



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:40 PM 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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

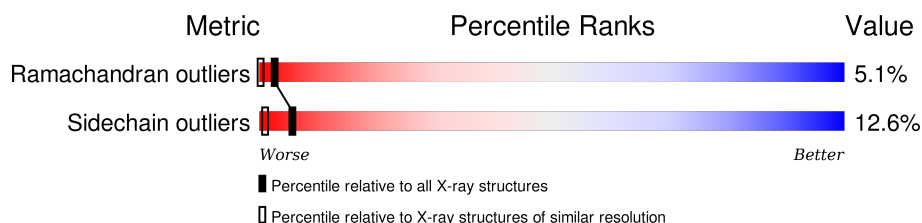
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	100387	7570 (1.80-1.76)
Sidechain outliers	100360	7569 (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. 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	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	

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Mol	Chain	Length	Quality of chain
1	17-A	418	 90% 6% 6%
1	18-A	418	 89% 6% 6%
1	19-A	418	 90% 6% 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% 6%
1	8-A	418	 88% 6% 6%
1	9-A	418	 89% 6% 6%

2 Entry composition [i](#)

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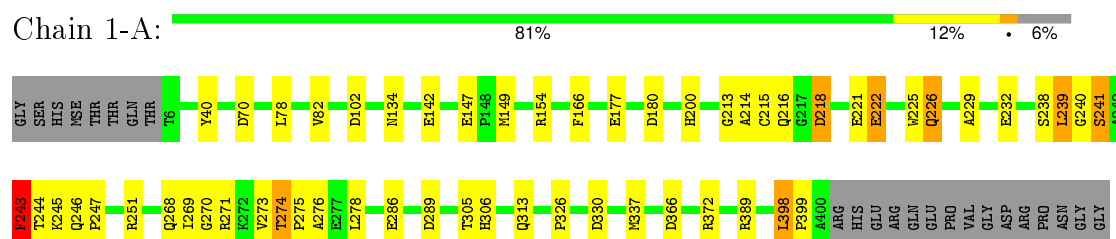
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	12-A	136	Total 136	O 136	0	136
3	13-A	135	Total 135	O 135	0	135
3	14-A	129	Total 129	O 129	0	129
3	15-A	121	Total 121	O 121	0	121
3	16-A	133	Total 133	O 133	0	133
3	17-A	132	Total 132	O 132	0	132
3	18-A	126	Total 126	O 126	0	126
3	19-A	134	Total 134	O 134	0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

3 Residue-property plots

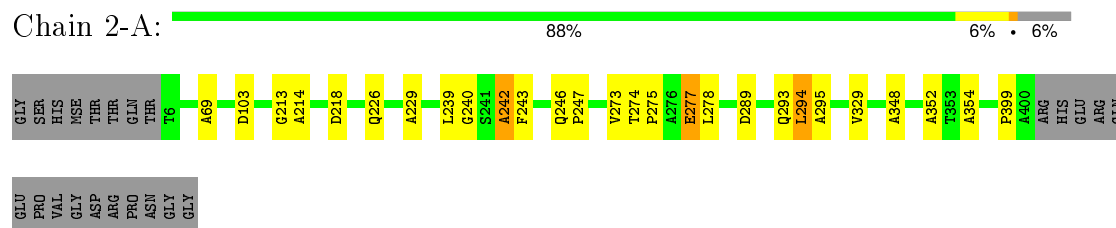
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

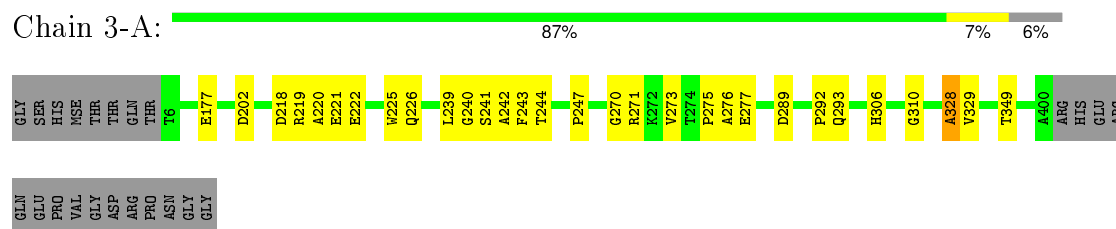
- Molecule 1: Oleandomycin glycosyltransferase



