



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 02:30 PM EDT

PDB ID : 3IDQ  
Title : Crystal structure of *S. cerevisiae* Get3 at 3.7 Angstrom resolution  
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Deposited on : 2009-07-21  
Resolution : 3.70 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](mailto: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>.

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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 : 2.35  
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) : 2.35

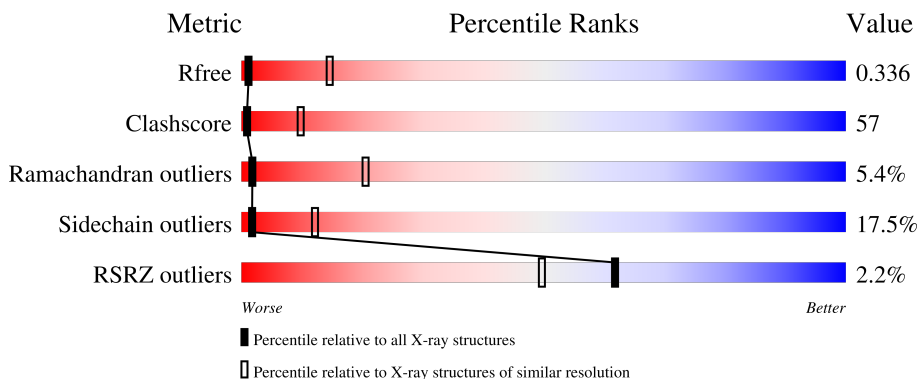
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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  $\geq 3$ , 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	369	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2186 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 ATPase GET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	272	2184	1387	366	417	14	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	GLY	-	expression tag	UNP Q12154
A	356	LEU	-	expression tag	UNP Q12154
A	357	VAL	-	expression tag	UNP Q12154
A	358	PRO	-	expression tag	UNP Q12154
A	359	ARG	-	expression tag	UNP Q12154
A	360	GLY	-	expression tag	UNP Q12154
A	361	SER	-	expression tag	UNP Q12154
A	362	LEU	-	expression tag	UNP Q12154
A	363	GLU	-	expression tag	UNP Q12154
A	364	HIS	-	expression tag	UNP Q12154
A	365	HIS	-	expression tag	UNP Q12154
A	366	HIS	-	expression tag	UNP Q12154
A	367	HIS	-	expression tag	UNP Q12154
A	368	HIS	-	expression tag	UNP Q12154
A	369	HIS	-	expression tag	UNP Q12154

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ni	0	0
			1	1		

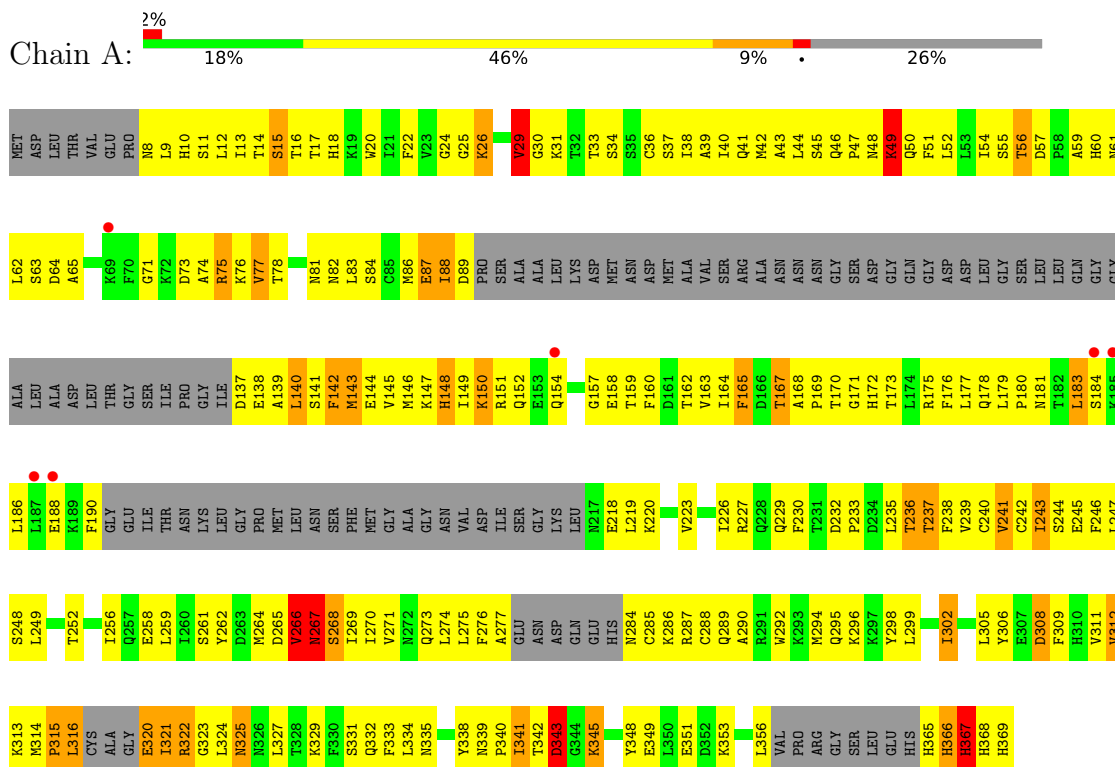
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	A	1	Total 1	Zn 1	0	0

