



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:54 AM UTC

PDB ID : 4M7P / pdb_00004m7p
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 X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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

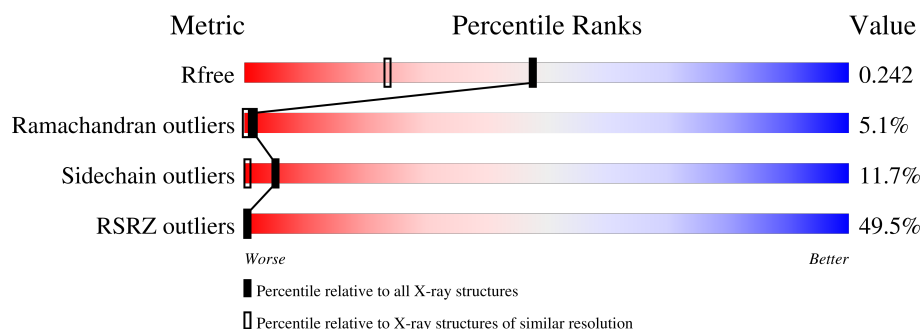
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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))
R_{free}	180053	1365 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	418	46% 82% 11% • 6%
1	10-A	418	89% 5% 6%
1	11-A	418	88% 6% 6%
1	12-A	418	89% 5% 6%
1	13-A	418	87% 7% 6%
1	14-A	418	90% • 6%

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Mol	Chain	Length	Quality of chain
1	15-A	418	 90% 5% 6%
1	16-A	418	 89% 6% 6%
1	17-A	418	 90% • 6%
1	18-A	418	 89% 6% 6%
1	19-A	418	 90% • 6%
1	2-A	418	 88% 6% • 6%
1	20-A	418	 88% 6% 6%
1	3-A	418	 87% 7% 6%
1	4-A	418	 90% 5% 6%
1	5-A	418	 90% 5% 6%
1	6-A	418	 89% 6% 6%
1	7-A	418	 90% • 6%
1	8-A	418	 88% 6% 6%
1	9-A	418	 89% 6% 6%

