UNP Q01217
C	53	HIS	-	expression tag	UNP Q01217
C	54	HIS	-	expression tag	UNP Q01217

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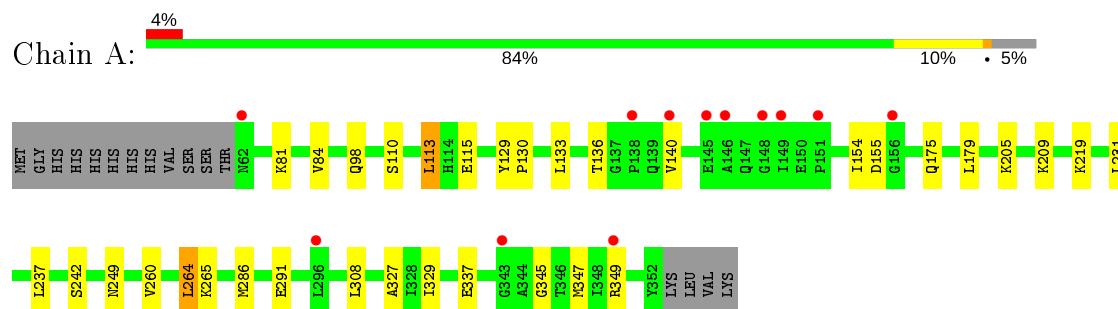
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Chain	Residue	Modelled	Actual	Comment	Reference
C	55	HIS	-	expression tag	UNP Q01217
C	56	HIS	-	expression tag	UNP Q01217
C	57	HIS	-	expression tag	UNP Q01217
D	50	MET	-	expression tag	UNP Q01217
D	51	GLY	-	expression tag	UNP Q01217
D	52	HIS	-	expression tag	UNP Q01217
D	53	HIS	-	expression tag	UNP Q01217
D	54	HIS	-	expression tag	UNP Q01217
D	55	HIS	-	expression tag	UNP Q01217
D	56	HIS	-	expression tag	UNP Q01217
D	57	HIS	-	expression tag	UNP Q01217

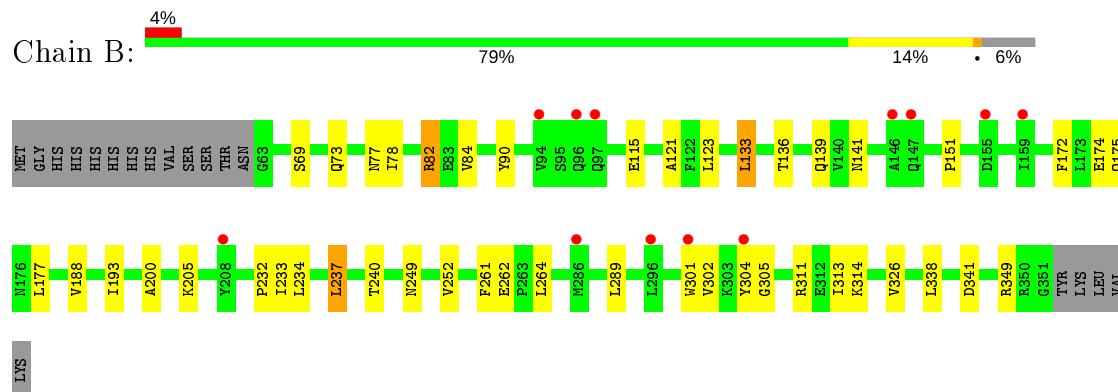
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

