



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:51 AM EDT

PDB ID : 5FRQ / pdb_00005frq
Title : Crystal Structure of Helicobacter pylori beta clamp bound to DNA ligase peptide
Authors : Pandey, P.; Gourinath, S.
Deposited on : 2015-12-21
Resolution : 2.90 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:

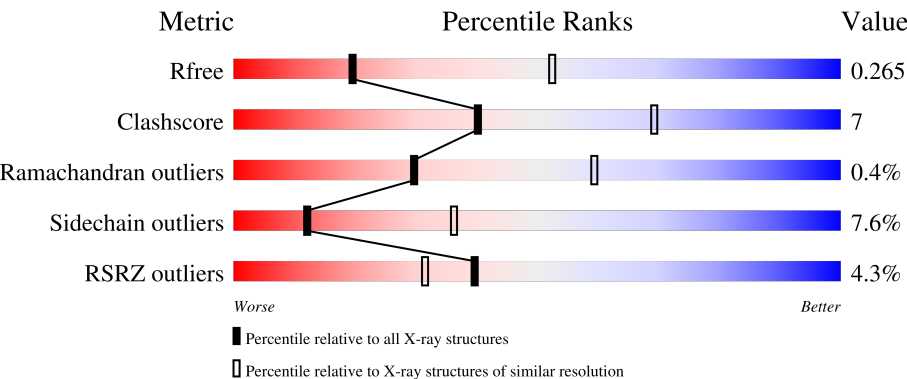
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	384	2% 79%13%7%
1	B	384	6% 77%14%5%
1	C	384	4% 76%16%7%
1	D	384	4% 78%12%7%
2	G	8	12% 50%25%25%

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Mol	Chain	Length	Quality of chain
2	L	8	25% 12% 50% 12% 25%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11507 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 DNA POLYMERASE III SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2837	1826	450	550	11			
1	B	364	Total	C	N	O	S	0	0	0
			2882	1854	458	559	11			
1	C	358	Total	C	N	O	S	0	0	0
			2840	1829	451	549	11			
1	D	357	Total	C	N	O	S	0	0	0
			2828	1820	448	549	11			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP O25242
A	0	ALA	-	expression tag	UNP O25242
A	375	GLU	-	expression tag	UNP O25242
A	376	LEU	-	expression tag	UNP O25242
A	377	HIS	-	expression tag	UNP O25242
A	378	HIS	-	expression tag	UNP O25242
A	379	HIS	-	expression tag	UNP O25242
A	380	HIS	-	expression tag	UNP O25242
A	381	HIS	-	expression tag	UNP O25242
A	382	HIS	-	expression tag	UNP O25242
B	-1	MET	-	expression tag	UNP O25242
B	0	ALA	-	expression tag	UNP O25242
B	375	GLU	-	expression tag	UNP O25242
B	376	LEU	-	expression tag	UNP O25242
B	377	HIS	-	expression tag	UNP O25242
B	378	HIS	-	expression tag	UNP O25242
B	379	HIS	-	expression tag	UNP O25242
B	380	HIS	-	expression tag	UNP O25242
B	381	HIS	-	expression tag	UNP O25242
B	382	HIS	-	expression tag	UNP O25242
C	-1	MET	-	expression tag	UNP O25242

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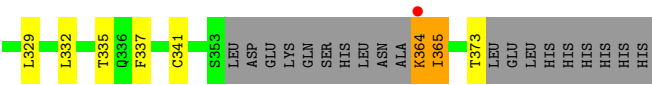
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ALA	-	expression tag	UNP O25242
C	375	GLU	-	expression tag	UNP O25242
C	376	LEU	-	expression tag	UNP O25242
C	377	HIS	-	expression tag	UNP O25242
C	378	HIS	-	expression tag	UNP O25242
C	379	HIS	-	expression tag	UNP O25242
C	380	HIS	-	expression tag	UNP O25242
C	381	HIS	-	expression tag	UNP O25242
C	382	HIS	-	expression tag	UNP O25242
D	-1	MET	-	expression tag	UNP O25242
D	0	ALA	-	expression tag	UNP O25242
D	375	GLU	-	expression tag	UNP O25242
D	376	LEU	-	expression tag	UNP O25242
D	377	HIS	-	expression tag	UNP O25242
D	378	HIS	-	expression tag	UNP O25242
D	379	HIS	-	expression tag	UNP O25242
D	380	HIS	-	expression tag	UNP O25242
D	381	HIS	-	expression tag	UNP O25242
D	382	HIS	-	expression tag	UNP O25242

