Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 01:09 PM EDT

PDB ID	:	4Q29
Title	:	Ensemble Refinement of plu4264 protein from Photorhabdus luminescens
Authors	:	Wang, F.; Michalska, K.; Li, H.; Jedrzejczak, R.; Babnigg, G.; Bingman, C.A.; Yennamalli, R.; Weerth, S.; Miller, M.D.; Thomas, M.G.; Joachimiak, A.; Phillips Jr., G.N.; Enzyme Discovery for Natural Product Biosynthesis (NatPro); Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2014-04-07
Resolution	:	1.35 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 (i) 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 (i)) were used in the production of this report:

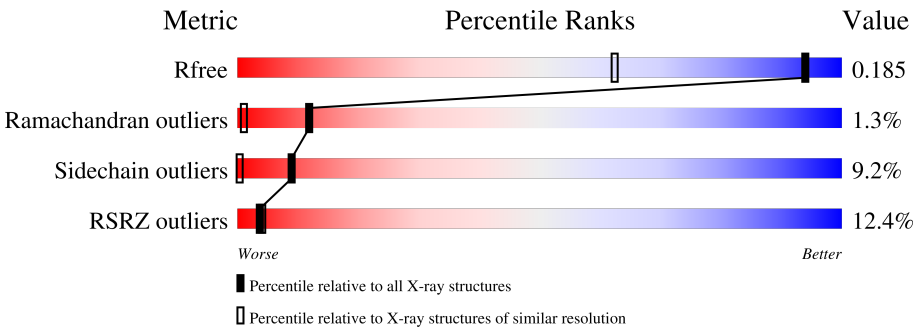
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.35 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}	130704	1385 (1.36-1.32)
Ramachandran outliers	138981	1397 (1.36-1.32)
Sidechain outliers	138945	1397 (1.36-1.32)
RSRZ outliers	127900	1369 (1.36-1.32)

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	1-A	128	13% 85% 9% • 5%
1	1-B	128	10% 84% 9% • 6%
1	10-A	128	13% 79% 14% • 5%
1	10-B	128	10% 82% 9% • 6%
1	11-A	128	13% 78% 13% • 5%
1	11-B	128	10% 84% 9% • 6%

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Mol	Chain	Length	Quality of chain
1	12-A	128	13% 88% 6% 5%
1	12-B	128	10% 84% 8% 6%
1	13-A	128	13% 84% 11% 5%
1	13-B	128	10% 88% 5% 6%
1	14-A	128	13% 77% 11% 5% 5%
1	14-B	128	10% 81% 11% 6%
1	15-A	128	13% 80% 13% 5%
1	15-B	128	10% 80% 14% 6%
1	16-A	128	13% 88% 7% 5%
1	16-B	128	10% 80% 12% 6%
1	17-A	128	13% 80% 12% 5%
1	17-B	128	10% 84% 8% 6%
1	18-A	128	13% 82% 12% 5%
1	18-B	128	10% 84% 8% 6%
1	19-A	128	13% 83% 12% 5%
1	19-B	128	10% 78% 14% 6%
1	2-A	128	13% 80% 12% 5%
1	2-B	128	10% 84% 9% 6%
1	20-A	128	13% 78% 16% 5%
1	20-B	128	10% 80% 12% 6%
1	3-A	128	13% 83% 9% 5%
1	3-B	128	10% 80% 13% 6%
1	4-A	128	13% 83% 10% 5%
1	4-B	128	10% 77% 15% 6%
1	5-A	128	13% 80% 14% 5%

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Mol	Chain	Length	Quality of chain
1	5-B	128	10% 84% 9% • 6%
1	6-A	128	13% 80% 12% • 5%
1	6-B	128	10% 84% 7% • 6%
1	7-A	128	13% 86% 9% 5%
1	7-B	128	10% 83% 10% • 6%
1	8-A	128	13% 84% 11% 5%
1	8-B	128	10% 84% 9% • 6%
1	9-A	128	13% 80% 14% • 5%
1	9-B	128	10% 83% 9% • 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 94724 atoms, of which 44279 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 plu4264 protein.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S	Se			
1	1-A	121	2195	718	1079	188	206	1	3	0	22	0
1	2-A	121	2195	718	1079	188	206	1	3	0	22	0
1	3-A	121	2195	718	1079	188	206	1	3	0	22	0
1	4-A	121	2195	718	1079	188	206	1	3	0	22	0
1	5-A	121	2195	718	1079	188	206	1	3	0	22	0
1	6-A	121	2195	718	1079	188	206	1	3	0	22	0
1	7-A	121	2195	718	1079	188	206	1	3	0	22	0
1	8-A	121	2195	718	1079	188	206	1	3	0	22	0
1	9-A	121	2195	718	1079	188	206	1	3	0	22	0
1	10-A	121	2195	718	1079	188	206	1	3	0	22	0
1	11-A	121	2195	718	1079	188	206	1	3	0	22	0
1	12-A	121	2195	718	1079	188	206	1	3	0	22	0
1	13-A	121	2195	718	1079	188	206	1	3	0	22	0
1	14-A	121	2195	718	1079	188	206	1	3	0	22	0
1	15-A	121	2195	718	1079	188	206	1	3	0	22	0
1	16-A	121	2195	718	1079	188	206	1	3	0	22	0

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S	Se			
1	17-A	121	2195	718	1079	188	206	1	3	0	22	0
1	18-A	121	2195	718	1079	188	206	1	3	0	22	0
1	19-A	121	2195	718	1079	188	206	1	3	0	22	0
1	20-A	121	2194	718	1078	188	206	1	3	0	21	0
1	1-B	120	2353	775	1135	209	230	1	3	0	33	0
1	2-B	120	2353	775	1135	209	230	1	3	0	33	0
1	3-B	120	2353	775	1135	209	230	1	3	0	33	0
1	4-B	120	2353	775	1135	209	230	1	3	0	33	0
1	5-B	120	2353	775	1135	209	230	1	3	0	33	0
1	6-B	120	2353	775	1135	209	230	1	3	0	33	0
1	7-B	120	2353	775	1135	209	230	1	3	0	33	0
1	8-B	120	2353	775	1135	209	230	1	3	0	33	0
1	9-B	120	2353	775	1135	209	230	1	3	0	33	0
1	10-B	120	2353	775	1135	209	230	1	3	0	33	0
1	11-B	120	2353	775	1135	209	230	1	3	0	33	0
1	12-B	120	2353	775	1135	209	230	1	3	0	33	0
1	13-B	120	2353	775	1135	209	230	1	3	0	33	0
1	14-B	120	2353	775	1135	209	230	1	3	0	33	0
1	15-B	120	2353	775	1135	209	230	1	3	0	33	0
1	16-B	120	2353	775	1135	209	230	1	3	0	33	0
1	17-B	120	2353	775	1135	209	230	1	3	0	33	0

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S	Se			
1	18-B	120	2353	775	1135	209	230	1	3	0	33	0
1	19-B	120	2353	775	1135	209	230	1	3	0	33	0
1	20-B	120	2353	775	1135	209	230	1	3	0	33	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	HIS	-	EXPRESSION TAG	UNP Q7MZL9
A	124	HIS	-	EXPRESSION TAG	UNP Q7MZL9
A	125	HIS	-	EXPRESSION TAG	UNP Q7MZL9
A	126	HIS	-	EXPRESSION TAG	UNP Q7MZL9
A	127	HIS	-	EXPRESSION TAG	UNP Q7MZL9
A	128	HIS	-	EXPRESSION TAG	UNP Q7MZL9
B	123	HIS	-	EXPRESSION TAG	UNP Q7MZL9
B	124	HIS	-	EXPRESSION TAG	UNP Q7MZL9
B	125	HIS	-	EXPRESSION TAG	UNP Q7MZL9
B	126	HIS	-	EXPRESSION TAG	UNP Q7MZL9
B	127	HIS	-	EXPRESSION TAG	UNP Q7MZL9
B	128	HIS	-	EXPRESSION TAG	UNP Q7MZL9

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
2	1-A	1	1	1	0	0
2	2-A	1	1	1	0	0
2	3-A	1	1	1	0	0
2	4-A	1	1	1	0	0
2	5-A	1	1	1	0	0
2	6-A	1	1	1	0	0
2	7-A	1	1	1	0	0
2	8-A	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
2	9-A	1	1	1	0	0
2	10-A	1	1	1	0	0
2	11-A	1	1	1	0	0
2	12-A	1	1	1	0	0
2	13-A	1	1	1	0	0
2	14-A	1	1	1	0	0
2	15-A	1	1	1	0	0
2	16-A	1	1	1	0	0
2	17-A	1	1	1	0	0
2	18-A	1	1	1	0	0
2	19-A	1	1	1	0	0
2	20-A	1	1	1	0	0
2	1-B	1	1	1	0	0
2	2-B	1	1	1	0	0
2	3-B	1	1	1	0	0
2	4-B	1	1	1	0	0
2	5-B	1	1	1	0	0
2	6-B	1	1	1	0	0
2	7-B	1	1	1	0	0
2	8-B	1	1	1	0	0
2	9-B	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
2	10-B	1	1	1	0	0
2	11-B	1	1	1	0	0
2	12-B	1	1	1	0	0
2	13-B	1	1	1	0	0
2	14-B	1	1	1	0	0
2	15-B	1	1	1	0	0
2	16-B	1	1	1	0	0
2	17-B	1	1	1	0	0
2	18-B	1	1	1	0	0
2	19-B	1	1	1	0	0
2	20-B	1	1	1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	1-A	1	1	1	0	0
3	2-A	1	1	1	0	0
3	3-A	1	1	1	0	0
3	4-A	1	1	1	0	0
3	5-A	1	1	1	0	0
3	6-A	1	1	1	0	0
3	7-A	1	1	1	0	0
3	8-A	1	1	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	9-A	1	Total Na 1 1	0	0
3	10-A	1	Total Na 1 1	0	0
3	11-A	1	Total Na 1 1	0	0
3	12-A	1	Total Na 1 1	0	0
3	13-A	1	Total Na 1 1	0	0
3	14-A	1	Total Na 1 1	0	0
3	15-A	1	Total Na 1 1	0	0
3	16-A	1	Total Na 1 1	0	0
3	17-A	1	Total Na 1 1	0	0
3	18-A	1	Total Na 1 1	0	0
3	19-A	1	Total Na 1 1	0	0
3	20-A	1	Total Na 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1-A	101	Total O 101 101	0	0
4	2-A	95	Total O 95 95	0	0
4	3-A	92	Total O 92 92	0	0
4	4-A	101	Total O 101 101	0	0
4	5-A	87	Total O 87 87	0	0
4	6-A	100	Total O 100 100	0	0
4	7-A	85	Total O 85 85	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	8-A	90	Total O 90 90	0	0
4	9-A	86	Total O 86 86	0	0
4	10-A	94	Total O 94 94	0	0
4	11-A	86	Total O 86 86	0	0
4	12-A	108	Total O 108 108	0	0
4	13-A	88	Total O 88 88	0	0
4	14-A	91	Total O 91 91	0	0
4	15-A	88	Total O 88 88	0	0
4	16-A	97	Total O 97 97	0	0
4	17-A	97	Total O 97 97	0	0
4	18-A	98	Total O 98 98	0	0
4	19-A	101	Total O 101 101	0	0
4	20-A	85	Total O 85 85	0	0
4	1-B	97	Total O 97 97	0	0
4	2-B	82	Total O 82 82	0	0
4	3-B	91	Total O 91 91	0	0
4	4-B	90	Total O 90 90	0	0
4	5-B	95	Total O 95 95	0	0
4	6-B	85	Total O 85 85	0	0
4	7-B	84	Total O 84 84	0	0
4	8-B	99	Total O 99 99	0	0

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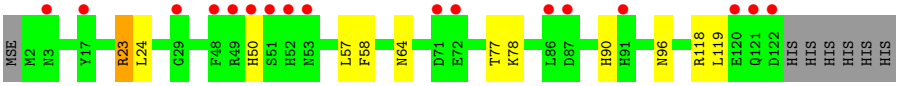
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	9-B	92	Total O 92 92	0	0
4	10-B	95	Total O 95 95	0	0
4	11-B	90	Total O 90 90	0	0
4	12-B	92	Total O 92 92	0	0
4	13-B	81	Total O 81 81	0	0
4	14-B	87	Total O 87 87	0	0
4	15-B	100	Total O 100 100	0	0
4	16-B	95	Total O 95 95	0	0
4	17-B	102	Total O 102 102	0	0
4	18-B	88	Total O 88 88	0	0
4	19-B	91	Total O 91 91	0	0
4	20-B	99	Total O 99 99	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.

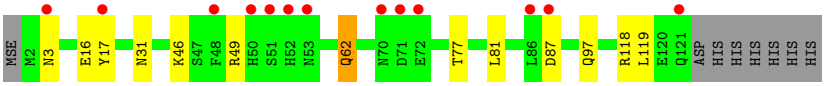
- Molecule 1: plu4264 protein

Chain 1-A:



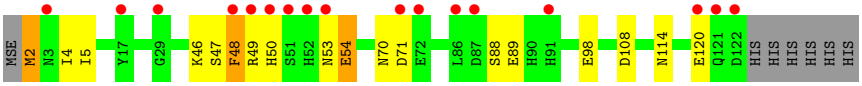
- Molecule 1: plu4264 protein

Chain 1-B:



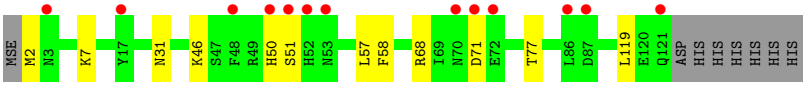
- Molecule 1: plu4264 protein

Chain 2-A:



- Molecule 1: plu4264 protein

Chain 2-B:

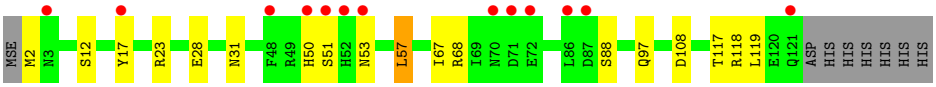


- Molecule 1: plu4264 protein

Chain 3-A:

- Molecule 1: plu4264 protein

Chain 3-B:

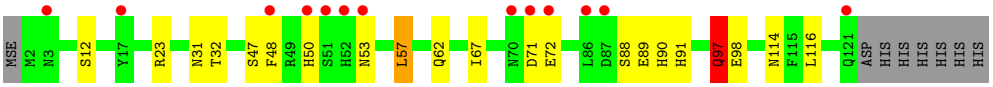


• Molecule 1: plu4264 protein

Chain 4-A:

• Molecule 1: plu4264 protein

Chain 4-B:

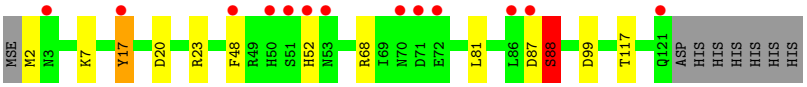


• Molecule 1: plu4264 protein

Chain 5-A:

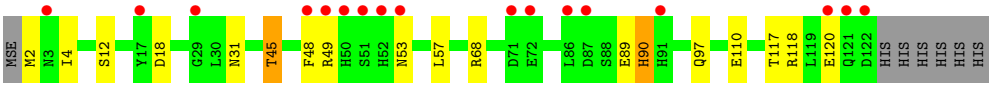
• Molecule 1: plu4264 protein

Chain 5-B:



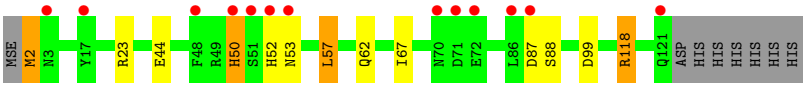
• Molecule 1: plu4264 protein

Chain 6-A:



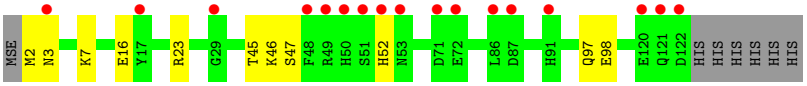
• Molecule 1: plu4264 protein

Chain 6-B:



• Molecule 1: plu4264 protein

Chain 7-A:



• Molecule 1: plu4264 protein

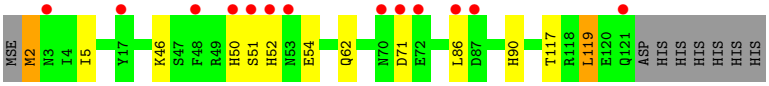
Chain 7-B:

• Molecule 1: plu4264 protein

Chain 8-A:

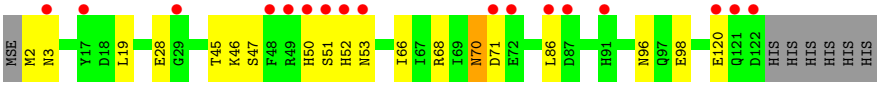
• Molecule 1: plu4264 protein

Chain 8-B:



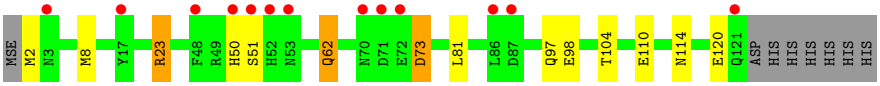
• Molecule 1: plu4264 protein

Chain 9-A:



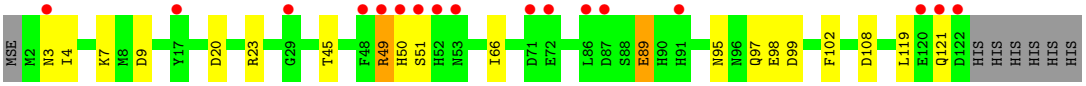
• Molecule 1: plu4264 protein

Chain 9-B:



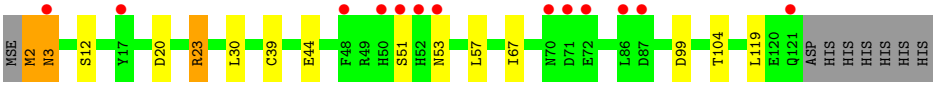
• Molecule 1: plu4264 protein

Chain 10-A:



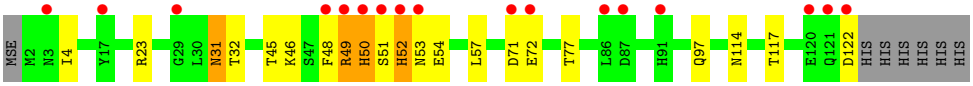
• Molecule 1: plu4264 protein

Chain 10-B:



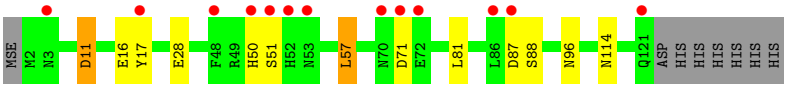
• Molecule 1: plu4264 protein

Chain 11-A:



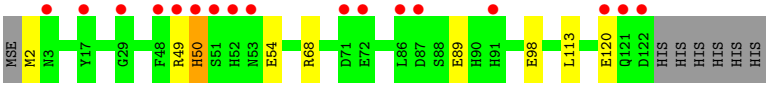
• Molecule 1: plu4264 protein

Chain 11-B:



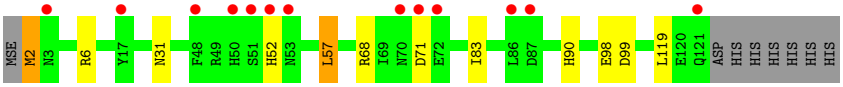
• Molecule 1: plu4264 protein

Chain 12-A:



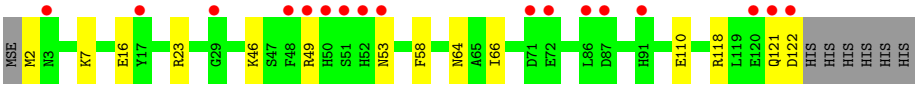
• Molecule 1: plu4264 protein

Chain 12-B:



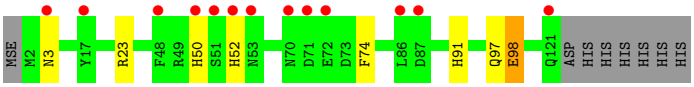
• Molecule 1: plu4264 protein

Chain 13-A:



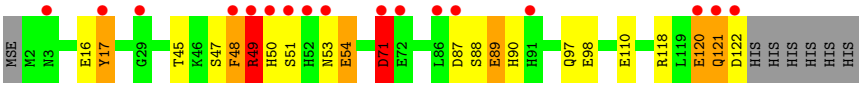
• Molecule 1: plu4264 protein

Chain 13-B:



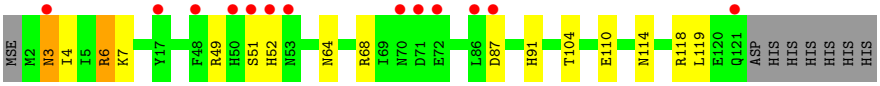
• Molecule 1: plu4264 protein

Chain 14-A:



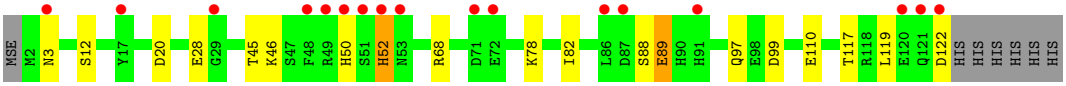
• Molecule 1: plu4264 protein

Chain 14-B:



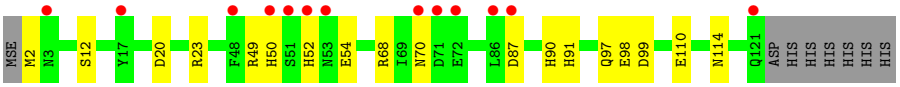
• Molecule 1: plu4264 protein

Chain 15-A:



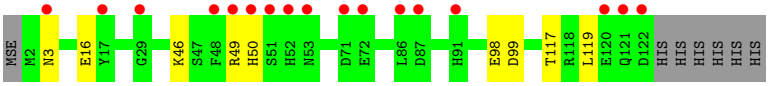
• Molecule 1: plu4264 protein

Chain 15-B:



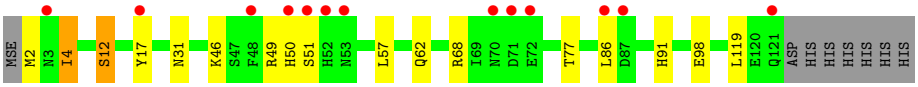
• Molecule 1: plu4264 protein

Chain 16-A:



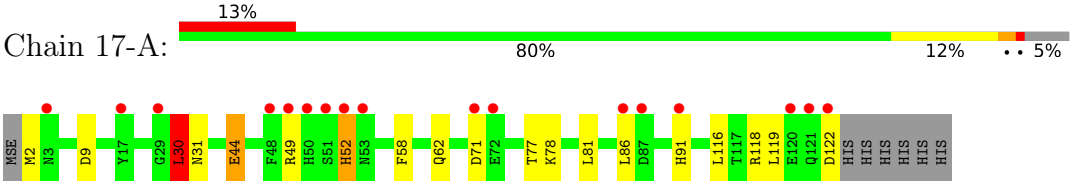
• Molecule 1: plu4264 protein

Chain 16-B:



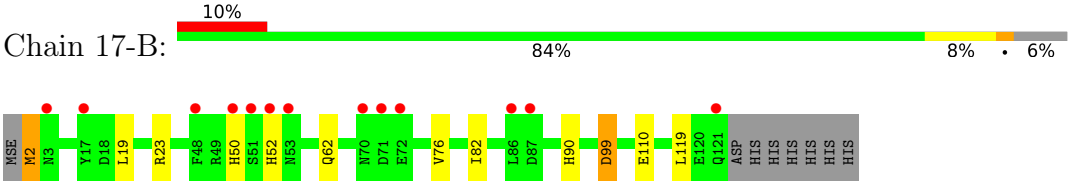
• Molecule 1: plu4264 protein

Chain 17-A:



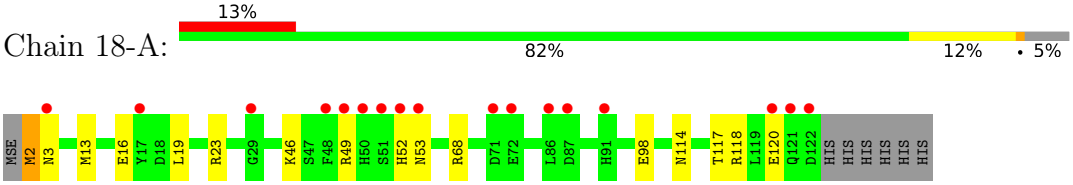
• Molecule 1: plu4264 protein

Chain 17-B:



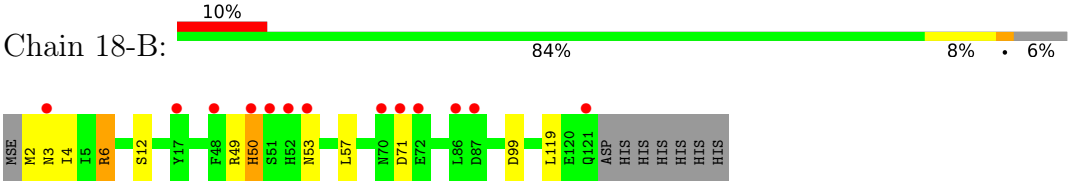
• Molecule 1: plu4264 protein

Chain 18-A:



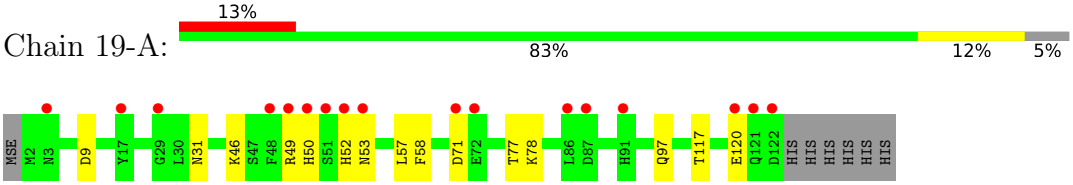
• Molecule 1: plu4264 protein

Chain 18-B:



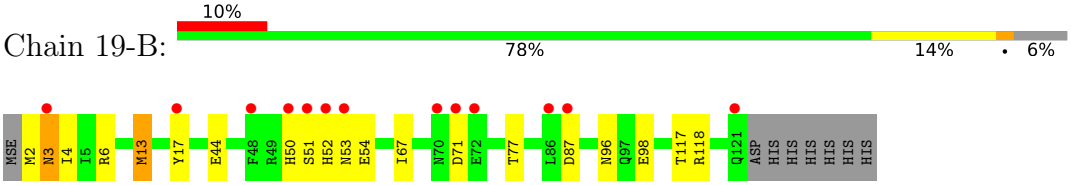
• Molecule 1: plu4264 protein

Chain 19-A:



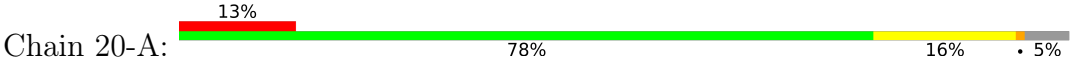
• Molecule 1: plu4264 protein

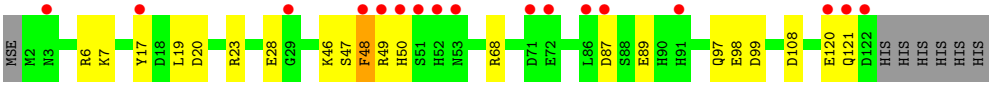
Chain 19-B:



• Molecule 1: plu4264 protein

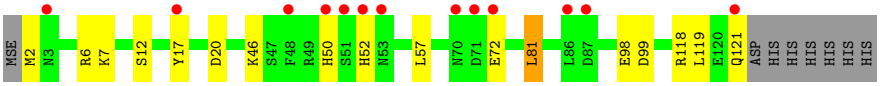
Chain 20-A:





- Molecule 1: plu4264 protein

Chain 20-B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	55.74Å 147.69Å 83.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.90 – 1.35 24.90 – 1.35	Depositor EDS
% Data completeness (in resolution range)	99.5 (24.90-1.35) 99.5 (24.90-1.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 1.35Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.126 , 0.155 0.162 , 0.185	Depositor DCC
R_{free} test set	1111 reflections (1.46%)	wwPDB-VP
Wilson B-factor (Å^2)	13.4	Xtriage
Anisotropy	0.734	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 262.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	94724	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 72.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.157*4*e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, NA

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	1-A	0.84	0/1237	1.05	7/1679 (0.4%)
1	1-B	0.85	1/1338 (0.1%)	0.90	0/1816
1	2-A	0.92	1/1237 (0.1%)	1.17	8/1679 (0.5%)
1	2-B	0.78	0/1338	0.99	3/1816 (0.2%)
1	3-A	0.85	1/1237 (0.1%)	1.09	7/1679 (0.4%)
1	3-B	0.84	0/1338	1.04	7/1816 (0.4%)
1	4-A	0.90	1/1237 (0.1%)	1.08	7/1679 (0.4%)
1	4-B	0.94	2/1338 (0.1%)	1.05	5/1816 (0.3%)
1	5-A	1.27	4/1237 (0.3%)	1.34	11/1679 (0.7%)
1	5-B	1.19	5/1338 (0.4%)	1.18	7/1816 (0.4%)
1	6-A	0.89	2/1237 (0.2%)	1.08	5/1679 (0.3%)
1	6-B	0.85	2/1338 (0.1%)	1.10	6/1816 (0.3%)
1	7-A	0.88	1/1237 (0.1%)	1.06	1/1679 (0.1%)
1	7-B	0.81	0/1338	0.96	5/1816 (0.3%)
1	8-A	0.84	0/1237	1.04	3/1679 (0.2%)
1	8-B	0.82	2/1338 (0.1%)	0.99	2/1816 (0.1%)
1	9-A	0.90	2/1237 (0.2%)	1.12	6/1679 (0.4%)
1	9-B	0.81	2/1338 (0.1%)	1.08	4/1816 (0.2%)
1	10-A	1.21	4/1237 (0.3%)	1.24	8/1679 (0.5%)
1	10-B	1.23	4/1338 (0.3%)	1.17	7/1816 (0.4%)
1	11-A	0.88	0/1237	1.10	4/1679 (0.2%)
1	11-B	0.85	1/1338 (0.1%)	1.08	3/1816 (0.2%)
1	12-A	0.93	3/1237 (0.2%)	1.09	6/1679 (0.4%)
1	12-B	0.85	1/1338 (0.1%)	1.05	5/1816 (0.3%)
1	13-A	0.86	1/1237 (0.1%)	1.03	6/1679 (0.4%)
1	13-B	0.84	1/1338 (0.1%)	0.94	1/1816 (0.1%)
1	14-A	1.12	5/1237 (0.4%)	1.25	10/1679 (0.6%)
1	14-B	0.98	1/1338 (0.1%)	1.20	6/1816 (0.3%)
1	15-A	1.32	3/1237 (0.2%)	1.26	7/1679 (0.4%)
1	15-B	1.13	1/1338 (0.1%)	1.11	5/1816 (0.3%)
1	16-A	0.85	1/1237 (0.1%)	1.01	1/1679 (0.1%)
1	16-B	0.86	1/1338 (0.1%)	1.07	3/1816 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	17-A	0.89	1/1237 (0.1%)	1.12	12/1679 (0.7%)
1	17-B	0.87	1/1338 (0.1%)	1.11	4/1816 (0.2%)
1	18-A	0.86	1/1237 (0.1%)	1.02	3/1679 (0.2%)
1	18-B	0.89	2/1338 (0.1%)	1.08	4/1816 (0.2%)
1	19-A	0.93	1/1237 (0.1%)	1.14	7/1679 (0.4%)
1	19-B	0.94	3/1338 (0.2%)	1.10	5/1816 (0.3%)
1	20-A	1.28	3/1229 (0.2%)	1.29	8/1668 (0.5%)
1	20-B	1.19	4/1338 (0.3%)	1.21	9/1816 (0.5%)
All	All	0.96	69/51492 (0.1%)	1.10	218/69889 (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	1-B	0	1
1	4-A	0	1
1	5-A	0	1
1	6-B	0	1
1	9-A	0	1
1	9-B	0	1
1	11-B	0	1
1	12-B	0	1
1	14-A	0	4
1	14-B	0	1
1	17-A	0	1
1	18-A	0	1
1	20-A	0	2
All	All	0	17

