



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:46 PM GMT

PDB ID : 4TZ5
Title : Ensemble refinement of the E502A variant of sacteLam55A from Streptomyces sp. SirexAA-E in complex with laminarihexaose
Authors : Bianchetti, C.M.; Takasuka, T.E.; Yik, E.J.; Bergeman, L.F.; Fox, B.G.
Deposited on : 2014-07-09
Resolution : 1.75 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 : **NOT EXECUTED**
Mogul : **NOT EXECUTED**
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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 1.75 Å.

There are no percentiles available for this entry.

MolProbity and EDS were not executed - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 427968 atoms, of which 195500 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 Putative secreted protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	2-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	3-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	4-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	5-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	6-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	7-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	8-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	9-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	10-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	11-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	12-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	13-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	14-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	15-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	16-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	18-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	19-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	20-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	21-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	22-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	23-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	24-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	25-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	1-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	2-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	3-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	4-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	5-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	6-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	7-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	8-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	9-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	10-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	11-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	12-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	13-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	14-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	15-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	16-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	17-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	18-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	19-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	20-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	21-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	22-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	23-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	24-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	25-B	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	502	ALA	GLU	engineered mutation	UNP G2NFJ9
B	502	ALA	GLU	engineered mutation	UNP G2NFJ9

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	1-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	2-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	3-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	4-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	5-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	6-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	7-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	8-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	9-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	10-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	11-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	12-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	13-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	14-A	1	Total	C	H	O	0	0
			10	2	6	2		

