



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 03:10 PM EDT

PDB ID : 6E09  
Title : Crystal Structure of Helicobacter pylori TlpA Chemoreceptor Ligand Binding Domain  
Authors : Remington, S.J.; Guillemin, K.; Sweeney, E.; Perkins, A.  
Deposited on : 2018-07-06  
Resolution : 2.30 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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
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) : 2.37.1

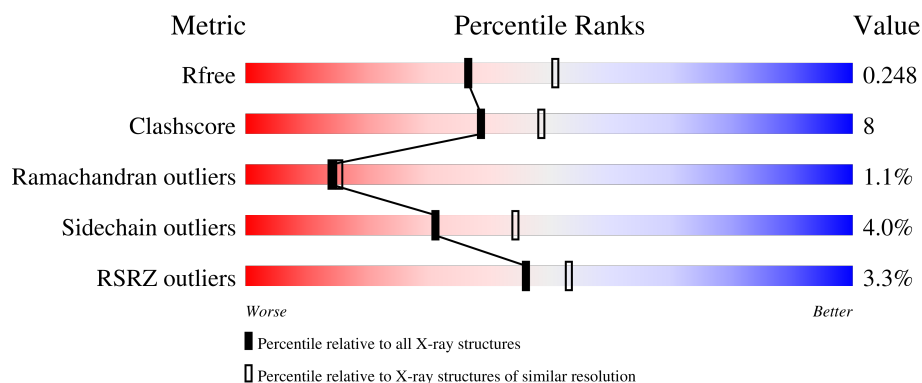
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	295	 2% 71% 14% 13%
1	B	295	 6% 64% 16% 18%
1	C	295	 2% 70% 15% 14%
1	D	295	 % 78% 9% 12%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8414 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 Methyl-accepting chemotaxis protein TlpA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	Se	0	0	0
			1985	1276	329	370	10			
1	B	241	Total	C	N	O	Se	0	0	0
			1855	1194	307	346	8			
1	C	255	Total	C	N	O	Se	0	0	0
			2004	1288	336	370	10			
1	D	260	Total	C	N	O	Se	0	0	0
			2041	1306	343	382	10			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	MSE	-	initiating methionine	UNP A0A1U9IS38
A	6	GLY	-	expression tag	UNP A0A1U9IS38
A	7	HIS	-	expression tag	UNP A0A1U9IS38
A	8	HIS	-	expression tag	UNP A0A1U9IS38
A	9	HIS	-	expression tag	UNP A0A1U9IS38
A	10	HIS	-	expression tag	UNP A0A1U9IS38
A	11	HIS	-	expression tag	UNP A0A1U9IS38
A	12	HIS	-	expression tag	UNP A0A1U9IS38
A	13	ASP	-	expression tag	UNP A0A1U9IS38
A	14	TYR	-	expression tag	UNP A0A1U9IS38
A	15	ASP	-	expression tag	UNP A0A1U9IS38
A	16	ILE	-	expression tag	UNP A0A1U9IS38
A	17	PRO	-	expression tag	UNP A0A1U9IS38
A	18	THR	-	expression tag	UNP A0A1U9IS38
A	19	THR	-	expression tag	UNP A0A1U9IS38
A	20	GLU	-	expression tag	UNP A0A1U9IS38
A	21	ASN	-	expression tag	UNP A0A1U9IS38
A	22	LEU	-	expression tag	UNP A0A1U9IS38
A	23	TYR	-	expression tag	UNP A0A1U9IS38
A	24	PHE	-	expression tag	UNP A0A1U9IS38
A	25	GLN	-	expression tag	UNP A0A1U9IS38