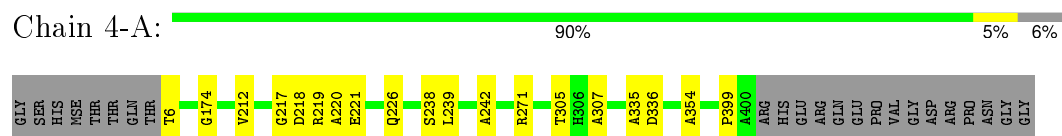
- Molecule 1: Oleandomycin glycosyltransferase



- Molecule 1: Oleandomycin glycosyltransferase



- Molecule 1: Oleandomycin glycosyltransferase



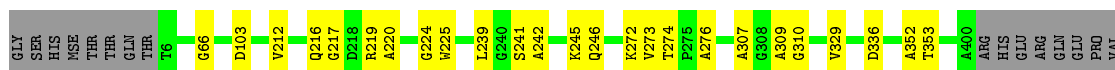
- Molecule 1: Oleandomycin glycosyltransferase

Chain 5-A:  90% 5% 6%



- Molecule 1: Oleandomycin glycosyltransferase

Chain 6-A:  89% 6% 6%




- Molecule 1: Oleandomycin glycosyltransferase

Chain 7-A:  90% 6% 6%




- Molecule 1: Oleandomycin glycosyltransferase

Chain 8-A:  88% 6% 6%



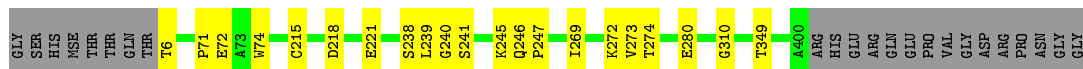
- Molecule 1: Oleandomycin glycosyltransferase

Chain 9-A:  89% 6% 6%



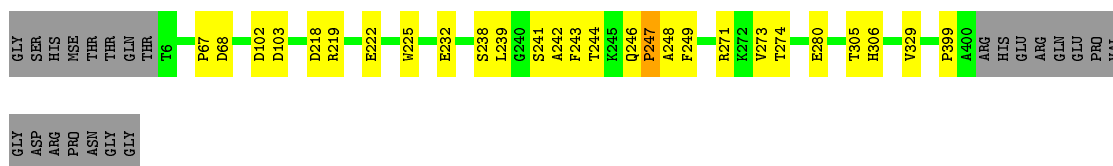
- Molecule 1: Oleandomycin glycosyltransferase

Chain 10-A:  89% 5% 6%



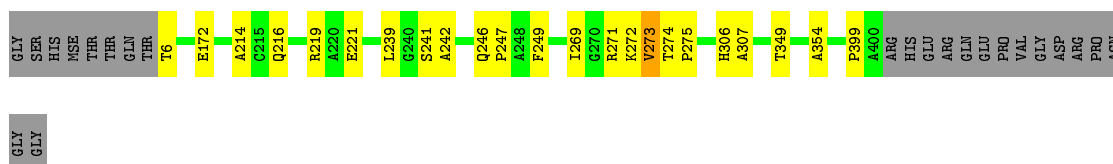
- Molecule 1: Oleandomycin glycosyltransferase

Chain 11-A:  88% 6% 6%



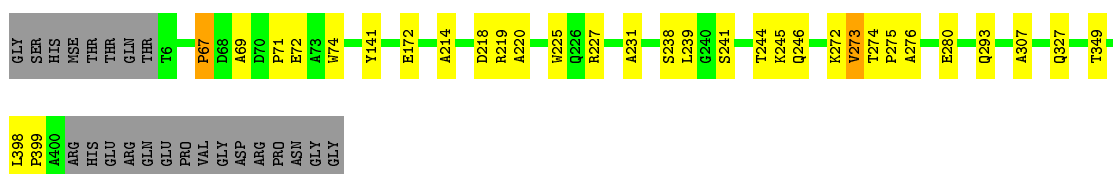
- Molecule 1: Oleandomycin glycosyltransferase