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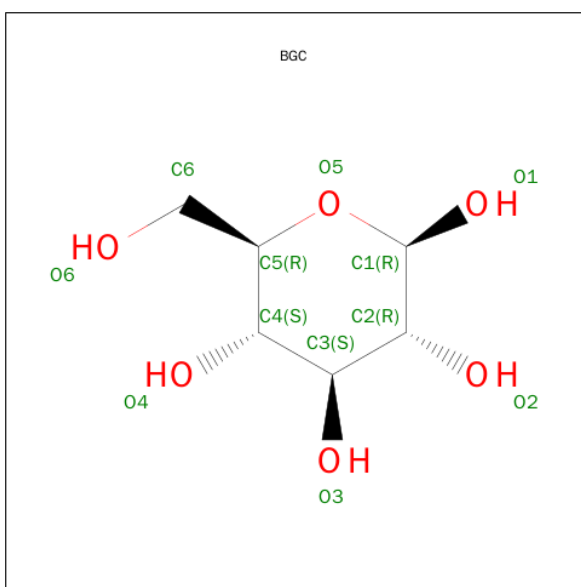
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	15-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	16-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	17-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	18-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	19-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	20-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	21-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	22-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	23-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	24-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	25-A	1	Total	C	H	O	0	0
			10	2	6	2		
2	1-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	2-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	3-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	4-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	5-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	6-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	7-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	8-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	9-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	10-B	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	11-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	12-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	13-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	14-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	15-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	16-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	17-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	18-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	19-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	20-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	21-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	22-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	23-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	24-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	25-B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 3 is BETA-D-GLUCOSE (three-letter code: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	1-A	1	Total	C	O	0	0
			11	6	5		
3	2-A	1	Total	C	O	0	0
			11	6	5		
3	3-A	1	Total	C	O	0	0
			11	6	5		
3	4-A	1	Total	C	O	0	0
			11	6	5		
3	5-A	1	Total	C	O	0	0
			11	6	5		
3	6-A	1	Total	C	O	0	0
			11	6	5		
3	7-A	1	Total	C	O	0	0
			11	6	5		
3	8-A	1	Total	C	O	0	0
			11	6	5		
3	9-A	1	Total	C	O	0	0
			11	6	5		
3	10-A	1	Total	C	O	0	0
			11	6	5		
3	11-A	1	Total	C	O	0	0
			11	6	5		
3	12-A	1	Total	C	O	0	0
			11	6	5		
3	13-A	1	Total	C	O	0	0
			11	6	5		
3	14-A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	15-A	1	Total	C	O	0	0
			11	6	5		
3	16-A	1	Total	C	O	0	0
			11	6	5		
3	17-A	1	Total	C	O	0	0
			11	6	5		
3	18-A	1	Total	C	O	0	0
			11	6	5		
3	19-A	1	Total	C	O	0	0
			11	6	5		
3	20-A	1	Total	C	O	0	0
			11	6	5		
3	21-A	1	Total	C	O	0	0
			11	6	5		
3	22-A	1	Total	C	O	0	0
			11	6	5		
3	23-A	1	Total	C	O	0	0
			11	6	5		
3	24-A	1	Total	C	O	0	0
			11	6	5		
3	25-A	1	Total	C	O	0	0
			11	6	5		
3	1-A	1	Total	C	O	0	0
			11	6	5		
3	2-A	1	Total	C	O	0	0
			11	6	5		
3	3-A	1	Total	C	O	0	0
			11	6	5		
3	4-A	1	Total	C	O	0	0
			11	6	5		
3	5-A	1	Total	C	O	0	0
			11	6	5		
3	6-A	1	Total	C	O	0	0
			11	6	5		
3	7-A	1	Total	C	O	0	0
			11	6	5		
3	8-A	1	Total	C	O	0	0
			11	6	5		
3	9-A	1	Total	C	O	0	0
			11	6	5		
3	10-A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	11-A	1	Total	C	O	0	0
			11	6	5		
3	12-A	1	Total	C	O	0	0
			11	6	5		
3	13-A	1	Total	C	O	0	0