### 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: ATPase GET3



## 4 Data and refinement statistics i

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.32Å 115.32Å 281.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.05 – 3.70 47.05 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.05-3.70) 99.7 (47.05-3.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 3.66Å)	Xtrriage
Refinement program	PHENIX 1.4_62	Depositor
R, $R_{free}$	0.283 , 0.335 0.280 , 0.336	Depositor DCC
$R_{free}$ test set	358 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	137.5	Xtrriage
Anisotropy	0.500	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 164.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.057 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k +1/3*l 0.057 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/ 3*k+1/3*l 0.056 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+ 1/3*l,-4/3*h+4/3*k+1/3*l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	2186	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	182.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NI

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	0.36	0/2222	0.57	0/2988

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	PHE	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	2184	0	2150	246	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
All	All	2186	0	2150	246	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 57.

All (246) 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:A:180:PRO:HB2	1:A:227:ARG:HD3	1.32	1.11
1:A:249:LEU:HD11	1:A:302:ILE:HD13	1.42	1.02
1:A:270:ILE:HD11	1:A:314:MET:HG3	1.52	0.89
1:A:170:THR:HB	1:A:172:HIS:HD2	1.40	0.85
1:A:88:ILE:HG22	1:A:89:ASP:H	1.42	0.84
1:A:218:GLU:HG3	1:A:219:LEU:H	1.42	0.82
1:A:267:ASN:HA	1:A:309:PHE:CD1	2.15	0.82
1:A:245:GLU:O	1:A:249:LEU:HD23	1.79	0.81
1:A:246:PHE:HB2	1:A:298:TYR:CZ	2.16	0.80
1:A:26:LYS:HB3	1:A:169:PRO:O	1.82	0.80
1:A:240:CYS:HB2	1:A:269:ILE:HG12	1.62	0.80
1:A:52:LEU:HD22	1:A:84:SER:HB3	1.64	0.77
1:A:37:SER:HA	1:A:40:ILE:HD12	1.65	0.77
1:A:179:LEU:HB3	1:A:180:PRO:HD3	1.67	0.76
1:A:13:ILE:HG12	1:A:335:ASN:HB2	1.66	0.75
1:A:38:ILE:HG22	1:A:334:LEU:HD21	1.69	0.75
1:A:259:LEU:HA	1:A:262:TYR:HD2	1.51	0.75
1:A:284:ASN:N	1:A:286:LYS:HD3	2.02	0.74
1:A:36:CYS:O	1:A:40:ILE:HG13	1.87	0.74
1:A:226:ILE:HA	1:A:229:GLN:HB2	1.68	0.74
