



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:37 AM UTC

PDB ID : 4Q29 / pdb_00004q29
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

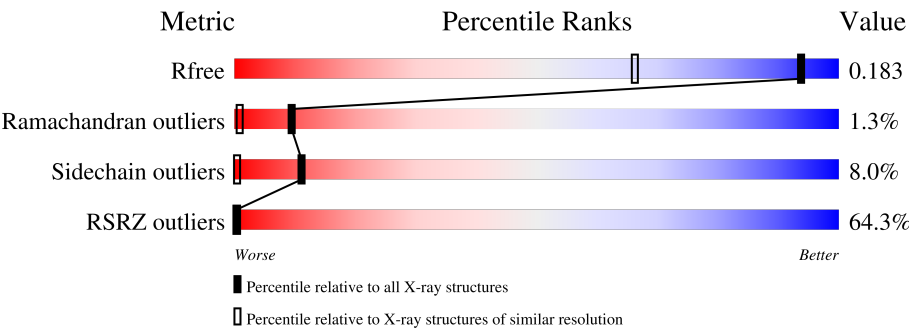
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2194 (1.36-1.32)
Ramachandran outliers	187476	2197 (1.36-1.32)
Sidechain outliers	187428	2197 (1.36-1.32)
RSRZ outliers	180081	2193 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	128	65% 88%7%5%
1	1-B	128	53% 84%9%6%
1	10-A	128	88%7%5%
1	10-B	128	85%8%6%
1	11-A	128	84%11%5%
1	11-B	128	84%10%6%

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Mol	Chain	Length	Quality of chain
1	12-A	128	 87% 8% 5%
1	12-B	128	 85% 9% 6%
1	13-A	128	 88% 7% 5%
1	13-B	128	 85% 9% 6%
1	14-A	128	 82% 12% 5%
1	14-B	128	 85% 8% 6%
1	15-A	128	 86% 9% 5%
1	15-B	128	 86% 8% 6%
1	16-A	128	 88% 6% 5%
1	16-B	128	 84% 10% 6%
1	17-A	128	 88% 6% 5%
1	17-B	128	 86% 8% 6%
1	18-A	128	 88% 7% 5%
1	18-B	128	 84% 9% 6%
1	19-A	128	 88% 6% 5%
1	19-B	128	 84% 10% 6%
1	2-A	128	 87% 8% 5%
1	2-B	128	 85% 9% 6%
1	20-A	128	 86% 9% 5%
1	20-B	128	 86% 8% 6%
1	3-A	128	 87% 8% 5%
1	3-B	128	 84% 10% 6%
1	4-A	128	 88% 7% 5%
1	4-B	128	 86% 7% 6%
1	5-A	128	 88% 5% 5%

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Mol	Chain	Length	Quality of chain
1	5-B	128	 84%9%6%
1	6-A	128	 88%5%5%
1	6-B	128	 84%10%6%
1	7-A	128	 88%6%5%
1	7-B	128	 84%9%6%
1	8-A	128	 88%6%5%
1	8-B	128	 85%9%6%
1	9-A	128	 85%9%5%
1	9-B	128	 84%10%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
1	1-A	121	Total	C	H	N	O	S	Se	0	22	0
			2195	718	1079	188	206	1	3			
1	2-A	121	Total	C	H	N	O	S	Se	0	22	0
			2195	718	1079	188	206	1	3			
1	3-A	121	Total	C	H	N	O	S	Se	0	22	0
			2195	718	1079	188	206	1	3			
1	4-A	121	Total	C	H	N	O	S	Se	0	22	0
			2195	718	1079	188	206	1	3			
1	5-A	121	Total	C	H	N	O	S	Se	0	22	0
			2195	718	1079	188	206	1	3			
1	6-A	121	Total	C	H	N	O	S	Se	0	22	0
			2195	718	1079	188	206	1	3			
1	7-A	121	Total	C	H	N	O	S	Se	0	22	0
			2195	718	1079	188	206	1	3			
1	8-A	121	Total	C	H	N	O	S	Se	0	22	0
			2195	718	1079	188	206	1	3			
1	9-A	121	Total	C	H	N	O	S	Se	0	22	0
			2195	718	1079	188	206	1	3			
1	10-A	121	Total	C	H	N	O	S	Se	0	22	0
			2195	718	1079	188	206	1	3			
1	11-A	121	Total	C	H	N	O	S	Se	0	22	0
			2195	718	1079	188	206	1	3			
1	12-A	121	Total	C	H	N	O	S	Se	0	22	0
			2195	718	1079	188	206	1	3			
1	13-A	121	Total	C	H	N	O	S	Se	0	22	0
			2195	718	1079	188	206	1	3			
1	14-A	121	Total	C	H	N	O	S	Se	0	22	0
			2195	718	1079	188	206	1	3			
1	15-A	121	Total	C	H	N	O	S	Se	0	22	0
			2195	718	1079	188	206	1	3			
1	16-A	121	Total	C	H	N	O	S	Se	0	22	0
			2195	718	1079	188	206	1	3			

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

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

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 (CCD ID: NI) (formula: Ni).

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

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

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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

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

- Molecule 4 is water.

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

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

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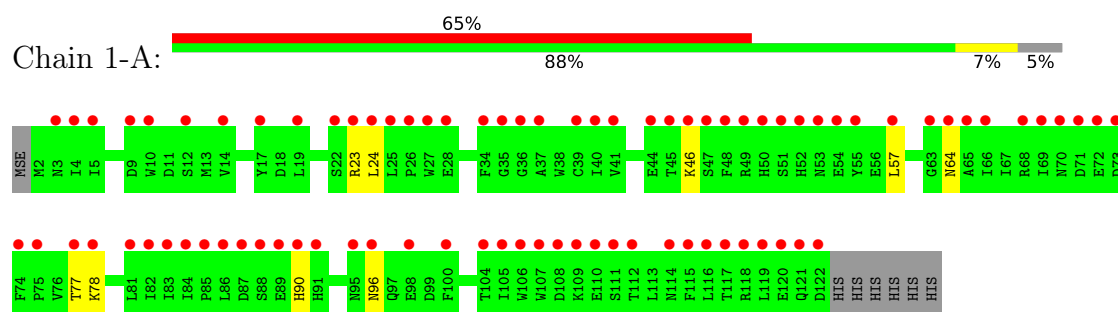
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	9-B	92	Total 92	O 92	0	0
4	10-B	95	Total 95	O 95	0	0
4	11-B	90	Total 90	O 90	0	0
4	12-B	92	Total 92	O 92	0	0
4	13-B	81	Total 81	O 81	0	0
4	14-B	87	Total 87	O 87	0	0
4	15-B	100	Total 100	O 100	0	0
4	16-B	95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