			11	6	5		
3	14-A	1	Total	C	O	0	0
			11	6	5		
3	15-A	1	Total	C	O	0	0
			11	6	5		
3	16-A	1	Total	C	O	0	0
			11	6	5		
3	17-A	1	Total	C	O	0	0
			11	6	5		
3	18-A	1	Total	C	O	0	0
			11	6	5		
3	19-A	1	Total	C	O	0	0
			11	6	5		
3	20-A	1	Total	C	O	0	0
			11	6	5		
3	21-A	1	Total	C	O	0	0
			11	6	5		
3	22-A	1	Total	C	O	0	0
			11	6	5		
3	23-A	1	Total	C	O	0	0
			11	6	5		
3	24-A	1	Total	C	O	0	0
			11	6	5		
3	25-A	1	Total	C	O	0	0
			11	6	5		
3	1-A	1	Total	C	O	0	0
			11	6	5		
3	2-A	1	Total	C	O	0	0
			11	6	5		
3	3-A	1	Total	C	O	0	0
			11	6	5		
3	4-A	1	Total	C	O	0	0
			11	6	5		
3	5-A	1	Total	C	O	0	0
			11	6	5		
3	6-A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	7-A	1	Total	C	O	0	0
			11	6	5		
3	8-A	1	Total	C	O	0	0
			11	6	5		
3	9-A	1	Total	C	O	0	0
			11	6	5		
3	10-A	1	Total	C	O	0	0
			11	6	5		
3	11-A	1	Total	C	O	0	0
			11	6	5		
3	12-A	1	Total	C	O	0	0
			11	6	5		
3	13-A	1	Total	C	O	0	0
			11	6	5		
3	14-A	1	Total	C	O	0	0
			11	6	5		
3	15-A	1	Total	C	O	0	0
			11	6	5		
3	16-A	1	Total	C	O	0	0
			11	6	5		
3	17-A	1	Total	C	O	0	0
			11	6	5		
3	18-A	1	Total	C	O	0	0
			11	6	5		
3	19-A	1	Total	C	O	0	0
			11	6	5		
3	20-A	1	Total	C	O	0	0
			11	6	5		
3	21-A	1	Total	C	O	0	0
			11	6	5		
3	22-A	1	Total	C	O	0	0
			11	6	5		
3	23-A	1	Total	C	O	0	0
			11	6	5		
3	24-A	1	Total	C	O	0	0
			11	6	5		
3	25-A	1	Total	C	O	0	0
			11	6	5		
3	1-A	1	Total	C	O	0	0
			11	6	5		
3	2-A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	3-A	1	Total	C	O	0	0
			11	6	5		
3	4-A	1	Total	C	O	0	0
			11	6	5		
3	5-A	1	Total	C	O	0	0
			11	6	5		
3	6-A	1	Total	C	O	0	0
			11	6	5		
3	7-A	1	Total	C	O	0	0
			11	6	5		
3	8-A	1	Total	C	O	0	0
			11	6	5		
3	9-A	1	Total	C	O	0	0
			11	6	5		
3	10-A	1	Total	C	O	0	0
			11	6	5		
3	11-A	1	Total	C	O	0	0
			11	6	5		
3	12-A	1	Total	C	O	0	0
			11	6	5		
3	13-A	1	Total	C	O	0	0
			11	6	5		
3	14-A	1	Total	C	O	0	0
			11	6	5		
3	15-A	1	Total	C	O	0	0
			11	6	5		
3	16-A	1	Total	C	O	0	0
			11	6	5		
3	17-A	1	Total	C	O	0	0
			11	6	5		
3	18-A	1	Total	C	O	0	0
			11	6	5		
3	19-A	1	Total	C	O	0	0
			11	6	5		
3	20-A	1	Total	C	O	0	0
			11	6	5		
3	21-A	1	Total	C	O	0	0
			11	6	5		
3	22-A	1	Total	C	O	0	0
			11	6	5		
3	23-A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	24-A	1	Total	C	O	0	0
			11	6	5		
3	25-A	1	Total	C	O	0	0
			11	6	5		
3	1-A	1	Total	C	O	0	0
			12	6	6		
3	2-A	1	Total	C	O	0	0
			12	6	6		
3	3-A	1	Total	C	O	0	0
			12	6	6		
3	4-A	1	Total	C	O	0	0
			12	6	6		
3	5-A	1	Total	C	O	0	0
			12	6	6		
3	6-A	1	Total	C	O	0	0
			12	6	6		
3	7-A	1	Total	C	O	0	0
			12	6	6		
3	8-A	1	Total	C	O	0	0
			12	6	6		
3	9-A	1	Total	C	O	0	0
			12	6	6		
3	10-A	1	Total	C	O	0	0
			12	6	6		
3	11-A	1	Total	C	O	0	0
			12	6	6		
3	12-A	1	Total	C	O	0	0
			12	6	6		
3	13-A	1	Total	C	O	0	0
			12	6	6		
3	14-A	1	Total	C	O	0	0
			12	6	6		
3	15-A	1	Total	C	O	0	0
			12	6	6		
3	16-A	1	Total	C	O	0	0
			12	6	6		
3	17-A	1	Total	C	O	0	0
			12	6	6		
3	18-A	1	Total	C	O	0	0
			12	6	6		
3	19-A	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	20-A	1	Total	C	O	0	0
			12	6	6		
3	21-A	1	Total	C	O	0	0
			12	6	6		
3	22-A	1	Total	C	O	0	0
			12	6	6		
3	23-A	1	Total	C	O	0	0
			12	6	6		
3	24-A	1	Total	C	O	0	0
			12	6	6		
3	25-A	1	Total	C	O	0	0
			12	6	6		
3	1-A	1	Total	C	O	0	0
			11	6	5		
3	2-A	1	Total	C	O	0	0
			11	6	5		
3	3-A	1	Total	C	O	0	0
			11	6	5		
3	4-A	1	Total	C	O	0	0
			11	6	5		
3	5-A	1	Total	C	O	0	0
			11	6	5		
3	6-A	1	Total	C	O	0	0
			11	6	5		
3	7-A	1	Total	C	O	0	0
			11	6	5		
3	8-A	1	Total	C	O	0	0
			11	6	5		
3	9-A	1	Total	C	O	0	0
			11	6	5		
3	10-A	1	Total	C	O	0	0
			11	6	5		
3	11-A	1	Total	C	O	0	0
			11	6	5		
3	12-A	1	Total	C	O	0	0
			11	6	5		
3	13-A	1	Total	C	O	0	0
			11	6	5		
3	14-A	1	Total	C	O	0	0
			11	6	5		