1:A:147:LYS:HG2	1:A:151:ARG:HG3	1.71	0.73
1:A:366:HIS:CG	1:A:367:HIS:H	2.05	0.73
1:A:40:ILE:O	1:A:44:LEU:HB2	1.88	0.73
1:A:181:ASN:HB2	1:A:227:ARG:HH11	1.55	0.72
1:A:43:ALA:HA	1:A:51:PHE:HE2	1.55	0.71
1:A:25:GLY:HA3	1:A:31:LYS:HG3	1.72	0.71
1:A:237:THR:HA	1:A:265:ASP:HB3	1.73	0.71
1:A:148:HIS:O	1:A:152:GLN:CB	2.40	0.70
1:A:181:ASN:HB2	1:A:227:ARG:NH1	2.07	0.70
1:A:242:CYS:HB2	1:A:271:VAL:HG12	1.72	0.69
1:A:148:HIS:O	1:A:152:GLN:HB2	1.92	0.69
1:A:252:THR:O	1:A:256:ILE:HG12	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:HIS:CE1	1:A:87:GLU:HB2	2.28	0.69
1:A:244:SER:CB	1:A:295:GLN:HG3	2.23	0.69
1:A:170:THR:HB	1:A:172:HIS:CD2	2.26	0.69
1:A:314:MET:HE1	1:A:333:PHE:O	1.92	0.68
1:A:232:ASP:HB3	1:A:235:LEU:HD12	1.76	0.68
1:A:34:SER:O	1:A:38:ILE:HG23	1.94	0.68
1:A:172:HIS:HE1	1:A:176:PHE:CZ	2.11	0.67
1:A:329:LYS:NZ	1:A:329:LYS:HB3	2.10	0.66
1:A:218:GLU:HG3	1:A:219:LEU:N	2.08	0.66
1:A:43:ALA:HA	1:A:51:PHE:CE2	2.31	0.66
1:A:172:HIS:HA	1:A:175:ARG:NH2	2.10	0.66
1:A:274:LEU:HD21	1:A:299:LEU:HD11	1.77	0.65
1:A:178:GLN:HA	1:A:227:ARG:HH12	1.59	0.65
1:A:246:PHE:HB2	1:A:298:TYR:CE1	2.31	0.65
1:A:284:ASN:C	1:A:286:LYS:H	1.98	0.65
1:A:316:LEU:HD12	1:A:316:LEU:H	1.62	0.65
1:A:145:VAL:O	1:A:148:HIS:HB3	1.97	0.65
1:A:168:ALA:H	1:A:173:THR:HG21	1.61	0.65
1:A:146:MET:O	1:A:149:ILE:HG12	1.97	0.64
1:A:329:LYS:HB3	1:A:329:LYS:HZ1	1.63	0.64
1:A:38:ILE:HD11	1:A:164:ILE:HG23	1.78	0.64
1:A:31:LYS:NZ	1:A:169:PRO:HG3	2.13	0.64
1:A:76:LYS:HA	1:A:84:SER:HA	1.80	0.64
1:A:52:LEU:HB3	1:A:84:SER:OG	1.98	0.64
1:A:143:MET:HB3	1:A:179:LEU:HD21	1.79	0.63
1:A:48:ASN:O	1:A:49:LYS:HB2	1.97	0.63
1:A:226:ILE:HD12	1:A:229:GLN:HB2	1.80	0.62
1:A:284:ASN:C	1:A:286:LYS:N	2.54	0.61
1:A:43:ALA:HB1	1:A:82:ASN:ND2	2.16	0.61
1:A:173:THR:HA	1:A:176:PHE:HB2	1.82	0.61
1:A:147:LYS:HE2	1:A:151:ARG:HE	1.65	0.61
1:A:18:HIS:CD2	1:A:237:THR:HG22	2.36	0.61
1:A:246:PHE:O	1:A:249:LEU:HB2	2.00	0.61
1:A:238:PHE:CD1	1:A:239:VAL:N	2.69	0.60
1:A:341:ILE:HG13	1:A:342:THR:H	1.66	0.60
1:A:226:ILE:HG13	1:A:230:PHE:CE1	2.36	0.60
1:A:148:HIS:C	1:A:148:HIS:CD2	2.75	0.60
1:A:36:CYS:HB3	1:A:40:ILE:HD11	1.84	0.60
1:A:157:GLY:C	1:A:158:GLU:HG3	2.21	0.59
1:A:142:PHE:O	1:A:146:MET:N	2.33	0.59
1:A:24:GLY:HA3	1:A:238:PHE:CZ	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLY:HA3	1:A:238:PHE:HZ	1.67	0.59
1:A:147:LYS:NZ	1:A:151:ARG:HH21	2.01	0.58
1:A:40:ILE:CD1	1:A:327:LEU:HG	2.33	0.58
