



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 01:52 AM GMT

PDB ID : 1ZC6
Title : Crystal Structure of Putative N-acetylglucosamine Kinase from *Chromobacterium violaceum*. Northeast Structural Genomics Target Cvr23.
Authors : Vorobiev, S.M.; Kuzin, A.; Forouhar, F.; Abashidze, M.; Acton, T.B.; Xiao, R.; Ma, L.-C.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2005-04-11
Resolution : 2.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

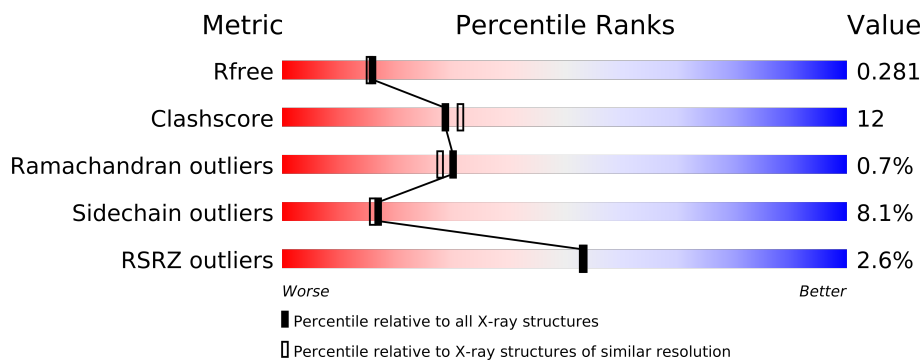
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.20 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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	305	
1	B	305	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4266 atoms, of which 0 are hydrogen and 0 are deuterium.

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 probable N-acetylglucosamine kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	Se	0	0	0
			2066	1293	378	389	2	4			
1	B	293	Total	C	N	O	S	Se	0	0	0
			2116	1323	388	398	2	5			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	MSE	MET	MODIFIED RESIDUE	UNP Q7NU07
A	37	MSE	MET	MODIFIED RESIDUE	UNP Q7NU07
A	173	MSE	MET	MODIFIED RESIDUE	UNP Q7NU07
A	199	MSE	MET	MODIFIED RESIDUE	UNP Q7NU07
A	199	MSE	MET	MODIFIED RESIDUE	UNP Q7NU07
A	298	LEU	-	CLONING ARTIFACT	UNP Q7NU07
A	299	GLU	-	CLONING ARTIFACT	UNP Q7NU07
A	300	HIS	-	CLONING ARTIFACT	UNP Q7NU07
A	301	HIS	-	CLONING ARTIFACT	UNP Q7NU07
A	302	HIS	-	CLONING ARTIFACT	UNP Q7NU07
A	303	HIS	-	CLONING ARTIFACT	UNP Q7NU07
A	304	HIS	-	CLONING ARTIFACT	UNP Q7NU07
A	305	HIS	-	CLONING ARTIFACT	UNP Q7NU07
B	6	MSE	MET	MODIFIED RESIDUE	UNP Q7NU07
B	37	MSE	MET	MODIFIED RESIDUE	UNP Q7NU07
B	173	MSE	MET	MODIFIED RESIDUE	UNP Q7NU07
B	199	MSE	MET	MODIFIED RESIDUE	UNP Q7NU07
B	199	MSE	MET	MODIFIED RESIDUE	UNP Q7NU07
B	298	LEU	-	CLONING ARTIFACT	UNP Q7NU07
B	299	GLU	-	CLONING ARTIFACT	UNP Q7NU07
B	300	HIS	-	CLONING ARTIFACT	UNP Q7NU07
B	301	HIS	-	CLONING ARTIFACT	UNP Q7NU07
B	302	HIS	-	CLONING ARTIFACT	UNP Q7NU07
B	303	HIS	-	CLONING ARTIFACT	UNP Q7NU07
B	304	HIS	-	CLONING ARTIFACT	UNP Q7NU07

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Chain	Residue	Modelled	Actual	Comment	Reference
B	305	HIS	-	CLONING ARTIFACT	UNP Q7NU07

- Molecule 2 is water.

