Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 01:32 am BST

PDB ID	:	5FRQ
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 following versions of software and data (see references ①) were used in the production of this report:

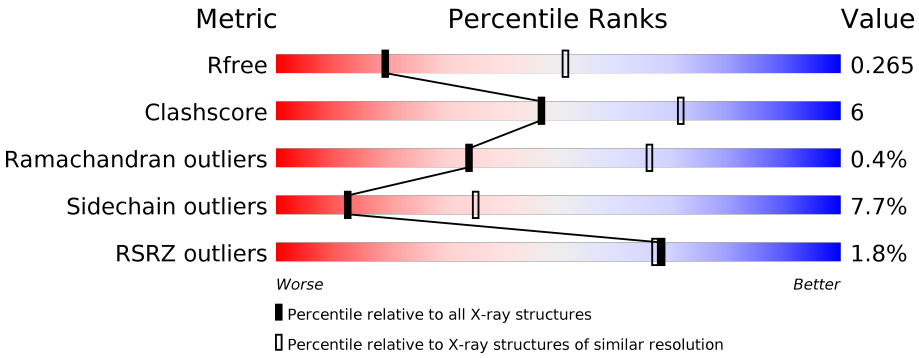
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 on 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 <=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% 12% • 7%
1	B	384	2% 77% 13% • • 5%
1	C	384	2% 77% 15% • 7%
1	D	384	% 78% 12% • • 7%
2	G	8	38% 38% 25%
2	L	8	13% 38% 25% 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.

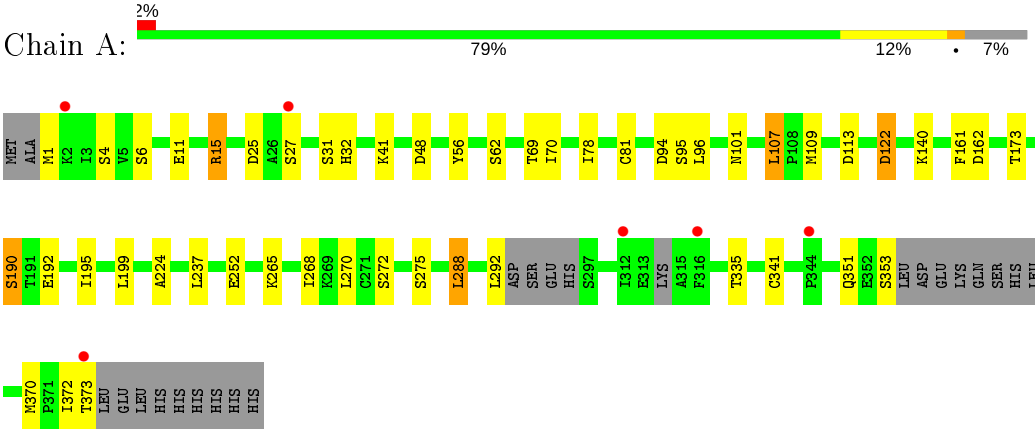
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	2	Total	O	0	0
			2	2		
3	C	3	Total	O	0	0
			3	3		
3	D	2	Total	O	0	0
			2	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

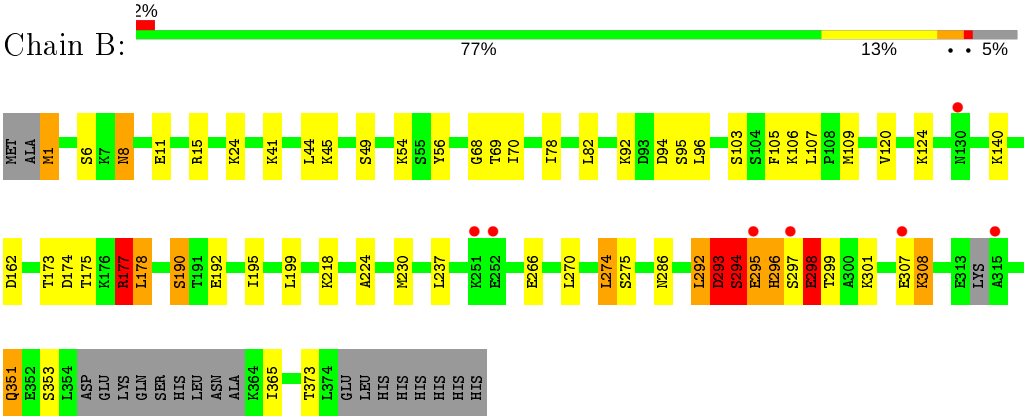
- Molecule 1: DNA POLYMERASE III SUBUNIT BETA

Chain A:



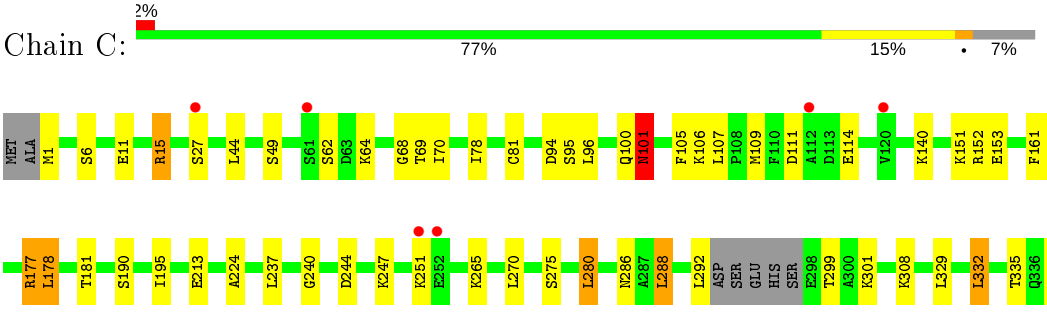
- Molecule 1: DNA POLYMERASE III SUBUNIT BETA

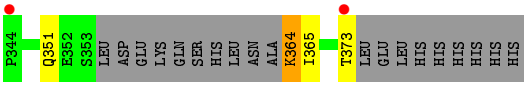
Chain B:



- Molecule 1: DNA POLYMERASE III SUBUNIT BETA

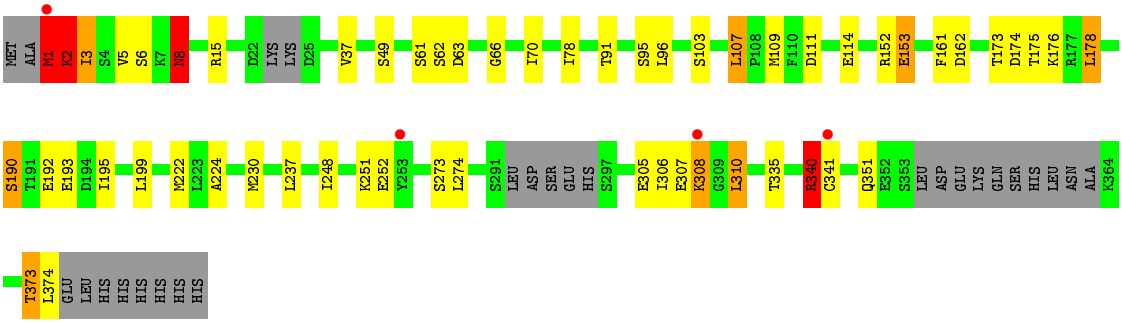
Chain C:





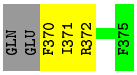
- Molecule 1: DNA POLYMERASE III SUBUNIT BETA

Chain D:



- Molecule 2: DNA LIGASE

Chain G:



- Molecule 2: DNA LIGASE

Chain L:

4 Data and refinement statistics (i)

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 42.64 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.3 (113.23-2.90) 94.3 (42.64-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.32 , 27.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.66	0/2883	0.88	12/3876 (0.3%)
1	B	0.67	0/2930	0.89	13/3942 (0.3%)
1	C	0.67	0/2887	0.91	11/3882 (0.3%)
1	D	0.71	1/2874 (0.0%)	0.92	10/3865 (0.3%)
2	G	0.67	0/56	0.98	0/73
2	L	0.84	0/56	1.13	1/73 (1.4%)
All	All	0.68	1/11686 (0.0%)	0.90	47/15711 (0.3%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	153	GLU	CD-OE1	5.16	1.31	1.25