1:A:20:TRP:CZ3	1:A:163:VAL:HB	2.39	0.58
1:A:173:THR:O	1:A:177:LEU:HD13	2.03	0.58
1:A:147:LYS:CE	1:A:151:ARG:HE	2.16	0.57
1:A:9:LEU:HD12	1:A:334:LEU:HD11	1.85	0.57
1:A:341:ILE:HG13	1:A:342:THR:N	2.20	0.57
1:A:246:PHE:C	1:A:246:PHE:CD2	2.78	0.57
1:A:71:GLY:O	1:A:86:MET:HG3	2.05	0.57
1:A:338:TYR:HB2	1:A:343:ASP:OD1	2.04	0.57
1:A:178:GLN:HB2	1:A:262:TYR:HE1	1.68	0.56
1:A:31:LYS:HZ1	1:A:169:PRO:HG3	1.70	0.56
1:A:178:GLN:HA	1:A:227:ARG:NH1	2.20	0.56
1:A:270:ILE:CD1	1:A:314:MET:HG3	2.30	0.55
1:A:342:THR:O	1:A:343:ASP:C	2.45	0.55
1:A:150:LYS:NZ	1:A:154:GLN:HE21	2.05	0.55
1:A:145:VAL:HA	1:A:148:HIS:HB3	1.88	0.55
1:A:60:HIS:CE1	1:A:88:ILE:O	2.61	0.54
1:A:137:ASP:O	1:A:140:LEU:HB3	2.06	0.54
1:A:168:ALA:HB3	1:A:173:THR:HG23	1.90	0.54
1:A:273:GLN:HA	1:A:316:LEU:HB3	1.89	0.54
1:A:139:ALA:HB1	1:A:179:LEU:HD13	1.89	0.53
1:A:11:SER:O	1:A:15:SER:HB2	2.09	0.53
1:A:48:ASN:O	1:A:49:LYS:HD3	2.08	0.53
1:A:147:LYS:HA	1:A:150:LYS:HB3	1.89	0.53
1:A:179:LEU:O	1:A:183:LEU:HB2	2.08	0.53
1:A:172:HIS:CE1	1:A:176:PHE:CZ	2.96	0.53
1:A:48:ASN:O	1:A:49:LYS:CB	2.56	0.53
1:A:143:MET:HB3	1:A:179:LEU:CD2	2.39	0.52
1:A:170:THR:CB	1:A:172:HIS:HD2	2.18	0.52
1:A:45:SER:O	1:A:47:PRO:HD3	2.09	0.52
1:A:230:PHE:HA	1:A:236:THR:OG1	2.10	0.52
1:A:271:VAL:HG22	1:A:312:VAL:O	2.10	0.52
1:A:316:LEU:HD12	1:A:316:LEU:N	2.24	0.52
1:A:341:ILE:O	1:A:345:LYS:HG3	2.10	0.52
1:A:311:VAL:HG23	1:A:311:VAL:O	2.10	0.52
1:A:290:ALA:O	1:A:294:MET:SD	2.68	0.51
1:A:40:ILE:HD11	1:A:327:LEU:HG	1.92	0.51
1:A:41:GLN:HB2	1:A:331:SER:HB2	1.91	0.51
1:A:180:PRO:HD2	1:A:227:ARG:NH2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LEU:HA	1:A:262:TYR:CD2	2.40	0.51
1:A:366:HIS:O	1:A:367:HIS:HB3	2.11	0.51
1:A:243:ILE:HD12	1:A:243:ILE:H	1.76	0.51
1:A:321:ILE:HD12	1:A:327:LEU:HA	1.92	0.51
1:A:29:VAL:HG11	1:A:243:ILE:HG13	1.93	0.50
1:A:87:GLU:C	1:A:88:ILE:HG12	2.32	0.50
1:A:60:HIS:ND1	1:A:87:GLU:HB2	2.25	0.50
1:A:331:SER:O	1:A:334:LEU:N	2.44	0.50
1:A:292:TRP:HA	1:A:295:GLN:HE21	1.77	0.50
1:A:56:THR:OG1	1:A:165:PHE:HE2	1.94	0.50
1:A:38:ILE:HG13	1:A:39:ALA:N	2.27	0.50
1:A:267:ASN:N	1:A:267:ASN:HD22	2.07	0.50
1:A:10:HIS:HA	1:A:13:ILE:HB	1.93	0.50
1:A:60:HIS:HE1	1:A:88:ILE:O	1.95	0.49
1:A:38:ILE:O	1:A:42:MET:HB2	2.12	0.49
1:A:267:ASN:HA	1:A:309:PHE:CE1	2.46	0.49
1:A:242:CYS:CB	1:A:271:VAL:HG12	2.39	0.49
1:A:275:LEU:O	1:A:276:PHE:CD2	2.66	0.49
1:A:81:ASN:H	1:A:81:ASN:HD22	1.59	0.49
1:A:10:HIS:O	1:A:10:HIS:ND1	2.45	0.49
