



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 2, 2024 – 07:32 PM EST

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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

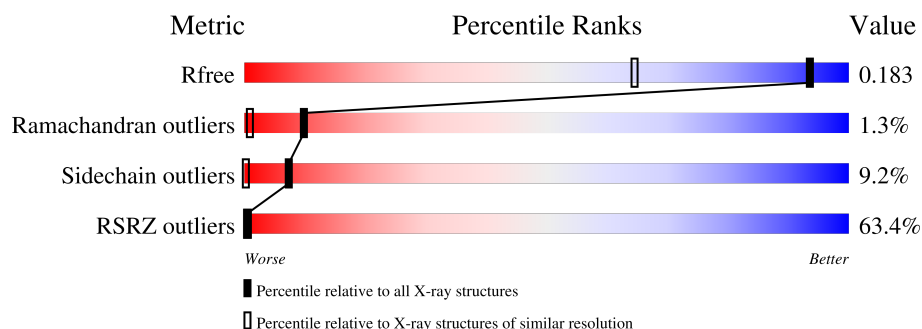
1 Overall quality at a glance ⓘ

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.














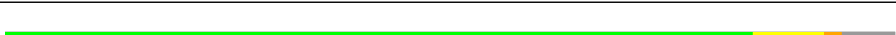

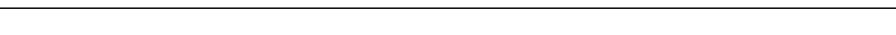
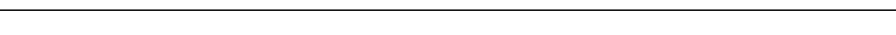
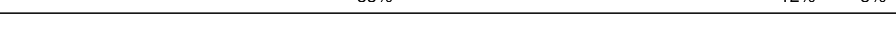

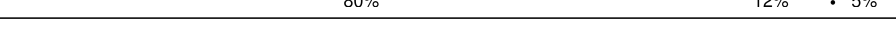







Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1904 (1.36-1.32)
Ramachandran outliers	177936	2016 (1.36-1.32)
Sidechain outliers	177891	2016 (1.36-1.32)
RSRZ outliers	164620	1903 (1.36-1.32)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1-A	128	<div> <div>63%</div> <div>85%</div> <div>9%</div> <div>5%</div> </div>
1	1-B	128	<div> <div>53%</div> <div>84%</div> <div>9%</div> <div>6%</div> </div>
1	10-A	128	<div> <div>79%</div> <div>14%</div> <div>5%</div> </div>
1	10-B	128	<div> <div>82%</div> <div>9%</div> <div>6%</div> </div>
1	11-A	128	<div> <div>78%</div> <div>13%</div> <div>5%</div> </div>
1	11-B	128	<div> <div>84%</div> <div>9%</div> <div>6%</div> </div>










Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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			

Continued on next page...

Continued from previous page...

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 (three-letter code: 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		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 (three-letter code: 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

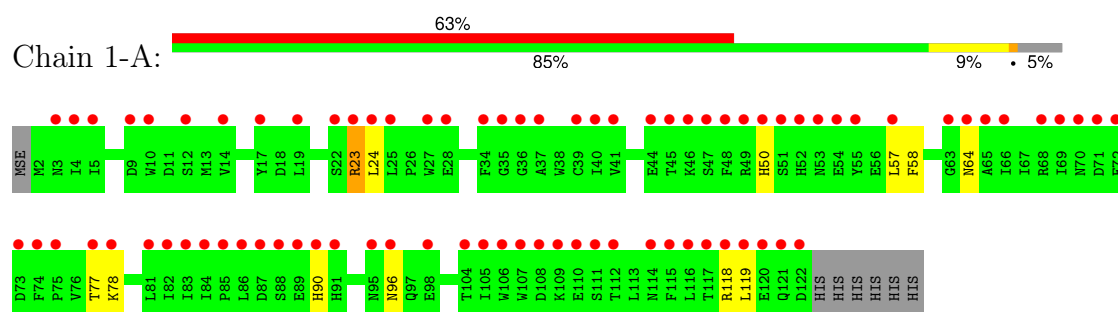
Continued from previous page...