3	15-A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	16-A	1	Total	C	O	0	0
			11	6	5		
3	17-A	1	Total	C	O	0	0
			11	6	5		
3	18-A	1	Total	C	O	0	0
			11	6	5		
3	19-A	1	Total	C	O	0	0
			11	6	5		
3	20-A	1	Total	C	O	0	0
			11	6	5		
3	21-A	1	Total	C	O	0	0
			11	6	5		
3	22-A	1	Total	C	O	0	0
			11	6	5		
3	23-A	1	Total	C	O	0	0
			11	6	5		
3	24-A	1	Total	C	O	0	0
			11	6	5		
3	25-A	1	Total	C	O	0	0
			11	6	5		
3	1-A	1	Total	C	O	0	0
			11	6	5		
3	2-A	1	Total	C	O	0	0
			11	6	5		
3	3-A	1	Total	C	O	0	0
			11	6	5		
3	4-A	1	Total	C	O	0	0
			11	6	5		
3	5-A	1	Total	C	O	0	0
			11	6	5		
3	6-A	1	Total	C	O	0	0
			11	6	5		
3	7-A	1	Total	C	O	0	0
			11	6	5		
3	8-A	1	Total	C	O	0	0
			11	6	5		
3	9-A	1	Total	C	O	0	0
			11	6	5		
3	10-A	1	Total	C	O	0	0
			11	6	5		
3	11-A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	12-A	1	Total	C	O	0	0
			11	6	5		
3	13-A	1	Total	C	O	0	0
			11	6	5		
3	14-A	1	Total	C	O	0	0
			11	6	5		
3	15-A	1	Total	C	O	0	0
			11	6	5		
3	16-A	1	Total	C	O	0	0
			11	6	5		
3	17-A	1	Total	C	O	0	0
			11	6	5		
3	18-A	1	Total	C	O	0	0
			11	6	5		
3	19-A	1	Total	C	O	0	0
			11	6	5		
3	20-A	1	Total	C	O	0	0
			11	6	5		
3	21-A	1	Total	C	O	0	0
			11	6	5		
3	22-A	1	Total	C	O	0	0
			11	6	5		
3	23-A	1	Total	C	O	0	0
			11	6	5		
3	24-A	1	Total	C	O	0	0
			11	6	5		
3	25-A	1	Total	C	O	0	0
			11	6	5		
3	1-A	1	Total	C	O	0	0
			11	6	5		
3	2-A	1	Total	C	O	0	0
			11	6	5		
3	3-A	1	Total	C	O	0	0
			11	6	5		
3	4-A	1	Total	C	O	0	0
			11	6	5		
3	5-A	1	Total	C	O	0	0
			11	6	5		
3	6-A	1	Total	C	O	0	0
			11	6	5		
3	7-A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	8-A	1	Total	C	O	0	0
			11	6	5		
3	9-A	1	Total	C	O	0	0
			11	6	5		
3	10-A	1	Total	C	O	0	0
			11	6	5		
3	11-A	1	Total	C	O	0	0
			11	6	5		
3	12-A	1	Total	C	O	0	0
			11	6	5		
3	13-A	1	Total	C	O	0	0
			11	6	5		
3	14-A	1	Total	C	O	0	0
			11	6	5		
3	15-A	1	Total	C	O	0	0
			11	6	5		
3	16-A	1	Total	C	O	0	0
			11	6	5		
3	17-A	1	Total	C	O	0	0
			11	6	5		
3	18-A	1	Total	C	O	0	0
			11	6	5		
3	19-A	1	Total	C	O	0	0
			11	6	5		
3	20-A	1	Total	C	O	0	0
			11	6	5		
3	21-A	1	Total	C	O	0	0
			11	6	5		
3	22-A	1	Total	C	O	0	0
			11	6	5		
3	23-A	1	Total	C	O	0	0
			11	6	5		
3	24-A	1	Total	C	O	0	0
			11	6	5		
3	25-A	1	Total	C	O	0	0
			11	6	5		
3	1-A	1	Total	C	O	0	0
			11	6	5		
3	2-A	1	Total	C	O	0	0
			11	6	5		
3	3-A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	4-A	1	Total	C	O	0	0
			11	6	5		
3	5-A	1	Total	C	O	0	0
			11	6	5		
3	6-A	1	Total	C	O	0	0
			11	6	5		
3	7-A	1	Total	C	O	0	0
			11	6	5		
3	8-A	1	Total	C	O	0	0
			11	6	5		
3	9-A	1	Total	C	O	0	0
			11	6	5		
3	10-A	1	Total	C	O	0	0
			11	6	5		
3	11-A	1	Total	C	O	0	0
			11	6	5		
3	12-A	1	Total	C	O	0	0
			11	6	5		
3	13-A	1	Total	C	O	0	0
			11	6	5		
3	14-A	1	Total	C	O	0	0
			11	6	5		
3	15-A	1	Total	C	O	0	0
			11	6	5		
3	16-A	1	Total	C	O	0	0
			11	6	5		
3	17-A	1	Total	C	O	0	0
			11	6	5		
3	18-A	1	Total	C	O	0	0
			11	6	5		
3	19-A	1	Total	C	O	0	0
			11	6	5		
3	20-A	1	Total	C	O	0	0
			11	6	5		
3	21-A	1	Total	C	O	0	0
			11	6	5		
3	22-A	1	Total	C	O	0	0
			11	6	5		
3	23-A	1	Total	C	O	0	0
			11	6	5		
3	24-A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	25-A	1	Total	C	O	0	0
			11	6	5		
3	1-A	1	Total	C	O	0	0
			11	6	5		
3	2-A	1	Total	C	O	0	0
			11	6	5		
3	3-A	1	Total	C	O	0	0
			11	6	5		
3	4-A	1	Total	C	O	0	0
			11	6	5		
3	5-A	1	Total	C	O	0	0
			11	6	5		
3	6-A	1	Total	C	O	0	0
			11	6	5		
3	7-A	1	Total	C	O	0	0
			11	6	5		
3	8-A	1	Total	C	O	0	0
			11	6	5		
3	9-A	1	Total	C	O	0	0
			11	6	5		
3	10-A	1	Total	C	O	0	0
			11	6	5		
3	11-A	1	Total	C	O	0	0
			11	6	5		
3	12-A	1	Total	C	O	0	0
			11	6	5		
3	13-A	1	Total	C	O	0	0
			11	6	5		
3	14-A	1	Total	C	O	0	0
			11	6	5		
3	15-A	1	Total	C	O	0	0
			11	6	5		
3	16-A	1	Total	C	O	0	0