1:A:37:SER:CB	1:A:331:SER:HB3	2.43	0.49
1:A:271:VAL:O	1:A:314:MET:HB2	2.11	0.49
1:A:178:GLN:HB2	1:A:262:TYR:CE1	2.47	0.48
1:A:315:PRO:HG3	1:A:343:ASP:OD2	2.12	0.48
1:A:179:LEU:CB	1:A:180:PRO:HD3	2.40	0.48
1:A:366:HIS:CG	1:A:367:HIS:N	2.75	0.48
1:A:270:ILE:HD12	1:A:334:LEU:HD13	1.96	0.48
1:A:320:GLU:N	1:A:320:GLU:OE1	2.46	0.48
1:A:26:LYS:HA	1:A:169:PRO:HA	1.95	0.48
1:A:240:CYS:HB2	1:A:269:ILE:CG1	2.39	0.48
1:A:147:LYS:HZ3	1:A:151:ARG:HH21	1.62	0.48
1:A:266:VAL:O	1:A:268:SER:N	2.46	0.47
1:A:26:LYS:HD3	1:A:171:GLY:CA	2.44	0.47
1:A:313:LYS:HB2	1:A:338:TYR:CZ	2.49	0.47
1:A:51:PHE:O	1:A:83:LEU:HA	2.14	0.47
1:A:163:VAL:HG12	1:A:163:VAL:O	2.13	0.47
1:A:220:LYS:O	1:A:223:VAL:HG12	2.14	0.47
1:A:62:LEU:O	1:A:65:ALA:HB3	2.14	0.47
1:A:65:ALA:O	1:A:322:ARG:O	2.31	0.47
1:A:286:LYS:HA	1:A:289:GLN:HB3	1.97	0.47
1:A:269:ILE:O	1:A:312:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:HIS:O	1:A:369:HIS:HB3	2.16	0.46
1:A:243:ILE:CD1	1:A:248:SER:HB3	2.46	0.46
1:A:306:TYR:HB3	1:A:309:PHE:CD2	2.50	0.46
1:A:8:ASN:ND2	1:A:335:ASN:O	2.47	0.46
1:A:77:VAL:HG23	1:A:78:THR:N	2.30	0.46
1:A:285:CYS:SG	1:A:288:CYS:HB2	2.55	0.46
1:A:142:PHE:CE2	1:A:146:MET:SD	3.09	0.46
1:A:246:PHE:HB2	1:A:298:TYR:OH	2.16	0.46
1:A:24:GLY:HA2	1:A:167:THR:OG1	2.16	0.46
1:A:249:LEU:HD12	1:A:302:ILE:HG23	1.97	0.46
1:A:273:GLN:HA	1:A:273:GLN:HE21	1.80	0.46
1:A:170:THR:C	1:A:172:HIS:H	2.19	0.45
1:A:52:LEU:HD22	1:A:84:SER:CB	2.41	0.45
1:A:331:SER:O	1:A:334:LEU:HB3	2.16	0.45
1:A:26:LYS:HD3	1:A:171:GLY:HA2	1.98	0.45
1:A:37:SER:CA	1:A:331:SER:HB3	2.47	0.45
1:A:148:HIS:HD2	1:A:149:ILE:N	2.15	0.45
1:A:258:GLU:O	1:A:261:SER:HB3	2.17	0.45
1:A:148:HIS:O	1:A:152:GLN:HB3	2.16	0.45
1:A:148:HIS:CD2	1:A:149:ILE:N	2.84	0.45
1:A:165:PHE:HD2	1:A:165:PHE:C	2.20	0.44
1:A:339:ASN:HA	1:A:340:PRO:HD3	1.79	0.44
1:A:56:THR:HB	1:A:168:ALA:HB2	1.99	0.44
1:A:244:SER:HB2	1:A:295:GLN:HG3	1.96	0.44
1:A:325:ASN:OD1	1:A:325:ASN:N	2.50	0.44
1:A:168:ALA:N	1:A:173:THR:HG21	2.30	0.44
1:A:341:ILE:CG1	1:A:342:THR:N	2.81	0.44
1:A:54:ILE:HD11	1:A:165:PHE:CD1	2.52	0.44
1:A:71:GLY:C	1:A:73:ASP:H	2.21	0.44
1:A:145:VAL:C	1:A:148:HIS:HB3	2.37	0.44
1:A:296:LYS:O	1:A:299:LEU:HB2	2.18	0.44
1:A:298:TYR:O	1:A:302:ILE:HG12	2.18	0.44
1:A:140:LEU:HG	1:A:141:SER:N	2.32	0.44
1:A:313:LYS:HB2	1:A:338:TYR:CE2	2.53	0.44
1:A:329:LYS:O	1:A:332:GLN:HB3	2.18	0.44
1:A:76:LYS:HA	1:A:83:LEU:O	2.17	0.43