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1	MET	CG-SD-CE	11.81	119.10	100.20
1	B	341	CYS	N-CA-C	9.69	137.16	111.00
1	C	280	LEU	CA-CB-CG	9.33	136.76	115.30
1	C	332	LEU	CB-CG-CD2	8.48	125.41	111.00
1	B	1	MET	CG-SD-CE	8.36	113.57	100.20
1	D	162	ASP	CB-CG-OD1	7.94	125.45	118.30
1	A	162	ASP	CB-CG-OD1	7.66	125.20	118.30
1	A	15	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	A	48	ASP	CB-CA-C	7.54	125.47	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	162	ASP	CB-CG-OD1	7.40	124.96	118.30
1	D	310	LEU	CA-CB-CG	7.18	131.82	115.30
1	C	15	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	C	174	ASP	N-CA-C	-7.05	91.96	111.00
1	B	92	LYS	CD-CE-NZ	7.01	127.82	111.70
1	A	122	ASP	N-CA-CB	6.76	122.76	110.60
1	C	162	ASP	CB-CG-OD2	6.65	124.28	118.30
1	A	288	LEU	CA-CB-CG	6.64	130.57	115.30
1	C	288	LEU	CA-CB-CG	6.62	130.53	115.30
1	C	1	MET	CG-SD-CE	6.57	110.71	100.20
1	A	199	LEU	CB-CG-CD1	6.38	121.84	111.00
1	D	310	LEU	CB-CG-CD1	-6.29	100.31	111.00
1	B	293	ASP	N-CA-C	6.17	127.66	111.00
1	D	2	LYS	CB-CA-C	6.10	122.60	110.40
1	C	177	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	D	199	LEU	CB-CG-CD1	6.02	121.23	111.00
1	A	15	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	162	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	A	162	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	1	MET	CG-SD-CE	5.81	109.50	100.20
1	B	340	ARG	CG-CD-NE	-5.76	99.70	111.80
1	A	109	MET	CG-SD-CE	5.61	109.18	100.20
1	C	174	ASP	CB-CA-C	5.59	121.59	110.40
1	C	15	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	159	MET	CG-SD-CE	-5.54	91.33	100.20
1	D	340	ARG	CG-CD-NE	-5.54	100.16	111.80
1	B	292	LEU	CB-CA-C	5.53	120.70	110.20
1	B	294	SER	N-CA-C	5.53	125.92	111.00
1	D	109	MET	CG-SD-CE	5.50	109.01	100.20
1	A	177	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	177	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	D	2	LYS	O-C-N	-5.33	114.18	122.70
1	D	222	MET	CG-SD-CE	5.29	108.66	100.20
1	B	230	MET	CG-SD-CE	5.28	108.65	100.20
1	B	298	GLU	CB-CA-C	-5.19	100.02	110.40
1	A	48	ASP	CB-CG-OD1	5.19	122.97	118.30
2	L	374	LEU	CA-CB-CG	5.12	127.08	115.30
1	C	101	ASN	CB-CA-C	-5.01	100.39	110.40

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 (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	2837	0	2901	22	0
1	B	2882	0	2942	58	0
1	C	2840	0	2910	37	0
1	D	2828	0	2888	43	0
2	G	55	0	57	3	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	144	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 6.

All (144) 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:HE3	1:D:2:LYS:O	1.47	1.13
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: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:D:1:MET:HE2	1:D:2:LYS:O	1.86	0.73
1:B:70:ILE:HD12	1:B:96:LEU:HD23	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:8:ASN:OD1	1:D:8:ASN:N	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:A:32:HIS:ND1	1:A:69:THR:HG22	2.16	0.60
1:B:159:MET:HE2	1:B:199:LEU:HD13	1.85	0.59
1:C:140:LYS:HD3	1:C:365:ILE:HD12	1.87	0.57
1:D:1:MET:HE2	1:D:2:LYS:HG3	1.85	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:5:VAL:HG23	1:D:61:SER:OG	2.06	0.55
1:D:1:MET:CE	1:D:91:THR:H	2.20	0.55
1:A:270:LEU:HD21	1:D:103:SER:OG	2.06	0.55
1:B:293:ASP:OD2	1:B:296:HIS:NE2	2.40	0.55
1:B:69:THR:H	1:B:109:MET:HE2	1.72	0.55
1:B:295:GLU:OE2	1:B:298:GLU:HB3	2.07	0.55
1:B:298:GLU:N	1:B:298:GLU:CD	2.59	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:N	1:C:94:ASP:OD1	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:CE	2.40	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:C:68:GLY:HA2	1:C:109:MET:HE2	1.93	0.50
1:A:25:ASP:O	1:A:31:SER:OG	2.29	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:68:GLY:HA3	1:B: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:OE1	1:D:252:GLU:HA	2.13	0.49
1:C:68:GLY:CA	1:C:109:MET:HE2	2.42	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:CG	1:D:2:LYS:O	2.56	0.48
1:D:307:GLU:HG3	1:D:308:LYS:N	2.28	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:C:69:THR:H	1:C:109:MET:HE2	1.80	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:B:68:GLY:HA2	1:B:109:MET:HE2	1.97	0.47
1:C:213:GLU:OE1	1:D:230:MET:HE3	2.15	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:B:68:GLY:CA	1:B:109:MET:HE2	2.44	0.46
1:D:174:ASP:O	1:D:175:THR:HB	2.15	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:C:68:GLY:HA3	1:C:109:MET:HE1	1.98	0.45
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: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:B:307:GLU:HB2	1:D:305:GLU:CD	2.38	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:140:LYS:CD	1:B:365:ILE:HD12	2.49	0.43
1:B:70:ILE:CD1	1:B:96:LEU:HD23	2.42	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:D:15:ARG:HB3	1:D:15:ARG:HH11	1.83	0.43
1:A:176:LYS:HD2	2:G:371:ILE:HB	2.01	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:C:11:GLU:O	1:C:15:ARG:HG3	2.19	0.42
1:C:100:GLN:O	1:C:101:ASN:C	2.57	0.42
1:C:152:ARG:HD2	1:C:152:ARG:HA	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:MET:HE2	1:B:199:LEU:CD1	2.51	0.41
1:B:173:THR:HB	1:B:178:LEU:HD12	2.01	0.41
1:B:8:ASN:HA	1:B:8:ASN:HD22	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:295:GLU:CD	1:B:298:GLU:HB3	2.42	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