Chain 12-A: 89% 5% 6%



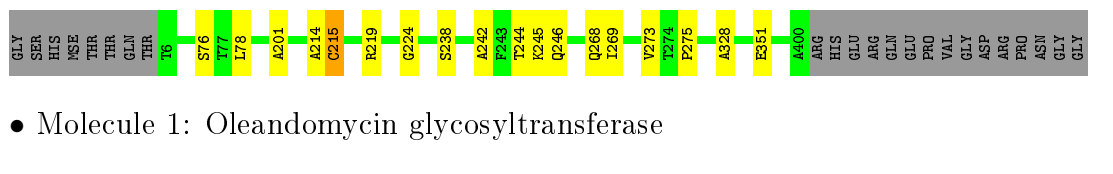
- Molecule 1: Oleandomycin glycosyltransferase

Chain 13-A: 87% 7% 6%



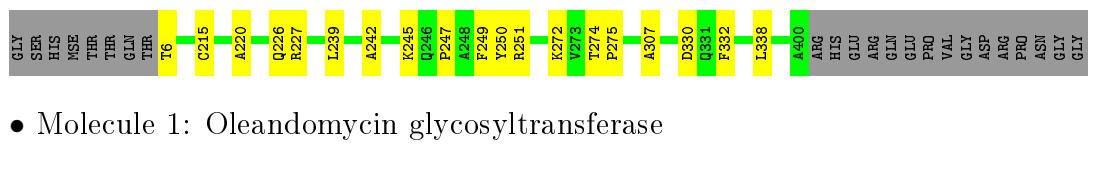
- Molecule 1: Oleandomycin glycosyltransferase

Chain 14-A: 90% 6%



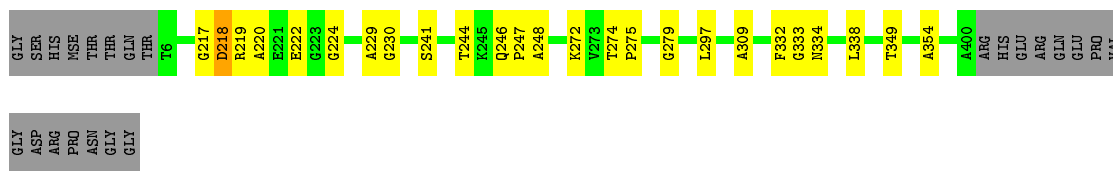
- Molecule 1: Oleandomycin glycosyltransferase

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

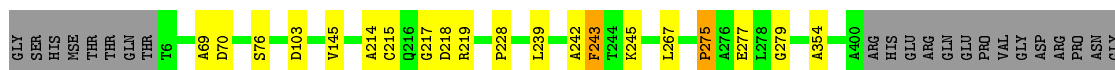
Chain 18-A:  89% 6% 6%



GLY
GLY

- Molecule 1: Oleandomycin glycosyltransferase

Chain 19-A:  90% 6%



GLY

- Molecule 1: Oleandomycin glycosyltransferase

Chain 20-A:  88% 6% 6%



ARG
GLN
GLU
PRO
VAL
GLY
GLY
ASP
ARG
PRO
ASN
GLY
GLY

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 ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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($^{\circ}$)	Ideal($^{\circ}$)
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.