- Molecule 2 is a protein called DNA LIGASE.

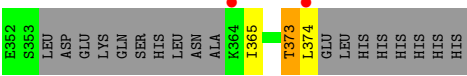
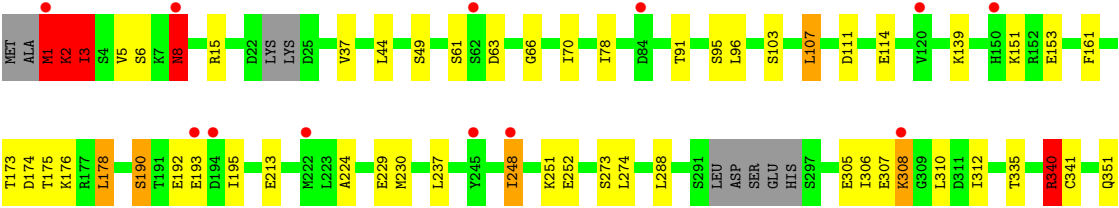
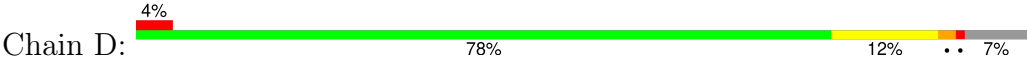
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	6	Total	C	N	O	0	0	0
			55	39	9	7			
2	L	6	Total	C	N	O	0	0	0
			55	39	9	7			

- Molecule 3 is water.

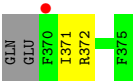
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	2	Total	O	0	0
			2	2		
3	C	3	Total	O	0	0
			3	3		
3	D	2	Total	O	0	0
			2	2		



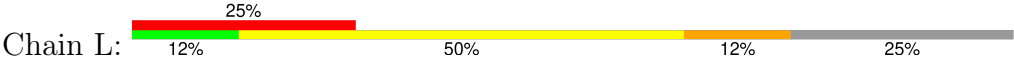
● Molecule 1: DNA POLYMERASE III SUBUNIT BETA



● Molecule 2: DNA LIGASE



● Molecule 2: DNA LIGASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.83Å 146.15Å 179.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.23 – 2.90 113.23 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.3 (113.23-2.90) 94.3 (113.23-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.231 , 0.262 0.236 , 0.265	Depositor DCC
R_{free} test set	1847 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11507	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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

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	0.83	0/2883	1.01	6/3876 (0.2%)
1	B	0.87	4/2930 (0.1%)	1.07	11/3942 (0.3%)
1	C	0.84	1/2887 (0.0%)	1.03	11/3882 (0.3%)
1	D	0.92	6/2874 (0.2%)	1.05	8/3865 (0.2%)
2	G	0.84	0/56	1.00	0/73
2	L	1.09	0/56	1.01	0/73
All	All	0.87	11/11686 (0.1%)	1.04	36/15711 (0.2%)