			11	6	5		
3	17-A	1	Total	C	O	0	0
			11	6	5		
3	18-A	1	Total	C	O	0	0
			11	6	5		
3	19-A	1	Total	C	O	0	0
			11	6	5		
3	20-A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	21-A	1	Total	C	O	0	0
			11	6	5		
3	22-A	1	Total	C	O	0	0
			11	6	5		
3	23-A	1	Total	C	O	0	0
			11	6	5		
3	24-A	1	Total	C	O	0	0
			11	6	5		
3	25-A	1	Total	C	O	0	0
			11	6	5		
3	1-A	1	Total	C	O	0	0
			12	6	6		
3	2-A	1	Total	C	O	0	0
			12	6	6		
3	3-A	1	Total	C	O	0	0
			12	6	6		
3	4-A	1	Total	C	O	0	0
			12	6	6		
3	5-A	1	Total	C	O	0	0
			12	6	6		
3	6-A	1	Total	C	O	0	0
			12	6	6		
3	7-A	1	Total	C	O	0	0
			12	6	6		
3	8-A	1	Total	C	O	0	0
			12	6	6		
3	9-A	1	Total	C	O	0	0
			12	6	6		
3	10-A	1	Total	C	O	0	0
			12	6	6		
3	11-A	1	Total	C	O	0	0
			12	6	6		
3	12-A	1	Total	C	O	0	0
			12	6	6		
3	13-A	1	Total	C	O	0	0
			12	6	6		
3	14-A	1	Total	C	O	0	0
			12	6	6		
3	15-A	1	Total	C	O	0	0
			12	6	6		
3	16-A	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	17-A	1	Total	C	O	0	0
			12	6	6		
3	18-A	1	Total	C	O	0	0
			12	6	6		
3	19-A	1	Total	C	O	0	0
			12	6	6		
3	20-A	1	Total	C	O	0	0
			12	6	6		
3	21-A	1	Total	C	O	0	0
			12	6	6		
3	22-A	1	Total	C	O	0	0
			12	6	6		
3	23-A	1	Total	C	O	0	0
			12	6	6		
3	24-A	1	Total	C	O	0	0
			12	6	6		
3	25-A	1	Total	C	O	0	0
			12	6	6		
3	1-B	1	Total	C	O	0	0
			11	6	5		
3	2-B	1	Total	C	O	0	0
			11	6	5		
3	3-B	1	Total	C	O	0	0
			11	6	5		
3	4-B	1	Total	C	O	0	0
			11	6	5		
3	5-B	1	Total	C	O	0	0
			11	6	5		
3	6-B	1	Total	C	O	0	0
			11	6	5		
3	7-B	1	Total	C	O	0	0
			11	6	5		
3	8-B	1	Total	C	O	0	0
			11	6	5		
3	9-B	1	Total	C	O	0	0
			11	6	5		
3	10-B	1	Total	C	O	0	0
			11	6	5		
3	11-B	1	Total	C	O	0	0
			11	6	5		
3	12-B	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	13-B	1	Total	C	O	0	0
			11	6	5		
3	14-B	1	Total	C	O	0	0
			11	6	5		
3	15-B	1	Total	C	O	0	0
			11	6	5		
3	16-B	1	Total	C	O	0	0
			11	6	5		
3	17-B	1	Total	C	O	0	0
			11	6	5		
3	18-B	1	Total	C	O	0	0
			11	6	5		
3	19-B	1	Total	C	O	0	0
			11	6	5		
3	20-B	1	Total	C	O	0	0
			11	6	5		
3	21-B	1	Total	C	O	0	0
			11	6	5		
3	22-B	1	Total	C	O	0	0
			11	6	5		
3	23-B	1	Total	C	O	0	0
			11	6	5		
3	24-B	1	Total	C	O	0	0
			11	6	5		
3	25-B	1	Total	C	O	0	0
			11	6	5		
3	1-B	1	Total	C	O	0	0
			11	6	5		
3	2-B	1	Total	C	O	0	0
			11	6	5		
3	3-B	1	Total	C	O	0	0
			11	6	5		
3	4-B	1	Total	C	O	0	0
			11	6	5		
3	5-B	1	Total	C	O	0	0
			11	6	5		
3	6-B	1	Total	C	O	0	0
			11	6	5		
3	7-B	1	Total	C	O	0	0
			11	6	5		
3	8-B	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	9-B	1	Total	C	O	0	0
			11	6	5		
3	10-B	1	Total	C	O	0	0
			11	6	5		
3	11-B	1	Total	C	O	0	0
			11	6	5		
3	12-B	1	Total	C	O	0	0
			11	6	5		
3	13-B	1	Total	C	O	0	0
			11	6	5		
3	14-B	1	Total	C	O	0	0
			11	6	5		
3	15-B	1	Total	C	O	0	0
			11	6	5		
3	16-B	1	Total	C	O	0	0
			11	6	5		
3	17-B	1	Total	C	O	0	0
			11	6	5		
3	18-B	1	Total	C	O	0	0
			11	6	5		
3	19-B	1	Total	C	O	0	0
			11	6	5		
3	20-B	1	Total	C	O	0	0
			11	6	5		
3	21-B	1	Total	C	O	0	0
			11	6	5		
3	22-B	1	Total	C	O	0	0
			11	6	5		
3	23-B	1	Total	C	O	0	0
			11	6	5		
3	24-B	1	Total	C	O	0	0
			11	6	5		
3	25-B	1	Total	C	O	0	0
			11	6	5		
3	1-B	1	Total	C	O	0	0
			11	6	5		
3	2-B	1	Total	C	O	0	0
			11	6	5		
3	3-B	1	Total	C	O	0	0
			11	6	5		
3	4-B	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	5-B	1	Total	C	O	0	0
			11	6	5		
3	6-B	1	Total	C	O	0	0
			11	6	5		
3	7-B	1	Total	C	O	0	0
			11	6	5		
3	8-B	1	Total	C	O	0	0
			11	6	5		
3	9-B	1	Total	C	O	0	0
			11	6	5		
3	10-B	1	Total	C	O	0	0
			11	6	5		
3	11-B	1	Total	C	O	0	0
			11	6	5		
3	12-B	1	Total	C	O	0	0
			11	6	5		
3	13-B	1	Total	C	O	0	0
			11	6	5		
3	14-B	1	Total	C	O	0	0
			11	6	5		
3	15-B	1	Total	C	O	0	0
			11	6	5		
3	16-B	1	Total	C	O	0	0
			11	6	5		
3	17-B	1	Total	C	O	0	0