All (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
1	1-A	276[A]	ALA	Peptide
1	10-A	215[J]	CYS	Peptide
1	10-A	238[J]	SER	Peptide
1	10-A	6[J]	THR	Peptide
1	11-A	102[K]	ASP	Peptide
1	11-A	222[K]	GLU	Peptide
1	11-A	238[K]	SER	Peptide
1	11-A	247[K]	PRO	Peptide
1	11-A	305[K]	THR	Peptide
1	12-A	242[L]	ALA	Peptide
1	12-A	271[L]	ARG	Peptide
1	12-A	273[L]	VAL	Peptide
1	12-A	399[L]	PRO	Peptide
1	12-A	6[L]	THR	Peptide
1	13-A	214[M]	ALA	Peptide
1	13-A	238[M]	SER	Peptide
1	13-A	273[M]	VAL	Peptide
1	13-A	293[M]	GLN	Peptide
1	13-A	327[M]	GLN	Peptide
1	13-A	67[M]	PRO	Peptide
1	14-A	215[N]	CYS	Peptide
1	14-A	238[N]	SER	Peptide
1	14-A	245[N]	LYS	Peptide
1	14-A	268[N]	GLN	Peptide
1	14-A	351[N]	GLU	Peptide
1	15-A	220[O]	ALA	Peptide
1	15-A	226[O]	GLN	Peptide
1	15-A	250[O]	TYR	Peptide
1	15-A	330[O]	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	15-A	6[O]	THR	Peptide
1	16-A	217[P]	GLY	Peptide
1	16-A	218[P]	ASP	Peptide
1	17-A	174[Q]	GLY	Peptide
1	17-A	214[Q]	ALA	Peptide
1	17-A	215[Q]	CYS	Peptide
1	17-A	227[Q]	ARG	Peptide
1	17-A	241[Q]	SER	Peptide
1	17-A	245[Q]	LYS	Peptide
1	17-A	308[Q]	GLY	Peptide
1	18-A	215[R]	CYS	Peptide
1	18-A	220[R]	ALA	Peptide
1	18-A	244[R]	THR	Peptide
1	18-A	269[R]	ILE	Peptide
1	18-A	270[R]	GLY	Peptide
1	18-A	6[R]	THR	Peptide
1	19-A	217[S]	GLY	Peptide
1	19-A	242[S]	ALA	Peptide
1	19-A	243[S]	PHE	Peptide
1	19-A	267[S]	LEU	Peptide
1	19-A	275[S]	PRO	Peptide
1	19-A	277[S]	GLU	Peptide
1	2-A	240[B]	GLY	Peptide
1	2-A	242[B]	ALA	Peptide
1	2-A	277[B]	GLU	Peptide
1	2-A	294[B]	LEU	Peptide
1	20-A	217[T]	GLY	Peptide
1	20-A	241[T]	SER	Peptide
1	20-A	247[T]	PRO	Peptide
1	3-A	221[C]	GLU	Peptide
1	3-A	244[C]	THR	Peptide
1	3-A	273[C]	VAL	Peptide
1	3-A	275[C]	PRO	Peptide
1	3-A	328[C]	ALA	Peptide
1	4-A	238[D]	SER	Peptide
1	4-A	305[D]	THR	Peptide
1	4-A	6[D]	THR	Peptide
1	5-A	217[E]	GLY	Peptide
1	5-A	244[E]	THR	Peptide
1	5-A	329[E]	VAL	Peptide
1	6-A	216[F]	GLN	Peptide
1	6-A	217[F]	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	7-A	221[G]	GLU	Peptide
1	7-A	239[G]	LEU	Peptide
1	7-A	245[G]	LYS	Peptide
1	7-A	246[G]	GLN	Peptide
1	7-A	350[G]	GLU	Peptide
1	8-A	215[H]	CYS	Peptide
1	8-A	348[H]	ALA	Peptide
1	8-A	6[H]	THR	Peptide
1	8-A	70[H]	ASP	Peptide
1	9-A	221[I]	GLU	Peptide
1	9-A	6[I]	THR	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	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%)	3	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%)	3	0
1	5-A	393/418 (94%)	345 (88%)	31 (8%)	17 (4%)	3	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%)	3	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%)	3	0
1	11-A	393/418 (94%)	341 (87%)	29 (7%)	23 (6%)	2	0
1	12-A	393/418 (94%)	343 (87%)	31 (8%)	19 (5%)	3	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%)	4	0
1	15-A	393/418 (94%)	344 (88%)	35 (9%)	14 (4%)	4	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%)	5	0
1	18-A	393/418 (94%)	340 (86%)	34 (9%)	19 (5%)	3	0
1	19-A	393/418 (94%)	347 (88%)	30 (8%)	16 (4%)	3	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%)	2	0

