Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2024 – 10:12 AM EDT

PDB ID	:	4LJK
Title	:	Structural insights into the unique single-stranded DNA binding mode of DNA processing protein A from Helicobacter pylori
Authors	:	Wang, W.
Deposited on	:	2013-07-05
Resolution	:	2.35 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:

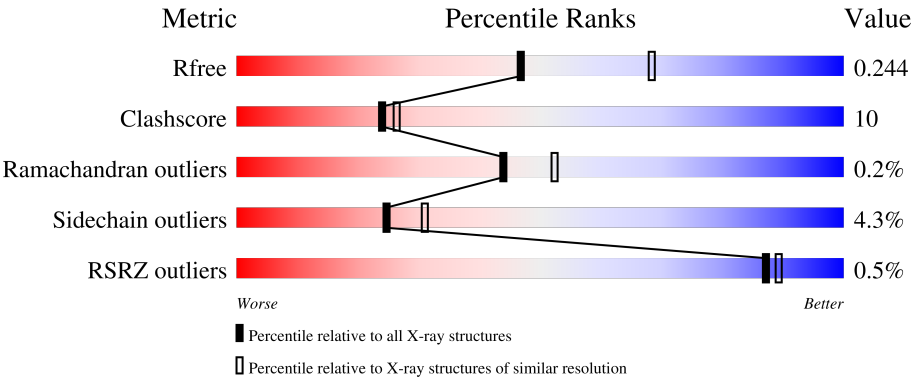
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.35 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}	164625	1460 (2.36-2.36)
Clashscore	180529	1571 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)
RSRZ outliers	164620	1460 (2.36-2.36)

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 <=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	229	74% 20% 6%
1	B	229	75% 17% • 5%
1	C	229	74% 19% • 6%
1	D	229	75% 17% • 6%
1	E	229	77% 17% 6%

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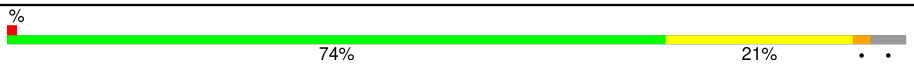
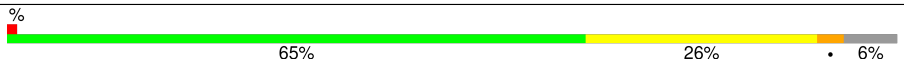
Mol	Chain	Length	Quality of chain
1	F	229	
1	G	229	
1	H	229	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13865 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 processing chain A (DprA).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	Se	0	0	0
			1689	1084	287	312	2	4			
1	B	217	Total	C	N	O	S	Se	0	0	0
			1698	1090	289	313	2	4			
1	E	216	Total	C	N	O	S	Se	0	0	0
			1689	1084	287	312	2	4			
1	F	220	Total	C	N	O	S	Se	0	0	0
			1722	1105	292	318	2	5			
1	H	215	Total	C	N	O	S	Se	0	0	0
			1681	1078	286	311	2	4			
1	C	216	Total	C	N	O	S	Se	0	0	0
			1689	1084	287	312	2	4			
1	D	215	Total	C	N	O	S	Se	0	0	0
			1681	1078	286	311	2	4			
1	G	214	Total	C	N	O	S	Se	0	0	0
			1671	1072	283	310	2	4			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	226	LEU	-	expression tag	UNP O25100
A	227	GLU	-	expression tag	UNP O25100
A	228	HIS	-	expression tag	UNP O25100
A	229	HIS	-	expression tag	UNP O25100
A	230	HIS	-	expression tag	UNP O25100
A	231	HIS	-	expression tag	UNP O25100
A	232	HIS	-	expression tag	UNP O25100
A	233	HIS	-	expression tag	UNP O25100
B	226	LEU	-	expression tag	UNP O25100
B	227	GLU	-	expression tag	UNP O25100
B	228	HIS	-	expression tag	UNP O25100
B	229	HIS	-	expression tag	UNP O25100
B	230	HIS	-	expression tag	UNP O25100

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Chain	Residue	Modelled	Actual	Comment	Reference
B	231	HIS	-	expression tag	UNP O25100
B	232	HIS	-	expression tag	UNP O25100
B	233	HIS	-	expression tag	UNP O25100
E	226	LEU	-	expression tag	UNP O25100
E	227	GLU	-	expression tag	UNP O25100
E	228	HIS	-	expression tag	UNP O25100
E	229	HIS	-	expression tag	UNP O25100
E	230	HIS	-	expression tag	UNP O25100
E	231	HIS	-	expression tag	UNP O25100
E	232	HIS	-	expression tag	UNP O25100
E	233	HIS	-	expression tag	UNP O25100
F	226	LEU	-	expression tag	UNP O25100
F	227	GLU	-	expression tag	UNP O25100
F	228	HIS	-	expression tag	UNP O25100
F	229	HIS	-	expression tag	UNP O25100
F	230	HIS	-	expression tag	UNP O25100
F	231	HIS	-	expression tag	UNP O25100
F	232	HIS	-	expression tag	UNP O25100
F	233	HIS	-	expression tag	UNP O25100
H	226	LEU	-	expression tag	UNP O25100
H	227	GLU	-	expression tag	UNP O25100
H	228	HIS	-	expression tag	UNP O25100
H	229	HIS	-	expression tag	UNP O25100
H	230	HIS	-	expression tag	UNP O25100
H	231	HIS	-	expression tag	UNP O25100
H	232	HIS	-	expression tag	UNP O25100
H	233	HIS	-	expression tag	UNP O25100
C	226	LEU	-	expression tag	UNP O25100
C	227	GLU	-	expression tag	UNP O25100
C	228	HIS	-	expression tag	UNP O25100
C	229	HIS	-	expression tag	UNP O25100
C	230	HIS	-	expression tag	UNP O25100
C	231	HIS	-	expression tag	UNP O25100
C	232	HIS	-	expression tag	UNP O25100
C	233	HIS	-	expression tag	UNP O25100
D	226	LEU	-	expression tag	UNP O25100
D	227	GLU	-	expression tag	UNP O25100
D	228	HIS	-	expression tag	UNP O25100
D	229	HIS	-	expression tag	UNP O25100
D	230	HIS	-	expression tag	UNP O25100
D	231	HIS	-	expression tag	UNP O25100
D	232	HIS	-	expression tag	UNP O25100