			11	6	5		
3	18-B	1	Total	C	O	0	0
			11	6	5		
3	19-B	1	Total	C	O	0	0
			11	6	5		
3	20-B	1	Total	C	O	0	0
			11	6	5		
3	21-B	1	Total	C	O	0	0
			11	6	5		
3	22-B	1	Total	C	O	0	0
			11	6	5		
3	23-B	1	Total	C	O	0	0
			11	6	5		
3	24-B	1	Total	C	O	0	0
			11	6	5		
3	25-B	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	1-B	1	Total	C	O	0	0
			11	6	5		
3	2-B	1	Total	C	O	0	0
			11	6	5		
3	3-B	1	Total	C	O	0	0
			11	6	5		
3	4-B	1	Total	C	O	0	0
			11	6	5		
3	5-B	1	Total	C	O	0	0
			11	6	5		
3	6-B	1	Total	C	O	0	0
			11	6	5		
3	7-B	1	Total	C	O	0	0
			11	6	5		
3	8-B	1	Total	C	O	0	0
			11	6	5		
3	9-B	1	Total	C	O	0	0
			11	6	5		
3	10-B	1	Total	C	O	0	0
			11	6	5		
3	11-B	1	Total	C	O	0	0
			11	6	5		
3	12-B	1	Total	C	O	0	0
			11	6	5		
3	13-B	1	Total	C	O	0	0
			11	6	5		
3	14-B	1	Total	C	O	0	0
			11	6	5		
3	15-B	1	Total	C	O	0	0
			11	6	5		
3	16-B	1	Total	C	O	0	0
			11	6	5		
3	17-B	1	Total	C	O	0	0
			11	6	5		
3	18-B	1	Total	C	O	0	0
			11	6	5		
3	19-B	1	Total	C	O	0	0
			11	6	5		
3	20-B	1	Total	C	O	0	0
			11	6	5		
3	21-B	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	22-B	1	Total	C	O	0	0
			11	6	5		
3	23-B	1	Total	C	O	0	0
			11	6	5		
3	24-B	1	Total	C	O	0	0
			11	6	5		
3	25-B	1	Total	C	O	0	0
			11	6	5		
3	1-B	1	Total	C	O	0	0
			12	6	6		
3	2-B	1	Total	C	O	0	0
			12	6	6		
3	3-B	1	Total	C	O	0	0
			12	6	6		
3	4-B	1	Total	C	O	0	0
			12	6	6		
3	5-B	1	Total	C	O	0	0
			12	6	6		
3	6-B	1	Total	C	O	0	0
			12	6	6		
3	7-B	1	Total	C	O	0	0
			12	6	6		
3	8-B	1	Total	C	O	0	0
			12	6	6		
3	9-B	1	Total	C	O	0	0
			12	6	6		
3	10-B	1	Total	C	O	0	0
			12	6	6		
3	11-B	1	Total	C	O	0	0
			12	6	6		
3	12-B	1	Total	C	O	0	0
			12	6	6		
3	13-B	1	Total	C	O	0	0
			12	6	6		
3	14-B	1	Total	C	O	0	0
			12	6	6		
3	15-B	1	Total	C	O	0	0
			12	6	6		
3	16-B	1	Total	C	O	0	0
			12	6	6		
3	17-B	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	18-B	1	Total	C	O	0	0
			12	6	6		
3	19-B	1	Total	C	O	0	0
			12	6	6		
3	20-B	1	Total	C	O	0	0
			12	6	6		
3	21-B	1	Total	C	O	0	0
			12	6	6		
3	22-B	1	Total	C	O	0	0
			12	6	6		
3	23-B	1	Total	C	O	0	0
			12	6	6		
3	24-B	1	Total	C	O	0	0
			12	6	6		
3	25-B	1	Total	C	O	0	0
			12	6	6		
3	1-B	1	Total	C	O	0	0
			11	6	5		
3	2-B	1	Total	C	O	0	0
			11	6	5		
3	3-B	1	Total	C	O	0	0
			11	6	5		
3	4-B	1	Total	C	O	0	0
			11	6	5		
3	5-B	1	Total	C	O	0	0
			11	6	5		
3	6-B	1	Total	C	O	0	0
			11	6	5		
3	7-B	1	Total	C	O	0	0
			11	6	5		
3	8-B	1	Total	C	O	0	0
			11	6	5		
3	9-B	1	Total	C	O	0	0
			11	6	5		
3	10-B	1	Total	C	O	0	0
			11	6	5		
3	11-B	1	Total	C	O	0	0
			11	6	5		
3	12-B	1	Total	C	O	0	0
			11	6	5		
3	13-B	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	14-B	1	Total	C	O	0	0
			11	6	5		
3	15-B	1	Total	C	O	0	0
			11	6	5		
3	16-B	1	Total	C	O	0	0
			11	6	5		
3	17-B	1	Total	C	O	0	0
			11	6	5		
3	18-B	1	Total	C	O	0	0
			11	6	5		
3	19-B	1	Total	C	O	0	0
			11	6	5		
3	20-B	1	Total	C	O	0	0
			11	6	5		
3	21-B	1	Total	C	O	0	0
			11	6	5		
3	22-B	1	Total	C	O	0	0
			11	6	5		
3	23-B	1	Total	C	O	0	0
			11	6	5		
3	24-B	1	Total	C	O	0	0
			11	6	5		
3	25-B	1	Total	C	O	0	0
			11	6	5		
3	1-B	1	Total	C	O	0	0
			11	6	5		
3	2-B	1	Total	C	O	0	0
			11	6	5		
3	3-B	1	Total	C	O	0	0
			11	6	5		
3	4-B	1	Total	C	O	0	0
			11	6	5		
3	5-B	1	Total	C	O	0	0
			11	6	5		
3	6-B	1	Total	C	O	0	0
			11	6	5		
3	7-B	1	Total	C	O	0	0
			11	6	5		
3	8-B	1	Total	C	O	0	0
			11	6	5		
3	9-B	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	10-B	1	Total	C	O	0	0
			11	6	5		
3	11-B	1	Total	C	O	0	0
			11	6	5		
3	12-B	1	Total	C	O	0	0
			11	6	5		
3	13-B	1	Total	C	O	0	0
			11	6	5		
3	14-B	1	Total	C	O	0	0
			11	6	5		
3	15-B	1	Total	C	O	0	0
			11	6	5		
3	16-B	1	Total	C	O	0	0
			11	6	5		
3	17-B	1	Total	C	O	0	0
			11	6	5		
