



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 26, 2020 – 08:41 pm GMT

PDB ID : 6ZQ8
Title : Crystal structure of Chaetomium thermophilum Glycerol Kinase in P3221 space group
Authors : Wilk, P.; Wator, E.; Malecki, P.; Tokarz, P.; Grudnik, P.
Deposited on : 2020-07-09
Resolution : 2.38 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 : 2.16
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) : 2.16

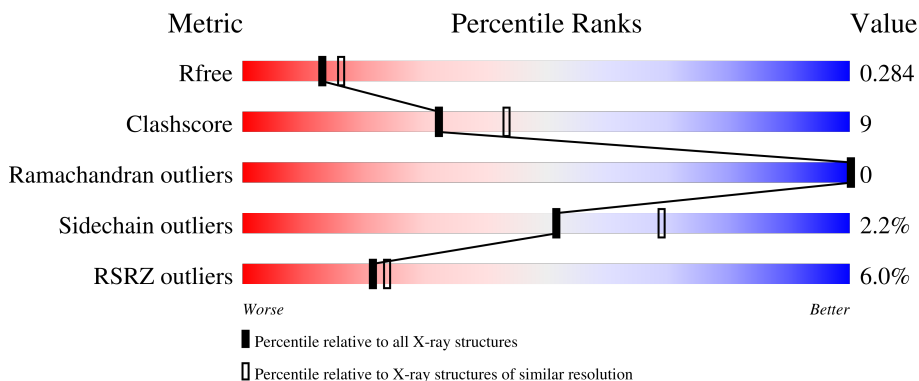
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	526	 9% 75% 22%
1	B	526	 2% 78% 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15608 atoms, of which 7725 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 Glycerol kinase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	B	512	7776	2474	3866	677	743	16	0	0	0
1	A	509	7758	2470	3859	675	738	16	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	65	GLY	-	expression tag	UNP G0SAG9
B	66	SER	-	expression tag	UNP G0SAG9
A	65	GLY	-	expression tag	UNP G0SAG9
A	66	SER	-	expression tag	UNP G0SAG9

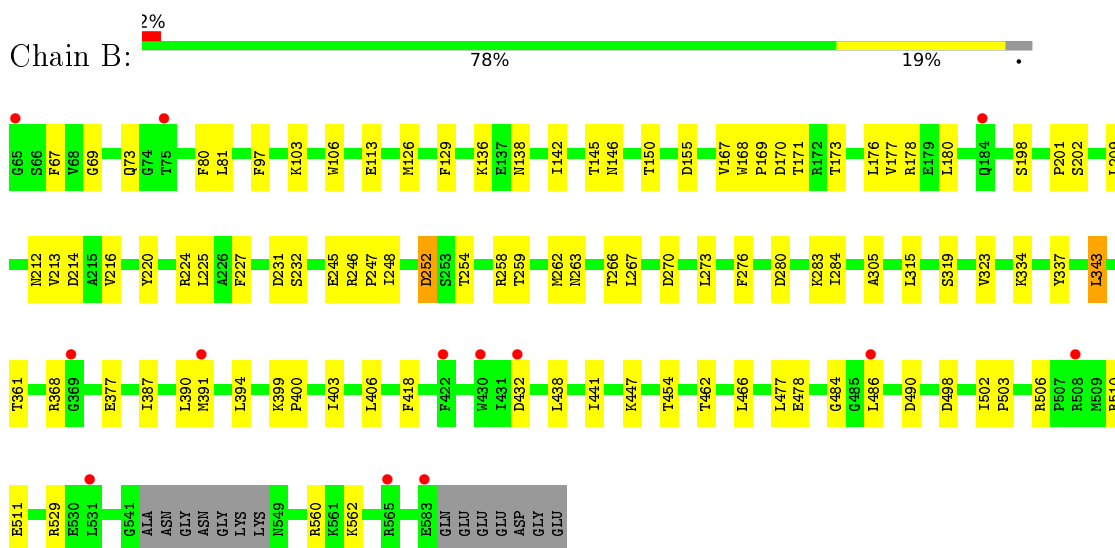
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	41	Total	O	0	0
			41	41		
2	A	33	Total	O	0	0
			33	33		

