



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2025 – 08:10 PM JST

PDB ID : 9JR1 / pdb\_00009jr1  
Title : Crystal structure of CtpA from Helicobacter pylori  
Authors : Sun, K.; Au, S.W.N.  
Deposited on : 2024-09-29  
Resolution : 3.40 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

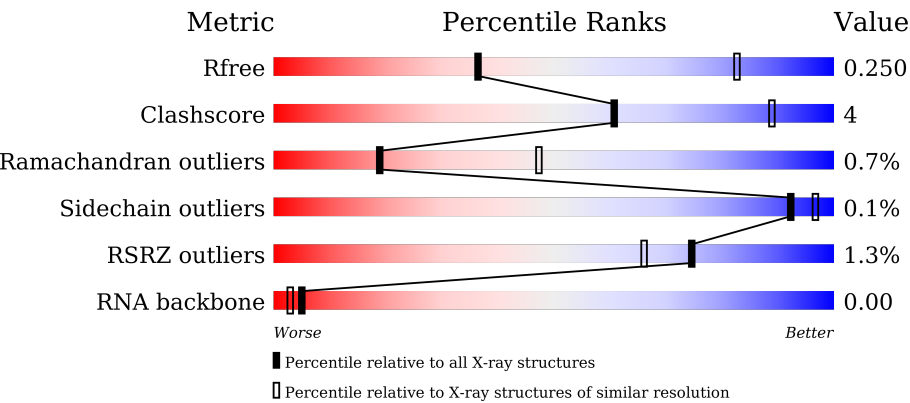
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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.












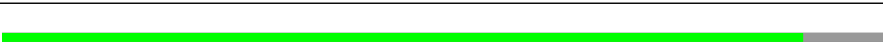
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	164625	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)
RNA backbone	3690	1033 (3.80-3.00)

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 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	416	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>75%12%13%</div></div>
1	B	416	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>79%8%13%</div></div>
1	C	416	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>81%10%9%</div></div>
1	D	416	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>78%8%13%</div></div>

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Mol	Chain	Length	Quality of chain
1	E	416	 % 80% 8% 11%
1	F	416	 % 74% 8% 17%
2	G	21	 48% 52%
2	H	21	 19% 81%
2	I	21	 81% 19%
2	J	21	 10% 5% 86%
2	K	21	 14% 86%
2	L	21	 14% 86%
2	N	21	 10% 90%
2	O	21	 5% 5% 90%
2	S	21	 52% 48%
2	T	21	 90% 10%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17123 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 Carboxyl-terminal protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	4	0	0
			2773	1768	471	526	8			
1	B	362	Total	C	N	O	S	0	0	0
			2781	1775	470	528	8			
1	C	380	Total	C	N	O	S	0	0	0
			2934	1870	497	559	8			
1	D	360	Total	C	N	O	S	0	0	0
			2765	1765	467	525	8			
1	F	344	Total	C	N	O	S	0	0	0
			2628	1680	445	496	7			
1	E	370	Total	C	N	O	S	0	0	0
			2849	1819	484	538	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	MET	-	initiating methionine	UNP B5Z8Z7
A	40	HIS	-	expression tag	UNP B5Z8Z7
A	41	HIS	-	expression tag	UNP B5Z8Z7
A	42	HIS	-	expression tag	UNP B5Z8Z7
A	43	HIS	-	expression tag	UNP B5Z8Z7
A	44	HIS	-	expression tag	UNP B5Z8Z7
A	45	HIS	-	expression tag	UNP B5Z8Z7
A	46	MET	-	expression tag	UNP B5Z8Z7
B	39	MET	-	initiating methionine	UNP B5Z8Z7
B	40	HIS	-	expression tag	UNP B5Z8Z7
B	41	HIS	-	expression tag	UNP B5Z8Z7
B	42	HIS	-	expression tag	UNP B5Z8Z7
B	43	HIS	-	expression tag	UNP B5Z8Z7
B	44	HIS	-	expression tag	UNP B5Z8Z7
B	45	HIS	-	expression tag	UNP B5Z8Z7
B	46	MET	-	expression tag	UNP B5Z8Z7
C	39	MET	-	initiating methionine	UNP B5Z8Z7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	40	HIS	-	expression tag	UNP B5Z8Z7
C	41	HIS	-	expression tag	UNP B5Z8Z7
C	42	HIS	-	expression tag	UNP B5Z8Z7
C	43	HIS	-	expression tag	UNP B5Z8Z7
C	44	HIS	-	expression tag	UNP B5Z8Z7
C	45	HIS	-	expression tag	UNP B5Z8Z7
C	46	MET	-	expression tag	UNP B5Z8Z7
D	39	MET	-	initiating methionine	UNP B5Z8Z7
D	40	HIS	-	expression tag	UNP B5Z8Z7
D	41	HIS	-	expression tag	UNP B5Z8Z7
D	42	HIS	-	expression tag	UNP B5Z8Z7
D	43	HIS	-	expression tag	UNP B5Z8Z7
D	44	HIS	-	expression tag	UNP B5Z8Z7
D	45	HIS	-	expression tag	UNP B5Z8Z7
D	46	MET	-	expression tag	UNP B5Z8Z7
F	39	MET	-	initiating methionine	UNP B5Z8Z7
F	40	HIS	-	expression tag	UNP B5Z8Z7
F	41	HIS	-	expression tag	UNP B5Z8Z7
F	42	HIS	-	expression tag	UNP B5Z8Z7
F	43	HIS	-	expression tag	UNP B5Z8Z7
F	44	HIS	-	expression tag	UNP B5Z8Z7
F	45	HIS	-	expression tag	UNP B5Z8Z7
F	46	MET	-	expression tag	UNP B5Z8Z7
E	39	MET	-	initiating methionine	UNP B5Z8Z7
E	40	HIS	-	expression tag	UNP B5Z8Z7
E	41	HIS	-	expression tag	UNP B5Z8Z7
E	42	HIS	-	expression tag	UNP B5Z8Z7
E	43	HIS	-	expression tag	UNP B5Z8Z7
E	44	HIS	-	expression tag	UNP B5Z8Z7
E	45	HIS	-	expression tag	UNP B5Z8Z7
E	46	MET	-	expression tag	UNP B5Z8Z7

