Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2023 – 10:10 PM JST

PDB ID	:	8IFJ
Title	:	Crystal structure of pyrrolysyl-tRNA synthetase from methanogenic archaeon ISO4-G1
Authors	:	Yanagisawa, T.; Tanabe, H.; Yokoyama, S.
Deposited on	:	2023-02-18
Resolution	:	2.78 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:

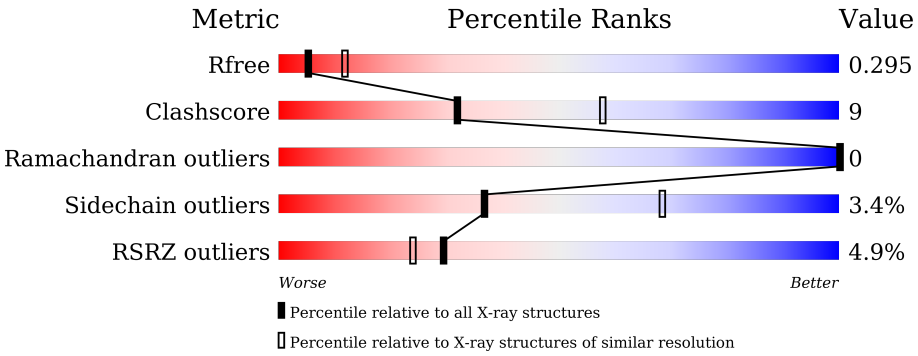
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 2.78 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	276	2% 78% 19% ••
1	B	276	2% 78% 20% •
1	C	276	3% 78% 20% ••
1	D	276	8% 73% 25% ••
1	E	276	3% 75% 24% ••
1	F	276	4% 77% 21% •

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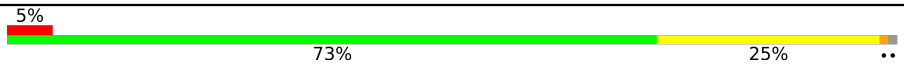
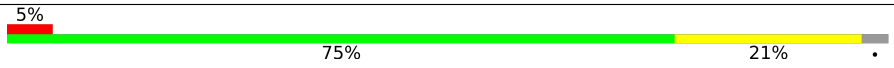
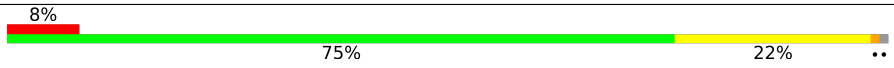
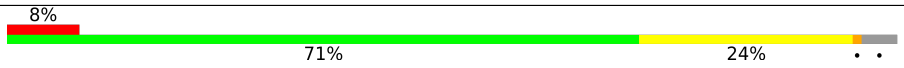
Mol	Chain	Length	Quality of chain
1	G	276	
1	H	276	
1	I	276	
1	J	276	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 21615 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 Pyrrolysyl-tRNA synthetase PylS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2163	1364	370	417	12			
1	B	272	Total	C	N	O	S	0	0	0
			2164	1364	370	418	12			
1	C	272	Total	C	N	O	S	0	0	0
			2164	1364	370	418	12			
1	D	273	Total	C	N	O	S	0	0	0
			2165	1363	371	418	13			
1	E	273	Total	C	N	O	S	0	0	0
			2172	1369	371	419	13			
1	F	273	Total	C	N	O	S	0	0	0
			2172	1369	371	419	13			
1	G	272	Total	C	N	O	S	0	0	0
			2164	1364	370	418	12			
1	H	268	Total	C	N	O	S	0	0	0
			2132	1342	366	412	12			
1	I	273	Total	C	N	O	S	0	0	0
			2172	1369	371	419	13			
1	J	264	Total	C	N	O	S	0	0	0
			2098	1321	361	404	12			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A126QV54
A	-1	SER	-	expression tag	UNP A0A126QV54
A	0	HIS	-	expression tag	UNP A0A126QV54
B	-2	GLY	-	expression tag	UNP A0A126QV54
B	-1	SER	-	expression tag	UNP A0A126QV54
B	0	HIS	-	expression tag	UNP A0A126QV54
C	-2	GLY	-	expression tag	UNP A0A126QV54
C	-1	SER	-	expression tag	UNP A0A126QV54
C	0	HIS	-	expression tag	UNP A0A126QV54

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP A0A126QV54
D	-1	SER	-	expression tag	UNP A0A126QV54
D	0	HIS	-	expression tag	UNP A0A126QV54
E	-2	GLY	-	expression tag	UNP A0A126QV54
E	-1	SER	-	expression tag	UNP A0A126QV54
E	0	HIS	-	expression tag	UNP A0A126QV54
F	-2	GLY	-	expression tag	UNP A0A126QV54
F	-1	SER	-	expression tag	UNP A0A126QV54
F	0	HIS	-	expression tag	UNP A0A126QV54
G	-2	GLY	-	expression tag	UNP A0A126QV54
G	-1	SER	-	expression tag	UNP A0A126QV54
G	0	HIS	-	expression tag	UNP A0A126QV54
H	-2	GLY	-	expression tag	UNP A0A126QV54
H	-1	SER	-	expression tag	UNP A0A126QV54
H	0	HIS	-	expression tag	UNP A0A126QV54
I	-2	GLY	-	expression tag	UNP A0A126QV54
I	-1	SER	-	expression tag	UNP A0A126QV54
I	0	HIS	-	expression tag	UNP A0A126QV54
J	-2	GLY	-	expression tag	UNP A0A126QV54
J	-1	SER	-	expression tag	UNP A0A126QV54
J	0	HIS	-	expression tag	UNP A0A126QV54

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	12	Total O 12 12	0	0
2	B	7	Total O 7 7	0	0
2	C	5	Total O 5 5	0	0
2	D	1	Total O 1 1	0	0
2	E	2	Total O 2 2	0	0
2	F	3	Total O 3 3	0	0
2	G	6	Total O 6 6	0	0
2	H	3	Total O 3 3	0	0
2	I	6	Total O 6 6	0	0

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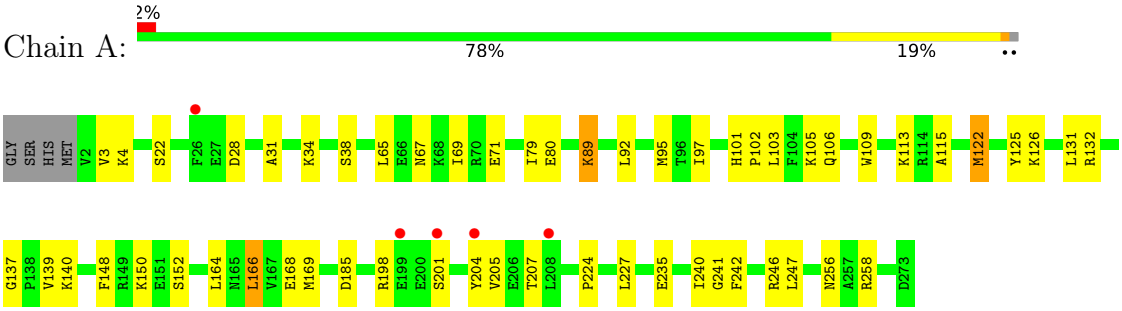
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	J	4	4	4	0	0

3 Residue-property plots

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.