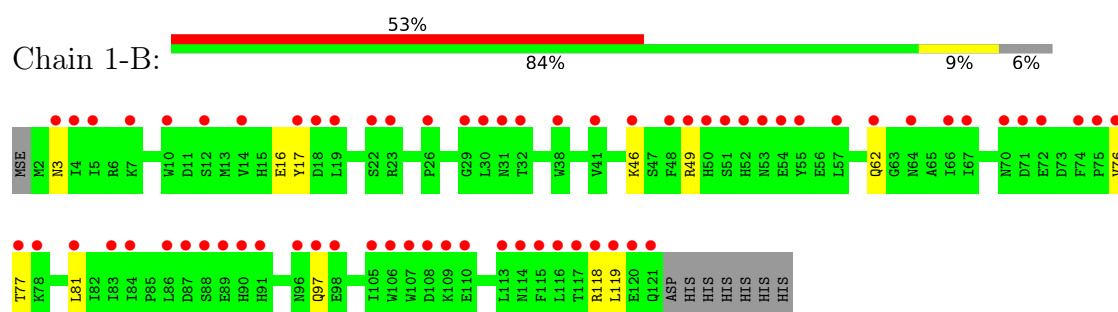
3 Residue-property plots [i](#)

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.

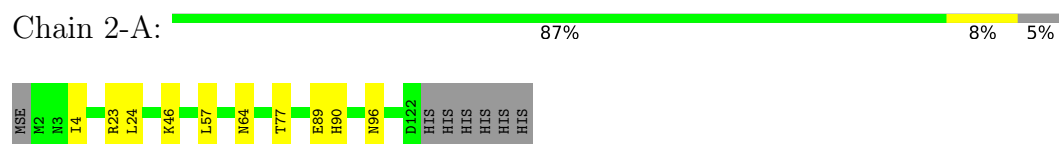
- Molecule 1: plu4264 protein



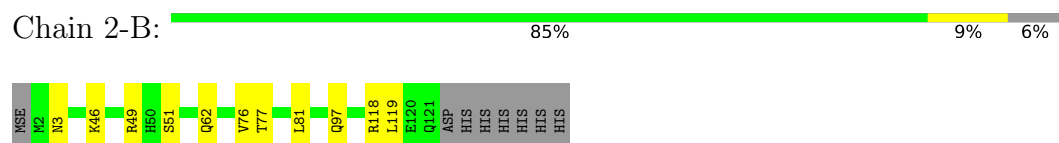
- Molecule 1: plu4264 protein



- Molecule 1: plu4264 protein



- Molecule 1: plu4264 protein



- Molecule 1: plu4264 protein

Chain 3-A:  87% 8% 5%



• Molecule 1: plu4264 protein

Chain 3-B:  84% 10% 6%



• Molecule 1: plu4264 protein

Chain 4-A:  88% 7% 5%



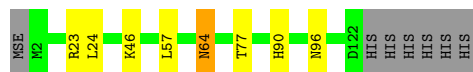
• Molecule 1: plu4264 protein

Chain 4-B:  86% 7% 6%



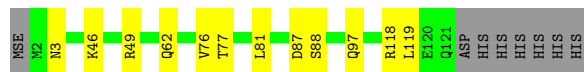
• Molecule 1: plu4264 protein

Chain 5-A:  88% 5% 5%



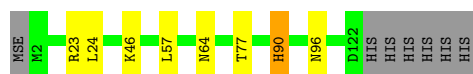
• Molecule 1: plu4264 protein

Chain 5-B:  84% 9% 6%



• Molecule 1: plu4264 protein

Chain 6-A:  88% 5% 5%



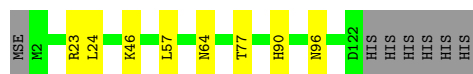
• Molecule 1: plu4264 protein

Chain 6-B:  84% 10% 6%



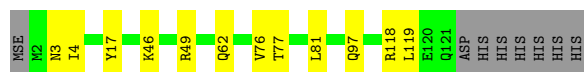
- Molecule 1: plu4264 protein

Chain 7-A:  88% 6% 5%



- Molecule 1: plu4264 protein

Chain 7-B:  84% 9% 6%



- Molecule 1: plu4264 protein

Chain 8-A:  88% 6% 5%



- Molecule 1: plu4264 protein

Chain 8-B:  85% 9% 6%



- Molecule 1: plu4264 protein

Chain 9-A:  85% 9% 5%

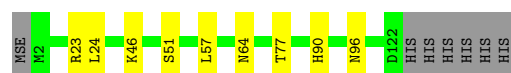


- Molecule 1: plu4264 protein

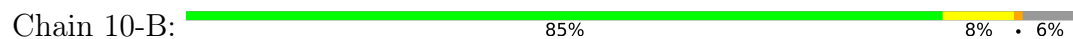
Chain 9-B:  84% 10% 6%



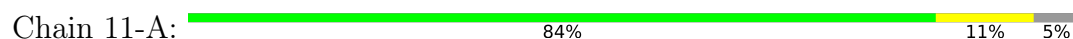
- Molecule 1: plu4264 protein



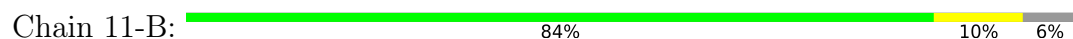
- Molecule 1: plu4264 protein



- Molecule 1: plu4264 protein



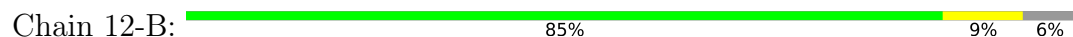
- Molecule 1: plu4264 protein



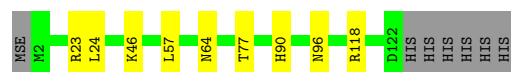
- Molecule 1: plu4264 protein



- Molecule 1: plu4264 protein

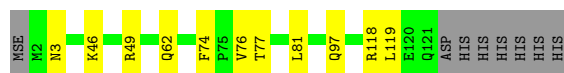


- Molecule 1: plu4264 protein



- Molecule 1: plu4264 protein

Chain 13-B:  85% 9% 6%



• Molecule 1: plu4264 protein

Chain 14-A:  82% 12% 5%



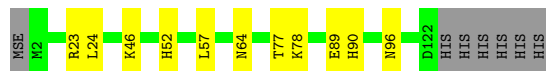
• Molecule 1: plu4264 protein

Chain 14-B:  85% 8% 6%



• Molecule 1: plu4264 protein

Chain 15-A:  86% 9% 5%



• Molecule 1: plu4264 protein

Chain 15-B:  86% 8% 6%



• Molecule 1: plu4264 protein

Chain 16-A:  88% 6% 5%



• Molecule 1: plu4264 protein

Chain 16-B:  84% 10% 6%



• Molecule 1: plu4264 protein

Chain 17-A:  88% 6% • 5%



- Molecule 1: plu4264 protein

Chain 17-B:  86% 8% 6%



- Molecule 1: plu4264 protein

Chain 18-A:  88% 7% 5%



- Molecule 1: plu4264 protein

Chain 18-B:  84% 9% • 6%



- Molecule 1: plu4264 protein

Chain 19-A:  88% 6% 5%



- Molecule 1: plu4264 protein

Chain 19-B:  84% 10% 6%



- Molecule 1: plu4264 protein

Chain 20-A:  86% 9% 5%



- Molecule 1: plu4264 protein

Chain 20-B: 86% 8% 6%



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 1.35Å)	Xtrriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.126 , 0.155 0.161 , 0.183	Depositor DCC
R_{free} test set	1111 reflections (1.46%)	wwPDB-VP
Wilson B-factor (Å ²)	13.4	Xtrriage
Anisotropy	0.734	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.02 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	94724	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtrriage'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 2.1574e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.40	0/1237	0.34	0/1679
1	1-B	0.35	0/1338	0.28	0/1816
1	2-A	0.40	0/1237	0.34	0/1679
1	2-B	0.35	0/1338	0.28	0/1816
1	3-A	0.40	0/1237	0.34	0/1679
