



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2024 – 10:51 AM JST

PDB ID : 5XWM  
Title : human ERp44 zinc-bound form  
Authors : Watanabe, S.; Harayama, M.; Inaba, K.  
Deposited on : 2017-06-30  
Resolution : 2.45 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 : 2.36  
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) : 2.36

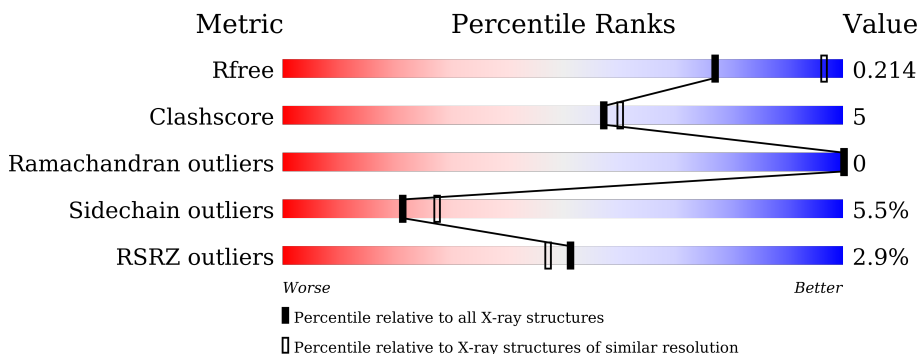
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	383	 2% 74% 15% • 10%
1	B	383	 2% 79% 13% • 8%
1	C	383	 2% 79% 10% • 9%
1	D	383	 4% 82% 13% • •

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 11949 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 Endoplasmic reticulum resident protein 44.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	346	2757	1749	469	524	15	0	1	0
1	B	354	2875	1825	491	545	14	0	0	0
1	C	348	2823	1795	480	534	14	0	0	0
1	D	368	2949	1869	505	561	14	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q9BS26
A	-4	SER	-	expression tag	UNP Q9BS26
A	-3	HIS	-	expression tag	UNP Q9BS26
A	-2	MET	-	expression tag	UNP Q9BS26
A	-1	ALA	-	expression tag	UNP Q9BS26
A	0	SER	-	expression tag	UNP Q9BS26
B	-5	GLY	-	expression tag	UNP Q9BS26
B	-4	SER	-	expression tag	UNP Q9BS26
B	-3	HIS	-	expression tag	UNP Q9BS26
B	-2	MET	-	expression tag	UNP Q9BS26
B	-1	ALA	-	expression tag	UNP Q9BS26
B	0	SER	-	expression tag	UNP Q9BS26
C	-5	GLY	-	expression tag	UNP Q9BS26
C	-4	SER	-	expression tag	UNP Q9BS26
C	-3	HIS	-	expression tag	UNP Q9BS26
C	-2	MET	-	expression tag	UNP Q9BS26
C	-1	ALA	-	expression tag	UNP Q9BS26
C	0	SER	-	expression tag	UNP Q9BS26
D	-5	GLY	-	expression tag	UNP Q9BS26
D	-4	SER	-	expression tag	UNP Q9BS26
D	-3	HIS	-	expression tag	UNP Q9BS26

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	MET	-	expression tag	UNP Q9BS26
D	-1	ALA	-	expression tag	UNP Q9BS26
D	0	SER	-	expression tag	UNP Q9BS26

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	Zn 3	0	0
2	B	3	Total 3	Zn 3	0	0
2	C	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Cl 2	0	0
3	B	2	Total 2	Cl 2	0	0
3	C	2	Total 2	Cl 2	0	0
3	D	2	Total 2	Cl 2	0	0