- Molecule 2 is a RNA chain called Unidentified protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	S	11	Total	C	N	O	0	0	0
			55	33	11	11			
2	T	19	Total	C	N	O	0	0	0
			95	57	19	19			
2	H	4	Total	C	N	O	0	0	0
			21	12	4	5			
2	G	10	Total	C	N	O	0	0	0
			50	30	10	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	3	Total	C	N	O	0	0	0
			16	9	3	4			
2	L	3	Total	C	N	O	0	0	0
			16	9	3	4			
2	I	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	J	3	Total	C	N	O	0	0	0
			15	9	3	3			
2	N	2	Total	C	N	O	0	0	0
			10	6	2	2			
2	O	2	Total	C	N	O	0	0	0
			10	6	2	2			







- Chain N:  10% 90%

UNK	UNK	UNK	UNK	X5	X6	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK
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● Molecule 2: Unidentified protein



UNK	UNK	UNK	UNK	UNK	UNK	UNK	X8	X9	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.70Å 229.09Å 116.58Å 90.00° 101.26° 90.00°	Depositor
Resolution (Å)	27.14 – 3.40 27.14 – 3.40	Depositor EDS
% Data completeness (in resolution range)	94.5 (27.14-3.40) 94.6 (27.14-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 3.38Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.193 , 0.250 0.193 , 0.250	Depositor DCC
$R_{free}$ test set	2010 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.3	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 51.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	17123	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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](#)

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	0.14	0/2814	0.38	0/3795
1	B	0.12	0/2821	0.36	0/3803
1	C	0.12	0/2977	0.37	0/4011
1	D	0.12	0/2805	0.39	0/3780
1	E	0.11	0/2890	0.35	0/3894
1	F	0.11	0/2665	0.35	0/3597
All	All	0.12	0/16972	0.37	0/22880

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	F	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	F	83	ASP	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	2773	0	2903	36	0
1	B	2781	0	2920	21	0
1	C	2934	0	3065	27	0
1	D	2765	0	2893	24	0
1	E	2849	0	2992	19	0
1	F	2628	0	2773	21	0
2	G	50	0	12	0	0
2	H	21	0	6	0	0
2	I	105	0	27	3	0
2	J	15	0	6	1	0
2	K	16	0	5	0	0
2	L	16	0	5	0	0
2	N	10	0	4	0	0
2	O	10	0	4	2	0
2	S	55	0	13	0	0
2	T	95	0	21	0	0
All	All	17123	0	17649	143	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 4.