1	3-B	0.35	0/1338	0.28	0/1816
1	4-A	0.40	0/1237	0.34	0/1679
1	4-B	0.35	0/1338	0.28	0/1816
1	5-A	0.40	0/1237	0.34	0/1679
1	5-B	0.35	0/1338	0.28	0/1816
1	6-A	0.40	0/1237	0.34	0/1679
1	6-B	0.35	0/1338	0.28	0/1816
1	7-A	0.40	0/1237	0.34	0/1679
1	7-B	0.35	0/1338	0.28	0/1816
1	8-A	0.40	0/1237	0.34	0/1679
1	8-B	0.35	0/1338	0.28	0/1816
1	9-A	0.40	0/1237	0.34	0/1679
1	9-B	0.35	0/1338	0.28	0/1816
1	10-A	0.40	0/1237	0.34	0/1679
1	10-B	0.35	0/1338	0.28	0/1816
1	11-A	0.40	0/1237	0.34	0/1679
1	11-B	0.35	0/1338	0.28	0/1816
1	12-A	0.40	0/1237	0.34	0/1679
1	12-B	0.35	0/1338	0.28	0/1816
1	13-A	0.40	0/1237	0.34	0/1679
1	13-B	0.35	0/1338	0.28	0/1816
1	14-A	0.40	0/1237	0.34	0/1679
1	14-B	0.35	0/1338	0.28	0/1816
1	15-A	0.40	0/1237	0.34	0/1679
1	15-B	0.35	0/1338	0.28	0/1816
1	16-A	0.40	0/1237	0.34	0/1679
1	16-B	0.35	0/1338	0.28	0/1816

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	17-A	0.40	0/1237	0.34	0/1679
1	17-B	0.35	0/1338	0.28	0/1816
1	18-A	0.40	0/1237	0.34	0/1679
1	18-B	0.35	0/1338	0.28	0/1816
1	19-A	0.40	0/1237	0.34	0/1679
1	19-B	0.35	0/1338	0.28	0/1816
1	20-A	0.40	0/1229	0.34	0/1668
1	20-B	0.35	0/1338	0.28	0/1816
All	All	0.37	0/51492	0.31	0/69889

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

There are no bond length outliers.

There are no bond angle outliers.

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

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Mol	Chain	Res	Type	Group
1	14-A	51	SER	Peptide
1	14-A	71	ASP	Peptide
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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	11-B	1218	1135	1045	0	0
1	12-A	1116	1079	982	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	12-B	1	0	0	0	0
2	13-A	1	0	0	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	3-B	91	0	0	0	0
4	4-A	101	0	0	0	0
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

5.3.1 Protein backbone

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%)	18	4
1	1-B	151/128 (118%)	143 (95%)	6 (4%)	2 (1%)	9	1
1	2-A	141/128 (110%)	134 (95%)	4 (3%)	3 (2%)	5	0
1	2-B	151/128 (118%)	138 (91%)	11 (7%)	2 (1%)	9	1
1	3-A	141/128 (110%)	137 (97%)	1 (1%)	3 (2%)	5	0
1	3-B	151/128 (118%)	137 (91%)	8 (5%)	6 (4%)	2	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%)	18	4
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%)	9	1
1	6-A	141/128 (110%)	133 (94%)	7 (5%)	1 (1%)	18	4
1	6-B	151/128 (118%)	141 (93%)	7 (5%)	3 (2%)	6	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%)	4	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%)	9	1
1	9-A	141/128 (110%)	131 (93%)	7 (5%)	3 (2%)	5	0
1	9-B	151/128 (118%)	133 (88%)	15 (10%)	3 (2%)	6	0
1	10-A	141/128 (110%)	136 (96%)	4 (3%)	1 (1%)	18	4
1	10-B	151/128 (118%)	140 (93%)	8 (5%)	3 (2%)	6	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%)	4	0
1	12-A	141/128 (110%)	137 (97%)	2 (1%)	2 (1%)	9	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%)	18	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	13-B	151/128 (118%)	142 (94%)	8 (5%)	1 (1%)	18	4
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%)	9	1
1	15-A	141/128 (110%)	132 (94%)	6 (4%)	3 (2%)	5	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%)	2	0
1	17-A	141/128 (110%)	136 (96%)	4 (3%)	1 (1%)	18	4
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%)	2	0
1	20-A	140/128 (109%)	136 (97%)	3 (2%)	1 (1%)	18	4
1	20-B	151/128 (118%)	140 (93%)	11 (7%)	0	100	100
All	All	5839/5120 (114%)	5473 (94%)	280 (5%)	86 (2%)	9	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 ⓘ