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 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 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 (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	1	Total	Na	0	1
			1	1		
2	2-A	1	Total	Na	0	1
			1	1		
2	3-A	1	Total	Na	0	1
			1	1		
2	4-A	1	Total	Na	0	1
			1	1		
2	5-A	1	Total	Na	0	1
			1	1		
2	6-A	1	Total	Na	0	1
			1	1		
2	7-A	1	Total	Na	0	1
			1	1		
2	8-A	1	Total	Na	0	1
			1	1		
2	9-A	1	Total	Na	0	1
			1	1		
2	10-A	1	Total	Na	0	1
			1	1		
2	11-A	1	Total	Na	0	1
			1	1		
2	12-A	1	Total	Na	0	1
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	13-A	1	Total 1	Na 1	0	1
2	14-A	1	Total 1	Na 1	0	1
2	15-A	1	Total 1	Na 1	0	1
2	16-A	1	Total 1	Na 1	0	1
2	17-A	1	Total 1	Na 1	0	1
2	18-A	1	Total 1	Na 1	0	1
2	19-A	1	Total 1	Na 1	0	1
2	20-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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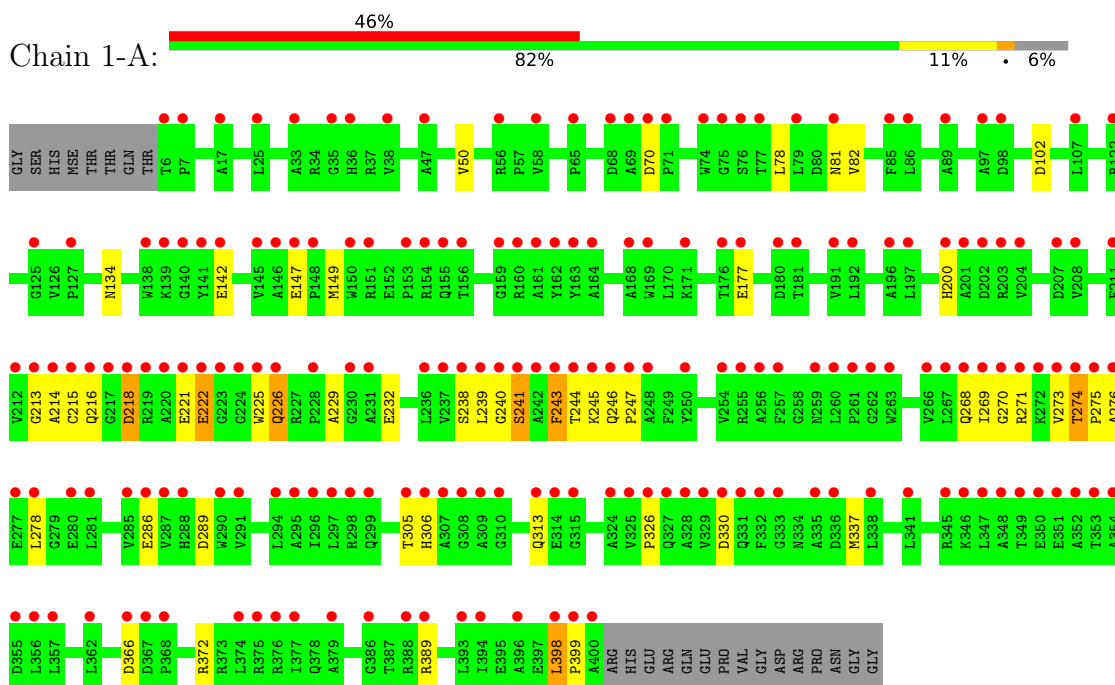
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	12-A	136	Total 136	O 136	0	136
3	13-A	135	Total 135	O 135	0	135
3	14-A	129	Total 129	O 129	0	129
3	15-A	121	Total 121	O 121	0	121
3	16-A	133	Total 133	O 133	0	133
3	17-A	132	Total 132	O 132	0	132
3	18-A	126	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

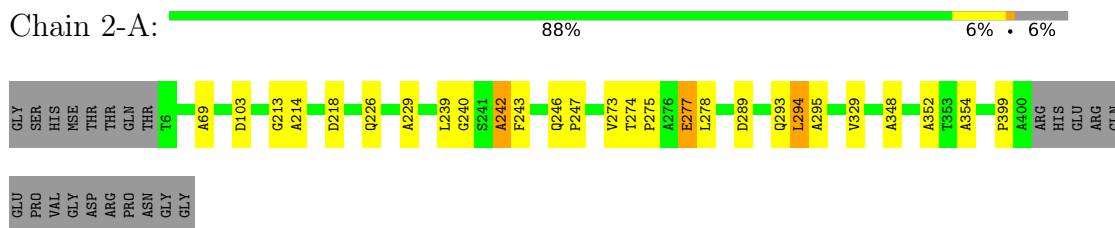
3 Residue-property plots [i](#)

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.

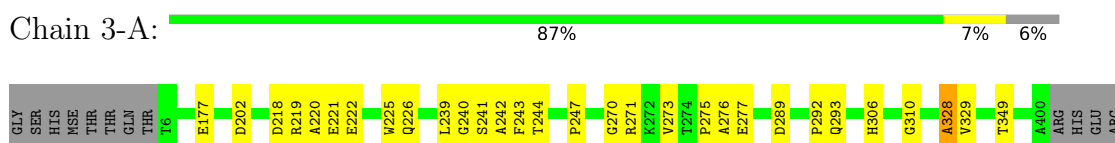
• Molecule 1: Oleandomycin glycosyltransferase