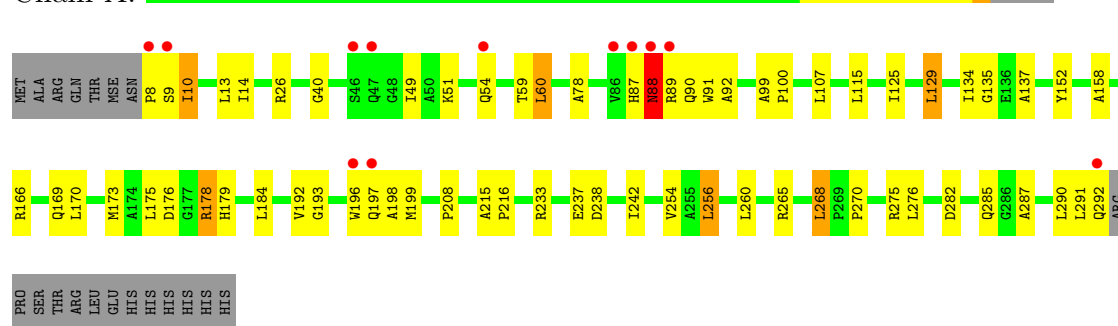
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total O 29 29	0	0
2	B	55	Total O 55 55	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

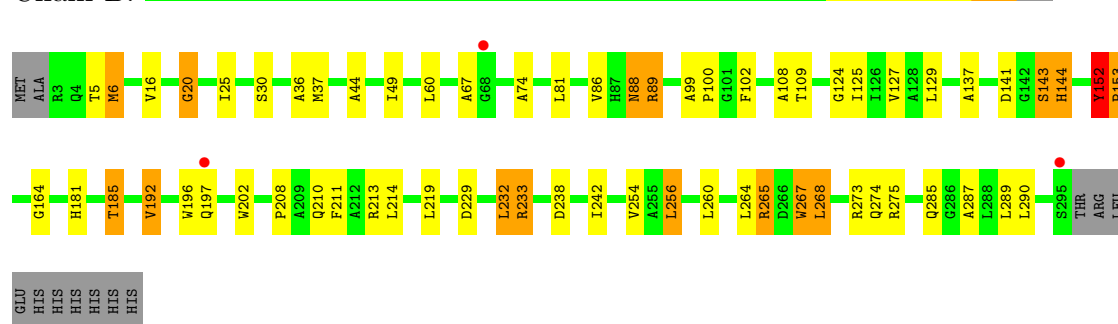
- Molecule 1: probable N-acetylglucosamine kinase

Chain A:



- Molecule 1: probable N-acetylglucosamine kinase

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	178.25Å 178.25Å 117.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.42 – 2.20 29.42 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.6 (29.42-2.20) 96.3 (29.42-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.241 , 0.267 0.254 , 0.281	Depositor DCC
R_{free} test set	1819 reflections (3.94%)	DCC
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 25.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 90884 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4266	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.40	0/2110	0.62	0/2867
1	B	0.44	1/2160 (0.0%)	0.66	1/2936 (0.0%)
All	All	0.42	1/4270 (0.0%)	0.64	1/5803 (0.0%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	6	MSE	CG-SE	-5.44	1.76	1.95