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

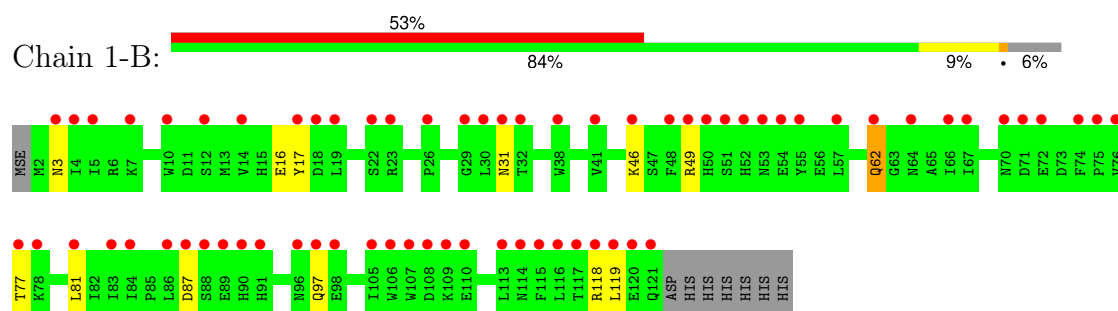
3 Residue-property plots [i](#)

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. 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. 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.

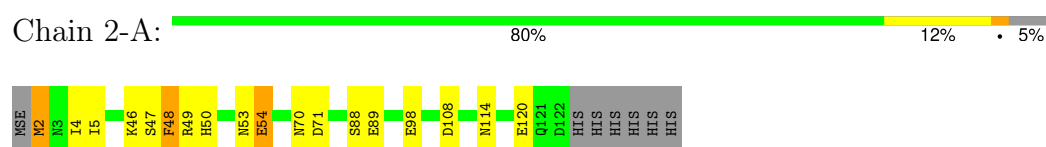
- Molecule 1: plu4264 protein



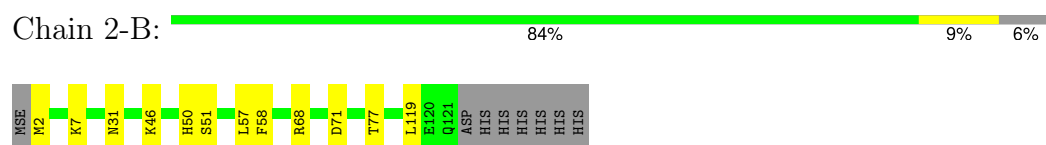
- Molecule 1: plu4264 protein



- Molecule 1: plu4264 protein



- Molecule 1: plu4264 protein

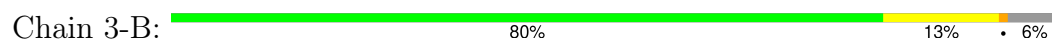


- Molecule 1: plu4264 protein

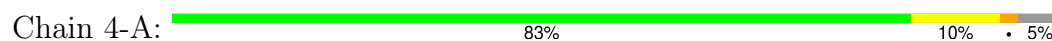




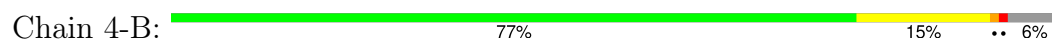
- Molecule 1: plu4264 protein



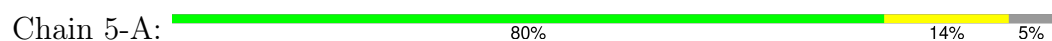
- Molecule 1: plu4264 protein



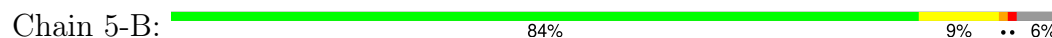
- Molecule 1: plu4264 protein



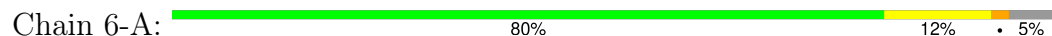
- Molecule 1: plu4264 protein



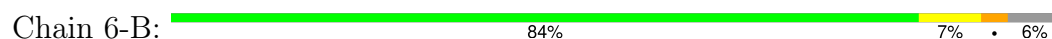
- Molecule 1: plu4264 protein



- Molecule 1: plu4264 protein



- Molecule 1: plu4264 protein

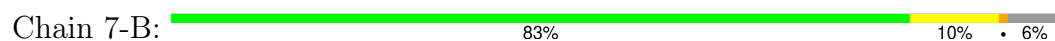




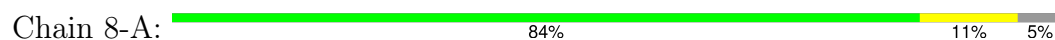
- Molecule 1: plu4264 protein



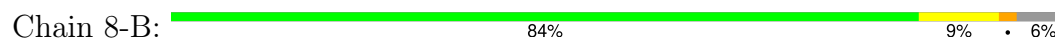
- Molecule 1: plu4264 protein



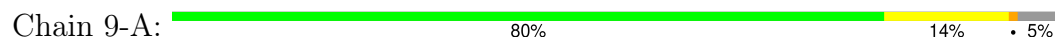
- Molecule 1: plu4264 protein



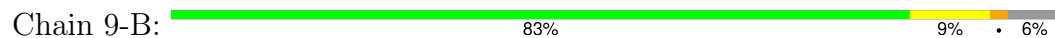
- Molecule 1: plu4264 protein



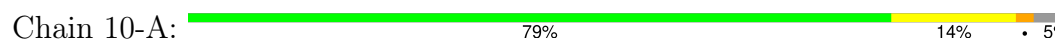
- Molecule 1: plu4264 protein



- Molecule 1: plu4264 protein



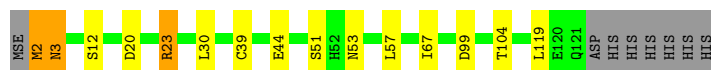
- Molecule 1: plu4264 protein





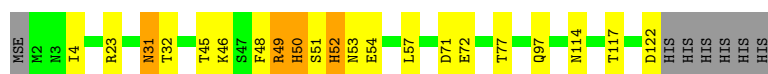
- Molecule 1: plu4264 protein

Chain 10-B: 82% 9% • 6%



- Molecule 1: plu4264 protein

Chain 11-A: 78% 13% • 5%



- Molecule 1: plu4264 protein

Chain 11-B: 84% 9% • 6%



- Molecule 1: plu4264 protein

Chain 12-A: 88% 6% • 5%



- Molecule 1: plu4264 protein

Chain 12-B: 84% 8% • 6%



- Molecule 1: plu4264 protein

Chain 13-A: 84% 11% • 5%



- Molecule 1: plu4264 protein

Chain 13-B: 88% 5% • 6%



- Molecule 1: plu4264 protein

Chain 14-A: 77% 11% 5% 5%



- Molecule 1: plu4264 protein

Chain 14-B: 81% 11% 6%



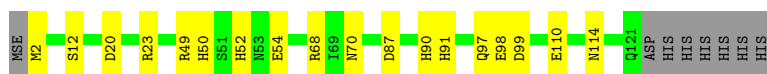
- Molecule 1: plu4264 protein

Chain 15-A: 80% 13% 5%



- Molecule 1: plu4264 protein

Chain 15-B: 80% 14% 6%



