



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:36 PM UTC

PDB ID : 6E09 / pdb_00006e09
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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

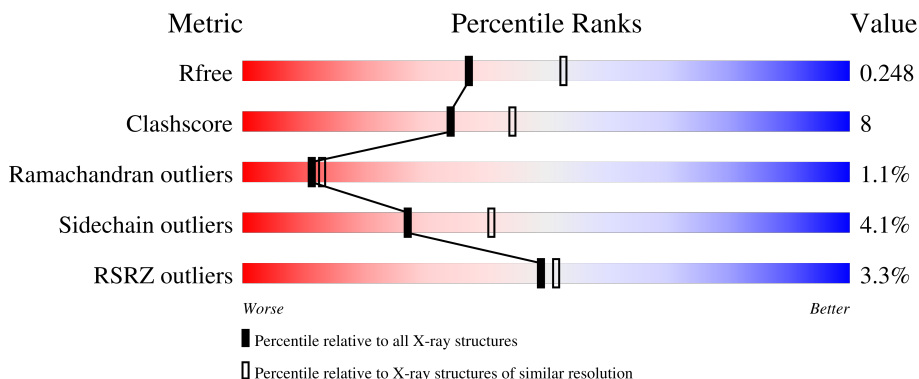
1 Overall quality at a glance

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 ≥ 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% 72% 13% • 13%
1	B	295	5% 63% 18% • 18%
1	C	295	• 70% 15% • 14%
1	D	295	2% 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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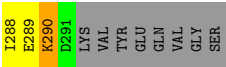
Chain	Residue	Modelled	Actual	Comment	Reference
C	22	LEU	-	expression tag	UNP A0A1U9IS38
C	23	TYR	-	expression tag	UNP A0A1U9IS38
C	24	PHE	-	expression tag	UNP A0A1U9IS38
C	25	GLN	-	expression tag	UNP A0A1U9IS38
C	26	GLY	-	expression tag	UNP A0A1U9IS38
C	27	SER	-	expression tag	UNP A0A1U9IS38
D	5	MSE	-	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.

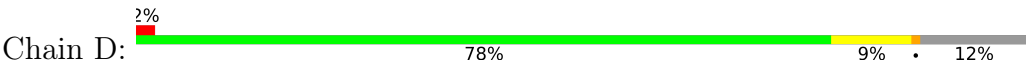
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	139	Total O 139 139	0	0
2	B	102	Total O 102 102	0	0
2	C	112	Total O 112 112	0	0
2	D	176	Total O 176 176	0	0

- 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, α , β , γ	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) 94.7 (26.70-2.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	27.7	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.71	0/2003	0.75	0/2685
1	B	0.59	0/1873	0.69	0/2517
1	C	0.57	0/2021	0.66	0/2699
1	D	0.72	0/2059	0.78	1/2756 (0.0%)
All	All	0.65	0/7956	0.72	1/10657 (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	D	46	MSE	N-CA-C	-5.13	106.53	112.89

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	1985	0	2025	29	0
1	B	1855	0	1876	38	0
1	C	2004	0	2094	33	0
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	3	0
2	D	176	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8414	0	8101	121	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 (121) 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:D:197:LYS:NZ	2:D:302:HOH:O	2.24	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:30:LEU:HD13	1:A:30:LEU:C	2.29	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ASN:ND2	1:A:133:ASN:N	2.55	0.54
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: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:B:210:LYS:NZ	1:B:221:ASP:OD1	2.41	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:A:145:ILE:O	1:A:145:ILE:HG23	2.12	0.48
1:D:103:MSE:HE3	1:D:111:LEU:HA	1.96	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:113:LEU:HD12	1:C:113:LEU:C	2.44	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:250:LEU:HD12	1:B:250:LEU:C	2.46	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%)	6	5
1	B	237/295 (80%)	217 (92%)	16 (7%)	4 (2%)	7	7
1	C	249/295 (84%)	239 (96%)	9 (4%)	1 (0%)	30	38
1	D	256/295 (87%)	245 (96%)	10 (4%)	1 (0%)	30	38
All	All	994/1180 (84%)	939 (94%)	44 (4%)	11 (1%)	11	13

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
1	C	197	LYS
1	A	275	GLU
1	B	276	SER
1	D	173	GLU

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Mol	Chain	Res	Type
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%)	207 (96%)	9 (4%)	26	40
1	B	201/256 (78%)	192 (96%)	9 (4%)	24	37
1	C	225/256 (88%)	216 (96%)	9 (4%)	28	42
1	D	228/256 (89%)	219 (96%)	9 (4%)	28	43
All	All	870/1024 (85%)	834 (96%)	36 (4%)	27	41

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	33	ARG
1	A	80	LYS
1	A	133	ASN
1	A	153	ARG
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	122	ILE
1	B	201	ASP
1	B	229	LYS
1	B	240	THR
1	B	246	SER
1	B	260	GLU
1	B	280	LEU
1	C	63	ASN

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Mol	Chain	Res	Type
1	C	116	LEU
1	C	122	ILE
1	C	124	LEU
1	C	154	LYS
1	C	167	LEU
1	C	214	SER
1	C	237	GLU
1	C	290	LYS
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. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	ASN
1	B	58	GLN
1	B	63	ASN
1	B	90	ASN
1	B	193	ASN
1	C	47	GLN
1	C	63	ASN
1	C	90	ASN
1	C	193	ASN
1	D	198	ASN
1	D	220	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 [i](#)

There are no oligosaccharides 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, 95th 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 ²)	Q<0.9
1	A	246/295 (83%)	0.17	7 (2%) 55 57	15, 32, 57, 74	0
1	B	232/295 (78%)	0.58	16 (6%) 23 25	19, 43, 71, 83	0
1	C	245/295 (83%)	0.31	4 (1%) 70 72	21, 37, 59, 73	0
1	D	250/295 (84%)	0.04	5 (2%) 65 66	10, 28, 56, 79	0
All	All	973/1180 (82%)	0.27	32 (3%) 49 51	10, 35, 62, 83	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	275	GLU	4.0
1	D	128	PRO	3.6
1	B	172	ASN	3.4
1	B	119	ASN	3.2
1	A	274	ALA	3.2
1	B	236	ASN	3.0
1	B	256	PHE	2.9
1	B	288	ILE	2.7
1	A	159	ALA	2.7
1	B	177	GLU	2.7
1	B	274	ALA	2.7
1	B	225	ALA	2.7
1	B	232	PRO	2.7
1	A	133	ASN	2.6
1	D	136	ALA	2.6
1	B	175	ALA	2.5
1	A	82	GLU	2.5
1	D	173	GLU	2.5
1	D	175	ALA	2.4
1	C	176	GLN	2.4
1	A	29	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	280	LEU	2.3
1	B	229	LYS	2.3
1	A	122	ILE	2.2
1	B	118	ASP	2.2
1	B	122	ILE	2.1
1	A	119	ASN	2.1
1	C	274	ALA	2.1
1	D	129	SER	2.0
1	B	231	VAL	2.0
1	C	197	LYS	2.0
1	B	219	LEU	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.