



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 9, 2025 – 02:56 pm BST

PDB ID : 9RP2 / pdb\_00009rp2  
Title : Ensemble refined structure of CotB2 F107A in complex with alendronate  
Authors : Helmer, C.P.O.; Loll, B.  
Deposited on : 2025-06-23  
Resolution : 1.93 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : **FAILED**  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

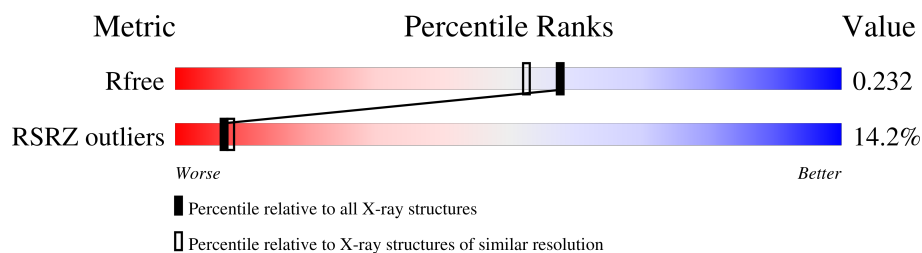
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.93 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1306 (1.94-1.94)
RSRZ outliers	164620	1306 (1.94-1.94)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 261865 atoms, of which 0 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 Cyclooctat-9-en-7-ol synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	2-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	3-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	4-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	5-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	6-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	7-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	8-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	9-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	10-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	11-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	12-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	13-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	14-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	15-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	16-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	17-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	18-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	19-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	20-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	21-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	22-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	23-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	24-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	25-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	26-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	27-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	28-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	29-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	30-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	31-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	32-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	33-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	34-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	35-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	36-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	37-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	38-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	39-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	40-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	41-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	42-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	43-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	44-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	45-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	46-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	47-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	48-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	49-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	50-A	295	Total	C	N	O	S	0	0	0
			2403	1525	408	453	17			
1	1-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	2-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	3-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	4-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	5-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	6-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	7-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	8-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	9-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	10-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	11-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	12-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	13-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	14-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	15-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	16-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	17-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	18-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	19-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	20-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	21-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	22-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	23-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	24-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	25-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	26-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	27-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	28-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	29-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			

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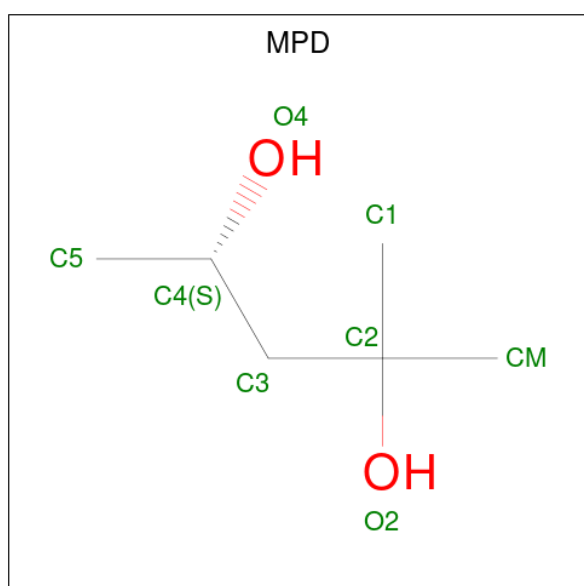
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	30-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	31-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	32-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	33-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	34-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	35-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	36-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	37-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	38-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	39-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	40-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	41-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	42-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	43-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	44-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	45-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	46-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	47-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	48-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	49-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			
1	50-B	296	Total	C	N	O	S	0	0	0
			2414	1532	409	456	17			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	ALA	PHE	engineered mutation	UNP C9K1X5
A	308	ALA	-	expression tag	UNP C9K1X5
A	309	ALA	-	expression tag	UNP C9K1X5
A	310	ALA	-	expression tag	UNP C9K1X5
A	311	LEU	-	expression tag	UNP C9K1X5
A	312	GLU	-	expression tag	UNP C9K1X5
A	313	HIS	-	expression tag	UNP C9K1X5
A	314	HIS	-	expression tag	UNP C9K1X5
A	315	HIS	-	expression tag	UNP C9K1X5
A	316	HIS	-	expression tag	UNP C9K1X5
A	317	HIS	-	expression tag	UNP C9K1X5
A	318	HIS	-	expression tag	UNP C9K1X5
B	107	ALA	PHE	engineered mutation	UNP C9K1X5
B	308	ALA	-	expression tag	UNP C9K1X5
B	309	ALA	-	expression tag	UNP C9K1X5
B	310	ALA	-	expression tag	UNP C9K1X5
B	311	LEU	-	expression tag	UNP C9K1X5
B	312	GLU	-	expression tag	UNP C9K1X5
B	313	HIS	-	expression tag	UNP C9K1X5
B	314	HIS	-	expression tag	UNP C9K1X5
B	315	HIS	-	expression tag	UNP C9K1X5
B	316	HIS	-	expression tag	UNP C9K1X5
B	317	HIS	-	expression tag	UNP C9K1X5
B	318	HIS	-	expression tag	UNP C9K1X5

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).





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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	23-A	1	Total	C	O	0	0
			8	6	2		
2	24-A	1	Total	C	O	0	0
			8	6	2		
2	25-A	1	Total	C	O	0	0
			8	6	2		
2	26-A	1	Total	C	O	0	0
			8	6	2		
2	27-A	1	Total	C	O	0	0
			8	6	2		
2	28-A	1	Total	C	O	0	0
			8	6	2		
2	29-A	1	Total	C	O	0	0
			8	6	2		
2	30-A	1	Total	C	O	0	0
			8	6	2		
2	31-A	1	Total	C	O	0	0
			8	6	2		
2	32-A	1	Total	C	O	0	0
			8	6	2		
2	33-A	1	Total	C	O	0	0
			8	6	2		
2	34-A	1	Total	C	O	0	0
			8	6	2		
2	35-A	1	Total	C	O	0	0
			8	6	2		
2	36-A	1	Total	C	O	0	0
			8	6	2		
2	37-A	1	Total	C	O	0	0
			8	6	2		
2	38-A	1	Total	C	O	0	0
			8	6	2		
2	39-A	1	Total	C	O	0	0
			8	6	2		
2	40-A	1	Total	C	O	0	0
			8	6	2		
2	41-A	1	Total	C	O	0	0
			8	6	2		
2	42-A	1	Total	C	O	0	0
			8	6	2		
2	43-A	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	44-A	1	Total	C	O	0	0
			8	6	2		
2	45-A	1	Total	C	O	0	0
			8	6	2		
2	46-A	1	Total	C	O	0	0
			8	6	2		
2	47-A	1	Total	C	O	0	0
			8	6	2		
2	48-A	1	Total	C	O	0	0
			8	6	2		
2	49-A	1	Total	C	O	0	0
			8	6	2		
2	50-A	1	Total	C	O	0	0
			8	6	2		
2	1-A	1	Total	C	O	0	0
			8	6	2		
2	2-A	1	Total	C	O	0	0
			8	6	2		
2	3-A	1	Total	C	O	0	0
			8	6	2		
2	4-A	1	Total	C	O	0	0
			8	6	2		
2	5-A	1	Total	C	O	0	0
			8	6	2		
2	6-A	1	Total	C	O	0	0
			8	6	2		
2	7-A	1	Total	C	O	0	0
			8	6	2		
2	8-A	1	Total	C	O	0	0
			8	6	2		
2	9-A	1	Total	C	O	0	0
			8	6	2		
2	10-A	1	Total	C	O	0	0
			8	6	2		
2	11-A	1	Total	C	O	0	0
			8	6	2		
2	12-A	1	Total	C	O	0	0
			8	6	2		
2	13-A	1	Total	C	O	0	0
			8	6	2		
2	14-A	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	15-A	1	Total	C	O	0	0
			8	6	2		
2	16-A	1	Total	C	O	0	0
			8	6	2		
2	17-A	1	Total	C	O	0	0
			8	6	2		
2	18-A	1	Total	C	O	0	0
			8	6	2		
2	19-A	1	Total	C	O	0	0
			8	6	2		
2	20-A	1	Total	C	O	0	0
			8	6	2		
2	21-A	1	Total	C	O	0	0
			8	6	2		
2	22-A	1	Total	C	O	0	0
			8	6	2		
2	23-A	1	Total	C	O	0	0
			8	6	2		
2	24-A	1	Total	C	O	0	0
			8	6	2		
2	25-A	1	Total	C	O	0	0
			8	6	2		
2	26-A	1	Total	C	O	0	0
			8	6	2		
2	27-A	1	Total	C	O	0	0
			8	6	2		
2	28-A	1	Total	C	O	0	0
			8	6	2		
2	29-A	1	Total	C	O	0	0
			8	6	2		
2	30-A	1	Total	C	O	0	0
			8	6	2		
2	31-A	1	Total	C	O	0	0
			8	6	2		
2	32-A	1	Total	C	O	0	0
			8	6	2		
2	33-A	1	Total	C	O	0	0
			8	6	2		
2	34-A	1	Total	C	O	0	0
			8	6	2		
2	35-A	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	36-A	1	Total	C	O	0	0
			8	6	2		
2	37-A	1	Total	C	O	0	0
			8	6	2		
2	38-A	1	Total	C	O	0	0
			8	6	2		
2	39-A	1	Total	C	O	0	0
			8	6	2		
2	40-A	1	Total	C	O	0	0
			8	6	2		
2	41-A	1	Total	C	O	0	0
			8	6	2		
2	42-A	1	Total	C	O	0	0
			8	6	2		
2	43-A	1	Total	C	O	0	0
			8	6	2		
2	44-A	1	Total	C	O	0	0
			8	6	2		
2	45-A	1	Total	C	O	0	0
			8	6	2		
2	46-A	1	Total	C	O	0	0
			8	6	2		
2	47-A	1	Total	C	O	0	0
			8	6	2		
2	48-A	1	Total	C	O	0	0
			8	6	2		
2	49-A	1	Total	C	O	0	0
			8	6	2		
2	50-A	1	Total	C	O	0	0
			8	6	2		
2	1-B	1	Total	C	O	0	0
			8	6	2		
2	2-B	1	Total	C	O	0	0
			8	6	2		
2	3-B	1	Total	C	O	0	0
			8	6	2		
2	4-B	1	Total	C	O	0	0
			8	6	2		
2	5-B	1	Total	C	O	0	0
			8	6	2		
2	6-B	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	7-B	1	Total	C	O	0	0
			8	6	2		
2	8-B	1	Total	C	O	0	0
			8	6	2		
2	9-B	1	Total	C	O	0	0
			8	6	2		
2	10-B	1	Total	C	O	0	0
			8	6	2		
2	11-B	1	Total	C	O	0	0
			8	6	2		
2	12-B	1	Total	C	O	0	0
			8	6	2		
2	13-B	1	Total	C	O	0	0
			8	6	2		
2	14-B	1	Total	C	O	0	0
			8	6	2		
2	15-B	1	Total	C	O	0	0
			8	6	2		
2	16-B	1	Total	C	O	0	0
			8	6	2		
2	17-B	1	Total	C	O	0	0
			8	6	2		
2	18-B	1	Total	C	O	0	0
			8	6	2		
2	19-B	1	Total	C	O	0	0
			8	6	2		
2	20-B	1	Total	C	O	0	0
			8	6	2		
2	21-B	1	Total	C	O	0	0
			8	6	2		
2	22-B	1	Total	C	O	0	0
			8	6	2		
2	23-B	1	Total	C	O	0	0
			8	6	2		
2	24-B	1	Total	C	O	0	0
			8	6	2		
2	25-B	1	Total	C	O	0	0
			8	6	2		
2	26-B	1	Total	C	O	0	0
			8	6	2		
2	27-B	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	28-B	1	Total	C	O	0	0
			8	6	2		
2	29-B	1	Total	C	O	0	0
			8	6	2		
2	30-B	1	Total	C	O	0	0
			8	6	2		
2	31-B	1	Total	C	O	0	0
			8	6	2		
2	32-B	1	Total	C	O	0	0
			8	6	2		
2	33-B	1	Total	C	O	0	0
			8	6	2		
2	34-B	1	Total	C	O	0	0
			8	6	2		
2	35-B	1	Total	C	O	0	0
			8	6	2		
2	36-B	1	Total	C	O	0	0
			8	6	2		
2	37-B	1	Total	C	O	0	0
			8	6	2		
2	38-B	1	Total	C	O	0	0
			8	6	2		
2	39-B	1	Total	C	O	0	0
			8	6	2		
2	40-B	1	Total	C	O	0	0
			8	6	2		
2	41-B	1	Total	C	O	0	0
			8	6	2		
2	42-B	1	Total	C	O	0	0
			8	6	2		
2	43-B	1	Total	C	O	0	0
			8	6	2		
2	44-B	1	Total	C	O	0	0
			8	6	2		
2	45-B	1	Total	C	O	0	0
			8	6	2		
2	46-B	1	Total	C	O	0	0
			8	6	2		
2	47-B	1	Total	C	O	0	0
			8	6	2		
2	48-B	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	49-B	1	Total	C	O	0	0
			8	6	2		
2	50-B	1	Total	C	O	0	0
			8	6	2		
2	1-B	1	Total	C	O	0	0
			8	6	2		
2	2-B	1	Total	C	O	0	0
			8	6	2		
2	3-B	1	Total	C	O	0	0
			8	6	2		
2	4-B	1	Total	C	O	0	0
			8	6	2		
2	5-B	1	Total	C	O	0	0
			8	6	2		
2	6-B	1	Total	C	O	0	0
			8	6	2		
2	7-B	1	Total	C	O	0	0
			8	6	2		
2	8-B	1	Total	C	O	0	0
			8	6	2		
2	9-B	1	Total	C	O	0	0
			8	6	2		
2	10-B	1	Total	C	O	0	0
			8	6	2		
2	11-B	1	Total	C	O	0	0
			8	6	2		
2	12-B	1	Total	C	O	0	0
			8	6	2		
2	13-B	1	Total	C	O	0	0
			8	6	2		
2	14-B	1	Total	C	O	0	0
			8	6	2		
2	15-B	1	Total	C	O	0	0
			8	6	2		
2	16-B	1	Total	C	O	0	0
			8	6	2		
2	17-B	1	Total	C	O	0	0
			8	6	2		
2	18-B	1	Total	C	O	0	0
			8	6	2		
2	19-B	1	Total	C	O	0	0
			8	6	2		