All (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
1	1-A	241[A]	SER
1	1-A	243[A]	PHE
1	1-A	274[A]	THR
1	1-A	398[A]	LEU
1	1-A	399[A]	PRO
1	2-A	69[B]	ALA
1	2-A	218[B]	ASP
1	2-A	242[B]	ALA
1	2-A	246[B]	GLN
1	2-A	247[B]	PRO
1	2-A	273[B]	VAL
1	2-A	274[B]	THR
1	2-A	275[B]	PRO
1	2-A	277[B]	GLU
1	2-A	278[B]	LEU
1	2-A	293[B]	GLN
1	2-A	294[B]	LEU
1	2-A	295[B]	ALA
1	2-A	348[B]	ALA
1	2-A	354[B]	ALA
1	2-A	399[B]	PRO
1	3-A	218[C]	ASP
1	3-A	222[C]	GLU
1	3-A	239[C]	LEU
1	3-A	241[C]	SER
1	3-A	293[C]	GLN
1	3-A	306[C]	HIS
1	3-A	329[C]	VAL
1	3-A	349[C]	THR
1	4-A	218[D]	ASP
1	4-A	219[D]	ARG
1	4-A	220[D]	ALA
1	4-A	239[D]	LEU
1	4-A	271[D]	ARG
1	4-A	307[D]	ALA
1	4-A	336[D]	ASP
1	5-A	69[E]	ALA

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Mol	Chain	Res	Type
1	5-A	77[E]	THR
1	5-A	218[E]	ASP
1	5-A	228[E]	PRO
1	5-A	231[E]	ALA
1	5-A	239[E]	LEU
1	5-A	273[E]	VAL
1	5-A	274[E]	THR
1	5-A	275[E]	PRO
1	5-A	280[E]	GLU
1	6-A	219[F]	ARG
1	6-A	241[F]	SER
1	6-A	242[F]	ALA
1	6-A	245[F]	LYS
1	6-A	246[F]	GLN
1	6-A	272[F]	LYS
1	6-A	274[F]	THR
1	6-A	307[F]	ALA
1	6-A	329[F]	VAL
1	6-A	352[F]	ALA
1	7-A	207[G]	ASP
1	7-A	219[G]	ARG
1	7-A	220[G]	ALA
1	7-A	238[G]	SER
1	7-A	239[G]	LEU
1	7-A	275[G]	PRO
1	7-A	276[G]	ALA
1	7-A	307[G]	ALA
1	7-A	312[G]	SER
1	8-A	70[H]	ASP
1	8-A	72[H]	GLU
1	8-A	239[H]	LEU
1	8-A	243[H]	PHE
1	8-A	275[H]	PRO
1	8-A	307[H]	ALA
1	8-A	329[H]	VAL
1	8-A	367[H]	ASP
1	9-A	216[I]	GLN
1	9-A	218[I]	ASP
1	9-A	221[I]	GLU
1	9-A	239[I]	LEU
1	9-A	244[I]	THR
1	9-A	271[I]	ARG

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Mol	Chain	Res	Type
1	9-A	277[I]	GLU
1	9-A	293[I]	GLN
1	9-A	306[I]	HIS
1	9-A	331[I]	GLN
1	10-A	71[J]	PRO
1	10-A	72[J]	GLU
1	10-A	221[J]	GLU
1	10-A	245[J]	LYS
1	10-A	246[J]	GLN
1	10-A	273[J]	VAL
1	10-A	349[J]	THR
1	11-A	67[K]	PRO
1	11-A	68[K]	ASP
1	11-A	218[K]	ASP
1	11-A	219[K]	ARG
1	11-A	239[K]	LEU
1	11-A	241[K]	SER
1	11-A	242[K]	ALA
1	11-A	244[K]	THR
1	11-A	246[K]	GLN
1	11-A	247[K]	PRO
1	11-A	248[K]	ALA
1	11-A	249[K]	PHE
1	11-A	274[K]	THR
1	11-A	399[K]	PRO
1	12-A	214[L]	ALA
1	12-A	216[L]	GLN
1	12-A	219[L]	ARG
1	12-A	221[L]	GLU
1	12-A	241[L]	SER
1	12-A	246[L]	GLN
1	12-A	247[L]	PRO
1	12-A	275[L]	PRO
1	12-A	307[L]	ALA
1	12-A	354[L]	ALA
1	13-A	67[M]	PRO
1	13-A	69[M]	ALA
1	13-A	218[M]	ASP
1	13-A	220[M]	ALA
1	13-A	239[M]	LEU
1	13-A	241[M]	SER
1	13-A	245[M]	LYS