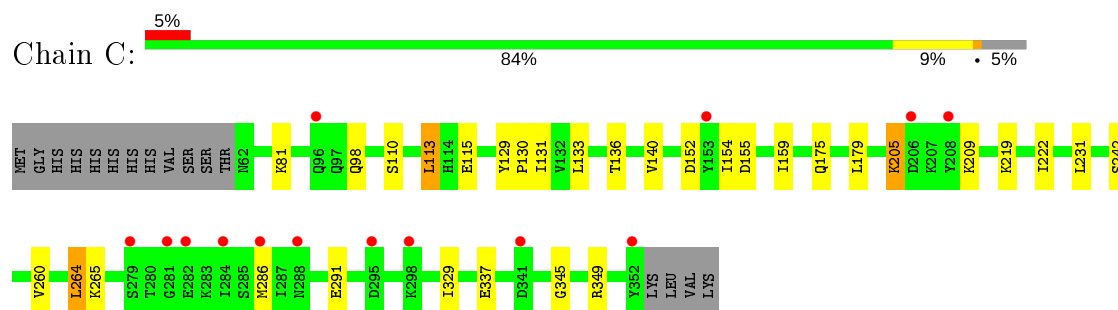
• Molecule 1: ACETYLGLUTAMATE KINASE



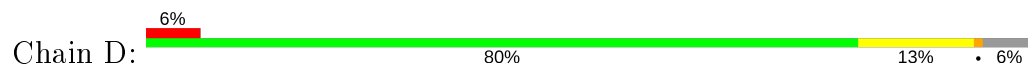
• Molecule 1: ACETYLGLUTAMATE KINASE

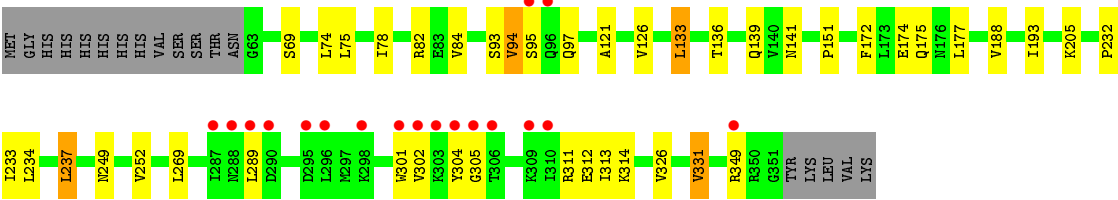


• Molecule 1: ACETYLGLUTAMATE KINASE



• Molecule 1: ACETYLGLUTAMATE KINASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.09Å 100.53Å 188.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.95 46.21 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.95) 99.7 (46.21-2.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.15 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.212 , 0.245 0.208 , 0.238	Depositor DCC
R_{free} test set	1403 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	71.1	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8978	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.43	0/2284	0.54	0/3087
1	B	0.48	0/2271	0.58	0/3069
1	C	0.44	0/2284	0.56	0/3087
1	D	0.45	0/2267	0.56	0/3065
All	All	0.45	0/9106	0.56	0/12308