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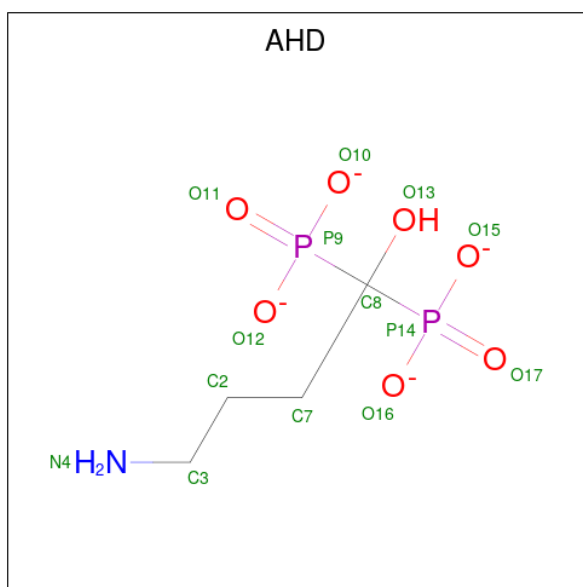
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	20-B	1	Total	C	O	0	0
			8	6	2		
2	21-B	1	Total	C	O	0	0
			8	6	2		
2	22-B	1	Total	C	O	0	0
			8	6	2		
2	23-B	1	Total	C	O	0	0
			8	6	2		
2	24-B	1	Total	C	O	0	0
			8	6	2		
2	25-B	1	Total	C	O	0	0
			8	6	2		
2	26-B	1	Total	C	O	0	0
			8	6	2		
2	27-B	1	Total	C	O	0	0
			8	6	2		
2	28-B	1	Total	C	O	0	0
			8	6	2		
2	29-B	1	Total	C	O	0	0
			8	6	2		
2	30-B	1	Total	C	O	0	0
			8	6	2		
2	31-B	1	Total	C	O	0	0
			8	6	2		
2	32-B	1	Total	C	O	0	0
			8	6	2		
2	33-B	1	Total	C	O	0	0
			8	6	2		
2	34-B	1	Total	C	O	0	0
			8	6	2		
2	35-B	1	Total	C	O	0	0
			8	6	2		
2	36-B	1	Total	C	O	0	0
			8	6	2		
2	37-B	1	Total	C	O	0	0
			8	6	2		
2	38-B	1	Total	C	O	0	0
			8	6	2		
2	39-B	1	Total	C	O	0	0
			8	6	2		
2	40-B	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	41-B	1	Total	C	O	0	0
			8	6	2		
2	42-B	1	Total	C	O	0	0
			8	6	2		
2	43-B	1	Total	C	O	0	0
			8	6	2		
2	44-B	1	Total	C	O	0	0
			8	6	2		
2	45-B	1	Total	C	O	0	0
			8	6	2		
2	46-B	1	Total	C	O	0	0
			8	6	2		
2	47-B	1	Total	C	O	0	0
			8	6	2		
2	48-B	1	Total	C	O	0	0
			8	6	2		
2	49-B	1	Total	C	O	0	0
			8	6	2		
2	50-B	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is 4-AMINO-1-HYDROXYBUTANE-1,1-DIYLDIPHOSPHONATE (CCD ID: AHD) (formula:  $C_4H_9NO_7P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	1-A	1	Total	C	N	O	P	0	0
			14	4	1	7	2		

