



## Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:42 am GMT

PDB ID : 2CWX  
Title : Crystal structure of octameric ribulose-1,5-bisphosphate carboxylase/oxygenase (Rubisco) from *Pyrococcus horikoshii* OT3 (form-1 crystal)  
Authors : Mizohata, E.; Mishima, C.; Akasaka, R.; Uda, H.; Terada, T.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2005-06-27  
Resolution : 2.00 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

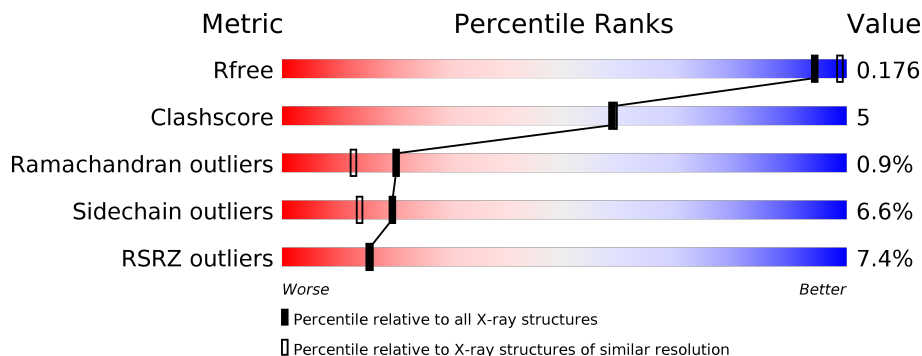
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	430	<div> <div>7%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>• •</div> </div> </div>
1	E	430	<div> <div>8%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>• 5%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6962 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 Ribulose biphosphate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3264	2093	562	594	15			
1	E	408	Total	C	N	O	S	0	0	0
			3229	2072	556	586	15			

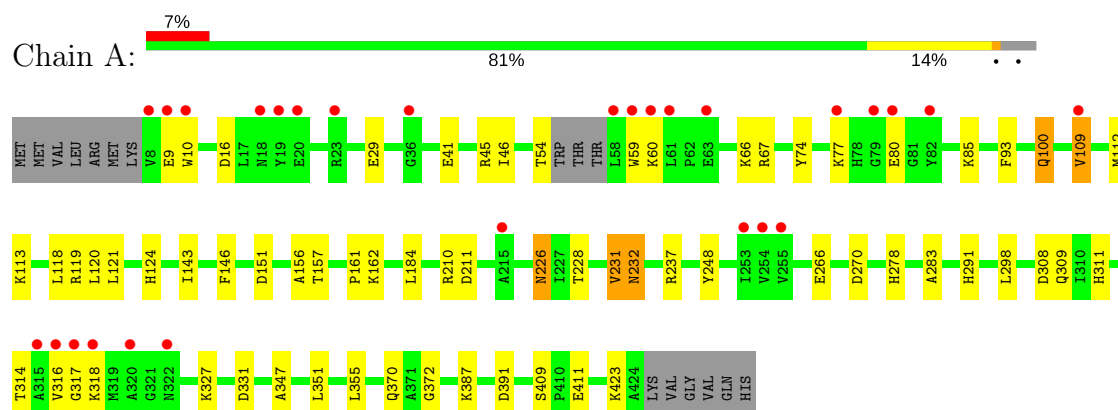
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	245	Total	O	0	0
			245	245		
2	E	224	Total	O	0	0
			224	224		

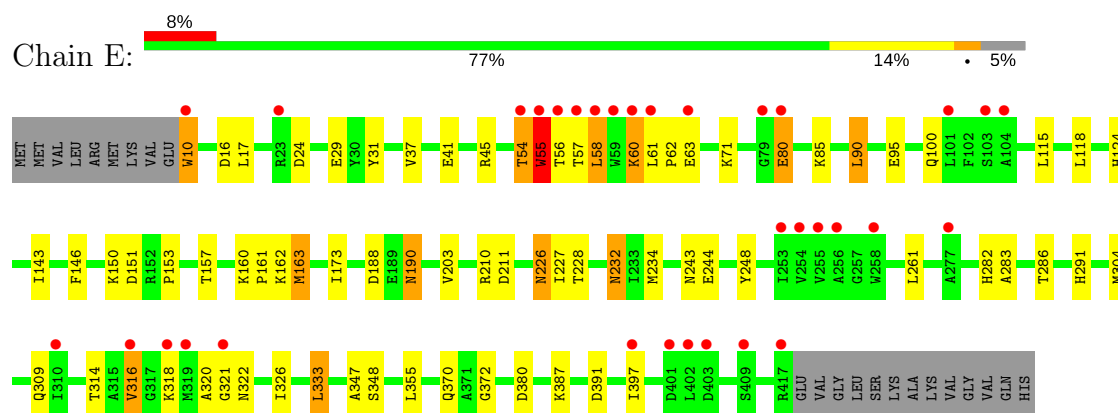
### 3 Residue-property plots [i](#)

