



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 08:47 AM GMT

PDB ID : 4M7P
Title : Ensemble refinement of protein crystal structure of macrolide glycosyltransferases OleD
Authors : Wang, F.; Helmich, K.E.; Xu, W.; Singh, S.; Olmos Jr., J.L.; Martinez iii, E.; Bingman, C.A.; Thorson, J.S.; Phillips Jr., G.N.; Enzyme Discovery for Natural Product Biosynthesis (NatPro)
Deposited on : 2013-08-12
Resolution : 1.77 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

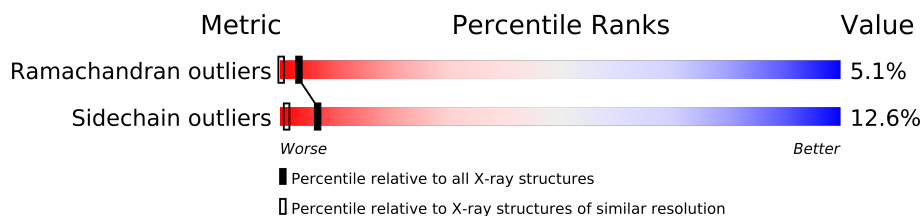
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	FAILED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.77 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	78287	6074 (1.80-1.76)
Sidechain outliers	78261	6073 (1.80-1.76)


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1-A	418	
1	10-A	418	
1	11-A	418	
1	12-A	418	
1	13-A	418	
1	14-A	418	
1	15-A	418	
1	16-A	418	
1	17-A	418	
1	18-A	418	
1	19-A	418	
1	2-A	418	
1	20-A	418	
1	3-A	418	
1	4-A	418	
1	5-A	418	
1	6-A	418	
1	7-A	418	
1	8-A	418	

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Mol	Chain	Length	Quality of chain
1	9-A	418	 A horizontal bar chart representing the quality of the chain. The bar is primarily green, indicating good quality, with a small yellow segment at the end, indicating some issues.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 120618 atoms, of which 57140 are hydrogens and 0 are deuterium.

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 Oleandomycin glycosyltransferase.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	1-A	395	Total	C	H	N	O	S	Se		0	395	0
			5899	1925	2857	543	567	2	5				
1	2-A	395	Total	C	H	N	O	S	Se		0	395	0
			5899	1925	2857	543	567	2	5				
1	3-A	395	Total	C	H	N	O	S	Se		0	395	0
			5899	1925	2857	543	567	2	5				
1	4-A	395	Total	C	H	N	O	S	Se		0	395	0
			5899	1925	2857	543	567	2	5				
1	5-A	395	Total	C	H	N	O	S	Se		0	395	0
			5899	1925	2857	543	567	2	5				
1	6-A	395	Total	C	H	N	O	S	Se		0	395	0
			5899	1925	2857	543	567	2	5				
1	7-A	395	Total	C	H	N	O	S	Se		0	395	0
			5899	1925	2857	543	567	2	5				
1	8-A	395	Total	C	H	N	O	S	Se		0	395	0
			5899	1925	2857	543	567	2	5				
1	9-A	395	Total	C	H	N	O	S	Se		0	395	0
			5899	1925	2857	543	567	2	5				
1	10-A	395	Total	C	H	N	O	S	Se		0	395	0
			5899	1925	2857	543	567	2	5				
1	11-A	395	Total	C	H	N	O	S	Se		0	395	0
			5899	1925	2857	543	567	2	5				
1	12-A	395	Total	C	H	N	O	S	Se		0	395	0
			5899	1925	2857	543	567	2	5				
1	13-A	395	Total	C	H	N	O	S	Se		0	395	0
			5899	1925	2857	543	567	2	5				
1	14-A	395	Total	C	H	N	O	S	Se		0	395	0
			5899	1925	2857	543	567	2	5				
1	15-A	395	Total	C	H	N	O	S	Se		0	395	0
			5899	1925	2857	543	567	2	5				
1	16-A	395	Total	C	H	N	O	S	Se		0	395	0
			5899	1925	2857	543	567	2	5				

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	17-A	395	Total	C	H	N	O	S	Se	0	395	0
			5899	1925	2857	543	567	2	5			
1	18-A	395	Total	C	H	N	O	S	Se	0	395	0
			5899	1925	2857	543	567	2	5			
1	19-A	395	Total	C	H	N	O	S	Se	0	395	0
			5899	1925	2857	543	567	2	5			
1	20-A	395	Total	C	H	N	O	S	Se	0	395	0
			5899	1925	2857	543	567	2	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q3HTL6
A	-1	SER	-	EXPRESSION TAG	UNP Q3HTL6
A	0	HIS	-	EXPRESSION TAG	UNP Q3HTL6