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Chain	Residue	Modelled	Actual	Comment	Reference
D	233	HIS	-	expression tag	UNP O25100
G	226	LEU	-	expression tag	UNP O25100
G	227	GLU	-	expression tag	UNP O25100
G	228	HIS	-	expression tag	UNP O25100
G	229	HIS	-	expression tag	UNP O25100
G	230	HIS	-	expression tag	UNP O25100
G	231	HIS	-	expression tag	UNP O25100
G	232	HIS	-	expression tag	UNP O25100
G	233	HIS	-	expression tag	UNP O25100

- Molecule 2 is water.

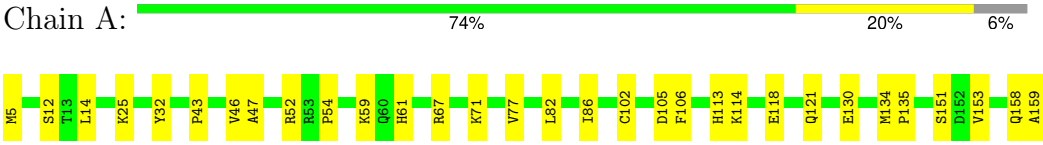
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	40	Total O 40 40	0	0
2	B	60	Total O 60 60	0	0
2	E	36	Total O 36 36	0	0
2	F	51	Total O 51 51	0	0
2	H	30	Total O 30 30	0	0
2	C	53	Total O 53 53	0	0
2	D	42	Total O 42 42	0	0
2	G	33	Total O 33 33	0	0

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.

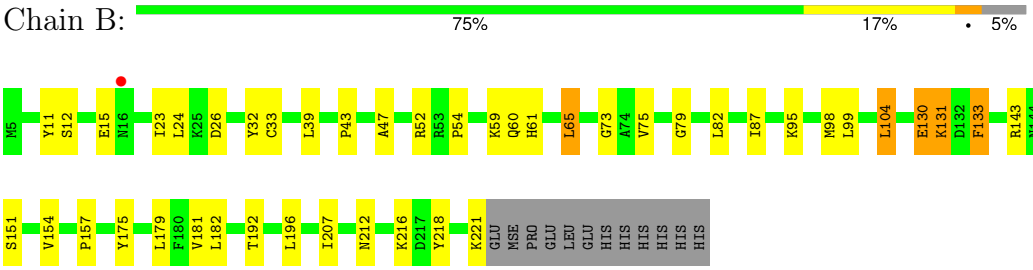
• Molecule 1: DNA processing chain A (DprA)

Chain A:



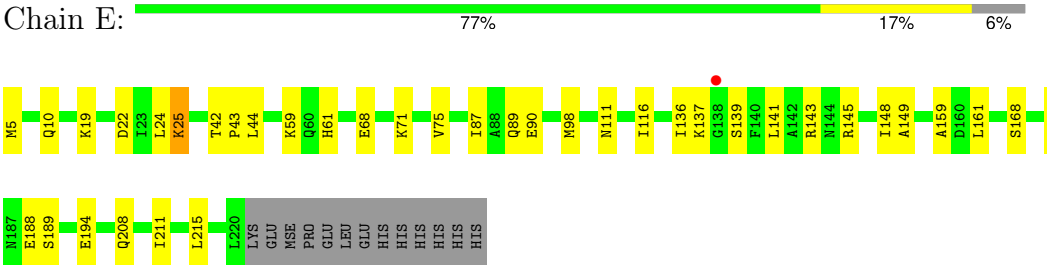
• Molecule 1: DNA processing chain A (DprA)

Chain B:



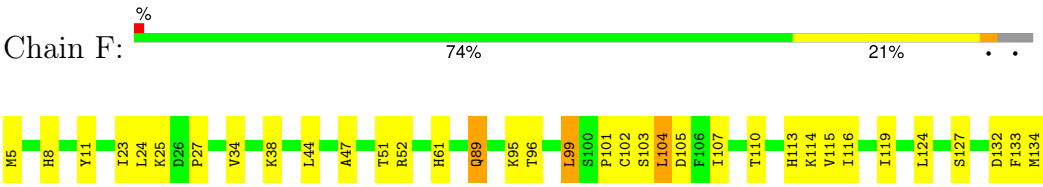
• Molecule 1: DNA processing chain A (DprA)

Chain E:



