



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:42 am GMT

PDB ID : 3G1N  
Title : Catalytic domain of the human E3 ubiquitin-protein ligase HUWE1  
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Deposited on : 2009-01-30  
Resolution : 2.60 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

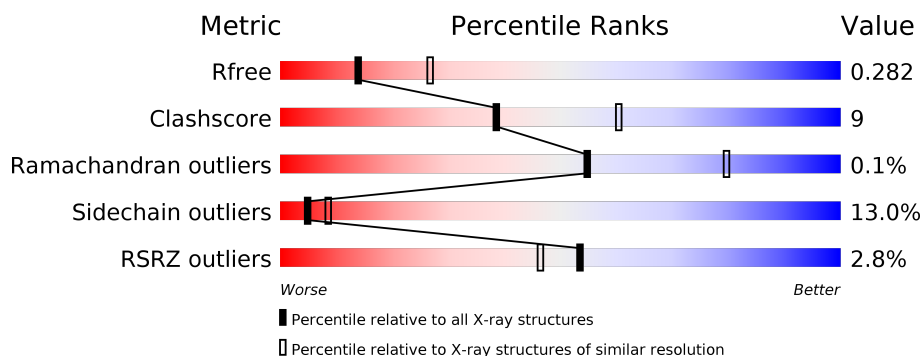
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	388	 3% 74% 19% . .
1	B	388	 3% 71% 19% 6% .

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6415 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 E3 ubiquitin-protein ligase HUWE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	5	0
			3130	1992	545	578	15			
1	B	371	Total	C	N	O	S	0	9	0
			3142	1999	548	578	17			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3987	MET	-	EXPRESSION TAG	UNP Q7Z6Z7
A	3988	HIS	-	EXPRESSION TAG	UNP Q7Z6Z7
A	3989	HIS	-	EXPRESSION TAG	UNP Q7Z6Z7
A	3990	HIS	-	EXPRESSION TAG	UNP Q7Z6Z7
A	3991	HIS	-	EXPRESSION TAG	UNP Q7Z6Z7
A	3992	HIS	-	EXPRESSION TAG	UNP Q7Z6Z7
A	3993	HIS	-	EXPRESSION TAG	UNP Q7Z6Z7
A	3994	SER	-	EXPRESSION TAG	UNP Q7Z6Z7
A	3995	SER	-	EXPRESSION TAG	UNP Q7Z6Z7
A	3996	GLY	-	EXPRESSION TAG	UNP Q7Z6Z7
A	3997	ARG	-	EXPRESSION TAG	UNP Q7Z6Z7
A	3998	GLU	-	EXPRESSION TAG	UNP Q7Z6Z7
A	3999	ASN	-	EXPRESSION TAG	UNP Q7Z6Z7
A	4000	LEU	-	EXPRESSION TAG	UNP Q7Z6Z7
A	4001	TYR	-	EXPRESSION TAG	UNP Q7Z6Z7
A	4002	PHE	-	EXPRESSION TAG	UNP Q7Z6Z7
A	4003	GLN	-	EXPRESSION TAG	UNP Q7Z6Z7
A	4004	GLY	-	EXPRESSION TAG	UNP Q7Z6Z7
B	3987	MET	-	EXPRESSION TAG	UNP Q7Z6Z7
B	3988	HIS	-	EXPRESSION TAG	UNP Q7Z6Z7
B	3989	HIS	-	EXPRESSION TAG	UNP Q7Z6Z7
B	3990	HIS	-	EXPRESSION TAG	UNP Q7Z6Z7
B	3991	HIS	-	EXPRESSION TAG	UNP Q7Z6Z7
B	3992	HIS	-	EXPRESSION TAG	UNP Q7Z6Z7
B	3993	HIS	-	EXPRESSION TAG	UNP Q7Z6Z7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3994	SER	-	EXPRESSION TAG	UNP Q7Z6Z7
B	3995	SER	-	EXPRESSION TAG	UNP Q7Z6Z7
B	3996	GLY	-	EXPRESSION TAG	UNP Q7Z6Z7
B	3997	ARG	-	EXPRESSION TAG	UNP Q7Z6Z7
B	3998	GLU	-	EXPRESSION TAG	UNP Q7Z6Z7
B	3999	ASN	-	EXPRESSION TAG	UNP Q7Z6Z7
B	4000	LEU	-	EXPRESSION TAG	UNP Q7Z6Z7
B	4001	TYR	-	EXPRESSION TAG	UNP Q7Z6Z7
B	4002	PHE	-	EXPRESSION TAG	UNP Q7Z6Z7
B	4003	GLN	-	EXPRESSION TAG	UNP Q7Z6Z7
B	4004	GLY	-	EXPRESSION TAG	UNP Q7Z6Z7