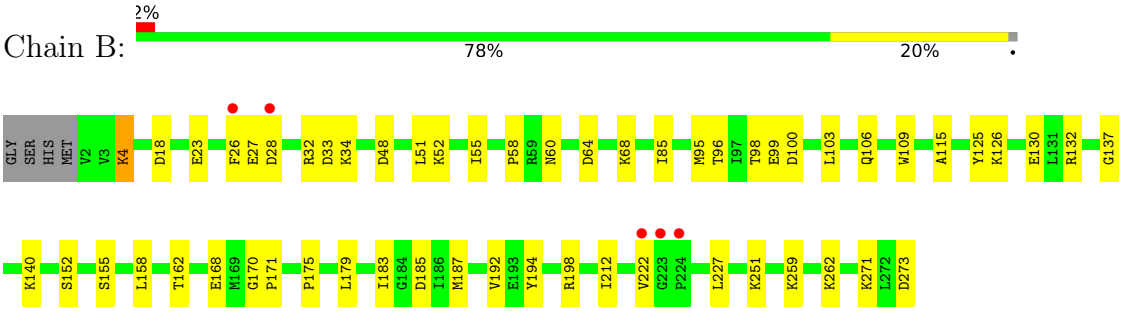
• Molecule 1: Pyrrolysyl-tRNA synthetase PylS

Chain A:



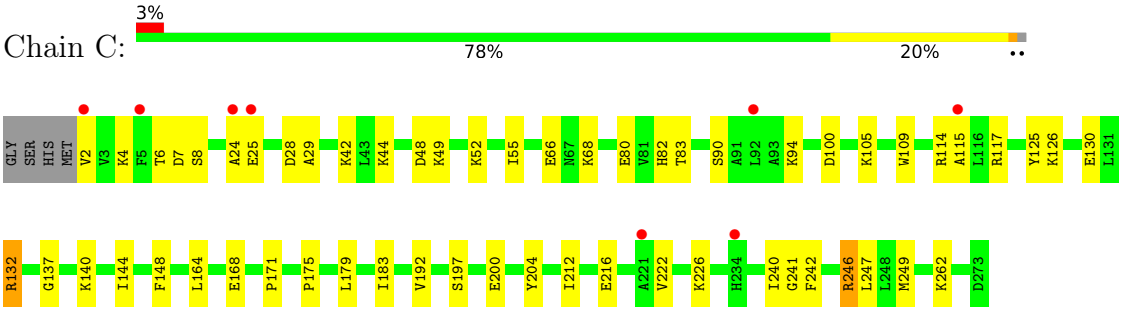
• Molecule 1: Pyrrolysyl-tRNA synthetase PylS

Chain B:



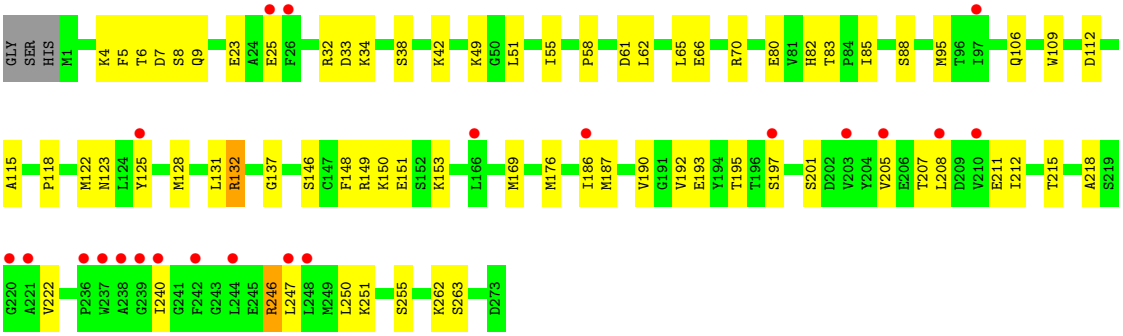
• Molecule 1: Pyrrolysyl-tRNA synthetase PylS

Chain C:

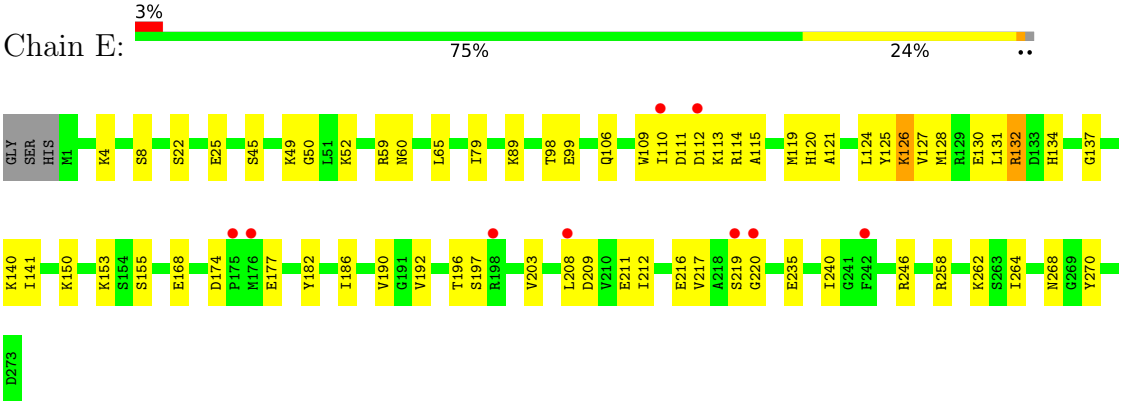


• Molecule 1: Pyrrolysyl-tRNA synthetase PylS

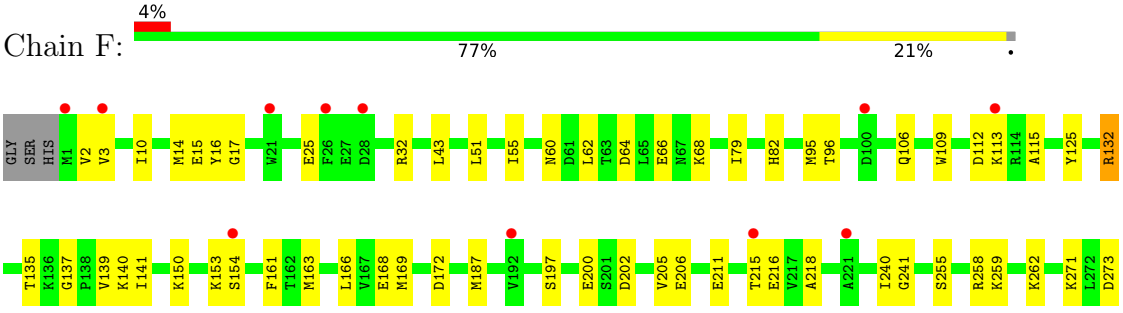
Chain D:



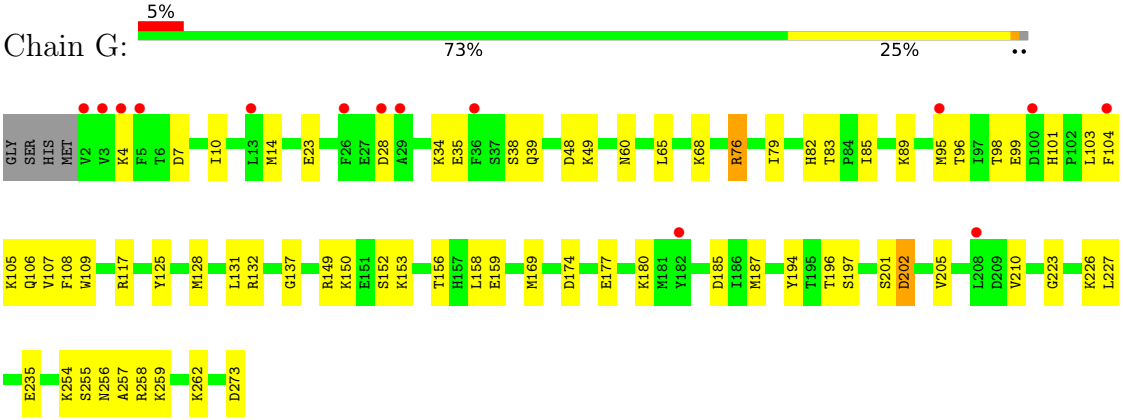
• Molecule 1: Pyrrolysyl-tRNA synthetase PylS