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	TYR	N-CA-C	5.78	126.60	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	152	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2066	0	2015	52	0
1	B	2116	0	2053	57	0
2	A	29	0	0	2	0
2	B	55	0	0	2	0
All	All	4266	0	4068	102	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (102) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:169:GLN:HG2	1:A:173:MSE:HE2	1.39	1.05
1:A:87:HIS:HB2	1:A:91:TRP:HB2	1.53	0.88
1:A:54:GLN:HB3	2:A:585:HOH:O	1.74	0.87
1:B:36:ALA:HB2	1:B:67:ALA:HB2	1.66	0.78
1:A:282:ASP:H	1:A:285:GLN:HE21	1.35	0.74
1:B:20:GLY:H	1:B:44:ALA:HB2	1.53	0.74
1:A:88:ASN:HA	1:A:92:ALA:HB3	1.68	0.73
1:A:125:ILE:HG13	1:A:254:VAL:HG13	1.72	0.71
1:B:254:VAL:HG21	2:B:552:HOH:O	1.91	0.71
1:B:256:LEU:HD12	1:B:268:LEU:HD21	1.73	0.70
1:B:229:ASP:OD1	1:B:267:TRP:HZ3	1.76	0.68
1:A:233:ARG:HG2	1:B:233:ARG:NH1	2.07	0.68
1:B:181:HIS:HA	1:B:185:THR:HG21	1.76	0.67
1:B:265:ARG:NH2	1:B:273:ARG:HH11	1.93	0.67
1:B:265:ARG:HB2	1:B:265:ARG:NH1	2.09	0.66
1:A:192:VAL:HG11	1:A:199:MSE:HA	1.78	0.66
1:A:233:ARG:CG	1:B:233:ARG:HD2	2.26	0.66
1:A:193:GLY:HA3	1:A:198:ALA:HB1	1.77	0.65
1:A:170:LEU:HA	1:A:173:MSE:HE3	1.78	0.64
1:A:87:HIS:HB3	1:A:90:GLN:HB3	1.80	0.64
1:B:210:GLN:HG3	1:B:213:ARG:NH2	2.14	0.63
1:B:5:THR:HG21	1:B:30:SER:HB2	1.81	0.63
1:B:125:ILE:HG13	1:B:137:ALA:HB2	1.80	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:282:ASP:H	1:A:285:GLN:NE2	1.98	0.62
1:B:197:GLN:HB3	2:B:502:HOH:O	2.00	0.61
1:B:181:HIS:CD2	1:B:185:THR:CG2	2.85	0.60
1:A:54:GLN:CB	2:A:585:HOH:O	2.39	0.59
1:A:291:LEU:HD12	1:A:292:GLN:HG3	1.83	0.58
1:B:49:ILE:HD12	1:B:49:ILE:N	2.17	0.58
1:A:233:ARG:HG2	1:B:233:ARG:HD2	1.86	0.57
1:A:40:GLY:HA3	1:A:59:THR:OG1	2.04	0.57
1:B:124:GLY:C	1:B:125:ILE:HD12	2.26	0.56
1:A:233:ARG:HG2	1:B:233:ARG:HH11	1.71	0.56
1:B:267:TRP:N	1:B:267:TRP:CD1	2.73	0.56
1:B:192:VAL:HG22	1:B:202:TRP:CG	2.41	0.55
1:A:176:ASP:OD1	1:A:178:ARG:HG2	2.07	0.54
1:A:197:GLN:CD	1:A:197:GLN:H	2.10	0.54
1:A:265:ARG:HA	1:A:268:LEU:HD22	1.90	0.54
1:B:256:LEU:CD1	1:B:268:LEU:HD21	2.38	0.53
1:B:219:LEU:HD23	1:B:232:LEU:HD21	1.91	0.53
1:A:256:LEU:HD12	1:A:268:LEU:HD21	1.91	0.53
1:A:51:LYS:HA	1:A:54:GLN:HE21	1.74	0.52
1:B:49:ILE:H	1:B:49:ILE:HD12	1.75	0.51
1:B:265:ARG:CZ	1:B:265:ARG:HB2	2.40	0.51
1:A:193:GLY:HA3	1:A:198:ALA:CB	2.41	0.51
1:B:287:ALA:O	1:B:290:LEU:HB2	2.11	0.51
1:B:129:LEU:HB3	1:B:260:LEU:HD12	1.93	0.51
1:A:8:PRO:HG2	1:A:9:SER:H	1.76	0.50
1:A:129:LEU:HD22	1:A:256:LEU:HD21	1.94	0.50
1:B:89:ARG:HH11	1:B:89:ARG:HB2	1.76	0.50
1:B:285:GLN:O	1:B:289:LEU:HD13	2.12	0.49
1:B:229:ASP:OD1	1:B:267:TRP:CZ3	2.63	0.49
1:A:125:ILE:HG22	1:A:137:ALA:CB	2.43	0.48
1:A:254:VAL:HG21	1:A:275:ARG:NH2	2.27	0.48
1:A:233:ARG:NE	1:B:233:ARG:HD2	2.28	0.48
1:B:152:TYR:CG	1:B:208:PRO:HG3	2.48	0.48
1:A:51:LYS:HD2	1:A:54:GLN:NE2	2.28	0.48
1:A:49:ILE:N	1:A:49:ILE:HD12	2.28	0.48
1:A:10:ILE:HG13	1:A:78:ALA:HB2	1.95	0.48
1:A:10:ILE:HD13	1:A:10:ILE:O	2.14	0.48
1:B:264:LEU:O	1:B:267:TRP:HD1	1.97	0.47
1:A:270:PRO:HD2	1:B:267:TRP:CZ3	2.49	0.47
1:A:129:LEU:HG	1:A:158:ALA:O	2.15	0.47
1:B:74:ALA:O	1:B:102:PHE:HA	2.15	0.47
1:A:87:HIS:O	1:A:88:ASN:C	2.54	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:173:MSE:HB3	1:A:179:HIS:HB2	1.96	0.46
1:A:134:ILE:HG12	1:A:135:GLY:N	2.30	0.46
1:A:10:ILE:HD11	1:A:13:LEU:HD21	1.98	0.45
1:A:287:ALA:O	1:A:290:LEU:HB3	2.16	0.45
1:B:89:ARG:HH11	1:B:89:ARG:CB	2.29	0.45
1:A:125:ILE:CG1	1:A:254:VAL:HG13	2.44	0.45
1:A:26:ARG:CD	1:A:285:GLN:HG3	2.47	0.45
1:A:14:ILE:HD13	1:A:60:LEU:HD11	1.98	0.44
1:B:233:ARG:HG3	1:B:233:ARG:HH11	1.83	0.44
1:B:232:LEU:HA	1:B:232:LEU:HD12	1.79	0.44
1:B:88:ASN:HD22	1:B:88:ASN:C	2.19	0.44
1:B:152:TYR:CG	1:B:153:PRO:N	2.86	0.44
1:B:274:GLN:HG3	1:B:275:ARG:HG3	2.00	0.43
1:A:87:HIS:O	1:A:90:GLN:HB3	2.17	0.43
1:A:152:TYR:CG	1:A:208:PRO:HG3	2.52	0.43
1:B:124:GLY:O	1:B:125:ILE:HD12	2.19	0.43
1:B:238:ASP:O	1:B:242:ILE:HG12	2.18	0.43
1:B:181:HIS:HD2	1:B:185:THR:CG2	2.30	0.42
1:B:141:ASP:OD1	1:B:143:SER:HB2	2.20	0.42
1:B:127:VAL:HG13	1:B:127:VAL:O	2.19	0.42
1:B:265:ARG:NH2	1:B:273:ARG:HD3	2.35	0.42
1:A:233:ARG:HE	1:B:233:ARG:HD2	1.84	0.42
1:B:86:VAL:HB	1:B:109:THR:HG22	2.02	0.42
1:A:99:ALA:HA	1:A:100:PRO:HD3	1.94	0.41
1:A:88:ASN:O	1:A:89:ARG:HB2	2.20	0.41
1:A:233:ARG:O	1:A:237:GLU:HG3	2.19	0.41
1:B:16:VAL:HG22	1:B:25:ILE:HG12	2.01	0.41
1:B:86:VAL:HG21	1:B:108:ALA:O	2.21	0.41
1:B:232:LEU:HG	1:B:264:LEU:HD23	2.01	0.41
1:B:6:MSE:HE2	1:B:6:MSE:HB3	1.99	0.41
1:B:260:LEU:HD13	1:B:264:LEU:HD12	2.03	0.41
1:A:238:ASP:O	1:A:242:ILE:HG12	2.21	0.41
1:B:99:ALA:HA	1:B:100:PRO:HD3	1.89	0.41
1:A:215:ALA:N	1:A:216:PRO:HD2	2.36	0.41
1:B:137:ALA:O	1:B:144:HIS:HA	2.22	0.40
1:B:164:GLY:HA3	1:B:211:PHE:O	2.22	0.40
1:A:178:ARG:H	1:A:178:ARG:HG2	1.78	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	283/305 (93%)	270 (95%)	12 (4%)	1 (0%)	43	45
1	B	291/305 (95%)	281 (97%)	7 (2%)	3 (1%)	22	18
All	All	574/610 (94%)	551 (96%)	19 (3%)	4 (1%)	30	28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	B	152	TYR
1	B	153	PRO
1	B	20	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	195/209 (93%)	180 (92%)	15 (8%)	18	18
1	B	199/209 (95%)	182 (92%)	17 (8%)	15	14
All	All	394/418 (94%)	362 (92%)	32 (8%)	17	16