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Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	expression tag	UNP A0A1U9IS38
A	27	SER	-	expression tag	UNP A0A1U9IS38
B	5	MSE	-	initiating methionine	UNP A0A1U9IS38
B	6	GLY	-	expression tag	UNP A0A1U9IS38
B	7	HIS	-	expression tag	UNP A0A1U9IS38
B	8	HIS	-	expression tag	UNP A0A1U9IS38
B	9	HIS	-	expression tag	UNP A0A1U9IS38
B	10	HIS	-	expression tag	UNP A0A1U9IS38
B	11	HIS	-	expression tag	UNP A0A1U9IS38
B	12	HIS	-	expression tag	UNP A0A1U9IS38
B	13	ASP	-	expression tag	UNP A0A1U9IS38
B	14	TYR	-	expression tag	UNP A0A1U9IS38
B	15	ASP	-	expression tag	UNP A0A1U9IS38
B	16	ILE	-	expression tag	UNP A0A1U9IS38
B	17	PRO	-	expression tag	UNP A0A1U9IS38
B	18	THR	-	expression tag	UNP A0A1U9IS38
B	19	THR	-	expression tag	UNP A0A1U9IS38
B	20	GLU	-	expression tag	UNP A0A1U9IS38
B	21	ASN	-	expression tag	UNP A0A1U9IS38
B	22	LEU	-	expression tag	UNP A0A1U9IS38
B	23	TYR	-	expression tag	UNP A0A1U9IS38
B	24	PHE	-	expression tag	UNP A0A1U9IS38
B	25	GLN	-	expression tag	UNP A0A1U9IS38
B	26	GLY	-	expression tag	UNP A0A1U9IS38
B	27	SER	-	expression tag	UNP A0A1U9IS38
C	5	MSE	-	initiating methionine	UNP A0A1U9IS38
C	6	GLY	-	expression tag	UNP A0A1U9IS38
C	7	HIS	-	expression tag	UNP A0A1U9IS38
C	8	HIS	-	expression tag	UNP A0A1U9IS38
C	9	HIS	-	expression tag	UNP A0A1U9IS38
C	10	HIS	-	expression tag	UNP A0A1U9IS38
C	11	HIS	-	expression tag	UNP A0A1U9IS38
C	12	HIS	-	expression tag	UNP A0A1U9IS38
C	13	ASP	-	expression tag	UNP A0A1U9IS38
C	14	TYR	-	expression tag	UNP A0A1U9IS38
C	15	ASP	-	expression tag	UNP A0A1U9IS38
C	16	ILE	-	expression tag	UNP A0A1U9IS38
C	17	PRO	-	expression tag	UNP A0A1U9IS38
C	18	THR	-	expression tag	UNP A0A1U9IS38
C	19	THR	-	expression tag	UNP A0A1U9IS38
C	20	GLU	-	expression tag	UNP A0A1U9IS38
C	21	ASN	-	expression tag	UNP A0A1U9IS38

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Chain	Residue	Modelled	Actual	Comment	Reference
C	22	LEU	-	expression tag	UNP A0A1U9IS38
C	23	TYR	-	expression tag	UNP A0A1U9IS38
C	24	PHE	-	expression tag	UNP A0A1U9IS38
C	25	GLN	-	expression tag	UNP A0A1U9IS38
C	26	GLY	-	expression tag	UNP A0A1U9IS38
C	27	SER	-	expression tag	UNP A0A1U9IS38
D	5	MSE	-	initiating methionine	UNP A0A1U9IS38
D	6	GLY	-	expression tag	UNP A0A1U9IS38
D	7	HIS	-	expression tag	UNP A0A1U9IS38
D	8	HIS	-	expression tag	UNP A0A1U9IS38
D	9	HIS	-	expression tag	UNP A0A1U9IS38
D	10	HIS	-	expression tag	UNP A0A1U9IS38
D	11	HIS	-	expression tag	UNP A0A1U9IS38
D	12	HIS	-	expression tag	UNP A0A1U9IS38
D	13	ASP	-	expression tag	UNP A0A1U9IS38
D	14	TYR	-	expression tag	UNP A0A1U9IS38
D	15	ASP	-	expression tag	UNP A0A1U9IS38
D	16	ILE	-	expression tag	UNP A0A1U9IS38
D	17	PRO	-	expression tag	UNP A0A1U9IS38
D	18	THR	-	expression tag	UNP A0A1U9IS38
D	19	THR	-	expression tag	UNP A0A1U9IS38
D	20	GLU	-	expression tag	UNP A0A1U9IS38
D	21	ASN	-	expression tag	UNP A0A1U9IS38
D	22	LEU	-	expression tag	UNP A0A1U9IS38
D	23	TYR	-	expression tag	UNP A0A1U9IS38
D	24	PHE	-	expression tag	UNP A0A1U9IS38
D	25	GLN	-	expression tag	UNP A0A1U9IS38
D	26	GLY	-	expression tag	UNP A0A1U9IS38
D	27	SER	-	expression tag	UNP A0A1U9IS38