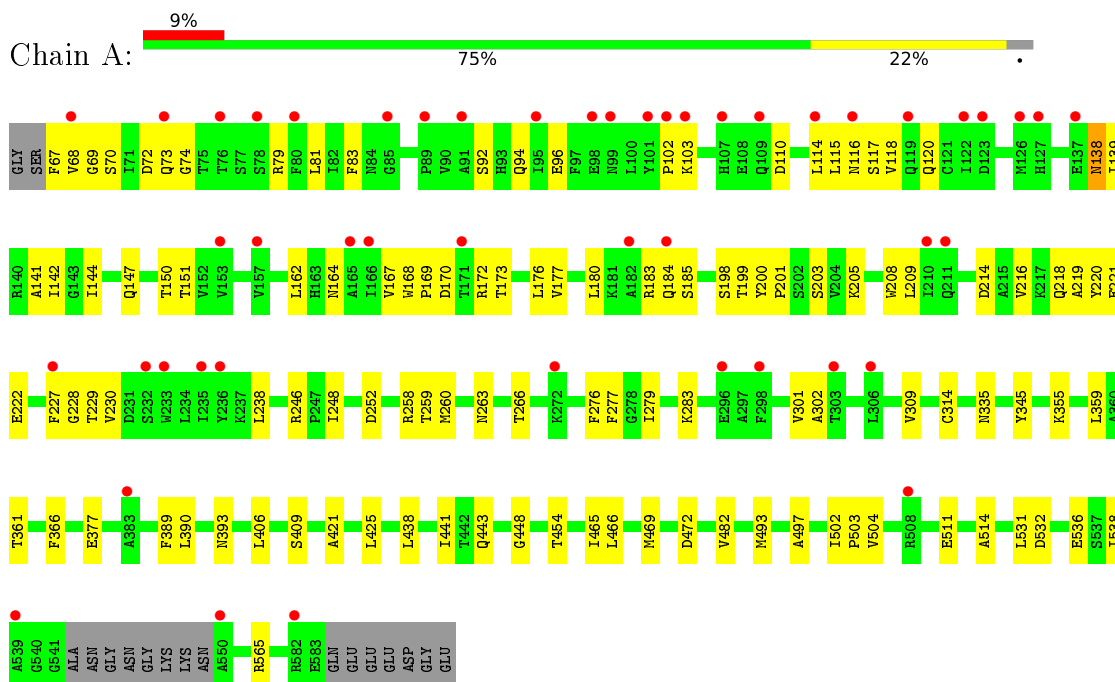
3 Residue-property plots [i](#)

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: Glycerol kinase-like protein



- Molecule 1: Glycerol kinase-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.14Å 92.14Å 232.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.04 – 2.38 47.04 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.04-2.38) 98.8 (47.04-2.38)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.39Å)	Xtrriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.244 , 0.284 0.244 , 0.284	Depositor DCC
R_{free} test set	2100 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtrriage
Anisotropy	0.193	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15608	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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	0.30	0/3985	0.49	0/5402
1	B	0.26	0/3992	0.47	0/5411
All	All	0.28	0/7977	0.48	0/10813

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	3899	3859	3859	78	0
1	B	3910	3866	3866	58	0
2	A	33	0	0	0	0
2	B	41	0	0	2	0
All	All	7883	7725	7725	136	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 9.