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	3-A	1	Total	Na	0	1
			1	1		
2	18-A	1	Total	Na	0	1
			1	1		
2	11-A	1	Total	Na	0	1
			1	1		
2	16-A	1	Total	Na	0	1
			1	1		
2	4-A	1	Total	Na	0	1
			1	1		
2	20-A	1	Total	Na	0	1
			1	1		
2	12-A	1	Total	Na	0	1
			1	1		
2	19-A	1	Total	Na	0	1
			1	1		
2	17-A	1	Total	Na	0	1
			1	1		
2	5-A	1	Total	Na	0	1
			1	1		
2	13-A	1	Total	Na	0	1
			1	1		
2	8-A	1	Total	Na	0	1
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	1	Total 1	Na 1	0	1
2	6-A	1	Total 1	Na 1	0	1
2	14-A	1	Total 1	Na 1	0	1
2	2-A	1	Total 1	Na 1	0	1
2	10-A	1	Total 1	Na 1	0	1
2	9-A	1	Total 1	Na 1	0	1
2	7-A	1	Total 1	Na 1	0	1
2	15-A	1	Total 1	Na 1	0	1

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	130	Total 130	O 130	0	130
3	2-A	128	Total 128	O 128	0	128
3	3-A	141	Total 141	O 141	0	141
3	4-A	119	Total 119	O 119	0	119
3	5-A	125	Total 125	O 125	0	125
3	6-A	120	Total 120	O 120	0	120
3	7-A	130	Total 130	O 130	0	130
3	8-A	146	Total 146	O 146	0	146
3	9-A	135	Total 135	O 135	0	135
3	10-A	146	Total 146	O 146	0	146
3	11-A	129	Total 129	O 129	0	129

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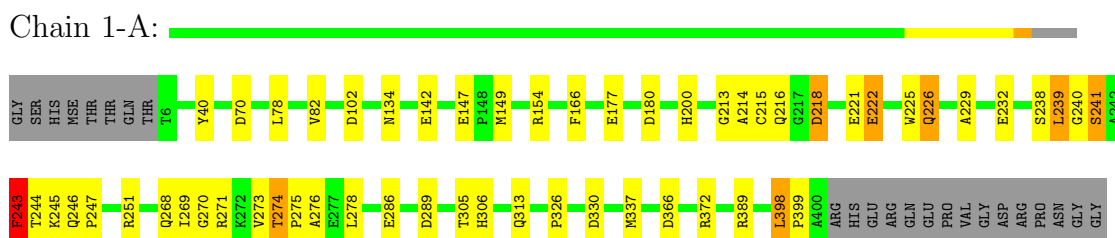
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	12-A	136	Total 136	O 136	0	136
3	13-A	135	Total 135	O 135	0	135
3	14-A	129	Total 129	O 129	0	129
3	15-A	121	Total 121	O 121	0	121
3	16-A	133	Total 133	O 133	0	133
3	17-A	132	Total 132	O 132	0	132
3	18-A	126	Total 126	O 126	0	126
3	19-A	134	Total 134	O 134	0	134
3	20-A	123	Total 123	O 123	0	123

3 Residue-property plots

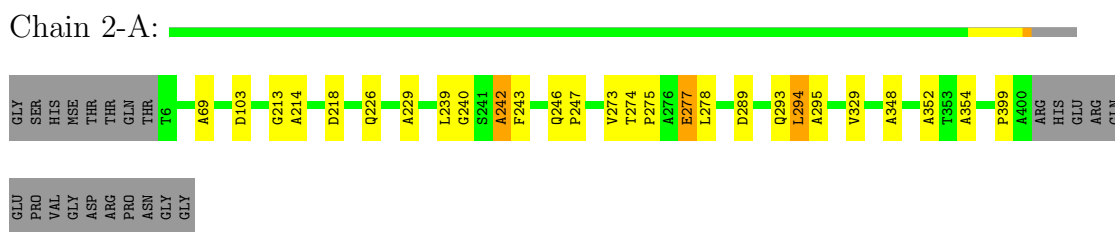
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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.