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Na 1 1	0	0
2	A	1	Total Na 1 1	0	0

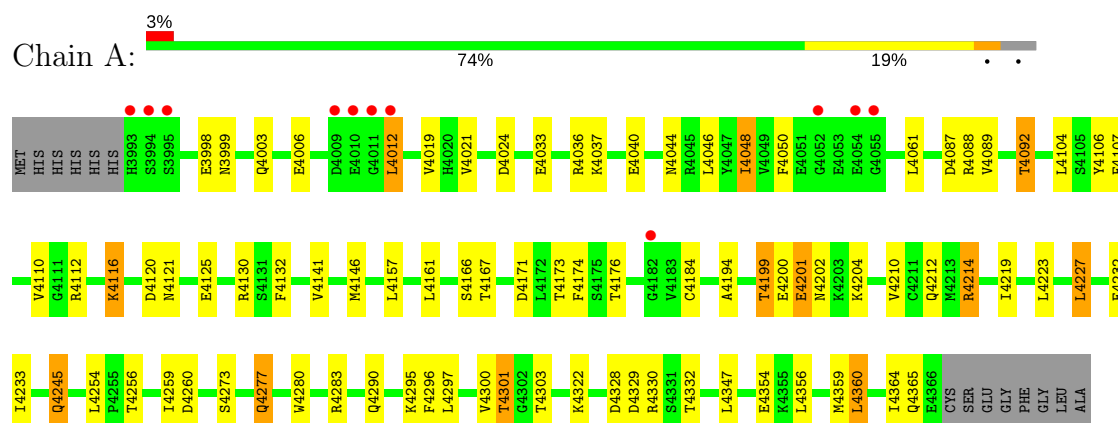
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	63	Total O 64 64	0	1
3	B	77	Total O 77 77	0	0

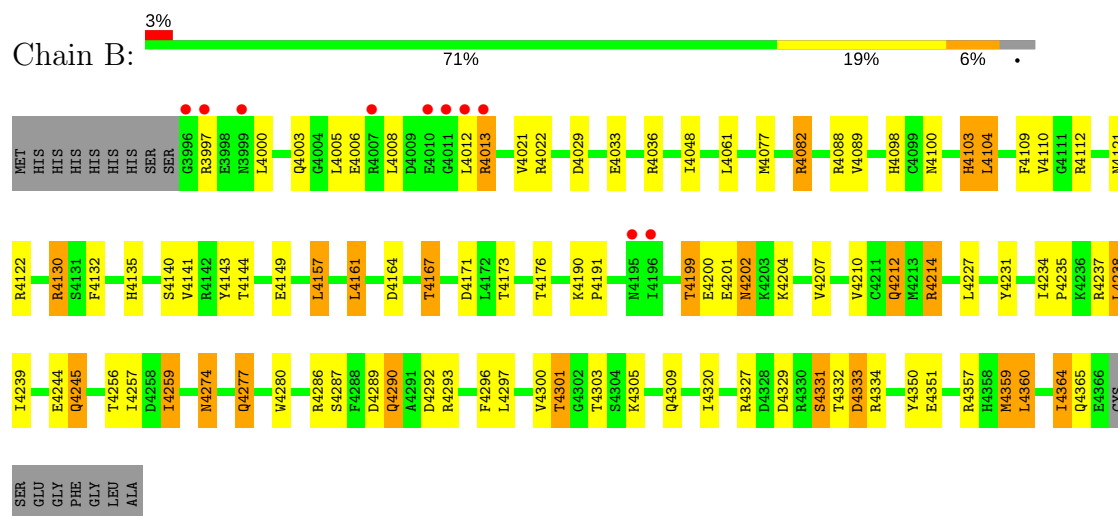
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: E3 ubiquitin-protein ligase HUWE1