• Molecule 1: Pyrrolysyl-tRNA synthetase PylS

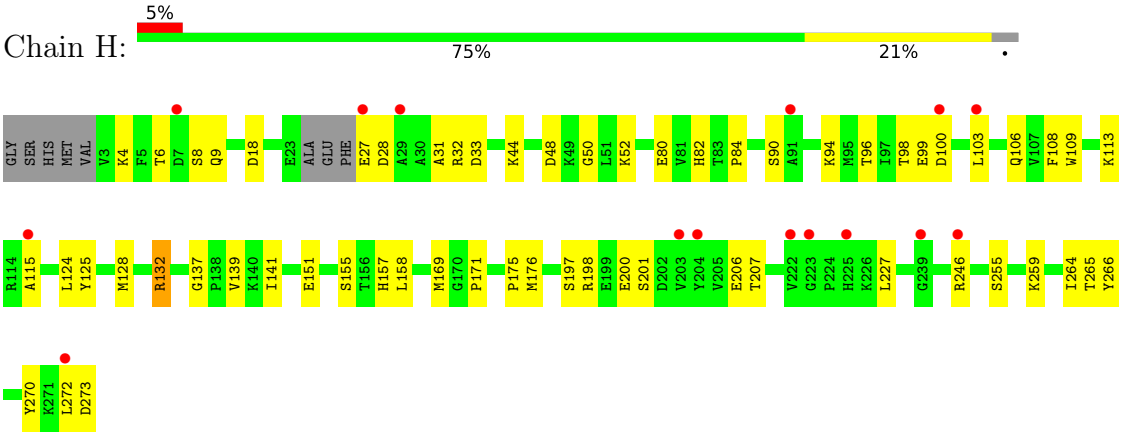


• Molecule 1: Pyrrolysyl-tRNA synthetase PylS



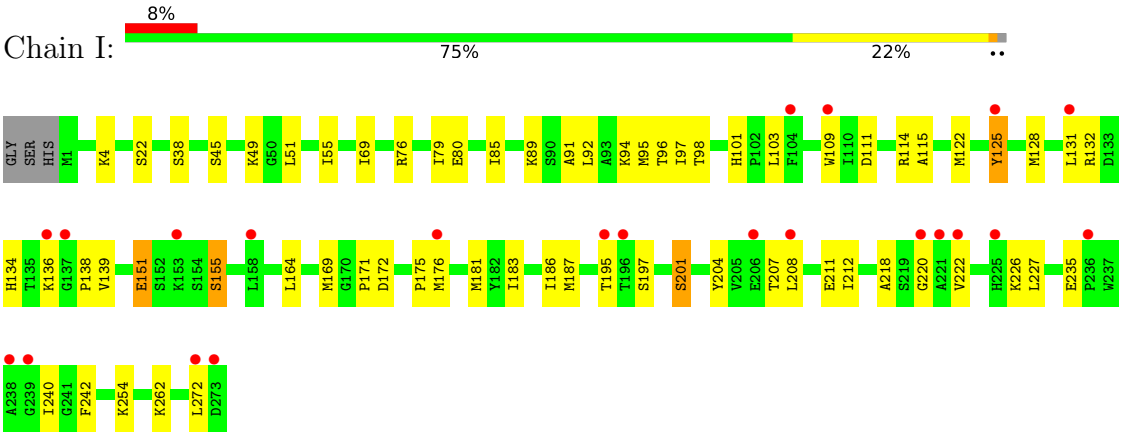
• Molecule 1: Pyrrolysyl-tRNA synthetase PylS

Chain H:



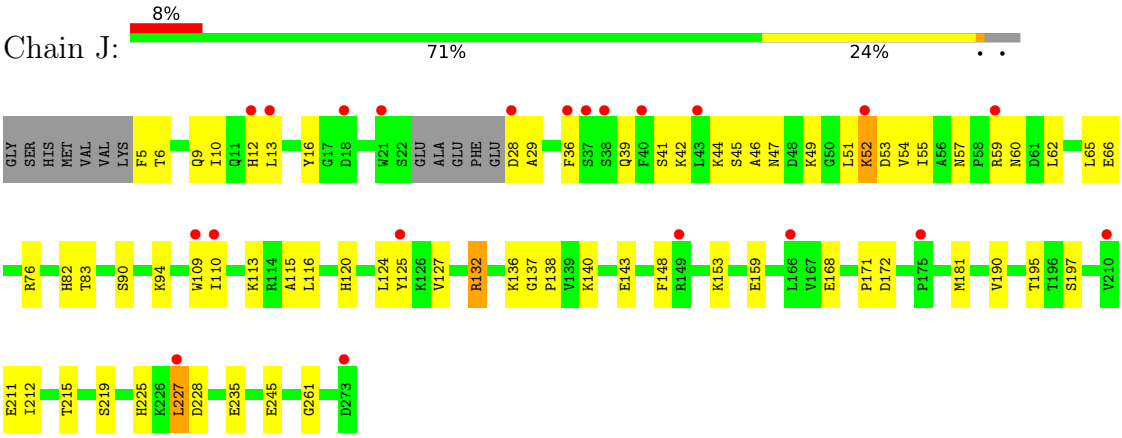
• Molecule 1: Pyrrolysyl-tRNA synthetase PylS

Chain I:



• Molecule 1: Pyrrolysyl-tRNA synthetase PylS

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	98.51Å 102.68Å 349.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.87 – 2.78 49.87 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.87-2.78) 90.8 (49.87-2.78)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.82 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.233 , 0.296 0.233 , 0.295	Depositor DCC
R_{free} test set	1999 reflections (2.22%)	wwPDB-VP
Wilson B-factor (Å^2)	68.5	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 61.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21615	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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	0.28	0/2207	0.47	0/2972
1	B	0.27	0/2208	0.45	0/2972
1	C	0.28	0/2208	0.46	0/2972
1	D	0.29	0/2208	0.47	0/2971
1	E	0.27	0/2216	0.44	0/2982
1	F	0.28	0/2216	0.48	0/2982
1	G	0.27	0/2208	0.46	0/2972
1	H	0.28	0/2174	0.45	0/2924
1	I	0.27	0/2216	0.47	0/2982
1	J	0.31	0/2140	0.49	0/2879
All	All	0.28	0/22001	0.46	0/29608

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	I	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	136	LYS	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	2163	0	2129	33	0
1	B	2164	0	2129	35	0
1	C	2164	0	2129	38	1
1	D	2165	0	2134	41	0
1	E	2172	0	2141	42	1
1	F	2172	0	2141	40	1
1	G	2164	0	2129	47	0
1	H	2132	0	2099	48	0
1	I	2172	0	2141	41	0
1	J	2098	0	2065	49	1
2	A	12	0	0	0	0
2	B	7	0	0	1	0
2	C	5	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	3	0	0	0	0
2	G	6	0	0	1	0
2	H	3	0	0	0	0
2	I	6	0	0	0	0
2	J	4	0	0	0	0
All	All	21615	0	21237	381	2

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 9.