All (143) 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:65:ILE:HD12	1:A:70:ILE:CG1	1.70	1.19
1:A:65:ILE:CD1	1:A:70:ILE:CG1	2.29	1.10
1:A:65:ILE:HD12	1:A:70:ILE:HG13	1.30	1.07
1:A:65:ILE:CD1	1:A:70:ILE:HG12	1.92	0.97
1:A:65:ILE:HD11	1:A:70:ILE:HD11	1.48	0.94
1:A:65:ILE:CD1	1:A:70:ILE:HD11	2.04	0.86
1:A:65:ILE:CD1	1:A:70:ILE:CD1	2.56	0.82
1:A:65:ILE:HD11	1:A:70:ILE:CD1	2.10	0.80
2:I:1:UNK:O	2:I:3:UNK:N	2.19	0.75
1:B:334:VAL:HG13	1:B:335:ASN:H	1.50	0.74
1:F:418:VAL:HG12	1:F:419:THR:H	1.55	0.71
1:A:65:ILE:HD12	1:A:70:ILE:CD1	2.20	0.71
1:F:214:PHE:HA	1:F:218:VAL:HG21	1.77	0.67
1:D:214:PHE:HA	1:D:218:VAL:HG21	1.78	0.66
1:A:254:SER:HB2	1:A:263:LEU:HD11	1.78	0.66
1:D:334:VAL:HG13	1:D:335:ASN:H	1.60	0.64
1:E:239:LEU:HD13	1:E:302:SER:HB3	1.79	0.64
1:C:284:PRO:O	1:C:286:THR:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:THR:HG22	1:D:49:ARG:HH22	1.63	0.63
1:A:65:ILE:HD13	1:A:70:ILE:HG12	1.82	0.61
1:F:204:THR:HG23	1:F:206:TYR:H	1.66	0.61
1:A:251:VAL:HG13	1:A:263:LEU:HD13	1.85	0.59
1:B:119:LEU:HD23	1:B:141:ILE:HB	1.85	0.58
1:A:237:LEU:HG	1:A:239:LEU:HD11	1.86	0.57
1:D:106:GLY:HA2	1:D:190:ILE:HA	1.86	0.57
1:B:214:PHE:HA	1:B:218:VAL:HG21	1.87	0.56
1:E:133:ALA:HB2	1:E:186:ILE:HD13	1.87	0.56
2:I:9:UNK:O	2:I:13:UNK:N	2.37	0.56
1:E:335:ASN:ND2	1:E:338:GLU:OE1	2.39	0.55
2:I:1:UNK:C	2:I:3:UNK:H	2.18	0.55
1:C:83:ASP:OD1	1:C:84:ALA:N	2.40	0.55
1:C:250:ALA:HB2	1:C:301:ALA:HB1	1.89	0.54
1:C:214:PHE:HA	1:C:218:VAL:HG21	1.88	0.54
1:C:47:PHE:CE1	1:C:49:ARG:HB2	2.43	0.53
1:D:255:ASN:O	1:D:255:ASN:ND2	2.40	0.53
1:F:154:ILE:HG12	1:F:155:ASP:H	1.72	0.53
1:C:49:ARG:NH1	1:C:52:ASN:OD1	2.42	0.53
1:E:290:ILE:HG23	1:E:315:ALA:HB2	1.90	0.53
1:A:72:THR:HG22	1:B:49:ARG:HH22	1.74	0.53
1:A:303:GLU:OE2	1:A:322:THR:OG1	2.23	0.53
1:C:83:ASP:HB3	1:C:86:SER:HB2	1.90	0.52
1:B:79:LEU:HD21	1:B:340:ILE:HD11	1.92	0.52
1:A:250:ALA:HB2	1:A:301:ALA:HB1	1.91	0.52
1:A:340:ILE:HD13	1:B:53:VAL:HG23	1.93	0.51
1:D:64:LYS:HG3	1:D:65:ILE:H	1.76	0.51
1:A:207:LEU:HD11	1:A:235:ILE:HG12	1.93	0.51
1:C:125:LEU:O	1:C:128:THR:HG22	2.10	0.51
1:D:101:THR:HG23	1:D:246:LEU:HD11	1.93	0.51
1:A:141:ILE:O	1:A:149:THR:HG21	2.11	0.50
1:A:110:ILE:HG23	1:A:130:ALA:CB	2.42	0.50
