



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:16 PM GMT

PDB ID : 4CBO
Title : Crystal structure of Complement Factor D mutant R202A after ensemble refinement
Authors : Forneris, F.; Burnley, B.T.; Gros, P.
Deposited on : 2013-10-15
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : **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 1.80 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 3 unique types of molecules in this entry. The entry contains 546299 atoms, of which 263032 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 COMPLEMENT FACTOR D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	2-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	3-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	4-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	5-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	6-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	7-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	8-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	9-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	10-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	11-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	12-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	13-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	14-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	15-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	16-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	18-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	19-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	20-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	21-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	22-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	23-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	24-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	25-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	26-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	27-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	28-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	29-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	30-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	31-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	32-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	33-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	34-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	35-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	36-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	37-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	38-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	39-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	40-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	41-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	42-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	43-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	44-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	45-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	46-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	47-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	48-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	49-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	50-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	51-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	52-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	53-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	54-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	55-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	56-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	57-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	58-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	59-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	60-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	61-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	62-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	63-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	64-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	65-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	66-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	67-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	68-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	69-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	70-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	71-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	72-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	73-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	74-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	75-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	76-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	77-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	1-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	2-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	3-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	4-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	5-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	6-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	7-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	8-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	9-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	10-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	11-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	12-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	13-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	14-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	15-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	16-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	17-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	18-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	19-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	20-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	21-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	22-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	23-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	24-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	25-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	26-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	27-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	28-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	29-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	30-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	31-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	32-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	33-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	34-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	35-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	36-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	37-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	38-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	39-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	40-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	41-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	42-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	43-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	44-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	45-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	46-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	47-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	48-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	49-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	50-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	51-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	52-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	53-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	54-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	55-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	56-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	57-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	58-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	59-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	60-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	61-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	62-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	63-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	64-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	65-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0

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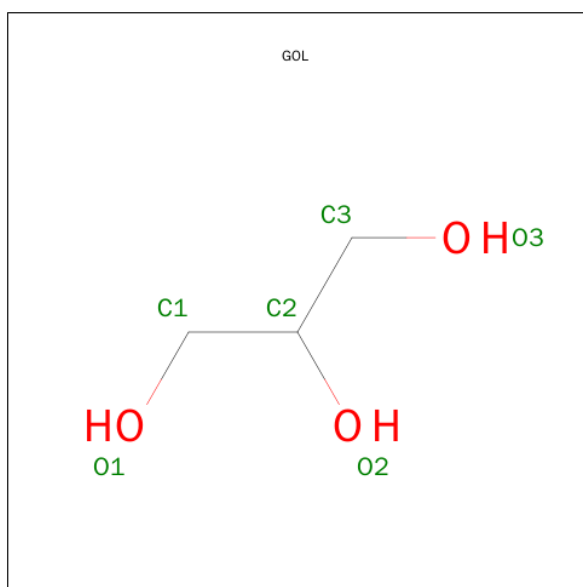
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	66-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	67-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	68-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	69-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	70-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	71-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	72-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	73-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	74-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	75-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	76-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	77-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	ALA	ARG	ENGINEERED MUTATION	UNP P00746
B	202	ALA	ARG	ENGINEERED MUTATION	UNP P00746