All (381) 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:C:4:LYS:HG2	1:C:25:GLU:HB3	1.57	0.86
1:D:6:THR:HG22	1:D:8:SER:H	1.43	0.84
1:E:196:THR:HG22	1:E:208:LEU:HD11	1.59	0.81
1:F:79:ILE:HB	1:F:141:ILE:HG22	1.64	0.79
1:G:153:LYS:H	1:G:153:LYS:HD2	1.47	0.77
1:F:132:ARG:NH2	1:F:137:GLY:O	2.19	0.76
1:H:32:ARG:NH1	1:H:33:ASP:OD1	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ILE:HG12	1:C:164:LEU:HD23	1.66	0.76
1:I:96:THR:HG23	1:I:227:LEU:HD21	1.70	0.73
1:F:135:THR:HG22	1:F:137:GLY:H	1.53	0.72
1:D:190:VAL:HG23	1:D:192:VAL:HG22	1.72	0.72
1:B:170:GLY:N	2:B:301:HOH:O	2.23	0.71
1:B:132:ARG:NH2	1:B:137:GLY:O	2.22	0.71
1:C:132:ARG:NH2	1:C:137:GLY:O	2.23	0.71
1:H:151:GLU:OE1	1:H:157:HIS:HB3	1.91	0.71
1:H:264:ILE:HD12	1:H:265:THR:HG23	1.73	0.70
1:H:264:ILE:CD1	1:H:265:THR:HG23	2.21	0.70
1:D:132:ARG:NH2	1:D:137:GLY:O	2.25	0.68
1:D:6:THR:HB	1:D:9:GLN:HG2	1.75	0.68
1:I:176:MET:HG2	1:I:222:VAL:HG21	1.75	0.67
1:J:110:ILE:HD11	1:J:116:LEU:HG	1.74	0.67
1:E:140:LYS:HG2	1:E:168:GLU:HG3	1.76	0.67
1:A:256:ASN:HD22	1:A:258:ARG:H	1.43	0.67
1:H:132:ARG:NH2	1:H:137:GLY:O	2.25	0.66
1:I:262:LYS:HG2	1:J:82:HIS:HB3	1.76	0.66
1:I:4:LYS:NZ	1:I:22:SER:O	2.27	0.66
1:J:52:LYS:HA	1:J:55:ILE:HD12	1.77	0.66
1:A:132:ARG:NH2	1:A:137:GLY:O	2.27	0.66
1:E:209:ASP:HA	1:E:219:SER:HB2	1.78	0.65
1:I:95:MET:HA	1:I:227:LEU:HD22	1.78	0.65
1:J:212:ILE:O	1:J:215:THR:OG1	2.12	0.65
1:B:4:LYS:HA	1:B:26:PHE:HD2	1.63	0.64
1:G:83:THR:OG1	1:G:117:ARG:NH1	2.31	0.64
1:D:95:MET:HG3	1:D:122:MET:HG3	1.80	0.64
1:G:76:ARG:NH1	1:G:185:ASP:OD2	2.31	0.63
1:I:114:ARG:NH1	1:J:159:GLU:OE1	2.27	0.63
1:C:66:GLU:HB2	1:C:144:ILE:HD13	1.79	0.63
1:J:245:GLU:HG2	1:J:261:GLY:HA2	1.79	0.63
1:D:262:LYS:HG2	1:F:82:HIS:HB3	1.81	0.63
1:D:32:ARG:NH1	1:D:33:ASP:OD1	2.32	0.62
1:G:174:ASP:HB3	1:G:177:GLU:HB3	1.80	0.62
1:A:201:SER:HB3	1:A:207:THR:HG23	1.80	0.62
1:F:153:LYS:HG2	1:F:154:SER:H	1.64	0.62
1:J:140:LYS:HG2	1:J:168:GLU:HG3	1.80	0.62
1:D:187:MET:HA	1:D:190:VAL:HG22	1.82	0.61
1:H:151:GLU:CD	1:H:157:HIS:HB3	2.21	0.61
1:F:218:ALA:HB1	1:F:240:ILE:HD11	1.81	0.61
1:B:32:ARG:NH1	1:B:33:ASP:OD1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:HIS:HB3	1:F:262:LYS:HG3	1.81	0.61
1:A:105:LYS:H	1:A:105:LYS:HD2	1.66	0.61
1:E:89:LYS:HD2	1:E:113:LYS:HA	1.83	0.60
1:A:102:PRO:HA	1:A:105:LYS:HE2	1.81	0.60
1:J:132:ARG:NH2	1:J:137:GLY:O	2.33	0.60
1:B:271:LYS:NZ	1:B:273:ASP:OD1	2.32	0.60
1:A:31:ALA:HA	1:A:34:LYS:HG2	1.83	0.60
1:E:106:GLN:HA	1:E:150:LYS:HB2	1.84	0.60
1:I:76:ARG:HH12	1:I:181:MET:HG2	1.67	0.60
1:C:140:LYS:HG2	1:C:168:GLU:HG3	1.84	0.59
1:J:52:LYS:C	1:J:52:LYS:HD3	2.22	0.59
1:J:9:GLN:HB3	1:J:36:PHE:CZ	2.38	0.59
1:H:28:ASP:HB2	1:H:31:ALA:HB2	1.84	0.59
1:B:171:PRO:HG2	1:B:175:PRO:HB3	1.83	0.59
1:H:18:ASP:OD1	1:H:259:LYS:NZ	2.36	0.59
1:H:171:PRO:HG3	1:H:175:PRO:HB3	1.85	0.59
1:D:65:LEU:HD11	1:D:190:VAL:HG12	1.85	0.58
1:E:134:HIS:NE2	1:H:272:LEU:O	2.36	0.58
1:C:183:ILE:HD11	1:C:240:ILE:HD13	1.84	0.58
1:D:83:THR:HG21	1:D:123:ASN:HB3	1.83	0.58
1:H:98:THR:HG22	1:H:99:GLU:H	1.68	0.58
1:C:114:ARG:NH1	1:G:159:GLU:OE1	2.35	0.58
1:B:198:ARG:NH2	1:D:7:ASP:OD2	2.36	0.58
1:C:6:THR:OG1	1:C:7:ASP:N	2.37	0.58
1:J:10:ILE:HA	1:J:13:LEU:HB3	1.86	0.58
1:E:98:THR:OG1	1:E:99:GLU:OE1	2.21	0.58
1:D:146:SER:OG	1:D:262:LYS:NZ	2.36	0.57
1:H:96:THR:HG23	1:H:227:LEU:HD21	1.87	0.57
1:D:38:SER:O	1:D:42:LYS:HG2	2.04	0.57
1:B:192:VAL:HG21	1:B:212:ILE:HD13	1.86	0.57
1:J:52:LYS:HD3	1:J:52:LYS:O	2.04	0.57
1:F:3:VAL:HG21	1:F:32:ARG:HB2	1.86	0.57
1:I:122:MET:SD	1:I:122:MET:N	2.78	0.57
1:A:139:VAL:HB	1:A:169:MET:HB3	1.86	0.56
1:A:132:ARG:NH1	1:A:235:GLU:OE1	2.38	0.56
1:B:152:SER:HB3	1:B:155:SER:HB2	1.87	0.56
1:G:65:LEU:HA	1:G:68:LYS:HE2	1.88	0.56
1:D:212:ILE:O	1:D:215:THR:OG1	2.24	0.56
1:A:4:LYS:NZ	1:A:22:SER:O	2.32	0.56
1:D:4:LYS:HG3	1:D:5:PHE:H	1.69	0.56
1:H:255:SER:HB3	1:H:259:LYS:HZ1	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:195:THR:OG1	1:J:211:GLU:HG2	2.05	0.55
1:H:264:ILE:HD12	1:H:265:THR:N	2.21	0.55
1:A:246:ARG:HG3	1:A:246:ARG:HH11	1.71	0.55
1:E:110:ILE:HG21	1:H:108:PHE:HD1	1.71	0.55
1:J:54:VAL:HG12	1:J:59:ARG:HH12	1.71	0.55
1:E:132:ARG:NH2	1:E:137:GLY:O	2.40	0.55
1:I:51:LEU:O	1:I:55:ILE:HG13	2.07	0.55
1:B:4:LYS:NZ	1:B:23:GLU:HA	2.22	0.54
1:I:89:LYS:NZ	1:I:97:ILE:O	2.32	0.54
1:I:272:LEU:HD11	1:J:127:VAL:HG13	1.89	0.54
1:G:38:SER:OG	1:G:39:GLN:N	2.39	0.54
1:B:48:ASP:OD1	1:B:52:LYS:NZ	2.33	0.54
1:J:120:HIS:HB3	1:J:124:LEU:CD1	2.38	0.54
1:B:103:LEU:HD12	1:B:106:GLN:HB2	1.89	0.54
1:H:151:GLU:OE2	1:H:157:HIS:ND1	2.41	0.53
1:I:91:ALA:HA	1:I:94:LYS:HE2	1.90	0.53
1:E:211:GLU:HG2	1:E:216:GLU:HA	1.91	0.53
1:I:89:LYS:HE3	1:I:98:THR:HG22	1.91	0.53
1:E:79:ILE:HB	1:E:141:ILE:HG22	1.91	0.53
1:G:101:HIS:HE1	1:G:103:LEU:HD12	1.74	0.53
1:H:264:ILE:HD12	1:H:264:ILE:C	2.30	0.53
1:I:101:HIS:CE1	1:I:103:LEU:HD13	2.43	0.53
1:G:226:LYS:HG3	1:G:227:LEU:HD23	1.90	0.52
1:F:166:LEU:HD11	1:F:240:ILE:HG22	1.91	0.52
1:D:195:THR:OG1	1:D:211:GLU:HB2	2.09	0.52
1:B:95:MET:O	1:B:96:THR:OG1	2.25	0.52
1:H:151:GLU:OE2	1:H:157:HIS:CG	2.63	0.52
1:I:208:LEU:O	1:I:220:GLY:N	2.29	0.52
1:J:39:GLN:HA	1:J:42:LYS:HB2	1.92	0.52
1:F:271:LYS:NZ	1:F:273:ASP:HB2	2.25	0.51
1:G:156:THR:HA	1:G:258:ARG:NH2	2.26	0.51
1:H:90:SER:O	1:H:94:LYS:HG3	2.10	0.51
1:C:4:LYS:HG2	1:C:25:GLU:CB	2.35	0.51
1:J:10:ILE:HG22	1:J:13:LEU:HD22	1.93	0.51
1:F:200:GLU:HA	1:F:206:GLU:HA	1.93	0.51
1:G:105:LYS:HG3	1:G:106:GLN:HG3	1.93	0.51
1:G:132:ARG:NH2	1:G:137:GLY:O	2.44	0.51
1:E:126:LYS:HE2	1:H:264:ILE:HD13	1.92	0.51
1:G:205:VAL:HB	1:G:223:GLY:HA3	1.93	0.51
1:A:106:GLN:HA	1:A:150:LYS:HB2	1.93	0.50
1:E:49:LYS:HA	1:E:52:LYS:HG3	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:89:LYS:HA	1:I:92:LEU:HB2	1.92	0.50
1:B:4:LYS:HA	1:B:26:PHE:CD2	2.45	0.50
1:F:106:GLN:HA	1:F:150:LYS:HB2	1.94	0.50
1:D:118:PRO:HB2	1:D:149:ARG:HE	1.77	0.50
1:H:176:MET:HG2	1:H:198:ARG:CZ	2.40	0.50
1:E:126:LYS:CE	1:H:264:ILE:HD13	2.41	0.50
1:J:120:HIS:O	1:J:124:LEU:HD12	2.11	0.50
1:F:140:LYS:HG2	1:F:168:GLU:HG3	1.93	0.50
1:G:101:HIS:CE1	1:G:103:LEU:HD12	2.47	0.50
1:I:132:ARG:C	1:I:134:HIS:H	2.15	0.50
1:B:109:TRP:CE3	1:B:115:ALA:HB2	2.47	0.50
1:C:90:SER:O	1:C:94:LYS:HG3	2.12	0.50
1:H:44:LYS:O	1:H:48:ASP:N	2.41	0.50
1:J:10:ILE:HA	1:J:13:LEU:CB	2.41	0.50
1:D:190:VAL:HG11	1:D:247:LEU:HD23	1.93	0.50
1:E:65:LEU:HD11	1:E:190:VAL:HG22	1.93	0.50
1:E:119:MET:HG3	1:E:121:ALA:H	1.77	0.50
1:I:139:VAL:HG22	1:I:169:MET:HB3	1.93	0.50
1:B:175:PRO:HB2	1:B:222:VAL:HG23	1.94	0.49
1:C:4:LYS:HB3	1:C:24:ALA:O	2.13	0.49
1:H:255:SER:HB3	1:H:259:LYS:NZ	2.27	0.49
1:I:128:MET:HG3	1:I:139:VAL:HG21	1.94	0.49
1:I:183:ILE:O	1:I:187:MET:HG2	2.13	0.49
1:C:204:TYR:OH	1:I:235:GLU:OE2	2.27	0.49
1:J:225:HIS:N	1:J:228:ASP:OD2	2.35	0.49
1:C:109:TRP:CE3	1:C:115:ALA:HB2	2.48	0.49
1:G:201:SER:OG	1:G:202:ASP:N	2.45	0.49
1:H:198:ARG:HE	1:H:206:GLU:CD	2.15	0.49
1:A:109:TRP:CE3	1:A:115:ALA:HB2	2.48	0.49
1:D:201:SER:HB2	1:D:207:THR:HG23	1.95	0.49
1:A:204:TYR:HB3	1:A:224:PRO:HG2	1.93	0.49
1:C:242:PHE:HB3	1:C:247:LEU:HD11	1.95	0.49
1:F:112:ASP:HB3	1:F:113:LYS:NZ	2.28	0.48
1:I:171:PRO:HG3	1:I:175:PRO:HB3	1.95	0.48
1:C:100:ASP:HB3	1:D:23:GLU:O	2.13	0.48
1:A:65:LEU:O	1:A:69:ILE:HG13	2.14	0.48
1:C:82:HIS:HB3	1:G:262:LYS:HG2	1.96	0.48
1:G:89:LYS:HG3	1:G:109:TRP:HH2	1.78	0.48
1:D:218:ALA:HB1	1:D:240:ILE:HD11	1.95	0.48
1:F:16:TYR:OH	1:F:273:ASP:OXT	2.31	0.48
1:G:7:ASP:HA	1:G:10:ILE:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:104:PHE:O	1:G:107:VAL:HG22	2.14	0.48
1:B:51:LEU:O	1:B:55:ILE:HG13	2.13	0.48
1:C:171:PRO:HG2	1:C:175:PRO:HB3	1.95	0.48
1:H:109:TRP:CE3	1:H:115:ALA:HB2	2.49	0.48
1:I:131:LEU:HD23	1:I:131:LEU:HA	1.58	0.48
1:J:41:SER:HA	1:J:44:LYS:HB2	1.95	0.48
1:A:256:ASN:HD21	1:A:258:ARG:HB2	1.78	0.48
1:G:28:ASP:OD1	1:G:28:ASP:N	2.46	0.48
1:G:255:SER:HB3	1:G:259:LYS:HE3	1.96	0.48
1:J:16:TYR:HD1	1:J:47:ASN:ND2	2.11	0.48
1:D:128:MET:HG3	1:D:169:MET:HE3	1.96	0.47
1:F:153:LYS:HG2	1:F:154:SER:N	2.28	0.47
1:A:34:LYS:HE3	1:A:34:LYS:HB2	1.56	0.47
1:C:148:PHE:HZ	1:G:85:ILE:HD12	1.79	0.47
1:J:138:PRO:HB2	1:J:140:LYS:HE3	1.95	0.47
1:G:106:GLN:HA	1:G:150:LYS:HB2	1.95	0.47
1:E:59:ARG:HG3	1:E:268:ASN:ND2	2.29	0.47
1:A:80:GLU:O	1:B:60:ASN:ND2	2.44	0.47
1:C:226:LYS:HB2	1:C:226:LYS:HE2	1.74	0.47
1:E:98:THR:OG1	1:E:99:GLU:N	2.48	0.47