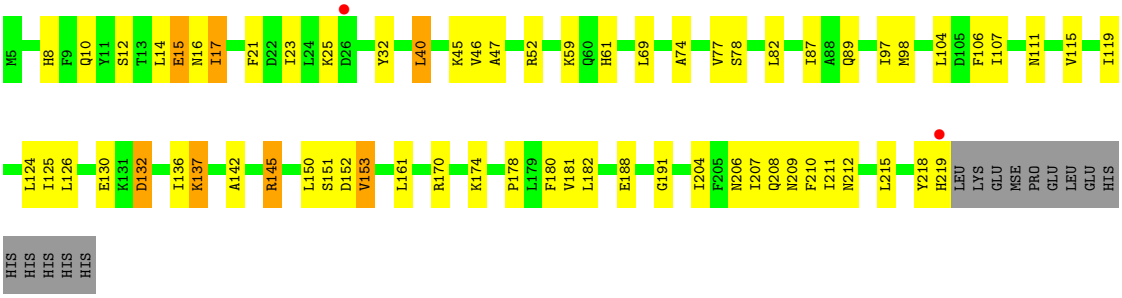
• Molecule 1: DNA processing chain A (DprA)

Chain F:



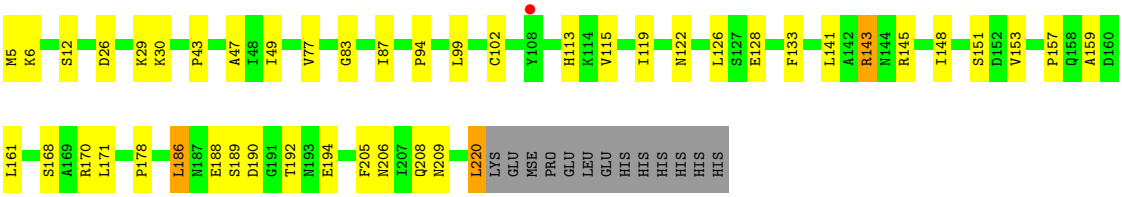
• Molecule 1: DNA processing chain A (DprA)

Chain H:



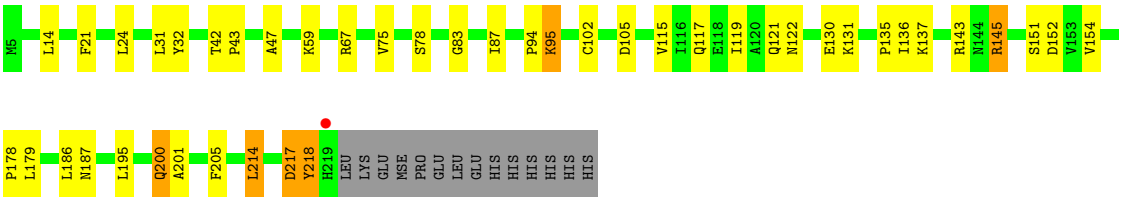
• Molecule 1: DNA processing chain A (DprA)

Chain C:



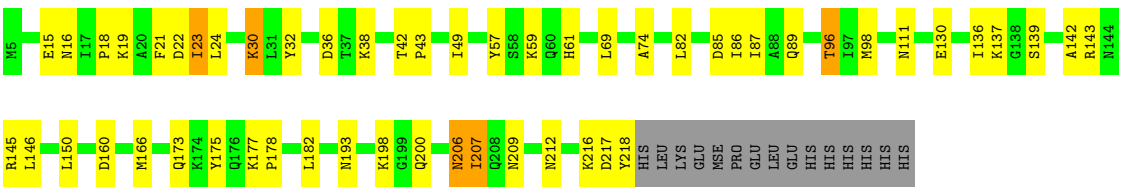
• Molecule 1: DNA processing chain A (DprA)

Chain D:



• Molecule 1: DNA processing chain A (DprA)

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	117.88Å 42.43Å 181.33Å 90.00° 108.65° 90.00°	Depositor
Resolution (Å)	59.23 – 2.35 59.23 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.9 (59.23-2.35) 98.9 (59.23-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.24 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.186 , 0.254 0.180 , 0.244	Depositor DCC
R_{free} test set	3585 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	36.9	Xtriage
Anisotropy	0.948	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13865	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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	0.40	0/1717	0.55	0/2319
1	B	0.37	0/1726	0.54	0/2330
1	C	0.40	0/1717	0.55	0/2319
1	D	0.40	0/1709	0.54	0/2308
1	E	0.38	0/1717	0.54	0/2319
1	F	0.40	0/1750	0.56	0/2361
1	G	0.36	0/1698	0.53	0/2293
1	H	0.35	0/1709	0.52	0/2308
All	All	0.38	0/13743	0.54	0/18557

There are no bond length outliers.

There are no bond angle outliers.

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	1689	0	1755	29	0
1	B	1698	0	1768	38	0
1	C	1689	0	1755	25	0
1	D	1681	0	1744	28	0
1	E	1689	0	1755	30	0
1	F	1722	0	1790	42	0
1	G	1671	0	1737	47	0
1	H	1681	0	1744	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	40	0	0	1	0
2	B	60	0	0	2	0
2	C	53	0	0	1	0
2	D	42	0	0	1	0
2	E	36	0	0	5	0
2	F	51	0	0	3	0
2	G	33	0	0	3	0
2	H	30	0	0	6	0
All	All	13865	0	14048	273	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 10.