#### • Molecule 1: E3 ubiquitin-protein ligase HUWE1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.53Å 72.21Å 77.24Å 90.00° 106.94° 90.00°	Depositor
Resolution (Å)	29.30 – 2.60 29.06 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.30-2.60) 98.9 (29.06-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0063	Depositor
R, $R_{free}$	0.214 , 0.279 0.228 , 0.282	Depositor DCC
$R_{free}$ test set	1443 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.9	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 36.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6415	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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:  
NA

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	0/3202	0.59	1/4317 (0.0%)
1	B	0.46	0/3213	0.60	0/4330
All	All	0.45	0/6415	0.59	1/8647 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4012	LEU	CA-CB-CG	5.20	127.26	115.30

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	3130	0	3042	54	0
1	B	3142	0	3057	57	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	64	0	0	4	0
3	B	77	0	0	4	0
All	All	6415	0	6099	106	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 (106) 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:4013[B]:ARG:HH11	1:B:4013[B]:ARG:CG	1.57	1.15
1:B:4013[B]:ARG:HG3	1:B:4013[B]:ARG:NH1	1.58	1.03
1:B:4013[B]:ARG:HH11	1:B:4013[B]:ARG:HG3	0.82	0.96
1:A:4199:THR:H	1:A:4202:ASN:HB2	1.33	0.94
1:A:4036[A]:ARG:HG3	3:A:5070:HOH:O	1.68	0.92
1:A:4141:VAL:H	1:A:4212:GLN:HE22	1.14	0.90
1:A:4245:GLN:HE21	1:A:4245:GLN:H	1.30	0.80
1:A:4199:THR:HB	1:A:4201:GLU:OE2	1.83	0.77
1:B:4274[A]:ASN:H	1:B:4274[A]:ASN:ND2	1.80	0.76
1:A:4048:ILE:HD11	1:A:4050:PHE:CE1	2.20	0.76
1:A:4141:VAL:N	1:A:4212:GLN:HE22	1.85	0.75
1:A:4116:LYS:HE2	1:A:4120:ASP:OD2	1.87	0.74
1:A:4141:VAL:H	1:A:4212:GLN:NE2	1.85	0.73
1:A:4260:ASP:HB3	1:B:4122:ARG:HD2	1.70	0.73
1:B:4199:THR:H	1:B:4202:ASN:HD21	1.37	0.71
1:B:4021:VAL:HG22	1:B:4048[A]:ILE:HD11	1.73	0.71
1:A:4040:GLU:HG2	3:A:5122:HOH:O	1.91	0.70
1:B:4199:THR:H	1:B:4202:ASN:ND2	1.90	0.69