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	D	0	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	2	LYS	CA-C	12.87	1.64	1.52
1	B	295	GLU	CA-C	6.39	1.61	1.52
1	B	296	HIS	N-CA	5.90	1.53	1.46
1	D	8	ASN	CA-C	5.84	1.62	1.52
1	D	3	ILE	C-O	-5.71	1.18	1.24
1	D	151	LYS	CA-CB	5.52	1.60	1.53
1	C	175	THR	N-CA	5.49	1.53	1.46
1	D	8	ASN	N-CA	5.46	1.52	1.46
1	D	1	MET	CG-SD	5.13	1.93	1.80
1	B	293	ASP	N-CA	5.13	1.52	1.46
1	B	294	SER	CA-C	5.09	1.59	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	341	CYS	N-CA-C	17.79	137.16	114.56
1	C	174	ASP	N-CA-C	-11.39	91.96	109.96
1	A	122	ASP	CB-CA-C	10.28	120.34	110.17
1	A	122	ASP	N-CA-CB	8.63	122.76	110.07
1	D	1	MET	CG-SD-CE	8.27	119.10	100.90
1	B	297	SER	N-CA-C	8.06	120.06	111.28
1	B	293	ASP	N-CA-C	7.92	127.66	110.80
1	A	48	ASP	CB-CA-C	7.57	125.47	110.42
1	B	294	SER	N-CA-C	7.10	125.92	110.80
1	B	312	ILE	N-CA-C	6.99	118.42	108.42
1	D	2	LYS	CB-CA-C	6.83	122.60	111.26
1	D	2	LYS	O-C-N	-6.64	114.18	121.95
1	B	292	LEU	CB-CA-C	6.64	120.70	109.75
1	B	298	GLU	N-CA-C	6.62	118.84	110.24
1	D	2	LYS	CA-C-N	-6.28	113.09	122.70
1	D	2	LYS	C-N-CA	-6.28	113.09	122.70
1	C	365	ILE	N-CA-C	5.91	116.81	108.36
1	B	266	GLU	CB-CA-C	-5.86	101.06	110.79
1	C	280	LEU	CA-CB-CG	5.84	136.76	116.30
1	B	1	MET	CG-SD-CE	5.76	113.57	100.90
1	C	174	ASP	CA-C-N	-5.66	112.83	122.56
1	C	174	ASP	C-N-CA	-5.66	112.83	122.56
1	B	340	ARG	CG-CD-NE	-5.59	99.70	112.00
1	D	3	ILE	N-CA-CB	5.51	120.14	111.99
1	C	102	LYS	N-CA-C	5.44	122.39	110.80
1	B	298	GLU	CB-CA-C	-5.43	100.02	109.64
1	D	340	ARG	CG-CD-NE	-5.38	100.16	112.00
1	A	49	SER	N-CA-C	-5.38	107.98	114.75
1	C	8	ASN	N-CA-C	5.37	116.81	111.07
1	C	194	ASP	N-CA-C	-5.35	103.63	110.53
1	D	365	ILE	N-CA-C	5.28	115.91	108.36
1	A	150	HIS	CA-CB-CG	5.27	119.07	113.80
1	C	147	GLN	CB-CA-C	-5.14	101.12	110.63
1	C	177	ARG	CB-CG-CD	5.14	123.11	111.30
1	A	263	GLU	CA-CB-CG	5.06	124.21	114.10
1	C	101	ASN	CB-CA-C	-5.04	100.39	110.42

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	1	MET	Peptide
1	D	8	ASN	Peptide

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	2837	0	2901	24	0
1	B	2882	0	2942	60	0
1	C	2840	0	2910	38	0
1	D	2828	0	2888	48	0
2	G	55	0	57	4	0
2	L	55	0	57	5	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
All	All	11507	0	11755	153	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 7.