All (273) 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:G:15:GLU:HG2	1:G:16:ASN:H	1.29	0.92
1:F:136:ILE:H	1:F:139:SER:HB3	1.36	0.89
1:H:215:LEU:O	1:H:219:HIS:HB2	1.73	0.89
1:G:173:GLN:HE22	1:G:200:GLN:HB3	1.38	0.88
1:B:73:GLY:HA2	1:B:95:LYS:HZ3	1.37	0.87
1:D:14:LEU:O	2:D:323:HOH:O	1.92	0.86
1:F:5:MSE:HE2	1:F:107:ILE:HD12	1.60	0.83
1:B:212:ASN:O	1:B:216:LYS:HD3	1.79	0.82
1:H:170:ARG:O	2:H:324:HOH:O	1.99	0.81
1:G:173:GLN:NE2	1:G:200:GLN:HB3	1.96	0.80
1:A:185:ARG:HB2	1:A:188:GLU:HG3	1.65	0.79
1:F:177:LYS:O	2:F:318:HOH:O	2.02	0.78
1:E:59:LYS:HG3	1:E:87:ILE:HD13	1.66	0.76
1:B:73:GLY:HA2	1:B:95:LYS:NZ	2.00	0.76
1:F:89:GLN:HG3	1:F:96:THR:OG1	1.85	0.76
1:F:11:TYR:HB3	1:F:34:VAL:CG2	2.15	0.76
1:F:134:MSE:HE3	1:F:135:PRO:HD2	1.70	0.73
1:F:102:CYS:SG	2:F:336:HOH:O	2.47	0.72
1:G:18:PRO:HG2	1:G:21:PHE:CE2	2.24	0.72
1:F:34:VAL:HG23	1:F:104:LEU:CD2	2.19	0.72
1:C:128:GLU:OE2	2:C:348:HOH:O	2.07	0.71
1:F:104:LEU:HD12	1:F:127:SER:HB3	1.73	0.71
1:G:15:GLU:HG2	1:G:16:ASN:N	2.06	0.70
1:A:61:HIS:HB2	1:A:182:LEU:HD21	1.73	0.70
1:F:99:LEU:O	1:F:143:ARG:HD3	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:GLU:HG2	1:B:131:LYS:HG2	1.74	0.70
1:D:102:CYS:HB3	1:D:135:PRO:HG3	1.75	0.69
1:B:11:TYR:HB2	1:B:33:CYS:O	1.93	0.68
1:D:195:LEU:HD23	1:D:200:GLN:HE21	1.60	0.67
1:F:103:SER:HB3	1:F:133:PHE:HB3	1.77	0.66
1:A:5:MSE:SE	1:C:178:PRO:HG3	2.46	0.66
1:H:59:LYS:HG3	1:H:87:ILE:HD13	1.78	0.66
1:G:24:LEU:HD21	1:G:145:ARG:HG3	1.77	0.65
1:G:206:ASN:HD22	1:G:207:ILE:N	1.95	0.64
1:F:142:ALA:O	1:F:145:ARG:HG2	1.98	0.63
1:G:160:ASP:OD1	2:G:302:HOH:O	2.15	0.63
1:H:180:PHE:HB3	1:H:204:ILE:HD11	1.80	0.62
1:B:23:ILE:HD12	1:B:175:TYR:HB3	1.82	0.62
1:H:150:LEU:O	1:H:150:LEU:HD23	2.00	0.62
1:F:11:TYR:HB3	1:F:34:VAL:HG22	1.81	0.61
1:D:42:THR:HG21	1:D:75:VAL:HG23	1.82	0.61
1:D:154:VAL:HB	1:D:179:LEU:HD12	1.83	0.61
1:G:23:ILE:CD1	1:G:175:TYR:HB3	2.31	0.61
1:G:89:GLN:HE21	1:G:96:THR:HG22	1.66	0.61
1:B:99:LEU:O	1:B:143:ARG:HD2	2.00	0.60
1:E:24:LEU:HD13	1:E:145:ARG:HD2	1.83	0.60
1:E:98:MSE:HE1	1:E:116:ILE:HD13	1.81	0.60
1:A:106:PHE:CD1	1:A:134:MSE:HE3	2.36	0.60
1:F:23:ILE:HD12	1:F:175:TYR:HB3	1.81	0.60
1:H:45:LYS:HD3	1:H:150:LEU:CD2	2.32	0.60
1:G:206:ASN:HB3	1:G:209:ASN:HB2	1.83	0.60
1:H:61:HIS:HB2	1:H:182:LEU:HD21	1.83	0.60
1:B:133:PHE:C	1:B:133:PHE:CD2	2.75	0.60
1:C:5:MSE:HE1	1:C:113:HIS:CD2	2.38	0.59
1:D:179:LEU:HD23	1:D:201:ALA:HB2	1.84	0.59
1:C:161:LEU:HD21	1:C:194:GLU:HG3	1.84	0.59
1:E:188:GLU:OE1	2:E:330:HOH:O	2.17	0.58
1:G:206:ASN:HD22	1:G:206:ASN:C	2.07	0.58
1:B:59:LYS:HG2	1:B:87:ILE:HD13	1.85	0.58
1:E:5:MSE:N	2:E:334:HOH:O	2.36	0.58
1:E:25:LYS:HD2	1:E:25:LYS:N	2.19	0.58
1:E:183:PRO:HG2	1:C:186:LEU:CD1	2.34	0.58
1:H:208:GLN:HE21	1:H:212:ASN:HD21	1.52	0.57
1:D:83:GLY:O	1:D:87:ILE:HG13	2.03	0.57
1:A:25:LYS:HD2	1:A:174:LYS:HZ1	1.68	0.57
1:F:104:LEU:HD12	1:F:127:SER:CB	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:TYR:CZ	1:B:130:GLU:HB2	2.40	0.57
1:H:208:GLN:NE2	1:H:212:ASN:HD21	2.03	0.57
1:F:89:GLN:HG2	1:F:119:ILE:CD1	2.35	0.57