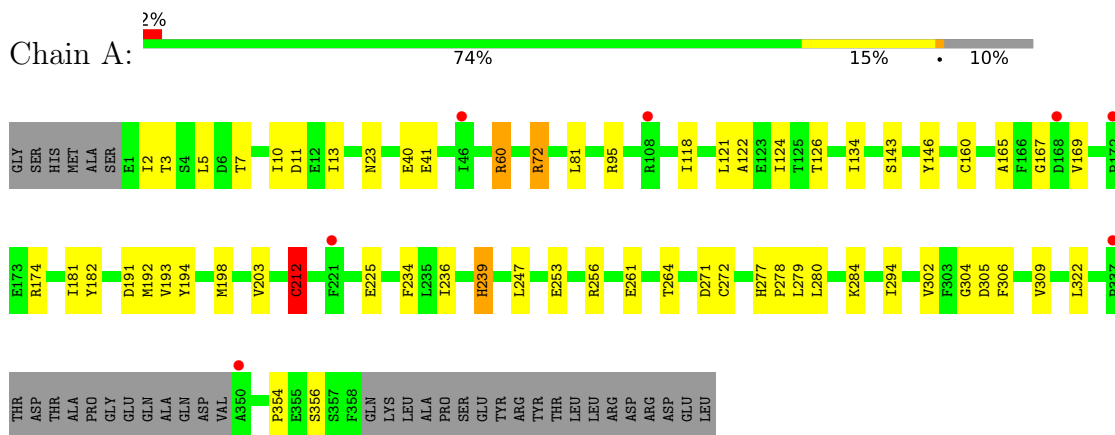
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total 42	O 42	0	0
4	B	152	Total 152	O 152	0	0
4	C	155	Total 155	O 155	0	0
4	D	178	Total 178	O 178	0	0

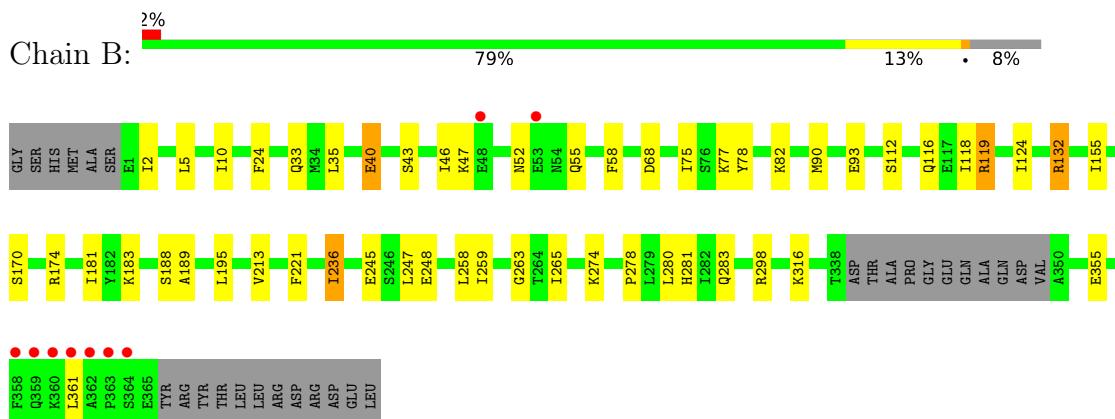
### 3 Residue-property plots [i](#)

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.

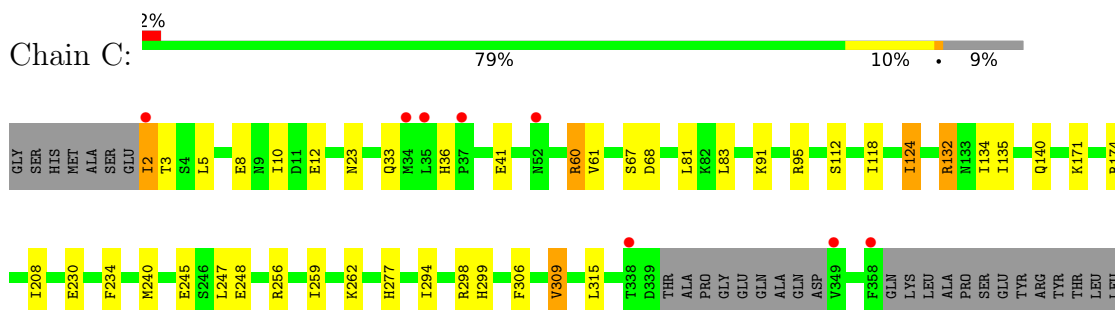
- Molecule 1: Endoplasmic reticulum resident protein 44



- Molecule 1: Endoplasmic reticulum resident protein 44



- Molecule 1: Endoplasmic reticulum resident protein 44



ARG  
ASP  
ARG  
ASP  
GLU  
LEU

- Molecule 1: Endoplasmic reticulum resident protein 44

Chain D: 4% 82% 13%

GLY  
SER  
HIS  
MET  
ALA  
S0  
L5  
D6  
T7  
I10  
D11  
E12  
R30  
L35  
F39  
K47  
N52  
Q85  
D68  
Q71  
F84  
M88  
M89  
R92  
E93  
Y94  
R95  
R98  
K101  
R119  
R129  
R132  
M135  
I134  
Y137  
F138  
F166  
E173