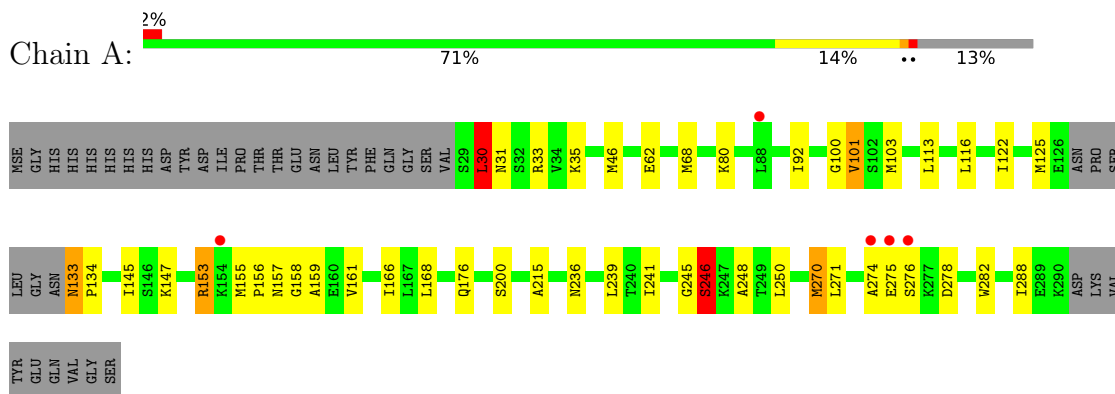
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	139	Total O 139 139	0	0
2	B	102	Total O 102 102	0	0
2	C	112	Total O 112 112	0	0
2	D	176	Total O 176 176	0	0

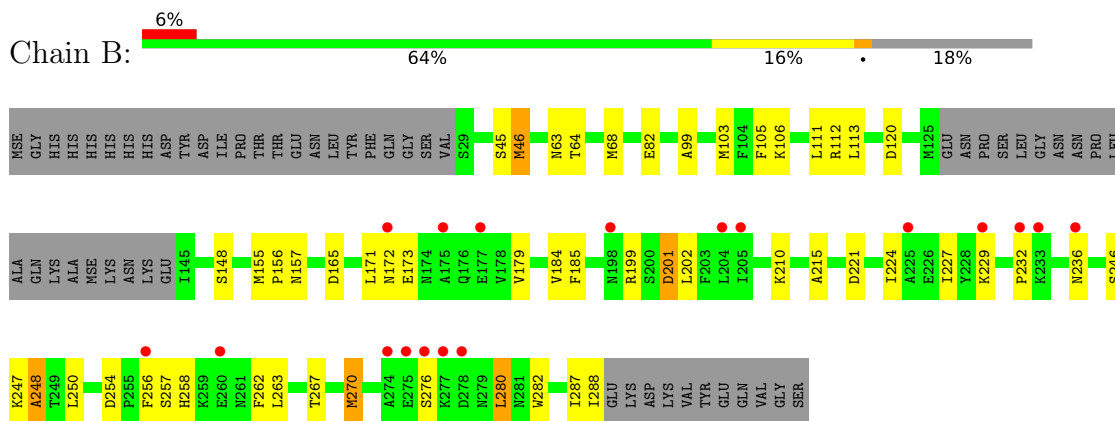
### 3 Residue-property plots [i](#)

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.