1:F:64:ASP:O	1:F:68:LYS:HG3	2.14	0.47
1:G:98:THR:OG1	1:G:99:GLU:N	2.47	0.47
1:I:85:ILE:HD12	1:J:148:PHE:HZ	1.79	0.47
1:J:28:ASP:OD1	1:J:29:ALA:N	2.47	0.47
1:J:76:ARG:NH1	1:J:181:MET:SD	2.88	0.47
1:J:132:ARG:HD2	1:J:235:GLU:OE2	2.14	0.47
1:H:151:GLU:OE1	1:H:157:HIS:CB	2.62	0.47
1:I:45:SER:O	1:I:49:LYS:HG2	2.13	0.47
1:E:50:GLY:HA3	1:E:270:TYR:CE1	2.50	0.47
1:E:212:ILE:HD12	1:E:217:VAL:HG11	1.96	0.47
1:C:175:PRO:HB2	1:C:222:VAL:HG21	1.97	0.47
1:C:216:GLU:OE2	1:D:49:LYS:NZ	2.47	0.47
1:D:58:PRO:HB3	1:F:79:ILE:HG13	1.96	0.47
1:F:109:TRP:CE3	1:F:115:ALA:HB2	2.50	0.47
1:F:211:GLU:HG2	1:F:216:GLU:HA	1.97	0.47
1:G:14:MET:HE2	1:G:255:SER:HB2	1.96	0.47
1:G:95:MET:O	1:G:96:THR:OG1	2.28	0.47
1:H:103:LEU:HD12	1:H:106:GLN:HB2	1.96	0.47
1:C:126:LYS:O	1:C:130:GLU:HG2	2.15	0.46
1:D:109:TRP:CE3	1:D:115:ALA:HB2	2.51	0.46
1:E:111:ASP:OD1	1:E:114:ARG:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:27:GLU:HG2	1:H:28:ASP:N	2.29	0.46
1:J:16:TYR:HD1	1:J:47:ASN:HD21	1.62	0.46
1:J:83:THR:N	1:J:143:GLU:OE2	2.37	0.46
1:H:128:MET:HB3	1:H:141:ILE:HD11	1.96	0.46
1:J:54:VAL:HG12	1:J:59:ARG:NH1	2.30	0.46
1:D:51:LEU:O	1:D:55:ILE:HG13	2.15	0.46
1:F:139:VAL:HG13	1:F:169:MET:HB3	1.98	0.46
1:H:6:THR:HG22	1:H:8:SER:H	1.80	0.46
1:G:196:THR:HG22	1:G:210:VAL:HG12	1.97	0.46
1:J:12:HIS:H	1:J:12:HIS:CD2	2.34	0.46
1:A:97:ILE:HD13	1:A:103:LEU:HD23	1.98	0.46
1:A:4:LYS:HB3	1:A:4:LYS:HZ2	1.81	0.46
1:J:53:ASP:O	1:J:57:ASN:N	2.46	0.46
1:B:187:MET:HG3	1:B:194:TYR:CD1	2.51	0.46
1:C:100:ASP:N	1:C:100:ASP:OD1	2.47	0.46
1:D:38:SER:O	1:D:42:LYS:HE2	2.15	0.46
1:E:127:VAL:O	1:E:131:LEU:HD12	2.15	0.46
1:B:162:THR:OG1	1:B:262:LYS:NZ	2.48	0.45
1:I:195:THR:OG1	1:I:211:GLU:HG2	2.15	0.45
1:F:202:ASP:HB3	1:F:205:VAL:HG12	1.98	0.45
1:H:48:ASP:O	1:H:52:LYS:HG3	2.16	0.45
1:A:166:LEU:HD21	1:A:240:ILE:HG22	1.96	0.45
1:C:164:LEU:O	1:C:241:GLY:HA2	2.17	0.45
1:G:273:ASP:OD1	1:G:273:ASP:N	2.45	0.45
1:H:4:LYS:HA	1:H:4:LYS:HE2	1.98	0.45
1:H:272:LEU:HD23	1:H:272:LEU:HA	1.66	0.45
1:J:47:ASN:O	1:J:51:LEU:HD12	2.17	0.45
1:H:106:GLN:OE1	1:H:151:GLU:HG2	2.17	0.45
1:I:80:GLU:O	1:J:60:ASN:ND2	2.43	0.45
1:E:49:LYS:HD2	1:E:49:LYS:O	2.16	0.45
1:F:15:GLU:HB3	1:F:271:LYS:HE3	1.97	0.45
1:H:139:VAL:HG22	1:H:169:MET:HB3	1.99	0.45
1:F:16:TYR:CZ	1:F:271:LYS:HD3	2.52	0.45
1:G:187:MET:HG3	1:G:194:TYR:CG	2.52	0.45
1:H:201:SER:HB3	1:H:207:THR:HG23	1.99	0.45
1:J:51:LEU:O	1:J:54:VAL:HG22	2.16	0.45
1:G:23:GLU:OE2	1:G:23:GLU:N	2.50	0.45
1:J:46:ALA:O	1:J:49:LYS:HB3	2.17	0.45
1:D:62:LEU:O	1:D:66:GLU:HG3	2.16	0.45
1:E:112:ASP:OD1	1:E:112:ASP:N	2.43	0.45
1:I:138:PRO:HG3	1:I:172:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:9:GLN:HB3	1:J:36:PHE:CE1	2.52	0.45
1:J:171:PRO:O	1:J:172:ASP:HB3	2.17	0.45
1:F:240:ILE:HD12	1:F:241:GLY:H	1.81	0.44
1:C:55:ILE:HD11	1:G:131:LEU:HD22	1.99	0.44
1:E:196:THR:CG2	1:E:208:LEU:HD11	2.40	0.44
1:H:264:ILE:CD1	1:H:264:ILE:C	2.86	0.44
1:I:186:ILE:HD11	1:I:242:PHE:CE2	2.52	0.44
1:E:59:ARG:HG3	1:E:268:ASN:HD21	1.82	0.44
1:E:132:ARG:NH1	1:E:235:GLU:OE1	2.51	0.44
1:E:262:LYS:HG2	1:H:82:HIS:HB3	2.00	0.44
1:H:98:THR:HB	1:H:100:ASP:OD1	2.18	0.44
1:I:187:MET:CE	1:I:212:ILE:HD11	2.48	0.44
1:I:254:LYS:HA	1:I:254:LYS:HD2	1.72	0.44
1:B:179:LEU:O	1:B:183:ILE:HG12	2.18	0.44
1:D:246:ARG:O	1:D:250:LEU:HG	2.17	0.44
1:A:3:VAL:HG11	1:A:28:ASP:HA	2.00	0.44
1:J:94:LYS:O	1:J:227:LEU:HD22	2.18	0.44
1:D:176:MET:SD	1:D:222:VAL:HG21	2.58	0.44
1:H:124:LEU:HD22	1:H:141:ILE:HD12	2.00	0.43
1:H:200:GLU:HA	1:H:206:GLU:HG3	1.99	0.43
1:J:109:TRP:CE3	1:J:115:ALA:HB2	2.53	0.43
1:A:79:ILE:HD12	1:A:140:LYS:O	2.18	0.43
1:A:101:HIS:CD2	1:A:102:PRO:HD2	2.53	0.43
1:F:258:ARG:HG2	1:F:258:ARG:HH11	1.83	0.43
1:G:128:MET:HE2	1:G:169:MET:HB2	2.00	0.43
1:G:256:ASN:OD1	1:G:257:ALA:N	2.52	0.43
1:J:132:ARG:NH1	1:J:235:GLU:OE1	2.51	0.43
1:E:153:LYS:HB2	1:E:153:LYS:HE2	1.72	0.43
1:E:220:GLY:N	1:E:240:ILE:HG13	2.34	0.43
1:F:161:PHE:HD2	1:F:163:MET:HG3	1.84	0.43
1:F:271:LYS:HZ2	1:F:273:ASP:HB2	1.83	0.43
1:D:205:VAL:HB	1:D:222:VAL:O	2.19	0.43
1:A:79:ILE:HG13	1:B:58:PRO:HB3	2.01	0.43
1:B:98:THR:OG1	1:B:99:GLU:N	2.52	0.43
1:C:28:ASP:CG	1:C:29:ALA:H	2.22	0.43
1:C:49:LYS:HB3	1:C:49:LYS:HE2	1.81	0.43
1:F:62:LEU:O	1:F:66:GLU:HG2	2.19	0.43
1:I:201:SER:OG	1:I:204:TYR:HB2	2.18	0.43
1:D:85:ILE:HD12	1:D:148:PHE:HE1	1.84	0.43
1:E:124:LEU:O	1:E:128:MET:HB2	2.19	0.43
1:E:130:GLU:CD	1:H:273:ASP:HB3	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:ILE:HG22	1:F:14:MET:HG2	2.01	0.43
1:G:108:PHE:CE1	1:G:150:LYS:HG2	2.54	0.43
1:I:95:MET:O	1:I:97:ILE:HG12	2.19	0.43
1:A:89:LYS:HG2	1:A:113:LYS:HD2	2.00	0.43
1:B:140:LYS:HG2	1:B:168:GLU:HG3	2.01	0.43
1:D:106:GLN:HA	1:D:150:LYS:HB2	2.00	0.43
1:G:158:LEU:O	2:G:301:HOH:O	2.21	0.43
1:C:55:ILE:HA	1:G:79:ILE:HD11	2.01	0.42
1:C:262:LYS:HG2	1:G:82:HIS:HB3	2.00	0.42
1:D:192:VAL:HG13	1:D:251:LYS:HD3	2.00	0.42
1:F:2:VAL:HG13	1:F:25:GLU:HB2	2.01	0.42
1:D:131:LEU:HD22	1:F:55:ILE:HD11	2.01	0.42
1:F:51:LEU:O	1:F:55:ILE:HG13	2.19	0.42
1:I:95:MET:HE1	1:I:125:TYR:HD2	1.84	0.42
1:C:246:ARG:HD3	1:C:249:MET:HE3	2.01	0.42
1:E:264:ILE:HG23	1:H:84:PRO:HD2	2.00	0.42
1:G:34:LYS:O	1:G:38:SER:N	2.50	0.42
1:B:96:THR:HG23	1:B:227:LEU:HD21	2.02	0.42
1:F:172:ASP:OD1	1:F:172:ASP:N	2.48	0.42
1:H:50:GLY:HA3	1:H:270:TYR:CE1	2.54	0.42
1:A:242:PHE:HB3	1:A:247:LEU:HD11	2.01	0.42
1:J:65:LEU:HD11	1:J:190:VAL:HG22	2.02	0.42
1:D:80:GLU:O	1:F:60:ASN:ND2	2.44	0.42
1:C:44:LYS:HE2	1:C:44:LYS:HB3	1.91	0.42
1:E:120:HIS:O	1:E:124:LEU:HB2	2.20	0.42
1:G:49:LYS:HA	1:G:49:LYS:HD3	1.68	0.42
1:B:126:LYS:O	1:B:130:GLU:HG3	2.19	0.42
1:E:4:LYS:HG2	1:E:25:GLU:HA	2.02	0.42
1:G:254:LYS:HE3	1:G:254:LYS:HB3	1.83	0.42
1:J:62:LEU:O	1:J:66:GLU:HG3	2.20	0.42
1:B:27:GLU:OE2	1:B:27:GLU:N	2.46	0.42
1:G:132:ARG:NH1	1:G:235:GLU:OE2	2.53	0.42
1:I:151:GLU:HG2	1:I:155:SER:OG	2.19	0.42
1:E:132:ARG:HD2	1:E:235:GLU:OE2	2.20	0.41
1:I:201:SER:HB3	1:I:207:THR:HG23	2.02	0.41
1:B:4:LYS:HZ1	1:B:23:GLU:HA	1.86	0.41
1:D:186:ILE:HD12	1:D:187:MET:HG3	2.01	0.41
1:I:69:ILE:HG21	1:I:164:LEU:HD22	2.03	0.41
1:I:109:TRP:CE3	1:I:115:ALA:HB2	2.55	0.41
1:J:6:THR:HB	1:J:9:GLN:HG3	2.03	0.41
1:A:67:ASN:O	1:A:71:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:MET:HA	1:A:227:LEU:HD13	2.03	0.41
1:B:4:LYS:HZ2	1:B:23:GLU:HA	1.85	0.41
1:B:18:ASP:OD1	1:B:259:LYS:NZ	2.42	0.41
1:F:95:MET:O	1:F:96:THR:OG1	2.32	0.41
1:F:255:SER:HB3	1:F:259:LYS:NZ	2.35	0.41
1:A:92:LEU:HD23	1:A:122:MET:SD	2.60	0.41
1:E:60:ASN:ND2	1:H:80:GLU:O	2.40	0.41
1:E:192:VAL:HG11	1:E:212:ILE:HD13	2.01	0.41
1:H:158:LEU:HD12	1:H:158:LEU:H	1.85	0.41
1:I:79:ILE:HD11	1:J:55:ILE:HA	2.03	0.41
1:J:42:LYS:HD2	1:J:42:LYS:HA	1.69	0.41
1:A:201:SER:OG	1:A:205:VAL:HB	2.21	0.41
1:E:182:TYR:O	1:E:186:ILE:HG12	2.21	0.41
1:G:48:ASP:HB3	1:G:49:LYS:HZ3	1.86	0.41
1:B:251:LYS:HA	1:B:251:LYS:HD2	1.93	0.41
1:C:2:VAL:HG11	1:C:25:GLU:OE2	2.21	0.41
1:A:148:PHE:HZ	1:B:85:ILE:HD12	1.85	0.41
1:F:211:GLU:HA	1:F:215:THR:O	2.21	0.41
1:J:10:ILE:O	1:J:13:LEU:HB3	2.21	0.41
1:B:28:ASP:OD1	1:B:28:ASP:N	2.53	0.41
1:D:193:GLU:H	1:D:193:GLU:HG2	1.75	0.41
1:E:109:TRP:CZ3	1:E:115:ALA:HB2	2.55	0.41
1:B:98:THR:HG23	1:B:100:ASP:OD1	2.21	0.41
1:C:192:VAL:HG21	1:C:212:ILE:HD13	2.03	0.41
1:D:176:MET:HE3	1:D:208:LEU:HD12	2.03	0.41
1:F:17:GLY:HA3	1:F:43:LEU:HD13	2.03	0.41
1:G:35:GLU:HA	1:G:38:SER:HB3	2.02	0.41
1:H:259:LYS:HD3	1:H:266:TYR:CE1	2.56	0.41
1:I:218:ALA:HB1	1:I:240:ILE:HD11	2.02	0.41
1:C:68:LYS:HA	1:C:68:LYS:HD3	1.80	0.40
1:G:4:LYS:NZ	1:G:23:GLU:HA	2.36	0.40
1:G:68:LYS:H	1:G:68:LYS:HG2	1.74	0.40
1:I:111:ASP:OD1	1:I:114:ARG:N	2.49	0.40
1:J:195:THR:OG1	1:J:211:GLU:O	2.37	0.40
1:C:80:GLU:O	1:G:60:ASN:ND2	2.38	0.40
1:C:83:THR:OG1	1:C:117:ARG:NH1	2.54	0.40
1:D:70:ARG:HE	1:D:80:GLU:CD	2.24	0.40
1:E:174:ASP:HB3	1:E:177:GLU:HB2	2.03	0.40
1:F:112:ASP:O	1:F:113:LYS:HD3	2.21	0.40
1:G:158:LEU:HD21	1:G:258:ARG:HA	2.03	0.40
1:A:164:LEU:O	1:A:241:GLY:HA2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:SER:HB3	1:E:258:ARG:HH22	1.87	0.40
1:A:131:LEU:HA	1:A:131:LEU:HD23	1.86	0.40
1:C:48:ASP:OD2	1:C:52:LYS:HE2	2.22	0.40
1:C:179:LEU:O	1:C:183:ILE:HG12	2.21	0.40
1:B:68:LYS:HB2	1:B:68:LYS:HE2	1.83	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:VAL:O	1:J:136:LYS:NZ[3_644]	2.14	0.06
1:C:42:LYS:NZ	1:F:200:GLU:O[4_465]	2.16	0.04