All (136) 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:432:ASP:OD2	2:B:601:HOH:O	1.92	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:PRO:O	1:A:103:LYS:HG3	1.84	0.77
1:A:482:VAL:HG21	1:A:493:MET:SD	2.26	0.76
1:B:258:ARG:HH11	1:B:361:THR:HG21	1.52	0.74
1:A:151:THR:HG23	1:A:227:PHE:HE1	1.51	0.74
1:A:151:THR:HG23	1:A:227:PHE:CE1	2.25	0.72
1:A:366:PHE:HE2	1:A:531:LEU:HD21	1.55	0.70
1:A:406:LEU:O	1:A:409:SER:HB3	1.94	0.66
1:B:490:ASP:OD1	1:B:506:ARG:NH2	2.26	0.66
1:B:258:ARG:NH1	1:B:361:THR:HG21	2.11	0.65
1:A:73:GLN:NE2	1:A:74:GLY:O	2.30	0.65
1:B:262:MET:HE2	1:B:267:LEU:HA	1.81	0.63
1:A:198:SER:OG	1:A:199:THR:N	2.31	0.62
1:A:502:ILE:HG13	1:A:503:PRO:HD2	1.81	0.62
1:A:366:PHE:CE2	1:A:531:LEU:HD21	2.35	0.61
1:A:216:VAL:HG22	1:A:219:ALA:HB3	1.82	0.61
1:A:199:THR:O	1:A:205:LYS:NZ	2.33	0.61
1:A:335:ASN:HB3	1:A:482:VAL:HG12	1.83	0.60
1:A:79:ARG:NH2	1:A:94:GLN:OE1	2.33	0.60
1:A:229:THR:HG22	1:A:230:VAL:H	1.66	0.60
1:A:208:TRP:HE3	1:A:209:LEU:HD12	1.67	0.59
1:B:81:LEU:HD21	1:B:511:GLU:HG3	1.84	0.59
1:B:387:ILE:HG13	1:B:486:LEU:HD11	1.83	0.59
1:B:368:ARG:NH2	1:B:529:ARG:O	2.35	0.59
1:B:247:PRO:O	1:B:248:ILE:HD13	2.03	0.58
1:B:103:LYS:HD3	1:B:106:TRP:CD2	2.39	0.58
1:A:114:LEU:HD12	1:A:115:LEU:N	2.19	0.57
1:B:173:THR:O	1:B:177:VAL:HG23	2.04	0.57
1:A:162:LEU:HD13	1:A:216:VAL:HG23	1.88	0.55
1:A:205:LYS:O	1:A:209:LEU:HD13	2.06	0.55
1:A:81:LEU:HD12	1:A:81:LEU:N	2.22	0.55
1:A:465:ILE:HG22	1:A:469:MET:HE2	1.88	0.55
1:B:180:LEU:HD22	1:B:276:PHE:CE1	2.41	0.55
1:B:155:ASP:OD2	1:B:224:ARG:NH2	2.40	0.55
1:A:218:GLN:O	1:A:222:GLU:N	2.35	0.55
1:A:532:ASP:O	1:A:536:GLU:HG3	2.06	0.55
1:A:68:VAL:HG12	1:A:69:GLY:H	1.70	0.54
1:A:173:THR:O	1:A:177:VAL:HG23	2.09	0.53
1:A:229:THR:HG22	1:A:230:VAL:N	2.23	0.53
1:A:438:LEU:HD23	1:A:441:ILE:HD11	1.90	0.52
1:A:406:LEU:O	1:A:448:GLY:HA2	2.10	0.52
1:A:162:LEU:HD13	1:A:216:VAL:CG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ASP:OD2	1:B:254:THR:OG1	2.16	0.52
1:B:103:LYS:HD3	1:B:106:TRP:CE2	2.45	0.52
1:A:147:GLN:OE1	1:A:150:THR:OG1	2.15	0.51
1:A:96:GLU:N	1:A:96:GLU:OE1	2.44	0.51
1:B:343:LEU:HD21	1:B:462:THR:HG23	1.93	0.51
1:A:258:ARG:NH1	1:A:361:THR:HG21	2.26	0.50
1:A:68:VAL:HG12	1:A:69:GLY:N	2.27	0.50
1:B:270:ASP:HB3	1:B:273:LEU:HD12	1.92	0.50
1:B:263:ASN:CG	1:B:266:THR:HG23	2.33	0.50
1:B:502:ILE:HG12	1:B:503:PRO:HD2	1.94	0.50
1:A:70:SER:HB3	1:A:83:PHE:HE1	1.77	0.49
1:B:478:GLU:C	1:B:502:ILE:HD11	2.33	0.49
1:A:115:LEU:O	1:A:118:VAL:HG12	2.13	0.49
1:B:390:LEU:HD11	1:B:454:THR:OG1	2.12	0.49
1:A:359:LEU:HB2	1:A:377:GLU:HB3	1.95	0.49
1:B:180:LEU:HD22	1:B:276:PHE:HE1	1.78	0.49
1:A:116:ASN:O	1:A:120:GLN:HG2	2.12	0.48
1:B:168:TRP:CG	1:B:169:PRO:HD3	2.47	0.48
1:B:466:LEU:HD22	1:B:477:LEU:HD13	1.95	0.48
1:A:72:ASP:HB2	1:A:514:ALA:HB2	1.94	0.48
1:A:81:LEU:HD21	1:A:511:GLU:HG3	1.96	0.48
1:B:126:MET:HA	1:B:129:PHE:CB	2.44	0.48
1:B:498:ASP:O	1:B:560:ARG:NH1	2.41	0.48
1:A:421:ALA:HB2	1:A:425:LEU:HG	1.96	0.48
1:A:70:SER:OG	1:A:514:ALA:HB1	2.13	0.48