1:A:4245:GLN:NE2	1:A:4245:GLN:H	1.91	0.68
1:A:4112:ARG:NH2	1:A:4232:GLU:OE1	2.28	0.66
1:B:4332:THR:HG21	1:B:4351:GLU:OE2	1.95	0.66
1:A:4037:LYS:O	1:A:4112:ARG:NH1	2.30	0.65
1:A:4044:ASN:O	1:A:4116:LYS:NZ	2.30	0.64
1:A:4360:LEU:O	1:A:4364:ILE:HG12	1.98	0.63
1:A:4354[A]:GLU:H	1:A:4354[A]:GLU:CD	2.01	0.62
1:B:4013[B]:ARG:NH1	1:B:4013[B]:ARG:CG	2.29	0.62
1:B:4121:ASN:HA	3:B:5031:HOH:O	2.00	0.61
1:A:4141:VAL:HG22	1:A:4212:GLN:NE2	2.16	0.61
1:A:4201:GLU:H	1:A:4201:GLU:CD	2.06	0.59
1:B:4141:VAL:H	1:B:4212:GLN:HE22	1.48	0.59
1:A:4297:LEU:O	1:A:4301:THR:HB	2.02	0.59
1:B:4364:ILE:HG22	1:B:4365:GLN:NE2	2.19	0.58
1:B:4289:ASP:HB2	1:B:4292:ASP:H	1.70	0.57
1:A:4121:ASN:HB2	1:B:4259:ILE:HG12	1.86	0.56
1:A:4283:ARG:HD2	1:B:4006:GLU:HG2	1.87	0.56
1:B:4130:ARG:HD3	1:B:4244:GLU:HG3	1.87	0.55
1:A:4019:VAL:HA	1:A:4033:GLU:HG2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4296:PHE:HA	1:A:4364:ILE:HD12	1.88	0.55
1:B:4082:ARG:HD3	3:B:5011:HOH:O	2.06	0.55
1:B:4164:ASP:O	1:B:4167:THR:HB	2.08	0.54
1:A:4301:THR:HG22	1:A:4303:THR:H	1.73	0.53
1:B:4297:LEU:O	1:B:4301:THR:HG22	2.09	0.53
1:A:4199:THR:HG22	1:A:4200:GLU:H	1.75	0.52
1:B:4327:ARG:HD2	1:B:4329:ASP:OD2	2.10	0.51
1:A:4173:THR:CG2	1:A:4194:ALA:HA	2.41	0.51
1:B:4021:VAL:CG2	1:B:4048[A]:ILE:HD11	2.38	0.51
1:B:4257:ILE:HD13	1:B:4293:ARG:HB3	1.91	0.51
1:B:4104:LEU:HB2	3:B:5093:HOH:O	2.11	0.51
1:A:4295:LYS:HB3	1:A:4364:ILE:HG22	1.94	0.50
1:A:4322:LYS:HE3	3:A:5105:HOH:O	2.12	0.49
1:A:4107:PHE:HA	1:A:4110:VAL:HG12	1.95	0.49
1:B:4202:ASN:HD22	1:B:4202:ASN:C	2.15	0.49
1:A:4087:ASP:O	1:A:4089:VAL:N	2.45	0.49
1:A:4173:THR:HG21	1:A:4194:ALA:HA	1.96	0.48
1:B:4190:LYS:HB2	1:B:4191:PRO:HD2	1.96	0.47
1:A:4290:GLN:NE2	1:B:4290:GLN:HG2	2.30	0.47
1:B:4089:VAL:CG1	1:B:4305:LYS:HD3	2.44	0.47
1:B:4274[A]:ASN:N	1:B:4274[A]:ASN:ND2	2.55	0.47
1:B:4287:SER:OG	1:B:4357:ARG:NH2	2.47	0.47
1:A:4223:LEU:HG	1:A:4227:LEU:HD22	1.95	0.46
1:A:4360:LEU:HD22	1:A:4364:ILE:HD11	1.96	0.46
1:B:4143:TYR:HB2	1:B:4157:LEU:HD23	1.98	0.46
1:B:4022:ARG:HD3	1:B:4029:ASP:OD2	2.15	0.45
1:A:4112:ARG:HD2	1:A:4233:ILE:CD1	2.47	0.45