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: Ribulose biphosphate carboxylase



#### • Molecule 1: Ribulose biphosphate carboxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.99Å 143.99Å 101.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 45.39 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.00) 99.7 (45.39-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.90 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.176 , 0.210 0.183 , 0.176	Depositor DCC
$R_{free}$ test set	3638 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.4	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 58.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6962	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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

### 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	0.75	2/3340 (0.1%)	0.83	10/4509 (0.2%)
1	E	0.73	0/3308	0.83	8/4470 (0.2%)
All	All	0.74	2/6648 (0.0%)	0.83	18/8979 (0.2%)

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	E	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	GLU	CD-OE1	6.55	1.32	1.25
1	A	231	VAL	CB-CG2	-5.43	1.41	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	ASP	CB-CG-OD2	6.80	124.42	118.30
1	E	391	ASP	CB-CG-OD2	6.36	124.02	118.30
1	E	16	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	151	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	231	VAL	CB-CA-C	-6.07	99.88	111.40
1	E	211	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	308	ASP	CB-CG-OD2	5.83	123.54	118.30
1	A	237	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	A	211	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	391	ASP	CB-CG-OD2	5.68	123.41	118.30
1	E	151	ASP	CB-CG-OD2	5.61	123.35	118.30
1	E	380	ASP	CB-CG-OD2	5.60	123.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	119	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	E	24	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	16	ASP	CB-CG-OD2	5.12	122.91	118.30
1	E	333	LEU	CB-CG-CD1	5.12	119.70	111.00
1	E	90	LEU	CB-CG-CD1	5.07	119.61	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	54	THR	Peptide

## 5.2 Too-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 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	3264	0	3255	34	0
1	E	3229	0	3213	41	0
2	A	245	0	0	2	0
2	E	224	0	0	2	1
All	All	6962	0	6468	71	1

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 5.