1:B:193:LEU:O	1:B:195:SER:N	2.44	0.50
1:B:270:ASN:HD22	1:B:272:GLU:HB3	1.77	0.49
1:B:334:VAL:HG13	1:B:335:ASN:N	2.24	0.49
1:E:346:ARG:NH1	1:E:356:GLN:OE1	2.45	0.49
1:E:240:ARG:NH1	1:E:428:GLN:OE1	2.42	0.49
1:A:72:THR:HA	1:A:75:ILE:HG22	1.93	0.49
1:F:259:LYS:O	1:F:281:GLY:HA2	2.13	0.49
1:F:366:ILE:HG13	1:F:431:THR:HG21	1.95	0.48
1:B:64:LYS:O	1:B:65:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:418:VAL:HG12	1:F:419:THR:N	2.28	0.48
1:A:56:GLU:HA	1:A:59:LYS:HG2	1.96	0.48
1:A:334:VAL:HG23	1:A:335:ASN:H	1.78	0.48
1:F:269:LYS:HD3	1:F:348:TYR:OH	2.13	0.48
1:E:276:GLU:OE1	1:E:278:LYS:NZ	2.39	0.48
1:C:169:ILE:HD12	1:C:188:ARG:HH21	1.79	0.47
1:E:214:PHE:HA	1:E:218:VAL:HG21	1.96	0.47
1:A:141:ILE:HB	1:A:171:ILE:HD11	1.97	0.47
1:B:434:ASP:O	1:B:438:THR:HG23	2.15	0.47
1:C:47:PHE:HE1	1:C:49:ARG:HB2	1.78	0.47
1:D:325:LYS:NZ	2:O:8:UNK:H2	2.13	0.46
1:E:250:ALA:HB2	1:E:301:ALA:HB1	1.97	0.46
1:F:344:THR:C	1:E:62:VAL:HG22	2.39	0.46
1:D:85:HIS:O	1:D:341:LYS:HE3	2.16	0.46
1:C:169:ILE:HD12	1:C:188:ARG:NH2	2.31	0.46
1:E:366:ILE:HG13	1:E:431:THR:HG21	1.98	0.45
1:C:57:ILE:HD13	1:D:82:LEU:HD11	1.99	0.45
1:E:111:THR:HG21	1:E:243:PRO:HB2	1.99	0.45
1:D:104:GLU:OE2	1:D:192:LYS:HE3	2.17	0.45
1:E:370:LYS:NZ	1:E:425:ASP:OD1	2.50	0.45
1:D:334:VAL:HG13	1:D:335:ASN:N	2.31	0.45
1:F:154:ILE:HG12	1:F:155:ASP:N	2.32	0.45
1:A:237:LEU:HG	1:A:239:LEU:CD1	2.47	0.44
1:A:285:TYR:HB3	1:A:288:LEU:HD22	1.99	0.44
1:B:270:ASN:ND2	1:B:272:GLU:HB3	2.33	0.44
1:C:362:PRO:HG2	1:C:365:VAL:HG22	1.99	0.44
1:E:215:ASP:O	1:E:249:GLN:HG3	2.17	0.44
1:A:247:LEU:HD13	1:A:304:ILE:HD13	1.99	0.44
1:A:196:VAL:HG21	1:A:222:VAL:HG22	1.99	0.44
1:A:362:PRO:HG2	1:A:365:VAL:HG22	1.99	0.44
1:C:215:ASP:O	1:C:216:LYS:CB	2.66	0.44
1:F:250:ALA:HB2	1:F:301:ALA:HB1	2.00	0.44
1:C:226:LEU:HD23	1:C:285:TYR:CD2	2.52	0.43
1:F:290:ILE:HG23	1:F:315:ALA:HB2	2.00	0.43
1:A:83:ASP:HB2	1:A:86:SER:HB2	1.99	0.43
1:B:170:GLN:OE1	1:B:185:ASN:ND2	2.49	0.43
1:A:59:LYS:HG3	1:A:60:LYS:HG2	2.01	0.43
1:F:259:LYS:HD2	1:F:283:ALA:HB3	2.00	0.43
1:B:332:LEU:HB2	1:B:340:ILE:HG22	2.00	0.43
1:F:202:LYS:NZ	1:F:203:GLU:OE2	2.45	0.43
1:E:289:PRO:HB3	1:E:439:TRP:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:VAL:HA	1:B:57:ILE:HG22	2.01	0.43
