



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:54 PM GMT

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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	FAILED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

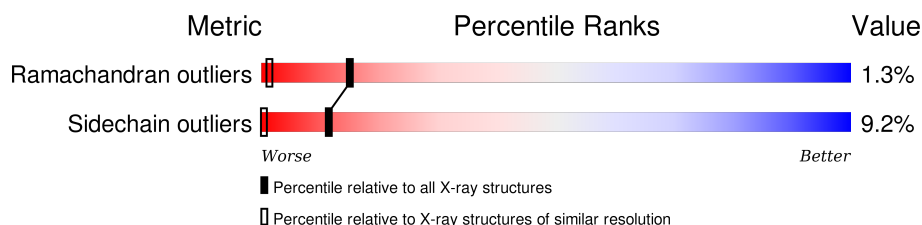
1 Overall quality at a glance

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))
Ramachandran outliers	100387	1749 (1.38-1.30)
Sidechain outliers	100360	1749 (1.38-1.30)


























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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1-A	128	
1	1-B	128	
1	10-A	128	
1	10-B	128	
1	11-A	128	
1	11-B	128	
1	12-A	128	
1	12-B	128	

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Mol	Chain	Length	Quality of chain
1	13-A	128	
1	13-B	128	
1	14-A	128	
1	14-B	128	
1	15-A	128	
1	15-B	128	
1	16-A	128	
1	16-B	128	
1	17-A	128	
1	17-B	128	
1	18-A	128	
1	18-B	128	
1	19-A	128	
1	19-B	128	
1	2-A	128	
1	2-B	128	
1	20-A	128	
1	20-B	128	
1	3-A	128	
1	3-B	128	
1	4-A	128	
1	4-B	128	
1	5-A	128	
1	5-B	128	
1	6-A	128	

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Mol	Chain	Length	Quality of chain
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			

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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 (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	19-B	1	Total	Ni	0	0
			1	1		
2	16-A	1	Total	Ni	0	0
			1	1		
2	20-B	1	Total	Ni	0	0
			1	1		
2	1-B	1	Total	Ni	0	0
			1	1		
2	5-A	1	Total	Ni	0	0
			1	1		
2	13-A	1	Total	Ni	0	0
			1	1		
2	8-A	1	Total	Ni	0	0
			1	1		
2	2-B	1	Total	Ni	0	0
			1	1		

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	17-A	1	Total 1	Na 1	0	0
3	5-A	1	Total 1	Na 1	0	0
3	13-A	1	Total 1	Na 1	0	0
3	8-A	1	Total 1	Na 1	0	0
3	1-A	1	Total 1	Na 1	0	0
3	6-A	1	Total 1	Na 1	0	0
3	14-A	1	Total 1	Na 1	0	0
3	2-A	1	Total 1	Na 1	0	0
3	10-A	1	Total 1	Na 1	0	0
3	9-A	1	Total 1	Na 1	0	0
3	7-A	1	Total 1	Na 1	0	0
3	15-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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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

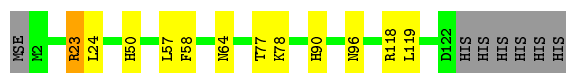
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.


Note EDS failed to run properly.

- Molecule 1: plu4264 protein

Chain 1-A: 




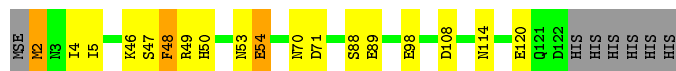
- Molecule 1: plu4264 protein

Chain 1-B: 




- Molecule 1: plu4264 protein

Chain 2-A: 




- Molecule 1: plu4264 protein

Chain 2-B: 




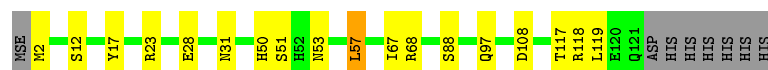
- Molecule 1: plu4264 protein

Chain 3-A: 