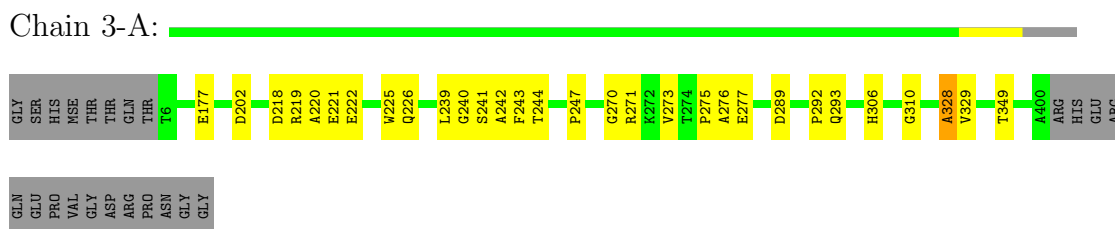
- Molecule 1: Oleandomycin glycosyltransferase



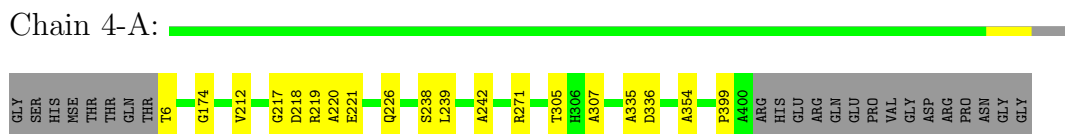
- Molecule 1: Oleandomycin glycosyltransferase



- Molecule 1: Oleandomycin glycosyltransferase



- Molecule 1: Oleandomycin glycosyltransferase



- Molecule 1: Oleandomycin glycosyltransferase





- Molecule 1: Oleandomycin glycosyltransferase

Chain 6-A:



- Molecule 1: Oleandomycin glycosyltransferase

Chain 7-A:



- Molecule 1: Oleandomycin glycosyltransferase

Chain 8-A:



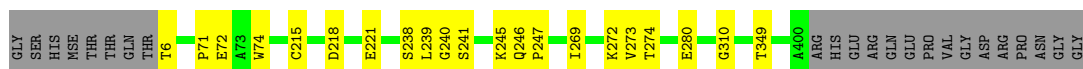
- Molecule 1: Oleandomycin glycosyltransferase

Chain 9-A:



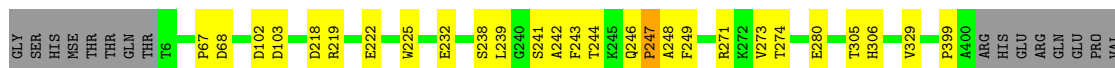
- Molecule 1: Oleandomycin glycosyltransferase

Chain 10-A:



- Molecule 1: Oleandomycin glycosyltransferase

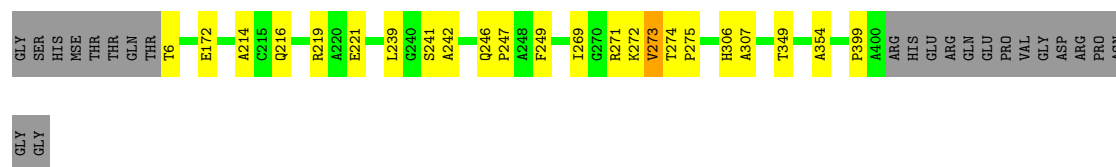
Chain 11-A:



GLY
ASP
ARG
PRO
ASN
GLY
GLY

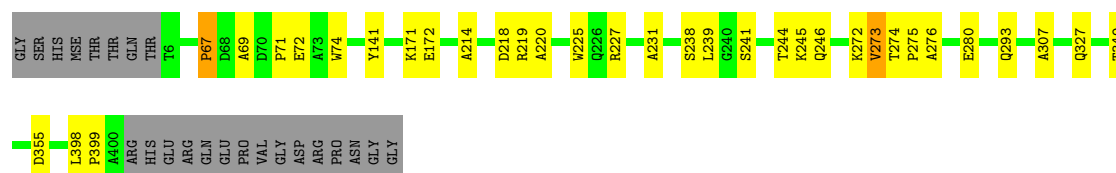
- Molecule 1: Oleandomycin glycosyltransferase

Chain 12-A: 



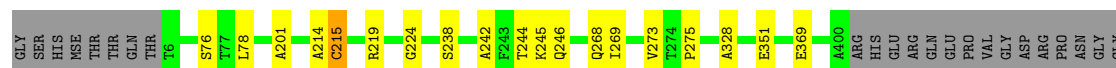
- Molecule 1: Oleandomycin glycosyltransferase

Chain 13-A: 