All (153) 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:1:MET:CE	1:D:2:LYS:O	1.78	1.32
1:D:1:MET:HE2	1:D:2:LYS:O	1.32	1.10
1:B:298:GLU:N	1:B:298:GLU:OE1	1.94	0.99
1:C:70:ILE:HD11	1:C:107:LEU:HD13	1.61	0.83
1:B:70:ILE:HD11	1:B:107:LEU:HD13	1.61	0.80
1:B:274:LEU:HD21	1:C:78:ILE:HD11	1.64	0.79
1:D:1:MET:HE1	1:D:2:LYS:HG3	1.65	0.78
1:B:340:ARG:NH1	1:B:351:GLN:OE1	2.19	0.75
1:C:70:ILE:HD12	1:C:96:LEU:HD23	1.69	0.75
1:A:70:ILE:HD12	1:A:96:LEU:HD23	1.68	0.74
1:D:70:ILE:HD12	1:D:96:LEU:HD23	1.69	0.73
1:B:70:ILE:HD12	1:B:96:LEU:HD23	1.69	0.73
1:D:176:LYS:HD3	2:L:371:ILE:HG21	1.71	0.72
1:D:1:MET:CE	1:D:2:LYS:HG3	2.22	0.69
1:B:298:GLU:HA	1:C:106:LYS:O	1.94	0.66
1:D:306:ILE:HD13	1:D:310:LEU:HD11	1.79	0.65
1:C:329:LEU:HA	1:C:332:LEU:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:ASN:N	1:D:8:ASN:OD1	2.32	0.63
1:C:70:ILE:HD11	1:C:107:LEU:CD1	2.28	0.63
1:B:70:ILE:HD11	1:B:107:LEU:CD1	2.29	0.62
1:B:307:GLU:OE1	1:D:305:GLU:HG3	1.98	0.62
1:A:370:MET:HG2	2:G:372:ARG:O	1.99	0.62
1:B:69:THR:H	1:B:109:MET:HE2	1.66	0.61
1:B:159:MET:HE1	1:B:217:PHE:CE2	2.36	0.61
1:D:1:MET:HE3	1:D:91:THR:H	1.65	0.61
1:A:32:HIS:ND1	1:A:69:THR:HG22	2.16	0.60
1:B:298:GLU:N	1:B:298:GLU:CD	2.59	0.59
1:C:69:THR:H	1:C:109:MET:HE2	1.68	0.58
1:C:140:LYS:HD3	1:C:365:ILE:HD12	1.87	0.57
1:D:229:GLU:HG2	1:D:230:MET:HE2	1.86	0.56
1:B:274:LEU:CD2	1:C:78:ILE:HD11	2.35	0.56
1:A:140:LYS:HD3	1:A:365:ILE:HD12	1.88	0.55
1:D:1:MET:CE	1:D:91:THR:H	2.20	0.55
1:D:5:VAL:HG23	1:D:61:SER:OG	2.06	0.55
1:A:270:LEU:HD21	1:D:103:SER:OG	2.06	0.55
1:A:370:MET:HE2	2:G:372:ARG:HB2	1.89	0.55
1:B:293:ASP:OD2	1:B:296:HIS:NE2	2.40	0.55
1:B:295:GLU:OE2	1:B:298:GLU:HB3	2.07	0.55
1:D:2:LYS:HB2	1:D:66:GLY:HA3	1.89	0.54
1:B:94:ASP:OD1	1:B:94:ASP:N	2.41	0.53
1:B:140:LYS:HD3	1:B:365:ILE:HD12	1.90	0.53
1:D:173:THR:HG21	2:L:375:PHE:CE2	2.43	0.53
1:D:190:SER:OG	1:D:192:GLU:O	2.27	0.53
1:A:190:SER:OG	1:A:192:GLU:O	2.27	0.52
1:B:68:GLY:CA	1:B:109:MET:CE	2.87	0.52
1:D:5:VAL:CG2	1:D:61:SER:OG	2.58	0.51
1:B:41:LYS:HE2	1:B:56:TYR:CE2	2.46	0.51
1:C:68:GLY:CA	1:C:109:MET:CE	2.88	0.51
1:D:78:ILE:CD1	1:D:107:LEU:HD11	2.40	0.51
1:B:45:LYS:HE2	1:B:54:LYS:HE2	1.93	0.51
1:B:270:LEU:HD12	1:C:81:CYS:HB3	1.92	0.51
1:C:94:ASP:OD1	1:C:94:ASP:N	2.41	0.51
1:B:106:LYS:HB2	1:C:299:THR:HB	1.93	0.50
1:A:101:ASN:HB2	1:B:335:THR:HG21	1.92	0.50