• Molecule 1: Oleandomycin glycosyltransferase



• Molecule 1: Oleandomycin glycosyltransferase



GLN
GLU
PRO
VAL
GLY
ASP
ARG
PRO
ASN
GLY
GLY

• Molecule 1: Oleandomycin glycosyltransferase

Chain 4-A: 90% 5% 6%

GLY SER HIS MSE THR THR THR T6 G174 D1212 G217 D218 R219 A220 E221 Q226 S238 L239 A242 R271 T305 H306 A307 A335 D336 A354 P399 A400 ARG HIS GLU ARG GLN GLU PRO VAL GLY ASP ARG PRO ASN GLY GLY

• Molecule 1: Oleandomycin glycosyltransferase

Chain 5-A: 90% 5% 6%

GLY SER HIS MSE THR THR THR T6 A69 D70 P71 T77 W150 R151 G217 D218 R219 A220 R227 P228 A231 L239 T244 V273 T274 P275 L278 G279 E280 A328 V329 A400 ARG HIS GLU ARG GLN GLU PRO VAL ASN ARG ASP PRO ASN GLY GLY

• Molecule 1: Oleandomycin glycosyltransferase

Chain 6-A: 89% 6% 6%

GLY SER HIS MSE THR THR THR T6 G66 D103 V212 Q216 G217 D218 R219 A220 G224 W225 L239 G240 S241 A242 K245 Q246 K272 V273 T274 P275 A276 A307 G308 A309 G310 V329 D336 A352 T353 A400 ARG HIS GLU ARG GLN GLU PRO VAL

GLY
ASP
ARG
PRO
ASN
GLY
GLY

• Molecule 1: Oleandomycin glycosyltransferase

Chain 7-A: 90% 6%

GLY SER HIS MSE THR THR THR T6 P194 D207 R219 A220 E221 V237 S238 L239 K245 Q246 G270 V273 T274 P275 A276 A295 A307 G311 S312 E350 P399 A400 ARG HIS GLU ARG GLN GLU PRO VAL GLY ASP ARG PRO ASN GLY GLY

• Molecule 1: Oleandomycin glycosyltransferase

Chain 8-A: 88% 6% 6%

GLY SER HIS MSE THR THR THR T6 D70 P71 E72 D103 M149 C215 Q216 D218 R219 A220 P228 A229 L239 F243 P275 V287 L294 A307 V329 G333 N334 A348 A352 D366 D367 A400 ARG HIS GLU ARG GLN GLU PRO

VAL
GLY
ASP
ARG
PRO
ASN
GLY
GLY

• Molecule 1: Oleandomycin glycosyltransferase

Chain 9-A: 89% 6% 6%

GLY SER HIS MSE THR THR THR T6 Y141 A214 C215 Q216 D218 E221 G224 W225 L239 G240 S241 A242 F243 T244 R271 P275 A276 E277 E280 E286 Q293 H306 Q331 F332 G333 A354 A400 ARG HIS GLU ARG GLN GLU PRO VAL GLY

ASP
ARG
PRO
ASN
GLY

- Molecule 1: Oleandomycin glycosyltransferase

Chain 10-A:  89% 5% 6%

GLY SER HIS MSE THR THR T6 P71 P73 W74 C215 D218 E221 S238 L239 G240 S241 K245 Q246 P247 L269 K272 V273 T274 E280 G310 T349 A400 ARG HIS GLU ARG GLN GLU PRO VAL GLY ASP ARG PRO GLY GLY

- Molecule 1: Oleandomycin glycosyltransferase

Chain 11-A:  88% 6% 6%

GLY SER HIS MSE THR GLN THR T6 P67 D68 D102 D103 R218 R219 E222 W225 E232 S238 L239 G240 S241 A242 F243 T244 K245 Q246 P247 A248 F249 R271 K272 V273 T274 E280 T305 H306 V329 P399 A400 ARG HIS GLU ARG GLN GLU PRO VAL