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Mol	Chain	Res	Type
1	13-A	246[M]	GLN
1	13-A	272[M]	LYS
1	13-A	275[M]	PRO
1	13-A	398[M]	LEU
1	13-A	399[M]	PRO
1	14-A	78[N]	LEU
1	14-A	219[N]	ARG
1	14-A	242[N]	ALA
1	14-A	246[N]	GLN
1	14-A	273[N]	VAL
1	14-A	328[N]	ALA
1	15-A	239[O]	LEU
1	15-A	242[O]	ALA
1	15-A	251[O]	ARG
1	15-A	332[O]	PHE
1	16-A	218[P]	ASP
1	16-A	219[P]	ARG
1	16-A	224[P]	GLY
1	16-A	229[P]	ALA
1	16-A	244[P]	THR
1	16-A	246[P]	GLN
1	16-A	247[P]	PRO
1	16-A	272[P]	LYS
1	16-A	274[P]	THR
1	16-A	275[P]	PRO
1	16-A	334[P]	ASN
1	16-A	338[P]	LEU
1	16-A	349[P]	THR
1	16-A	354[P]	ALA
1	17-A	240[Q]	GLY
1	17-A	273[Q]	VAL
1	18-A	70[R]	ASP
1	18-A	218[R]	ASP
1	18-A	219[R]	ARG
1	18-A	220[R]	ALA
1	18-A	221[R]	GLU
1	18-A	223[R]	GLY
1	18-A	273[R]	VAL
1	18-A	275[R]	PRO
1	18-A	276[R]	ALA
1	18-A	277[R]	GLU
1	18-A	349[R]	THR

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Mol	Chain	Res	Type
1	19-A	70[S]	ASP
1	19-A	215[S]	CYS
1	19-A	218[S]	ASP
1	19-A	219[S]	ARG
1	19-A	354[S]	ALA
1	20-A	69[T]	ALA
1	20-A	70[T]	ASP
1	20-A	71[T]	PRO
1	20-A	218[T]	ASP
1	20-A	225[T]	TRP
1	20-A	243[T]	PHE
1	20-A	244[T]	THR
1	20-A	247[T]	PRO
1	20-A	268[T]	GLN
1	20-A	272[T]	LYS
1	20-A	274[T]	THR
1	20-A	275[T]	PRO
1	1-A	229[A]	ALA
1	1-A	247[A]	PRO
1	1-A	278[A]	LEU
1	1-A	326[A]	PRO
1	2-A	103[B]	ASP
1	2-A	243[B]	PHE
1	3-A	177[C]	GLU
1	3-A	240[C]	GLY
1	3-A	270[C]	GLY
1	3-A	276[C]	ALA
1	3-A	277[C]	GLU
1	3-A	310[C]	GLY
1	4-A	174[D]	GLY
1	4-A	335[D]	ALA
1	5-A	220[E]	ALA
1	6-A	220[F]	ALA
1	6-A	224[F]	GLY
1	6-A	309[F]	ALA
1	7-A	237[G]	VAL
1	7-A	295[G]	ALA
1	7-A	311[G]	GLY
1	8-A	103[H]	ASP
1	8-A	217[H]	GLY
1	8-A	218[H]	ASP
1	8-A	220[H]	ALA

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Mol	Chain	Res	Type
1	8-A	229[H]	ALA
1	8-A	287[H]	VAL
1	8-A	294[H]	LEU
1	8-A	333[H]	GLY
1	8-A	334[H]	ASN
1	8-A	352[H]	ALA
1	9-A	141[I]	TYR
1	9-A	214[I]	ALA
1	9-A	275[I]	PRO
1	9-A	276[I]	ALA
1	9-A	280[I]	GLU
1	9-A	286[I]	GLU
1	9-A	332[I]	PHE
1	9-A	333[I]	GLY
1	10-A	74[J]	TRP
1	10-A	241[J]	SER
1	10-A	247[J]	PRO
1	10-A	272[J]	LYS
1	10-A	274[J]	THR
1	10-A	310[J]	GLY
1	11-A	225[K]	TRP
1	11-A	232[K]	GLU
1	11-A	243[K]	PHE
1	11-A	306[K]	HIS
1	12-A	239[L]	LEU
1	12-A	269[L]	ILE
1	12-A	272[L]	LYS
1	12-A	273[L]	VAL
1	12-A	274[L]	THR
1	13-A	74[M]	TRP
1	13-A	141[M]	TYR
1	13-A	273[M]	VAL
1	14-A	214[N]	ALA
1	14-A	215[N]	CYS
1	14-A	224[N]	GLY
1	15-A	245[O]	LYS
1	15-A	272[O]	LYS
1	15-A	275[O]	PRO
1	15-A	338[O]	LEU
1	16-A	220[P]	ALA
1	16-A	222[P]	GLU
1	16-A	248[P]	ALA