1:B:68:GLY:HA3	1:B:109:MET:HE1	1.93	0.50
1:B:68:GLY:HA3	1:B:109:MET:CE	2.40	0.50
1:B:159:MET:HE1	1:B:217:PHE:CZ	2.46	0.50
1:B:307:GLU:HG3	1:B:308:LYS:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:ASP:HB3	1:C:247:LYS:HD2	1.93	0.50
1:A:78:ILE:CD1	1:A:107:LEU:HD11	2.41	0.50
1:A:25:ASP:O	1:A:31:SER:OG	2.29	0.50
1:C:213:GLU:OE1	1:D:230:MET:HE1	2.12	0.50
1:C:68:GLY:HA3	1:C:109:MET:CE	2.41	0.50
1:B:293:ASP:OD2	1:B:296:HIS:CD2	2.65	0.49
1:B:307:GLU:HB2	1:D:305:GLU:CD	2.38	0.49
1:C:68:GLY:HA3	1:C:109:MET:HE1	1.95	0.49
1:A:41:LYS:HE2	1:A:56:TYR:CE2	2.47	0.49
1:D:224:ALA:HB2	1:D:237:LEU:HD21	1.93	0.49
1:D:252:GLU:HA	1:D:252:GLU:OE1	2.13	0.49
1:C:78:ILE:CD1	1:C:107:LEU:HD11	2.43	0.49
1:B:307:GLU:OE1	1:D:305:GLU:CG	2.61	0.49
1:A:224:ALA:HB2	1:A:237:LEU:HD21	1.95	0.48
1:B:190:SER:OG	1:B:192:GLU:O	2.29	0.48
1:B:307:GLU:CG	1:B:308:LYS:HD3	2.43	0.48
1:D:1:MET:SD	1:D:91:THR:OG1	2.65	0.48
1:D:1:MET:CG	1:D:2:LYS:O	2.56	0.48
1:C:230:MET:HE1	1:D:213:GLU:OE1	2.14	0.48
1:D:307:GLU:HG3	1:D:308:LYS:N	2.28	0.48
1:A:229:GLU:OE1	1:A:230:MET:HE2	2.13	0.48
1:B:224:ALA:HB2	1:B:237:LEU:HD21	1.95	0.48
1:B:161:PHE:HB2	1:B:195:ILE:HG23	1.96	0.47
1:C:332:LEU:CD2	1:C:337:PHE:HB2	2.44	0.47
1:C:224:ALA:HB2	1:C:237:LEU:HD21	1.95	0.47
1:D:1:MET:SD	1:D:91:THR:HG23	2.54	0.47
1:B:78:ILE:CD1	1:B:107:LEU:HD11	2.44	0.47
1:B:299:THR:O	1:C:105:PHE:HA	2.14	0.47
1:B:159:MET:CE	1:B:199:LEU:CD1	2.93	0.47
1:D:111:ASP:O	1:D:114:GLU:HG2	2.15	0.47
1:B:45:LYS:HE2	1:B:54:LYS:CE	2.44	0.47
1:C:100:GLN:O	1:C:101:ASN:C	2.57	0.47
1:D:70:ILE:CD1	1:D:96:LEU:HD23	2.42	0.47
1:C:161:PHE:HB2	1:C:195:ILE:HG23	1.97	0.47
1:A:70:ILE:HD11	1:A:107:LEU:HD13	1.97	0.46
1:D:174:ASP:O	1:D:175:THR:HB	2.15	0.46
1:D:229:GLU:CG	1:D:230:MET:HE2	2.46	0.46
1:C:70:ILE:CD1	1:C:96:LEU:HD23	2.42	0.46
1:A:70:ILE:CD1	1:A:96:LEU:HD23	2.41	0.46
1:D:340:ARG:NH1	1:D:351:GLN:NE2	2.64	0.45
1:D:373:THR:OG1	2:L:372:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:HA	1:D:37:VAL:HG23	1.97	0.45
1:A:81:CYS:SG	1:D:273:SER:HB3	2.57	0.45
1:B:295:GLU:CD	1:B:298:GLU:HB3	2.42	0.45
1:D:70:ILE:HD11	1:D:107:LEU:HD13	1.98	0.45
1:C:111:ASP:O	1:C:114:GLU:HG2	2.17	0.45
1:A:173:THR:HB	1:A:178:LEU:HD12	1.99	0.45
1:D:161:PHE:HB2	1:D:195:ILE:HG23	1.98	0.44
1:A:140:LYS:CD	1:A:365:ILE:HD12	2.47	0.44