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	23-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	24-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	25-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	26-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	27-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	28-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	29-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	30-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	31-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	32-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	33-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	34-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	35-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	36-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	37-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	38-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	39-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	40-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	41-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	42-A	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	43-A	1	Total 14	C 4	N 1	O 7	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	44-A	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	45-A	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	46-A	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	47-A	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	48-A	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	49-A	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	50-A	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	1-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	2-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	3-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	4-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	5-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	6-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	7-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	8-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	9-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	10-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	11-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	12-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	13-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	14-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	15-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	16-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	17-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	18-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	19-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	20-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	21-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	22-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	23-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	24-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	25-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	26-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	27-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	28-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	29-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	30-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	31-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	32-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	33-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	34-B	1	Total 14	C 4	N 1	O 7	P 2	0	0
3	35-B	1	Total 14	C 4	N 1	O 7	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	36-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	37-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	38-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	39-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	40-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	41-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	42-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	43-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	44-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	45-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	46-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	47-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	48-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	49-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
3	50-B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-A	3	Total	Mg	0	0
			3	3		
4	2-A	3	Total	Mg	0	0
			3	3		
4	3-A	3	Total	Mg	0	0
			3	3		
4	4-A	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	5-A	3	Total 3	Mg 3	0	0
4	6-A	3	Total 3	Mg 3	0	0
4	7-A	3	Total 3	Mg 3	0	0
4	8-A	3	Total 3	Mg 3	0	0
4	9-A	3	Total 3	Mg 3	0	0
4	10-A	3	Total 3	Mg 3	0	0
4	11-A	3	Total 3	Mg 3	0	0
4	12-A	3	Total 3	Mg 3	0	0
4	13-A	3	Total 3	Mg 3	0	0
4	14-A	3	Total 3	Mg 3	0	0
4	15-A	3	Total 3	Mg 3	0	0
4	16-A	3	Total 3	Mg 3	0	0
4	17-A	3	Total 3	Mg 3	0	0
4	18-A	3	Total 3	Mg 3	0	0
4	19-A	3	Total 3	Mg 3	0	0
4	20-A	3	Total 3	Mg 3	0	0
4	21-A	3	Total 3	Mg 3	0	0
4	22-A	3	Total 3	Mg 3	0	0
4	23-A	3	Total 3	Mg 3	0	0
4	24-A	3	Total 3	Mg 3	0	0
4	25-A	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	26-A	3	Total 3	Mg 3	0	0
4	27-A	3	Total 3	Mg 3	0	0
4	28-A	3	Total 3	Mg 3	0	0
4	29-A	3	Total 3	Mg 3	0	0
4	30-A	3	Total 3	Mg 3	0	0
4	31-A	3	Total 3	Mg 3	0	0
4	32-A	3	Total 3	Mg 3	0	0
4	33-A	3	Total 3	Mg 3	0	0
4	34-A	3	Total 3	Mg 3	0	0
4	35-A	3	Total 3	Mg 3	0	0
4	36-A	3	Total 3	Mg 3	0	0
4	37-A	3	Total 3	Mg 3	0	0
4	38-A	3	Total 3	Mg 3	0	0
4	39-A	3	Total 3	Mg 3	0	0
4	40-A	3	Total 3	Mg 3	0	0
4	41-A	3	Total 3	Mg 3	0	0
4	42-A	3	Total 3	Mg 3	0	0
4	43-A	3	Total 3	Mg 3	0	0
4	44-A	3	Total 3	Mg 3	0	0
4	45-A	3	Total 3	Mg 3	0	0
4	46-A	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	47-A	3	Total 3	Mg 3	0	0
4	48-A	3	Total 3	Mg 3	0	0
4	49-A	3	Total 3	Mg 3	0	0
4	50-A	3	Total 3	Mg 3	0	0
4	1-B	3	Total 3	Mg 3	0	0
4	2-B	3	Total 3	Mg 3	0	0
4	3-B	3	Total 3	Mg 3	0	0
4	4-B	3	Total 3	Mg 3	0	0
4	5-B	3	Total 3	Mg 3	0	0
4	6-B	3	Total 3	Mg 3	0	0
4	7-B	3	Total 3	Mg 3	0	0
4	8-B	3	Total 3	Mg 3	0	0
4	9-B	3	Total 3	Mg 3	0	0
4	10-B	3	Total 3	Mg 3	0	0
4	11-B	3	Total 3	Mg 3	0	0
4	12-B	3	Total 3	Mg 3	0	0
4	13-B	3	Total 3	Mg 3	0	0
4	14-B	3	Total 3	Mg 3	0	0
4	15-B	3	Total 3	Mg 3	0	0
4	16-B	3	Total 3	Mg 3	0	0
4	17-B	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	18-B	3	Total 3	Mg 3	0	0
4	19-B	3	Total 3	Mg 3	0	0
4	20-B	3	Total 3	Mg 3	0	0
4	21-B	3	Total 3	Mg 3	0	0
4	22-B	3	Total 3	Mg 3	0	0
4	23-B	3	Total 3	Mg 3	0	0
4	24-B	3	Total 3	Mg 3	0	0
4	25-B	3	Total 3	Mg 3	0	0
4	26-B	3	Total 3	Mg 3	0	0
4	27-B	3	Total 3	Mg 3	0	0
4	28-B	3	Total 3	Mg 3	0	0
4	29-B	3	Total 3	Mg 3	0	0
4	30-B	3	Total 3	Mg 3	0	0
4	31-B	3	Total 3	Mg 3	0	0
4	32-B	3	Total 3	Mg 3	0	0
4	33-B	3	Total 3	Mg 3	0	0
4	34-B	3	Total 3	Mg 3	0	0
4	35-B	3	Total 3	Mg 3	0	0
4	36-B	3	Total 3	Mg 3	0	0
4	37-B	3	Total 3	Mg 3	0	0
4	38-B	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	39-B	3	Total 3	Mg 3	0	0
4	40-B	3	Total 3	Mg 3	0	0
4	41-B	3	Total 3	Mg 3	0	0
4	42-B	3	Total 3	Mg 3	0	0
4	43-B	3	Total 3	Mg 3	0	0
4	44-B	3	Total 3	Mg 3	0	0
4	45-B	3	Total 3	Mg 3	0	0
4	46-B	3	Total 3	Mg 3	0	0
4	47-B	3	Total 3	Mg 3	0	0
4	48-B	3	Total 3	Mg 3	0	0
4	49-B	3	Total 3	Mg 3	0	0
4	50-B	3	Total 3	Mg 3	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1-A	1	Total 1	Cl 1	0	0
5	2-A	1	Total 1	Cl 1	0	0
5	3-A	1	Total 1	Cl 1	0	0
5	4-A	1	Total 1	Cl 1	0	0
5	5-A	1	Total 1	Cl 1	0	0
5	6-A	1	Total 1	Cl 1	0	0
5	7-A	1	Total 1	Cl 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	8-A	1	Total 1	Cl 1	0	0
5	9-A	1	Total 1	Cl 1	0	0
5	10-A	1	Total 1	Cl 1	0	0
5	11-A	1	Total 1	Cl 1	0	0
5	12-A	1	Total 1	Cl 1	0	0
5	13-A	1	Total 1	Cl 1	0	0
5	14-A	1	Total 1	Cl 1	0	0
5	15-A	1	Total 1	Cl 1	0	0
5	16-A	1	Total 1	Cl 1	0	0
5	17-A	1	Total 1	Cl 1	0	0
5	18-A	1	Total 1	Cl 1	0	0
5	19-A	1	Total 1	Cl 1	0	0
5	20-A	1	Total 1	Cl 1	0	0
5	21-A	1	Total 1	Cl 1	0	0
5	22-A	1	Total 1	Cl 1	0	0
5	23-A	1	Total 1	Cl 1	0	0
5	24-A	1	Total 1	Cl 1	0	0
5	25-A	1	Total 1	Cl 1	0	0
5	26-A	1	Total 1	Cl 1	0	0
5	27-A	1	Total 1	Cl 1	0	0
5	28-A	1	Total 1	Cl 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	29-A	1	Total	Cl	0	0
			1	1		
5	30-A	1	Total	Cl	0	0
			1	1		
5	31-A	1	Total	Cl	0	0
			1	1		
5	32-A	1	Total	Cl	0	0
			1	1		
5	33-A	1	Total	Cl	0	0
			1	1		
5	34-A	1	Total	Cl	0	0
			1	1		
5	35-A	1	Total	Cl	0	0
			1	1		
5	36-A	1	Total	Cl	0	0
			1	1		
5	37-A	1	Total	Cl	0	0
			1	1		
5	38-A	1	Total	Cl	0	0
			1	1		
5	39-A	1	Total	Cl	0	0
			1	1		
5	40-A	1	Total	Cl	0	0
			1	1		
5	41-A	1	Total	Cl	0	0
			1	1		
5	42-A	1	Total	Cl	0	0
			1	1		
5	43-A	1	Total	Cl	0	0
			1	1		
5	44-A	1	Total	Cl	0	0
			1	1		
5	45-A	1	Total	Cl	0	0
			1	1		
5	46-A	1	Total	Cl	0	0
			1	1		
5	47-A	1	Total	Cl	0	0
			1	1		
5	48-A	1	Total	Cl	0	0
			1	1		
5	49-A	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	50-A	1	Total 1	Cl 1	0	0
5	1-B	1	Total 1	Cl 1	0	0
5	2-B	1	Total 1	Cl 1	0	0
5	3-B	1	Total 1	Cl 1	0	0
5	4-B	1	Total 1	Cl 1	0	0
5	5-B	1	Total 1	Cl 1	0	0
5	6-B	1	Total 1	Cl 1	0	0
5	7-B	1	Total 1	Cl 1	0	0
5	8-B	1	Total 1	Cl 1	0	0
5	9-B	1	Total 1	Cl 1	0	0
5	10-B	1	Total 1	Cl 1	0	0
5	11-B	1	Total 1	Cl 1	0	0
5	12-B	1	Total 1	Cl 1	0	0
5	13-B	1	Total 1	Cl 1	0	0
5	14-B	1	Total 1	Cl 1	0	0
5	15-B	1	Total 1	Cl 1	0	0
5	16-B	1	Total 1	Cl 1	0	0
5	17-B	1	Total 1	Cl 1	0	0
5	18-B	1	Total 1	Cl 1	0	0
5	19-B	1	Total 1	Cl 1	0	0
5	20-B	1	Total 1	Cl 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	21-B	1	Total 1	Cl 1	0	0
5	22-B	1	Total 1	Cl 1	0	0
5	23-B	1	Total 1	Cl 1	0	0
5	24-B	1	Total 1	Cl 1	0	0
5	25-B	1	Total 1	Cl 1	0	0
5	26-B	1	Total 1	Cl 1	0	0
5	27-B	1	Total 1	Cl 1	0	0
5	28-B	1	Total 1	Cl 1	0	0
5	29-B	1	Total 1	Cl 1	0	0
5	30-B	1	Total 1	Cl 1	0	0
5	31-B	1	Total 1	Cl 1	0	0
5	32-B	1	Total 1	Cl 1	0	0
5	33-B	1	Total 1	Cl 1	0	0
5	34-B	1	Total 1	Cl 1	0	0
5	35-B	1	Total 1	Cl 1	0	0
5	36-B	1	Total 1	Cl 1	0	0
5	37-B	1	Total 1	Cl 1	0	0
5	38-B	1	Total 1	Cl 1	0	0
5	39-B	1	Total 1	Cl 1	0	0
5	40-B	1	Total 1	Cl 1	0	0
5	41-B	1	Total 1	Cl 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	42-B	1	Total 1	Cl 1	0	0
5	43-B	1	Total 1	Cl 1	0	0
5	44-B	1	Total 1	Cl 1	0	0
5	45-B	1	Total 1	Cl 1	0	0
5	46-B	1	Total 1	Cl 1	0	0
5	47-B	1	Total 1	Cl 1	0	0
5	48-B	1	Total 1	Cl 1	0	0
5	49-B	1	Total 1	Cl 1	0	0
5	50-B	1	Total 1	Cl 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1-A	232	Total 232	O 232	0	0
6	2-A	241	Total 241	O 241	0	0
6	3-A	242	Total 242	O 242	0	0
6	4-A	221	Total 221	O 221	0	0
6	5-A	236	Total 236	O 236	0	0
6	6-A	239	Total 239	O 239	0	0
6	7-A	228	Total 228	O 228	0	0
6	8-A	226	Total 226	O 226	0	0
6	9-A	229	Total 229	O 229	0	0
6	10-A	234	Total 234	O 234	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	11-A	236	Total 236	O 236	0	0
6	12-A	221	Total 221	O 221	0	0
6	13-A	221	Total 221	O 221	0	0
6	14-A	229	Total 229	O 229	0	0
6	15-A	230	Total 230	O 230	0	0
6	16-A	246	Total 246	O 246	0	0
6	17-A	229	Total 229	O 229	0	0
6	18-A	234	Total 234	O 234	0	0
6	19-A	231	Total 231	O 231	0	0
6	20-A	226	Total 226	O 226	0	0
6	21-A	227	Total 227	O 227	0	0
6	22-A	238	Total 238	O 238	0	0
6	23-A	236	Total 236	O 236	0	0
6	24-A	221	Total 221	O 221	0	0
6	25-A	230	Total 230	O 230	0	0
6	26-A	230	Total 230	O 230	0	0
6	27-A	236	Total 236	O 236	0	0
6	28-A	222	Total 222	O 222	0	0
6	29-A	222	Total 222	O 222	0	0
6	30-A	227	Total 227	O 227	0	0
6	31-A	211	Total 211	O 211	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	32-A	227	Total 227	O 227	0	0
6	33-A	224	Total 224	O 224	0	0
6	34-A	240	Total 240	O 240	0	0
6	35-A	231	Total 231	O 231	0	0
6	36-A	225	Total 225	O 225	0	0
6	37-A	221	Total 221	O 221	0	0
6	38-A	225	Total 225	O 225	0	0
6	39-A	235	Total 235	O 235	0	0
6	40-A	226	Total 226	O 226	0	0
6	41-A	226	Total 226	O 226	0	0
6	42-A	229	Total 229	O 229	0	0
6	43-A	241	Total 241	O 241	0	0
6	44-A	250	Total 250	O 250	0	0
6	45-A	253	Total 253	O 253	0	0
6	46-A	240	Total 240	O 240	0	0
6	47-A	224	Total 224	O 224	0	0
6	48-A	226	Total 226	O 226	0	0
6	49-A	250	Total 250	O 250	0	0
6	50-A	242	Total 242	O 242	0	0
6	1-B	121	Total 121	O 121	0	0
6	2-B	124	Total 124	O 124	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	3-B	126	Total 126	O 126	0	0
6	4-B	116	Total 116	O 116	0	0
6	5-B	122	Total 122	O 122	0	0
6	6-B	124	Total 124	O 124	0	0
6	7-B	120	Total 120	O 120	0	0
6	8-B	119	Total 119	O 119	0	0
6	9-B	120	Total 120	O 120	0	0
6	10-B	121	Total 121	O 121	0	0
6	11-B	122	Total 122	O 122	0	0
6	12-B	117	Total 117	O 117	0	0
6	13-B	116	Total 116	O 116	0	0
6	14-B	120	Total 120	O 120	0	0
6	15-B	120	Total 120	O 120	0	0
6	16-B	129	Total 129	O 129	0	0
6	17-B	120	Total 120	O 120	0	0
6	18-B	121	Total 121	O 121	0	0
6	19-B	121	Total 121	O 121	0	0
6	20-B	119	Total 119	O 119	0	0
6	21-B	120	Total 120	O 120	0	0
6	22-B	122	Total 122	O 122	0	0
6	23-B	122	Total 122	O 122	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	24-B	118	Total 118	O 118	0	0
6	25-B	120	Total 120	O 120	0	0
6	26-B	120	Total 120	O 120	0	0
6	27-B	121	Total 121	O 121	0	0
6	28-B	118	Total 118	O 118	0	0
6	29-B	118	Total 118	O 118	0	0
6	30-B	120	Total 120	O 120	0	0
6	31-B	113	Total 113	O 113	0	0
6	32-B	120	Total 120	O 120	0	0
6	33-B	119	Total 119	O 119	0	0
6	34-B	124	Total 124	O 124	0	0
6	35-B	120	Total 120	O 120	0	0
6	36-B	119	Total 119	O 119	0	0
6	37-B	116	Total 116	O 116	0	0
6	38-B	119	Total 119	O 119	0	0
6	39-B	121	Total 121	O 121	0	0
6	40-B	119	Total 119	O 119	0	0
6	41-B	120	Total 120	O 120	0	0
6	42-B	120	Total 120	O 120	0	0
6	43-B	125	Total 125	O 125	0	0
6	44-B	129	Total 129	O 129	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	45-B	130	Total 130	O 130	0	0
6	46-B	124	Total 124	O 124	0	0
6	47-B	119	Total 119	O 119	0	0
6	48-B	119	Total 119	O 119	0	0
6	49-B	129	Total 129	O 129	0	0
6	50-B	127	Total 127	O 127	0	0

MolProbity failed to run properly - this section is therefore empty.

### 3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.81Å 98.05Å 106.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.48 – 1.93 16.48 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.4 (16.48-1.93) 99.4 (16.48-1.93)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.08 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.179 , 0.216 0.191 , 0.232	Depositor DCC
$R_{free}$ test set	2100 reflections (4.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.9	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.01 , 32.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	261865	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4957e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