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	60	LEU
1	A	88	ASN
1	A	107	LEU
1	A	115	LEU

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Mol	Chain	Res	Type
1	A	129	LEU
1	A	166	ARG
1	A	175	LEU
1	A	178	ARG
1	A	184	LEU
1	A	196	TRP
1	A	256	LEU
1	A	260	LEU
1	A	268	LEU
1	A	276	LEU
1	B	37	MSE
1	B	60	LEU
1	B	81	LEU
1	B	88	ASN
1	B	89	ARG
1	B	143	SER
1	B	144	HIS
1	B	185	THR
1	B	192	VAL
1	B	196	TRP
1	B	214	LEU
1	B	232	LEU
1	B	233	ARG
1	B	256	LEU
1	B	265	ARG
1	B	267	TRP
1	B	268	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	90	GLN
1	A	172	GLN
1	A	181	HIS
1	A	285	GLN
1	B	28	HIS
1	B	66	GLN
1	B	88	ASN
1	B	165	GLN
1	B	169	GLN
1	B	179	HIS

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Mol	Chain	Res	Type
1	B	181	HIS
1	B	210	GLN
1	B	280	GLN
1	B	285	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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	285/305 (93%)	0.11	12 (4%) 35 35	26, 40, 60, 88	0
1	B	293/305 (96%)	-0.02	3 (1%) 79 80	22, 37, 58, 67	0
All	All	578/610 (94%)	0.04	15 (2%) 53 53	22, 39, 60, 88	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	ARG	8.6
1	A	88	ASN	5.9
1	A	8	PRO	4.5
1	A	9	SER	3.0
1	A	292	GLN	2.9
1	A	86	VAL	2.7
1	A	47	GLN	2.6
1	A	196	TRP	2.6
1	A	87	HIS	2.5
1	A	197	GLN	2.2
1	B	68	GLY	2.2
1	B	197	GLN	2.2
1	A	46	SER	2.2
1	B	295	SER	2.2
1	A	54	GLN	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 ⓘ

There are no carbohydrates 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.