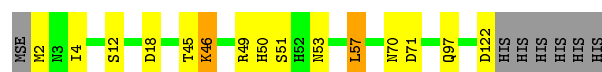
- Molecule 1: plu4264 protein

Chain 3-B:  80% 13% • 6%




- Molecule 1: plu4264 protein

Chain 4-A:  83% 10% • 5%




- Molecule 1: plu4264 protein

Chain 4-B:  77% 15% •• 6%




- Molecule 1: plu4264 protein

Chain 5-A:  80% 14% 5%




- Molecule 1: plu4264 protein

Chain 5-B:  84% 9% •• 6%




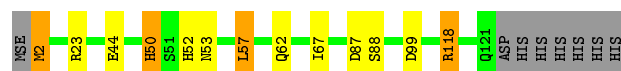
- Molecule 1: plu4264 protein

Chain 6-A:  80% 13% • 5%




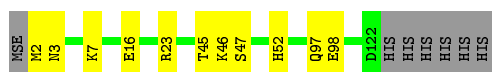
- Molecule 1: plu4264 protein

Chain 6-B:  84% 7% • 6%



- Molecule 1: plu4264 protein

Chain 7-A:  86% 9% 5%



- Molecule 1: plu4264 protein

Chain 7-B: 83% 10% 6%



- Molecule 1: plu4264 protein

Chain 8-A: 84% 11% 5%



- Molecule 1: plu4264 protein

Chain 8-B: 84% 9% 6%



- Molecule 1: plu4264 protein

Chain 9-A: 80% 14% 5%



- Molecule 1: plu4264 protein

Chain 9-B: 83% 9% 6%



- Molecule 1: plu4264 protein

Chain 10-A: 79% 14% 5%




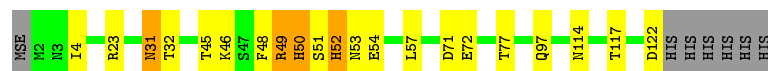
- Molecule 1: plu4264 protein

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% 13% 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% 13% 6%

4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

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	Depositor
% Data completeness (in resolution range)	99.5 (24.90-1.35)	Depositor
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 (phenix.ensemble_refinement: 1.8.4_1496)	Depositor
R, R_{free}	0.126 , 0.155	Depositor
Wilson B-factor (Å ²)	13.4	Xtriage
Anisotropy	0.734	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 75927 reflections (0.003%)	Xtriage
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.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.84	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

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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

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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