1:F:259:LYS:HD3	1:F:286:THR:HB	2.01	0.43
1:D:157:ALA:HB1	1:D:161:MET:HE2	2.00	0.43
1:B:247:LEU:HB3	2:J:0:UNK:HA	2.00	0.42
1:D:64:LYS:O	1:D:65:ILE:HG12	2.19	0.42
1:D:318:ILE:HD12	1:D:432:ALA:HA	2.01	0.42
1:A:139:ASP:HB3	1:A:173:ILE:HD12	2.02	0.42
1:A:108:LEU:HD11	1:A:186:ILE:HB	2.01	0.42
1:E:83:ASP:OD1	1:E:86:SER:HB3	2.19	0.42
1:D:85:HIS:CE1	1:D:325:LYS:HE2	2.54	0.42
1:B:84:ALA:HB1	1:C:385:LEU:HD23	2.02	0.42
1:C:100:GLN:O	1:C:101:THR:OG1	2.30	0.42
1:F:206:TYR:CD1	1:F:234:GLY:HA3	2.55	0.42
1:B:85:HIS:CG	1:B:325:LYS:HE3	2.55	0.42
1:B:124:PRO:HG3	1:B:135:VAL:O	2.20	0.41
1:D:223:LEU:HD13	1:D:256:LEU:HD11	2.01	0.41
1:F:293:LEU:HD21	1:F:432:ALA:HB2	2.02	0.41
1:C:128:THR:HG23	1:C:131:TYR:H	1.84	0.41
1:C:215:ASP:O	1:C:216:LYS:HB3	2.20	0.41
1:C:251:VAL:HG13	1:C:263:LEU:HD12	2.03	0.41
1:B:289:PRO:HB3	1:B:439:TRP:CG	2.55	0.41
1:E:143:LYS:HB3	1:E:172:THR:OG1	2.21	0.41
1:A:106:GLY:O	1:A:162:ARG:HG3	2.21	0.41
1:A:434:ASP:O	1:A:438:THR:HG23	2.20	0.41
1:A:105:PHE:O	1:A:165:PRO:HD3	2.21	0.41
1:B:303:GLU:OE2	1:B:322:THR:OG1	2.32	0.41
1:C:52:ASN:C	1:C:52:ASN:HD22	2.25	0.41
1:D:325:LYS:HZ1	2:O:8:UNK:H2	1.69	0.41
1:F:215:ASP:O	1:F:249:GLN:HG3	2.21	0.41
1:D:85:HIS:NE2	1:D:325:LYS:HE2	2.36	0.41
1:F:304:ILE:HD11	1:F:347:TYR:CD2	2.56	0.41
1:C:196:VAL:HA	1:C:210:ARG:O	2.21	0.40
1:C:208:TYR:CE2	1:C:210:ARG:HB2	2.56	0.40
1:C:369:GLY:O	1:C:427:ILE:HG13	2.21	0.40
1:D:208:TYR:CE2	1:D:210:ARG:HB2	2.56	0.40
1:D:108:LEU:HD11	1:D:186:ILE:HD11	2.02	0.40
1:D:139:ASP:HB3	1:D:173:ILE:HD12	2.03	0.40
1:D:288:LEU:HD12	1:D:289:PRO:HD2	2.01	0.40
1:C:189:ASP:OD1	1:C:190:ILE:N	2.54	0.40
1:E:382:GLU:HA	1:E:385:LEU:HG	2.04	0.40
1:C:332:LEU:HD13	1:D:60:LYS:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:82:LEU:O	1:E:61:TYR:OH	2.30	0.40
1:F:255:ASN:O	1:F:255:ASN:ND2	2.51	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	357/416 (86%)	342 (96%)	14 (4%)	1 (0%)	37	66
1	B	358/416 (86%)	342 (96%)	15 (4%)	1 (0%)	37	66
1	C	376/416 (90%)	345 (92%)	25 (7%)	6 (2%)	8	29
1	D	354/416 (85%)	333 (94%)	18 (5%)	3 (1%)	16	44
1	E	364/416 (88%)	346 (95%)	17 (5%)	1 (0%)	37	66
1	F	338/416 (81%)	317 (94%)	17 (5%)	4 (1%)	11	35
All	All	2147/2496 (86%)	2025 (94%)	106 (5%)	16 (1%)	19	47