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-B	98	GLU	CG-CD	12.88	1.71	1.51
1	15-A	45	THR	CB-CG2	-12.85	1.09	1.52
1	20-A	98	GLU	CG-CD	-12.32	1.33	1.51
1	12-A	98	GLU	CD-OE2	11.86	1.38	1.25
1	20-A	98	GLU	CD-OE2	-11.31	1.13	1.25
1	19-B	13	MSE	CB-CG	10.34	1.83	1.52
1	9-B	62	GLN	CB-CG	-10.20	1.25	1.52
1	20-B	12	SER	CB-OG	10.12	1.55	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-B	98	GLU	CB-CG	9.84	1.70	1.52
1	5-A	54	GLU	CD-OE2	9.72	1.36	1.25
1	18-B	12	SER	CB-OG	9.41	1.54	1.42
1	18-B	12	SER	CA-CB	9.37	1.67	1.52
1	11-B	11	ASP	CG-OD2	8.96	1.46	1.25
1	5-B	23	ARG	CZ-NH2	-8.61	1.21	1.33
1	5-B	17[A]	TYR	CD2-CE2	-8.40	1.26	1.39
1	5-B	17[B]	TYR	CD2-CE2	-8.40	1.26	1.39
1	16-A	98	GLU	CG-CD	-8.31	1.39	1.51
1	9-A	120	GLU	CB-CG	8.23	1.67	1.52
1	12-A	98	GLU	CB-CG	7.94	1.67	1.52
1	15-A	89	GLU	N-CA	7.68	1.61	1.46
1	10-B	3	ASN	CB-CG	7.65	1.68	1.51
1	1-B	62	GLN	CG-CD	-7.36	1.34	1.51
1	8-B	62	GLN	CG-CD	7.34	1.68	1.51
1	19-B	44	GLU	CB-CG	7.29	1.66	1.52
1	2-A	54	GLU	CB-CG	7.17	1.65	1.52
1	10-B	44	GLU	CG-CD	-7.12	1.41	1.51
1	16-B	12	SER	CA-CB	7.03	1.63	1.52
1	14-A	17	TYR	CD2-CE2	6.90	1.49	1.39
1	10-A	97[A]	GLN	CB-CG	6.71	1.70	1.52
1	10-A	97[B]	GLN	CB-CG	6.71	1.70	1.52
1	17-A	44	GLU	CB-CG	-6.68	1.39	1.52
1	20-B	12	SER	CA-CB	6.64	1.62	1.52
1	5-A	44	GLU	CD-OE2	6.62	1.32	1.25
1	10-B	23	ARG	CG-CD	6.55	1.68	1.51
1	15-A	28	GLU	CB-CG	6.54	1.64	1.52
1	3-A	45	THR	CB-CG2	-6.26	1.31	1.52
1	20-A	17	TYR	CE2-CZ	-6.21	1.30	1.38
1	5-B	88	SER	N-CA	6.18	1.58	1.46
1	5-B	23	ARG	CG-CD	6.17	1.67	1.51
1	12-A	98	GLU	CG-CD	6.10	1.61	1.51
1	9-B	8	MSE	CB-CG	5.82	1.70	1.52
1	17-B	76	VAL	CB-CG1	5.81	1.65	1.52
1	14-A	120	GLU	CB-CG	5.77	1.63	1.52
1	12-B	98	GLU	CG-CD	5.75	1.60	1.51
1	8-B	62	GLN	CB-CG	5.72	1.68	1.52
1	19-A	117	THR	CB-CG2	5.67	1.71	1.52
1	14-A	47	SER	CA-C	5.65	1.67	1.52
1	6-B	62	GLN	CG-CD	5.63	1.64	1.51
1	18-A	98	GLU	CG-CD	-5.58	1.43	1.51
1	14-A	89	GLU	CB-CG	5.51	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	15-B	98	GLU	CD-OE2	5.49	1.31	1.25
1	7-A	98	GLU	CB-CG	5.44	1.62	1.52
1	5-A	54	GLU	CG-CD	5.38	1.60	1.51
1	4-A	46	LYS	CB-CG	5.36	1.67	1.52
1	10-A	98	GLU	CG-CD	-5.35	1.44	1.51
1	6-B	44	GLU	CD-OE1	5.27	1.31	1.25
1	13-A	16	GLU	CB-CG	-5.22	1.42	1.52
1	5-A	87	ASP	CB-CG	5.21	1.62	1.51
1	9-A	45	THR	CB-CG2	-5.21	1.35	1.52
1	10-A	89	GLU	CB-CG	5.21	1.62	1.52
1	13-B	98	GLU	CB-CG	5.18	1.61	1.52
1	10-B	39	CYS	CB-SG	-5.16	1.73	1.81
1	14-A	98	GLU	CG-CD	5.15	1.59	1.51
1	14-B	110	GLU	CG-CD	5.12	1.59	1.51
1	20-B	17[A]	TYR	CD2-CE2	-5.10	1.31	1.39
1	20-B	17[B]	TYR	CD2-CE2	-5.10	1.31	1.39
1	6-A	31	ASN	CB-CG	-5.09	1.39	1.51
1	19-B	44	GLU	CG-CD	5.09	1.59	1.51
1	6-A	12	SER	CA-CB	5.01	1.60	1.52

All (218) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	11-B	11	ASP	CB-CG-OD1	-16.17	103.75	118.30
1	18-B	6	ARG	NE-CZ-NH1	-15.12	112.74	120.30
1	6-B	57	LEU	CB-CG-CD2	-11.07	92.17	111.00
1	17-B	99	ASP	CB-CG-OD2	10.49	127.74	118.30
1	6-B	57	LEU	CB-CG-CD1	10.18	128.30	111.00
1	5-A	23	ARG	NE-CZ-NH2	-10.10	115.25	120.30
1	20-B	118	ARG	NE-CZ-NH2	-9.95	115.33	120.30
1	14-B	118	ARG	NE-CZ-NH2	-9.74	115.43	120.30
1	2-A	48	PHE	CB-CG-CD1	-9.55	114.11	120.80
1	11-B	57	LEU	CB-CG-CD1	9.44	127.04	111.00
1	14-B	118	ARG	NE-CZ-NH1	9.41	125.00	120.30
1	18-B	6	ARG	NE-CZ-NH2	9.07	124.84	120.30
1	12-A	2	MSE	CG-SE-CE	-9.06	78.97	98.90
1	14-B	6	ARG	NE-CZ-NH1	-9.04	115.78	120.30
1	2-A	48	PHE	CB-CG-CD2	8.91	127.04	120.80
1	11-B	11	ASP	CB-CG-OD2	8.89	126.30	118.30
1	8-B	2	MSE	CB-CG-SE	-8.51	87.16	112.70
1	15-A	68	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	17-A	30	LEU	CA-CB-CG	8.46	134.75	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	20-A	108	ASP	CB-CG-OD1	8.23	125.71	118.30
1	5-A	23	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	4-B	97	GLN	CA-CB-CG	8.18	131.39	113.40
1	19-B	13	MSE	CA-CB-CG	8.14	127.14	113.30
1	5-B	23	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	15-A	45	THR	N-CA-CB	-8.05	95.01	110.30
1	19-B	6	ARG	NE-CZ-NH1	7.65	124.12	120.30
1	15-A	20	ASP	CB-CG-OD1	7.60	125.14	118.30
1	10-A	20	ASP	CB-CG-OD1	7.50	125.05	118.30
1	17-A	52	HIS	CB-CA-C	-7.43	95.53	110.40
1	15-A	89	GLU	N-CA-CB	7.41	123.93	110.60
1	5-A	20	ASP	CB-CG-OD1	7.33	124.89	118.30
1	16-B	31	ASN	CB-CA-C	-7.31	95.79	110.40
1	5-B	23	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	17-A	9	ASP	CB-CG-OD1	7.28	124.86	118.30
1	3-B	57	LEU	CA-CB-CG	7.27	132.03	115.30
1	14-A	49	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	19-A	78	LYS	CD-CE-NZ	7.21	128.29	111.70
1	3-B	57	LEU	CB-CG-CD1	-7.17	98.81	111.00
1	12-B	57	LEU	CA-CB-CG	7.16	131.78	115.30
1	10-B	44	GLU	OE1-CD-OE2	7.16	131.89	123.30
1	3-B	23	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	17-A	9	ASP	CB-CG-OD2	-7.05	111.96	118.30
1	9-B	62	GLN	CB-CA-C	-7.04	96.31	110.40
1	14-B	68	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	20-B	20	ASP	CB-CG-OD1	7.01	124.61	118.30
1	2-A	108	ASP	CB-CG-OD1	7.00	124.60	118.30
1	17-B	23	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	20-A	68	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	3-B	68	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	10-A	108	ASP	CB-CG-OD1	6.86	124.48	118.30
1	20-A	23	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	5-B	20	ASP	CB-CG-OD1	6.84	124.45	118.30
1	1-A	118	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	10-A	23	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	7-B	7	LYS	CD-CE-NZ	-6.72	96.24	111.70
1	14-A	118	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	16-B	68	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	12-A	98	GLU	CG-CD-OE1	-6.65	105.01	118.30
1	15-B	68	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	6-B	118	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	20-B	57	LEU	CB-CG-CD2	-6.63	99.73	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	6-A	45	THR	OG1-CB-CG2	6.58	125.14	110.00
1	1-A	23	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	5-B	99	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	20-A	20	ASP	CB-CG-OD1	6.51	124.16	118.30
1	15-A	89	GLU	CB-CA-C	-6.49	97.42	110.40
1	2-B	68	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	5-A	68	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	2-A	88	SER	N-CA-C	6.41	128.31	111.00
1	14-A	47	SER	N-CA-C	6.41	128.31	111.00
1	3-A	45	THR	CB-CA-C	-6.40	94.33	111.60
1	3-A	45	THR	N-CA-CB	6.35	122.37	110.30
1	5-A	108	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	18-B	6	ARG	CD-NE-CZ	6.34	132.48	123.60
1	15-B	23	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	4-B	98	GLU	OE1-CD-OE2	-6.33	115.70	123.30
1	17-B	99	ASP	CB-CG-OD1	-6.33	112.60	118.30
1	19-A	58[A]	PHE	CB-CG-CD2	-6.29	116.40	120.80
1	19-A	58[B]	PHE	CB-CG-CD2	-6.29	116.40	120.80
1	5-A	18	ASP	CB-CG-OD2	-6.26	112.66	118.30
1	12-A	113[A]	LEU	CA-CB-CG	-6.21	101.01	115.30
1	12-A	113[B]	LEU	CA-CB-CG	-6.21	101.01	115.30
1	19-A	71	ASP	CB-CG-OD1	6.21	123.89	118.30
1	5-B	68	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	3-B	118	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	1-A	118	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	10-A	49	ARG	CG-CD-NE	6.17	124.76	111.80
1	9-A	68	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	11-A	52	HIS	N-CA-C	6.15	127.61	111.00
1	8-A	68	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	6-B	23	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	4-A	4[A]	ILE	CB-CA-C	-6.12	99.36	111.60
1	4-A	4[B]	ILE	CB-CA-C	-6.12	99.36	111.60
1	15-A	88	SER	C-N-CA	-6.11	106.43	121.70
1	19-B	6	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	20-B	6	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	15-B	20	ASP	CB-CG-OD1	5.99	123.69	118.30
1	9-A	86	LEU	CA-CB-CG	-5.97	101.56	115.30
1	4-A	46	LYS	CA-CB-CG	5.96	126.51	113.40
1	19-A	58[A]	PHE	CB-CG-CD1	5.94	124.96	120.80
1	19-A	58[B]	PHE	CB-CG-CD1	5.94	124.96	120.80
1	7-A	23	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	14-A	54	GLU	N-CA-C	-5.88	95.14	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5-A	108	ASP	CB-CG-OD1	5.86	123.58	118.30
1	9-A	45	THR	OG1-CB-CG2	-5.86	96.53	110.00
1	3-A	86	LEU	CA-CB-CG	5.82	128.68	115.30
1	17-A	78	LYS	CD-CE-NZ	-5.81	98.35	111.70
1	5-A	4[A]	ILE	CB-CA-C	-5.80	100.01	111.60
1	5-A	4[B]	ILE	CB-CA-C	-5.80	100.01	111.60
1	14-B	64	ASN	CB-CA-C	-5.77	98.86	110.40
1	20-B	119	LEU	CA-CB-CG	5.75	128.53	115.30
1	6-B	118	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	3-A	119	LEU	CA-CB-CG	5.71	128.44	115.30
1	2-A	70[A]	ASN	N-CA-C	5.70	126.38	111.00
1	2-A	70[B]	ASN	N-CA-C	5.70	126.38	111.00
1	5-A	18	ASP	CB-CG-OD1	5.67	123.40	118.30
1	6-B	99	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	7-B	49[A]	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	7-B	49[B]	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	15-B	23	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	18-A	23	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	17-A	58[A]	PHE	CB-CG-CD2	-5.63	116.86	120.80
1	17-A	58[B]	PHE	CB-CG-CD2	-5.63	116.86	120.80
1	14-A	118	ARG	NE-CZ-NH1	-5.63	117.49	120.30
1	10-B	30	LEU	CA-CB-CG	5.61	128.21	115.30
1	5-B	99	ASP	CB-CG-OD1	5.60	123.34	118.30
1	11-A	51	SER	CB-CA-C	-5.59	99.48	110.10
1	4-A	57[A]	LEU	CA-CB-CG	5.59	128.15	115.30
1	4-A	57[B]	LEU	CA-CB-CG	5.59	128.15	115.30
1	2-B	2	MSE	CG-SE-CE	-5.58	86.62	98.90
1	1-A	23	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	5-A	115	PHE	CB-CG-CD2	5.58	124.70	120.80
1	11-A	23	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	4-B	12	SER	N-CA-CB	-5.55	102.17	110.50
1	17-A	58[A]	PHE	CB-CG-CD1	5.51	124.66	120.80
1	17-A	58[B]	PHE	CB-CG-CD1	5.51	124.66	120.80
1	10-A	45	THR	OG1-CB-CG2	-5.51	97.33	110.00
1	12-B	99	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	13-A	16	GLU	CB-CA-C	-5.50	99.41	110.40
1	20-A	108	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	15-B	99	ASP	CB-CG-OD1	5.48	123.23	118.30
1	14-A	71	ASP	N-CA-C	5.46	125.75	111.00
1	19-B	67	ILE	CB-CA-C	5.46	122.51	111.60
1	12-A	2	MSE	CB-CG-SE	5.45	129.05	112.70
1	12-B	57	LEU	CB-CG-CD2	5.45	120.26	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	14-A	97[A]	GLN	CG-CD-OE1	-5.44	110.72	121.60
1	14-A	97[B]	GLN	CG-CD-OE1	-5.44	110.72	121.60
1	10-B	20	ASP	CB-CG-OD1	5.44	123.20	118.30
1	12-B	6	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	6-A	90	HIS	N-CA-C	5.42	125.63	111.00
1	20-A	6[A]	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	20-A	6[B]	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	19-A	117	THR	OG1-CB-CG2	5.39	122.41	110.00
1	7-B	118	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	9-A	70[A]	ASN	N-CA-C	5.38	125.52	111.00
1	9-A	70[B]	ASN	N-CA-C	5.38	125.52	111.00
1	8-A	23	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	10-A	102	PHE	CB-CG-CD1	5.35	124.55	120.80
1	6-A	18	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	12-B	31	ASN	N-CA-CB	-5.34	100.99	110.60
1	10-B	3	ASN	N-CA-CB	5.33	120.19	110.60
1	12-A	68	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	9-B	73[A]	ASP	N-CA-C	5.32	125.37	111.00
1	9-B	73[B]	ASP	N-CA-C	5.32	125.37	111.00
1	17-A	119	LEU	CA-CB-CG	5.32	127.54	115.30
1	9-B	23	ARG	CG-CD-NE	5.32	122.97	111.80
1	17-A	118	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	18-A	13	MSE	CG-SE-CE	-5.31	87.22	98.90
1	10-B	2	MSE	CB-CG-SE	5.30	128.62	112.70
1	20-B	99	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	10-B	57	LEU	CB-CG-CD2	5.29	120.00	111.00
1	13-A	58[A]	PHE	CB-CG-CD2	-5.28	117.10	120.80
1	13-A	58[B]	PHE	CB-CG-CD2	-5.28	117.10	120.80
1	13-A	23	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	20-B	57	LEU	CA-CB-CG	5.26	127.39	115.30
1	2-A	48	PHE	CB-CA-C	5.25	120.91	110.40
1	15-A	99	ASP	CB-CG-OD1	5.25	123.02	118.30
1	18-A	68	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	10-A	49	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	2-B	58	PHE	CB-CG-CD2	-5.23	117.14	120.80
1	20-B	118	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	20-A	99	ASP	CB-CG-OD1	5.20	122.98	118.30
1	4-B	23	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	4-A	70[A]	ASN	CB-CA-C	5.19	120.78	110.40
1	4-A	70[B]	ASN	CB-CA-C	5.19	120.78	110.40
1	1-A	58[A]	PHE	CB-CG-CD2	-5.18	117.17	120.80
1	1-A	58[B]	PHE	CB-CG-CD2	-5.18	117.17	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	9-A	66	ILE	CB-CA-C	5.17	121.94	111.60
1	7-B	86	LEU	CA-CB-CG	5.17	127.19	115.30
1	16-A	99	ASP	CB-CG-OD1	5.15	122.94	118.30
1	8-A	23	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	13-B	23	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	1-A	119	LEU	CA-CB-CG	5.13	127.09	115.30
1	20-B	81	LEU	CB-CG-CD1	5.12	119.71	111.00
1	3-B	108	ASP	CB-CG-OD2	5.12	122.91	118.30
1	14-B	87	ASP	CB-CG-OD2	5.12	122.90	118.30
1	6-A	89	GLU	N-CA-C	5.11	124.81	111.00
1	10-A	99	ASP	CB-CG-OD1	5.11	122.90	118.30
1	13-A	58[A]	PHE	CB-CG-CD1	5.11	124.38	120.80
1	13-A	58[B]	PHE	CB-CG-CD1	5.11	124.38	120.80
1	18-B	99	ASP	CB-CG-OD1	5.10	122.89	118.30
1	8-B	119	LEU	CA-CB-CG	5.09	127.01	115.30
1	5-B	88	SER	N-CA-C	5.08	124.72	111.00
1	3-A	71	ASP	CB-CG-OD2	5.07	122.86	118.30
1	11-A	31	ASN	CB-CA-C	5.07	120.54	110.40
1	14-A	97[A]	GLN	CA-CB-CG	-5.05	102.28	113.40
1	14-A	97[B]	GLN	CA-CB-CG	-5.05	102.28	113.40
1	17-A	116	LEU	CB-CG-CD1	-5.05	102.42	111.00
1	3-B	68	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	4-B	57	LEU	CB-CG-CD2	5.03	119.56	111.00
1	3-A	57[A]	LEU	CB-CG-CD1	-5.03	102.45	111.00
1	3-A	57[B]	LEU	CB-CG-CD1	-5.03	102.45	111.00
1	16-B	68	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	10-B	99	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	19-B	3	ASN	CB-CA-C	5.02	120.44	110.40
1	6-A	68	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	2-A	2	MSE	CG-SE-CE	-5.01	87.88	98.90
1	17-B	2	MSE	CA-CB-CG	5.00	121.81	113.30