1:C:206:ASN:HB3	1:C:209:ASN:HB2	1.87	0.56
1:C:29:LYS:HG3	1:C:30:LYS:N	2.20	0.56
1:G:136:ILE:H	1:G:139:SER:HB3	1.69	0.56
1:E:183:PRO:HG2	1:C:186:LEU:HD13	1.86	0.56
1:D:218:TYR:N	1:D:218:TYR:CD2	2.73	0.56
1:B:79:GLY:O	1:B:98:MSE:HE3	2.05	0.56
1:G:89:GLN:HE21	1:G:96:THR:CG2	2.18	0.56
1:H:188:GLU:OE1	2:H:316:HOH:O	2.18	0.55
1:B:54:PRO:HG2	1:B:59:LYS:HD2	1.89	0.55
1:B:32:TYR:OH	1:B:130:GLU:HB2	2.06	0.55
1:G:212:ASN:O	1:G:216:LYS:HG2	2.07	0.55
1:B:130:GLU:HG2	1:B:131:LYS:CG	2.36	0.55
1:G:21:PHE:O	1:G:24:LEU:HB2	2.07	0.55
1:G:89:GLN:HE22	1:G:98:MSE:HB2	1.71	0.55
1:F:34:VAL:HG23	1:F:104:LEU:HD23	1.89	0.54
1:B:47:ALA:HB2	1:B:151:SER:OG	2.06	0.54
1:E:42:THR:HG21	1:E:75:VAL:HG23	1.90	0.54
1:B:133:PHE:C	1:B:133:PHE:HD2	2.11	0.54
1:G:24:LEU:CD2	1:G:145:ARG:HG3	2.38	0.53
1:A:102:CYS:HB3	1:A:135:PRO:HG3	1.92	0.53
1:E:143:ARG:HD2	1:E:143:ARG:C	2.29	0.53
1:E:136:ILE:HD12	1:E:139:SER:H	1.75	0.52
1:F:115:VAL:O	1:F:119:ILE:HG13	2.09	0.52
1:F:61:HIS:HB2	1:F:182:LEU:HD21	1.90	0.52
1:A:54:PRO:HG2	1:A:59:LYS:HE2	1.91	0.52
1:C:99:LEU:HD13	1:C:126:LEU:HB2	1.92	0.52
1:A:158:GLN:HG3	1:A:189:SER:HB3	1.92	0.52
1:A:32:TYR:CE1	1:A:130:GLU:HG3	2.46	0.51
1:C:49:ILE:O	1:C:157:PRO:HD2	2.10	0.51
1:H:46:VAL:HG22	1:H:153:VAL:HG13	1.91	0.51
1:H:69:LEU:HB3	1:H:74:ALA:HB3	1.93	0.51
1:G:18:PRO:HG2	1:G:21:PHE:HE2	1.70	0.51
1:H:106:PHE:HE2	1:H:132:ASP:HA	1.76	0.51
1:B:216:LYS:HD3	1:B:216:LYS:H	1.76	0.51
1:F:110:THR:O	1:F:113:HIS:HB3	2.10	0.50
1:B:12:SER:HB2	2:B:360:HOH:O	2.10	0.50
1:C:190:ASP:O	1:C:194:GLU:HB2	2.11	0.50
1:E:111:ASN:ND2	2:E:325:HOH:O	2.33	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:VAL:HB	1:B:179:LEU:HD23	1.94	0.50
1:E:61:HIS:ND1	2:E:310:HOH:O	2.35	0.50
1:E:42:THR:HG23	1:E:43:PRO:HD2	1.93	0.50
1:D:94:PRO:HB3	1:D:122:ASN:HB3	1.93	0.50
1:G:216:LYS:C	1:G:218:TYR:H	2.14	0.50
1:B:43:PRO:HB3	1:B:218:TYR:OH	2.12	0.49
1:F:107:ILE:HG23	1:F:116:ILE:HG21	1.93	0.49
1:D:218:TYR:H	1:D:218:TYR:HD2	1.56	0.49
1:H:181:VAL:O	1:H:204:ILE:HD12	2.12	0.49
1:G:69:LEU:O	1:G:74:ALA:HB3	2.12	0.49
1:C:47:ALA:HB2	1:C:151:SER:OG	2.13	0.49
1:F:101:PRO:O	1:F:139:SER:OG	2.30	0.49
1:D:217:ASP:N	1:D:217:ASP:OD1	2.45	0.49
1:H:25:LYS:HE3	1:H:174:LYS:NZ	2.28	0.48
1:G:36:ASP:OD1	1:G:38:LYS:HB2	2.12	0.48
1:G:150:LEU:O	1:G:150:LEU:HG	2.13	0.48
1:E:211:ILE:O	1:E:215:LEU:HG	2.13	0.48
1:F:24:LEU:O	1:F:27:PRO:HD3	2.13	0.48
1:B:24:LEU:HD21	1:B:149:ALA:HB2	1.95	0.48
1:F:89:GLN:HG2	1:F:119:ILE:HD11	1.96	0.48
1:A:5:MSE:HE1	1:A:113:HIS:CG	2.49	0.48
1:D:145:ARG:HE	1:D:145:ARG:HB3	1.44	0.48
1:G:32:TYR:CE2	1:G:130:GLU:HA	2.49	0.48
1:H:211:ILE:O	1:H:215:LEU:HG	2.13	0.48
1:A:105:ASP:HA	2:A:316:HOH:O	2.12	0.48
1:H:8:HIS:N	2:H:313:HOH:O	2.05	0.48
1:H:115:VAL:O	1:H:119:ILE:HG13	2.13	0.48
1:C:170:ARG:HA	1:C:170:ARG:HD3	1.74	0.47
1:B:32:TYR:CE2	1:B:130:GLU:HA	2.49	0.47
1:H:47:ALA:HB2	1:H:151:SER:OG	2.14	0.47
1:F:185:ARG:HB3	1:G:57:TYR:CE1	2.49	0.47
1:G:42:THR:CG2	1:G:43:PRO:HD2	2.45	0.47
1:E:148:ILE:HD11	1:E:168:SER:HB3	1.96	0.47
1:F:102:CYS:HB2	1:F:133:PHE:O	2.14	0.47
1:C:43:PRO:HG2	1:C:220:LEU:HD11	1.96	0.47