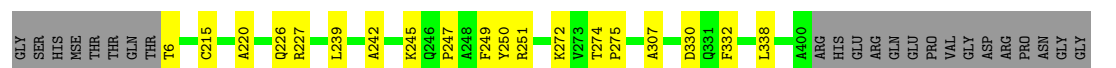
- Molecule 1: Oleandomycin glycosyltransferase

Chain 14-A: 



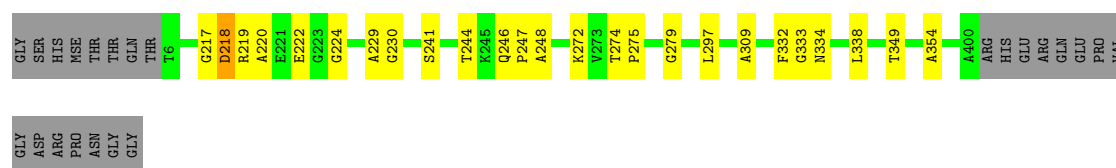
- Molecule 1: Oleandomycin glycosyltransferase

Chain 15-A: 



- Molecule 1: Oleandomycin glycosyltransferase

Chain 16-A: 



- Molecule 1: Oleandomycin glycosyltransferase

Chain 17-A: 



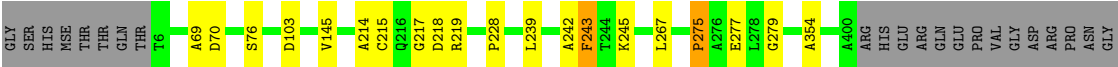
- Molecule 1: Oleandomycin glycosyltransferase

Chain 18-A: 



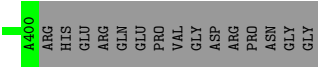
● Molecule 1: Oleandomycin glycosyltransferase

Chain 19-A: 



● Molecule 1: Oleandomycin glycosyltransferase

Chain 20-A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	124.13Å 124.13Å 67.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.08 – 1.77	Depositor
% Data completeness (in resolution range)	100.0 (42.08-1.77)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 1.77Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble.refinement:dev_1420)	Depositor
R, R_{free}	0.150 , 0.188	Depositor
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.297	Xtriage
Estimated twinning fraction	0.022 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 37890 reflections	Xtriage
Total number of atoms	120618	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.58	0/3115	0.83	2/4251 (0.0%)

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-A	0	6
1	2-A	0	4
1	3-A	0	5
1	4-A	0	3
1	5-A	0	3
1	6-A	0	2
1	7-A	0	5
1	8-A	0	4
1	9-A	0	2
1	10-A	0	3
1	11-A	0	5
1	12-A	0	5
1	13-A	0	6
1	14-A	0	5
1	15-A	0	5
1	16-A	0	2
1	17-A	0	7
1	18-A	0	6
1	19-A	0	6
1	20-A	0	3
All	All	0	87

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	239[A]	LEU	CB-CG-CD2	5.63	120.58	111.00
1	1-A	243[A]	PHE	CB-CG-CD1	5.38	124.56	120.80

There are no chirality outliers.

5 of 87 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	213[A]	GLY	Peptide
1	1-A	215[A]	CYS	Peptide
1	1-A	241[A]	SER	Peptide
1	1-A	268[A]	GLN	Peptide
1	1-A	275[A]	PRO	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	3042	2857	0	0	0
1	2-A	3042	2857	0	0	0
1	3-A	3042	2857	0	0	0
1	4-A	3042	2857	0	0	0
1	5-A	3042	2857	0	0	0
1	6-A	3042	2857	0	0	0
1	7-A	3042	2857	0	0	0
1	8-A	3042	2857	0	0	1
1	9-A	3042	2857	0	0	0
1	10-A	3042	2857	0	0	0
1	11-A	3042	2857	0	0	0
1	12-A	3042	2857	0	0	0
1	13-A	3042	2857	0	0	1
1	14-A	3042	2857	0	0	1
1	15-A	3042	2857	0	0	0
1	16-A	3042	2857	0	0	0
1	17-A	3042	2857	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	18-A	3042	2857	0	0	1
1	19-A	3042	2857	0	0	0
1	20-A	3042	2857	0	0	2
2	1-A	1	0	0	0	0
2	2-A	1	0	0	0	0
2	3-A	1	0	0	0	0
2	4-A	1	0	0	0	0
2	5-A	1	0	0	0	0
2	6-A	1	0	0	0	0
2	7-A	1	0	0	0	0
2	8-A	1	0	0	0	0
2	9-A	1	0	0	0	0
2	10-A	1	0	0	0	0
2	11-A	1	0	0	0	0
2	12-A	1	0	0	0	0
2	13-A	1	0	0	0	0
2	14-A	1	0	0	0	0
2	15-A	1	0	0	0	0
2	16-A	1	0	0	0	0
2	17-A	1	0	0	0	0
2	18-A	1	0	0	0	0
2	19-A	1	0	0	0	0
2	20-A	1	0	0	0	0
3	1-A	130	0	0	0	0
3	2-A	128	0	0	0	0
3	3-A	141	0	0	0	0
3	4-A	119	0	0	0	0
3	5-A	125	0	0	0	0
3	6-A	120	0	0	0	0
3	7-A	130	0	0	0	0
3	8-A	146	0	0	0	0
3	9-A	135	0	0	0	0
3	10-A	146	0	0	0	0
3	11-A	129	0	0	0	1
3	12-A	136	0	0	0	0
3	13-A	135	0	0	0	0
3	14-A	129	0	0	0	1
3	15-A	121	0	0	0	0
3	16-A	133	0	0	0	0
3	17-A	132	0	0	0	0
3	18-A	126	0	0	0	0
3	19-A	134	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	20-A	123	0	0	0	0
All	All	63478	57140	0	0	7