1:B:295:GLU:HG2	1:B:298:GLU:OE1	2.16	0.44
1:B:105:PHE:HZ	1:C:270:LEU:HD22	1.83	0.44
1:B:307:GLU:HG3	1:B:308:LYS:HD3	2.00	0.44
1:D:173:THR:HB	1:D:178:LEU:HD12	1.99	0.44
1:C:173:THR:HB	1:C:178:LEU:HD12	2.00	0.44
1:B:294:SER:HB2	1:B:298:GLU:HG3	2.00	0.44
1:B:296:HIS:N	1:B:298:GLU:OE2	2.50	0.44
1:B:295:GLU:N	1:B:298:GLU:OE2	2.48	0.43
1:B:70:ILE:CD1	1:B:96:LEU:HD23	2.42	0.43
1:B:140:LYS:CD	1:B:365:ILE:HD12	2.49	0.43
1:D:307:GLU:CG	1:D:308:LYS:HD3	2.49	0.43
1:A:161:PHE:HB2	1:A:195:ILE:HG23	2.00	0.43
1:B:82:LEU:HD23	1:C:270:LEU:HD21	2.00	0.43
1:A:176:LYS:HD2	2:G:371:ILE:HB	2.01	0.43
1:D:15:ARG:HB3	1:D:15:ARG:HH11	1.83	0.43
1:B:294:SER:O	1:B:295:GLU:HB3	2.18	0.43
1:C:140:LYS:CD	1:C:365:ILE:HD12	2.47	0.42
1:B:222:MET:HE3	1:B:222:MET:HB3	1.94	0.42
1:C:11:GLU:O	1:C:15:ARG:HG3	2.19	0.42
1:C:68:GLY:CA	1:C:109:MET:HE2	2.49	0.42
1:C:152:ARG:HA	1:C:152:ARG:HD2	1.90	0.42
1:A:11:GLU:O	1:A:15:ARG:HG3	2.20	0.42
1:B:144:VAL:HG13	1:B:177:ARG:HG3	2.02	0.42
1:B:68:GLY:CA	1:B:109:MET:HE2	2.48	0.42
1:B:159:MET:CE	1:B:199:LEU:HD13	2.50	0.42
1:B:307:GLU:CB	1:D:305:GLU:HG3	2.49	0.42
1:C:332:LEU:CD2	1:C:337:PHE:CB	2.98	0.42
1:D:1:MET:SD	1:D:1:MET:O	2.78	0.42
1:B:159:MET:HE2	1:B:199:LEU:HD13	2.02	0.41
1:A:268:ILE:O	1:A:272:SER:HB2	2.20	0.41
1:B:174:ASP:O	1:B:175:THR:HB	2.20	0.41
1:C:181:THR:OG1	1:C:364:LYS:HG3	2.20	0.41
1:D:1:MET:HE3	1:D:91:THR:N	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:ILE:HG12	1:D:63:ASP:HB2	2.02	0.41
1:A:372:ILE:HG12	2:G:371:ILE:HG12	2.01	0.41
1:D:340:ARG:NH1	1:D:351:GLN:HE21	2.18	0.41
1:B:11:GLU:O	1:B:15:ARG:HG3	2.21	0.41
1:B:68:GLY:HA2	1:B:109:MET:HE2	2.03	0.41
1:B:173:THR:HB	1:B:178:LEU:HD12	2.01	0.41
1:B:8:ASN:HD22	1:B:8:ASN:HA	1.68	0.41
1:D:248:ILE:HD12	2:L:374:LEU:HG	2.02	0.41
1:A:32:HIS:HB3	1:A:69:THR:CG2	2.51	0.40
1:C:332:LEU:HD22	1:C:337:PHE:HB3	2.03	0.40
1:B:103:SER:OG	1:C:270:LEU:HD13	2.21	0.40
2:L:372:ARG:HB2	2:L:372:ARG:NH1	2.36	0.40
1:C:162:ASP:OD1	1:C:162:ASP:C	2.64	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	350/384 (91%)	334 (95%)	16 (5%)	0	100	100
1	B	358/384 (93%)	338 (94%)	16 (4%)	4 (1%)	11	36
1	C	352/384 (92%)	335 (95%)	15 (4%)	2 (1%)	21	51
1	D	349/384 (91%)	331 (95%)	18 (5%)	0	100	100
2	G	4/8 (50%)	4 (100%)	0	0	100	100
2	L	4/8 (50%)	4 (100%)	0	0	100	100
All	All	1417/1552 (91%)	1346 (95%)	65 (5%)	6 (0%)	30	59