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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 [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%)	26	5
1	1-B	151/128 (118%)	143 (95%)	6 (4%)	2 (1%)	15	1
1	2-A	141/128 (110%)	134 (95%)	4 (3%)	3 (2%)	9	0
1	2-B	151/128 (118%)	138 (91%)	11 (7%)	2 (1%)	15	1
1	3-A	141/128 (110%)	137 (97%)	1 (1%)	3 (2%)	9	0
1	3-B	151/128 (118%)	137 (91%)	8 (5%)	6 (4%)	4	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%)	26	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%)	15	1
1	6-A	141/128 (110%)	133 (94%)	7 (5%)	1 (1%)	26	5
1	6-B	151/128 (118%)	141 (93%)	7 (5%)	3 (2%)	9	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%)	7	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%)	15	1
1	9-A	141/128 (110%)	131 (93%)	7 (5%)	3 (2%)	9	0
1	9-B	151/128 (118%)	133 (88%)	15 (10%)	3 (2%)	9	0
1	10-A	141/128 (110%)	136 (96%)	4 (3%)	1 (1%)	26	5
1	10-B	151/128 (118%)	140 (93%)	8 (5%)	3 (2%)	9	0
1	11-A	141/128 (110%)	134 (95%)	1 (1%)	6 (4%)	3	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	11-B	151/128 (118%)	139 (92%)	8 (5%)	4 (3%)	7	0
1	12-A	141/128 (110%)	137 (97%)	2 (1%)	2 (1%)	14	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%)	26	5
1	13-B	151/128 (118%)	142 (94%)	8 (5%)	1 (1%)	26	5
1	14-A	141/128 (110%)	131 (93%)	4 (3%)	6 (4%)	3	0
1	14-B	151/128 (118%)	135 (89%)	14 (9%)	2 (1%)	15	1
1	15-A	141/128 (110%)	132 (94%)	6 (4%)	3 (2%)	9	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%)	4	0
1	17-A	141/128 (110%)	136 (96%)	4 (3%)	1 (1%)	26	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%)	3	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%)	4	0
1	20-A	140/128 (109%)	136 (97%)	3 (2%)	1 (1%)	26	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%)	15	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%)	17	1
1	1-B	145/116 (125%)	131 (90%)	14 (10%)	10	0
1	2-A	135/116 (116%)	121 (90%)	14 (10%)	9	0
1	2-B	145/116 (125%)	133 (92%)	12 (8%)	14	0
1	3-A	135/116 (116%)	121 (90%)	14 (10%)	9	0
1	3-B	145/116 (125%)	133 (92%)	12 (8%)	14	0
1	4-A	135/116 (116%)	121 (90%)	14 (10%)	9	0
1	4-B	145/116 (125%)	118 (81%)	27 (19%)	2	0
1	5-A	135/116 (116%)	127 (94%)	8 (6%)	24	1
1	5-B	145/116 (125%)	134 (92%)	11 (8%)	16	1
1	6-A	135/116 (116%)	120 (89%)	15 (11%)	8	0
1	6-B	145/116 (125%)	134 (92%)	11 (8%)	16	1
1	7-A	135/116 (116%)	124 (92%)	11 (8%)	15	1
1	7-B	145/116 (125%)	134 (92%)	11 (8%)	16	1
1	8-A	135/116 (116%)	120 (89%)	15 (11%)	8	0
1	8-B	145/116 (125%)	127 (88%)	18 (12%)	6	0
1	9-A	135/116 (116%)	123 (91%)	12 (9%)	12	0
1	9-B	145/116 (125%)	133 (92%)	12 (8%)	14	0
1	10-A	135/116 (116%)	122 (90%)	13 (10%)	10	0
1	10-B	145/116 (125%)	137 (94%)	8 (6%)	27	2
1	11-A	135/116 (116%)	116 (86%)	19 (14%)	4	0
1	11-B	145/116 (125%)	133 (92%)	12 (8%)	14	0
1	12-A	135/116 (116%)	131 (97%)	4 (3%)	48	10
1	12-B	145/116 (125%)	133 (92%)	12 (8%)	14	0
1	13-A	135/116 (116%)	124 (92%)	11 (8%)	15	1
1	13-B	145/116 (125%)	136 (94%)	9 (6%)	23	1
1	14-A	135/116 (116%)	122 (90%)	13 (10%)	10	0
1	14-B	145/116 (125%)	131 (90%)	14 (10%)	10	0
1	15-A	135/116 (116%)	122 (90%)	13 (10%)	10	0
1	15-B	145/116 (125%)	125 (86%)	20 (14%)	4	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	16-A	135/116 (116%)	128 (95%)	7 (5%)	29	3
1	16-B	145/116 (125%)	126 (87%)	19 (13%)	5	0
1	17-A	135/116 (116%)	121 (90%)	14 (10%)	9	0
1	17-B	145/116 (125%)	130 (90%)	15 (10%)	9	0
1	18-A	135/116 (116%)	123 (91%)	12 (9%)	12	0
1	18-B	145/116 (125%)	135 (93%)	10 (7%)	19	1
1	19-A	135/116 (116%)	122 (90%)	13 (10%)	10	0
1	19-B	145/116 (125%)	125 (86%)	20 (14%)	4	0
1	20-A	134/116 (116%)	121 (90%)	13 (10%)	10	0
1	20-B	145/116 (125%)	132 (91%)	13 (9%)	12	0
All	All	5599/4640 (121%)	5074 (91%)	525 (9%)	11	0

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

Mol	Chain	Res	Type
1	9-B	98	GLU
1	12-A	50	HIS
1	19-B	52[B]	HIS
1	10-A	7[A]	LYS
1	11-A	45	THR

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

Mol	Chain	Res	Type
1	9-A	62	GLN
1	10-B	64	ASN
1	20-A	31	ASN
1	9-A	64	ASN
1	9-B	121	GLN

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 carbohydrates 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 ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.