1:A:466:LEU:HD23	1:A:469:MET:HE3	1.95	0.48
1:A:277:PHE:HB2	1:A:279:ILE:HD13	1.96	0.47
1:B:126:MET:HA	1:B:129:PHE:HB2	1.96	0.47
1:A:201:PRO:HB3	1:A:260:MET:HG3	1.97	0.47
1:A:301:VAL:HG23	1:A:309:VAL:O	2.14	0.47
1:A:238:LEU:O	1:A:302:ALA:N	2.47	0.47
1:B:176:LEU:HD23	1:B:180:LEU:CD1	2.45	0.47
1:B:220:TYR:O	1:B:283:LYS:HG2	2.15	0.47
1:A:168:TRP:CG	1:A:169:PRO:HD3	2.50	0.46
1:B:262:MET:CE	1:B:267:LEU:HA	2.45	0.46
1:B:80:PHE:C	1:B:81:LEU:HD12	2.36	0.46
1:A:114:LEU:HA	1:A:117:SER:HB3	1.97	0.46
1:A:200:TYR:N	1:A:201:PRO:CD	2.79	0.46
1:B:209:LEU:O	1:B:213:VAL:HB	2.16	0.45
1:B:399:LYS:HG2	1:B:400:PRO:HD2	1.98	0.45
1:A:203:SER:HB3	1:A:259:THR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ARG:NH1	1:A:511:GLU:OE1	2.49	0.45
1:A:389:PHE:O	1:A:393:ASN:HB2	2.16	0.45
1:B:390:LEU:HD23	1:B:394:LEU:HD12	1.99	0.45
1:A:390:LEU:HD11	1:A:454:THR:OG1	2.16	0.45
1:A:538:ILE:O	1:A:538:ILE:HG22	2.17	0.45
1:B:280:ASP:OD1	1:B:283:LYS:HB3	2.17	0.44
1:A:246:ARG:HD2	1:A:248:ILE:HD11	1.98	0.44
1:A:259:THR:O	1:A:260:MET:HB2	2.17	0.44
1:A:141:ALA:O	1:A:142:ILE:HD13	2.17	0.44
1:B:319:SER:O	1:B:323:VAL:HG23	2.18	0.44
1:B:562:LYS:NZ	2:B:610:HOH:O	2.51	0.44
1:A:170:ASP:OD2	1:A:172:ARG:NH2	2.50	0.44
1:A:227:PHE:CG	1:A:228:GLY:N	2.86	0.44
1:B:67:PHE:N	1:B:138:ASN:O	2.47	0.44
1:B:406:LEU:HD21	1:B:447:LYS:HE3	1.99	0.44
1:A:144:ILE:O	1:A:314:CYS:HA	2.18	0.43
1:A:497:ALA:HB2	1:A:504:VAL:HG23	2.00	0.43
1:B:263:ASN:HB3	1:B:266:THR:OG1	2.18	0.43
1:A:167:VAL:HG12	1:A:168:TRP:H	1.82	0.43
1:B:258:ARG:NH1	1:B:377:GLU:OE1	2.46	0.43
1:B:337:TYR:HB2	1:B:484:GLY:O	2.18	0.43
1:A:220:TYR:O	1:A:283:LYS:HB3	2.19	0.43
1:A:96:GLU:N	1:A:96:GLU:CD	2.72	0.43
1:B:69:GLY:HA3	1:B:142:ILE:HD13	2.01	0.43
1:A:184:GLN:N	1:A:184:GLN:OE1	2.40	0.43
1:B:150:THR:HG23	1:B:167:VAL:HA	2.00	0.42
1:B:213:VAL:HG12	1:B:216:VAL:H	1.84	0.42
1:B:225:LEU:HD22	1:B:284:ILE:HG13	2.01	0.42
1:B:202:SER:HB2	1:B:259:THR:HG22	2.01	0.42
1:A:502:ILE:CG1	1:A:503:PRO:HD2	2.47	0.42
1:B:438:LEU:HD23	1:B:441:ILE:HD11	2.01	0.42
1:A:183:ARG:NH1	1:A:276:PHE:O	2.53	0.42
1:B:198:SER:HB2	1:B:201:PRO:HD3	2.02	0.42
1:B:97:PHE:HB2	1:B:113:GLU:HG3	2.01	0.42
1:A:110:ASP:HA	1:A:164:ASN:OD1	2.20	0.42
1:A:355:LYS:HB3	1:A:355:LYS:HE2	1.80	0.42
1:B:399:LYS:CG	1:B:400:PRO:HD2	2.50	0.42
1:B:478:GLU:O	1:B:502:ILE:HD11	2.20	0.42
1:A:184:GLN:HG2	1:A:185:SER:N	2.35	0.41
1:A:355:LYS:HG2	1:A:472:ASP:OD1	2.20	0.41
1:A:345:TYR:HB2	1:A:469:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:GLU:O	1:B:246:ARG:HB2	2.21	0.41
1:A:176:LEU:HD11	1:A:180:LEU:HD11	2.01	0.41
1:A:218:GLN:HA	1:A:221:GLU:HB2	2.03	0.41
1:B:136:LYS:HD2	1:B:305:ALA:O	2.20	0.41
1:A:69:GLY:CA	1:A:142:ILE:HD12	2.51	0.41
1:A:263:ASN:CG	1:A:266:THR:HG23	2.41	0.41
1:A:465:ILE:HG22	1:A:469:MET:CE	2.51	0.41
1:A:138:ASN:C	1:A:139:ILE:HD12	2.41	0.41
1:B:146:ASN:OD1	1:B:231:ASP:HB3	2.21	0.41
1:B:170:ASP:OD1	1:B:171:THR:N	2.54	0.40
1:B:145:THR:HA	1:B:315:LEU:O	2.21	0.40
1:B:391:MET:HG2	1:B:403:ILE:HD11	2.03	0.40