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Mol	Chain	Res	Type
1	16-A	297[P]	LEU
1	16-A	333[P]	GLY
1	17-A	139[Q]	LYS
1	17-A	215[Q]	CYS
1	17-A	225[Q]	TRP
1	17-A	276[Q]	ALA
1	17-A	308[Q]	GLY
1	18-A	338[R]	LEU
1	18-A	399[R]	PRO
1	19-A	69[S]	ALA
1	19-A	214[S]	ALA
1	19-A	243[S]	PHE
1	19-A	245[S]	LYS
1	19-A	279[S]	GLY
1	20-A	214[T]	ALA
1	20-A	229[T]	ALA
1	20-A	239[T]	LEU
1	20-A	245[T]	LYS
1	20-A	276[T]	ALA
1	20-A	309[T]	ALA
1	20-A	334[T]	ASN
1	2-A	214[B]	ALA
1	2-A	229[B]	ALA
1	2-A	239[B]	LEU
1	2-A	289[B]	ASP
1	2-A	329[B]	VAL
1	2-A	352[B]	ALA
1	3-A	202[C]	ASP
1	3-A	242[C]	ALA
1	3-A	247[C]	PRO
1	3-A	289[C]	ASP
1	4-A	242[D]	ALA
1	5-A	150[E]	TRP
1	6-A	336[F]	ASP
1	8-A	366[H]	ASP
1	9-A	225[I]	TRP
1	9-A	241[I]	SER
1	9-A	242[I]	ALA
1	10-A	218[J]	ASP
1	11-A	280[K]	GLU
1	12-A	172[L]	GLU
1	12-A	249[L]	PHE

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Mol	Chain	Res	Type
1	12-A	349[L]	THR
1	13-A	72[M]	GLU
1	13-A	172[M]	GLU
1	13-A	225[M]	TRP
1	13-A	244[M]	THR
1	13-A	276[M]	ALA
1	13-A	307[M]	ALA
1	13-A	349[M]	THR
1	14-A	275[N]	PRO
1	15-A	215[O]	CYS
1	15-A	247[O]	PRO
1	15-A	249[O]	PHE
1	15-A	307[O]	ALA
1	16-A	230[P]	GLY
1	16-A	241[P]	SER
1	16-A	332[P]	PHE
1	17-A	229[Q]	ALA
1	17-A	271[Q]	ARG
1	19-A	76[S]	SER
1	19-A	103[S]	ASP
1	20-A	220[T]	ALA
1	20-A	349[T]	THR
1	1-A	200[A]	HIS
1	1-A	226[A]	GLN
1	1-A	273[A]	VAL
1	3-A	243[C]	PHE
1	4-A	221[D]	GLU
1	5-A	151[E]	ARG
1	5-A	278[E]	LEU
1	6-A	66[F]	GLY
1	6-A	103[F]	ASP
1	6-A	225[F]	TRP
1	6-A	239[F]	LEU
1	6-A	276[F]	ALA
1	6-A	353[F]	THR
1	7-A	194[G]	PRO
1	7-A	246[G]	GLN
1	8-A	71[H]	PRO
1	8-A	149[H]	MSE
1	8-A	219[H]	ARG
1	9-A	354[I]	ALA
1	10-A	239[J]	LEU