1:B:4088:ARG:HA	1:B:4088:ARG:CZ	2.47	0.45
1:B:4296:PHE:HA	1:B:4364:ILE:CG1	2.48	0.44
1:A:4328:ASP:OD2	1:A:4329:ASP:N	2.51	0.44
1:B:4234:ILE:HG21	1:B:4239:ILE:HD13	1.98	0.44
1:A:4256:THR:HG23	3:A:5102:HOH:O	2.18	0.44
1:B:4301:THR:HG23	1:B:4303:THR:H	1.82	0.44
1:A:4210:VAL:O	1:A:4214:ARG:HB2	2.17	0.44
1:B:4277:GLN:HA	1:B:4280:TRP:HB2	1.99	0.44
1:A:4106:TYR:O	1:A:4110:VAL:HG12	2.18	0.44
1:A:4219[A]:ILE:HG22	1:A:4223:LEU:HB2	2.01	0.43
1:B:4109:PHE:O	1:B:4112:ARG:HB3	2.19	0.43
1:B:4296:PHE:HD1	1:B:4364:ILE:HD11	1.83	0.43
1:A:4328:ASP:O	1:A:4329:ASP:HB2	2.19	0.43
1:B:4161:LEU:HD13	1:B:4207:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4210:VAL:O	1:B:4214:ARG:HB2	2.18	0.42
1:A:4347:LEU:HD21	1:A:4356:LEU:HD11	2.00	0.42
1:B:4231:TYR:HA	1:B:4234:ILE:O	2.19	0.42
1:A:4260:ASP:CB	1:B:4122:ARG:HD2	2.45	0.42
1:A:4087:ASP:C	1:A:4089:VAL:H	2.23	0.42
1:B:4350:TYR:OH	1:B:4359:MET:HG2	2.20	0.42
1:A:4245:GLN:HE21	1:A:4245:GLN:N	2.09	0.42
1:A:4295:LYS:HB3	1:A:4364:ILE:CG2	2.50	0.41
1:B:4021:VAL:HG22	1:B:4048[A]:ILE:CD1	2.48	0.41
1:A:4173:THR:CG2	1:A:4174:PHE:N	2.83	0.41
1:A:4171:ASP:N	1:A:4171:ASP:OD2	2.54	0.41
1:B:4103:HIS:CE1	1:B:4104:LEU:HD13	2.56	0.41
1:B:4235:PRO:HG2	1:B:4238:LEU:HD22	2.02	0.41
1:A:4277:GLN:HA	1:A:4280:TRP:HB2	2.02	0.41
1:A:4254:LEU:HD13	1:A:4290:GLN:HE21	1.85	0.41
1:B:4132:PHE:HA	1:B:4135:HIS:CD2	2.55	0.41
1:B:4333:ASP:HB2	3:B:5140:HOH:O	2.19	0.41
1:B:4360:LEU:HD22	1:B:4364:ILE:HD13	2.03	0.41
1:A:4199:THR:H	1:A:4202:ASN:CB	2.17	0.41
1:B:4000:LEU:HA	1:B:4003:GLN:HE21	1.86	0.41
1:B:4149:GLU:OE1	1:B:4149:GLU:HA	2.21	0.41
1:B:4331:SER:O	1:B:4334:ARG:HG2	2.21	0.41
1:B:4245:GLN:H	1:B:4245:GLN:NE2	2.19	0.40
1:A:4092:THR:HG23	1:A:4132:PHE:HB2	2.03	0.40
1:A:4199:THR:N	1:A:4202:ASN:HB2	2.16	0.40
1:B:4098:HIS:C	1:B:4100:ASN:N	2.74	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	377/388 (97%)	361 (96%)	15 (4%)	1 (0%)	44	70
1	B	378/388 (97%)	357 (94%)	21 (6%)	0	100	100
All	All	755/776 (97%)	718 (95%)	36 (5%)	1 (0%)	55	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4088	ARG