1:B:26:ASP:O	1:B:145:ARG:NH1	2.41	0.47
1:F:34:VAL:O	1:F:124:LEU:HD12	2.15	0.47
1:H:206:ASN:HB3	1:H:209:ASN:HB2	1.96	0.47
1:F:89:GLN:HG2	1:F:119:ILE:HD13	1.96	0.46
1:E:137:LYS:HA	1:E:137:LYS:HD2	1.64	0.46
1:F:11:TYR:HB3	1:F:34:VAL:HG23	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:136:ILE:O	1:G:137:LYS:C	2.52	0.46
1:A:114:LYS:O	1:A:118:GLU:HG3	2.15	0.46
1:E:42:THR:HG22	1:E:44:LEU:H	1.79	0.46
1:D:32:TYR:CE1	1:D:130:GLU:HG3	2.50	0.46
1:F:136:ILE:H	1:F:139:SER:CB	2.17	0.46
1:D:59:LYS:HG3	1:D:87:ILE:HD13	1.97	0.46
1:G:61:HIS:HB2	1:G:182:LEU:HD21	1.98	0.46
1:E:24:LEU:HD21	1:E:149:ALA:HB2	1.98	0.46
1:C:115:VAL:O	1:C:119:ILE:HG13	2.15	0.46
1:G:21:PHE:CE1	1:G:146:LEU:HD22	2.51	0.46
1:G:30:LYS:HE3	1:G:32:TYR:OH	2.16	0.46
1:E:136:ILE:HD12	1:E:136:ILE:C	2.36	0.46
1:F:135:PRO:O	1:F:136:ILE:HD13	2.16	0.46
1:A:159:ALA:H	1:A:189:SER:HB2	1.81	0.45
1:F:47:ALA:HB2	1:F:151:SER:OG	2.17	0.45
1:G:89:GLN:HB3	1:G:96:THR:HG21	1.97	0.45
1:D:42:THR:HA	1:D:43:PRO:HD2	1.78	0.45
1:G:218:TYR:O	2:G:324:HOH:O	2.21	0.45
1:A:43:PRO:HG3	1:A:220:LEU:HD21	1.99	0.45
1:H:15:GLU:HG2	2:H:320:HOH:O	2.17	0.45
1:F:52:ARG:CZ	1:F:52:ARG:HB2	2.47	0.45
1:C:159:ALA:H	1:C:189:SER:HB2	1.82	0.45
1:G:23:ILE:HD11	1:G:175:TYR:HB3	1.98	0.45
1:G:89:GLN:CB	1:G:96:THR:HG21	2.47	0.45
1:B:32:TYR:CE2	1:B:130:GLU:CA	2.99	0.45
1:A:159:ALA:O	1:A:189:SER:HB2	2.17	0.45
1:B:52:ARG:NH2	2:B:345:HOH:O	2.29	0.45
1:E:90:GLU:OE1	2:E:315:HOH:O	2.21	0.45
1:F:44:LEU:HB3	1:F:220:LEU:HD11	1.98	0.45
1:G:136:ILE:O	1:G:139:SER:N	2.48	0.45
1:G:166:MSE:HE2	1:G:166:MSE:HA	1.98	0.45
1:H:207:ILE:O	1:H:211:ILE:HG13	2.16	0.44
1:D:115:VAL:O	1:D:119:ILE:HG13	2.17	0.44
1:E:68:GLU:HA	1:E:68:GLU:OE1	2.17	0.44
1:D:21:PHE:O	1:D:24:LEU:HB2	2.17	0.44
1:H:14:LEU:HD12	2:H:320:HOH:O	2.17	0.44
1:B:52:ARG:HA	1:B:82:LEU:O	2.18	0.44
1:D:136:ILE:O	1:D:137:LYS:C	2.56	0.44
1:F:222:GLU:HG3	2:F:346:HOH:O	2.18	0.44
1:H:52:ARG:HG2	2:H:318:HOH:O	2.16	0.44
1:G:216:LYS:N	1:G:216:LYS:HD2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:77:VAL:HA	1:H:97:ILE:O	2.17	0.44
1:G:19:LYS:O	1:G:22:ASP:HB2	2.18	0.44
1:A:153:VAL:HG21	1:A:214:LEU:HD21	1.99	0.43
1:B:39:LEU:HD22	1:B:75:VAL:HG21	2.00	0.43
1:F:38:LYS:HB2	1:F:38:LYS:HE3	1.59	0.43
1:H:104:LEU:HD21	1:H:125:ILE:HG22	2.00	0.43
1:C:83:GLY:O	1:C:87:ILE:HG13	2.18	0.43
1:G:137:LYS:HE3	1:G:137:LYS:HB2	1.81	0.43
1:D:105:ASP:OD1	1:D:105:ASP:N	2.40	0.43
1:G:198:LYS:O	1:G:198:LYS:HG3	2.18	0.43
1:A:179:LEU:HD21	1:A:195:LEU:HD13	2.00	0.43
1:B:216:LYS:H	1:B:216:LYS:CD	2.30	0.43
1:E:186:LEU:HD21	1:C:205:PHE:HA	2.00	0.43
1:B:216:LYS:CD	1:B:216:LYS:N	2.82	0.43
1:E:161:LEU:HD21	1:E:194:GLU:OE2	2.18	0.43
1:H:124:LEU:HD21	1:H:126:LEU:HD21	2.01	0.43
1:A:47:ALA:HB2	1:A:151:SER:OG	2.17	0.43
1:A:186:LEU:O	1:A:187:ASN:HB2	2.19	0.43
1:B:15:GLU:H	1:B:15:GLU:HG2	1.62	0.43
1:H:142:ALA:O	1:H:145:ARG:HG3	2.19	0.43
1:F:11:TYR:CB	1:F:34:VAL:HG22	2.47	0.43
1:F:136:ILE:HG22	1:F:137:LYS:N	2.33	0.43
1:H:40:LEU:HD12	1:H:40:LEU:HA	1.83	0.43
1:A:67:ARG:O	1:A:71:LYS:HB2	2.18	0.43