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2252	0	2308	18	0
1	B	2239	0	2300	22	0
1	C	2252	0	2308	16	0
1	D	2235	0	2289	23	0
All	All	8978	0	9205	78	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 (78) 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:B:90:TYR:CE2	1:B:264:LEU:HD22	2.20	0.76
1:A:264:LEU:HD12	1:A:265:LYS:HD3	1.72	0.72
1:B:193:ILE:HB	1:B:234:LEU:HD22	1.73	0.71
1:D:193:ILE:HB	1:D:234:LEU:HD22	1.72	0.70
1:C:264:LEU:HD12	1:C:265:LYS:HD3	1.76	0.68
1:B:82:ARG:NH2	1:B:341:ASP:HB2	2.14	0.61
1:B:121:ALA:HA	1:B:188:VAL:HG21	1.84	0.60
1:D:94:VAL:HG13	1:D:95:SER:H	1.67	0.59
1:A:249:ASN:HD22	1:A:308:LEU:HD23	1.67	0.58
1:A:329:ILE:HG22	1:A:345:GLY:HA3	1.86	0.58
1:C:219:LYS:CE	1:C:260:VAL:HG12	2.34	0.57
1:D:133:LEU:C	1:D:133:LEU:HD13	2.25	0.57
1:A:219:LYS:CE	1:A:260:VAL:HG12	2.35	0.57
1:D:121:ALA:HA	1:D:188:VAL:HG21	1.87	0.56
1:D:313:ILE:HG23	1:D:326:VAL:HG21	1.89	0.54
1:C:329:ILE:HG22	1:C:345:GLY:HA3	1.90	0.54
1:D:289:LEU:HD13	1:D:314:LYS:HA	1.89	0.54
1:D:136:THR:O	1:D:136:THR:HG23	2.08	0.54
1:B:289:LEU:HD13	1:B:314:LYS:HA	1.90	0.54
1:B:123:LEU:HD11	1:B:338:LEU:CD1	2.39	0.53
1:B:136:THR:O	1:B:136:THR:HG23	2.09	0.51
1:B:172:PHE:CE2	1:B:237:LEU:HD13	2.45	0.51
1:C:133:LEU:HD13	1:C:133:LEU:C	2.31	0.50
1:D:172:PHE:CE2	1:D:237:LEU:HD13	2.46	0.50
1:A:329:ILE:HG21	1:A:337:GLU:HG3	1.93	0.50
1:B:172:PHE:CD2	1:B:237:LEU:HD13	2.46	0.50
1:A:98:GLN:NE2	1:A:129:TYR:O	2.44	0.50
1:A:219:LYS:HE3	1:A:260:VAL:HG12	1.93	0.50
1:B:141:ASN:HD22	1:B:151:PRO:CG	2.25	0.49
1:C:329:ILE:HG21	1:C:337:GLU:HG3	1.94	0.49
1:D:172:PHE:CD2	1:D:237:LEU:HD13	2.47	0.49
1:B:301:TRP:CZ3	1:B:302:VAL:HG22	2.48	0.48
1:D:301:TRP:CZ3	1:D:302:VAL:HG22	2.48	0.48
1:C:113:LEU:HD21	1:C:179:LEU:HA	1.96	0.48
1:A:113:LEU:HD21	1:A:179:LEU:HA	1.96	0.47
1:C:130:PRO:HD2	1:C:231:LEU:HD22	1.95	0.47
1:B:73:GLN:O	1:B:77:ASN:ND2	2.46	0.47
1:A:133:LEU:C	1:A:133:LEU:HD13	2.35	0.47
1:C:219:LYS:HE3	1:C:260:VAL:HG12	1.96	0.47
1:D:249:ASN:HB3	1:D:252:VAL:HG22	1.97	0.47
1:B:90:TYR:HE2	1:B:264:LEU:HD22	1.74	0.46
1:D:141:ASN:HD22	1:D:151:PRO:CG	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:THR:HG21	1:A:140:VAL:HG21	1.97	0.46
1:C:136:THR:HG23	1:C:136:THR:O	2.16	0.45
1:D:232:PRO:O	1:D:233:ILE:HD13	2.16	0.45
1:C:154:ILE:HG22	1:C:155:ASP:OD1	2.16	0.45
1:A:154:ILE:HG22	1:A:155:ASP:OD1	2.17	0.45
1:A:130:PRO:HD2	1:A:231:LEU:HD22	1.99	0.45
1:B:249:ASN:HB3	1:B:252:VAL:HG22	1.97	0.45
1:B:133:LEU:HD13	1:B:133:LEU:C	2.37	0.44
1:D:304:TYR:HD1	1:D:305:GLY:N	2.16	0.44
1:A:205:LYS:O	1:A:209:LYS:HA	2.16	0.44
1:D:78:ILE:CG2	1:D:84:VAL:HG22	2.48	0.44
1:A:84:VAL:HG13	1:D:75:LEU:HB3	2.00	0.44
1:D:78:ILE:HG21	1:D:84:VAL:HG22	2.00	0.44
1:B:304:TYR:HD1	1:B:305:GLY:N	2.16	0.44
1:D:269:LEU:HD13	1:D:331:VAL:HG23	1.99	0.44
1:D:74:LEU:HD13	1:D:126:VAL:HG11	2.00	0.44
1:D:252:VAL:HG12	1:D:312:GLU:HB2	2.00	0.43
1:C:98:GLN:NE2	1:C:129:TYR:O	2.51	0.43
1:C:136:THR:HG21	1:C:140:VAL:HG21	2.01	0.43
1:C:152:ASP:CB	1:C:159:ILE:HD12	2.49	0.43
1:A:329:ILE:HD13	1:A:337:GLU:HG3	2.00	0.43
1:A:327:ALA:CA	1:A:347:MET:HE3	2.49	0.42
1:B:232:PRO:O	1:B:233:ILE:HD13	2.19	0.42
1:D:133:LEU:CD1	1:D:133:LEU:C	2.87	0.42
1:D:93:SER:O	1:D:94:VAL:HG12	2.20	0.42
1:C:205:LYS:O	1:C:209:LYS:HA	2.20	0.42
1:B:177:LEU:HA	1:B:177:LEU:HD12	1.81	0.42
1:A:136:THR:OG1	1:A:140:VAL:HG23	2.20	0.41
1:B:200:ALA:O	1:B:240:THR:HA	2.20	0.41
1:A:237:LEU:HD23	1:A:237:LEU:HA	1.94	0.41
1:C:329:ILE:HD13	1:C:337:GLU:HG3	2.02	0.41
1:C:131:ILE:HG12	1:C:222:ILE:HG21	2.03	0.41
1:D:177:LEU:HD12	1:D:177:LEU:HA	1.88	0.41
1:B:261:PHE:O	1:B:262:GLU:C	2.59	0.41
1:B:313:ILE:HG23	1:B:326:VAL:HG21	2.02	0.40
1:B:78:ILE:HG21	1:B:84:VAL:HG22	2.04	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	289/307 (94%)	275 (95%)	14 (5%)	0	100	100
1	B	287/307 (94%)	276 (96%)	11 (4%)	0	100	100
1	C	289/307 (94%)	275 (95%)	14 (5%)	0	100	100
1	D	287/307 (94%)	273 (95%)	13 (4%)	1 (0%)	41	73
All	All	1152/1228 (94%)	1099 (95%)	52 (4%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	94	VAL