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Mol	Chain	Res	Type
1	11-A	103[K]	ASP
1	11-A	271[K]	ARG
1	12-A	306[L]	HIS
1	13-A	219[M]	ARG
1	13-A	231[M]	ALA
1	13-A	280[M]	GLU
1	14-A	201[N]	ALA
1	15-A	227[O]	ARG
1	15-A	274[O]	THR
1	16-A	309[P]	ALA
1	18-A	69[R]	ALA
1	18-A	76[R]	SER
1	18-A	242[R]	ALA
1	18-A	278[R]	LEU
1	19-A	145[S]	VAL
1	19-A	275[S]	PRO
1	20-A	78[T]	LEU
1	20-A	228[T]	PRO
1	2-A	226[B]	GLN
1	3-A	219[C]	ARG
1	3-A	220[C]	ALA
1	3-A	225[C]	TRP
1	3-A	328[C]	ALA
1	4-A	212[D]	VAL
1	4-A	354[D]	ALA
1	4-A	399[D]	PRO
1	5-A	227[E]	ARG
1	5-A	328[E]	ALA
1	7-A	273[G]	VAL
1	7-A	399[G]	PRO
1	10-A	280[J]	GLU
1	14-A	244[N]	THR
1	17-A	216[Q]	GLN
1	17-A	268[Q]	GLN
1	18-A	293[R]	GLN
1	18-A	348[R]	ALA
1	19-A	228[S]	PRO
1	19-A	239[S]	LEU
1	20-A	352[T]	ALA
1	3-A	226[C]	GLN
1	3-A	271[C]	ARG
1	4-A	217[D]	GLY

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Mol	Chain	Res	Type
1	4-A	226[D]	GLN
1	8-A	228[H]	PRO
1	9-A	224[I]	GLY
1	11-A	273[K]	VAL
1	13-A	71[M]	PRO
1	14-A	76[N]	SER
1	14-A	269[N]	ILE
1	16-A	279[P]	GLY
1	20-A	227[T]	ARG
1	7-A	270[G]	GLY
1	13-A	227[M]	ARG
1	10-A	269[J]	ILE
1	17-A	274[Q]	THR
1	20-A	224[T]	GLY
1	1-A	270[A]	GLY
1	6-A	212[F]	VAL
1	6-A	273[F]	VAL
1	6-A	310[F]	GLY
1	1-A	147[A]	GLU
1	2-A	213[B]	GLY
1	5-A	71[E]	PRO
1	10-A	240[J]	GLY
1	17-A	246[Q]	GLN
1	3-A	292[C]	PRO
1	11-A	329[K]	VAL
1	13-A	274[M]	THR

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%)	5 1

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	40[A]	TYR
1	1-A	70[A]	ASP
1	1-A	78[A]	LEU
1	1-A	82[A]	VAL
1	1-A	102[A]	ASP
1	1-A	134[A]	ASN
1	1-A	142[A]	GLU
1	1-A	149[A]	MSE
1	1-A	154[A]	ARG
1	1-A	166[A]	PHE
1	1-A	177[A]	GLU
1	1-A	180[A]	ASP
1	1-A	216[A]	GLN
1	1-A	218[A]	ASP
1	1-A	221[A]	GLU
1	1-A	222[A]	GLU
1	1-A	225[A]	TRP
1	1-A	226[A]	GLN
1	1-A	238[A]	SER
1	1-A	239[A]	LEU
1	1-A	243[A]	PHE
1	1-A	244[A]	THR
1	1-A	245[A]	LYS
1	1-A	246[A]	GLN
1	1-A	251[A]	ARG
1	1-A	269[A]	ILE
1	1-A	271[A]	ARG
1	1-A	274[A]	THR
1	1-A	286[A]	GLU
1	1-A	289[A]	ASP
1	1-A	305[A]	THR
1	1-A	306[A]	HIS
1	1-A	313[A]	GLN
1	1-A	330[A]	ASP
1	1-A	337[A]	MSE
1	1-A	366[A]	ASP
1	1-A	372[A]	ARG
1	1-A	389[A]	ARG
1	1-A	398[A]	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	18[A]	HIS
1	1-A	81[A]	ASN
1	1-A	246[A]	GLN
1	1-A	264[A]	HIS
1	1-A	293[A]	GLN
1	1-A	331[A]	GLN
1	1-A	339[A]	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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.

No monomer is involved in short contacts.

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.