1:H:136:ILE:O	1:H:137:LYS:C	2.57	0.43
1:G:216:LYS:C	1:G:218:TYR:N	2.72	0.43
1:E:24:LEU:HD22	1:E:145:ARG:HG3	2.01	0.42
1:C:47:ALA:HA	1:C:77:VAL:O	2.20	0.42
1:A:43:PRO:CG	1:A:220:LEU:HD21	2.49	0.42
1:B:196:LEU:HD13	1:D:205:PHE:CE1	2.55	0.42
1:C:99:LEU:HB3	1:C:143:ARG:HG2	2.01	0.42
1:F:107:ILE:HG21	1:F:113:HIS:HA	2.00	0.42
1:F:166:MSE:HA	1:F:166:MSE:HE2	2.01	0.42
1:C:6:LYS:HD2	1:C:6:LYS:HA	1.85	0.42
1:D:152:ASP:O	1:D:178:PRO:HD2	2.18	0.42
1:C:148:ILE:HD11	1:C:168:SER:HB3	2.01	0.42
1:D:117:GLN:O	1:D:121:GLN:HG3	2.19	0.42
1:B:11:TYR:CD2	1:B:104:LEU:HB3	2.54	0.42
1:E:159:ALA:H	1:E:189:SER:HB2	1.84	0.42
1:A:47:ALA:HA	1:A:77:VAL:O	2.19	0.42
1:H:32:TYR:CE2	1:H:130:GLU:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:PRO:HB3	1:B:182:LEU:HD22	2.02	0.42
1:H:204:ILE:HG23	1:H:210:PHE:HB2	2.02	0.42
1:A:52:ARG:HA	1:A:82:LEU:O	2.19	0.41
1:E:19:LYS:O	1:E:22:ASP:HB2	2.20	0.41
1:H:218:TYR:O	1:H:219:HIS:O	2.38	0.41
1:H:161:LEU:HD23	1:H:191:GLY:HA2	2.02	0.41
1:C:171:LEU:HD23	1:C:171:LEU:HA	1.90	0.41
1:B:59:LYS:O	1:B:60:GLN:C	2.59	0.41
1:D:95:LYS:HE2	1:D:95:LYS:HB3	1.90	0.41
1:A:166:MSE:O	1:A:170:ARG:HG3	2.20	0.41
1:E:89:GLN:HE22	1:E:98:MSE:HB2	1.84	0.41
1:H:152:ASP:O	1:H:178:PRO:HD2	2.20	0.41
1:G:49:ILE:HA	1:G:85:ASP:OD1	2.20	0.41
1:G:59:LYS:HG3	1:G:87:ILE:HD13	2.02	0.41
1:F:105:ASP:OD2	1:F:132:ASP:N	2.32	0.41
1:G:86:ILE:HD12	1:G:86:ILE:HA	1.90	0.41
1:A:46:VAL:HG22	1:A:153:VAL:HG22	2.03	0.41
1:B:61:HIS:HB2	1:B:182:LEU:HD21	2.02	0.41
1:E:159:ALA:O	1:E:189:SER:HB2	2.20	0.41
1:D:214:LEU:HD12	1:D:214:LEU:HA	1.88	0.41
1:G:177:LYS:HA	1:G:178:PRO:HD3	1.88	0.41
1:H:89:GLN:HE22	1:H:98:MSE:HB2	1.85	0.41
1:A:61:HIS:HB3	1:A:207:ILE:HD11	2.03	0.41
1:B:181:VAL:HG11	1:B:192:THR:HB	2.03	0.41
1:C:94:PRO:HB3	1:C:122:ASN:HB3	2.03	0.41
1:D:47:ALA:HB2	1:D:151:SER:OG	2.21	0.41
1:G:142:ALA:HB1	1:G:145:ARG:HH21	1.85	0.41
1:A:14:LEU:HD12	1:A:14:LEU:HA	1.88	0.41
1:B:43:PRO:HB3	1:B:218:TYR:CZ	2.56	0.41
1:E:136:ILE:HD12	1:E:139:SER:N	2.36	0.40
1:A:46:VAL:HG13	1:A:153:VAL:HG23	2.03	0.40
1:H:17:ILE:HG13	1:H:21:PHE:HD2	1.86	0.40
1:H:106:PHE:CE2	1:H:132:ASP:HA	2.54	0.40
1:A:86:ILE:HD12	1:A:86:ILE:HA	1.88	0.40
1:B:65:LEU:CD1	1:B:207:ILE:HG23	2.51	0.40
1:H:82:LEU:HD21	1:H:111:ASN:HB2	2.02	0.40
1:H:204:ILE:HG23	1:H:210:PHE:CB	2.50	0.40
1:D:143:ARG:HD2	1:D:143:ARG:C	2.42	0.40
1:G:193:ASN:ND2	2:G:304:HOH:O	2.48	0.40
1:F:11:TYR:CB	1:F:34:VAL:CG2	2.94	0.40
1:C:102:CYS:HB2	1:C:133:PHE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:CYS:HB3	1:D:135:PRO:CG	2.49	0.40
1:D:186:LEU:O	1:D:187:ASN:HB2	2.21	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	214/229 (93%)	210 (98%)	4 (2%)	0	100	100
1	B	215/229 (94%)	207 (96%)	7 (3%)	1 (0%)	25	28
1	C	214/229 (93%)	207 (97%)	7 (3%)	0	100	100
1	D	213/229 (93%)	207 (97%)	6 (3%)	0	100	100
1	E	214/229 (93%)	208 (97%)	6 (3%)	0	100	100
1	F	218/229 (95%)	210 (96%)	7 (3%)	1 (0%)	25	28
1	G	212/229 (93%)	200 (94%)	10 (5%)	2 (1%)	14	14
1	H	213/229 (93%)	202 (95%)	11 (5%)	0	100	100
All	All	1713/1832 (94%)	1651 (96%)	58 (3%)	4 (0%)	44	52