### 4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

Of 700 ligands modelled in this entry, 400 are monoatomic - leaving 300 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	AHD	16-B	706	4	13,13,13	1.84	5 (38%)	19,21,21	1.69	4 (21%)
2	MPD	23-A	401	-	7,7,7	0.47	0	9,10,10	0.65	0
3	AHD	31-A	402	4	13,13,13	2.00	6 (46%)	19,21,21	1.32	3 (15%)
3	AHD	21-A	402	4	13,13,13	1.68	3 (23%)	19,21,21	1.59	6 (31%)
2	MPD	20-A	403	-	7,7,7	0.31	0	9,10,10	0.66	0
2	MPD	24-A	403	-	7,7,7	0.34	0	9,10,10	0.46	0
2	MPD	20-B	707	-	7,7,7	0.41	0	9,10,10	1.08	1 (11%)
2	MPD	12-B	707	-	7,7,7	0.42	0	9,10,10	0.78	0
2	MPD	14-B	701	-	7,7,7	0.48	0	9,10,10	1.87	2 (22%)
2	MPD	45-A	403	-	7,7,7	0.32	0	9,10,10	0.86	0
3	AHD	2-A	402	4	13,13,13	1.81	4 (30%)	19,21,21	1.80	6 (31%)
3	AHD	28-B	706	4	13,13,13	1.81	6 (46%)	19,21,21	1.29	2 (10%)
2	MPD	47-A	403	-	7,7,7	0.19	0	9,10,10	0.54	0
2	MPD	50-A	401	-	7,7,7	0.61	0	9,10,10	0.67	0
2	MPD	42-A	401	-	7,7,7	0.33	0	9,10,10	0.45	0
3	AHD	12-A	402	4	13,13,13	1.85	4 (30%)	19,21,21	1.41	3 (15%)
3	AHD	47-B	706	4	13,13,13	1.81	6 (46%)	19,21,21	1.52	4 (21%)
3	AHD	49-B	706	4	13,13,13	1.84	5 (38%)	19,21,21	1.45	5 (26%)
2	MPD	47-B	707	-	7,7,7	0.33	0	9,10,10	0.91	0
2	MPD	45-A	401	-	7,7,7	0.54	0	9,10,10	0.80	0
2	MPD	29-A	403	-	7,7,7	0.18	0	9,10,10	0.68	0
3	AHD	14-A	402	4	13,13,13	1.87	4 (30%)	19,21,21	2.03	9 (47%)
3	AHD	5-B	706	4	13,13,13	2.03	6 (46%)	19,21,21	1.51	3 (15%)
2	MPD	19-A	401	-	7,7,7	0.44	0	9,10,10	0.85	0
2	MPD	6-B	707	-	7,7,7	0.51	0	9,10,10	1.12	1 (11%)
3	AHD	29-A	402	4	13,13,13	1.95	6 (46%)	19,21,21	1.69	4 (21%)
2	MPD	6-A	403	-	7,7,7	0.32	0	9,10,10	0.75	0
3	AHD	39-B	706	4	13,13,13	1.78	5 (38%)	19,21,21	1.44	4 (21%)
3	AHD	33-A	402	4	13,13,13	1.78	4 (30%)	19,21,21	1.39	2 (10%)
3	AHD	9-B	706	4	13,13,13	1.71	6 (46%)	19,21,21	1.45	1 (5%)
3	AHD	20-A	402	4	13,13,13	1.70	4 (30%)	19,21,21	1.78	3 (15%)
2	MPD	14-A	403	-	7,7,7	0.30	0	9,10,10	0.39	0
2	MPD	8-B	701	-	7,7,7	0.39	0	9,10,10	0.93	1 (11%)
2	MPD	29-B	701	-	7,7,7	0.45	0	9,10,10	0.81	0
3	AHD	35-B	706	4	13,13,13	1.82	6 (46%)	19,21,21	1.53	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MPD	3-A	403	-	7,7,7	0.35	0	9,10,10	0.68	0
3	AHD	24-B	706	4	13,13,13	1.81	5 (38%)	19,21,21	1.72	3 (15%)
2	MPD	46-A	401	-	7,7,7	0.31	0	9,10,10	0.82	0
2	MPD	27-B	707	-	7,7,7	0.35	0	9,10,10	0.72	0
2	MPD	35-B	707	-	7,7,7	0.30	0	9,10,10	0.96	0
2	MPD	41-B	707	-	7,7,7	0.38	0	9,10,10	0.86	0
3	AHD	14-B	706	4	13,13,13	1.89	4 (30%)	19,21,21	1.32	4 (21%)
3	AHD	18-B	706	4	13,13,13	1.89	6 (46%)	19,21,21	1.48	4 (21%)
2	MPD	31-B	707	-	7,7,7	0.58	0	9,10,10	0.99	0
2	MPD	21-B	707	-	7,7,7	0.50	0	9,10,10	0.70	0
3	AHD	50-B	706	4	13,13,13	1.83	6 (46%)	19,21,21	1.56	5 (26%)
2	MPD	44-B	701	-	7,7,7	0.36	0	9,10,10	0.87	0
2	MPD	5-B	701	-	7,7,7	0.76	0	9,10,10	0.80	0
3	AHD	4-B	706	4	13,13,13	1.89	5 (38%)	19,21,21	1.35	5 (26%)
3	AHD	26-B	706	4	13,13,13	1.90	6 (46%)	19,21,21	1.71	4 (21%)
2	MPD	48-A	403	-	7,7,7	0.58	0	9,10,10	0.77	0
2	MPD	27-A	403	-	7,7,7	0.26	0	9,10,10	0.75	0
2	MPD	23-A	403	-	7,7,7	0.36	0	9,10,10	0.99	1 (11%)
2	MPD	11-A	401	-	7,7,7	0.38	0	9,10,10	0.76	0
2	MPD	41-B	701	-	7,7,7	0.47	0	9,10,10	0.79	0
2	MPD	39-A	403	-	7,7,7	0.71	0	9,10,10	1.19	1 (11%)
2	MPD	28-B	707	-	7,7,7	0.47	0	9,10,10	0.95	0
2	MPD	9-B	701	-	7,7,7	0.61	0	9,10,10	0.67	0
2	MPD	46-A	403	-	7,7,7	0.29	0	9,10,10	0.66	0
2	MPD	35-B	701	-	7,7,7	0.43	0	9,10,10	1.06	0
2	MPD	13-B	701	-	7,7,7	0.61	0	9,10,10	1.15	0
2	MPD	4-A	401	-	7,7,7	0.32	0	9,10,10	0.93	0
2	MPD	32-A	401	-	7,7,7	0.48	0	9,10,10	0.53	0
2	MPD	11-B	707	-	7,7,7	0.34	0	9,10,10	0.67	0
3	AHD	31-B	706	4	13,13,13	1.69	4 (30%)	19,21,21	1.64	5 (26%)
3	AHD	23-B	706	4	13,13,13	1.86	6 (46%)	19,21,21	1.72	4 (21%)
2	MPD	23-B	701	-	7,7,7	0.57	0	9,10,10	1.17	1 (11%)
2	MPD	1-A	401	-	7,7,7	0.44	0	9,10,10	0.77	0
2	MPD	13-A	403	-	7,7,7	0.29	0	9,10,10	1.09	1 (11%)
3	AHD	30-A	402	4	13,13,13	1.73	4 (30%)	19,21,21	1.70	6 (31%)
2	MPD	28-B	701	-	7,7,7	0.55	0	9,10,10	0.79	1 (11%)
2	MPD	40-A	401	-	7,7,7	0.48	0	9,10,10	0.63	0
2	MPD	46-B	707	-	7,7,7	0.45	0	9,10,10	0.53	0
2	MPD	38-A	403	-	7,7,7	0.30	0	9,10,10	0.57	0
2	MPD	39-A	401	-	7,7,7	0.28	0	9,10,10	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MPD	26-B	701	-	7,7,7	0.73	0	9,10,10	0.77	0
2	MPD	11-A	403	-	7,7,7	0.60	0	9,10,10	0.76	0
2	MPD	18-A	401	-	7,7,7	0.31	0	9,10,10	0.70	0
2	MPD	28-A	403	-	7,7,7	0.54	0	9,10,10	0.37	0
2	MPD	48-B	701	-	7,7,7	0.56	0	9,10,10	0.80	0
2	MPD	19-B	707	-	7,7,7	0.24	0	9,10,10	1.11	1 (11%)
2	MPD	33-A	401	-	7,7,7	0.35	0	9,10,10	0.74	0
3	AHD	47-A	402	4	13,13,13	1.78	5 (38%)	19,21,21	1.47	5 (26%)
3	AHD	25-B	706	4	13,13,13	1.77	6 (46%)	19,21,21	1.47	3 (15%)
2	MPD	31-A	403	-	7,7,7	0.50	0	9,10,10	0.91	0
2	MPD	37-A	401	-	7,7,7	0.32	0	9,10,10	0.71	0
2	MPD	38-A	401	-	7,7,7	0.46	0	9,10,10	0.88	0
2	MPD	28-A	401	-	7,7,7	0.32	0	9,10,10	0.53	0
2	MPD	6-B	701	-	7,7,7	0.26	0	9,10,10	0.89	0
2	MPD	17-B	701	-	7,7,7	0.54	0	9,10,10	0.82	0
2	MPD	17-A	403	-	7,7,7	0.58	0	9,10,10	1.52	1 (11%)
3	AHD	6-A	402	4	13,13,13	1.80	5 (38%)	19,21,21	1.65	5 (26%)
2	MPD	7-B	707	-	7,7,7	0.42	0	9,10,10	2.70	2 (22%)
3	AHD	45-A	402	4	13,13,13	1.85	4 (30%)	19,21,21	1.63	3 (15%)
2	MPD	5-B	707	-	7,7,7	0.33	0	9,10,10	1.24	1 (11%)
2	MPD	43-B	707	-	7,7,7	0.32	0	9,10,10	1.04	0
3	AHD	6-B	706	4	13,13,13	1.81	5 (38%)	19,21,21	1.30	2 (10%)
2	MPD	9-A	403	-	7,7,7	0.41	0	9,10,10	0.82	0
2	MPD	34-B	707	-	7,7,7	0.58	0	9,10,10	1.53	1 (11%)
2	MPD	33-A	403	-	7,7,7	0.39	0	9,10,10	0.82	1 (11%)
2	MPD	42-A	403	-	7,7,7	0.44	0	9,10,10	0.68	0
2	MPD	24-B	701	-	7,7,7	0.75	0	9,10,10	0.71	0
3	AHD	22-A	402	4	13,13,13	1.76	4 (30%)	19,21,21	1.75	5 (26%)
2	MPD	48-A	401	-	7,7,7	0.38	0	9,10,10	0.69	0
3	AHD	45-B	706	4	13,13,13	1.73	5 (38%)	19,21,21	1.54	1 (5%)
3	AHD	3-A	402	4	13,13,13	2.00	6 (46%)	19,21,21	1.73	3 (15%)
2	MPD	39-B	701	-	7,7,7	0.42	0	9,10,10	0.77	0
2	MPD	5-A	403	-	7,7,7	0.57	0	9,10,10	0.63	0
2	MPD	20-B	701	-	7,7,7	0.57	0	9,10,10	0.85	0
2	MPD	21-A	401	-	7,7,7	0.57	0	9,10,10	0.80	0
2	MPD	4-B	701	-	7,7,7	0.79	0	9,10,10	1.08	0
2	MPD	23-B	707	-	7,7,7	0.50	0	9,10,10	0.51	0
3	AHD	41-B	706	4	13,13,13	1.75	5 (38%)	19,21,21	1.48	2 (10%)
3	AHD	36-A	402	4	13,13,13	2.09	6 (46%)	19,21,21	1.83	6 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	AHD	46-A	402	4	13,13,13	1.92	4 (30%)	19,21,21	1.81	6 (31%)
2	MPD	29-B	707	-	7,7,7	0.35	0	9,10,10	0.65	0
3	AHD	12-B	706	4	13,13,13	1.82	6 (46%)	19,21,21	1.42	5 (26%)
3	AHD	21-B	706	4	13,13,13	1.85	6 (46%)	19,21,21	1.59	2 (10%)
2	MPD	47-B	701	-	7,7,7	0.64	0	9,10,10	0.88	1 (11%)
3	AHD	27-A	402	4	13,13,13	1.75	4 (30%)	19,21,21	1.56	2 (10%)
2	MPD	35-A	403	-	7,7,7	0.32	0	9,10,10	0.73	0
2	MPD	14-A	401	-	7,7,7	0.53	0	9,10,10	0.66	0
2	MPD	13-A	401	-	7,7,7	0.47	0	9,10,10	1.53	2 (22%)
2	MPD	35-A	401	-	7,7,7	0.63	0	9,10,10	1.00	1 (11%)
2	MPD	36-A	403	-	7,7,7	0.33	0	9,10,10	0.81	0
2	MPD	22-A	401	-	7,7,7	0.31	0	9,10,10	1.04	0
2	MPD	8-B	707	-	7,7,7	0.48	0	9,10,10	1.09	1 (11%)
3	AHD	17-A	402	4	13,13,13	1.74	5 (38%)	19,21,21	1.72	4 (21%)
2	MPD	44-A	403	-	7,7,7	0.40	0	9,10,10	1.37	1 (11%)
3	AHD	38-A	402	4	13,13,13	1.76	5 (38%)	19,21,21	1.81	6 (31%)
2	MPD	25-B	707	-	7,7,7	0.45	0	9,10,10	0.49	0
3	AHD	1-B	706	4	13,13,13	1.72	5 (38%)	19,21,21	1.52	2 (10%)
3	AHD	22-B	706	4	13,13,13	1.94	5 (38%)	19,21,21	0.85	0
2	MPD	16-A	401	-	7,7,7	0.38	0	9,10,10	0.88	0
2	MPD	25-A	403	-	7,7,7	0.44	0	9,10,10	0.74	0
2	MPD	46-B	701	-	7,7,7	1.06	1 (14%)	9,10,10	1.96	3 (33%)
2	MPD	7-B	701	-	7,7,7	0.68	0	9,10,10	1.57	2 (22%)
2	MPD	44-A	401	-	7,7,7	0.38	0	9,10,10	1.52	1 (11%)
3	AHD	33-B	706	4	13,13,13	1.96	6 (46%)	19,21,21	1.50	4 (21%)
2	MPD	34-B	701	-	7,7,7	0.79	0	9,10,10	0.62	0
2	MPD	25-A	401	-	7,7,7	0.51	0	9,10,10	0.73	0
3	AHD	7-A	402	4	13,13,13	2.02	6 (46%)	19,21,21	1.37	5 (26%)
3	AHD	24-A	402	4	13,13,13	1.83	4 (30%)	19,21,21	1.72	4 (21%)
3	AHD	4-A	402	4	13,13,13	1.77	4 (30%)	19,21,21	1.60	3 (15%)
3	AHD	48-B	706	4	13,13,13	1.85	6 (46%)	19,21,21	1.74	2 (10%)
2	MPD	33-B	707	-	7,7,7	0.36	0	9,10,10	0.61	0
2	MPD	39-B	707	-	7,7,7	0.31	0	9,10,10	1.06	1 (11%)
3	AHD	34-A	402	4	13,13,13	1.88	5 (38%)	19,21,21	1.86	5 (26%)
3	AHD	38-B	706	4	13,13,13	1.77	5 (38%)	19,21,21	1.68	4 (21%)
2	MPD	18-B	707	-	7,7,7	0.27	0	9,10,10	1.07	1 (11%)
2	MPD	3-B	701	-	7,7,7	0.50	0	9,10,10	1.20	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MPD	37-B	701	-	7,7,7	0.75	0	9,10,10	0.81	0
2	MPD	48-B	707	-	7,7,7	0.30	0	9,10,10	0.81	0
2	MPD	9-A	401	-	7,7,7	0.28	0	9,10,10	1.07	1 (11%)
2	MPD	50-B	707	-	7,7,7	0.44	0	9,10,10	0.84	0
2	MPD	49-A	403	-	7,7,7	0.44	0	9,10,10	0.52	0
2	MPD	26-A	401	-	7,7,7	0.37	0	9,10,10	1.23	2 (22%)
2	MPD	16-B	701	-	7,7,7	0.57	0	9,10,10	1.06	1 (11%)