1:A:165:PHE:C	1:A:165:PHE:CD2	2.91	0.43
1:A:323:GLY:O	1:A:327:LEU:HB2	2.18	0.43
1:A:146:MET:HE2	1:A:147:LYS:N	2.33	0.43
1:A:54:ILE:HA	1:A:86:MET:O	2.18	0.43
1:A:286:LYS:HG3	1:A:289:GLN:HE21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:LEU:O	1:A:302:ILE:HG13	2.18	0.43
1:A:63:SER:HB3	1:A:87:GLU:OE2	2.18	0.43
1:A:314:MET:HA	1:A:314:MET:CE	2.49	0.43
1:A:351:GLU:C	1:A:353:LYS:N	2.72	0.43
1:A:8:ASN:C	1:A:8:ASN:OD1	2.56	0.43
1:A:139:ALA:HB1	1:A:143:MET:SD	2.59	0.43
1:A:247:LEU:HD12	1:A:247:LEU:O	2.19	0.43
1:A:284:ASN:O	1:A:286:LYS:N	2.52	0.43
1:A:339:ASN:OD1	1:A:339:ASN:C	2.57	0.43
1:A:59:ALA:O	1:A:60:HIS:HB2	2.18	0.43
1:A:12:LEU:C	1:A:14:THR:N	2.71	0.42
1:A:138:GLU:OE2	1:A:172:HIS:HB2	2.18	0.42
1:A:286:LYS:HG3	1:A:289:GLN:NE2	2.33	0.42
1:A:36:CYS:C	1:A:40:ILE:HG13	2.40	0.42
1:A:232:ASP:HA	1:A:233:PRO:HD3	1.60	0.42
1:A:74:ALA:O	1:A:75:ARG:HG3	2.19	0.42
1:A:88:ILE:HG22	1:A:89:ASP:N	2.21	0.42
1:A:238:PHE:HE1	1:A:240:CYS:HG	1.65	0.42
1:A:305:LEU:HD12	1:A:305:LEU:O	2.18	0.42
1:A:31:LYS:HE3	1:A:31:LYS:HB3	1.61	0.42
1:A:143:MET:HG2	1:A:144:GLU:H	1.83	0.42
1:A:223:VAL:O	1:A:227:ARG:HB2	2.19	0.42
1:A:168:ALA:H	1:A:173:THR:CG2	2.29	0.42
1:A:25:GLY:O	1:A:26:LYS:C	2.58	0.42
1:A:145:VAL:CA	1:A:148:HIS:HB3	2.50	0.42
1:A:223:VAL:HA	1:A:226:ILE:HG22	2.01	0.42
1:A:55:SER:C	1:A:57:ASP:N	2.74	0.42
1:A:313:LYS:O	1:A:314:MET:HE3	2.21	0.41
1:A:37:SER:O	1:A:41:GLN:HB2	2.19	0.41
1:A:145:VAL:HA	1:A:148:HIS:CB	2.50	0.41
1:A:264:MET:HG2	1:A:265:ASP:N	2.34	0.41
1:A:313:LYS:HG3	1:A:338:TYR:OH	2.19	0.41
1:A:267:ASN:HA	1:A:309:PHE:HD1	1.77	0.41
1:A:296:LYS:HA	1:A:299:LEU:HD22	2.02	0.41
1:A:75:ARG:H	1:A:84:SER:HB2	1.84	0.41
1:A:241:VAL:HA	1:A:270:ILE:O	2.19	0.41
1:A:314:MET:O	1:A:315:PRO:O	2.39	0.41
1:A:22:PHE:HD1	1:A:167:THR:HG23	1.86	0.41
1:A:142:PHE:HD2	1:A:179:LEU:HD22	1.85	0.41
1:A:39:ALA:HB2	1:A:164:ILE:HD13	2.03	0.41
1:A:61:ASN:O	1:A:64:ASP:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASN:HB2	1:A:308:ASP:O	2.21	0.41
1:A:277:ALA:HA	1:A:289:GLN:OE1	2.21	0.41
1:A:184:SER:O	1:A:188:GLU:HG3	2.20	0.40
1:A:37:SER:HA	1:A:331:SER:HB3	2.02	0.40
1:A:38:ILE:CG1	1:A:39:ALA:N	2.84	0.40
1:A:321:ILE:H	1:A:321:ILE:HG12	1.56	0.40
1:A:51:PHE:HD1	1:A:162:THR:HG23	1.86	0.40
1:A:178:GLN:O	1:A:178:GLN:CG	2.70	0.40
1:A:30:GLY:O	1:A:33:THR:N	2.55	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	260/369 (70%)	202 (78%)	44 (17%)	14 (5%)	<b>2</b> <b>20</b>