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-B	16[B]	GLU	Peptide
1	11-B	16[B]	GLU	Peptide
1	12-B	2	MSE	Peptide
1	14-A	50	HIS	Peptide
1	14-A	51	SER	Peptide
1	14-A	71	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	14-B	3	ASN	Peptide
1	17-A	30	LEU	Peptide
1	18-A	2	MSE	Peptide
1	20-A	47	SER	Peptide
1	20-A	48	PHE	Peptide
1	4-A	2	MSE	Peptide
1	5-A	64	ASN	Sidechain
1	6-B	2	MSE	Peptide
1	9-A	3	ASN	Peptide
1	9-B	2	MSE	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	1-A	1116	1079	982	0	0
1	1-B	1218	1135	1045	0	0
1	2-A	1116	1079	982	0	0
1	2-B	1218	1135	1045	0	0
1	3-A	1116	1079	982	0	0
1	3-B	1218	1135	1045	0	0
1	4-A	1116	1079	982	0	0
1	4-B	1218	1135	1045	0	0
1	5-A	1116	1079	982	0	0
1	5-B	1218	1135	1045	0	0
1	6-A	1116	1079	982	0	0
1	6-B	1218	1135	1045	0	0
1	7-A	1116	1079	982	0	0
1	7-B	1218	1135	1045	0	0
1	8-A	1116	1079	982	0	0
1	8-B	1218	1135	1045	0	0
1	9-A	1116	1079	982	0	0
1	9-B	1218	1135	1045	0	0
1	10-A	1116	1079	982	0	0
1	10-B	1218	1135	1045	0	0
1	11-A	1116	1079	982	0	0
1	11-B	1218	1135	1045	0	0
1	12-A	1116	1079	982	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	12-B	1218	1135	1045	0	0
1	13-A	1116	1079	982	0	0
1	13-B	1218	1135	1045	0	0
1	14-A	1116	1079	982	0	0
1	14-B	1218	1135	1045	0	0
1	15-A	1116	1079	982	0	0
1	15-B	1218	1135	1045	0	0
1	16-A	1116	1079	982	0	0
1	16-B	1218	1135	1045	0	0
1	17-A	1116	1079	982	0	0
1	17-B	1218	1135	1045	0	0
1	18-A	1116	1079	982	0	0
1	18-B	1218	1135	1045	0	0
1	19-A	1116	1079	982	0	0
1	19-B	1218	1135	1045	0	0
1	20-A	1116	1078	987	0	0
1	20-B	1218	1135	1045	0	0
2	1-A	1	0	0	0	0
2	1-B	1	0	0	0	0
2	2-A	1	0	0	0	0
2	2-B	1	0	0	0	0
2	3-A	1	0	0	0	0
2	3-B	1	0	0	0	0
2	4-A	1	0	0	0	0
2	4-B	1	0	0	0	0
2	5-A	1	0	0	0	0
2	5-B	1	0	0	0	0
2	6-A	1	0	0	0	0
2	6-B	1	0	0	0	0
2	7-A	1	0	0	0	0
2	7-B	1	0	0	0	0
2	8-A	1	0	0	0	0
2	8-B	1	0	0	0	0
2	9-A	1	0	0	0	0
2	9-B	1	0	0	0	0
2	10-A	1	0	0	0	0
2	10-B	1	0	0	0	0
2	11-A	1	0	0	0	0
2	11-B	1	0	0	0	0
2	12-A	1	0	0	0	0
2	12-B	1	0	0	0	0
2	13-A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	13-B	1	0	0	0	0
2	14-A	1	0	0	0	0
2	14-B	1	0	0	0	0
2	15-A	1	0	0	0	0
2	15-B	1	0	0	0	0
2	16-A	1	0	0	0	0
2	16-B	1	0	0	0	0
2	17-A	1	0	0	0	0
2	17-B	1	0	0	0	0
2	18-A	1	0	0	0	0
2	18-B	1	0	0	0	0
2	19-A	1	0	0	0	0
2	19-B	1	0	0	0	0
2	20-A	1	0	0	0	0
2	20-B	1	0	0	0	0
3	1-A	1	0	0	0	0
3	2-A	1	0	0	0	0
3	3-A	1	0	0	0	0
3	4-A	1	0	0	0	0
3	5-A	1	0	0	0	0
3	6-A	1	0	0	0	0
3	7-A	1	0	0	0	0
3	8-A	1	0	0	0	0
3	9-A	1	0	0	0	0
3	10-A	1	0	0	0	0
3	11-A	1	0	0	0	0
3	12-A	1	0	0	0	0
3	13-A	1	0	0	0	0
3	14-A	1	0	0	0	0
3	15-A	1	0	0	0	0
3	16-A	1	0	0	0	0
3	17-A	1	0	0	0	0
3	18-A	1	0	0	0	0
3	19-A	1	0	0	0	0
3	20-A	1	0	0	0	0
4	1-A	101	0	0	0	0
4	1-B	97	0	0	0	0
4	2-A	95	0	0	0	0
4	2-B	82	0	0	0	0
4	3-A	92	0	0	0	0
4	3-B	91	0	0	0	0
4	4-A	101	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	4-B	90	0	0	0	0
4	5-A	87	0	0	0	0
4	5-B	95	0	0	0	0
4	6-A	100	0	0	0	0
4	6-B	85	0	0	0	0
4	7-A	85	0	0	0	0
4	7-B	84	0	0	0	0
4	8-A	90	0	0	0	0
4	8-B	99	0	0	0	0
4	9-A	86	0	0	0	0
4	9-B	92	0	0	0	0
4	10-A	94	0	0	0	0
4	10-B	95	0	0	0	0
4	11-A	86	0	0	0	0
4	11-B	90	0	0	0	0
4	12-A	108	0	0	0	0
4	12-B	92	0	0	0	0
4	13-A	88	0	0	0	0
4	13-B	81	0	0	0	0
4	14-A	91	0	0	0	0
4	14-B	87	0	0	0	0
4	15-A	88	0	0	0	0
4	15-B	100	0	0	0	0
4	16-A	97	0	0	0	0
4	16-B	95	0	0	0	0
4	17-A	97	0	0	0	0
4	17-B	102	0	0	0	0
4	18-A	98	0	0	0	0
4	18-B	88	0	0	0	0
4	19-A	101	0	0	0	0
4	19-B	91	0	0	0	0
4	20-A	85	0	0	0	0
4	20-B	99	0	0	0	0
All	All	50445	44279	40545	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	1-A	141/128 (110%)	139 (99%)	1 (1%)	1 (1%)	22	5
1	1-B	151/128 (118%)	143 (95%)	6 (4%)	2 (1%)	12	1
1	2-A	141/128 (110%)	134 (95%)	4 (3%)	3 (2%)	7	0
1	2-B	151/128 (118%)	138 (91%)	11 (7%)	2 (1%)	12	1
1	3-A	141/128 (110%)	137 (97%)	1 (1%)	3 (2%)	7	0
1	3-B	151/128 (118%)	137 (91%)	8 (5%)	6 (4%)	3	0
1	4-A	141/128 (110%)	137 (97%)	4 (3%)	0	100	100
1	4-B	151/128 (118%)	138 (91%)	12 (8%)	1 (1%)	22	5
1	5-A	141/128 (110%)	137 (97%)	4 (3%)	0	100	100
1	5-B	151/128 (118%)	140 (93%)	9 (6%)	2 (1%)	12	1
1	6-A	141/128 (110%)	133 (94%)	7 (5%)	1 (1%)	22	5
1	6-B	151/128 (118%)	141 (93%)	7 (5%)	3 (2%)	7	0
1	7-A	141/128 (110%)	133 (94%)	8 (6%)	0	100	100
1	7-B	151/128 (118%)	140 (93%)	7 (5%)	4 (3%)	5	0
1	8-A	141/128 (110%)	135 (96%)	6 (4%)	0	100	100
1	8-B	151/128 (118%)	143 (95%)	6 (4%)	2 (1%)	12	1
1	9-A	141/128 (110%)	131 (93%)	7 (5%)	3 (2%)	7	0
1	9-B	151/128 (118%)	133 (88%)	15 (10%)	3 (2%)	7	0
1	10-A	141/128 (110%)	136 (96%)	4 (3%)	1 (1%)	22	5
1	10-B	151/128 (118%)	140 (93%)	8 (5%)	3 (2%)	7	0
1	11-A	141/128 (110%)	134 (95%)	1 (1%)	6 (4%)	2	0
1	11-B	151/128 (118%)	139 (92%)	8 (5%)	4 (3%)	5	0
1	12-A	141/128 (110%)	137 (97%)	2 (1%)	2 (1%)	11	1
1	12-B	151/128 (118%)	140 (93%)	11 (7%)	0	100	100
1	13-A	141/128 (110%)	132 (94%)	8 (6%)	1 (1%)	22	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	13-B	151/128 (118%)	142 (94%)	8 (5%)	1 (1%)	22	5
1	14-A	141/128 (110%)	131 (93%)	4 (3%)	6 (4%)	2	0
1	14-B	151/128 (118%)	135 (89%)	14 (9%)	2 (1%)	12	1
1	15-A	141/128 (110%)	132 (94%)	6 (4%)	3 (2%)	7	0
1	15-B	151/128 (118%)	140 (93%)	11 (7%)	0	100	100
1	16-A	141/128 (110%)	138 (98%)	3 (2%)	0	100	100
1	16-B	151/128 (118%)	133 (88%)	12 (8%)	6 (4%)	3	0
1	17-A	141/128 (110%)	136 (96%)	4 (3%)	1 (1%)	22	5
1	17-B	151/128 (118%)	142 (94%)	9 (6%)	0	100	100
1	18-A	141/128 (110%)	132 (94%)	9 (6%)	0	100	100
1	18-B	151/128 (118%)	134 (89%)	10 (7%)	7 (5%)	2	0
1	19-A	141/128 (110%)	135 (96%)	6 (4%)	0	100	100
1	19-B	151/128 (118%)	140 (93%)	5 (3%)	6 (4%)	3	0
1	20-A	140/128 (109%)	136 (97%)	3 (2%)	1 (1%)	22	5
1	20-B	151/128 (118%)	140 (93%)	11 (7%)	0	100	100
All	All	5839/5120 (114%)	5473 (94%)	280 (5%)	86 (2%)	12	1