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	270/276 (98%)	260 (96%)	10 (4%)	0	100	100
1	B	270/276 (98%)	264 (98%)	6 (2%)	0	100	100
1	C	270/276 (98%)	262 (97%)	8 (3%)	0	100	100
1	D	271/276 (98%)	260 (96%)	11 (4%)	0	100	100
1	E	271/276 (98%)	257 (95%)	14 (5%)	0	100	100
1	F	271/276 (98%)	260 (96%)	11 (4%)	0	100	100
1	G	270/276 (98%)	260 (96%)	10 (4%)	0	100	100
1	H	264/276 (96%)	255 (97%)	9 (3%)	0	100	100
1	I	271/276 (98%)	259 (96%)	12 (4%)	0	100	100
1	J	260/276 (94%)	246 (95%)	14 (5%)	0	100	100
All	All	2688/2760 (97%)	2583 (96%)	105 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	236/239 (99%)	226 (96%)	10 (4%)	30	60
1	B	236/239 (99%)	230 (98%)	6 (2%)	47	77
1	C	236/239 (99%)	229 (97%)	7 (3%)	41	72
1	D	236/239 (99%)	223 (94%)	13 (6%)	21	49
1	E	237/239 (99%)	229 (97%)	8 (3%)	37	68
1	F	237/239 (99%)	233 (98%)	4 (2%)	60	85
1	G	236/239 (99%)	229 (97%)	7 (3%)	41	72
1	H	233/239 (98%)	226 (97%)	7 (3%)	41	72
1	I	237/239 (99%)	230 (97%)	7 (3%)	41	72
1	J	229/239 (96%)	218 (95%)	11 (5%)	25	55
All	All	2353/2390 (98%)	2273 (97%)	80 (3%)	37	68