### 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	338/347 (97%)	300 (89%)	38 (11%)	7	12
1	B	339/347 (98%)	287 (85%)	52 (15%)	3	5
All	All	677/694 (98%)	587 (87%)	90 (13%)	5	8

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3998	GLU
1	A	3999	ASN
1	A	4003	GLN
1	A	4006	GLU
1	A	4012	LEU
1	A	4021	VAL
1	A	4024	ASP
1	A	4046	LEU
1	A	4048	ILE
1	A	4061	LEU
1	A	4092	THR
1	A	4104	LEU
1	A	4116	LYS
1	A	4125	GLU
1	A	4130	ARG

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Mol	Chain	Res	Type
1	A	4146	MET
1	A	4157	LEU
1	A	4161	LEU
1	A	4166	SER
1	A	4167	THR
1	A	4176	THR
1	A	4184	CYS
1	A	4199	THR
1	A	4201	GLU
1	A	4204	LYS
1	A	4214	ARG
1	A	4227	LEU
1	A	4245	GLN
1	A	4259	ILE
1	A	4273	SER
1	A	4277	GLN
1	A	4300	VAL
1	A	4301	THR
1	A	4330	ARG
1	A	4332	THR
1	A	4359	MET
1	A	4360	LEU
1	A	4365	GLN
1	B	3997	ARG
1	B	4005	LEU
1	B	4008	LEU
1	B	4012	LEU
1	B	4013[A]	ARG
1	B	4013[B]	ARG
1	B	4033	GLU
1	B	4036[A]	ARG
1	B	4036[B]	ARG
1	B	4061	LEU
1	B	4077[A]	MET
1	B	4077[B]	MET
1	B	4082	ARG
1	B	4103	HIS
1	B	4104	LEU
1	B	4110	VAL
1	B	4130	ARG
1	B	4140	SER
1	B	4144	THR

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Mol	Chain	Res	Type
1	B	4157	LEU
1	B	4161	LEU
1	B	4167	THR
1	B	4171	ASP
1	B	4173	THR
1	B	4176	THR
1	B	4199	THR
1	B	4200	GLU
1	B	4201	GLU
1	B	4202	ASN
1	B	4204	LYS
1	B	4212	GLN
1	B	4214	ARG
1	B	4227	LEU
1	B	4237	ARG
1	B	4238	LEU
1	B	4245	GLN
1	B	4256	THR
1	B	4259	ILE
1	B	4274[A]	ASN
1	B	4274[B]	ASN
1	B	4277	GLN
1	B	4286	ARG
1	B	4290	GLN
1	B	4300	VAL
1	B	4301	THR
1	B	4309	GLN
1	B	4320	ILE
1	B	4331	SER
1	B	4333	ASP
1	B	4359	MET
1	B	4360	LEU
1	B	4364	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4098	HIS
1	A	4102	ASN
1	A	4103	HIS
1	A	4121	ASN
1	A	4212	GLN

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Mol	Chain	Res	Type
1	A	4245	GLN
1	A	4290	GLN
1	A	4358	HIS
1	B	4003	GLN
1	B	4121	ASN
1	B	4155	GLN
1	B	4179	GLN
1	B	4202	ASN
1	B	4212	GLN
1	B	4245	GLN
1	B	4290	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 ⓘ

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 ⓘ

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 [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	374/388 (96%)	-0.11	11 (2%) 52 45	20, 34, 52, 67	0
1	B	371/388 (95%)	-0.14	10 (2%) 55 48	22, 34, 52, 62	0
All	All	745/776 (96%)	-0.12	21 (2%) 53 46	20, 34, 52, 67	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4011	GLY	6.6
1	A	3993	HIS	4.3
1	B	4012	LEU	3.9
1	A	4011	GLY	3.2
1	A	3994	SER	3.1
1	A	3995	SER	3.1
1	A	4055	GLY	3.0
1	A	4052	GLY	3.0
1	A	4054	GLU	2.7
1	B	4013[A]	ARG	2.7
1	A	4010	GLU	2.7
1	B	3996	GLY	2.6
1	B	4010	GLU	2.6
1	A	4012	LEU	2.5
1	B	3997	ARG	2.4
1	B	4195	ASN	2.3
1	B	3999	ASN	2.2
1	A	4182	GLY	2.2
1	B	4196	ILE	2.2
1	A	4009	ASP	2.0
1	B	4007	ARG	2.0



## 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NA	A	5001	1/1	0.96	0.18	1.08	27,27,27,27	0
2	NA	B	5002	1/1	0.85	0.16	0.34	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.