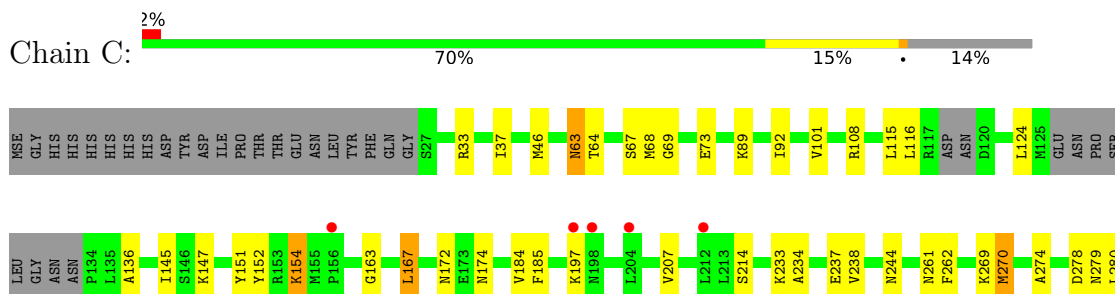
- Molecule 1: Methyl-accepting chemotaxis protein TlpA

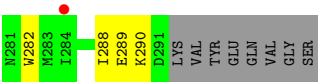


- Molecule 1: Methyl-accepting chemotaxis protein TlpA

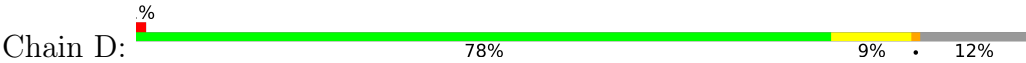


- Molecule 1: Methyl-accepting chemotaxis protein TlpA





● Molecule 1: Methyl-accepting chemotaxis protein TlpA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.50Å 72.35Å 132.92Å 90.00° 93.26° 90.00°	Depositor
Resolution (Å)	26.70 – 2.30 26.70 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.5 (26.70-2.30) 94.5 (26.70-2.30)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.190 , 0.246 0.198 , 0.248	Depositor DCC
$R_{free}$ test set	2006 reflections (3.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 53.2	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	0.93	EDS
Total number of atoms	8414	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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	0.72	1/2003 (0.0%)	0.76	1/2685 (0.0%)
1	B	0.59	0/1873	0.72	0/2517
1	C	0.61	0/2021	0.68	0/2699
1	D	0.71	0/2059	0.78	1/2756 (0.0%)
All	All	0.66	1/7956 (0.0%)	0.73	2/10657 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	VAL	CB-CG1	-6.19	1.39	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	LEU	CA-CB-CG	5.33	127.56	115.30
1	D	182	LEU	CB-CG-CD2	-5.29	102.01	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	1985	0	2025	29	0
1	B	1855	0	1876	37	0
1	C	2004	0	2094	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2041	0	2106	22	0
2	A	139	0	0	5	0
2	B	102	0	0	5	0
2	C	112	0	0	4	0
2	D	176	0	0	5	0
All	All	8414	0	8101	120	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 8.