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	89	LYS
1	A	122	MET
1	A	125	TYR
1	A	126	LYS
1	A	152	SER
1	A	166	LEU
1	A	168	GLU
1	A	185	ASP
1	A	198	ARG
1	B	4	LYS
1	B	34	LYS
1	B	64	ASP
1	B	125	TYR

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Mol	Chain	Res	Type
1	B	158	LEU
1	B	185	ASP
1	C	8	SER
1	C	105	LYS
1	C	125	TYR
1	C	132	ARG
1	C	197	SER
1	C	200	GLU
1	C	246	ARG
1	D	25	GLU
1	D	34	LYS
1	D	61	ASP
1	D	88	SER
1	D	112	ASP
1	D	125	TYR
1	D	132	ARG
1	D	151	GLU
1	D	153	LYS
1	D	197	SER
1	D	246	ARG
1	D	255	SER
1	D	263	SER
1	E	8	SER
1	E	22	SER
1	E	45	SER
1	E	125	TYR
1	E	126	LYS
1	E	132	ARG
1	E	197	SER
1	E	246	ARG
1	F	125	TYR
1	F	132	ARG
1	F	187	MET
1	F	197	SER
1	G	76	ARG
1	G	125	TYR
1	G	149	ARG
1	G	152	SER
1	G	180	LYS
1	G	197	SER
1	G	202	ASP
1	H	9	GLN