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-B	17[A]	TYR
1	1-B	17[B]	TYR
1	2-A	4[A]	ILE
1	2-A	4[B]	ILE
1	2-B	51[A]	SER
1	2-B	51[B]	SER
1	3-B	17[A]	TYR
1	3-B	17[B]	TYR
1	3-B	53[A]	ASN
1	3-B	53[B]	ASN
1	5-B	87	ASP
1	8-B	51[A]	SER
1	8-B	51[B]	SER
1	9-A	52	HIS
1	9-A	53	ASN
1	10-A	51	SER
1	10-B	3	ASN

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Mol	Chain	Res	Type
1	10-B	51[A]	SER
1	10-B	51[B]	SER
1	11-A	48	PHE
1	11-A	49	ARG
1	11-A	50	HIS
1	11-A	52	HIS
1	11-A	54	GLU
1	12-A	49	ARG
1	12-A	50	HIS
1	14-A	48	PHE
1	14-A	49	ARG
1	14-A	89	GLU
1	14-A	90	HIS
1	14-B	4[A]	ILE
1	14-B	4[B]	ILE
1	15-A	52	HIS
1	16-B	4[A]	ILE
1	16-B	4[B]	ILE
1	16-B	17[A]	TYR
1	16-B	17[B]	TYR
1	18-B	4[A]	ILE
1	18-B	4[B]	ILE
1	19-B	17[A]	TYR
1	19-B	17[B]	TYR
1	19-B	50[A]	HIS
1	19-B	50[B]	HIS
1	2-A	89	GLU
1	3-A	71	ASP
1	4-B	97	GLN
1	6-B	50[A]	HIS
1	6-B	50[B]	HIS
1	9-B	73[A]	ASP
1	9-B	73[B]	ASP
1	11-A	71	ASP
1	11-B	17[A]	TYR
1	11-B	17[B]	TYR
1	13-A	118	ARG
1	14-A	17	TYR
1	14-A	121	GLN
1	16-B	51[A]	SER
1	16-B	51[B]	SER
1	18-B	71[A]	ASP

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Mol	Chain	Res	Type
1	18-B	71[B]	ASP
1	19-B	4[A]	ILE
1	19-B	4[B]	ILE
1	1-A	78	LYS
1	3-A	70[A]	ASN
1	3-A	70[B]	ASN
1	6-A	90	HIS
1	7-B	17[A]	TYR
1	7-B	17[B]	TYR
1	9-A	71	ASP
1	9-B	110	GLU
1	11-B	51[A]	SER
1	11-B	51[B]	SER
1	15-A	78	LYS
1	18-B	3	ASN
1	6-B	88	SER
1	15-A	89	GLU
1	17-A	30	LEU
1	20-A	49	ARG
1	5-B	88	SER
1	18-B	50[A]	HIS
1	18-B	50[B]	HIS
1	3-B	51[A]	SER
1	3-B	51[B]	SER
1	7-B	4[A]	ILE
1	7-B	4[B]	ILE
1	13-B	74	PHE

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	1-A	135/116 (116%)	125 (93%)	10 (7%)	13 1
1	1-B	145/116 (125%)	131 (90%)	14 (10%)	8 0
1	2-A	135/116 (116%)	121 (90%)	14 (10%)	7 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2-B	145/116 (125%)	133 (92%)	12 (8%)	11	0
1	3-A	135/116 (116%)	121 (90%)	14 (10%)	7	0
1	3-B	145/116 (125%)	133 (92%)	12 (8%)	11	0
1	4-A	135/116 (116%)	121 (90%)	14 (10%)	7	0
1	4-B	145/116 (125%)	118 (81%)	27 (19%)	1	0
1	5-A	135/116 (116%)	127 (94%)	8 (6%)	19	1
1	5-B	145/116 (125%)	134 (92%)	11 (8%)	13	1
1	6-A	135/116 (116%)	120 (89%)	15 (11%)	6	0
1	6-B	145/116 (125%)	134 (92%)	11 (8%)	13	1
1	7-A	135/116 (116%)	124 (92%)	11 (8%)	11	0
1	7-B	145/116 (125%)	134 (92%)	11 (8%)	13	1
1	8-A	135/116 (116%)	120 (89%)	15 (11%)	6	0
1	8-B	145/116 (125%)	127 (88%)	18 (12%)	4	0
1	9-A	135/116 (116%)	123 (91%)	12 (9%)	9	0
1	9-B	145/116 (125%)	133 (92%)	12 (8%)	11	0
1	10-A	135/116 (116%)	122 (90%)	13 (10%)	8	0
1	10-B	145/116 (125%)	137 (94%)	8 (6%)	21	1
1	11-A	135/116 (116%)	116 (86%)	19 (14%)	3	0
1	11-B	145/116 (125%)	133 (92%)	12 (8%)	11	0
1	12-A	135/116 (116%)	131 (97%)	4 (3%)	41	8
1	12-B	145/116 (125%)	133 (92%)	12 (8%)	11	0
1	13-A	135/116 (116%)	124 (92%)	11 (8%)	11	0
1	13-B	145/116 (125%)	136 (94%)	9 (6%)	18	1
1	14-A	135/116 (116%)	122 (90%)	13 (10%)	8	0
1	14-B	145/116 (125%)	131 (90%)	14 (10%)	8	0
1	15-A	135/116 (116%)	122 (90%)	13 (10%)	8	0
1	15-B	145/116 (125%)	125 (86%)	20 (14%)	3	0
1	16-A	135/116 (116%)	128 (95%)	7 (5%)	23	2
1	16-B	145/116 (125%)	126 (87%)	19 (13%)	4	0
1	17-A	135/116 (116%)	121 (90%)	14 (10%)	7	0
1	17-B	145/116 (125%)	130 (90%)	15 (10%)	7	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	18-A	135/116 (116%)	123 (91%)	12 (9%)	9 0
1	18-B	145/116 (125%)	135 (93%)	10 (7%)	15 1
1	19-A	135/116 (116%)	122 (90%)	13 (10%)	8 0
1	19-B	145/116 (125%)	125 (86%)	20 (14%)	3 0
1	20-A	134/116 (116%)	121 (90%)	13 (10%)	8 0
1	20-B	145/116 (125%)	132 (91%)	13 (9%)	9 0
All	All	5599/4640 (121%)	5074 (91%)	525 (9%)	9 0

All (525) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	23	ARG
1	1-A	24	LEU
1	1-A	50	HIS
1	1-A	57[A]	LEU
1	1-A	57[B]	LEU
1	1-A	64	ASN
1	1-A	77	THR
1	1-A	90	HIS
1	1-A	96[A]	ASN
1	1-A	96[B]	ASN
1	1-B	3	ASN
1	1-B	31	ASN
1	1-B	46[A]	LYS
1	1-B	46[B]	LYS
1	1-B	49[A]	ARG
1	1-B	49[B]	ARG
1	1-B	62	GLN
1	1-B	77[A]	THR
1	1-B	77[B]	THR
1	1-B	81	LEU
1	1-B	87	ASP
1	1-B	97	GLN
1	1-B	118	ARG
1	1-B	119	LEU
1	2-A	2	MSE
1	2-A	5[A]	ILE
1	2-A	5[B]	ILE
1	2-A	46	LYS
1	2-A	47	SER

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Mol	Chain	Res	Type
1	2-A	48	PHE
1	2-A	49	ARG
1	2-A	50	HIS
1	2-A	53	ASN
1	2-A	54	GLU
1	2-A	71	ASP
1	2-A	98	GLU
1	2-A	114	ASN
1	2-A	120	GLU
1	2-B	7	LYS
1	2-B	31	ASN
1	2-B	46[A]	LYS
1	2-B	46[B]	LYS
1	2-B	50[A]	HIS
1	2-B	50[B]	HIS
1	2-B	57	LEU
1	2-B	71[A]	ASP
1	2-B	71[B]	ASP
1	2-B	77[A]	THR
1	2-B	77[B]	THR
1	2-B	119	LEU
1	3-A	3	ASN
1	3-A	4[A]	ILE
1	3-A	4[B]	ILE
1	3-A	7[A]	LYS
1	3-A	7[B]	LYS
1	3-A	12	SER
1	3-A	45	THR
1	3-A	46	LYS
1	3-A	50	HIS
1	3-A	71	ASP
1	3-A	75	PRO
1	3-A	86	LEU
1	3-A	91	HIS
1	3-A	110	GLU
1	3-B	2	MSE
1	3-B	12	SER
1	3-B	28	GLU
1	3-B	31	ASN
1	3-B	50[A]	HIS
1	3-B	50[B]	HIS
1	3-B	57	LEU

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Mol	Chain	Res	Type
1	3-B	67	ILE
1	3-B	88	SER
1	3-B	97	GLN
1	3-B	117	THR
1	3-B	119	LEU
1	4-A	12	SER
1	4-A	18	ASP
1	4-A	45	THR
1	4-A	46	LYS
1	4-A	49	ARG
1	4-A	50	HIS
1	4-A	51	SER
1	4-A	53	ASN
1	4-A	57[A]	LEU
1	4-A	57[B]	LEU
1	4-A	71	ASP
1	4-A	97[A]	GLN
1	4-A	97[B]	GLN
1	4-A	122	ASP
1	4-B	31	ASN
1	4-B	32	THR
1	4-B	47[A]	SER
1	4-B	47[B]	SER
1	4-B	48[A]	PHE
1	4-B	48[B]	PHE
1	4-B	50[A]	HIS
1	4-B	50[B]	HIS
1	4-B	53[A]	ASN
1	4-B	53[B]	ASN
1	4-B	57	LEU
1	4-B	62	GLN
1	4-B	67	ILE
1	4-B	71[A]	ASP
1	4-B	71[B]	ASP
1	4-B	72[A]	GLU
1	4-B	72[B]	GLU
1	4-B	88	SER
1	4-B	89[A]	GLU
1	4-B	89[B]	GLU
1	4-B	90[A]	HIS
1	4-B	90[B]	HIS
1	4-B	91[A]	HIS

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Mol	Chain	Res	Type
1	4-B	91[B]	HIS
1	4-B	97	GLN
1	4-B	114	ASN
1	4-B	116	LEU
1	5-A	2	MSE
1	5-A	16	GLU
1	5-A	19	LEU
1	5-A	52	HIS
1	5-A	53	ASN
1	5-A	57[A]	LEU
1	5-A	57[B]	LEU
1	5-A	110	GLU
1	5-B	2	MSE
1	5-B	7	LYS
1	5-B	17[A]	TYR
1	5-B	17[B]	TYR
1	5-B	48[A]	PHE
1	5-B	48[B]	PHE
1	5-B	52[A]	HIS
1	5-B	52[B]	HIS
1	5-B	81	LEU
1	5-B	88	SER
1	5-B	117	THR
1	6-A	2	MSE
1	6-A	4[A]	ILE
1	6-A	4[B]	ILE
1	6-A	45	THR
1	6-A	48	PHE
1	6-A	49	ARG
1	6-A	53	ASN
1	6-A	57[A]	LEU
1	6-A	57[B]	LEU
1	6-A	97[A]	GLN
1	6-A	97[B]	GLN
1	6-A	110	GLU
1	6-A	117	THR
1	6-A	118	ARG
1	6-A	120	GLU
1	6-B	2	MSE
1	6-B	50[A]	HIS
1	6-B	50[B]	HIS
1	6-B	52[A]	HIS

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Mol	Chain	Res	Type
1	6-B	52[B]	HIS
1	6-B	53[A]	ASN
1	6-B	53[B]	ASN
1	6-B	57	LEU
1	6-B	67	ILE
1	6-B	87	ASP
1	6-B	118	ARG
1	7-A	2	MSE
1	7-A	3	ASN
1	7-A	7[A]	LYS
1	7-A	7[B]	LYS
1	7-A	16	GLU
1	7-A	45	THR
1	7-A	46	LYS
1	7-A	47	SER
1	7-A	52	HIS
1	7-A	97[A]	GLN
1	7-A	97[B]	GLN
1	7-B	2	MSE
1	7-B	7	LYS
1	7-B	12	SER
1	7-B	54[A]	GLU
1	7-B	54[B]	GLU
1	7-B	57	LEU
1	7-B	70[A]	ASN
1	7-B	70[B]	ASN
1	7-B	87	ASP
1	7-B	110	GLU
1	7-B	117	THR
1	8-A	3	ASN
1	8-A	4[A]	ILE
1	8-A	4[B]	ILE
1	8-A	7[A]	LYS
1	8-A	7[B]	LYS
1	8-A	45	THR
1	8-A	46	LYS
1	8-A	49	ARG
1	8-A	50	HIS
1	8-A	51	SER
1	8-A	53	ASN
1	8-A	87	ASP
1	8-A	97[A]	GLN

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Mol	Chain	Res	Type
1	8-A	97[B]	GLN
1	8-A	117	THR
1	8-B	2	MSE
1	8-B	5[A]	ILE
1	8-B	5[B]	ILE
1	8-B	46[A]	LYS
1	8-B	46[B]	LYS
1	8-B	50[A]	HIS
1	8-B	50[B]	HIS
1	8-B	52[A]	HIS
1	8-B	52[B]	HIS
1	8-B	54[A]	GLU
1	8-B	54[B]	GLU
1	8-B	71[A]	ASP
1	8-B	71[B]	ASP
1	8-B	86	LEU
1	8-B	90[A]	HIS
1	8-B	90[B]	HIS
1	8-B	117	THR
1	8-B	119	LEU
1	9-A	2	MSE
1	9-A	19	LEU
1	9-A	28	GLU
1	9-A	46	LYS
1	9-A	47	SER
1	9-A	50	HIS
1	9-A	51	SER
1	9-A	70[A]	ASN
1	9-A	70[B]	ASN
1	9-A	96[A]	ASN
1	9-A	96[B]	ASN
1	9-A	98	GLU
1	9-B	23	ARG
1	9-B	50[A]	HIS
1	9-B	50[B]	HIS
1	9-B	51[A]	SER
1	9-B	51[B]	SER
1	9-B	62	GLN
1	9-B	81	LEU
1	9-B	97	GLN
1	9-B	98	GLU
1	9-B	104	THR

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Mol	Chain	Res	Type
1	9-B	114	ASN
1	9-B	120	GLU
1	10-A	3	ASN
1	10-A	4[A]	ILE
1	10-A	4[B]	ILE
1	10-A	7[A]	LYS
1	10-A	7[B]	LYS
1	10-A	9	ASP
1	10-A	49	ARG
1	10-A	50	HIS
1	10-A	66	ILE
1	10-A	89	GLU
1	10-A	95	ASN
1	10-A	119	LEU
1	10-A	121	GLN
1	10-B	2	MSE
1	10-B	12	SER
1	10-B	23	ARG
1	10-B	53[A]	ASN
1	10-B	53[B]	ASN
1	10-B	67	ILE
1	10-B	104	THR
1	10-B	119	LEU
1	11-A	4[A]	ILE
1	11-A	4[B]	ILE
1	11-A	31	ASN
1	11-A	32	THR
1	11-A	45	THR
1	11-A	46	LYS
1	11-A	49	ARG
1	11-A	50	HIS
1	11-A	53	ASN
1	11-A	57[A]	LEU
1	11-A	57[B]	LEU
1	11-A	72[A]	GLU
1	11-A	72[B]	GLU
1	11-A	77	THR
1	11-A	97[A]	GLN
1	11-A	97[B]	GLN
1	11-A	114	ASN
1	11-A	117	THR
1	11-A	122	ASP