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 0
1	1-B	145/116 (125%)	132 (91%)	13 (9%)	9 0
1	2-A	135/116 (116%)	125 (93%)	10 (7%)	13 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2-B	145/116 (125%)	132 (91%)	13 (9%)	9	0
1	3-A	135/116 (116%)	125 (93%)	10 (7%)	13	0
1	3-B	145/116 (125%)	132 (91%)	13 (9%)	9	0
1	4-A	135/116 (116%)	125 (93%)	10 (7%)	13	0
1	4-B	145/116 (125%)	132 (91%)	13 (9%)	9	0
1	5-A	135/116 (116%)	125 (93%)	10 (7%)	13	0
1	5-B	145/116 (125%)	132 (91%)	13 (9%)	9	0
1	6-A	135/116 (116%)	125 (93%)	10 (7%)	13	0
1	6-B	145/116 (125%)	132 (91%)	13 (9%)	9	0
1	7-A	135/116 (116%)	125 (93%)	10 (7%)	13	0
1	7-B	145/116 (125%)	132 (91%)	13 (9%)	9	0
1	8-A	135/116 (116%)	125 (93%)	10 (7%)	13	0
1	8-B	145/116 (125%)	132 (91%)	13 (9%)	9	0
1	9-A	135/116 (116%)	125 (93%)	10 (7%)	13	0
1	9-B	145/116 (125%)	132 (91%)	13 (9%)	9	0
1	10-A	135/116 (116%)	125 (93%)	10 (7%)	13	0
1	10-B	145/116 (125%)	132 (91%)	13 (9%)	9	0
1	11-A	135/116 (116%)	125 (93%)	10 (7%)	13	0
1	11-B	145/116 (125%)	132 (91%)	13 (9%)	9	0
1	12-A	135/116 (116%)	125 (93%)	10 (7%)	13	0
1	12-B	145/116 (125%)	132 (91%)	13 (9%)	9	0
1	13-A	135/116 (116%)	125 (93%)	10 (7%)	13	0
1	13-B	145/116 (125%)	132 (91%)	13 (9%)	9	0
1	14-A	135/116 (116%)	125 (93%)	10 (7%)	13	0
1	14-B	145/116 (125%)	132 (91%)	13 (9%)	9	0
1	15-A	135/116 (116%)	125 (93%)	10 (7%)	13	0
1	15-B	145/116 (125%)	132 (91%)	13 (9%)	9	0
1	16-A	135/116 (116%)	125 (93%)	10 (7%)	13	0
1	16-B	145/116 (125%)	132 (91%)	13 (9%)	9	0
1	17-A	135/116 (116%)	125 (93%)	10 (7%)	13	0
1	17-B	145/116 (125%)	132 (91%)	13 (9%)	9	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	18-A	135/116 (116%)	125 (93%)	10 (7%)	13	0
1	18-B	145/116 (125%)	132 (91%)	13 (9%)	9	0
1	19-A	135/116 (116%)	125 (93%)	10 (7%)	13	0
1	19-B	145/116 (125%)	132 (91%)	13 (9%)	9	0
1	20-A	134/116 (116%)	124 (92%)	10 (8%)	12	0
1	20-B	145/116 (125%)	132 (91%)	13 (9%)	9	0
All	All	5599/4640 (121%)	5139 (92%)	460 (8%)	11	0

All (460) 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	46	LYS
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	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	76	VAL
1	1-B	77[A]	THR
1	1-B	77[B]	THR
1	1-B	81	LEU
1	1-B	97	GLN
1	1-B	118	ARG
1	1-B	119	LEU
1	2-A	23	ARG
1	2-A	24	LEU
1	2-A	46	LYS
1	2-A	57[A]	LEU
1	2-A	57[B]	LEU
1	2-A	64	ASN

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Mol	Chain	Res	Type
1	2-A	77	THR
1	2-A	90	HIS
1	2-A	96[A]	ASN
1	2-A	96[B]	ASN
1	2-B	3	ASN
1	2-B	46[A]	LYS
1	2-B	46[B]	LYS
1	2-B	49[A]	ARG
1	2-B	49[B]	ARG
1	2-B	62	GLN
1	2-B	76	VAL
1	2-B	77[A]	THR
1	2-B	77[B]	THR
1	2-B	81	LEU
1	2-B	97	GLN
1	2-B	118	ARG
1	2-B	119	LEU
1	3-A	23	ARG
1	3-A	24	LEU
1	3-A	46	LYS
1	3-A	57[A]	LEU
1	3-A	57[B]	LEU
1	3-A	64	ASN
1	3-A	77	THR
1	3-A	90	HIS
1	3-A	96[A]	ASN
1	3-A	96[B]	ASN
1	3-B	3	ASN
1	3-B	46[A]	LYS
1	3-B	46[B]	LYS
1	3-B	49[A]	ARG
1	3-B	49[B]	ARG
1	3-B	62	GLN
1	3-B	76	VAL
1	3-B	77[A]	THR
1	3-B	77[B]	THR
1	3-B	81	LEU
1	3-B	97	GLN
1	3-B	118	ARG
1	3-B	119	LEU
1	4-A	23	ARG
1	4-A	24	LEU

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Mol	Chain	Res	Type
1	4-A	46	LYS
1	4-A	57[A]	LEU
1	4-A	57[B]	LEU
1	4-A	64	ASN
1	4-A	77	THR
1	4-A	90	HIS
1	4-A	96[A]	ASN
1	4-A	96[B]	ASN
1	4-B	3	ASN
1	4-B	46[A]	LYS
1	4-B	46[B]	LYS
1	4-B	49[A]	ARG
1	4-B	49[B]	ARG
1	4-B	62	GLN
1	4-B	76	VAL
1	4-B	77[A]	THR
1	4-B	77[B]	THR
1	4-B	81	LEU
1	4-B	97	GLN
1	4-B	118	ARG
1	4-B	119	LEU
1	5-A	23	ARG
1	5-A	24	LEU
1	5-A	46	LYS
1	5-A	57[A]	LEU
1	5-A	57[B]	LEU
1	5-A	64	ASN
1	5-A	77	THR
1	5-A	90	HIS
1	5-A	96[A]	ASN
1	5-A	96[B]	ASN
1	5-B	3	ASN
1	5-B	46[A]	LYS
1	5-B	46[B]	LYS
1	5-B	49[A]	ARG
1	5-B	49[B]	ARG
1	5-B	62	GLN
1	5-B	76	VAL
1	5-B	77[A]	THR
1	5-B	77[B]	THR
1	5-B	81	LEU
1	5-B	97	GLN