- Molecule 1: plu4264 protein

Chain 16-A: 88% 7% 5%



- Molecule 1: plu4264 protein

Chain 16-B: 80% 12% 6%




- Molecule 1: plu4264 protein

Chain 17-A: 80% 12% 5%



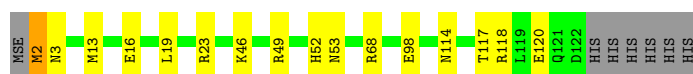
- Molecule 1: plu4264 protein

Chain 17-B:  84% 8% 6%




- Molecule 1: plu4264 protein

Chain 18-A:  82% 12% 5%




- Molecule 1: plu4264 protein

Chain 18-B:  84% 8% 6%




- Molecule 1: plu4264 protein

Chain 19-A:  83% 12% 5%




- Molecule 1: plu4264 protein

Chain 19-B:  78% 14% 6%




- Molecule 1: plu4264 protein

Chain 20-A:  78% 16% 5%



- Molecule 1: plu4264 protein

Chain 20-B:  80% 12% 6%

MSE	M2	R6	K7	S12	Y17	D20	K46	H50	S51	H52	L57	E72	L81	E98	D99	R118	L119	E120	Q121	ASP	HIS	HIS	HIS	HIS	HIS	HIS
-----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	-----	-----	-----	-----	-----	-----	-----

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)	Xtriage
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	Xtriage
Anisotropy	0.734	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.02 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

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 2.1574e-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: NA, NI

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

The worst 5 of 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

The worst 5 of 218 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-B	16[B]	GLU	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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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%)	19	4
1	1-B	151/128 (118%)	143 (95%)	6 (4%)	2 (1%)	10	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%)	10	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%)	19	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%)	10	1
1	6-A	141/128 (110%)	133 (94%)	7 (5%)	1 (1%)	19	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%)	10	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%)	19	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	19	4
1	13-B	151/128 (118%)	142 (94%)	8 (5%)	1 (1%)	19	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%)	10	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%)	19	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%)	19	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%)	10	1