Y182  
L195  
V213  
F234  
E242  
L258  
I259  
S260  
E261  
I265  
H277  
P278  
H281  
I294  
D295  
S296  
F297  
V302  
V309  
L315  
H323  
H333  
T338  
D339  
T340  
A341  
P342  
G343  
E344  
Q345  
ALA  
GLN  
ASP  
V349  
A350  
S351  
P354  
F358  
GLN  
LYS  
LEU  
ALA  
PRO

SER  
GLU  
Y366  
R367  
Y368  
T369  
L370  
L371  
R372  
D375  
E376  
L377

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	175.15Å 175.15Å 407.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.06 – 2.45 44.06 – 2.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.06-2.45) 100.0 (44.06-2.45)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.59 (at 2.45Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.182 , 0.214 0.182 , 0.214	Depositor DCC
$R_{free}$ test set	6621 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.9	Xtrriage
Anisotropy	0.009	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 54.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.20$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11949	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.90% 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, CL

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	0.39	1/2824 (0.0%)	0.53	0/3833
1	B	0.43	0/2945	0.59	0/3984
1	C	0.45	0/2892	0.59	0/3915
1	D	0.43	0/3018	0.62	0/4087
All	All	0.43	1/11679 (0.0%)	0.58	0/15819

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	CYS	CB-SG	-6.46	1.71	1.82

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	2757	0	2587	33	0
1	B	2875	0	2761	28	0
1	C	2823	0	2703	24	0
1	D	2949	0	2798	31	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	2	0	0	1	0
3	B	2	0	0	2	0
3	C	2	0	0	1	0
3	D	2	0	0	2	0
4	A	42	0	0	0	0
4	B	152	0	0	1	0
4	C	155	0	0	0	0
4	D	178	0	0	4	0
All	All	11949	0	10849	109	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 5.