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Mol	Chain	Res	Type
1	5-B	118	ARG
1	5-B	119	LEU
1	6-A	23	ARG
1	6-A	24	LEU
1	6-A	46	LYS
1	6-A	57[A]	LEU
1	6-A	57[B]	LEU
1	6-A	64	ASN
1	6-A	77	THR
1	6-A	90	HIS
1	6-A	96[A]	ASN
1	6-A	96[B]	ASN
1	6-B	3	ASN
1	6-B	46[A]	LYS
1	6-B	46[B]	LYS
1	6-B	49[A]	ARG
1	6-B	49[B]	ARG
1	6-B	62	GLN
1	6-B	76	VAL
1	6-B	77[A]	THR
1	6-B	77[B]	THR
1	6-B	81	LEU
1	6-B	97	GLN
1	6-B	118	ARG
1	6-B	119	LEU
1	7-A	23	ARG
1	7-A	24	LEU
1	7-A	46	LYS
1	7-A	57[A]	LEU
1	7-A	57[B]	LEU
1	7-A	64	ASN
1	7-A	77	THR
1	7-A	90	HIS
1	7-A	96[A]	ASN
1	7-A	96[B]	ASN
1	7-B	3	ASN
1	7-B	46[A]	LYS
1	7-B	46[B]	LYS
1	7-B	49[A]	ARG
1	7-B	49[B]	ARG
1	7-B	62	GLN
1	7-B	76	VAL

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Mol	Chain	Res	Type
1	7-B	77[A]	THR
1	7-B	77[B]	THR
1	7-B	81	LEU
1	7-B	97	GLN
1	7-B	118	ARG
1	7-B	119	LEU
1	8-A	23	ARG
1	8-A	24	LEU
1	8-A	46	LYS
1	8-A	57[A]	LEU
1	8-A	57[B]	LEU
1	8-A	64	ASN
1	8-A	77	THR
1	8-A	90	HIS
1	8-A	96[A]	ASN
1	8-A	96[B]	ASN
1	8-B	3	ASN
1	8-B	46[A]	LYS
1	8-B	46[B]	LYS
1	8-B	49[A]	ARG
1	8-B	49[B]	ARG
1	8-B	62	GLN
1	8-B	76	VAL
1	8-B	77[A]	THR
1	8-B	77[B]	THR
1	8-B	81	LEU
1	8-B	97	GLN
1	8-B	118	ARG
1	8-B	119	LEU
1	9-A	23	ARG
1	9-A	24	LEU
1	9-A	46	LYS
1	9-A	57[A]	LEU
1	9-A	57[B]	LEU
1	9-A	64	ASN
1	9-A	77	THR
1	9-A	90	HIS
1	9-A	96[A]	ASN
1	9-A	96[B]	ASN
1	9-B	3	ASN
1	9-B	46[A]	LYS
1	9-B	46[B]	LYS

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Mol	Chain	Res	Type
1	9-B	49[A]	ARG
1	9-B	49[B]	ARG
1	9-B	62	GLN
1	9-B	76	VAL
1	9-B	77[A]	THR
1	9-B	77[B]	THR
1	9-B	81	LEU
1	9-B	97	GLN
1	9-B	118	ARG
1	9-B	119	LEU
1	10-A	23	ARG
1	10-A	24	LEU
1	10-A	46	LYS
1	10-A	57[A]	LEU
1	10-A	57[B]	LEU
1	10-A	64	ASN
1	10-A	77	THR
1	10-A	90	HIS
1	10-A	96[A]	ASN
1	10-A	96[B]	ASN
1	10-B	3	ASN
1	10-B	46[A]	LYS
1	10-B	46[B]	LYS
1	10-B	49[A]	ARG
1	10-B	49[B]	ARG
1	10-B	62	GLN
1	10-B	76	VAL
1	10-B	77[A]	THR
1	10-B	77[B]	THR
1	10-B	81	LEU
1	10-B	97	GLN
1	10-B	118	ARG
1	10-B	119	LEU
1	11-A	23	ARG
1	11-A	24	LEU
1	11-A	46	LYS
1	11-A	57[A]	LEU
1	11-A	57[B]	LEU
1	11-A	64	ASN
1	11-A	77	THR
1	11-A	90	HIS
1	11-A	96[A]	ASN

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Mol	Chain	Res	Type
1	11-A	96[B]	ASN
1	11-B	3	ASN
1	11-B	46[A]	LYS
1	11-B	46[B]	LYS
1	11-B	49[A]	ARG
1	11-B	49[B]	ARG
1	11-B	62	GLN
1	11-B	76	VAL
1	11-B	77[A]	THR
1	11-B	77[B]	THR
1	11-B	81	LEU
1	11-B	97	GLN
1	11-B	118	ARG
1	11-B	119	LEU
1	12-A	23	ARG
1	12-A	24	LEU
1	12-A	46	LYS
1	12-A	57[A]	LEU
1	12-A	57[B]	LEU
1	12-A	64	ASN
1	12-A	77	THR
1	12-A	90	HIS
1	12-A	96[A]	ASN
1	12-A	96[B]	ASN
1	12-B	3	ASN
1	12-B	46[A]	LYS
1	12-B	46[B]	LYS
1	12-B	49[A]	ARG
1	12-B	49[B]	ARG
1	12-B	62	GLN
1	12-B	76	VAL
1	12-B	77[A]	THR
1	12-B	77[B]	THR
1	12-B	81	LEU
1	12-B	97	GLN
1	12-B	118	ARG
1	12-B	119	LEU
1	13-A	23	ARG
1	13-A	24	LEU
1	13-A	46	LYS
1	13-A	57[A]	LEU
1	13-A	57[B]	LEU

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Mol	Chain	Res	Type
1	13-A	64	ASN
1	13-A	77	THR
1	13-A	90	HIS
1	13-A	96[A]	ASN
1	13-A	96[B]	ASN
1	13-B	3	ASN
1	13-B	46[A]	LYS
1	13-B	46[B]	LYS
1	13-B	49[A]	ARG
1	13-B	49[B]	ARG
1	13-B	62	GLN
1	13-B	76	VAL
1	13-B	77[A]	THR
1	13-B	77[B]	THR
1	13-B	81	LEU
1	13-B	97	GLN
1	13-B	118	ARG
1	13-B	119	LEU
1	14-A	23	ARG
1	14-A	24	LEU
1	14-A	46	LYS
1	14-A	57[A]	LEU
1	14-A	57[B]	LEU
1	14-A	64	ASN
1	14-A	77	THR
1	14-A	90	HIS
1	14-A	96[A]	ASN
1	14-A	96[B]	ASN
1	14-B	3	ASN
1	14-B	46[A]	LYS
1	14-B	46[B]	LYS
1	14-B	49[A]	ARG
1	14-B	49[B]	ARG
1	14-B	62	GLN
1	14-B	76	VAL
1	14-B	77[A]	THR
1	14-B	77[B]	THR
1	14-B	81	LEU
1	14-B	97	GLN
1	14-B	118	ARG
1	14-B	119	LEU
1	15-A	23	ARG