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	246/262 (94%)	236 (96%)	10 (4%)	30	64
1	B	245/262 (94%)	234 (96%)	11 (4%)	27	61
1	C	246/262 (94%)	235 (96%)	11 (4%)	27	61
1	D	244/262 (93%)	232 (95%)	12 (5%)	25	58
All	All	981/1048 (94%)	937 (96%)	44 (4%)	27	61

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	LYS
1	A	110	SER
1	A	113	LEU
1	A	115	GLU
1	A	175	GLN
1	A	242	SER
1	A	264	LEU
1	A	286	MET
1	A	291	GLU
1	A	349	ARG
1	B	69	SER
1	B	82	ARG
1	B	115	GLU
1	B	133	LEU
1	B	139	GLN
1	B	174	GLU
1	B	175	GLN
1	B	205	LYS
1	B	237	LEU
1	B	311	ARG
1	B	349	ARG
1	C	81	LYS
1	C	110	SER
1	C	113	LEU
1	C	115	GLU
1	C	175	GLN
1	C	205	LYS
1	C	242	SER
1	C	264	LEU
1	C	286	MET
1	C	291	GLU
1	C	349	ARG
1	D	69	SER
1	D	82	ARG
1	D	97	GLN
1	D	133	LEU
1	D	139	GLN
1	D	174	GLU
1	D	175	GLN
1	D	205	LYS
1	D	237	LEU
1	D	311	ARG
1	D	331	VAL

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Mol	Chain	Res	Type
1	D	349	ARG

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	62	ASN
1	A	139	GLN
1	A	175	GLN
1	A	277	ASN
1	A	332	GLN
1	B	98	GLN
1	B	139	GLN
1	B	141	ASN
1	B	147	GLN
1	B	163	HIS
1	B	332	GLN
1	C	62	ASN
1	C	139	GLN
1	C	175	GLN
1	C	277	ASN
1	C	332	GLN
1	D	96	GLN
1	D	97	GLN
1	D	139	GLN
1	D	141	ASN
1	D	147	GLN
1	D	163	HIS
1	D	332	GLN

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 carbohydrates 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	291/307 (94%)	0.07	12 (4%)	37 24	41, 76, 132, 175	0
1	B	289/307 (94%)	0.14	12 (4%)	36 23	34, 64, 129, 165	0
1	C	291/307 (94%)	0.21	14 (4%)	30 19	41, 75, 164, 240	0
1	D	289/307 (94%)	0.14	18 (6%)	20 12	41, 74, 129, 163	0
All	All	1160/1228 (94%)	0.14	56 (4%)	30 19	34, 73, 137, 240	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	304	TYR	6.0
1	D	305	GLY	5.4
1	D	296	LEU	5.2
1	D	306	THR	5.0
1	D	310	ILE	4.8
1	B	97	GLN	4.7
1	C	352	TYR	4.7
1	D	302	VAL	4.6
1	B	296	LEU	4.4
1	D	301	TRP	3.9
1	C	279	SER	3.4
1	A	151	PRO	3.4
1	D	288	ASN	3.4
1	D	290	ASP	3.3
1	D	295	ASP	3.2
1	B	208	TYR	3.1
1	C	295	ASP	3.1
1	D	349	ARG	3.1
1	A	146	ALA	3.1
1	A	62	ASN	3.1
1	B	146	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	96	GLN	3.0
1	A	343	GLY	2.9
1	D	287	ILE	2.9
1	A	148	GLY	2.8
1	C	288	ASN	2.8
1	D	303	LYS	2.8
1	D	298	LYS	2.7
1	B	286	MET	2.6
1	B	159	ILE	2.6
1	B	301	TRP	2.6
1	A	156	GLY	2.4
1	C	282	GLU	2.4
1	B	96	GLN	2.4
1	A	149	ILE	2.4
1	C	284	ILE	2.4
1	D	96	GLN	2.3
1	C	341	ASP	2.3
1	D	309	LYS	2.2
1	D	95	SER	2.2
1	A	145	GLU	2.2
1	C	153	TYR	2.2
1	C	206	ASP	2.1
1	B	94	VAL	2.1
1	B	304	TYR	2.1
1	B	147	GLN	2.1
1	B	155	ASP	2.1
1	A	138	PRO	2.1
1	A	349	ARG	2.1
1	C	298	LYS	2.1
1	A	140	VAL	2.0
1	A	296	LEU	2.0
1	D	289	LEU	2.0
1	C	286	MET	2.0
1	C	281	GLY	2.0
1	C	208	TYR	2.0

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 [i](#)

There are no carbohydrates 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.