All (120) 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:D:64:THR:HG22	1:D:68:MSE:HE3	1.57	0.87
1:A:46:MSE:HE2	1:A:288:ILE:HD12	1.64	0.80
1:A:92:ILE:HD11	1:A:101:VAL:HG22	1.63	0.80
1:B:201:ASP:OD1	1:B:201:ASP:N	2.16	0.79
1:D:68:MSE:HE1	1:D:184:VAL:HG11	1.65	0.79
1:D:68:MSE:CE	1:D:184:VAL:HG11	2.14	0.77
1:C:68:MSE:HE2	1:C:184:VAL:HG11	1.71	0.73
1:B:112:ARG:O	1:B:113:LEU:HD23	1.89	0.73
1:C:136:ALA:HA	1:C:167:LEU:HD22	1.72	0.71
1:A:30:LEU:HD13	1:A:31:ASN:N	2.07	0.69
1:B:68:MSE:HE2	1:B:184:VAL:HG11	1.73	0.69
1:D:68:MSE:HE2	1:D:184:VAL:HG21	1.76	0.67
1:A:103:MSE:HE2	1:A:113:LEU:HD12	1.77	0.66
1:D:103:MSE:HE2	1:D:113:LEU:HD12	1.79	0.65
1:B:64:THR:HG22	1:B:68:MSE:HE3	1.77	0.65
1:A:155:MSE:HE2	1:A:161:VAL:HB	1.79	0.63
1:C:68:MSE:CE	1:C:184:VAL:HG11	2.29	0.63
1:D:102:SER:HB2	1:D:183:MSE:HG2	1.80	0.63
1:B:64:THR:HG22	1:B:68:MSE:CE	2.29	0.62
1:B:254:ASP:O	1:B:258:HIS:N	2.32	0.62
1:C:64:THR:HG22	1:C:68:MSE:HE3	1.81	0.61
1:B:254:ASP:OD1	1:B:257:SER:N	2.32	0.61
1:B:250:LEU:HD11	1:B:263:LEU:HD23	1.83	0.61
1:B:63:ASN:OD1	1:C:63:ASN:ND2	2.36	0.58
1:C:92:ILE:HD11	1:C:101:VAL:HG12	1.86	0.57
1:A:153:ARG:NH2	2:A:307:HOH:O	2.37	0.57
1:C:269:LYS:NZ	1:C:279:ASN:O	2.30	0.56
1:A:46:MSE:HE2	1:A:288:ILE:CD1	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ALA:HB3	1:B:185:PHE:CD2	2.41	0.55
1:C:46:MSE:HE1	1:C:288:ILE:HG21	1.88	0.55
1:A:68:MSE:HE3	1:A:168:LEU:HD21	1.87	0.55
1:A:133:ASN:ND2	1:A:133:ASN:N	2.55	0.54
1:A:30:LEU:HD13	1:A:30:LEU:C	2.29	0.53
1:D:145:ILE:CD1	2:D:476:HOH:O	2.57	0.53
1:C:68:MSE:HE2	1:C:184:VAL:HG21	1.91	0.52
1:A:133:ASN:N	1:A:133:ASN:HD22	2.08	0.51
1:B:232:PRO:O	1:B:236:ASN:HB2	2.11	0.50
1:D:270:MSE:HG3	1:D:282:TRP:CE2	2.47	0.50
1:A:145:ILE:O	1:A:145:ILE:HG23	2.12	0.49
1:A:245:GLY:O	1:A:246:SER:CB	2.61	0.49
1:C:46:MSE:CE	1:C:288:ILE:HG21	2.41	0.49
1:B:82:GLU:HB2	2:B:356:HOH:O	2.12	0.49
1:B:262:PHE:HB2	1:B:288:ILE:HG22	1.95	0.49
1:A:157:ASN:O	1:A:159:ALA:N	2.45	0.48
1:A:80:LYS:NZ	2:A:315:HOH:O	2.45	0.48
1:D:103:MSE:HE3	1:D:111:LEU:HA	1.96	0.48
1:B:210:LYS:NZ	1:B:221:ASP:OD1	2.41	0.48
1:D:172:ASN:ND2	2:D:312:HOH:O	2.47	0.48
1:D:110:ASP:OD1	1:D:110:ASP:N	2.47	0.47
1:A:100:GLY:HA3	1:A:116:LEU:HD23	1.96	0.47
1:B:172:ASN:CB	1:B:179:VAL:HG11	2.45	0.47
1:A:270:MSE:HE3	1:A:282:TRP:CZ3	2.49	0.47
1:A:103:MSE:CE	1:A:113:LEU:HD12	2.44	0.47
1:B:263:LEU:HD13	1:B:287:ILE:HG22	1.97	0.47
1:C:33:ARG:O	1:C:37:ILE:HG12	2.14	0.47
1:A:241:ILE:HD13	1:A:248:ALA:HB3	1.97	0.47
1:C:261:ASN:OD1	1:C:289:GLU:HA	2.14	0.46
1:B:103:MSE:HE3	1:B:113:LEU:HD12	1.97	0.46
1:B:263:LEU:HD13	1:B:287:ILE:CG2	2.46	0.46
1:B:106:LYS:O	1:B:112:ARG:NH2	2.49	0.46
1:A:176:GLN:O	2:A:301:HOH:O	2.20	0.46
1:B:215:ALA:O	2:B:301:HOH:O	2.20	0.46
1:B:254:ASP:HB3	1:B:257:SER:OG	2.16	0.46