GLY
ASP
ARG
PRO
ASN
GLY

- Molecule 1: Oleandomycin glycosyltransferase

Chain 12-A:  89% 5% 6%

GLY SER HIS MSE THR GLN THR T6 E172 A214 G215 Q216 R219 A220 E221 L239 G240 S241 A242 Q246 P247 F249 L269 G270 R271 K272 T274 P275 H306 A307 T349 A354 P399 A400 ARG HIS GLU ARG GLN GLU PRO VAL GLY ASP ARG ASN

GLY
GLY

- Molecule 1: Oleandomycin glycosyltransferase

Chain 13-A:  87% 7% 6%

GLY SER HIS MSE THR THR T6 P67 D68 A69 D70 P71 E72 A73 W74 Y141 E172 A214 D218 R219 A220 W225 Q226 R227 A231 S238 L239 G240 S241 T244 K245 Q246 K272 V273 T274 P275 A276 E280 Q293 A307 Q327 T349

L398 P399 A400 ARG HIS GLU ARG GLN GLU PRO VAL GLY ASP ARG ASN GLY

- Molecule 1: Oleandomycin glycosyltransferase

Chain 14-A:  90% 6%

GLY SER HIS MSE THR GLN THR T6 S76 S77 L78 A201 A214 C215 R219 G224 S238 A242 F243 T244 K245 Q246 Q268 L269 V273 T274 P275 A328 E351 A400 ARG HIS GLU ARG GLN GLU PRO VAL GLY ASP ARG PRO ASN GLY

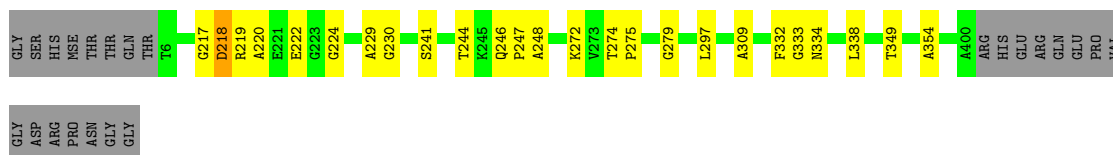
- Molecule 1: Oleandomycin glycosyltransferase

Chain 15-A:  90% 5% 6%



- Molecule 1: Oleandomycin glycosyltransferase

Chain 16-A: 89% 6% 6%



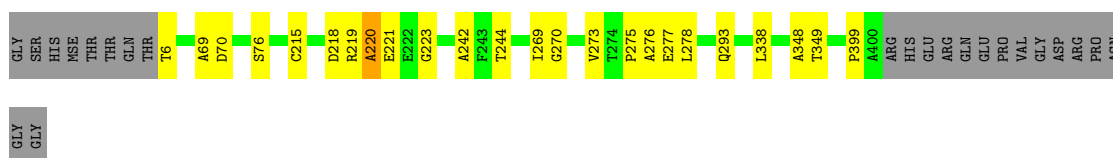
- Molecule 1: Oleandomycin glycosyltransferase

Chain 17-A: 90% 6%



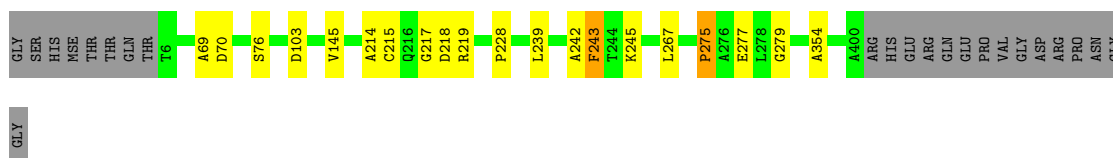
- Molecule 1: Oleandomycin glycosyltransferase