2	MPD	8-A	403	-	7,7,7	0.27	0	9,10,10	0.64	0
2	MPD	19-A	403	-	7,7,7	0.34	0	9,10,10	0.39	0
2	MPD	45-B	701	-	7,7,7	0.45	0	9,10,10	1.24	1 (11%)
2	MPD	15-B	707	-	7,7,7	0.40	0	9,10,10	0.65	0
3	AHD	26-A	402	4	13,13,13	1.70	3 (23%)	19,21,21	1.49	4 (21%)
3	AHD	46-B	706	4	13,13,13	1.78	5 (38%)	19,21,21	1.49	4 (21%)
3	AHD	40-A	402	4	13,13,13	1.83	4 (30%)	19,21,21	1.86	6 (31%)
3	AHD	2-B	706	4	13,13,13	1.86	5 (38%)	19,21,21	1.50	5 (26%)
3	AHD	19-B	706	4	13,13,13	2.02	6 (46%)	19,21,21	1.62	1 (5%)
2	MPD	49-B	701	-	7,7,7	0.61	0	9,10,10	1.25	1 (11%)
2	MPD	4-B	707	-	7,7,7	0.35	0	9,10,10	0.71	0
2	MPD	49-A	401	-	7,7,7	0.65	0	9,10,10	1.28	1 (11%)
2	MPD	21-A	403	-	7,7,7	0.43	0	9,10,10	0.74	0
2	MPD	2-B	707	-	7,7,7	0.50	0	9,10,10	0.38	0
2	MPD	13-B	707	-	7,7,7	0.39	0	9,10,10	0.81	0
2	MPD	27-B	701	-	7,7,7	0.59	0	9,10,10	1.18	1 (11%)
2	MPD	41-A	401	-	7,7,7	0.53	0	9,10,10	0.70	0
3	AHD	37-A	402	4	13,13,13	1.89	5 (38%)	19,21,21	1.77	4 (21%)
2	MPD	25-B	701	-	7,7,7	0.36	0	9,10,10	0.52	0
2	MPD	26-B	707	-	7,7,7	0.43	0	9,10,10	1.09	1 (11%)
3	AHD	29-B	706	4	13,13,13	1.97	6 (46%)	19,21,21	1.91	6 (31%)
3	AHD	32-B	706	4	13,13,13	1.90	6 (46%)	19,21,21	1.76	4 (21%)
3	AHD	10-A	402	4	13,13,13	1.75	4 (30%)	19,21,21	1.68	3 (15%)
2	MPD	12-A	403	-	7,7,7	0.82	0	9,10,10	0.79	0
2	MPD	43-B	701	-	7,7,7	0.46	0	9,10,10	1.01	1 (11%)
2	MPD	32-B	707	-	7,7,7	0.35	0	9,10,10	0.75	0
3	AHD	19-A	402	4	13,13,13	1.83	5 (38%)	19,21,21	1.37	3 (15%)
2	MPD	22-A	403	-	7,7,7	0.43	0	9,10,10	0.94	0
2	MPD	12-B	701	-	7,7,7	0.69	0	9,10,10	1.08	0
2	MPD	15-A	401	-	7,7,7	0.34	0	9,10,10	0.84	0
3	AHD	35-A	402	4	13,13,13	1.87	4 (30%)	19,21,21	1.82	6 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	AHD	48-A	402	4	13,13,13	1.78	5 (38%)	19,21,21	1.88	4 (21%)
2	MPD	21-B	701	-	7,7,7	0.55	0	9,10,10	0.77	0
2	MPD	36-B	707	-	7,7,7	0.31	0	9,10,10	0.97	0
2	MPD	19-B	701	-	7,7,7	0.80	0	9,10,10	0.80	0
2	MPD	50-B	701	-	7,7,7	0.52	0	9,10,10	0.67	0
2	MPD	10-A	403	-	7,7,7	0.31	0	9,10,10	0.52	0
2	MPD	30-B	707	-	7,7,7	0.33	0	9,10,10	0.99	0
3	AHD	3-B	706	4	13,13,13	1.94	5 (38%)	19,21,21	1.43	3 (15%)
3	AHD	15-B	706	4	13,13,13	1.84	6 (46%)	19,21,21	1.58	5 (26%)
2	MPD	29-A	401	-	7,7,7	0.44	0	9,10,10	0.74	0
2	MPD	3-B	707	-	7,7,7	0.45	0	9,10,10	0.53	0
2	MPD	10-A	401	-	7,7,7	0.42	0	9,10,10	1.64	2 (22%)
2	MPD	34-A	403	-	7,7,7	0.33	0	9,10,10	0.52	0
2	MPD	33-B	701	-	7,7,7	0.76	0	9,10,10	0.89	0
3	AHD	27-B	706	4	13,13,13	1.89	6 (46%)	19,21,21	1.27	3 (15%)
2	MPD	12-A	401	-	7,7,7	0.81	0	9,10,10	1.44	2 (22%)
2	MPD	37-B	707	-	7,7,7	0.37	0	9,10,10	0.76	0
3	AHD	15-A	402	4	13,13,13	1.67	4 (30%)	19,21,21	1.58	3 (15%)
2	MPD	5-A	401	-	7,7,7	0.44	0	9,10,10	0.86	0
2	MPD	36-B	701	-	7,7,7	0.67	0	9,10,10	1.22	1 (11%)
2	MPD	1-A	403	-	7,7,7	0.67	0	9,10,10	0.72	0
2	MPD	17-A	401	-	7,7,7	0.59	0	9,10,10	0.82	0
2	MPD	10-B	701	-	7,7,7	0.30	0	9,10,10	1.12	0
2	MPD	22-B	707	-	7,7,7	0.44	0	9,10,10	0.45	0
2	MPD	34-A	401	-	7,7,7	0.62	0	9,10,10	1.77	2 (22%)
3	AHD	7-B	706	4	13,13,13	1.78	6 (46%)	19,21,21	1.58	3 (15%)
2	MPD	24-A	401	-	7,7,7	0.50	0	9,10,10	0.75	0
2	MPD	7-A	403	-	7,7,7	0.37	0	9,10,10	0.78	0
2	MPD	42-B	701	-	7,7,7	0.53	0	9,10,10	0.63	0
2	MPD	30-B	701	-	7,7,7	0.62	0	9,10,10	1.67	1 (11%)
3	AHD	43-B	706	4	13,13,13	1.85	6 (46%)	19,21,21	1.45	2 (10%)
2	MPD	18-A	403	-	7,7,7	0.50	0	9,10,10	0.66	0
3	AHD	34-B	706	4	13,13,13	1.81	5 (38%)	19,21,21	1.87	5 (26%)
3	AHD	44-B	706	4	13,13,13	1.86	6 (46%)	19,21,21	1.55	4 (21%)
2	MPD	20-A	401	-	7,7,7	0.41	0	9,10,10	1.03	0
3	AHD	40-B	706	4	13,13,13	1.97	6 (46%)	19,21,21	1.72	5 (26%)
2	MPD	31-B	701	-	7,7,7	0.59	0	9,10,10	0.71	0
2	MPD	9-B	707	-	7,7,7	0.38	0	9,10,10	0.66	0
2	MPD	40-B	701	-	7,7,7	0.57	0	9,10,10	1.38	2 (22%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	AHD	41-A	402	4	13,13,13	1.88	5 (38%)	19,21,21	1.62	3 (15%)
2	MPD	42-B	707	-	7,7,7	0.30	0	9,10,10	0.76	0
3	AHD	25-A	402	4	13,13,13	1.97	5 (38%)	19,21,21	1.78	5 (26%)
3	AHD	32-A	402	4	13,13,13	1.76	4 (30%)	19,21,21	2.30	7 (36%)
2	MPD	18-B	701	-	7,7,7	0.59	0	9,10,10	0.91	0
2	MPD	47-A	401	-	7,7,7	0.34	0	9,10,10	0.74	0
3	AHD	8-B	706	4	13,13,13	1.80	6 (46%)	19,21,21	1.34	2 (10%)
3	AHD	11-B	706	4	13,13,13	1.71	5 (38%)	19,21,21	1.73	3 (15%)
2	MPD	2-B	701	-	7,7,7	0.64	0	9,10,10	1.13	1 (11%)
2	MPD	11-B	701	-	7,7,7	0.33	0	9,10,10	1.18	1 (11%)
2	MPD	16-B	707	-	7,7,7	0.47	0	9,10,10	0.61	0
2	MPD	24-B	707	-	7,7,7	0.47	0	9,10,10	0.74	0
2	MPD	16-A	403	-	7,7,7	0.38	0	9,10,10	0.59	0
3	AHD	1-A	402	4	13,13,13	1.73	4 (30%)	19,21,21	1.73	4 (21%)
3	AHD	9-A	402	4	13,13,13	1.93	5 (38%)	19,21,21	1.82	6 (31%)
2	MPD	14-B	707	-	7,7,7	0.40	0	9,10,10	0.75	0
2	MPD	6-A	401	-	7,7,7	0.49	0	9,10,10	1.34	2 (22%)
2	MPD	32-A	403	-	7,7,7	0.61	0	9,10,10	1.21	1 (11%)
3	AHD	50-A	402	4	13,13,13	1.73	4 (30%)	19,21,21	1.61	3 (15%)
2	MPD	1-B	701	-	7,7,7	0.60	0	9,10,10	0.90	0
2	MPD	36-A	401	-	7,7,7	0.38	0	9,10,10	0.78	0
3	AHD	39-A	402	4	13,13,13	1.72	4 (30%)	19,21,21	1.47	3 (15%)
2	MPD	43-A	403	-	7,7,7	0.43	0	9,10,10	0.54	0
3	AHD	30-B	706	4	13,13,13	1.75	4 (30%)	19,21,21	1.51	6 (31%)
2	MPD	8-A	401	-	7,7,7	0.50	0	9,10,10	0.52	0
2	MPD	50-A	403	-	7,7,7	0.38	0	9,10,10	0.62	0
3	AHD	17-B	706	4	13,13,13	1.89	5 (38%)	19,21,21	1.54	3 (15%)
2	MPD	2-A	403	-	7,7,7	0.34	0	9,10,10	1.77	2 (22%)
3	AHD	28-A	402	4	13,13,13	1.75	4 (30%)	19,21,21	1.66	5 (26%)
2	MPD	17-B	707	-	7,7,7	0.53	0	9,10,10	1.29	1 (11%)
3	AHD	49-A	402	4	13,13,13	1.80	4 (30%)	19,21,21	1.29	3 (15%)
2	MPD	32-B	701	-	7,7,7	0.42	0	9,10,10	1.24	0
2	MPD	4-A	403	-	7,7,7	0.25	0	9,10,10	0.67	0
2	MPD	2-A	401	-	7,7,7	0.31	0	9,10,10	0.71	0
2	MPD	27-A	401	-	7,7,7	0.26	0	9,10,10	1.07	0
2	MPD	37-A	403	-	7,7,7	0.37	0	9,10,10	0.70	0
2	MPD	15-B	701	-	7,7,7	0.38	0	9,10,10	1.19	1 (11%)
3	AHD	36-B	706	4	13,13,13	1.85	6 (46%)	19,21,21	1.57	6 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MPD	49-B	707	-	7,7,7	0.38	0	9,10,10	1.00	0
2	MPD	31-A	401	-	7,7,7	0.44	0	9,10,10	0.55	0
3	AHD	20-B	706	4	13,13,13	1.77	6 (46%)	19,21,21	1.48	4 (21%)
3	AHD	43-A	402	4	13,13,13	1.83	6 (46%)	19,21,21	1.83	5 (26%)
2	MPD	43-A	401	-	7,7,7	0.40	0	9,10,10	0.65	0
3	AHD	23-A	402	4	13,13,13	1.75	3 (23%)	19,21,21	1.33	4 (21%)
2	MPD	40-B	707	-	7,7,7	0.31	0	9,10,10	0.77	0
2	MPD	3-A	401	-	7,7,7	0.36	0	9,10,10	0.73	0
3	AHD	37-B	706	4	13,13,13	1.83	6 (46%)	19,21,21	1.62	4 (21%)
2	MPD	15-A	403	-	7,7,7	0.42	0	9,10,10	0.47	0
2	MPD	30-A	403	-	7,7,7	0.38	0	9,10,10	0.65	0
2	MPD	44-B	707	-	7,7,7	0.43	0	9,10,10	0.67	0
2	MPD	38-B	707	-	7,7,7	0.39	0	9,10,10	0.84	0
3	AHD	18-A	402	4	13,13,13	1.60	4 (30%)	19,21,21	1.55	4 (21%)
3	AHD	5-A	402	4	13,13,13	1.73	4 (30%)	19,21,21	1.86	6 (31%)
2	MPD	7-A	401	-	7,7,7	0.37	0	9,10,10	0.88	0
2	MPD	22-B	701	-	7,7,7	0.27	0	9,10,10	1.14	1 (11%)
2	MPD	26-A	403	-	7,7,7	0.38	0	9,10,10	0.67	0
3	AHD	10-B	706	4	13,13,13	1.69	5 (38%)	19,21,21	1.50	2 (10%)
2	MPD	1-B	707	-	7,7,7	0.45	0	9,10,10	0.60	0
3	AHD	8-A	402	4	13,13,13	1.70	5 (38%)	19,21,21	1.51	3 (15%)
2	MPD	30-A	401	-	7,7,7	0.38	0	9,10,10	0.82	0
2	MPD	40-A	403	-	7,7,7	0.62	0	9,10,10	0.81	0
2	MPD	10-B	707	-	7,7,7	0.39	0	9,10,10	0.83	0
3	AHD	11-A	402	4	13,13,13	1.75	4 (30%)	19,21,21	1.26	1 (5%)
3	AHD	13-A	402	4	13,13,13	2.00	5 (38%)	19,21,21	1.79	4 (21%)
3	AHD	42-A	402	4	13,13,13	1.76	5 (38%)	19,21,21	1.68	6 (31%)
2	MPD	45-B	707	-	7,7,7	0.59	0	9,10,10	1.15	1 (11%)
2	MPD	38-B	701	-	7,7,7	0.24	0	9,10,10	0.91	0
3	AHD	42-B	706	4	13,13,13	1.77	6 (46%)	19,21,21	1.37	3 (15%)
2	MPD	41-A	403	-	7,7,7	0.34	0	9,10,10	0.67	0
3	AHD	44-A	402	4	13,13,13	1.84	4 (30%)	19,21,21	1.79	5 (26%)
3	AHD	16-A	402	4	13,13,13	1.76	5 (38%)	19,21,21	1.67	4 (21%)
3	AHD	13-B	706	4	13,13,13	1.99	7 (53%)	19,21,21	1.62	5 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AHD	16-B	706	4	-	2/23/23/23	-
2	MPD	23-A	401	-	-	5/5/5/5	-
3	AHD	31-A	402	4	-	4/23/23/23	-
3	AHD	21-A	402	4	-	0/23/23/23	-
2	MPD	20-A	403	-	-	1/5/5/5	-
2	MPD	24-A	403	-	-	0/5/5/5	-
2	MPD	20-B	707	-	-	0/5/5/5	-
2	MPD	12-B	707	-	-	1/5/5/5	-
2	MPD	14-B	701	-	-	3/5/5/5	-
2	MPD	45-A	403	-	-	1/5/5/5	-
3	AHD	2-A	402	4	-	4/23/23/23	-
3	AHD	28-B	706	4	-	3/23/23/23	-
2	MPD	47-A	403	-	-	0/5/5/5	-
2	MPD	50-A	401	-	-	2/5/5/5	-
2	MPD	42-A	401	-	-	5/5/5/5	-
3	AHD	12-A	402	4	-	1/23/23/23	-
3	AHD	47-B	706	4	-	4/23/23/23	-
3	AHD	49-B	706	4	-	2/23/23/23	-
2	MPD	47-B	707	-	-	0/5/5/5	-
2	MPD	45-A	401	-	-	4/5/5/5	-
2	MPD	29-A	403	-	-	0/5/5/5	-
3	AHD	14-A	402	4	-	3/23/23/23	-
3	AHD	5-B	706	4	-	0/23/23/23	-
2	MPD	19-A	401	-	-	2/5/5/5	-
2	MPD	6-B	707	-	-	1/5/5/5	-
3	AHD	29-A	402	4	-	0/23/23/23	-
2	MPD	6-A	403	-	-	0/5/5/5	-
3	AHD	39-B	706	4	-	4/23/23/23	-
3	AHD	33-A	402	4	-	1/23/23/23	-