All (109) 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:52:ASN:HB2	1:B:55:GLN:HG3	1.69	0.76
1:A:253:GLU:HG2	1:A:309:VAL:HG12	1.69	0.75
1:A:118:ILE:HD11	1:A:165:ALA:HB2	1.72	0.71
1:A:306:PHE:O	1:A:309:VAL:HG23	1.92	0.69
1:D:281:HIS:HD1	1:D:366:TYR:HA	1.59	0.66
1:C:2:ILE:HD11	1:C:60:ARG:HD2	1.78	0.66
1:B:278:PRO:HG3	1:D:372:ARG:HG2	1.77	0.65
1:D:369:THR:O	1:D:369:THR:OG1	2.15	0.64
1:C:33:GLN:HA	1:C:36:HIS:HD2	1.62	0.64
1:B:90:MET:HE1	1:B:155:ILE:HA	1.80	0.63
1:D:261:GLU:HG2	4:D:529:HOH:O	1.99	0.62
1:A:122:ALA:O	1:A:126:THR:HG22	2.00	0.61
1:D:88:MET:SD	4:D:676:HOH:O	2.57	0.60
1:A:294:ILE:HG21	1:A:322:LEU:HD22	1.84	0.58
1:B:2:ILE:HG13	1:B:40:GLU:HG2	1.86	0.58
1:B:78:TYR:O	1:D:333:HIS:HE1	1.87	0.58
1:D:242:GLU:H	1:D:242:GLU:CD	2.07	0.58
1:A:121:LEU:O	1:A:124:ILE:HG12	2.03	0.57
3:B:405:CL:CL	3:D:404:CL:CL	2.96	0.57
1:C:306:PHE:O	1:C:309:VAL:HG22	2.04	0.56
1:B:132:ARG:NH2	1:C:248:GLU:OE1	2.36	0.56
1:C:118:ILE:HD13	1:C:124:ILE:HD11	1.88	0.56
1:A:181:ILE:HD11	1:A:191:ASP:OD2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ASN:HA	1:A:81:LEU:HD23	1.87	0.55
1:A:277:HIS:HE2	1:C:277:HIS:CD2	2.14	0.54
1:D:134:ILE:HD13	1:D:182:TYR:HA	1.90	0.54
1:B:5:LEU:HD13	1:B:10:ILE:HG13	1.91	0.53
1:B:283:GLN:HG2	1:B:361:LEU:CB	2.38	0.53
1:B:258:LEU:HD21	1:B:316:LYS:HA	1.91	0.52
1:B:82:LYS:HD3	1:B:93:GLU:HB2	1.90	0.52
1:D:5:LEU:HD13	1:D:10:ILE:HG13	1.90	0.52
1:A:2:ILE:HG22	1:A:60:ARG:HG2	1.93	0.50
1:A:354:PRO:O	1:C:95:ARG:NH1	2.37	0.49
1:D:265:ILE:HD11	1:D:323:HIS:CE1	2.48	0.49
1:C:2:ILE:O	1:C:2:ILE:HG13	2.12	0.49
1:D:35:LEU:HD22	1:D:39:PHE:HB2	1.93	0.49
3:A:405:CL:CL	3:C:404:CL:CL	3.04	0.49
1:D:84:PHE:CE2	1:D:89:MET:HB2	2.48	0.49
1:B:118:ILE:HD13	1:B:124:ILE:HD11	1.95	0.49
1:D:234:PHE:HB2	1:D:295:ASP:HB3	1.95	0.49
1:B:77:LYS:HD2	1:D:354:PRO:HB2	1.95	0.48
1:A:160:CYS:HB2	1:A:212:CYS:SG	2.52	0.48
1:A:277:HIS:NE2	1:C:277:HIS:CD2	2.80	0.48
1:C:259:ILE:O	1:C:262:LYS:HB2	2.14	0.48
1:D:281:HIS:ND1	1:D:366:TYR:HA	2.27	0.48
1:B:259:ILE:HD12	1:B:259:ILE:HA	1.79	0.48
1:C:5:LEU:HB2	1:C:61:VAL:HG22	1.96	0.48
1:A:277:HIS:O	1:A:280:LEU:HB3	2.13	0.47
1:A:272:CYS:HB2	1:A:279:LEU:HD11	1.95	0.47
1:C:171:LYS:HA	1:C:174:ARG:NH1	2.30	0.47
1:B:248:GLU:OE1	1:C:132:ARG:NH2	2.48	0.47
3:B:404:CL:CL	3:D:403:CL:CL	3.08	0.46
1:A:302:VAL:HG12	1:A:304:GLY:H	1.81	0.46
1:B:281:HIS:HD1	1:D:370:LEU:H	1.62	0.46
1:C:134:ILE:HD13	1:C:208:ILE:HG23	1.98	0.46
1:C:5:LEU:HD13	1:C:10:ILE:HG13	1.98	0.46
1:C:298:ARG:HG2	1:C:299:HIS:CD2	2.51	0.46
1:A:239:HIS:HE1	1:A:247:LEU:HD22	1.81	0.46
1:B:170:SER:OG	1:B:174:ARG:HD3	2.16	0.46
1:D:129:ARG:HA	1:D:129:ARG:HD2	1.74	0.46
1:A:121:LEU:HD12	1:A:121:LEU:H	1.80	0.45
1:A:11:ASP:OD1	1:A:72:ARG:NH2	2.49	0.45
1:A:284:LYS:HD3	1:A:284:LYS:HA	1.81	0.45
1:A:277:HIS:HD2	1:A:280:LEU:HD23	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ASN:HA	1:C:81:LEU:HD23	1.97	0.45
1:B:188:SER:OG	1:B:189:ALA:N	2.50	0.45
1:D:281:HIS:HD1	1:D:366:TYR:CA	2.25	0.45
1:B:119:ARG:HA	1:B:119:ARG:HD2	1.75	0.45
1:B:118:ILE:CD1	1:B:124:ILE:HD11	2.47	0.45
1:B:24:PHE:CD2	1:B:75:ILE:HG13	2.52	0.45
1:D:349:VAL:N	4:D:507:HOH:O	2.50	0.45
1:A:121:LEU:HD11	1:A:169:VAL:O	2.17	0.45
1:C:68:ASP:OD1	1:C:68:ASP:N	2.50	0.45
1:A:194:TYR:OH	1:A:203:VAL:HG12	2.17	0.44
1:C:91:LYS:HB3	1:C:230:GLU:HG2	1.98	0.44
1:A:198:MET:HE3	1:A:198:MET:HB3	1.90	0.44
1:D:259:ILE:HD13	1:D:259:ILE:HA	1.76	0.44
1:A:3:THR:HG21	1:A:13:ILE:HD13	2.00	0.44
1:A:143:SER:HB2	1:A:146:TYR:H	1.82	0.43
1:D:68:ASP:N	1:D:68:ASP:OD1	2.51	0.43
1:A:277:HIS:HB3	1:A:278:PRO:HD3	2.00	0.43
1:B:47:LYS:HA	1:B:47:LYS:HD2	1.83	0.43
1:D:234:PHE:O	1:D:294:ILE:HA	2.19	0.43
1:A:167:GLY:O	1:A:174:ARG:NH2	2.50	0.43
1:B:68:ASP:OD1	1:B:68:ASP:N	2.52	0.42
1:A:261:GLU:OE1	1:A:264:THR:OG1	2.35	0.42
1:D:138:PHE:O	1:D:166:PHE:HA	2.19	0.42
1:C:315:LEU:HD12	1:C:315:LEU:HA	1.80	0.42
1:D:137:TYR:CE2	1:D:173:GLU:HG3	2.54	0.42
1:C:83:LEU:HD12	1:C:83:LEU:HA	1.87	0.42
1:D:333:HIS:CD2	1:D:333:HIS:H	2.37	0.42
1:D:258:LEU:HD11	1:D:315:LEU:HG	2.00	0.42
1:A:5:LEU:HD13	1:A:10:ILE:HD12	2.01	0.42
1:B:236:ILE:HD13	1:B:236:ILE:HG21	1.80	0.41
1:A:134:ILE:HG12	1:A:182:TYR:HD1	1.86	0.41
1:A:234:PHE:O	1:A:294:ILE:HA	2.20	0.41
1:B:43:SER:HB3	1:B:58:PHE:CD2	2.55	0.41
1:B:263:GLY:N	4:B:501:HOH:O	2.15	0.41
1:D:52:ASN:HB2	1:D:55:GLN:HG2	2.02	0.41
1:D:92:ARG:HD2	4:D:665:HOH:O	2.19	0.41
1:C:124:ILE:HG12	1:C:135:ILE:HD13	2.03	0.41
1:D:296:SER:O	1:D:297:PHE:HB2	2.20	0.41
1:B:181:ILE:HD12	1:B:181:ILE:HG23	1.83	0.41
1:C:36:HIS:CE1	1:C:60:ARG:HH21	2.39	0.41
1:A:253:GLU:OE2	1:A:256:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ARG:O	1:D:369:THR:HG21	2.20	0.41
1:B:221:PHE:HZ	1:B:274:LYS:O	2.04	0.40
1:C:234:PHE:O	1:C:294:ILE:HA	2.22	0.40
1:D:277:HIS:HB3	1:D:278:PRO:HD3	2.02	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	343/383 (90%)	332 (97%)	11 (3%)	0	100	100
1	B	350/383 (91%)	344 (98%)	6 (2%)	0	100	100
1	C	344/383 (90%)	338 (98%)	6 (2%)	0	100	100
1	D	362/383 (94%)	350 (97%)	12 (3%)	0	100	100
All	All	1399/1532 (91%)	1364 (98%)	35 (2%)	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	296/344 (86%)	281 (95%)	15 (5%)	24	31
1	B	316/344 (92%)	299 (95%)	17 (5%)	22	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	310/344 (90%)	294 (95%)	16 (5%)	23	30
1	D	318/344 (92%)	298 (94%)	20 (6%)	18	22
All	All	1240/1376 (90%)	1172 (94%)	68 (6%)	21	27