Chain 18-A: 89% 6% 6%



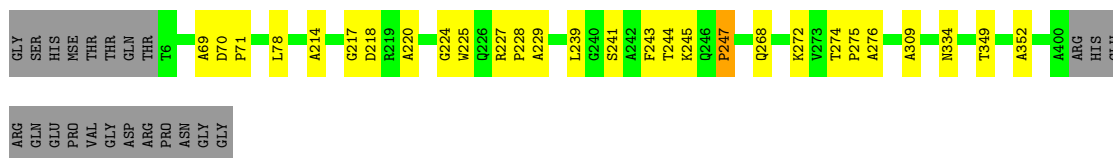
- Molecule 1: Oleandomycin glycosyltransferase

Chain 19-A: 90% 6%



- Molecule 1: Oleandomycin glycosyltransferase

Chain 20-A: 88% 6% 6%



4 Data and refinement statistics

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 42.08 – 1.77	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.08-1.77) 93.4 (42.08-1.77)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.93 (at 1.77Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement: dev_1420)	Depositor
R, R_{free}	0.150 , 0.188 0.200 , 0.242	Depositor DCC
R_{free} test set	2004 reflections (5.29%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.02 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
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.

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

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	0.22	0/3115	0.27	0/4251

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.

There are no bond angle outliers.

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 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	3042	2857	2982	0	0
1	2-A	3042	2857	2982	0	0
1	3-A	3042	2857	2982	0	0
1	4-A	3042	2857	2982	0	0
1	5-A	3042	2857	2982	0	0
1	6-A	3042	2857	2982	0	0
1	7-A	3042	2857	2982	0	0
1	8-A	3042	2857	2982	0	0
1	9-A	3042	2857	2982	0	0
1	10-A	3042	2857	2982	0	0
1	11-A	3042	2857	2982	0	0
1	12-A	3042	2857	2982	0	0
1	13-A	3042	2857	2982	0	0
1	14-A	3042	2857	2982	0	0
1	15-A	3042	2857	2982	0	0
1	16-A	3042	2857	2982	0	0
1	17-A	3042	2857	2982	0	0
1	18-A	3042	2857	2982	0	0
1	19-A	3042	2857	2982	0	0
1	20-A	3042	2857	2982	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0
3	12-A	136	0	0	0	0
3	13-A	135	0	0	0	0
3	14-A	129	0	0	0	0
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
3	20-A	123	0	0	0	0
All	All	63478	57140	59640	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	393/418 (94%)	347 (88%)	27 (7%)	19 (5%)	2	0
1	2-A	393/418 (94%)	337 (86%)	30 (8%)	26 (7%)	1	0
1	3-A	393/418 (94%)	344 (88%)	23 (6%)	26 (7%)	1	0
1	4-A	393/418 (94%)	342 (87%)	35 (9%)	16 (4%)	2	0
1	5-A	393/418 (94%)	345 (88%)	31 (8%)	17 (4%)	2	0
1	6-A	393/418 (94%)	340 (86%)	30 (8%)	23 (6%)	1	0
1	7-A	393/418 (94%)	351 (89%)	25 (6%)	17 (4%)	2	0
1	8-A	393/418 (94%)	332 (84%)	38 (10%)	23 (6%)	1	0
1	9-A	393/418 (94%)	333 (85%)	37 (9%)	23 (6%)	1	0
1	10-A	393/418 (94%)	346 (88%)	29 (7%)	18 (5%)	2	0
1	11-A	393/418 (94%)	341 (87%)	29 (7%)	23 (6%)	1	0
1	12-A	393/418 (94%)	343 (87%)	31 (8%)	19 (5%)	2	0
1	13-A	393/418 (94%)	329 (84%)	36 (9%)	28 (7%)	1	0
1	14-A	393/418 (94%)	344 (88%)	35 (9%)	14 (4%)	2	0
1	15-A	393/418 (94%)	344 (88%)	35 (9%)	14 (4%)	2	0
1	16-A	393/418 (94%)	338 (86%)	31 (8%)	24 (6%)	1	0
1	17-A	393/418 (94%)	344 (88%)	36 (9%)	13 (3%)	3	0
1	18-A	393/418 (94%)	340 (86%)	34 (9%)	19 (5%)	2	0
1	19-A	393/418 (94%)	347 (88%)	30 (8%)	16 (4%)	2	0
1	20-A	393/418 (94%)	337 (86%)	30 (8%)	26 (7%)	1	0
All	All	7860/8360 (94%)	6824 (87%)	632 (8%)	404 (5%)	1	0