3	AHD	9-B	706	4	-	4/23/23/23	-
3	AHD	20-A	402	4	-	4/23/23/23	-
2	MPD	14-A	403	-	-	0/5/5/5	-
2	MPD	8-B	701	-	-	1/5/5/5	-
2	MPD	29-B	701	-	-	0/5/5/5	-
3	AHD	35-B	706	4	-	2/23/23/23	-
2	MPD	3-A	403	-	-	1/5/5/5	-
3	AHD	24-B	706	4	-	4/23/23/23	-
2	MPD	46-A	401	-	-	2/5/5/5	-
2	MPD	27-B	707	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	35-B	707	-	-	0/5/5/5	-
2	MPD	41-B	707	-	-	0/5/5/5	-
3	AHD	14-B	706	4	-	4/23/23/23	-
3	AHD	18-B	706	4	-	4/23/23/23	-
2	MPD	31-B	707	-	-	0/5/5/5	-
2	MPD	21-B	707	-	-	1/5/5/5	-
3	AHD	50-B	706	4	-	1/23/23/23	-
2	MPD	44-B	701	-	-	2/5/5/5	-
2	MPD	5-B	701	-	-	3/5/5/5	-
3	AHD	4-B	706	4	-	4/23/23/23	-
3	AHD	26-B	706	4	-	3/23/23/23	-
2	MPD	48-A	403	-	-	0/5/5/5	-
2	MPD	27-A	403	-	-	0/5/5/5	-
2	MPD	23-A	403	-	-	0/5/5/5	-
2	MPD	11-A	401	-	-	3/5/5/5	-
2	MPD	41-B	701	-	-	4/5/5/5	-
2	MPD	39-A	403	-	-	2/5/5/5	-
2	MPD	28-B	707	-	-	0/5/5/5	-
2	MPD	9-B	701	-	-	2/5/5/5	-
2	MPD	46-A	403	-	-	0/5/5/5	-
2	MPD	35-B	701	-	-	1/5/5/5	-
2	MPD	13-B	701	-	-	2/5/5/5	-
2	MPD	4-A	401	-	-	3/5/5/5	-
2	MPD	32-A	401	-	-	4/5/5/5	-
2	MPD	11-B	707	-	-	0/5/5/5	-
3	AHD	31-B	706	4	-	4/23/23/23	-
3	AHD	23-B	706	4	-	4/23/23/23	-
2	MPD	23-B	701	-	-	2/5/5/5	-
2	MPD	1-A	401	-	-	2/5/5/5	-
2	MPD	13-A	403	-	-	0/5/5/5	-
3	AHD	30-A	402	4	-	4/23/23/23	-
2	MPD	28-B	701	-	-	1/5/5/5	-
2	MPD	40-A	401	-	-	4/5/5/5	-
2	MPD	46-B	707	-	-	1/5/5/5	-
2	MPD	38-A	403	-	-	0/5/5/5	-
2	MPD	39-A	401	-	-	1/5/5/5	-
2	MPD	26-B	701	-	-	1/5/5/5	-
2	MPD	11-A	403	-	-	1/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	18-A	401	-	-	2/5/5/5	-
2	MPD	28-A	403	-	-	4/5/5/5	-
2	MPD	48-B	701	-	-	4/5/5/5	-
2	MPD	19-B	707	-	-	1/5/5/5	-
2	MPD	33-A	401	-	-	2/5/5/5	-
3	AHD	47-A	402	4	-	4/23/23/23	-
3	AHD	25-B	706	4	-	0/23/23/23	-
2	MPD	31-A	403	-	-	2/5/5/5	-
2	MPD	37-A	401	-	-	3/5/5/5	-
2	MPD	38-A	401	-	-	4/5/5/5	-
2	MPD	28-A	401	-	-	3/5/5/5	-
2	MPD	6-B	701	-	-	4/5/5/5	-
2	MPD	17-B	701	-	-	0/5/5/5	-
2	MPD	17-A	403	-	-	1/5/5/5	-
3	AHD	6-A	402	4	-	4/23/23/23	-
2	MPD	7-B	707	-	-	0/5/5/5	-
3	AHD	45-A	402	4	-	3/23/23/23	-
2	MPD	5-B	707	-	-	3/5/5/5	-
2	MPD	43-B	707	-	-	0/5/5/5	-
3	AHD	6-B	706	4	-	5/23/23/23	-
2	MPD	9-A	403	-	-	0/5/5/5	-
2	MPD	34-B	707	-	-	0/5/5/5	-
2	MPD	33-A	403	-	-	0/5/5/5	-
2	MPD	42-A	403	-	-	1/5/5/5	-
2	MPD	24-B	701	-	-	3/5/5/5	-
3	AHD	22-A	402	4	-	3/23/23/23	-
2	MPD	48-A	401	-	-	3/5/5/5	-
3	AHD	45-B	706	4	-	3/23/23/23	-
3	AHD	3-A	402	4	-	4/23/23/23	-
2	MPD	39-B	701	-	-	1/5/5/5	-
2	MPD	5-A	403	-	-	3/5/5/5	-
2	MPD	20-B	701	-	-	1/5/5/5	-
2	MPD	21-A	401	-	-	1/5/5/5	-
2	MPD	4-B	701	-	-	2/5/5/5	-
2	MPD	23-B	707	-	-	0/5/5/5	-
3	AHD	41-B	706	4	-	6/23/23/23	-
3	AHD	36-A	402	4	-	3/23/23/23	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AHD	46-A	402	4	-	3/23/23/23	-
2	MPD	29-B	707	-	-	0/5/5/5	-
3	AHD	12-B	706	4	-	4/23/23/23	-
3	AHD	21-B	706	4	-	0/23/23/23	-
2	MPD	47-B	701	-	-	4/5/5/5	-
3	AHD	27-A	402	4	-	3/23/23/23	-
2	MPD	35-A	403	-	-	0/5/5/5	-
2	MPD	14-A	401	-	-	4/5/5/5	-
2	MPD	13-A	401	-	-	2/5/5/5	-
2	MPD	35-A	401	-	-	4/5/5/5	-
2	MPD	36-A	403	-	-	1/5/5/5	-
2	MPD	22-A	401	-	-	2/5/5/5	-
2	MPD	8-B	707	-	-	0/5/5/5	-
3	AHD	17-A	402	4	-	4/23/23/23	-
2	MPD	44-A	403	-	-	0/5/5/5	-
3	AHD	38-A	402	4	-	3/23/23/23	-
2	MPD	25-B	707	-	-	0/5/5/5	-
3	AHD	1-B	706	4	-	4/23/23/23	-
3	AHD	22-B	706	4	-	5/23/23/23	-
2	MPD	16-A	401	-	-	3/5/5/5	-
2	MPD	25-A	403	-	-	0/5/5/5	-
2	MPD	46-B	701	-	-	1/5/5/5	-
2	MPD	7-B	701	-	-	1/5/5/5	-
2	MPD	44-A	401	-	-	5/5/5/5	-
3	AHD	33-B	706	4	-	4/23/23/23	-
2	MPD	34-B	701	-	-	2/5/5/5	-
2	MPD	25-A	401	-	-	1/5/5/5	-
3	AHD	7-A	402	4	-	2/23/23/23	-
3	AHD	24-A	402	4	-	4/23/23/23	-
3	AHD	4-A	402	4	-	3/23/23/23	-
3	AHD	48-B	706	4	-	1/23/23/23	-
2	MPD	33-B	707	-	-	0/5/5/5	-
2	MPD	39-B	707	-	-	0/5/5/5	-
3	AHD	34-A	402	4	-	4/23/23/23	-
3	AHD	38-B	706	4	-	4/23/23/23	-
2	MPD	18-B	707	-	-	1/5/5/5	-
2	MPD	3-B	701	-	-	1/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	37-B	701	-	-	4/5/5/5	-
2	MPD	48-B	707	-	-	0/5/5/5	-
2	MPD	9-A	401	-	-	5/5/5/5	-
2	MPD	50-B	707	-	-	0/5/5/5	-
2	MPD	49-A	403	-	-	2/5/5/5	-
2	MPD	26-A	401	-	-	5/5/5/5	-
2	MPD	16-B	701	-	-	2/5/5/5	-
2	MPD	8-A	403	-	-	0/5/5/5	-
2	MPD	19-A	403	-	-	0/5/5/5	-
2	MPD	45-B	701	-	-	2/5/5/5	-
2	MPD	15-B	707	-	-	0/5/5/5	-
3	AHD	26-A	402	4	-	3/23/23/23	-
3	AHD	46-B	706	4	-	4/23/23/23	-
3	AHD	40-A	402	4	-	3/23/23/23	-
3	AHD	2-B	706	4	-	1/23/23/23	-
3	AHD	19-B	706	4	-	2/23/23/23	-
2	MPD	49-B	701	-	-	0/5/5/5	-
2	MPD	4-B	707	-	-	2/5/5/5	-
2	MPD	49-A	401	-	-	1/5/5/5	-
2	MPD	21-A	403	-	-	3/5/5/5	-
2	MPD	2-B	707	-	-	0/5/5/5	-
2	MPD	13-B	707	-	-	2/5/5/5	-
2	MPD	27-B	701	-	-	5/5/5/5	-
2	MPD	41-A	401	-	-	4/5/5/5	-
3	AHD	37-A	402	4	-	6/23/23/23	-
2	MPD	25-B	701	-	-	2/5/5/5	-
2	MPD	26-B	707	-	-	2/5/5/5	-
3	AHD	29-B	706	4	-	4/23/23/23	-
3	AHD	32-B	706	4	-	4/23/23/23	-
3	AHD	10-A	402	4	-	2/23/23/23	-
2	MPD	12-A	403	-	-	3/5/5/5	-
2	MPD	43-B	701	-	-	3/5/5/5	-
2	MPD	32-B	707	-	-	1/5/5/5	-
3	AHD	19-A	402	4	-	2/23/23/23	-
2	MPD	22-A	403	-	-	0/5/5/5	-
2	MPD	12-B	701	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	15-A	401	-	-	2/5/5/5	-
3	AHD	35-A	402	4	-	9/23/23/23	-
3	AHD	48-A	402	4	-	4/23/23/23	-
2	MPD	21-B	701	-	-	4/5/5/5	-
2	MPD	36-B	707	-	-	0/5/5/5	-
2	MPD	19-B	701	-	-	1/5/5/5	-
2	MPD	50-B	701	-	-	2/5/5/5	-
2	MPD	10-A	403	-	-	1/5/5/5	-
2	MPD	30-B	707	-	-	0/5/5/5	-
3	AHD	3-B	706	4	-	3/23/23/23	-
3	AHD	15-B	706	4	-	3/23/23/23	-
2	MPD	29-A	401	-	-	2/5/5/5	-
2	MPD	3-B	707	-	-	0/5/5/5	-
2	MPD	10-A	401	-	-	4/5/5/5	-
2	MPD	34-A	403	-	-	1/5/5/5	-
2	MPD	33-B	701	-	-	3/5/5/5	-
3	AHD	27-B	706	4	-	4/23/23/23	-
2	MPD	12-A	401	-	-	4/5/5/5	-
2	MPD	37-B	707	-	-	0/5/5/5	-
3	AHD	15-A	402	4	-	1/23/23/23	-
2	MPD	5-A	401	-	-	4/5/5/5	-
2	MPD	36-B	701	-	-	1/5/5/5	-
2	MPD	1-A	403	-	-	2/5/5/5	-
2	MPD	17-A	401	-	-	1/5/5/5	-
2	MPD	10-B	701	-	-	4/5/5/5	-
2	MPD	22-B	707	-	-	1/5/5/5	-
2	MPD	34-A	401	-	-	2/5/5/5	-
3	AHD	7-B	706	4	-	0/23/23/23	-
2	MPD	24-A	401	-	-	4/5/5/5	-
2	MPD	7-A	403	-	-	0/5/5/5	-
2	MPD	42-B	701	-	-	1/5/5/5	-
2	MPD	30-B	701	-	-	4/5/5/5	-
3	AHD	43-B	706	4	-	4/23/23/23	-
2	MPD	18-A	403	-	-	0/5/5/5	-
3	AHD	34-B	706	4	-	1/23/23/23	-
3	AHD	44-B	706	4	-	4/23/23/23	-
2	MPD	20-A	401	-	-	1/5/5/5	-
3	AHD	40-B	706	4	-	0/23/23/23	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	31-B	701	-	-	2/5/5/5	-
2	MPD	9-B	707	-	-	3/5/5/5	-
2	MPD	40-B	701	-	-	2/5/5/5	-
3	AHD	41-A	402	4	-	4/23/23/23	-
2	MPD	42-B	707	-	-	1/5/5/5	-
3	AHD	25-A	402	4	-	6/23/23/23	-
3	AHD	32-A	402	4	-	4/23/23/23	-
2	MPD	18-B	701	-	-	0/5/5/5	-
2	MPD	47-A	401	-	-	4/5/5/5	-
3	AHD	8-B	706	4	-	3/23/23/23	-
3	AHD	11-B	706	4	-	4/23/23/23	-
2	MPD	2-B	701	-	-	2/5/5/5	-
2	MPD	11-B	701	-	-	3/5/5/5	-
2	MPD	16-B	707	-	-	0/5/5/5	-
2	MPD	24-B	707	-	-	0/5/5/5	-
2	MPD	16-A	403	-	-	0/5/5/5	-
3	AHD	1-A	402	4	-	5/23/23/23	-
3	AHD	9-A	402	4	-	5/23/23/23	-
2	MPD	14-B	707	-	-	0/5/5/5	-
2	MPD	6-A	401	-	-	1/5/5/5	-
2	MPD	32-A	403	-	-	2/5/5/5	-
3	AHD	50-A	402	4	-	4/23/23/23	-
2	MPD	1-B	701	-	-	1/5/5/5	-
2	MPD	36-A	401	-	-	3/5/5/5	-
3	AHD	39-A	402	4	-	3/23/23/23	-
2	MPD	43-A	403	-	-	2/5/5/5	-
3	AHD	30-B	706	4	-	3/23/23/23	-
2	MPD	8-A	401	-	-	4/5/5/5	-
2	MPD	50-A	403	-	-	0/5/5/5	-
3	AHD	17-B	706	4	-	3/23/23/23	-
2	MPD	2-A	403	-	-	0/5/5/5	-
3	AHD	28-A	402	4	-	5/23/23/23	-
2	MPD	17-B	707	-	-	2/5/5/5	-
3	AHD	49-A	402	4	-	4/23/23/23	-
2	MPD	32-B	701	-	-	2/5/5/5	-
2	MPD	4-A	403	-	-	1/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	2-A	401	-	-	4/5/5/5	-
2	MPD	27-A	401	-	-	5/5/5/5	-
2	MPD	37-A	403	-	-	1/5/5/5	-
2	MPD	15-B	701	-	-	4/5/5/5	-
3	AHD	36-B	706	4	-	1/23/23/23	-
2	MPD	49-B	707	-	-	0/5/5/5	-
2	MPD	31-A	401	-	-	1/5/5/5	-
3	AHD	20-B	706	4	-	4/23/23/23	-
3	AHD	43-A	402	4	-	0/23/23/23	-
2	MPD	43-A	401	-	-	4/5/5/5	-
3	AHD	23-A	402	4	-	4/23/23/23	-
2	MPD	40-B	707	-	-	0/5/5/5	-
2	MPD	3-A	401	-	-	5/5/5/5	-
3	AHD	37-B	706	4	-	4/23/23/23	-
2	MPD	15-A	403	-	-	0/5/5/5	-
2	MPD	30-A	403	-	-	1/5/5/5	-
2	MPD	44-B	707	-	-	0/5/5/5	-
2	MPD	38-B	707	-	-	3/5/5/5	-
3	AHD	18-A	402	4	-	3/23/23/23	-
3	AHD	5-A	402	4	-	8/23/23/23	-
2	MPD	7-A	401	-	-	4/5/5/5	-
2	MPD	22-B	701	-	-	1/5/5/5	-
2	MPD	26-A	403	-	-	0/5/5/5	-
3	AHD	10-B	706	4	-	2/23/23/23	-
2	MPD	1-B	707	-	-	2/5/5/5	-
3	AHD	8-A	402	4	-	4/23/23/23	-
2	MPD	30-A	401	-	-	2/5/5/5	-
2	MPD	40-A	403	-	-	3/5/5/5	-
2	MPD	10-B	707	-	-	0/5/5/5	-
3	AHD	11-A	402	4	-	3/23/23/23	-
3	AHD	13-A	402	4	-	4/23/23/23	-
3	AHD	42-A	402	4	-	2/23/23/23	-
2	MPD	45-B	707	-	-	0/5/5/5	-
2	MPD	38-B	701	-	-	2/5/5/5	-
3	AHD	42-B	706	4	-	0/23/23/23	-
2	MPD	41-A	403	-	-	0/5/5/5	-
3	AHD	44-A	402	4	-	1/23/23/23	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AHD	16-A	402	4	-	4/23/23/23	-
3	AHD	13-B	706	4	-	3/23/23/23	-