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Mol	Chain	Res	Type
1	11-B	11	ASP
1	11-B	28	GLU
1	11-B	50[A]	HIS
1	11-B	50[B]	HIS
1	11-B	57	LEU
1	11-B	71[A]	ASP
1	11-B	71[B]	ASP
1	11-B	81	LEU
1	11-B	87	ASP
1	11-B	88	SER
1	11-B	96	ASN
1	11-B	114	ASN
1	12-A	50	HIS
1	12-A	54	GLU
1	12-A	89	GLU
1	12-A	120	GLU
1	12-B	2	MSE
1	12-B	52[A]	HIS
1	12-B	52[B]	HIS
1	12-B	57	LEU
1	12-B	68	ARG
1	12-B	71[A]	ASP
1	12-B	71[B]	ASP
1	12-B	83[A]	ILE
1	12-B	83[B]	ILE
1	12-B	90[A]	HIS
1	12-B	90[B]	HIS
1	12-B	119	LEU
1	13-A	2	MSE
1	13-A	7[A]	LYS
1	13-A	7[B]	LYS
1	13-A	46	LYS
1	13-A	49	ARG
1	13-A	53	ASN
1	13-A	64	ASN
1	13-A	66	ILE
1	13-A	110	GLU
1	13-A	121	GLN
1	13-A	122	ASP
1	13-B	3	ASN
1	13-B	50[A]	HIS
1	13-B	50[B]	HIS

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Mol	Chain	Res	Type
1	13-B	52[A]	HIS
1	13-B	52[B]	HIS
1	13-B	91[A]	HIS
1	13-B	91[B]	HIS
1	13-B	97	GLN
1	13-B	98	GLU
1	14-A	16	GLU
1	14-A	45	THR
1	14-A	48	PHE
1	14-A	49	ARG
1	14-A	53	ASN
1	14-A	54	GLU
1	14-A	71	ASP
1	14-A	87	ASP
1	14-A	88	SER
1	14-A	110	GLU
1	14-A	120	GLU
1	14-A	121	GLN
1	14-A	122	ASP
1	14-B	3	ASN
1	14-B	6	ARG
1	14-B	7	LYS
1	14-B	49[A]	ARG
1	14-B	49[B]	ARG
1	14-B	51[A]	SER
1	14-B	51[B]	SER
1	14-B	52[A]	HIS
1	14-B	52[B]	HIS
1	14-B	91[A]	HIS
1	14-B	91[B]	HIS
1	14-B	104	THR
1	14-B	114	ASN
1	14-B	119	LEU
1	15-A	3	ASN
1	15-A	12	SER
1	15-A	46	LYS
1	15-A	50	HIS
1	15-A	52	HIS
1	15-A	82[A]	ILE
1	15-A	82[B]	ILE
1	15-A	97[A]	GLN
1	15-A	97[B]	GLN

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Mol	Chain	Res	Type
1	15-A	110	GLU
1	15-A	117	THR
1	15-A	119	LEU
1	15-A	122	ASP
1	15-B	2	MSE
1	15-B	12	SER
1	15-B	49[A]	ARG
1	15-B	49[B]	ARG
1	15-B	50[A]	HIS
1	15-B	50[B]	HIS
1	15-B	52[A]	HIS
1	15-B	52[B]	HIS
1	15-B	54[A]	GLU
1	15-B	54[B]	GLU
1	15-B	70[A]	ASN
1	15-B	70[B]	ASN
1	15-B	87	ASP
1	15-B	90[A]	HIS
1	15-B	90[B]	HIS
1	15-B	91[A]	HIS
1	15-B	91[B]	HIS
1	15-B	97	GLN
1	15-B	110	GLU
1	15-B	114	ASN
1	16-A	3	ASN
1	16-A	16	GLU
1	16-A	46	LYS
1	16-A	49	ARG
1	16-A	50	HIS
1	16-A	117	THR
1	16-A	119	LEU
1	16-B	2	MSE
1	16-B	4[A]	ILE
1	16-B	4[B]	ILE
1	16-B	12	SER
1	16-B	46[A]	LYS
1	16-B	46[B]	LYS
1	16-B	49[A]	ARG
1	16-B	49[B]	ARG
1	16-B	50[A]	HIS
1	16-B	50[B]	HIS
1	16-B	57	LEU

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Mol	Chain	Res	Type
1	16-B	62	GLN
1	16-B	77[A]	THR
1	16-B	77[B]	THR
1	16-B	86	LEU
1	16-B	91[A]	HIS
1	16-B	91[B]	HIS
1	16-B	98	GLU
1	16-B	119	LEU
1	17-A	2	MSE
1	17-A	30	LEU
1	17-A	31	ASN
1	17-A	44	GLU
1	17-A	49	ARG
1	17-A	52	HIS
1	17-A	62	GLN
1	17-A	71	ASP
1	17-A	77	THR
1	17-A	81[A]	LEU
1	17-A	81[B]	LEU
1	17-A	86	LEU
1	17-A	91	HIS
1	17-A	122	ASP
1	17-B	2	MSE
1	17-B	19[A]	LEU
1	17-B	19[B]	LEU
1	17-B	50[A]	HIS
1	17-B	50[B]	HIS
1	17-B	52[A]	HIS
1	17-B	52[B]	HIS
1	17-B	62	GLN
1	17-B	82[A]	ILE
1	17-B	82[B]	ILE
1	17-B	90[A]	HIS
1	17-B	90[B]	HIS
1	17-B	99	ASP
1	17-B	110	GLU
1	17-B	119	LEU
1	18-A	2	MSE
1	18-A	3	ASN
1	18-A	16	GLU
1	18-A	19	LEU
1	18-A	46	LYS

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Mol	Chain	Res	Type
1	18-A	49	ARG
1	18-A	52	HIS
1	18-A	53	ASN
1	18-A	114	ASN
1	18-A	117	THR
1	18-A	118	ARG
1	18-A	120	GLU
1	18-B	2	MSE
1	18-B	6	ARG
1	18-B	49[A]	ARG
1	18-B	49[B]	ARG
1	18-B	50[A]	HIS
1	18-B	50[B]	HIS
1	18-B	53[A]	ASN
1	18-B	53[B]	ASN
1	18-B	57	LEU
1	18-B	119	LEU
1	19-A	9	ASP
1	19-A	31	ASN
1	19-A	46	LYS
1	19-A	49	ARG
1	19-A	50	HIS
1	19-A	52	HIS
1	19-A	53	ASN
1	19-A	57[A]	LEU
1	19-A	57[B]	LEU
1	19-A	77	THR
1	19-A	97[A]	GLN
1	19-A	97[B]	GLN
1	19-A	120	GLU
1	19-B	2	MSE
1	19-B	3	ASN
1	19-B	13	MSE
1	19-B	51[A]	SER
1	19-B	51[B]	SER
1	19-B	52[A]	HIS
1	19-B	52[B]	HIS
1	19-B	53[A]	ASN
1	19-B	53[B]	ASN
1	19-B	54[A]	GLU
1	19-B	54[B]	GLU
1	19-B	71[A]	ASP

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Mol	Chain	Res	Type
1	19-B	71[B]	ASP
1	19-B	77[A]	THR
1	19-B	77[B]	THR
1	19-B	87	ASP
1	19-B	96	ASN
1	19-B	98	GLU
1	19-B	117	THR
1	19-B	118	ARG
1	20-A	7[A]	LYS
1	20-A	7[B]	LYS
1	20-A	19	LEU
1	20-A	28	GLU
1	20-A	46	LYS
1	20-A	48	PHE
1	20-A	50	HIS
1	20-A	87	ASP
1	20-A	89	GLU
1	20-A	97[A]	GLN
1	20-A	97[B]	GLN
1	20-A	120	GLU
1	20-A	121	GLN
1	20-B	2	MSE
1	20-B	7	LYS
1	20-B	46[A]	LYS
1	20-B	46[B]	LYS
1	20-B	50[A]	HIS
1	20-B	50[B]	HIS
1	20-B	52[A]	HIS
1	20-B	52[B]	HIS
1	20-B	72[A]	GLU
1	20-B	72[B]	GLU
1	20-B	81	LEU
1	20-B	98	GLU
1	20-B	121	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	95	ASN
1	1-B	31	ASN
1	1-B	64	ASN
1	1-B	97	GLN

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Mol	Chain	Res	Type
1	1-B	114	ASN
1	2-A	31	ASN
1	2-A	50	HIS
1	2-A	95	ASN
1	2-B	31	ASN
1	2-B	62	GLN
1	2-B	64	ASN
1	2-B	97	GLN
1	3-A	90	HIS
1	3-A	95	ASN
1	3-B	31	ASN
1	3-B	64	ASN
1	3-B	97	GLN
1	4-A	90	HIS
1	4-B	31	ASN
1	4-B	64	ASN
1	4-B	97	GLN
1	4-B	114	ASN
1	5-A	62	GLN
1	5-A	95	ASN
1	5-A	121	GLN
1	5-B	3	ASN
1	5-B	96	ASN
1	5-B	97	GLN
1	6-A	62	GLN
1	6-B	3	ASN
1	6-B	31	ASN
1	6-B	62	GLN
1	6-B	97	GLN
1	7-A	31	ASN
1	7-A	50	HIS
1	7-A	62	GLN
1	7-A	64	ASN
1	7-B	64	ASN
1	7-B	96	ASN
1	8-A	31	ASN
1	8-A	50	HIS
1	8-B	31	ASN
1	8-B	64	ASN
1	9-A	53	ASN
1	9-A	62	GLN
1	9-A	64	ASN

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Mol	Chain	Res	Type
1	9-A	95	ASN
1	9-B	3	ASN
1	9-B	64	ASN
1	9-B	121	GLN
1	10-A	53	ASN
1	10-A	64	ASN
1	10-A	91	HIS
1	10-A	95	ASN
1	10-B	64	ASN
1	11-A	114	ASN
1	11-B	96	ASN
1	11-B	114	ASN
1	12-A	50	HIS
1	12-B	3	ASN
1	12-B	64	ASN
1	12-B	96	ASN
1	13-A	50	HIS
1	13-A	62	GLN
1	13-A	64	ASN
1	13-A	91	HIS
1	13-B	114	ASN
1	14-B	3	ASN
1	15-B	62	GLN
1	15-B	64	ASN
1	15-B	121	GLN
1	16-A	31	ASN
1	16-A	53	ASN
1	16-A	64	ASN
1	17-A	31	ASN
1	17-A	52	HIS
1	17-A	62	GLN
1	17-A	91	HIS
1	17-A	101	HIS
1	17-B	62	GLN
1	17-B	121	GLN
1	18-A	31	ASN
1	18-A	52	HIS
1	18-A	53	ASN
1	18-A	62	GLN
1	19-A	31	ASN
1	19-A	62	GLN
1	19-A	91	HIS

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Mol	Chain	Res	Type
1	19-A	114	ASN
1	19-A	121	GLN
1	20-A	31	ASN
1	20-A	50	HIS
1	20-A	53	ASN
1	20-A	62	GLN
1	20-A	70	ASN
1	20-A	121	GLN
1	20-B	31	ASN
1	20-B	62	GLN

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)

Of 60 ligands modelled in this entry, 60 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	1-A	118/128 (92%)	0.55	17 (14%)	2	2	11, 16, 25, 40	118 (100%)
1	1-B	117/128 (91%)	0.53	13 (11%)	5	6	11, 16, 26, 42	117 (100%)
1	2-A	118/128 (92%)	0.55	17 (14%)	2	2	11, 16, 25, 40	118 (100%)
1	2-B	117/128 (91%)	0.53	13 (11%)	5	6	11, 16, 26, 42	117 (100%)
1	3-A	118/128 (92%)	0.55	17 (14%)	2	2	11, 16, 25, 40	118 (100%)
1	3-B	117/128 (91%)	0.53	13 (11%)	5	6	11, 16, 26, 42	117 (100%)
1	4-A	118/128 (92%)	0.55	17 (14%)	2	2	11, 16, 25, 40	118 (100%)
1	4-B	117/128 (91%)	0.53	13 (11%)	5	6	11, 16, 26, 42	117 (100%)
1	5-A	118/128 (92%)	0.55	17 (14%)	2	2	11, 16, 25, 40	118 (100%)
1	5-B	117/128 (91%)	0.53	13 (11%)	5	6	11, 16, 26, 42	117 (100%)
1	6-A	118/128 (92%)	0.55	17 (14%)	2	2	11, 16, 25, 40	118 (100%)
1	6-B	117/128 (91%)	0.53	13 (11%)	5	6	11, 16, 26, 42	117 (100%)
1	7-A	118/128 (92%)	0.55	17 (14%)	2	2	11, 16, 25, 40	118 (100%)
1	7-B	117/128 (91%)	0.53	13 (11%)	5	6	11, 16, 26, 42	117 (100%)
1	8-A	118/128 (92%)	0.55	17 (14%)	2	2	11, 16, 25, 40	118 (100%)
1	8-B	117/128 (91%)	0.53	13 (11%)	5	6	11, 16, 26, 42	117 (100%)
1	9-A	118/128 (92%)	0.55	17 (14%)	2	2	11, 16, 25, 40	118 (100%)
1	9-B	117/128 (91%)	0.53	13 (11%)	5	6	11, 16, 26, 42	117 (100%)
1	10-A	118/128 (92%)	0.55	17 (14%)	2	2	11, 16, 25, 40	118 (100%)
1	10-B	117/128 (91%)	0.53	13 (11%)	5	6	11, 16, 26, 42	117 (100%)
1	11-A	118/128 (92%)	0.55	17 (14%)	2	2	11, 16, 25, 40	118 (100%)
1	11-B	117/128 (91%)	0.53	13 (11%)	5	6	11, 16, 26, 42	117 (100%)
1	12-A	118/128 (92%)	0.55	17 (14%)	2	2	11, 16, 25, 40	118 (100%)
1	12-B	117/128 (91%)	0.53	13 (11%)	5	6	11, 16, 26, 42	117 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	13-A	118/128 (92%)	0.55	17 (14%)	2	2	11, 16, 25, 40	118 (100%)
1	13-B	117/128 (91%)	0.53	13 (11%)	5	6	11, 16, 26, 42	117 (100%)
1	14-A	118/128 (92%)	0.55	17 (14%)	2	2	11, 16, 25, 40	118 (100%)
1	14-B	117/128 (91%)	0.53	13 (11%)	5	6	11, 16, 26, 42	117 (100%)
1	15-A	118/128 (92%)	0.55	17 (14%)	2	2	11, 16, 25, 40	118 (100%)
1	15-B	117/128 (91%)	0.53	13 (11%)	5	6	11, 16, 26, 42	117 (100%)
1	16-A	118/128 (92%)	0.55	17 (14%)	2	2	11, 16, 25, 40	118 (100%)
1	16-B	117/128 (91%)	0.53	13 (11%)	5	6	11, 16, 26, 42	117 (100%)
1	17-A	118/128 (92%)	0.55	17 (14%)	2	2	11, 16, 25, 40	118 (100%)
1	17-B	117/128 (91%)	0.53	13 (11%)	5	6	11, 16, 26, 42	117 (100%)
1	18-A	118/128 (92%)	0.55	17 (14%)	2	2	11, 16, 25, 40	118 (100%)
1	18-B	117/128 (91%)	0.53	13 (11%)	5	6	11, 16, 26, 42	117 (100%)
1	19-A	118/128 (92%)	0.55	17 (14%)	2	2	11, 16, 25, 40	118 (100%)
1	19-B	117/128 (91%)	0.53	13 (11%)	5	6	11, 16, 26, 42	117 (100%)
1	20-A	118/128 (92%)	0.55	17 (14%)	2	2	11, 16, 25, 40	118 (100%)
1	20-B	117/128 (91%)	0.53	13 (11%)	5	6	11, 16, 26, 42	117 (100%)
All	All	4700/5120 (91%)	0.54	600 (12%)	4	3	11, 16, 26, 42	4700 (100%)