1:C:270:MSE:HG3	1:C:282:TRP:CE2	2.51	0.46
1:D:145:ILE:HD12	2:D:476:HOH:O	2.14	0.46
1:A:166:ILE:HD12	1:A:271:LEU:HD21	1.98	0.45
1:C:115:LEU:HD12	1:C:115:LEU:N	2.31	0.45
1:C:244:ASN:OD1	2:C:301:HOH:O	2.21	0.45
1:C:280:LEU:HD23	1:C:280:LEU:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:MSE:HE3	1:A:282:TRP:CH2	2.52	0.45
1:B:254:ASP:OD1	1:B:256:PHE:N	2.50	0.45
1:D:68:MSE:HE2	1:D:184:VAL:HG11	1.95	0.44
1:C:145:ILE:HG21	1:C:274:ALA:HB1	2.00	0.44
1:D:251:GLU:OE1	1:D:290:LYS:HE3	2.17	0.44
1:C:64:THR:HG22	1:C:68:MSE:CE	2.45	0.44
1:B:224:ILE:HA	1:B:227:ILE:HB	2.00	0.44
1:D:197:LYS:NZ	2:D:302:HOH:O	2.24	0.44
1:B:202:LEU:O	2:B:302:HOH:O	2.21	0.43
1:C:163:GLY:HA3	1:C:185:PHE:CZ	2.53	0.43
1:A:133:ASN:N	1:A:134:PRO:HD3	2.33	0.43
1:A:200:SER:HA	1:A:215:ALA:HB2	1.99	0.43
1:C:234:ALA:O	1:C:238:VAL:HG23	2.18	0.43
1:B:99:ALA:HB3	1:B:185:PHE:HD2	1.82	0.43
1:D:47:GLN:HG2	2:D:408:HOH:O	2.19	0.43
1:A:122:ILE:HD12	1:A:156:PRO:HB3	1.99	0.43
1:B:270:MSE:HG3	1:B:282:TRP:CE2	2.54	0.43
1:D:64:THR:CG2	1:D:68:MSE:HE3	2.38	0.43
1:A:245:GLY:O	1:A:246:SER:HB3	2.19	0.42
1:B:46:MSE:HE1	1:B:288:ILE:HG21	2.01	0.42
1:C:147:LYS:HG2	1:C:278:ASP:HB3	2.02	0.42
1:C:233:LYS:NZ	2:C:319:HOH:O	2.52	0.42
1:B:46:MSE:HE1	1:B:288:ILE:CG2	2.49	0.42
1:B:199:ARG:NH1	2:B:309:HOH:O	2.53	0.42
1:B:280:LEU:HD12	1:B:280:LEU:H	1.83	0.41
1:A:62:GLU:OE1	2:A:302:HOH:O	2.21	0.41
1:B:267:THR:HA	1:B:282:TRP:O	2.20	0.41
1:B:171:LEU:O	1:B:172:ASN:CB	2.67	0.41
1:C:172:ASN:ND2	1:C:174:ASN:OD1	2.53	0.41
1:B:247:LYS:O	1:B:248:ALA:HB2	2.21	0.41
1:C:69:GLY:O	1:C:73:GLU:HG2	2.21	0.41
1:D:103:MSE:HE3	1:D:111:LEU:CA	2.50	0.41
1:B:120:ASP:HB3	2:B:317:HOH:O	2.20	0.41
1:C:154:LYS:H	1:C:154:LYS:CD	2.34	0.41
1:C:46:MSE:HE2	1:C:46:MSE:HB3	1.99	0.41
1:C:108:ARG:HA	2:C:331:HOH:O	2.20	0.41
1:C:151:TYR:HD1	1:C:152:TYR:O	2.03	0.41
1:C:207:VAL:HG13	1:C:207:VAL:O	2.21	0.41
1:C:89:LYS:HE3	1:C:89:LYS:HB2	1.97	0.41
1:D:103:MSE:HE2	1:D:113:LEU:CD1	2.49	0.41
1:A:125:MSE:HB3	2:A:332:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:SER:HB3	1:B:165:ASP:HB2	2.03	0.41
1:C:262:PHE:CE1	1:C:290:LYS:HD2	2.56	0.41
1:D:112:ARG:O	1:D:113:LEU:HD23	2.20	0.41
1:B:105:PHE:CD1	1:B:111:LEU:HB3	2.56	0.40
1:B:155:MSE:O	1:B:157:ASN:N	2.54	0.40
1:D:253:LEU:HB2	1:D:260:GLU:OE2	2.21	0.40
1:A:147:LYS:HG2	1:A:278:ASP:HB3	2.03	0.40
1:C:89:LYS:HA	1:C:92:ILE:HD12	2.04	0.40
1:C:174:ASN:O	2:C:302:HOH:O	2.22	0.40
1:D:103:MSE:HE3	1:D:111:LEU:HB3	2.03	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	252/295 (85%)	238 (94%)	9 (4%)	5 (2%)	7	6
1	B	237/295 (80%)	217 (92%)	16 (7%)	4 (2%)	9	8
1	C	249/295 (84%)	239 (96%)	9 (4%)	1 (0%)	34	42
1	D	256/295 (87%)	245 (96%)	10 (4%)	1 (0%)	34	42
All	All	994/1180 (84%)	939 (94%)	44 (4%)	11 (1%)	14	15