3	18-B	1	Total	C	O	0	0
			11	6	5		
3	19-B	1	Total	C	O	0	0
			11	6	5		
3	20-B	1	Total	C	O	0	0
			11	6	5		
3	21-B	1	Total	C	O	0	0
			11	6	5		
3	22-B	1	Total	C	O	0	0
			11	6	5		
3	23-B	1	Total	C	O	0	0
			11	6	5		
3	24-B	1	Total	C	O	0	0
			11	6	5		
3	25-B	1	Total	C	O	0	0
			11	6	5		
3	1-B	1	Total	C	O	0	0
			11	6	5		
3	2-B	1	Total	C	O	0	0
			11	6	5		
3	3-B	1	Total	C	O	0	0
			11	6	5		
3	4-B	1	Total	C	O	0	0
			11	6	5		
3	5-B	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	6-B	1	Total	C	O	0	0
			11	6	5		
3	7-B	1	Total	C	O	0	0
			11	6	5		
3	8-B	1	Total	C	O	0	0
			11	6	5		
3	9-B	1	Total	C	O	0	0
			11	6	5		
3	10-B	1	Total	C	O	0	0
			11	6	5		
3	11-B	1	Total	C	O	0	0
			11	6	5		
3	12-B	1	Total	C	O	0	0
			11	6	5		
3	13-B	1	Total	C	O	0	0
			11	6	5		
3	14-B	1	Total	C	O	0	0
			11	6	5		
3	15-B	1	Total	C	O	0	0
			11	6	5		
3	16-B	1	Total	C	O	0	0
			11	6	5		
3	17-B	1	Total	C	O	0	0
			11	6	5		
3	18-B	1	Total	C	O	0	0
			11	6	5		
3	19-B	1	Total	C	O	0	0
			11	6	5		
3	20-B	1	Total	C	O	0	0
			11	6	5		
3	21-B	1	Total	C	O	0	0
			11	6	5		
3	22-B	1	Total	C	O	0	0
			11	6	5		
3	23-B	1	Total	C	O	0	0
			11	6	5		
3	24-B	1	Total	C	O	0	0
			11	6	5		
3	25-B	1	Total	C	O	0	0
			11	6	5		
3	1-B	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	2-B	1	Total	C	O	0	0
			11	6	5		
3	3-B	1	Total	C	O	0	0
			11	6	5		
3	4-B	1	Total	C	O	0	0
			11	6	5		
3	5-B	1	Total	C	O	0	0
			11	6	5		
3	6-B	1	Total	C	O	0	0
			11	6	5		
3	7-B	1	Total	C	O	0	0
			11	6	5		
3	8-B	1	Total	C	O	0	0
			11	6	5		
3	9-B	1	Total	C	O	0	0
			11	6	5		
3	10-B	1	Total	C	O	0	0
			11	6	5		
3	11-B	1	Total	C	O	0	0
			11	6	5		
3	12-B	1	Total	C	O	0	0
			11	6	5		
3	13-B	1	Total	C	O	0	0
			11	6	5		
3	14-B	1	Total	C	O	0	0
			11	6	5		
3	15-B	1	Total	C	O	0	0
			11	6	5		
3	16-B	1	Total	C	O	0	0
			11	6	5		
3	17-B	1	Total	C	O	0	0
			11	6	5		
3	18-B	1	Total	C	O	0	0
			11	6	5		
3	19-B	1	Total	C	O	0	0
			11	6	5		
3	20-B	1	Total	C	O	0	0
			11	6	5		
3	21-B	1	Total	C	O	0	0
			11	6	5		
3	22-B	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	23-B	1	Total	C	O	0	0
			11	6	5		
3	24-B	1	Total	C	O	0	0
			11	6	5		
3	25-B	1	Total	C	O	0	0
			11	6	5		
3	1-B	1	Total	C	O	0	0
			11	6	5		
3	2-B	1	Total	C	O	0	0
			11	6	5		
3	3-B	1	Total	C	O	0	0
			11	6	5		
3	4-B	1	Total	C	O	0	0
			11	6	5		
3	5-B	1	Total	C	O	0	0
			11	6	5		
3	6-B	1	Total	C	O	0	0
			11	6	5		
3	7-B	1	Total	C	O	0	0
			11	6	5		
3	8-B	1	Total	C	O	0	0
			11	6	5		
3	9-B	1	Total	C	O	0	0
			11	6	5		
3	10-B	1	Total	C	O	0	0
			11	6	5		
3	11-B	1	Total	C	O	0	0
			11	6	5		
3	12-B	1	Total	C	O	0	0
			11	6	5		
3	13-B	1	Total	C	O	0	0
			11	6	5		
3	14-B	1	Total	C	O	0	0
			11	6	5		
3	15-B	1	Total	C	O	0	0
			11	6	5		
3	16-B	1	Total	C	O	0	0
			11	6	5		
3	17-B	1	Total	C	O	0	0
			11	6	5		
3	18-B	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	19-B	1	Total	C	O	0	0
			11	6	5		
3	20-B	1	Total	C	O	0	0
			11	6	5		
3	21-B	1	Total	C	O	0	0
			11	6	5		
3	22-B	1	Total	C	O	0	0
			11	6	5		
3	23-B	1	Total	C	O	0	0
			11	6	5		
3	24-B	1	Total	C	O	0	0
			11	6	5		
3	25-B	1	Total	C	O	0	0
			11	6	5		
3	1-B	1	Total	C	O	0	0
			12	6	6		
3	2-B	1	Total	C	O	0	0
			12	6	6		
3	3-B	1	Total	C	O	0	0
			12	6	6		
3	4-B	1	Total	C	O	0	0
			12	6	6		
3	5-B	1	Total	C	O	0	0
			12	6	6		
3	6-B	1	Total	C	O	0	0
			12	6	6		
3	7-B	1	Total	C	O	0	0
			12	6	6		
3	8-B	1	Total	C	O	0	0
			12	6	6		
3	9-B	1	Total	C	O	0	0
			12	6	6		
3	10-B	1	Total	C	O	0	0
			12	6	6		
3	11-B	1	Total	C	O	0	0
			12	6	6		
3	12-B	1	Total	C	O	0	0
			12	6	6		
3	13-B	1	Total	C	O	0	0
			12	6	6		
3	14-B	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	15-B	1	Total	C	O	0	0
			12	6	6		
3	16-B	1	Total	C	O	0	0
			12	6	6		
3	17-B	1	Total	C	O	0	0
			12	6	6		
3	18-B	1	Total	C	O	0	0
			12	6	6		