5 of 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

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%)	11	0
1	1-B	145/116 (125%)	131 (90%)	14 (10%)	6	0
1	2-A	135/116 (116%)	121 (90%)	14 (10%)	5	0
1	2-B	145/116 (125%)	133 (92%)	12 (8%)	9	0
1	3-A	135/116 (116%)	121 (90%)	14 (10%)	5	0
1	3-B	145/116 (125%)	133 (92%)	12 (8%)	9	0
1	4-A	135/116 (116%)	121 (90%)	14 (10%)	5	0
1	4-B	145/116 (125%)	118 (81%)	27 (19%)	1	0
1	5-A	135/116 (116%)	127 (94%)	8 (6%)	16	1
1	5-B	145/116 (125%)	134 (92%)	11 (8%)	11	0
1	6-A	135/116 (116%)	120 (89%)	15 (11%)	5	0
1	6-B	145/116 (125%)	134 (92%)	11 (8%)	11	0
1	7-A	135/116 (116%)	124 (92%)	11 (8%)	9	0
1	7-B	145/116 (125%)	134 (92%)	11 (8%)	11	0
1	8-A	135/116 (116%)	120 (89%)	15 (11%)	5	0
1	8-B	145/116 (125%)	127 (88%)	18 (12%)	4	0
1	9-A	135/116 (116%)	123 (91%)	12 (9%)	8	0
1	9-B	145/116 (125%)	133 (92%)	12 (8%)	9	0
1	10-A	135/116 (116%)	122 (90%)	13 (10%)	7	0
1	10-B	145/116 (125%)	137 (94%)	8 (6%)	18	1
1	11-A	135/116 (116%)	116 (86%)	19 (14%)	3	0
1	11-B	145/116 (125%)	133 (92%)	12 (8%)	9	0
1	12-A	135/116 (116%)	131 (97%)	4 (3%)	36	6
1	12-B	145/116 (125%)	133 (92%)	12 (8%)	9	0
1	13-A	135/116 (116%)	124 (92%)	11 (8%)	9	0
1	13-B	145/116 (125%)	136 (94%)	9 (6%)	15	1
1	14-A	135/116 (116%)	122 (90%)	13 (10%)	7	0
1	14-B	145/116 (125%)	131 (90%)	14 (10%)	6	0
1	15-A	135/116 (116%)	122 (90%)	13 (10%)	7	0
1	15-B	145/116 (125%)	125 (86%)	20 (14%)	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	16-A	135/116 (116%)	128 (95%)	7 (5%)	19	2
1	16-B	145/116 (125%)	126 (87%)	19 (13%)	3	0
1	17-A	135/116 (116%)	121 (90%)	14 (10%)	5	0
1	17-B	145/116 (125%)	130 (90%)	15 (10%)	6	0
1	18-A	135/116 (116%)	123 (91%)	12 (9%)	8	0
1	18-B	145/116 (125%)	135 (93%)	10 (7%)	13	0
1	19-A	135/116 (116%)	122 (90%)	13 (10%)	7	0
1	19-B	145/116 (125%)	125 (86%)	20 (14%)	3	0
1	20-A	134/116 (116%)	121 (90%)	13 (10%)	6	0
1	20-B	145/116 (125%)	132 (91%)	13 (9%)	8	0
All	All	5599/4640 (121%)	5074 (91%)	525 (9%)	7	0

5 of 525 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	18-B	53[B]	ASN
1	19-A	97[A]	GLN
1	18-B	53[A]	ASN
1	20-B	72[A]	GLU
1	8-A	53	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
1	11-B	114	ASN
1	16-A	31	ASN
1	12-B	3	ASN
1	13-A	91	HIS
1	17-A	52	HIS

5.3.3 RNA ⓘ

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 oligosaccharides 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Warning: The R factor obtained from EDS is 0.3184, which does not match the depositor's R factor of 0.1264. Please interpret the results in this section carefully.

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%)	3.02	81 (68%) 0 0	0, 1, 1, 2	118 (100%)
1	1-B	117/128 (91%)	2.79	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	-	-	-	-

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	15-B	0/128	-	-	-	-
1	16-A	0/128	-	-	-	-
1	16-B	0/128	-	-	-	-
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%)	2.91	149 (63%) 0 0	0, 1, 1, 2	235 (100%)

The worst 5 of 149 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	48[A]	PHE	11.7
1	1-B	87	ASP	8.2
1	1-A	49	ARG	8.2
1	1-A	90	HIS	7.9
1	1-A	48	PHE	7.8

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](#)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers [i](#)

There are no such residues in this entry.