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	40	GLU
1	A	41	GLU
1	A	60	ARG
1	A	72	ARG
1	A	95	ARG
1	A	192	MET
1	A	193	VAL
1	A	212	CYS
1	A	225	GLU
1	A	236	ILE
1	A	239	HIS
1	A	271	ASP
1	A	305	ASP
1	A	356	SER
1	B	33	GLN
1	B	35	LEU
1	B	40	GLU
1	B	46	ILE
1	B	112	SER
1	B	116	GLN
1	B	119	ARG
1	B	132	ARG
1	B	183	LYS
1	B	195	LEU
1	B	213	VAL
1	B	236	ILE
1	B	245	GLU
1	B	247	LEU
1	B	265	ILE
1	B	280	LEU
1	B	355	GLU
1	C	2	ILE
1	C	3	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	8	GLU
1	C	12	GLU
1	C	41	GLU
1	C	60	ARG
1	C	67	SER
1	C	112	SER
1	C	124	ILE
1	C	132	ARG
1	C	140	GLN
1	C	240	MET
1	C	245	GLU
1	C	247	LEU
1	C	256	ARG
1	C	309	VAL
1	D	7	THR
1	D	12	GLU
1	D	30	ARG
1	D	35	LEU
1	D	47	LYS
1	D	55	GLN
1	D	71	GLN
1	D	93	GLU
1	D	95	ARG
1	D	98	ARG
1	D	101	LYS
1	D	119	ARG
1	D	132	ARG
1	D	195	LEU
1	D	213	VAL
1	D	259	ILE
1	D	302	VAL
1	D	309	VAL
1	D	369	THR
1	D	372	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	97	GLN
1	B	97	GLN
1	C	36	HIS
1	C	97	GLN