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	356	GLN
1	C	285	TYR
1	C	356	GLN
1	D	65	ILE
1	D	144	ILE
1	B	65	ILE
1	C	284	PRO
1	C	372	PRO
1	D	145	ASN
1	F	154	ILE

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Mol	Chain	Res	Type
1	E	356	GLN
1	C	376	ASN
1	C	194	PRO
1	F	284	PRO
1	F	334	VAL
1	F	418	VAL

### 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	308/360 (86%)	307 (100%)	1 (0%)	91	95
1	B	309/360 (86%)	309 (100%)	0	100	100
1	C	326/360 (91%)	326 (100%)	0	100	100
1	D	307/360 (85%)	307 (100%)	0	100	100
1	E	317/360 (88%)	317 (100%)	0	100	100
1	F	293/360 (81%)	293 (100%)	0	100	100
All	All	1860/2160 (86%)	1859 (100%)	1 (0%)	92	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	A	185	ASN
1	A	329	GLN
1	B	217	ASN
1	D	329	GLN
1	F	170	GLN

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Mol	Chain	Res	Type
1	F	185	ASN
1	F	248	ASN
1	F	335	ASN
1	E	98	GLN
1	E	145	ASN
1	E	387	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	0/21	-	-
2	H	0/21	-	-
2	I	0/21	-	-
2	J	0/21	-	-
2	K	0/21	-	-
2	L	0/21	-	-
2	N	0/21	-	-
2	O	0/21	-	-
2	S	0/21	-	-
2	T	0/21	-	-
All	All	0/210	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

## 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 oligosaccharides 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	360/416 (86%)	-0.03	6 (1%) 69 59	22, 59, 98, 133	0
1	B	362/416 (87%)	-0.21	2 (0%) 85 80	15, 51, 98, 128	0
1	C	380/416 (91%)	-0.16	6 (1%) 70 61	19, 51, 86, 139	0
1	D	360/416 (86%)	-0.12	6 (1%) 69 59	20, 54, 108, 128	0
1	E	370/416 (88%)	-0.14	3 (0%) 82 75	20, 53, 98, 129	0
1	F	344/416 (82%)	-0.01	5 (1%) 71 62	22, 55, 128, 145	0
2	G	0/21	-	-	-	-
2	H	0/21	-	-	-	-
2	I	0/21	-	-	-	-
2	J	0/21	-	-	-	-
2	K	0/21	-	-	-	-
2	L	0/21	-	-	-	-
2	N	0/21	-	-	-	-
2	O	0/21	-	-	-	-
2	S	0/21	-	-	-	-
2	T	0/21	-	-	-	-
All	All	2176/2706 (80%)	-0.11	28 (1%) 74 66	15, 54, 110, 145	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	99	ALA	3.6
1	C	101	THR	3.6
1	D	137	SER	3.6
1	F	84	ALA	3.0
1	B	415	GLU	3.0
1	C	374	ASN	3.0
1	D	153	SER	2.9
1	E	66	SER	2.9
1	D	154	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	104	GLU	2.7
1	D	181	PRO	2.7
1	F	152	MET	2.7
1	C	439	TRP	2.6
1	C	373	GLU	2.4
1	A	337	ASP	2.2
1	D	108	LEU	2.2
1	F	85	HIS	2.2
1	A	434	ASP	2.2
1	B	439	TRP	2.2
1	A	195	SER	2.2
1	F	145	ASN	2.2
1	E	155	ASP	2.2
1	F	120	THR	2.2
1	E	386	LYS	2.1
1	A	105	PHE	2.1
1	A	91	GLU	2.1
1	D	215	ASP	2.1
1	C	392	GLU	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 oligosaccharides 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.