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	15-A	1	Total 14	C 3	H 8	O 3	0	0
2	16-A	1	Total 14	C 3	H 8	O 3	0	0
2	17-A	1	Total 14	C 3	H 8	O 3	0	0
2	18-A	1	Total 14	C 3	H 8	O 3	0	0
2	19-A	1	Total 14	C 3	H 8	O 3	0	0
2	20-A	1	Total 14	C 3	H 8	O 3	0	0
2	21-A	1	Total 14	C 3	H 8	O 3	0	0
2	22-A	1	Total 14	C 3	H 8	O 3	0	0
2	23-A	1	Total 14	C 3	H 8	O 3	0	0
2	24-A	1	Total 14	C 3	H 8	O 3	0	0
2	25-A	1	Total 14	C 3	H 8	O 3	0	0
2	26-A	1	Total 14	C 3	H 8	O 3	0	0
2	27-A	1	Total 14	C 3	H 8	O 3	0	0
2	28-A	1	Total 14	C 3	H 8	O 3	0	0
2	29-A	1	Total 14	C 3	H 8	O 3	0	0
2	30-A	1	Total 14	C 3	H 8	O 3	0	0
2	31-A	1	Total 14	C 3	H 8	O 3	0	0
2	32-A	1	Total 14	C 3	H 8	O 3	0	0
2	33-A	1	Total 14	C 3	H 8	O 3	0	0
2	34-A	1	Total 14	C 3	H 8	O 3	0	0
2	35-A	1	Total 14	C 3	H 8	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	36-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	37-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	38-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	39-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	40-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	41-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	42-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	43-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	44-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	45-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	46-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	47-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	48-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	49-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	50-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	51-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	52-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	53-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	54-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	55-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	56-A	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	57-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	58-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	59-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	60-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	61-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	62-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	63-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	64-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	65-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	66-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	67-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	68-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	69-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	70-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	71-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	72-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	73-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	74-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	75-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	76-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	77-A	1	Total	C	H	O	0	0
			14	3	8	3		

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	22-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	23-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	24-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	25-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	26-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	27-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	28-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	29-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	30-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	31-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	32-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	33-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	34-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	35-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	36-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	37-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	38-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	39-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	40-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	41-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	42-B	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	43-B	1	Total 14	C 3	H 8	O 3	0	0
2	44-B	1	Total 14	C 3	H 8	O 3	0	0
2	45-B	1	Total 14	C 3	H 8	O 3	0	0
2	46-B	1	Total 14	C 3	H 8	O 3	0	0
2	47-B	1	Total 14	C 3	H 8	O 3	0	0
2	48-B	1	Total 14	C 3	H 8	O 3	0	0
2	49-B	1	Total 14	C 3	H 8	O 3	0	0
2	50-B	1	Total 14	C 3	H 8	O 3	0	0
2	51-B	1	Total 14	C 3	H 8	O 3	0	0
2	52-B	1	Total 14	C 3	H 8	O 3	0	0
2	53-B	1	Total 14	C 3	H 8	O 3	0	0
2	54-B	1	Total 14	C 3	H 8	O 3	0	0
2	55-B	1	Total 14	C 3	H 8	O 3	0	0
2	56-B	1	Total 14	C 3	H 8	O 3	0	0
2	57-B	1	Total 14	C 3	H 8	O 3	0	0
2	58-B	1	Total 14	C 3	H 8	O 3	0	0
2	59-B	1	Total 14	C 3	H 8	O 3	0	0
2	60-B	1	Total 14	C 3	H 8	O 3	0	0
2	61-B	1	Total 14	C 3	H 8	O 3	0	0
2	62-B	1	Total 14	C 3	H 8	O 3	0	0
2	63-B	1	Total 14	C 3	H 8	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	64-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	65-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	66-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	67-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	68-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	69-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	70-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	71-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	72-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	73-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	74-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	75-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	76-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	77-B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	148	Total	O	0	0
			148	148		
3	2-A	139	Total	O	0	0
			139	139		
3	3-A	142	Total	O	0	0
			142	142		
3	4-A	129	Total	O	0	0
			129	129		
3	5-A	128	Total	O	0	1
			129	129		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	6-A	135	Total 136	O 136	0	1
3	7-A	134	Total 134	O 134	0	0
3	8-A	136	Total 136	O 136	0	0
3	9-A	138	Total 138	O 138	0	0
3	10-A	135	Total 135	O 135	0	0
3	11-A	123	Total 123	O 123	0	0
3	12-A	145	Total 145	O 145	0	0
3	13-A	164	Total 165	O 165	0	1
3	14-A	157	Total 157	O 157	0	0
3	15-A	142	Total 142	O 142	0	0
3	16-A	135	Total 135	O 135	0	0
3	17-A	142	Total 142	O 142	0	0
3	18-A	147	Total 147	O 147	0	0
3	19-A	127	Total 127	O 127	0	0
3	20-A	131	Total 131	O 131	0	0
3	21-A	144	Total 144	O 144	0	0
3	22-A	142	Total 143	O 143	0	1
3	23-A	142	Total 142	O 142	0	0
3	24-A	127	Total 127	O 127	0	0
3	25-A	136	Total 137	O 137	0	1
3	26-A	144	Total 145	O 145	0	1