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	207	ILE
1	B	130	GLU
1	F	51	THR
1	G	217	ASP

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	189/197 (96%)	186 (98%)	3 (2%)	58	71
1	B	190/197 (96%)	184 (97%)	6 (3%)	34	43
1	C	189/197 (96%)	178 (94%)	11 (6%)	17	19
1	D	188/197 (95%)	178 (95%)	10 (5%)	19	23
1	E	189/197 (96%)	183 (97%)	6 (3%)	34	43
1	F	193/197 (98%)	184 (95%)	9 (5%)	22	27
1	G	187/197 (95%)	180 (96%)	7 (4%)	29	38
1	H	188/197 (95%)	175 (93%)	13 (7%)	13	13
All	All	1513/1576 (96%)	1448 (96%)	65 (4%)	25	31

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	121	GLN
1	A	208	GLN
1	B	65	LEU
1	B	104	LEU
1	B	131	LYS
1	B	133	PHE
1	B	145	ARG
1	B	221	LYS
1	E	10	GLN
1	E	25	LYS
1	E	71	LYS
1	E	141	LEU
1	E	182	LEU
1	E	208	GLN
1	F	8	HIS
1	F	25	LYS
1	F	89	GLN
1	F	95	LYS

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Mol	Chain	Res	Type
1	F	99	LEU
1	F	104	LEU
1	F	114	LYS
1	F	182	LEU
1	F	194	GLU
1	H	10	GLN
1	H	12	SER
1	H	15	GLU
1	H	16	ASN
1	H	17	ILE
1	H	23	ILE
1	H	40	LEU
1	H	78	SER
1	H	107	ILE
1	H	132	ASP
1	H	137	LYS
1	H	145	ARG
1	H	153	VAL
1	C	12	SER
1	C	26	ASP
1	C	141	LEU
1	C	143	ARG
1	C	145	ARG
1	C	153	VAL
1	C	186	LEU
1	C	188	GLU
1	C	192	THR
1	C	208	GLN
1	C	220	LEU
1	D	31	LEU
1	D	67	ARG
1	D	78	SER
1	D	95	LYS
1	D	131	LYS
1	D	145	ARG
1	D	200	GLN
1	D	214	LEU
1	D	217	ASP
1	D	218	TYR
1	G	23	ILE
1	G	30	LYS
1	G	82	LEU

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Mol	Chain	Res	Type
1	G	96	THR
1	G	111	ASN
1	G	143	ARG
1	G	206	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	B	113	HIS
1	B	121	GLN
1	E	117	GLN
1	E	208	GLN
1	F	113	HIS
1	H	208	GLN
1	C	10	GLN
1	C	91	ASN
1	C	113	HIS
1	C	212	ASN
1	D	111	ASN
1	D	176	GLN
1	D	200	GLN
1	D	219	HIS
1	G	72	ASN
1	G	89	GLN
1	G	112	ASN
1	G	173	GLN
1	G	206	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 oligosaccharides 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	212/229 (92%)	-0.37	0 100 100	23, 39, 62, 77	0
1	B	213/229 (93%)	-0.31	1 (0%) 87 89	20, 37, 68, 91	0
1	C	212/229 (92%)	-0.25	1 (0%) 87 89	21, 38, 64, 87	0
1	D	211/229 (92%)	-0.28	1 (0%) 87 89	20, 40, 67, 97	0
1	E	212/229 (92%)	-0.27	1 (0%) 87 89	23, 41, 68, 87	0
1	F	215/229 (93%)	-0.25	3 (1%) 73 77	23, 40, 70, 91	0
1	G	210/229 (91%)	0.06	0 100 100	24, 49, 79, 90	0
1	H	211/229 (92%)	-0.00	2 (0%) 81 84	27, 52, 85, 106	0
All	All	1696/1832 (92%)	-0.21	9 (0%) 87 89	20, 42, 74, 106	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	136	ILE	3.5
1	F	224	PRO	3.3
1	D	219	HIS	3.0
1	H	219	HIS	2.6
1	C	108	TYR	2.5
1	B	16	ASN	2.4
1	H	26	ASP	2.3
1	F	141	LEU	2.3
1	E	138	GLY	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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.