All (600) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	53[A]	ASN	8.0
1	2-B	53[A]	ASN	8.0
1	3-B	53[A]	ASN	8.0
1	4-B	53[A]	ASN	8.0
1	5-B	53[A]	ASN	8.0
1	6-B	53[A]	ASN	8.0
1	7-B	53[A]	ASN	8.0
1	8-B	53[A]	ASN	8.0
1	9-B	53[A]	ASN	8.0
1	10-B	53[A]	ASN	8.0
1	11-B	53[A]	ASN	8.0
1	12-B	53[A]	ASN	8.0
1	13-B	53[A]	ASN	8.0
1	14-B	53[A]	ASN	8.0
1	15-B	53[A]	ASN	8.0

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Mol	Chain	Res	Type	RSRZ
1	16-B	53[A]	ASN	8.0
1	17-B	53[A]	ASN	8.0
1	18-B	53[A]	ASN	8.0
1	19-B	53[A]	ASN	8.0
1	20-B	53[A]	ASN	8.0
1	1-A	122	ASP	7.9
1	2-A	122	ASP	7.9
1	3-A	122	ASP	7.9
1	4-A	122	ASP	7.9
1	5-A	122	ASP	7.9
1	6-A	122	ASP	7.9
1	7-A	122	ASP	7.9
1	8-A	122	ASP	7.9
1	9-A	122	ASP	7.9
1	10-A	122	ASP	7.9
1	11-A	122	ASP	7.9
1	12-A	122	ASP	7.9
1	13-A	122	ASP	7.9
1	14-A	122	ASP	7.9
1	15-A	122	ASP	7.9
1	16-A	122	ASP	7.9
1	17-A	122	ASP	7.9
1	18-A	122	ASP	7.9
1	19-A	122	ASP	7.9
1	20-A	122	ASP	7.9
1	1-A	49	ARG	6.2
1	2-A	49	ARG	6.2
1	3-A	49	ARG	6.2
1	4-A	49	ARG	6.2
1	5-A	49	ARG	6.2
1	6-A	49	ARG	6.2
1	7-A	49	ARG	6.2
1	8-A	49	ARG	6.2
1	9-A	49	ARG	6.2
1	10-A	49	ARG	6.2
1	11-A	49	ARG	6.2
1	12-A	49	ARG	6.2
1	13-A	49	ARG	6.2
1	14-A	49	ARG	6.2
1	15-A	49	ARG	6.2
1	16-A	49	ARG	6.2
1	17-A	49	ARG	6.2

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Mol	Chain	Res	Type	RSRZ
1	18-A	49	ARG	6.2
1	19-A	49	ARG	6.2
1	20-A	49	ARG	6.2
1	1-B	51[A]	SER	5.8
1	2-B	51[A]	SER	5.8
1	3-B	51[A]	SER	5.8
1	4-B	51[A]	SER	5.8
1	5-B	51[A]	SER	5.8
1	6-B	51[A]	SER	5.8
1	7-B	51[A]	SER	5.8
1	8-B	51[A]	SER	5.8
1	9-B	51[A]	SER	5.8
1	10-B	51[A]	SER	5.8
1	11-B	51[A]	SER	5.8
1	12-B	51[A]	SER	5.8
1	13-B	51[A]	SER	5.8
1	14-B	51[A]	SER	5.8
1	15-B	51[A]	SER	5.8
1	16-B	51[A]	SER	5.8
1	17-B	51[A]	SER	5.8
1	18-B	51[A]	SER	5.8
1	19-B	51[A]	SER	5.8
1	20-B	51[A]	SER	5.8
1	1-A	48	PHE	5.5
1	2-A	48	PHE	5.5
1	3-A	48	PHE	5.5
1	4-A	48	PHE	5.5
1	5-A	48	PHE	5.5
1	6-A	48	PHE	5.5
1	7-A	48	PHE	5.5
1	8-A	48	PHE	5.5
1	9-A	48	PHE	5.5
1	10-A	48	PHE	5.5
1	11-A	48	PHE	5.5
1	12-A	48	PHE	5.5
1	13-A	48	PHE	5.5
1	14-A	48	PHE	5.5
1	15-A	48	PHE	5.5
1	16-A	48	PHE	5.5
1	17-A	48	PHE	5.5
1	18-A	48	PHE	5.5
1	19-A	48	PHE	5.5

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Mol	Chain	Res	Type	RSRZ
1	20-A	48	PHE	5.5
1	1-B	71[A]	ASP	5.2
1	2-B	71[A]	ASP	5.2
1	3-B	71[A]	ASP	5.2
1	4-B	71[A]	ASP	5.2
1	5-B	71[A]	ASP	5.2
1	6-B	71[A]	ASP	5.2
1	7-B	71[A]	ASP	5.2
1	8-B	71[A]	ASP	5.2
1	9-B	71[A]	ASP	5.2
1	10-B	71[A]	ASP	5.2
1	11-B	71[A]	ASP	5.2
1	12-B	71[A]	ASP	5.2
1	13-B	71[A]	ASP	5.2
1	14-B	71[A]	ASP	5.2
1	15-B	71[A]	ASP	5.2
1	16-B	71[A]	ASP	5.2
1	17-B	71[A]	ASP	5.2
1	18-B	71[A]	ASP	5.2
1	19-B	71[A]	ASP	5.2
1	20-B	71[A]	ASP	5.2
1	1-A	17	TYR	5.0
1	2-A	17	TYR	5.0
1	3-A	17	TYR	5.0
1	4-A	17	TYR	5.0
1	5-A	17	TYR	5.0
1	6-A	17	TYR	5.0
1	7-A	17	TYR	5.0
1	8-A	17	TYR	5.0
1	9-A	17	TYR	5.0
1	10-A	17	TYR	5.0
1	11-A	17	TYR	5.0
1	12-A	17	TYR	5.0
1	13-A	17	TYR	5.0
1	14-A	17	TYR	5.0
1	15-A	17	TYR	5.0
1	16-A	17	TYR	5.0
1	17-A	17	TYR	5.0
1	18-A	17	TYR	5.0
1	19-A	17	TYR	5.0
1	20-A	17	TYR	5.0
1	1-B	52[A]	HIS	4.8

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Mol	Chain	Res	Type	RSRZ
1	2-B	52[A]	HIS	4.8
1	3-B	52[A]	HIS	4.8
1	4-B	52[A]	HIS	4.8
1	5-B	52[A]	HIS	4.8
1	6-B	52[A]	HIS	4.8
1	7-B	52[A]	HIS	4.8
1	8-B	52[A]	HIS	4.8
1	9-B	52[A]	HIS	4.8
1	10-B	52[A]	HIS	4.8
1	11-B	52[A]	HIS	4.8
1	12-B	52[A]	HIS	4.8
1	13-B	52[A]	HIS	4.8
1	14-B	52[A]	HIS	4.8
1	15-B	52[A]	HIS	4.8
1	16-B	52[A]	HIS	4.8
1	17-B	52[A]	HIS	4.8
1	18-B	52[A]	HIS	4.8
1	19-B	52[A]	HIS	4.8
1	20-B	52[A]	HIS	4.8
1	1-B	70[A]	ASN	4.7
1	2-B	70[A]	ASN	4.7
1	3-B	70[A]	ASN	4.7
1	4-B	70[A]	ASN	4.7
1	5-B	70[A]	ASN	4.7
1	6-B	70[A]	ASN	4.7
1	7-B	70[A]	ASN	4.7
1	8-B	70[A]	ASN	4.7
1	9-B	70[A]	ASN	4.7
1	10-B	70[A]	ASN	4.7
1	11-B	70[A]	ASN	4.7
1	12-B	70[A]	ASN	4.7
1	13-B	70[A]	ASN	4.7
1	14-B	70[A]	ASN	4.7
1	15-B	70[A]	ASN	4.7
1	16-B	70[A]	ASN	4.7
1	17-B	70[A]	ASN	4.7
1	18-B	70[A]	ASN	4.7
1	19-B	70[A]	ASN	4.7
1	20-B	70[A]	ASN	4.7
1	1-A	121	GLN	4.5
1	2-A	121	GLN	4.5
1	3-A	121	GLN	4.5

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Mol	Chain	Res	Type	RSRZ
1	4-A	121	GLN	4.5
1	5-A	121	GLN	4.5
1	6-A	121	GLN	4.5
1	7-A	121	GLN	4.5
1	8-A	121	GLN	4.5
1	9-A	121	GLN	4.5
1	10-A	121	GLN	4.5
1	11-A	121	GLN	4.5
1	12-A	121	GLN	4.5
1	13-A	121	GLN	4.5
1	14-A	121	GLN	4.5
1	15-A	121	GLN	4.5
1	16-A	121	GLN	4.5
1	17-A	121	GLN	4.5
1	18-A	121	GLN	4.5
1	19-A	121	GLN	4.5
1	20-A	121	GLN	4.5
1	1-A	72[A]	GLU	4.4
1	2-A	72[A]	GLU	4.4
1	3-A	72[A]	GLU	4.4
1	4-A	72[A]	GLU	4.4
1	5-A	72[A]	GLU	4.4
1	6-A	72[A]	GLU	4.4
1	7-A	72[A]	GLU	4.4
1	8-A	72[A]	GLU	4.4
1	9-A	72[A]	GLU	4.4
1	10-A	72[A]	GLU	4.4
1	11-A	72[A]	GLU	4.4
1	12-A	72[A]	GLU	4.4
1	13-A	72[A]	GLU	4.4
1	14-A	72[A]	GLU	4.4
1	15-A	72[A]	GLU	4.4
1	16-A	72[A]	GLU	4.4
1	17-A	72[A]	GLU	4.4
1	18-A	72[A]	GLU	4.4
1	19-A	72[A]	GLU	4.4
1	20-A	72[A]	GLU	4.4
1	1-A	50	HIS	4.4
1	2-A	50	HIS	4.4
1	3-A	50	HIS	4.4
1	4-A	50	HIS	4.4
1	5-A	50	HIS	4.4