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	293	ASP
1	B	294	SER
1	B	295	GLU
1	B	296	HIS
1	C	101	ASN
1	C	240	GLY

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	327/351 (93%)	304 (93%)	23 (7%)	14	40
1	B	332/351 (95%)	305 (92%)	27 (8%)	11	33
1	C	327/351 (93%)	304 (93%)	23 (7%)	14	40
1	D	326/351 (93%)	301 (92%)	25 (8%)	12	35
2	G	6/8 (75%)	6 (100%)	0	100	100
2	L	6/8 (75%)	4 (67%)	2 (33%)	0	0
All	All	1324/1420 (93%)	1224 (92%)	100 (8%)	12	36

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	6	SER
1	A	27	SER
1	A	44	LEU
1	A	94	ASP
1	A	95	SER
1	A	107	LEU
1	A	113	ASP
1	A	122	ASP
1	A	178	LEU
1	A	190	SER
1	A	248	ILE
1	A	252	GLU

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Mol	Chain	Res	Type
1	A	265	LYS
1	A	270	LEU
1	A	275	SER
1	A	288	LEU
1	A	292	LEU
1	A	305	GLU
1	A	335	THR
1	A	341	CYS
1	A	353	SER
1	A	373	THR
1	B	6	SER
1	B	8	ASN
1	B	24	LYS
1	B	44	LEU
1	B	49	SER
1	B	95	SER
1	B	120	VAL
1	B	124	LYS
1	B	178	LEU
1	B	190	SER
1	B	218	LYS
1	B	248	ILE
1	B	266	GLU
1	B	270	LEU
1	B	274	LEU
1	B	286	ASN
1	B	292	LEU
1	B	294	SER
1	B	297	SER
1	B	298	GLU
1	B	301	LYS
1	B	308	LYS
1	B	335	THR
1	B	340	ARG
1	B	341	CYS
1	B	353	SER
1	B	373	THR
1	C	6	SER
1	C	27	SER
1	C	44	LEU
1	C	49	SER
1	C	64	LYS