The worst 5 of 502 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	46-A	402	AHD	O13-C8	-4.92	1.38	1.44
3	12-A	402	AHD	O13-C8	-4.46	1.39	1.44
3	37-A	402	AHD	O13-C8	-4.23	1.39	1.44
3	9-A	402	AHD	O13-C8	-4.20	1.39	1.44
3	33-A	402	AHD	O13-C8	-4.18	1.39	1.44

The worst 5 of 455 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7-B	707	MPD	CM-C2-C1	-6.50	97.02	110.57
3	32-A	402	AHD	C2-C7-C8	-6.11	104.86	116.07
3	34-B	706	AHD	C2-C7-C8	-5.72	105.57	116.07
3	21-B	706	AHD	C2-C7-C8	-5.54	105.89	116.07
3	29-B	706	AHD	C2-C7-C8	-5.34	106.26	116.07

There are no chirality outliers.

5 of 644 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1-A	401	MPD	C2-C3-C4-O4
2	2-A	401	MPD	O2-C2-C3-C4
2	2-A	401	MPD	C2-C3-C4-O4
2	3-A	401	MPD	C2-C3-C4-O4
2	4-A	401	MPD	C2-C3-C4-O4

There are no ring outliers.

No monomer is involved in short contacts.

## 4.7 Other polymers ⓘ

There are no such residues in this entry.

## 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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1-A	295/318 (92%)	1.04	41 (13%) 7 9	0, 0, 1, 1	295 (100%)
1	1-B	296/318 (93%)	1.03	43 (14%) 7 8	0, 0, 1, 1	296 (100%)
1	2-A	0/318	-	-	-	-
1	2-B	0/318	-	-	-	-
1	3-A	0/318	-	-	-	-
1	3-B	0/318	-	-	-	-
1	4-A	0/318	-	-	-	-
1	4-B	0/318	-	-	-	-
1	5-A	0/318	-	-	-	-
1	5-B	0/318	-	-	-	-
1	6-A	0/318	-	-	-	-
1	6-B	0/318	-	-	-	-
1	7-A	0/318	-	-	-	-
1	7-B	0/318	-	-	-	-
1	8-A	0/318	-	-	-	-
1	8-B	0/318	-	-	-	-
1	9-A	0/318	-	-	-	-
1	9-B	0/318	-	-	-	-
1	10-A	0/318	-	-	-	-
1	10-B	0/318	-	-	-	-
1	11-A	0/318	-	-	-	-
1	11-B	0/318	-	-	-	-
1	12-A	0/318	-	-	-	-
1	12-B	0/318	-	-	-	-
1	13-A	0/318	-	-	-	-
1	13-B	0/318	-	-	-	-
1	14-A	0/318	-	-	-	-
1	14-B	0/318	-	-	-	-
1	15-A	0/318	-	-	-	-
1	15-B	0/318	-	-	-	-
1	16-A	0/318	-	-	-	-
1	16-B	0/318	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	17-A	0/318	-	-	-	-
1	17-B	0/318	-	-	-	-
1	18-A	0/318	-	-	-	-
1	18-B	0/318	-	-	-	-
1	19-A	0/318	-	-	-	-
1	19-B	0/318	-	-	-	-
1	20-A	0/318	-	-	-	-
1	20-B	0/318	-	-	-	-
1	21-A	0/318	-	-	-	-
1	21-B	0/318	-	-	-	-
1	22-A	0/318	-	-	-	-
1	22-B	0/318	-	-	-	-
1	23-A	0/318	-	-	-	-
1	23-B	0/318	-	-	-	-
1	24-A	0/318	-	-	-	-
1	24-B	0/318	-	-	-	-
1	25-A	0/318	-	-	-	-
1	25-B	0/318	-	-	-	-
1	26-A	0/318	-	-	-	-
1	26-B	0/318	-	-	-	-
1	27-A	0/318	-	-	-	-
1	27-B	0/318	-	-	-	-
1	28-A	0/318	-	-	-	-
1	28-B	0/318	-	-	-	-
1	29-A	0/318	-	-	-	-
1	29-B	0/318	-	-	-	-
1	30-A	0/318	-	-	-	-
1	30-B	0/318	-	-	-	-
1	31-A	0/318	-	-	-	-
1	31-B	0/318	-	-	-	-
1	32-A	0/318	-	-	-	-
1	32-B	0/318	-	-	-	-
1	33-A	0/318	-	-	-	-
1	33-B	0/318	-	-	-	-
1	34-A	0/318	-	-	-	-
1	34-B	0/318	-	-	-	-
1	35-A	0/318	-	-	-	-
1	35-B	0/318	-	-	-	-
1	36-A	0/318	-	-	-	-
1	36-B	0/318	-	-	-	-
1	37-A	0/318	-	-	-	-
1	37-B	0/318	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	38-A	0/318	-	-	-	-
1	38-B	0/318	-	-	-	-
1	39-A	0/318	-	-	-	-
1	39-B	0/318	-	-	-	-
1	40-A	0/318	-	-	-	-
1	40-B	0/318	-	-	-	-
1	41-A	0/318	-	-	-	-
1	41-B	0/318	-	-	-	-
1	42-A	0/318	-	-	-	-
1	42-B	0/318	-	-	-	-
1	43-A	0/318	-	-	-	-
1	43-B	0/318	-	-	-	-
1	44-A	0/318	-	-	-	-
1	44-B	0/318	-	-	-	-
1	45-A	0/318	-	-	-	-
1	45-B	0/318	-	-	-	-
1	46-A	0/318	-	-	-	-
1	46-B	0/318	-	-	-	-
1	47-A	0/318	-	-	-	-
1	47-B	0/318	-	-	-	-
1	48-A	0/318	-	-	-	-
1	48-B	0/318	-	-	-	-
1	49-A	0/318	-	-	-	-
1	49-B	0/318	-	-	-	-
1	50-A	0/318	-	-	-	-
1	50-B	0/318	-	-	-	-
All	All	591/31800 (1%)	1.04	84 (14%) 7 8	0, 0, 1, 1	591 (100%)