All (71) 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:314:THR:HG22	1:A:347:ALA:HB1	1.55	0.86
1:E:163:MET:SD	1:E:190:ASN:ND2	2.60	0.74
1:E:203:VAL:CG1	1:E:244:GLU:HG3	2.17	0.74
1:A:278:HIS:CD2	1:A:311:HIS:HE1	2.04	0.74
1:E:188:ASP:OD1	1:E:190:ASN:ND2	2.21	0.72
1:E:95:GLU:O	2:E:585:HOH:O	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ILE:HD13	1:A:309:GLN:HE21	1.59	0.66
1:E:63:GLU:O	2:E:535:HOH:O	2.14	0.65
1:E:143:ILE:HD13	1:E:309:GLN:HE21	1.62	0.64
1:E:41:GLU:OE1	1:E:45:ARG:NH1	2.31	0.64
1:E:203:VAL:HG12	1:E:244:GLU:HG3	1.78	0.64
1:A:232:ASN:H	1:A:232:ASN:HD22	1.45	0.63
1:E:232:ASN:HD22	1:E:232:ASN:H	1.46	0.63
1:A:411:GLU:HG3	2:A:576:HOH:O	1.98	0.62
1:A:157:THR:HG23	1:A:372:GLY:HA2	1.82	0.62
1:E:61:LEU:HD13	1:E:62:PRO:O	2.00	0.61
1:E:37:VAL:HG11	1:E:45:ARG:NH1	2.15	0.61
1:A:278:HIS:CD2	1:A:311:HIS:CE1	2.88	0.60
1:A:316:VAL:HG12	1:A:317:GLY:N	2.17	0.60
1:E:227:ILE:O	1:E:234:MET:HG2	2.02	0.60
1:E:54:THR:O	1:E:55:TRP:HB2	2.06	0.56
1:E:348:SER:HB3	1:E:370:GLN:HB3	1.86	0.56
1:A:283:ALA:O	1:E:291:HIS:HE1	1.88	0.56
1:A:370:GLN:HG2	2:A:609:HOH:O	2.05	0.55
1:A:248:TYR:OH	1:A:309:GLN:NE2	2.39	0.55
1:A:29:GLU:OE1	1:A:124:HIS:HE1	1.91	0.54
1:E:282:HIS:HD2	1:E:286:THR:OG1	1.92	0.53
1:A:291:HIS:HE1	1:E:283:ALA:O	1.92	0.53
1:A:109:VAL:HG13	1:A:118:LEU:CD2	2.39	0.52
1:E:248:TYR:OH	1:E:309:GLN:NE2	2.41	0.52
1:A:10:TRP:NE1	1:A:54:THR:HA	2.25	0.51
1:E:226:ASN:ND2	1:E:228:THR:H	2.08	0.51
1:A:316:VAL:HG13	1:A:355:LEU:HD13	1.93	0.50
1:A:41:GLU:OE1	1:A:45:ARG:NH1	2.43	0.50
1:E:226:ASN:HD21	1:E:228:THR:CB	2.25	0.49
1:E:55:TRP:CZ3	1:E:58:LEU:O	2.66	0.49
1:A:314:THR:HG21	1:A:351:LEU:HD11	1.95	0.48
1:E:157:THR:HG23	1:E:372:GLY:HA2	1.94	0.48
1:E:314:THR:HG23	1:E:348:SER:O	2.14	0.48
1:E:203:VAL:HG13	1:E:244:GLU:HG3	1.95	0.48
1:A:298:LEU:HD23	1:A:298:LEU:O	2.13	0.48
1:A:93:PHE:HA	1:A:100:GLN:HE22	1.80	0.47
1:E:316:VAL:HG11	1:E:355:LEU:HD11	1.97	0.47
1:A:118:LEU:H	1:A:291:HIS:HD2	1.62	0.47
1:E:153:PRO:HD2	1:E:397:ILE:HD11	1.97	0.47
1:E:210:ARG:HD2	1:E:210:ARG:C	2.36	0.46
1:A:316:VAL:HG13	1:A:355:LEU:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:VAL:HG12	1:A:317:GLY:H	1.80	0.45
1:E:29:GLU:HG2	1:E:85:LYS:HG2	1.98	0.45
1:E:226:ASN:HD22	1:E:228:THR:H	1.64	0.45
1:A:109:VAL:HG13	1:A:118:LEU:HD21	1.98	0.45
1:A:156:ALA:HA	1:A:184:LEU:O	2.16	0.45
1:A:210:ARG:C	1:A:210:ARG:HD2	2.38	0.45
1:A:10:TRP:HE1	1:A:54:THR:HA	1.83	0.44
1:E:56:THR:O	1:E:56:THR:HG23	2.17	0.44
1:A:161:PRO:HG2	1:E:62:PRO:HG2	1.99	0.44
1:E:314:THR:HG22	1:E:347:ALA:HB1	2.00	0.44
1:A:74:TYR:HB3	1:A:85:LYS:HB2	2.00	0.44
1:A:298:LEU:HD23	1:A:298:LEU:C	2.39	0.43
1:A:59:TRP:CD1	1:E:173:ILE:HD11	2.54	0.43
1:A:314:THR:CG2	1:A:347:ALA:HB1	2.37	0.43
1:E:80:GLU:CD	1:E:80:GLU:H	2.23	0.42
1:A:226:ASN:ND2	1:A:228:THR:H	2.17	0.42
1:E:118:LEU:H	1:E:291:HIS:HD2	1.68	0.42
1:E:232:ASN:HD22	1:E:232:ASN:N	2.17	0.42
1:E:10:TRP:HE1	1:E:56:THR:HG22	1.84	0.42
1:E:160:LYS:HA	1:E:161:PRO:C	2.39	0.42
1:E:304:MET:HE2	1:E:304:MET:HB2	1.70	0.42
1:E:31:TYR:OH	1:E:80:GLU:HG2	2.20	0.41
1:A:46:ILE:HA	1:A:112:MET:HE1	2.02	0.41
1:E:29:GLU:OE2	1:E:124:HIS:HE1	2.04	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:609:HOH:O	2:E:651:HOH:O[4_555]	2.17	0.03

## 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	410/430 (95%)	394 (96%)	15 (4%)	1 (0%)	51	48
1	E	406/430 (94%)	387 (95%)	13 (3%)	6 (2%)	12	5
All	All	816/860 (95%)	781 (96%)	28 (3%)	7 (1%)	20	12