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Mol	Chain	Res	Type
1	15-A	24	LEU
1	15-A	46	LYS
1	15-A	57[A]	LEU
1	15-A	57[B]	LEU
1	15-A	64	ASN
1	15-A	77	THR
1	15-A	90	HIS
1	15-A	96[A]	ASN
1	15-A	96[B]	ASN
1	15-B	3	ASN
1	15-B	46[A]	LYS
1	15-B	46[B]	LYS
1	15-B	49[A]	ARG
1	15-B	49[B]	ARG
1	15-B	62	GLN
1	15-B	76	VAL
1	15-B	77[A]	THR
1	15-B	77[B]	THR
1	15-B	81	LEU
1	15-B	97	GLN
1	15-B	118	ARG
1	15-B	119	LEU
1	16-A	23	ARG
1	16-A	24	LEU
1	16-A	46	LYS
1	16-A	57[A]	LEU
1	16-A	57[B]	LEU
1	16-A	64	ASN
1	16-A	77	THR
1	16-A	90	HIS
1	16-A	96[A]	ASN
1	16-A	96[B]	ASN
1	16-B	3	ASN
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	62	GLN
1	16-B	76	VAL
1	16-B	77[A]	THR
1	16-B	77[B]	THR
1	16-B	81	LEU

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Mol	Chain	Res	Type
1	16-B	97	GLN
1	16-B	118	ARG
1	16-B	119	LEU
1	17-A	23	ARG
1	17-A	24	LEU
1	17-A	46	LYS
1	17-A	57[A]	LEU
1	17-A	57[B]	LEU
1	17-A	64	ASN
1	17-A	77	THR
1	17-A	90	HIS
1	17-A	96[A]	ASN
1	17-A	96[B]	ASN
1	17-B	3	ASN
1	17-B	46[A]	LYS
1	17-B	46[B]	LYS
1	17-B	49[A]	ARG
1	17-B	49[B]	ARG
1	17-B	62	GLN
1	17-B	76	VAL
1	17-B	77[A]	THR
1	17-B	77[B]	THR
1	17-B	81	LEU
1	17-B	97	GLN
1	17-B	118	ARG
1	17-B	119	LEU
1	18-A	23	ARG
1	18-A	24	LEU
1	18-A	46	LYS
1	18-A	57[A]	LEU
1	18-A	57[B]	LEU
1	18-A	64	ASN
1	18-A	77	THR
1	18-A	90	HIS
1	18-A	96[A]	ASN
1	18-A	96[B]	ASN
1	18-B	3	ASN
1	18-B	46[A]	LYS
1	18-B	46[B]	LYS
1	18-B	49[A]	ARG
1	18-B	49[B]	ARG
1	18-B	62	GLN

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Mol	Chain	Res	Type
1	18-B	76	VAL
1	18-B	77[A]	THR
1	18-B	77[B]	THR
1	18-B	81	LEU
1	18-B	97	GLN
1	18-B	118	ARG
1	18-B	119	LEU
1	19-A	23	ARG
1	19-A	24	LEU
1	19-A	46	LYS
1	19-A	57[A]	LEU
1	19-A	57[B]	LEU
1	19-A	64	ASN
1	19-A	77	THR
1	19-A	90	HIS
1	19-A	96[A]	ASN
1	19-A	96[B]	ASN
1	19-B	3	ASN
1	19-B	46[A]	LYS
1	19-B	46[B]	LYS
1	19-B	49[A]	ARG
1	19-B	49[B]	ARG
1	19-B	62	GLN
1	19-B	76	VAL
1	19-B	77[A]	THR
1	19-B	77[B]	THR
1	19-B	81	LEU
1	19-B	97	GLN
1	19-B	118	ARG
1	19-B	119	LEU
1	20-A	23	ARG
1	20-A	24	LEU
1	20-A	46	LYS
1	20-A	57[A]	LEU
1	20-A	57[B]	LEU
1	20-A	64	ASN
1	20-A	77	THR
1	20-A	90	HIS
1	20-A	96[A]	ASN
1	20-A	96[B]	ASN
1	20-B	3	ASN
1	20-B	46[A]	LYS

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Mol	Chain	Res	Type
1	20-B	46[B]	LYS
1	20-B	49[A]	ARG
1	20-B	49[B]	ARG
1	20-B	62	GLN
1	20-B	76	VAL
1	20-B	77[A]	THR
1	20-B	77[B]	THR
1	20-B	81	LEU
1	20-B	97	GLN
1	20-B	118	ARG
1	20-B	119	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	95	ASN
1	1-A	114	ASN
1	1-B	3	ASN
1	1-B	31	ASN
1	1-B	64	ASN
1	1-B	97	GLN
1	2-A	50	HIS
1	2-A	91	HIS
1	2-A	95	ASN
1	2-B	3	ASN
1	2-B	31	ASN
1	2-B	62	GLN
1	2-B	64	ASN
1	3-A	3	ASN
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-A	95	ASN
1	4-A	114	ASN
1	4-B	31	ASN
1	4-B	64	ASN
1	4-B	97	GLN
1	5-A	62	GLN
1	5-A	114	ASN

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Mol	Chain	Res	Type
1	5-A	121	GLN
1	5-B	3	ASN
1	5-B	31	ASN
1	5-B	96	ASN
1	5-B	97	GLN
1	6-A	50	HIS
1	6-A	62	GLN
1	6-A	91	HIS
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	53	ASN
1	7-A	62	GLN
1	7-A	64	ASN
1	7-A	91	HIS
1	7-B	64	ASN
1	7-B	96	ASN
1	7-B	114	ASN
1	8-A	31	ASN
1	8-A	64	ASN
1	8-A	95	ASN
1	8-B	31	ASN
1	8-B	62	GLN
1	8-B	64	ASN
1	8-B	114	ASN
1	9-A	53	ASN
1	9-A	62	GLN
1	9-A	64	ASN
1	9-A	95	ASN
1	9-B	3	ASN
1	9-B	64	ASN
1	9-B	96	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	62	GLN
1	10-B	64	ASN

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Mol	Chain	Res	Type
1	11-A	3	ASN
1	11-A	91	HIS
1	11-A	114	ASN
1	11-B	96	ASN
1	11-B	114	ASN
1	12-A	50	HIS
1	12-A	53	ASN
1	12-A	95	ASN
1	12-B	3	ASN
1	12-B	64	ASN
1	12-B	96	ASN
1	12-B	121	GLN
1	13-A	50	HIS
1	13-A	62	GLN
1	13-A	64	ASN
1	13-A	91	HIS
1	13-B	3	ASN
1	13-B	114	ASN
1	14-A	90	HIS
1	14-B	3	ASN
1	15-A	91	HIS
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	16-B	96	ASN
1	17-A	31	ASN
1	17-A	52	HIS
1	17-A	62	GLN
1	17-A	91	HIS
1	17-B	62	GLN
1	18-A	31	ASN
1	18-A	52	HIS
1	18-A	53	ASN
1	18-A	62	GLN
1	18-A	95	ASN
1	18-B	96	ASN
1	19-A	31	ASN
1	19-A	53	ASN
1	19-A	62	GLN