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%)	14 42
1	C	352/384 (92%)	335 (95%)	15 (4%)	2 (1%)	25 58
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%)	34 66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	293	ASP
1	B	294	SER
1	B	295	GLU

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Mol	Chain	Res	Type
1	B	296	HIS
1	C	101	ASN
1	C	240	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	327/351 (93%)	305 (93%)	22 (7%)	16 43
1	B	332/351 (95%)	303 (91%)	29 (9%)	10 30
1	C	327/351 (93%)	301 (92%)	26 (8%)	12 33
1	D	326/351 (93%)	304 (93%)	22 (7%)	16 43
2	G	6/8 (75%)	5 (83%)	1 (17%)	2 6
2	L	6/8 (75%)	4 (67%)	2 (33%)	0 0
All	All	1324/1420 (93%)	1222 (92%)	102 (8%)	13 35

All (102) 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	62	SER
1	A	94	ASP
1	A	95	SER
1	A	107	LEU
1	A	113	ASP
1	A	122	ASP
1	A	177	ARG
1	A	178	LEU
1	A	190	SER
1	A	252	GLU
1	A	265	LYS
1	A	275	SER

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Mol	Chain	Res	Type
1	A	288	LEU
1	A	292	LEU
1	A	335	THR
1	A	341	CYS
1	A	351	GLN
1	A	353	SER
1	A	373	THR
1	B	1	MET
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	177	ARG
1	B	178	LEU
1	B	190	SER
1	B	218	LYS
1	B	266	GLU
1	B	274	LEU
1	B	275	SER
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	351	GLN
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	62	SER
1	C	64	LYS

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Mol	Chain	Res	Type
1	C	95	SER
1	C	151	LYS
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	308	LYS
1	C	335	THR
1	C	341	CYS
1	C	351	GLN
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	49	SER
1	D	62	SER
1	D	95	SER
1	D	107	LEU
1	D	152	ARG
1	D	153	GLU
1	D	178	LEU
1	D	190	SER
1	D	193	GLU
1	D	251	LYS
1	D	274	LEU
1	D	308	LYS
1	D	335	THR
1	D	340	ARG
1	D	341	CYS
1	D	373	THR
1	D	374	LEU

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Mol	Chain	Res	Type
2	G	370	PHE
2	L	372	ARG
2	L	373	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	8	ASN
1	B	165	HIS
1	D	130	ASN
1	D	241	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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%)	0.17	6 (1%) 70 69	49, 59, 69, 77	0
1	B	364/384 (94%)	0.16	7 (1%) 66 65	53, 64, 81, 90	0
1	C	358/384 (93%)	0.23	9 (2%) 57 55	54, 64, 75, 85	0
1	D	357/384 (92%)	0.13	4 (1%) 80 80	51, 60, 71, 78	0
2	G	6/8 (75%)	0.33	0 100 100	62, 66, 70, 75	0
2	L	6/8 (75%)	0.73	0 100 100	75, 77, 80, 86	0
All	All	1449/1552 (93%)	0.17	26 (1%) 68 67	49, 62, 75, 90	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	4.3
1	A	344	PRO	3.5
1	C	252	GLU	3.3
1	A	316	PHE	3.2
1	A	312	ILE	3.1
1	B	130	ASN	3.1
1	C	344	PRO	3.1
1	C	112	ALA	3.0
1	C	120	VAL	2.7
1	C	27	SER	2.6
1	D	308	LYS	2.5
1	B	307	GLU	2.5
1	C	373	THR	2.4
1	A	2	LYS	2.3
1	B	251	LYS	2.3
1	B	315	ALA	2.2
1	C	341	CYS	2.2
1	C	251	LYS	2.2
1	A	373	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	252	GLU	2.1
1	B	297	SER	2.1
1	D	341	CYS	2.1
1	D	253	TYR	2.1
1	B	295	GLU	2.0
1	A	27	SER	2.0
1	C	61	SER	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 carbohydrates 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.