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	ALA
1	B	173	GLU
1	A	158	GLY
1	A	246	SER
1	A	276	SER

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Mol	Chain	Res	Type
1	C	197	LYS
1	A	275	GLU
1	B	276	SER
1	D	173	GLU
1	B	248	ALA
1	B	156	PRO

### 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	216/256 (84%)	206 (95%)	10 (5%)	27	38
1	B	201/256 (78%)	194 (96%)	7 (4%)	36	50
1	C	225/256 (88%)	216 (96%)	9 (4%)	31	44
1	D	228/256 (89%)	219 (96%)	9 (4%)	32	46
All	All	870/1024 (85%)	835 (96%)	35 (4%)	31	44

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	33	ARG
1	A	35	LYS
1	A	133	ASN
1	A	153	ARG
1	A	236	ASN
1	A	239	LEU
1	A	246	SER
1	A	250	LEU
1	A	270	MSE
1	B	45	SER
1	B	46	MSE
1	B	201	ASP
1	B	229	LYS
1	B	246	SER

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Mol	Chain	Res	Type
1	B	270	MSE
1	B	280	LEU
1	C	63	ASN
1	C	67	SER
1	C	116	LEU
1	C	124	LEU
1	C	154	LYS
1	C	167	LEU
1	C	214	SER
1	C	237	GLU
1	C	270	MSE
1	D	32	SER
1	D	44	ARG
1	D	68	MSE
1	D	75	LEU
1	D	125	MSE
1	D	137	GLN
1	D	183	MSE
1	D	250	LEU
1	D	275	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

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	246/295 (83%)	-0.06	5 (2%) 65 71	15, 32, 57, 74	0
1	B	232/295 (78%)	0.23	18 (7%) 13 17	19, 43, 71, 83	0
1	C	245/295 (83%)	0.00	6 (2%) 59 66	21, 37, 59, 73	0
1	D	250/295 (84%)	-0.17	3 (1%) 79 83	10, 28, 56, 79	0
All	All	973/1180 (82%)	-0.00	32 (3%) 46 53	10, 35, 62, 83	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	275	GLU	7.4
1	B	205	ILE	3.7
1	D	175	ALA	3.6
1	B	232	PRO	3.6
1	A	274	ALA	3.6
1	B	172	ASN	3.5
1	B	276	SER	3.4
1	B	274	ALA	3.4
1	B	198	ASN	3.0
1	D	173	GLU	2.9
1	B	229	LYS	2.9
1	C	197	LYS	2.8
1	C	198	ASN	2.6
1	B	233	LYS	2.6
1	B	260	GLU	2.5
1	B	256	PHE	2.5
1	B	175	ALA	2.4
1	B	204	LEU	2.4
1	C	284	ILE	2.4
1	B	225	ALA	2.4
1	B	277	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	156	PRO	2.2
1	B	236	ASN	2.2
1	C	212	LEU	2.2
1	A	275	GLU	2.2
1	A	88	LEU	2.2
1	C	204	LEU	2.2
1	B	278	ASP	2.1
1	A	276	SER	2.1
1	B	177	GLU	2.1
1	A	154	LYS	2.1
1	D	205	ILE	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 monosaccharides 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.