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Mol	Chain	Res	Type
1	19-A	91	HIS
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	62	GLN
1	20-B	95	ASN
1	20-B	114	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	118/128 (92%)	3.05	83 (70%) 0 0	0, 1, 1, 2	118 (100%)
1	1-B	117/128 (91%)	2.82	68 (58%) 0 0	0, 1, 1, 2	117 (100%)
1	2-A	0/128	-	-	-	-
1	2-B	0/128	-	-	-	-
1	3-A	0/128	-	-	-	-
1	3-B	0/128	-	-	-	-
1	4-A	0/128	-	-	-	-
1	4-B	0/128	-	-	-	-
1	5-A	0/128	-	-	-	-
1	5-B	0/128	-	-	-	-
1	6-A	0/128	-	-	-	-
1	6-B	0/128	-	-	-	-
1	7-A	0/128	-	-	-	-
1	7-B	0/128	-	-	-	-
1	8-A	0/128	-	-	-	-
1	8-B	0/128	-	-	-	-
1	9-A	0/128	-	-	-	-
1	9-B	0/128	-	-	-	-
1	10-A	0/128	-	-	-	-
1	10-B	0/128	-	-	-	-
1	11-A	0/128	-	-	-	-
1	11-B	0/128	-	-	-	-
1	12-A	0/128	-	-	-	-
1	12-B	0/128	-	-	-	-
1	13-A	0/128	-	-	-	-
1	13-B	0/128	-	-	-	-
1	14-A	0/128	-	-	-	-
1	14-B	0/128	-	-	-	-
1	15-A	0/128	-	-	-	-
1	15-B	0/128	-	-	-	-
1	16-A	0/128	-	-	-	-
1	16-B	0/128	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	17-A	0/128	-	-	-	-
1	17-B	0/128	-	-	-	-
1	18-A	0/128	-	-	-	-
1	18-B	0/128	-	-	-	-
1	19-A	0/128	-	-	-	-
1	19-B	0/128	-	-	-	-
1	20-A	0/128	-	-	-	-
1	20-B	0/128	-	-	-	-
All	All	235/5120 (4%)	2.93	151 (64%) 0 0	0, 1, 1, 2	235 (100%)

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	48[A]	PHE	11.9
1	1-B	87	ASP	8.3
1	1-A	49	ARG	8.2
1	1-A	48	PHE	7.8
1	1-B	53[A]	ASN	7.7
1	1-A	90	HIS	7.6
1	1-B	49[A]	ARG	7.5
1	1-A	96[A]	ASN	7.5
1	1-A	71	ASP	7.5
1	1-A	122	ASP	7.5
1	1-A	4[A]	ILE	7.4
1	1-A	64	ASN	7.2
1	1-A	72[A]	GLU	6.8
1	1-B	74	PHE	6.8
1	1-B	96	ASN	6.7
1	1-A	65	ALA	6.3
1	1-B	121	GLN	6.2
1	1-B	17[A]	TYR	6.1
1	1-B	119	LEU	6.1
1	1-A	89	GLU	6.0
1	1-B	97	GLN	6.0
1	1-B	3	ASN	5.9
1	1-A	86	LEU	5.9
1	1-A	3	ASN	5.7
1	1-A	69[A]	ILE	5.7
1	1-B	118	ARG	5.6
1	1-B	84	ILE	5.5
1	1-B	70[A]	ASN	5.4
1	1-B	120	GLU	5.3