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Mol	Chain	Res	Type	RSRZ
1	6-A	50	HIS	4.4
1	7-A	50	HIS	4.4
1	8-A	50	HIS	4.4
1	9-A	50	HIS	4.4
1	10-A	50	HIS	4.4
1	11-A	50	HIS	4.4
1	12-A	50	HIS	4.4
1	13-A	50	HIS	4.4
1	14-A	50	HIS	4.4
1	15-A	50	HIS	4.4
1	16-A	50	HIS	4.4
1	17-A	50	HIS	4.4
1	18-A	50	HIS	4.4
1	19-A	50	HIS	4.4
1	20-A	50	HIS	4.4
1	1-B	17[A]	TYR	4.1
1	2-B	17[A]	TYR	4.1
1	3-B	17[A]	TYR	4.1
1	4-B	17[A]	TYR	4.1
1	5-B	17[A]	TYR	4.1
1	6-B	17[A]	TYR	4.1
1	7-B	17[A]	TYR	4.1
1	8-B	17[A]	TYR	4.1
1	9-B	17[A]	TYR	4.1
1	10-B	17[A]	TYR	4.1
1	11-B	17[A]	TYR	4.1
1	12-B	17[A]	TYR	4.1
1	13-B	17[A]	TYR	4.1
1	14-B	17[A]	TYR	4.1
1	15-B	17[A]	TYR	4.1
1	16-B	17[A]	TYR	4.1
1	17-B	17[A]	TYR	4.1
1	18-B	17[A]	TYR	4.1
1	19-B	17[A]	TYR	4.1
1	20-B	17[A]	TYR	4.1
1	1-A	91	HIS	4.0
1	2-A	91	HIS	4.0
1	3-A	91	HIS	4.0
1	4-A	91	HIS	4.0
1	5-A	91	HIS	4.0
1	6-A	91	HIS	4.0
1	7-A	91	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
1	8-A	91	HIS	4.0
1	9-A	91	HIS	4.0
1	10-A	91	HIS	4.0
1	11-A	91	HIS	4.0
1	12-A	91	HIS	4.0
1	13-A	91	HIS	4.0
1	14-A	91	HIS	4.0
1	15-A	91	HIS	4.0
1	16-A	91	HIS	4.0
1	17-A	91	HIS	4.0
1	18-A	91	HIS	4.0
1	19-A	91	HIS	4.0
1	20-A	91	HIS	4.0
1	1-B	48[A]	PHE	3.8
1	2-B	48[A]	PHE	3.8
1	3-B	48[A]	PHE	3.8
1	4-B	48[A]	PHE	3.8
1	5-B	48[A]	PHE	3.8
1	6-B	48[A]	PHE	3.8
1	7-B	48[A]	PHE	3.8
1	8-B	48[A]	PHE	3.8
1	9-B	48[A]	PHE	3.8
1	10-B	48[A]	PHE	3.8
1	11-B	48[A]	PHE	3.8
1	12-B	48[A]	PHE	3.8
1	13-B	48[A]	PHE	3.8
1	14-B	48[A]	PHE	3.8
1	15-B	48[A]	PHE	3.8
1	16-B	48[A]	PHE	3.8
1	17-B	48[A]	PHE	3.8
1	18-B	48[A]	PHE	3.8
1	19-B	48[A]	PHE	3.8
1	20-B	48[A]	PHE	3.8
1	1-A	53	ASN	3.7
1	2-A	53	ASN	3.7
1	3-A	53	ASN	3.7
1	4-A	53	ASN	3.7
1	5-A	53	ASN	3.7
1	6-A	53	ASN	3.7
1	7-A	53	ASN	3.7
1	8-A	53	ASN	3.7
1	9-A	53	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	10-A	53	ASN	3.7
1	11-A	53	ASN	3.7
1	12-A	53	ASN	3.7
1	13-A	53	ASN	3.7
1	14-A	53	ASN	3.7
1	15-A	53	ASN	3.7
1	16-A	53	ASN	3.7
1	17-A	53	ASN	3.7
1	18-A	53	ASN	3.7
1	19-A	53	ASN	3.7
1	20-A	53	ASN	3.7
1	1-B	121	GLN	3.4
1	2-B	121	GLN	3.4
1	3-B	121	GLN	3.4
1	4-B	121	GLN	3.4
1	5-B	121	GLN	3.4
1	6-B	121	GLN	3.4
1	7-B	121	GLN	3.4
1	8-B	121	GLN	3.4
1	9-B	121	GLN	3.4
1	10-B	121	GLN	3.4
1	11-B	121	GLN	3.4
1	12-B	121	GLN	3.4
1	13-B	121	GLN	3.4
1	14-B	121	GLN	3.4
1	15-B	121	GLN	3.4
1	16-B	121	GLN	3.4
1	17-B	121	GLN	3.4
1	18-B	121	GLN	3.4
1	19-B	121	GLN	3.4
1	20-B	121	GLN	3.4
1	1-A	29	GLY	3.4
1	2-A	29	GLY	3.4
1	3-A	29	GLY	3.4
1	4-A	29	GLY	3.4
1	5-A	29	GLY	3.4
1	6-A	29	GLY	3.4
1	7-A	29	GLY	3.4
1	8-A	29	GLY	3.4
1	9-A	29	GLY	3.4
1	10-A	29	GLY	3.4
1	11-A	29	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	12-A	29	GLY	3.4
1	13-A	29	GLY	3.4
1	14-A	29	GLY	3.4
1	15-A	29	GLY	3.4
1	16-A	29	GLY	3.4
1	17-A	29	GLY	3.4
1	18-A	29	GLY	3.4
1	19-A	29	GLY	3.4
1	20-A	29	GLY	3.4
1	1-B	87	ASP	3.3
1	2-B	87	ASP	3.3
1	3-B	87	ASP	3.3
1	4-B	87	ASP	3.3
1	5-B	87	ASP	3.3
1	6-B	87	ASP	3.3
1	7-B	87	ASP	3.3
1	8-B	87	ASP	3.3
1	9-B	87	ASP	3.3
1	10-B	87	ASP	3.3
1	11-B	87	ASP	3.3
1	12-B	87	ASP	3.3
1	13-B	87	ASP	3.3
1	14-B	87	ASP	3.3
1	15-B	87	ASP	3.3
1	16-B	87	ASP	3.3
1	17-B	87	ASP	3.3
1	18-B	87	ASP	3.3
1	19-B	87	ASP	3.3
1	20-B	87	ASP	3.3
1	1-A	71	ASP	3.3
1	2-A	71	ASP	3.3
1	3-A	71	ASP	3.3
1	4-A	71	ASP	3.3
1	5-A	71	ASP	3.3
1	6-A	71	ASP	3.3
1	7-A	71	ASP	3.3
1	8-A	71	ASP	3.3
1	9-A	71	ASP	3.3
1	10-A	71	ASP	3.3
1	11-A	71	ASP	3.3
1	12-A	71	ASP	3.3
1	13-A	71	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	14-A	71	ASP	3.3
1	15-A	71	ASP	3.3
1	16-A	71	ASP	3.3
1	17-A	71	ASP	3.3
1	18-A	71	ASP	3.3
1	19-A	71	ASP	3.3
1	20-A	71	ASP	3.3
1	1-B	3	ASN	3.1
1	2-B	3	ASN	3.1
1	3-B	3	ASN	3.1
1	4-B	3	ASN	3.1
1	5-B	3	ASN	3.1
1	6-B	3	ASN	3.1
1	7-B	3	ASN	3.1
1	8-B	3	ASN	3.1
1	9-B	3	ASN	3.1
1	10-B	3	ASN	3.1
1	11-B	3	ASN	3.1
1	12-B	3	ASN	3.1
1	13-B	3	ASN	3.1
1	14-B	3	ASN	3.1
1	15-B	3	ASN	3.1
1	16-B	3	ASN	3.1
1	17-B	3	ASN	3.1
1	18-B	3	ASN	3.1
1	19-B	3	ASN	3.1
1	20-B	3	ASN	3.1
1	1-A	51	SER	2.8
1	2-A	51	SER	2.8
1	3-A	51	SER	2.8
1	4-A	51	SER	2.8
1	5-A	51	SER	2.8
1	6-A	51	SER	2.8
1	7-A	51	SER	2.8
1	8-A	51	SER	2.8
1	9-A	51	SER	2.8
1	10-A	51	SER	2.8
1	11-A	51	SER	2.8
1	12-A	51	SER	2.8
1	13-A	51	SER	2.8
1	14-A	51	SER	2.8
1	15-A	51	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	16-A	51	SER	2.8
1	17-A	51	SER	2.8
1	18-A	51	SER	2.8
1	19-A	51	SER	2.8
1	20-A	51	SER	2.8
1	1-B	50[A]	HIS	2.7
1	2-B	50[A]	HIS	2.7
1	3-B	50[A]	HIS	2.7
1	4-B	50[A]	HIS	2.7
1	5-B	50[A]	HIS	2.7
1	6-B	50[A]	HIS	2.7
1	7-B	50[A]	HIS	2.7
1	8-B	50[A]	HIS	2.7
1	9-B	50[A]	HIS	2.7
1	10-B	50[A]	HIS	2.7
1	11-B	50[A]	HIS	2.7
1	12-B	50[A]	HIS	2.7
1	13-B	50[A]	HIS	2.7
1	14-B	50[A]	HIS	2.7
1	15-B	50[A]	HIS	2.7
1	16-B	50[A]	HIS	2.7
1	17-B	50[A]	HIS	2.7
1	18-B	50[A]	HIS	2.7
1	19-B	50[A]	HIS	2.7
1	20-B	50[A]	HIS	2.7
1	1-A	86	LEU	2.7
1	2-A	86	LEU	2.7
1	3-A	86	LEU	2.7
1	4-A	86	LEU	2.7
1	5-A	86	LEU	2.7
1	6-A	86	LEU	2.7
1	7-A	86	LEU	2.7
1	8-A	86	LEU	2.7
1	9-A	86	LEU	2.7
1	10-A	86	LEU	2.7
1	11-A	86	LEU	2.7
1	12-A	86	LEU	2.7
1	13-A	86	LEU	2.7
1	14-A	86	LEU	2.7
1	15-A	86	LEU	2.7
1	16-A	86	LEU	2.7
1	17-A	86	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	18-A	86	LEU	2.7
1	19-A	86	LEU	2.7
1	20-A	86	LEU	2.7
1	1-B	72[A]	GLU	2.5
1	2-B	72[A]	GLU	2.5
1	3-B	72[A]	GLU	2.5
1	4-B	72[A]	GLU	2.5
1	5-B	72[A]	GLU	2.5
1	6-B	72[A]	GLU	2.5
1	7-B	72[A]	GLU	2.5
1	8-B	72[A]	GLU	2.5
1	9-B	72[A]	GLU	2.5
1	10-B	72[A]	GLU	2.5
1	11-B	72[A]	GLU	2.5
1	12-B	72[A]	GLU	2.5
1	13-B	72[A]	GLU	2.5
1	14-B	72[A]	GLU	2.5
1	15-B	72[A]	GLU	2.5
1	16-B	72[A]	GLU	2.5
1	17-B	72[A]	GLU	2.5
1	18-B	72[A]	GLU	2.5
1	19-B	72[A]	GLU	2.5
1	20-B	72[A]	GLU	2.5
1	1-B	86	LEU	2.2
1	2-B	86	LEU	2.2
1	3-B	86	LEU	2.2
1	4-B	86	LEU	2.2
1	5-B	86	LEU	2.2
1	6-B	86	LEU	2.2
1	7-B	86	LEU	2.2
1	8-B	86	LEU	2.2
1	9-B	86	LEU	2.2
1	10-B	86	LEU	2.2
1	11-B	86	LEU	2.2
1	12-B	86	LEU	2.2
1	13-B	86	LEU	2.2
1	14-B	86	LEU	2.2
1	15-B	86	LEU	2.2
1	16-B	86	LEU	2.2
1	17-B	86	LEU	2.2
1	18-B	86	LEU	2.2
1	19-B	86	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	20-B	86	LEU	2.2
1	1-A	120	GLU	2.1
1	2-A	120	GLU	2.1
1	3-A	120	GLU	2.1
1	4-A	120	GLU	2.1
1	5-A	120	GLU	2.1
1	6-A	120	GLU	2.1
1	7-A	120	GLU	2.1
1	8-A	120	GLU	2.1
1	9-A	120	GLU	2.1
1	10-A	120	GLU	2.1
1	11-A	120	GLU	2.1
1	12-A	120	GLU	2.1
1	13-A	120	GLU	2.1
1	14-A	120	GLU	2.1
1	15-A	120	GLU	2.1
1	16-A	120	GLU	2.1
1	17-A	120	GLU	2.1
1	18-A	120	GLU	2.1
1	19-A	120	GLU	2.1
1	20-A	120	GLU	2.1
1	1-A	52	HIS	2.1
1	2-A	52	HIS	2.1
1	3-A	52	HIS	2.1
1	4-A	52	HIS	2.1
1	5-A	52	HIS	2.1
1	6-A	52	HIS	2.1
1	7-A	52	HIS	2.1
1	8-A	52	HIS	2.1
1	9-A	52	HIS	2.1
1	10-A	52	HIS	2.1
1	11-A	52	HIS	2.1
1	12-A	52	HIS	2.1
1	13-A	52	HIS	2.1
1	14-A	52	HIS	2.1
1	15-A	52	HIS	2.1
1	16-A	52	HIS	2.1
1	17-A	52	HIS	2.1
1	18-A	52	HIS	2.1
1	19-A	52	HIS	2.1
1	20-A	52	HIS	2.1
1	1-A	87	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	2-A	87	ASP	2.1
1	3-A	87	ASP	2.1
1	4-A	87	ASP	2.1
1	5-A	87	ASP	2.1
1	6-A	87	ASP	2.1
1	7-A	87	ASP	2.1
1	8-A	87	ASP	2.1
1	9-A	87	ASP	2.1
1	10-A	87	ASP	2.1
1	11-A	87	ASP	2.1
1	12-A	87	ASP	2.1
1	13-A	87	ASP	2.1
1	14-A	87	ASP	2.1
1	15-A	87	ASP	2.1
1	16-A	87	ASP	2.1
1	17-A	87	ASP	2.1
1	18-A	87	ASP	2.1
1	19-A	87	ASP	2.1
1	20-A	87	ASP	2.1
1	1-A	3	ASN	2.1
1	2-A	3	ASN	2.1
1	3-A	3	ASN	2.1
1	4-A	3	ASN	2.1
1	5-A	3	ASN	2.1
1	6-A	3	ASN	2.1
1	7-A	3	ASN	2.1
1	8-A	3	ASN	2.1
1	9-A	3	ASN	2.1
1	10-A	3	ASN	2.1
1	11-A	3	ASN	2.1
1	12-A	3	ASN	2.1
1	13-A	3	ASN	2.1
1	14-A	3	ASN	2.1
1	15-A	3	ASN	2.1
1	16-A	3	ASN	2.1
1	17-A	3	ASN	2.1
1	18-A	3	ASN	2.1
1	19-A	3	ASN	2.1
1	20-A	3	ASN	2.1

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NA	1-A	202	1/1	0.99	0.08	9,9,9,9	1
3	NA	2-A	202	1/1	0.99	0.08	9,9,9,9	1
3	NA	3-A	202	1/1	0.99	0.08	9,9,9,9	1
3	NA	4-A	202	1/1	0.99	0.08	9,9,9,9	1
3	NA	5-A	202	1/1	0.99	0.08	9,9,9,9	1
3	NA	6-A	202	1/1	0.99	0.08	9,9,9,9	1
3	NA	7-A	202	1/1	0.99	0.08	9,9,9,9	1
3	NA	8-A	202	1/1	0.99	0.08	9,9,9,9	1
3	NA	9-A	202	1/1	0.99	0.08	9,9,9,9	1
3	NA	10-A	202	1/1	0.99	0.08	9,9,9,9	1
3	NA	11-A	202	1/1	0.99	0.08	9,9,9,9	1
3	NA	12-A	202	1/1	0.99	0.08	9,9,9,9	1
3	NA	13-A	202	1/1	0.99	0.08	9,9,9,9	1
3	NA	14-A	202	1/1	0.99	0.08	9,9,9,9	1
3	NA	15-A	202	1/1	0.99	0.08	9,9,9,9	1
3	NA	16-A	202	1/1	0.99	0.08	9,9,9,9	1
3	NA	17-A	202	1/1	0.99	0.08	9,9,9,9	1
3	NA	18-A	202	1/1	0.99	0.08	9,9,9,9	1
3	NA	19-A	202	1/1	0.99	0.08	9,9,9,9	1
3	NA	20-A	202	1/1	0.99	0.08	9,9,9,9	1
2	NI	1-B	201	1/1	1.00	0.03	16,16,16,16	1
2	NI	2-B	201	1/1	1.00	0.03	16,16,16,16	1
2	NI	3-B	201	1/1	1.00	0.03	16,16,16,16	1
2	NI	4-B	201	1/1	1.00	0.03	16,16,16,16	1
2	NI	5-B	201	1/1	1.00	0.03	16,16,16,16	1
2	NI	6-B	201	1/1	1.00	0.03	16,16,16,16	1
2	NI	7-B	201	1/1	1.00	0.03	16,16,16,16	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NI	8-B	201	1/1	1.00	0.03	16,16,16,16	1
2	NI	9-B	201	1/1	1.00	0.03	16,16,16,16	1
2	NI	10-B	201	1/1	1.00	0.03	16,16,16,16	1
2	NI	11-B	201	1/1	1.00	0.03	16,16,16,16	1
2	NI	12-B	201	1/1	1.00	0.03	16,16,16,16	1
2	NI	13-B	201	1/1	1.00	0.03	16,16,16,16	1
2	NI	14-B	201	1/1	1.00	0.03	16,16,16,16	1
2	NI	15-B	201	1/1	1.00	0.03	16,16,16,16	1
2	NI	16-B	201	1/1	1.00	0.03	16,16,16,16	1
2	NI	17-B	201	1/1	1.00	0.03	16,16,16,16	1
2	NI	18-B	201	1/1	1.00	0.03	16,16,16,16	1
2	NI	19-B	201	1/1	1.00	0.03	16,16,16,16	1
2	NI	20-B	201	1/1	1.00	0.03	16,16,16,16	1
2	NI	1-A	201	1/1	1.00	0.02	16,16,16,16	1
2	NI	2-A	201	1/1	1.00	0.02	16,16,16,16	1
2	NI	3-A	201	1/1	1.00	0.02	16,16,16,16	1
2	NI	4-A	201	1/1	1.00	0.02	16,16,16,16	1
2	NI	5-A	201	1/1	1.00	0.02	16,16,16,16	1
2	NI	6-A	201	1/1	1.00	0.02	16,16,16,16	1
2	NI	7-A	201	1/1	1.00	0.02	16,16,16,16	1
2	NI	8-A	201	1/1	1.00	0.02	16,16,16,16	1
2	NI	9-A	201	1/1	1.00	0.02	16,16,16,16	1
2	NI	10-A	201	1/1	1.00	0.02	16,16,16,16	1
2	NI	11-A	201	1/1	1.00	0.02	16,16,16,16	1
2	NI	12-A	201	1/1	1.00	0.02	16,16,16,16	1
2	NI	13-A	201	1/1	1.00	0.02	16,16,16,16	1
2	NI	14-A	201	1/1	1.00	0.02	16,16,16,16	1
2	NI	15-A	201	1/1	1.00	0.02	16,16,16,16	1
2	NI	16-A	201	1/1	1.00	0.02	16,16,16,16	1
2	NI	17-A	201	1/1	1.00	0.02	16,16,16,16	1
2	NI	18-A	201	1/1	1.00	0.02	16,16,16,16	1
2	NI	19-A	201	1/1	1.00	0.02	16,16,16,16	1
2	NI	20-A	201	1/1	1.00	0.02	16,16,16,16	1

6.5 Other polymers (i)

There are no such residues in this entry.