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:221[T]:GLU:OE2	1:A:271[T]:ARG:NH1[2.655]	1.88	0.32
1:A:221[R]:GLU:O	1:A:271[R]:ARG:NH2[2.655]	1.91	0.29
1:A:171[M]:LYS:NZ	1:A:355[M]:ASP:OD1[1.554]	2.07	0.13
3:A:653[K]:HOH:O	3:A:654[K]:HOH:O[1.554]	2.14	0.06
1:A:369[N]:GLU:OE2	3:A:619[N]:HOH:O[5.555]	2.16	0.04

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	393/418 (94%)	347 (88%)	27 (7%)	19 (5%)	4	0
1	2-A	393/418 (94%)	337 (86%)	30 (8%)	26 (7%)	2	0
1	3-A	393/418 (94%)	344 (88%)	23 (6%)	26 (7%)	2	0
1	4-A	393/418 (94%)	342 (87%)	35 (9%)	16 (4%)	4	0
1	5-A	393/418 (94%)	345 (88%)	31 (8%)	17 (4%)	4	0
1	6-A	393/418 (94%)	340 (86%)	30 (8%)	23 (6%)	2	0
1	7-A	393/418 (94%)	351 (89%)	25 (6%)	17 (4%)	4	0
1	8-A	393/418 (94%)	332 (84%)	38 (10%)	23 (6%)	2	0
1	9-A	393/418 (94%)	333 (85%)	37 (9%)	23 (6%)	2	0
1	10-A	393/418 (94%)	346 (88%)	29 (7%)	18 (5%)	4	0
1	11-A	393/418 (94%)	341 (87%)	29 (7%)	23 (6%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	12-A	393/418 (94%)	343 (87%)	31 (8%)	19 (5%)	4	0
1	13-A	393/418 (94%)	329 (84%)	36 (9%)	28 (7%)	2	0
1	14-A	393/418 (94%)	344 (88%)	35 (9%)	14 (4%)	5	0
1	15-A	393/418 (94%)	344 (88%)	35 (9%)	14 (4%)	5	0
1	16-A	393/418 (94%)	338 (86%)	31 (8%)	24 (6%)	2	0
1	17-A	393/418 (94%)	344 (88%)	36 (9%)	13 (3%)	6	0
1	18-A	393/418 (94%)	340 (86%)	34 (9%)	19 (5%)	4	0
1	19-A	393/418 (94%)	347 (88%)	30 (8%)	16 (4%)	4	0
1	20-A	393/418 (94%)	337 (86%)	30 (8%)	26 (7%)	2	0
All	All	7860/8360 (94%)	6824 (87%)	632 (8%)	404 (5%)	3	0

5 of 404 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	214[A]	ALA
1	1-A	218[A]	ASP
1	1-A	222[A]	GLU
1	1-A	232[A]	GLU
1	1-A	240[A]	GLY

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	309/322 (96%)	270 (87%)	39 (13%)	7	1

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	226[A]	GLN
1	1-A	244[A]	THR
1	1-A	372[A]	ARG
1	1-A	238[A]	SER
1	1-A	239[A]	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	216[A]	GLN
1	1-A	339[A]	GLN
1	1-A	264[A]	HIS
1	1-A	81[A]	ASN
1	1-A	334[A]	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 20 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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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.