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Mol	Chain	Res	Type	RSRZ
1	1-A	17	TYR	5.2
1	1-A	108	ASP	5.0
1	1-B	67	ILE	5.0
1	1-B	50[A]	HIS	4.9
1	1-A	77	THR	4.9
1	1-A	57[A]	LEU	4.7
1	1-A	119	LEU	4.7
1	1-B	71[A]	ASP	4.7
1	1-A	83[A]	ILE	4.7
1	1-B	54[A]	GLU	4.6
1	1-B	98	GLU	4.6
1	1-A	53	ASN	4.5
1	1-A	120	GLU	4.4
1	1-B	77[A]	THR	4.3
1	1-A	74	PHE	4.3
1	1-B	4[A]	ILE	4.2
1	1-A	28	GLU	4.1
1	1-A	50	HIS	4.0
1	1-B	88	SER	4.0
1	1-A	12	SER	4.0
1	1-A	51	SER	4.0
1	1-A	75	PRO	4.0
1	1-A	24	LEU	4.0
1	1-B	72[A]	GLU	3.9
1	1-B	52[A]	HIS	3.9
1	1-A	115	PHE	3.9
1	1-B	51[A]	SER	3.9
1	1-A	55	TYR	3.8
1	1-A	121	GLN	3.8
1	1-A	110	GLU	3.7
1	1-A	66	ILE	3.6
1	1-A	84[A]	ILE	3.6
1	1-B	116	LEU	3.5
1	1-A	109	LYS	3.5
1	1-B	81	LEU	3.5
1	1-A	88	SER	3.4
1	1-A	112[A]	THR	3.3
1	1-A	106[A]	TRP	3.3
1	1-A	44	GLU	3.3
1	1-B	62	GLN	3.3
1	1-A	23	ARG	3.3
1	1-A	118	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	1-A	14	VAL	3.3
1	1-B	7	LYS	3.3
1	1-B	78[A]	LYS	3.2
1	1-B	22	SER	3.2
1	1-A	27	TRP	3.2
1	1-B	106[A]	TRP	3.2
1	1-A	19	LEU	3.2
1	1-B	90[A]	HIS	3.1
1	1-B	86	LEU	3.1
1	1-B	41	VAL	3.1
1	1-A	87	ASP	3.1
1	1-A	54	GLU	3.0
1	1-B	30	LEU	3.0
1	1-B	91[A]	HIS	3.0
1	1-B	108	ASP	3.0
1	1-B	83[A]	ILE	3.0
1	1-B	75	PRO	2.9
1	1-B	66	ILE	2.9
1	1-B	46[A]	LYS	2.9
1	1-A	52	HIS	2.9
1	1-A	107	TRP	2.8
1	1-A	116	LEU	2.8
1	1-B	115	PHE	2.8
1	1-B	64	ASN	2.7
1	1-B	14	VAL	2.7
1	1-A	34	PHE	2.7
1	1-A	82[A]	ILE	2.7
1	1-A	91	HIS	2.6
1	1-B	29	GLY	2.6
1	1-A	5[A]	ILE	2.6
1	1-B	107	TRP	2.6
1	1-A	36	GLY	2.6
1	1-A	70[A]	ASN	2.6
1	1-A	78	LYS	2.5
1	1-A	68	ARG	2.5
1	1-A	63	GLY	2.5
1	1-A	46	LYS	2.5
1	1-A	10	TRP	2.5
1	1-A	117	THR	2.5
1	1-A	40	ILE	2.5
1	1-A	73[A]	ASP	2.5
1	1-B	18[A]	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	1-A	41	VAL	2.5
1	1-B	57	LEU	2.4
1	1-B	31	ASN	2.4
1	1-B	32	THR	2.4
1	1-B	12	SER	2.3
1	1-B	76	VAL	2.3
1	1-A	114	ASN	2.3
1	1-B	26	PRO	2.3
1	1-B	109	LYS	2.3
1	1-B	10	TRP	2.3
1	1-A	81[A]	LEU	2.3
1	1-A	105[A]	ILE	2.3
1	1-A	85	PRO	2.3
1	1-A	37	ALA	2.2
1	1-B	105[A]	ILE	2.2
1	1-A	111	SER	2.2
1	1-A	45	THR	2.2
1	1-B	117	THR	2.2
1	1-A	25	LEU	2.2
1	1-B	113[A]	LEU	2.2
1	1-B	114	ASN	2.2
1	1-A	9	ASP	2.2
1	1-A	35	GLY	2.2
1	1-B	110	GLU	2.2
1	1-B	38	TRP	2.1
1	1-A	98	GLU	2.1
1	1-A	39	CYS	2.1
1	1-A	104	THR	2.1
1	1-A	22	SER	2.1
1	1-A	47	SER	2.1
1	1-A	95	ASN	2.1
1	1-B	5[A]	ILE	2.1
1	1-B	55[A]	TYR	2.1
1	1-B	19[A]	LEU	2.1
1	1-B	89[A]	GLU	2.1
1	1-A	26	PRO	2.1
1	1-B	23	ARG	2.0
1	1-A	100	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
2	NI	1-B	201	1/1	0.97	0.16	16,16,16,16	1
2	NI	2-A	201	1/1	-	-	16,16,16,16	1
2	NI	3-A	201	1/1	-	-	16,16,16,16	1
2	NI	4-A	201	1/1	-	-	16,16,16,16	1
2	NI	5-A	201	1/1	-	-	16,16,16,16	1
2	NI	6-A	201	1/1	-	-	16,16,16,16	1
2	NI	7-A	201	1/1	-	-	16,16,16,16	1
2	NI	8-A	201	1/1	-	-	16,16,16,16	1
2	NI	9-A	201	1/1	-	-	16,16,16,16	1
2	NI	10-A	201	1/1	-	-	16,16,16,16	1
2	NI	11-A	201	1/1	-	-	16,16,16,16	1
2	NI	12-A	201	1/1	-	-	16,16,16,16	1
2	NI	13-A	201	1/1	-	-	16,16,16,16	1
2	NI	14-A	201	1/1	-	-	16,16,16,16	1
2	NI	15-A	201	1/1	-	-	16,16,16,16	1
2	NI	16-A	201	1/1	-	-	16,16,16,16	1
2	NI	17-A	201	1/1	-	-	16,16,16,16	1
2	NI	18-A	201	1/1	-	-	16,16,16,16	1
2	NI	19-A	201	1/1	-	-	16,16,16,16	1
2	NI	20-A	201	1/1	-	-	16,16,16,16	1
3	NA	1-A	202	1/1	0.97	0.36	9,9,9,9	1
2	NI	2-B	201	1/1	-	-	16,16,16,16	1
2	NI	3-B	201	1/1	-	-	16,16,16,16	1
2	NI	4-B	201	1/1	-	-	16,16,16,16	1
2	NI	5-B	201	1/1	-	-	16,16,16,16	1
2	NI	6-B	201	1/1	-	-	16,16,16,16	1
2	NI	7-B	201	1/1	-	-	16,16,16,16	1
2	NI	8-B	201	1/1	-	-	16,16,16,16	1
2	NI	9-B	201	1/1	-	-	16,16,16,16	1
2	NI	10-B	201	1/1	-	-	16,16,16,16	1
2	NI	11-B	201	1/1	-	-	16,16,16,16	1
2	NI	12-B	201	1/1	-	-	16,16,16,16	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NI	13-B	201	1/1	-	-	16,16,16,16	1
2	NI	14-B	201	1/1	-	-	16,16,16,16	1
2	NI	15-B	201	1/1	-	-	16,16,16,16	1
2	NI	16-B	201	1/1	-	-	16,16,16,16	1
2	NI	17-B	201	1/1	-	-	16,16,16,16	1
2	NI	18-B	201	1/1	-	-	16,16,16,16	1
2	NI	19-B	201	1/1	-	-	16,16,16,16	1
2	NI	20-B	201	1/1	-	-	16,16,16,16	1
2	NI	1-A	201	1/1	0.98	0.10	16,16,16,16	1
3	NA	2-A	202	1/1	-	-	9,9,9,9	1
3	NA	3-A	202	1/1	-	-	9,9,9,9	1
3	NA	4-A	202	1/1	-	-	9,9,9,9	1
3	NA	5-A	202	1/1	-	-	9,9,9,9	1
3	NA	6-A	202	1/1	-	-	9,9,9,9	1
3	NA	7-A	202	1/1	-	-	9,9,9,9	1
3	NA	8-A	202	1/1	-	-	9,9,9,9	1
3	NA	9-A	202	1/1	-	-	9,9,9,9	1
3	NA	10-A	202	1/1	-	-	9,9,9,9	1
3	NA	11-A	202	1/1	-	-	9,9,9,9	1
3	NA	12-A	202	1/1	-	-	9,9,9,9	1
3	NA	13-A	202	1/1	-	-	9,9,9,9	1
3	NA	14-A	202	1/1	-	-	9,9,9,9	1
3	NA	15-A	202	1/1	-	-	9,9,9,9	1
3	NA	16-A	202	1/1	-	-	9,9,9,9	1
3	NA	17-A	202	1/1	-	-	9,9,9,9	1
3	NA	18-A	202	1/1	-	-	9,9,9,9	1
3	NA	19-A	202	1/1	-	-	9,9,9,9	1
3	NA	20-A	202	1/1	-	-	9,9,9,9	1

6.5 Other polymers [i](#)

There are no such residues in this entry.