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	60	LYS
1	E	316	VAL
1	E	321	GLY
1	E	55	TRP
1	E	57	THR
1	A	318	LYS
1	E	320	ALA

### 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	336/351 (96%)	316 (94%)	20 (6%)	22	17
1	E	332/351 (95%)	308 (93%)	24 (7%)	17	11
All	All	668/702 (95%)	624 (93%)	44 (7%)	19	14

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

Mol	Chain	Res	Type
1	A	9	GLU
1	A	60	LYS
1	A	66	LYS
1	A	67	ARG
1	A	77	LYS
1	A	80	GLU
1	A	100	GLN

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Mol	Chain	Res	Type
1	A	109	VAL
1	A	113	LYS
1	A	120	LEU
1	A	121	LEU
1	A	146	PHE
1	A	162	LYS
1	A	226	ASN
1	A	231	VAL
1	A	232	ASN
1	A	327	LYS
1	A	387	LYS
1	A	409	SER
1	A	423	LYS
1	E	10	TRP
1	E	17	LEU
1	E	55	TRP
1	E	58	LEU
1	E	60	LYS
1	E	71	LYS
1	E	80	GLU
1	E	90	LEU
1	E	100	GLN
1	E	115	LEU
1	E	146	PHE
1	E	150	LYS
1	E	162	LYS
1	E	163	MET
1	E	190	ASN
1	E	226	ASN
1	E	232	ASN
1	E	243	ASN
1	E	261	LEU
1	E	318	LYS
1	E	322	ASN
1	E	326	ILE
1	E	333	LEU
1	E	387	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN

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Mol	Chain	Res	Type
1	A	100	GLN
1	A	124	HIS
1	A	132	HIS
1	A	226	ASN
1	A	232	ASN
1	A	291	HIS
1	A	309	GLN
1	A	322	ASN
1	A	330	ASN
1	E	35	ASN
1	E	100	GLN
1	E	124	HIS
1	E	132	HIS
1	E	226	ASN
1	E	232	ASN
1	E	282	HIS
1	E	291	HIS
1	E	309	GLN
1	E	330	ASN
1	E	370	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 [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

### 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, 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	414/430 (96%)	0.26	28 (6%) 18 18	19, 27, 45, 77	0
1	E	408/430 (94%)	0.41	33 (8%) 13 13	19, 27, 51, 78	0
All	All	822/860 (95%)	0.33	61 (7%) 15 15	19, 27, 50, 78	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	57	THR	9.8
1	E	316	VAL	7.1
1	E	319	MET	6.7
1	E	55	TRP	6.4
1	A	316	VAL	5.9
1	E	60	LYS	5.5
1	A	59	TRP	5.4
1	E	59	TRP	5.3
1	E	56	THR	5.0
1	A	320	ALA	4.9
1	A	318	LYS	4.9
1	A	60	LYS	4.6
1	A	10	TRP	4.4
1	A	80	GLU	4.2
1	E	80	GLU	4.2
1	A	61	LEU	3.9
1	E	58	LEU	3.5
1	A	58	LEU	3.4
1	E	10	TRP	3.4
1	A	19	TYR	3.3
1	E	397	ILE	3.2
1	A	63	GLU	3.2
1	A	255	VAL	3.1
1	E	258	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	417	ARG	3.1
1	A	23	ARG	3.0
1	E	253	ILE	2.9
1	E	79	GLY	2.9
1	A	20	GLU	2.8
1	E	63	GLU	2.8
1	A	9	GLU	2.8
1	E	256	ALA	2.6
1	A	77	LYS	2.6
1	E	254	VAL	2.6
1	A	79	GLY	2.6
1	E	23	ARG	2.6
1	A	18	ASN	2.5
1	A	8	VAL	2.5
1	E	402	LEU	2.4
1	E	403	ASP	2.4
1	E	401	ASP	2.4
1	E	277	ALA	2.4
1	E	103	SER	2.4
1	E	61	LEU	2.4
1	A	315	ALA	2.4
1	E	104	ALA	2.3
1	E	321	GLY	2.3
1	A	215	ALA	2.3
1	A	82	TYR	2.3
1	A	109	VAL	2.2
1	E	310	ILE	2.2
1	E	409	SER	2.2
1	E	318	LYS	2.2
1	E	255	VAL	2.2
1	A	317	GLY	2.2
1	A	254	VAL	2.1
1	A	36	GLY	2.1
1	E	101	LEU	2.0
1	E	54	THR	2.0
1	A	253	ILE	2.0
1	A	322	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 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.