5 of 404 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	214[A]	ALA

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Mol	Chain	Res	Type
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%)	273 (88%)	36 (12%)	5 0

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	306[A]	HIS
1	1-A	398[A]	LEU
1	1-A	313[A]	GLN
1	1-A	366[A]	ASP
1	1-A	221[A]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	293[A]	GLN
1	1-A	331[A]	GLN
1	1-A	339[A]	GLN
1	1-A	81[A]	ASN
1	1-A	18[A]	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 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.

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	390/418 (93%)	2.46	193 (49%) 0 0	1, 1, 2, 3	390 (100%)
1	2-A	0/418	-	-	-	-
1	3-A	0/418	-	-	-	-
1	4-A	0/418	-	-	-	-
1	5-A	0/418	-	-	-	-
1	6-A	0/418	-	-	-	-
1	7-A	0/418	-	-	-	-
1	8-A	0/418	-	-	-	-
1	9-A	0/418	-	-	-	-
1	10-A	0/418	-	-	-	-
1	11-A	0/418	-	-	-	-
1	12-A	0/418	-	-	-	-
1	13-A	0/418	-	-	-	-
1	14-A	0/418	-	-	-	-
1	15-A	0/418	-	-	-	-
1	16-A	0/418	-	-	-	-
1	17-A	0/418	-	-	-	-
1	18-A	0/418	-	-	-	-
1	19-A	0/418	-	-	-	-
1	20-A	0/418	-	-	-	-
All	All	390/8360 (4%)	2.46	193 (49%) 0 0	1, 1, 2, 3	390 (100%)

The worst 5 of 193 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	274[A]	THR	12.7
1	1-A	240[A]	GLY	11.9
1	1-A	238[A]	SER	10.4
1	1-A	247[A]	PRO	10.0
1	1-A	222[A]	GLU	8.7

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NA	1-A	501[A]	1/1	0.64	0.24	28,28,28,28	1
2	NA	2-A	501[B]	1/1	-	-	28,28,28,28	1
2	NA	3-A	501[C]	1/1	-	-	28,28,28,28	1
2	NA	4-A	501[D]	1/1	-	-	28,28,28,28	1
2	NA	5-A	501[E]	1/1	-	-	28,28,28,28	1
2	NA	6-A	501[F]	1/1	-	-	28,28,28,28	1
2	NA	7-A	501[G]	1/1	-	-	29,29,29,29	1
2	NA	8-A	501[H]	1/1	-	-	29,29,29,29	1
2	NA	9-A	501[I]	1/1	-	-	29,29,29,29	1
2	NA	10-A	501[J]	1/1	-	-	28,28,28,28	1
2	NA	11-A	501[K]	1/1	-	-	28,28,28,28	1
2	NA	12-A	501[L]	1/1	-	-	28,28,28,28	1
2	NA	13-A	501[M]	1/1	-	-	28,28,28,28	1
2	NA	14-A	501[N]	1/1	-	-	28,28,28,28	1
2	NA	15-A	501[O]	1/1	-	-	28,28,28,28	1
2	NA	16-A	501[P]	1/1	-	-	28,28,28,28	1
2	NA	17-A	501[Q]	1/1	-	-	28,28,28,28	1
2	NA	18-A	501[R]	1/1	-	-	27,27,27,27	1
2	NA	19-A	501[S]	1/1	-	-	28,28,28,28	1
2	NA	20-A	501[T]	1/1	-	-	28,28,28,28	1

6.5 Other polymers [i](#)

There are no such residues in this entry.