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Mol	Chain	Res	Type
1	D	33	GLN

### 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 18 ligands modelled in this entry, 18 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

### 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	346/383 (90%)	-0.08	7 (2%) 65 62	43, 74, 108, 135	0
1	B	354/383 (92%)	-0.26	9 (2%) 57 53	27, 52, 104, 192	0
1	C	348/383 (90%)	-0.30	8 (2%) 60 56	25, 51, 105, 134	0
1	D	368/383 (96%)	-0.20	17 (4%) 32 30	25, 50, 119, 169	0
All	All	1416/1532 (92%)	-0.21	41 (2%) 51 47	25, 57, 109, 192	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	377	LEU	7.3
1	D	343	GLY	6.6
1	B	361	LEU	6.3
1	D	368	TYR	5.2
1	B	362	ALA	4.9
1	D	342	PRO	4.7
1	B	359	GLN	4.6
1	D	351	SER	4.4
1	D	375	ASP	4.3
1	D	370	LEU	4.1
1	D	350	ALA	4.0
1	A	168	ASP	3.8
1	B	360	LYS	3.8
1	D	0	SER	3.6
1	A	350	ALA	3.5
1	D	349	VAL	3.2
1	A	337	PRO	3.1
1	C	349	VAL	3.0
1	A	221	PHE	2.9
1	C	358	PHE	2.8
1	A	46	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	371	LEU	2.8
1	D	338	THR	2.7
1	C	34	MET	2.7
1	D	341	ALA	2.6
1	B	53	GLU	2.6
1	D	369	THR	2.6
1	C	52	ASN	2.6
1	B	363	PRO	2.5
1	D	372	ARG	2.5
1	A	108	ARG	2.5
1	B	358	PHE	2.5
1	A	172	PRO	2.4
1	B	48	GLU	2.4
1	D	339	ASP	2.4
1	C	338	THR	2.4
1	C	2	ILE	2.3
1	D	344	GLU	2.3
1	B	364	SER	2.2
1	C	37	PRO	2.2
1	C	35	LEU	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
2	ZN	B	401	1/1	0.96	0.12	72,72,72,72	0
3	CL	B	404	1/1	0.97	0.12	57,57,57,57	0
3	CL	B	405	1/1	0.97	0.08	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	D	403	1/1	0.97	0.16	53,53,53,53	0
3	CL	D	404	1/1	0.98	0.06	62,62,62,62	0
2	ZN	C	402	1/1	0.99	0.14	65,65,65,65	0
2	ZN	D	401	1/1	0.99	0.21	46,46,46,46	0
2	ZN	D	402	1/1	0.99	0.17	45,45,45,45	0
3	CL	A	404	1/1	0.99	0.13	58,58,58,58	0
3	CL	A	405	1/1	0.99	0.06	75,75,75,75	0
2	ZN	A	403	1/1	0.99	0.16	53,53,53,53	0
2	ZN	B	402	1/1	0.99	0.19	43,43,43,43	0
3	CL	C	403	1/1	0.99	0.15	60,60,60,60	0
3	CL	C	404	1/1	0.99	0.09	78,78,78,78	0
2	ZN	B	403	1/1	0.99	0.13	48,48,48,48	0
2	ZN	C	401	1/1	0.99	0.21	50,50,50,50	0
2	ZN	A	401	1/1	1.00	0.20	50,50,50,50	0
2	ZN	A	402	1/1	1.00	0.07	80,80,80,80	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.