3	19-B	1	Total	C	O	0	0
			12	6	6		
3	20-B	1	Total	C	O	0	0
			12	6	6		
3	21-B	1	Total	C	O	0	0
			12	6	6		
3	22-B	1	Total	C	O	0	0
			12	6	6		
3	23-B	1	Total	C	O	0	0
			12	6	6		
3	24-B	1	Total	C	O	0	0
			12	6	6		
3	25-B	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-A	355	Total	O	0	0
			355	355		
4	2-A	362	Total	O	0	0
			362	362		
4	3-A	360	Total	O	0	0
			360	360		
4	4-A	370	Total	O	0	0
			370	370		
4	5-A	364	Total	O	0	0
			364	364		
4	6-A	356	Total	O	0	0
			356	356		
4	7-A	325	Total	O	0	0
			325	325		
4	8-A	356	Total	O	0	0
			356	356		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	9-A	327	Total 327	O 327	0	0
4	10-A	365	Total 365	O 365	0	0
4	11-A	361	Total 361	O 361	0	0
4	12-A	360	Total 360	O 360	0	0
4	13-A	335	Total 335	O 335	0	0
4	14-A	359	Total 359	O 359	0	0
4	15-A	348	Total 348	O 348	0	0
4	16-A	369	Total 369	O 369	0	0
4	17-A	351	Total 351	O 351	0	0
4	18-A	349	Total 349	O 349	0	0
4	19-A	346	Total 346	O 346	0	0
4	20-A	324	Total 324	O 324	0	0
4	21-A	347	Total 347	O 347	0	0
4	22-A	338	Total 338	O 338	0	0
4	23-A	366	Total 366	O 366	0	0
4	24-A	364	Total 364	O 364	0	0
4	25-A	359	Total 359	O 359	0	0
4	1-B	381	Total 381	O 381	0	0
4	2-B	369	Total 369	O 369	0	0
4	3-B	348	Total 348	O 348	0	0
4	4-B	377	Total 377	O 377	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	5-B	350	Total 350	O 350	0	0
4	6-B	364	Total 364	O 364	0	0
4	7-B	377	Total 377	O 377	0	0
4	8-B	372	Total 372	O 372	0	0
4	9-B	353	Total 353	O 353	0	0
4	10-B	367	Total 367	O 367	0	0
4	11-B	357	Total 357	O 357	0	0
4	12-B	379	Total 379	O 379	0	0
4	13-B	360	Total 360	O 360	0	0
4	14-B	392	Total 392	O 392	0	0
4	15-B	373	Total 373	O 373	0	0
4	16-B	361	Total 361	O 361	0	0
4	17-B	377	Total 377	O 377	0	0
4	18-B	373	Total 373	O 373	0	0
4	19-B	355	Total 355	O 355	0	0
4	20-B	372	Total 372	O 372	0	0
4	21-B	370	Total 370	O 370	0	0
4	22-B	386	Total 386	O 386	0	0
4	23-B	332	Total 332	O 332	0	0
4	24-B	360	Total 360	O 360	0	0
4	25-B	372	Total 372	O 372	0	0

MolProbity and EDS were not executed - this section will therefore be empty.

3 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.10 Å 100.96 Å 104.18 Å 90.00° 91.10° 90.00°	Depositor
Resolution (Å)	30.30 – 1.75	Depositor
% Data completeness (in resolution range)	99.7 (30.30-1.75)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX (phenix.ensemble_refinement: 1.9_1692)	Depositor
R, R_{free}	0.122 , 0.163	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	427968	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity was not executed - this section will therefore be empty.

4.2 Too-close contacts [i](#)

MolProbity was not executed - this section will therefore be empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity was not executed - this section will therefore be empty.

4.3.2 Protein sidechains [i](#)

MolProbity was not executed - this section will therefore be empty.

4.3.3 RNA [i](#)

MolProbity was not executed - this section will therefore be empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

validation-pack and Mogul were not executed - this section will therefore be empty.

4.5 Carbohydrates [i](#)

validation-pack and Mogul were not executed - this section will therefore be empty.

4.6 Ligand geometry [i](#)

validation-pack and Mogul were not executed - this section will therefore be empty.

4.7 Other polymers [i](#)

validation-pack and Mogul were not executed - this section will therefore be empty.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

5.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

5.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

5.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.