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	506/526 (96%)	484 (96%)	22 (4%)	0	100	100
1	B	508/526 (97%)	490 (96%)	18 (4%)	0	100	100
All	All	1014/1052 (96%)	974 (96%)	40 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	409/420 (97%)	402 (98%)	7 (2%)	60	76
1	B	410/420 (98%)	399 (97%)	11 (3%)	44	62
All	All	819/840 (98%)	801 (98%)	18 (2%)	52	69

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	73	GLN
1	B	178	ARG
1	B	212	ASN
1	B	214	ASP
1	B	227	PHE
1	B	232	SER
1	B	252	ASP
1	B	334	LYS
1	B	343	LEU
1	B	418	PHE
1	B	510	ARG
1	A	67	PHE
1	A	92	SER
1	A	138	ASN
1	A	214	ASP
1	A	252	ASP
1	A	443	GLN
1	A	565	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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	509/526 (96%)	0.65	48 (9%) 8 9	38, 83, 131, 175	0
1	B	512/526 (97%)	0.30	13 (2%) 57 59	37, 68, 119, 142	0
All	All	1021/1052 (97%)	0.48	61 (5%) 21 24	37, 75, 128, 175	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	101	TYR	7.0
1	A	137	GLU	6.9
1	A	165	ALA	6.4
1	A	550	ALA	5.2
1	A	303	THR	4.2
1	A	68	VAL	4.1
1	A	91	ALA	4.1
1	A	235	ILE	4.0
1	A	211	GLN	3.9
1	A	508	ARG	3.9
1	A	122	ILE	3.7
1	A	126	MET	3.4
1	A	78	SER	3.3
1	A	119	GLN	3.3
1	A	233	TRP	3.2
1	A	80	PHE	3.1
1	A	123	ASP	3.1
1	A	127	HIS	3.1
1	A	582	ARG	3.1
1	A	95	ILE	2.9
1	A	116	ASN	2.8
1	B	65	GLY	2.8
1	A	166	ILE	2.8
1	A	109	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	107	HIS	2.7
1	A	236	TYR	2.7
1	A	153	VAL	2.7
1	A	306	LEU	2.7
1	B	184	GLN	2.7
1	B	422	PHE	2.7
1	B	369	GLY	2.7
1	A	184	GLN	2.6
1	A	89	PRO	2.6
1	A	227	PHE	2.6
1	A	76	THR	2.5
1	A	73	GLN	2.5
1	B	583	GLU	2.5
1	A	298	PHE	2.5
1	A	539	ALA	2.4
1	A	103	LYS	2.4
1	A	171	THR	2.4
1	B	508	ARG	2.4
1	B	391	MET	2.3
1	A	157	VAL	2.3
1	A	102	PRO	2.3
1	B	486	LEU	2.2
1	A	210	ILE	2.2
1	A	114	LEU	2.2
1	A	98	GLU	2.2
1	A	272	LYS	2.2
1	B	531	LEU	2.2
1	A	232	SER	2.2
1	B	432	ASP	2.2
1	B	75	THR	2.1
1	A	182	ALA	2.1
1	A	383	ALA	2.1
1	A	85	GLY	2.1
1	A	296	GLU	2.1
1	B	565	ARG	2.0
1	B	430	TRP	2.0
1	A	99	ASN	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 monosaccharides 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.