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	49	LYS
1	A	75	ARG
1	A	267	ASN
1	A	315	PRO
1	A	366	HIS
1	A	367	HIS
1	A	29	VAL
1	A	142	PHE
1	A	15	SER
1	A	343	ASP
1	A	268	SER

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Mol	Chain	Res	Type
1	A	88	ILE
1	A	266	VAL

### 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	246/322 (76%)	203 (82%)	43 (18%)	<b>2</b> <b>12</b>

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	17	THR
1	A	26	LYS
1	A	29	VAL
1	A	49	LYS
1	A	50	GLN
1	A	56	THR
1	A	77	VAL
1	A	87	GLU
1	A	140	LEU
1	A	143	MET
1	A	148	HIS
1	A	150	LYS
1	A	159	THR
1	A	165	PHE
1	A	167	THR
1	A	183	LEU
1	A	186	LEU
1	A	190	PHE
1	A	236	THR
1	A	237	THR
1	A	241	VAL
1	A	243	ILE
1	A	266	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	267	ASN
1	A	287	ARG
1	A	302	ILE
1	A	308	ASP
1	A	312	VAL
1	A	316	LEU
1	A	320	GLU
1	A	321	ILE
1	A	322	ARG
1	A	324	LEU
1	A	325	ASN
1	A	341	ILE
1	A	343	ASP
1	A	345	LYS
1	A	348	TYR
1	A	349	GLU
1	A	356	LEU
1	A	365	HIS
1	A	367	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	50	GLN
1	A	60	HIS
1	A	81	ASN
1	A	82	ASN
1	A	148	HIS
1	A	154	GLN
1	A	172	HIS
1	A	178	GLN
1	A	217	ASN
1	A	257	GLN
1	A	267	ASN
1	A	272	ASN
1	A	273	GLN
1	A	284	ASN
1	A	289	GLN
1	A	295	GLN
1	A	301	GLN
1	A	326	ASN



### 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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	272/369 (73%)	-0.05	6 (2%) 62 50	92, 172, 267, 401	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	154	GLN	3.8
1	A	184	SER	2.3
1	A	69	LYS	2.3
1	A	188	GLU	2.3
1	A	187	LEU	2.1
1	A	185	LYS	2.1

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	A	371	1/1	0.96	0.12	141,141,141,141	0
2	NI	A	370	1/1	0.97	0.02	59,59,59,59	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.