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Mol	Chain	Res	Type
1	H	113	LYS
1	H	125	TYR
1	H	132	ARG
1	H	155	SER
1	H	197	SER
1	H	246	ARG
1	I	38	SER
1	I	125	TYR
1	I	151	GLU
1	I	155	SER
1	I	197	SER
1	I	201	SER
1	I	226	LYS
1	J	5	PHE
1	J	45	SER
1	J	52	LYS
1	J	90	SER
1	J	113	LYS
1	J	125	TYR
1	J	132	ARG
1	J	153	LYS
1	J	197	SER
1	J	219	SER
1	J	227	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	256	ASN
1	F	106	GLN
1	I	165	ASN
1	J	12	HIS
1	J	47	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	272/276 (98%)	0.34	5 (1%) 68 65	48, 73, 130, 164	0
1	B	272/276 (98%)	0.27	5 (1%) 68 65	45, 78, 136, 168	0
1	C	272/276 (98%)	0.49	8 (2%) 51 46	58, 87, 148, 192	0
1	D	273/276 (98%)	0.60	22 (8%) 12 8	64, 107, 168, 202	0
1	E	273/276 (98%)	0.46	9 (3%) 46 41	57, 96, 154, 207	0
1	F	273/276 (98%)	0.42	11 (4%) 38 33	59, 94, 145, 217	0
1	G	272/276 (98%)	0.48	14 (5%) 28 22	62, 103, 159, 203	0
1	H	268/276 (97%)	0.52	15 (5%) 24 19	64, 99, 164, 199	0
1	I	273/276 (98%)	0.57	22 (8%) 12 8	54, 101, 156, 192	0
1	J	264/276 (95%)	0.61	21 (7%) 12 8	62, 112, 180, 208	0
All	All	2712/2760 (98%)	0.48	132 (4%) 29 24	45, 95, 158, 217	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	21	TRP	8.9
1	I	104	PHE	5.7
1	F	1	MET	5.0
1	D	125	TYR	4.6
1	J	38	SER	4.5
1	J	43	LEU	4.5
1	F	21	TRP	4.5
1	A	201	SER	4.2
1	G	13	LEU	4.0
1	F	26	PHE	4.0
1	I	153	LYS	3.9
1	I	220	GLY	3.6
1	D	166	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	2	VAL	3.5
1	I	208	LEU	3.4
1	D	242	PHE	3.4
1	D	25	GLU	3.4
1	E	220	GLY	3.4
1	H	7	ASP	3.3
1	D	236	PRO	3.3
1	C	25	GLU	3.2
1	J	40	PHE	3.2
1	D	247	LEU	3.2
1	D	221	ALA	3.2
1	J	52	LYS	3.1
1	D	239	GLY	3.1
1	H	115	ALA	3.1
1	J	37	SER	3.0
1	F	100	ASP	3.0
1	G	4	LYS	3.0
1	I	136	LYS	2.9
1	D	186	ILE	2.9
1	G	3	VAL	2.9
1	H	100	ASP	2.9
1	D	240	ILE	2.9
1	G	36	PHE	2.9
1	D	244	LEU	2.9
1	H	27	GLU	2.8
1	J	36	PHE	2.8
1	D	210	VAL	2.8
1	F	3	VAL	2.8
1	H	91	ALA	2.8
1	G	208	LEU	2.8
1	H	239	GLY	2.8
1	E	198	ARG	2.8
1	I	131	LEU	2.8
1	J	210	VAL	2.8
1	G	28	ASP	2.8
1	E	176	MET	2.7
1	H	203	VAL	2.7
1	I	221	ALA	2.7
1	A	199	GLU	2.7
1	D	208	LEU	2.7
1	I	196	THR	2.7
1	B	223	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	154	SER	2.7
1	J	110	ILE	2.7
1	E	219	SER	2.6
1	E	208	LEU	2.6
1	D	205	VAL	2.6
1	F	215	THR	2.6
1	H	29	ALA	2.6
1	H	204	TYR	2.6
1	J	12	HIS	2.6
1	G	5	PHE	2.6
1	I	236	PRO	2.5
1	F	192	VAL	2.5
1	E	110	ILE	2.5
1	F	28	ASP	2.5
1	H	222	VAL	2.5
1	I	222	VAL	2.5
1	D	203	VAL	2.5
1	G	182	TYR	2.5
1	A	26	PHE	2.5
1	C	2	VAL	2.5
1	D	238	ALA	2.5
1	H	272	LEU	2.4
1	D	220	GLY	2.4
1	I	272	LEU	2.4
1	F	113	LYS	2.4
1	I	273	ASP	2.4
1	F	221	ALA	2.4
1	B	28	ASP	2.4
1	I	206	GLU	2.4
1	I	158	LEU	2.4
1	I	195	THR	2.4
1	B	26	PHE	2.4
1	I	125	TYR	2.4
1	C	115	ALA	2.3
1	J	125	TYR	2.3
1	J	13	LEU	2.3
1	H	246	ARG	2.3
1	C	5	PHE	2.3
1	D	26	PHE	2.3
1	H	223	GLY	2.3
1	E	175	PRO	2.3
1	C	24	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	208	LEU	2.3
1	G	104	PHE	2.2
1	G	100	ASP	2.2
1	G	95	MET	2.2
1	J	18	ASP	2.2
1	G	26	PHE	2.2
1	J	227	LEU	2.2
1	B	224	PRO	2.2
1	C	92	LEU	2.2
1	J	175	PRO	2.2
1	I	239	GLY	2.2
1	B	222	VAL	2.2
1	D	97	ILE	2.1
1	A	204	TYR	2.1
1	J	149	ARG	2.1
1	G	29	ALA	2.1
1	D	237	TRP	2.1
1	J	109	TRP	2.1
1	E	242	PHE	2.1
1	J	28	ASP	2.1
1	J	59	ARG	2.1
1	J	166	LEU	2.1
1	C	221	ALA	2.1
1	I	176	MET	2.1
1	D	197	SER	2.1
1	E	112	ASP	2.1
1	I	238	ALA	2.1
1	I	109	TRP	2.1
1	I	137	GLY	2.1
1	J	273	ASP	2.1
1	H	103	LEU	2.0
1	D	248	LEU	2.0
1	H	225	HIS	2.0
1	I	225	HIS	2.0
1	C	234	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.