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	27-A	139	Total 139	O 139	0	0
3	28-A	136	Total 137	O 137	0	1
3	29-A	134	Total 135	O 135	0	1
3	30-A	149	Total 149	O 149	0	0
3	31-A	146	Total 146	O 146	0	0
3	32-A	135	Total 135	O 135	0	0
3	33-A	133	Total 133	O 133	0	0
3	34-A	139	Total 139	O 139	0	0
3	35-A	125	Total 125	O 125	0	0
3	36-A	130	Total 130	O 130	0	0
3	37-A	138	Total 138	O 138	0	0
3	38-A	133	Total 134	O 134	0	1
3	39-A	130	Total 130	O 130	0	0
3	40-A	127	Total 128	O 128	0	1
3	41-A	139	Total 139	O 139	0	0
3	42-A	128	Total 128	O 128	0	0
3	43-A	154	Total 155	O 155	0	1
3	44-A	143	Total 143	O 143	0	0
3	45-A	140	Total 140	O 140	0	0
3	46-A	131	Total 131	O 131	0	0
3	47-A	127	Total 127	O 127	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	48-A	141	Total 141	O 141	0	0
3	49-A	121	Total 121	O 121	0	0
3	50-A	138	Total 139	O 139	0	1
3	51-A	137	Total 137	O 137	0	0
3	52-A	145	Total 145	O 145	0	0
3	53-A	141	Total 141	O 141	0	0
3	54-A	137	Total 137	O 137	0	0
3	55-A	135	Total 136	O 136	0	1
3	56-A	152	Total 153	O 153	0	1
3	57-A	124	Total 124	O 124	0	0
3	58-A	133	Total 133	O 133	0	0
3	59-A	142	Total 143	O 143	0	1
3	60-A	132	Total 132	O 132	0	0
3	61-A	138	Total 138	O 138	0	0
3	62-A	136	Total 137	O 137	0	1
3	63-A	151	Total 151	O 151	0	0
3	64-A	142	Total 142	O 142	0	0
3	65-A	148	Total 149	O 149	0	1
3	66-A	135	Total 135	O 135	0	0
3	67-A	143	Total 143	O 143	0	0
3	68-A	137	Total 137	O 137	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	69-A	131	Total 131	O 131	0	0
3	70-A	136	Total 136	O 136	0	0
3	71-A	137	Total 138	O 138	0	1
3	72-A	135	Total 135	O 135	0	0
3	73-A	134	Total 134	O 134	0	0
3	74-A	153	Total 153	O 153	0	0
3	75-A	147	Total 147	O 147	0	0
3	76-A	145	Total 145	O 145	0	0
3	77-A	131	Total 131	O 131	0	0
3	1-B	113	Total 113	O 113	0	0
3	2-B	122	Total 122	O 122	0	0
3	3-B	96	Total 96	O 96	0	0
3	4-B	108	Total 108	O 108	0	0
3	5-B	109	Total 109	O 109	0	0
3	6-B	111	Total 111	O 111	0	0
3	7-B	111	Total 111	O 111	0	0
3	8-B	104	Total 104	O 104	0	0
3	9-B	118	Total 119	O 119	0	1
3	10-B	117	Total 117	O 117	0	0
3	11-B	118	Total 118	O 118	0	0
3	12-B	114	Total 115	O 115	0	1