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Mol	Chain	Res	Type
1	C	95	SER
1	C	153	GLU
1	C	177	ARG
1	C	178	LEU
1	C	190	SER
1	C	251	LYS
1	C	265	LYS
1	C	275	SER
1	C	280	LEU
1	C	286	ASN
1	C	288	LEU
1	C	292	LEU
1	C	301	LYS
1	C	312	ILE
1	C	335	THR
1	C	341	CYS
1	C	364	LYS
1	C	373	THR
1	D	1	MET
1	D	2	LYS
1	D	3	ILE
1	D	6	SER
1	D	8	ASN
1	D	44	LEU
1	D	49	SER
1	D	95	SER
1	D	107	LEU
1	D	139	LYS
1	D	153	GLU
1	D	178	LEU
1	D	190	SER
1	D	193	GLU
1	D	248	ILE
1	D	251	LYS
1	D	274	LEU
1	D	288	LEU
1	D	308	LYS
1	D	312	ILE
1	D	335	THR
1	D	340	ARG
1	D	341	CYS
1	D	373	THR

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Mol	Chain	Res	Type
1	D	374	LEU
2	L	372	ARG
2	L	373	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	HIS
1	B	8	ASN
1	B	34	HIS
1	B	130	ASN
1	B	214	ASN
1	B	317	HIS
1	C	34	HIS
1	C	130	ASN
1	C	214	ASN
1	C	317	HIS
1	D	34	HIS
1	D	160	GLN
1	D	241	ASN
1	D	285	ASN
1	D	317	HIS

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 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, 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	358/384 (93%)	0.46	9 (2%) 58 48	49, 59, 69, 77	0
1	B	364/384 (94%)	0.65	23 (6%) 26 20	53, 64, 81, 90	0
1	C	358/384 (93%)	0.60	14 (3%) 43 35	54, 64, 75, 85	0
1	D	357/384 (92%)	0.59	14 (3%) 43 35	51, 60, 71, 78	0
2	G	6/8 (75%)	0.96	1 (16%) 4 3	62, 66, 70, 75	0
2	L	6/8 (75%)	1.94	2 (33%) 1 1	75, 77, 80, 86	0
All	All	1449/1552 (93%)	0.58	63 (4%) 40 31	49, 62, 75, 90	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	4.4
1	B	374	LEU	3.8
1	C	61	SER	3.6
1	B	297	SER	3.5
1	D	374	LEU	3.5
1	A	297	SER	3.4
1	B	343	GLU	3.3
1	B	130	ASN	3.3
1	C	150	HIS	3.2
2	L	375	PHE	3.1
1	C	62	SER	3.0
1	D	194	ASP	3.0
2	L	370	PHE	3.0
1	B	296	HIS	2.8
1	C	241	ASN	2.8
1	B	120	VAL	2.8
1	B	245	TYR	2.8
1	C	27	SER	2.8
1	C	298	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	312	ILE	2.7
1	D	62	SER	2.7
1	B	354	LEU	2.7
1	C	112	ALA	2.7
1	D	222	MET	2.7
1	D	248	ILE	2.6
1	B	310	LEU	2.5
1	B	313	GLU	2.5
1	A	81	CYS	2.5
1	B	114	GLU	2.5
1	D	8	ASN	2.5
1	D	193	GLU	2.4
1	B	364	LYS	2.4
1	C	299	THR	2.4
1	B	307	GLU	2.4
1	D	245	TYR	2.4
1	B	341	CYS	2.4
1	D	120	VAL	2.4
1	B	294	SER	2.4
2	G	370	PHE	2.4
1	D	364	LYS	2.3
1	A	84	ASP	2.3
1	B	84	ASP	2.3
1	C	191	THR	2.3
1	A	373	THR	2.2
1	B	230	MET	2.2
1	D	150	HIS	2.2
1	B	272	SER	2.2
1	B	298	GLU	2.2
1	C	193	GLU	2.2
1	D	308	LYS	2.2
1	A	353	SER	2.2
1	A	26	ALA	2.1
1	A	184	GLU	2.1
1	C	97	ALA	2.1
1	B	295	GLU	2.1
1	C	63	ASP	2.1
1	A	149	SER	2.1
1	C	364	LYS	2.0
1	C	8	ASN	2.0
1	B	26	ALA	2.0
1	D	84	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	150	HIS	2.0
1	B	293	ASP	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.