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	13-B	109	Total 109	O 109	0	0
3	14-B	115	Total 115	O 115	0	0
3	15-B	113	Total 113	O 113	0	0
3	16-B	117	Total 117	O 117	0	0
3	17-B	121	Total 122	O 122	0	1
3	18-B	111	Total 111	O 111	0	0
3	19-B	117	Total 117	O 117	0	0
3	20-B	122	Total 123	O 123	0	1
3	21-B	103	Total 103	O 103	0	0
3	22-B	122	Total 122	O 122	0	0
3	23-B	113	Total 113	O 113	0	0
3	24-B	116	Total 116	O 116	0	0
3	25-B	120	Total 120	O 120	0	0
3	26-B	114	Total 114	O 114	0	0
3	27-B	114	Total 114	O 114	0	0
3	28-B	123	Total 123	O 123	0	0
3	29-B	132	Total 132	O 132	0	0
3	30-B	115	Total 115	O 115	0	0
3	31-B	117	Total 117	O 117	0	0
3	32-B	127	Total 127	O 127	0	0
3	33-B	119	Total 119	O 119	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	34-B	109	Total 109	O 109	0	0
3	35-B	102	Total 102	O 102	0	0
3	36-B	119	Total 120	O 120	0	1
3	37-B	110	Total 110	O 110	0	0
3	38-B	118	Total 118	O 118	0	0
3	39-B	112	Total 112	O 112	0	0
3	40-B	118	Total 118	O 118	0	0
3	41-B	106	Total 106	O 106	0	0
3	42-B	123	Total 124	O 124	0	1
3	43-B	125	Total 125	O 125	0	0
3	44-B	118	Total 118	O 118	0	0
3	45-B	108	Total 108	O 108	0	0
3	46-B	105	Total 105	O 105	0	0
3	47-B	117	Total 118	O 118	0	1
3	48-B	128	Total 129	O 129	0	1
3	49-B	109	Total 109	O 109	0	0
3	50-B	111	Total 111	O 111	0	0
3	51-B	130	Total 131	O 131	0	1
3	52-B	119	Total 119	O 119	0	0
3	53-B	113	Total 113	O 113	0	0
3	54-B	109	Total 109	O 109	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	55-B	120	Total 120	O 120	0	0
3	56-B	127	Total 127	O 127	0	0
3	57-B	122	Total 122	O 122	0	0
3	58-B	121	Total 122	O 122	0	1
3	59-B	117	Total 117	O 117	0	0
3	60-B	116	Total 116	O 116	0	0
3	61-B	118	Total 119	O 119	0	1
3	62-B	121	Total 121	O 121	0	0
3	63-B	122	Total 123	O 123	0	1
3	64-B	121	Total 121	O 121	0	0
3	65-B	128	Total 128	O 128	0	0
3	66-B	112	Total 112	O 112	0	0
3	67-B	124	Total 125	O 125	0	1
3	68-B	126	Total 126	O 126	0	0
3	69-B	112	Total 112	O 112	0	0
3	70-B	122	Total 123	O 123	0	1
3	71-B	122	Total 122	O 122	0	0
3	72-B	121	Total 121	O 121	0	0
3	73-B	131	Total 132	O 132	0	1
3	74-B	113	Total 113	O 113	0	0
3	75-B	111	Total 111	O 111	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	76-B	105	Total	O	0	0
			105	105		
3	77-B	119	Total	O	0	0
			119	119		

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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.14Å 67.31Å 133.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.33 – 1.80	Depositor
% Data completeness (in resolution range)	98.7 (47.33-1.80)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX (PHENIX.ENSEMBLE_REFINEMENT: DEV_1259)	Depositor
R, R_{free}	0.163 , 0.212	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	546299	wwPDB-V
Average B, all atoms (Å ²)	26.0	wwPDB-V

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 [i](#)

5.1 Protein, DNA and RNA chains [i](#)

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

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

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

5.3 Carbohydrates [i](#)

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

5.4 Ligands [i](#)

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

5.5 Other polymers [i](#)

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