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	303	ASN	14.3
1	1-A	308	ALA	13.3
1	1-B	306	ILE	12.6
1	1-A	306	ILE	12.1
1	1-A	298	ALA	11.5

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

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

### 5.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MPD	1-B	707	8/8	0.48	0.25	17,17,18,18	8
2	MPD	2-A	401	8/8	-	-	18,19,19,20	8
2	MPD	3-A	401	8/8	-	-	18,19,19,20	8
2	MPD	4-A	401	8/8	-	-	18,19,19,20	8
2	MPD	5-A	401	8/8	-	-	18,19,19,20	8
2	MPD	6-A	401	8/8	-	-	18,19,19,20	8
2	MPD	7-A	401	8/8	-	-	18,19,19,20	8
2	MPD	8-A	401	8/8	-	-	18,19,19,20	8
2	MPD	9-A	401	8/8	-	-	18,19,19,20	8
2	MPD	10-A	401	8/8	-	-	18,19,19,20	8
2	MPD	11-A	401	8/8	-	-	18,19,19,20	8
2	MPD	12-A	401	8/8	-	-	18,19,19,20	8
2	MPD	13-A	401	8/8	-	-	18,19,19,20	8
2	MPD	14-A	401	8/8	-	-	18,19,19,20	8
2	MPD	15-A	401	8/8	-	-	18,19,19,20	8
2	MPD	16-A	401	8/8	-	-	18,19,19,20	8
2	MPD	17-A	401	8/8	-	-	18,19,19,20	8
2	MPD	18-A	401	8/8	-	-	18,19,19,20	8
2	MPD	19-A	401	8/8	-	-	18,19,19,20	8
2	MPD	20-A	401	8/8	-	-	18,19,19,20	8
2	MPD	21-A	401	8/8	-	-	18,19,19,20	8
2	MPD	22-A	401	8/8	-	-	18,19,19,20	8
2	MPD	23-A	401	8/8	-	-	18,19,19,20	8
2	MPD	24-A	401	8/8	-	-	18,19,19,20	8
2	MPD	25-A	401	8/8	-	-	18,19,19,20	8
2	MPD	26-A	401	8/8	-	-	18,19,19,20	8
2	MPD	27-A	401	8/8	-	-	18,19,19,20	8
2	MPD	28-A	401	8/8	-	-	18,19,19,20	8
2	MPD	29-A	401	8/8	-	-	18,19,19,20	8
2	MPD	30-A	401	8/8	-	-	18,19,19,20	8
2	MPD	31-A	401	8/8	-	-	18,19,19,20	8
2	MPD	32-A	401	8/8	-	-	18,19,19,20	8

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MPD	33-A	401	8/8	-	-	18,19,19,20	8
2	MPD	34-A	401	8/8	-	-	18,19,19,20	8
2	MPD	35-A	401	8/8	-	-	18,19,19,20	8
2	MPD	36-A	401	8/8	-	-	18,19,19,20	8
2	MPD	37-A	401	8/8	-	-	18,19,19,20	8
2	MPD	38-A	401	8/8	-	-	18,19,19,20	8
2	MPD	39-A	401	8/8	-	-	18,19,19,20	8
2	MPD	40-A	401	8/8	-	-	18,19,19,20	8
2	MPD	41-A	401	8/8	-	-	18,19,19,20	8
2	MPD	42-A	401	8/8	-	-	18,19,19,20	8
2	MPD	43-A	401	8/8	-	-	18,19,19,20	8
2	MPD	44-A	401	8/8	-	-	18,19,19,20	8
2	MPD	45-A	401	8/8	-	-	18,19,19,20	8
2	MPD	46-A	401	8/8	-	-	18,19,19,20	8
2	MPD	47-A	401	8/8	-	-	18,19,19,20	8
2	MPD	48-A	401	8/8	-	-	18,19,19,20	8
2	MPD	49-A	401	8/8	-	-	18,19,19,20	8
2	MPD	50-A	401	8/8	-	-	18,19,19,20	8
2	MPD	1-A	401	8/8	0.55	0.23	18,19,19,20	8
2	MPD	2-A	403	8/8	-	-	16,17,17,17	8
2	MPD	3-A	403	8/8	-	-	16,17,17,17	8
2	MPD	4-A	403	8/8	-	-	16,17,17,17	8
2	MPD	5-A	403	8/8	-	-	16,17,17,17	8
2	MPD	6-A	403	8/8	-	-	16,17,17,17	8
2	MPD	7-A	403	8/8	-	-	16,17,17,17	8
2	MPD	8-A	403	8/8	-	-	16,17,17,17	8
2	MPD	9-A	403	8/8	-	-	16,17,17,17	8
2	MPD	10-A	403	8/8	-	-	16,17,17,17	8
2	MPD	11-A	403	8/8	-	-	16,17,17,17	8
2	MPD	12-A	403	8/8	-	-	16,17,17,17	8
2	MPD	13-A	403	8/8	-	-	16,17,17,17	8
2	MPD	14-A	403	8/8	-	-	16,17,17,17	8
2	MPD	15-A	403	8/8	-	-	16,17,17,17	8
2	MPD	16-A	403	8/8	-	-	16,17,17,17	8
2	MPD	17-A	403	8/8	-	-	16,17,17,17	8
2	MPD	18-A	403	8/8	-	-	16,17,17,17	8
2	MPD	19-A	403	8/8	-	-	16,17,17,17	8
2	MPD	20-A	403	8/8	-	-	16,17,17,17	8
2	MPD	21-A	403	8/8	-	-	16,17,17,17	8
2	MPD	22-A	403	8/8	-	-	16,17,17,17	8
2	MPD	23-A	403	8/8	-	-	16,17,17,17	8
2	MPD	24-A	403	8/8	-	-	16,17,17,17	8

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MPD	25-A	403	8/8	-	-	16,17,17,17	8
2	MPD	26-A	403	8/8	-	-	16,17,17,17	8
2	MPD	27-A	403	8/8	-	-	16,17,17,17	8
2	MPD	28-A	403	8/8	-	-	16,17,17,17	8
2	MPD	29-A	403	8/8	-	-	16,17,17,17	8
2	MPD	30-A	403	8/8	-	-	16,17,17,17	8
2	MPD	31-A	403	8/8	-	-	16,17,17,17	8
2	MPD	32-A	403	8/8	-	-	16,17,17,17	8
2	MPD	33-A	403	8/8	-	-	16,17,17,17	8
2	MPD	34-A	403	8/8	-	-	16,17,17,17	8
2	MPD	35-A	403	8/8	-	-	16,17,17,17	8
2	MPD	36-A	403	8/8	-	-	16,17,17,17	8
2	MPD	37-A	403	8/8	-	-	16,17,17,17	8
2	MPD	38-A	403	8/8	-	-	16,17,17,17	8
2	MPD	39-A	403	8/8	-	-	16,17,17,17	8
2	MPD	40-A	403	8/8	-	-	16,17,17,17	8
2	MPD	41-A	403	8/8	-	-	16,17,17,17	8
2	MPD	42-A	403	8/8	-	-	16,17,17,17	8
2	MPD	43-A	403	8/8	-	-	16,17,17,17	8
2	MPD	44-A	403	8/8	-	-	16,17,17,17	8
2	MPD	45-A	403	8/8	-	-	16,17,17,17	8
2	MPD	46-A	403	8/8	-	-	16,17,17,17	8
2	MPD	47-A	403	8/8	-	-	16,17,17,17	8
2	MPD	48-A	403	8/8	-	-	16,17,17,17	8
2	MPD	49-A	403	8/8	-	-	16,17,17,17	8
2	MPD	50-A	403	8/8	-	-	16,17,17,17	8
2	MPD	1-A	403	8/8	0.74	0.18	16,17,17,17	8
2	MPD	2-B	701	8/8	-	-	15,15,16,16	8
2	MPD	3-B	701	8/8	-	-	15,15,16,16	8
2	MPD	4-B	701	8/8	-	-	15,15,16,16	8
2	MPD	5-B	701	8/8	-	-	15,15,16,16	8
2	MPD	6-B	701	8/8	-	-	15,15,16,16	8
2	MPD	7-B	701	8/8	-	-	15,15,16,16	8
2	MPD	8-B	701	8/8	-	-	15,15,16,16	8
2	MPD	9-B	701	8/8	-	-	15,15,16,16	8
2	MPD	10-B	701	8/8	-	-	15,15,16,16	8
2	MPD	11-B	701	8/8	-	-	15,15,16,16	8
2	MPD	12-B	701	8/8	-	-	15,15,16,16	8
2	MPD	13-B	701	8/8	-	-	15,15,16,16	8
2	MPD	14-B	701	8/8	-	-	15,15,16,16	8
2	MPD	15-B	701	8/8	-	-	15,15,16,16	8
2	MPD	16-B	701	8/8	-	-	15,15,16,16	8

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MPD	17-B	701	8/8	-	-	15,15,16,16	8
2	MPD	18-B	701	8/8	-	-	15,15,16,16	8
2	MPD	19-B	701	8/8	-	-	15,15,16,16	8
2	MPD	20-B	701	8/8	-	-	15,15,16,16	8
2	MPD	21-B	701	8/8	-	-	15,15,16,16	8
2	MPD	22-B	701	8/8	-	-	15,15,16,16	8
2	MPD	23-B	701	8/8	-	-	15,15,16,16	8
2	MPD	24-B	701	8/8	-	-	15,15,16,16	8
2	MPD	25-B	701	8/8	-	-	15,15,16,16	8
2	MPD	26-B	701	8/8	-	-	15,15,16,16	8
2	MPD	27-B	701	8/8	-	-	15,15,16,16	8
2	MPD	28-B	701	8/8	-	-	15,15,16,16	8
2	MPD	29-B	701	8/8	-	-	15,15,16,16	8
2	MPD	30-B	701	8/8	-	-	15,15,16,16	8
2	MPD	31-B	701	8/8	-	-	15,15,16,16	8
2	MPD	32-B	701	8/8	-	-	15,15,16,16	8
2	MPD	33-B	701	8/8	-	-	15,15,16,16	8
2	MPD	34-B	701	8/8	-	-	15,15,16,16	8
2	MPD	35-B	701	8/8	-	-	15,15,16,16	8
2	MPD	36-B	701	8/8	-	-	15,15,16,16	8
2	MPD	37-B	701	8/8	-	-	15,15,16,16	8
2	MPD	38-B	701	8/8	-	-	15,15,16,16	8
2	MPD	39-B	701	8/8	-	-	15,15,16,16	8
2	MPD	40-B	701	8/8	-	-	15,15,16,16	8
2	MPD	41-B	701	8/8	-	-	15,15,16,16	8
2	MPD	42-B	701	8/8	-	-	15,15,16,16	8
2	MPD	43-B	701	8/8	-	-	15,15,16,16	8
2	MPD	44-B	701	8/8	-	-	15,15,16,16	8
2	MPD	45-B	701	8/8	-	-	15,15,16,16	8
2	MPD	46-B	701	8/8	-	-	15,15,16,16	8
2	MPD	47-B	701	8/8	-	-	15,15,16,16	8
2	MPD	48-B	701	8/8	-	-	15,15,16,16	8
2	MPD	49-B	701	8/8	-	-	15,15,16,16	8
2	MPD	50-B	701	8/8	-	-	15,15,16,16	8
2	MPD	1-B	701	8/8	0.75	0.23	15,15,16,16	8
2	MPD	2-B	707	8/8	-	-	17,17,18,18	8
2	MPD	3-B	707	8/8	-	-	17,17,18,18	8
2	MPD	4-B	707	8/8	-	-	17,17,18,18	8
2	MPD	5-B	707	8/8	-	-	17,17,18,18	8
2	MPD	6-B	707	8/8	-	-	17,17,18,18	8
2	MPD	7-B	707	8/8	-	-	17,17,18,18	8
2	MPD	8-B	707	8/8	-	-	17,17,18,18	8

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MPD	9-B	707	8/8	-	-	17,17,18,18	8
2	MPD	10-B	707	8/8	-	-	17,17,18,18	8
2	MPD	11-B	707	8/8	-	-	17,17,18,18	8
2	MPD	12-B	707	8/8	-	-	17,17,18,18	8
2	MPD	13-B	707	8/8	-	-	17,17,18,18	8
2	MPD	14-B	707	8/8	-	-	17,17,18,18	8
2	MPD	15-B	707	8/8	-	-	17,17,18,18	8
2	MPD	16-B	707	8/8	-	-	17,17,18,18	8
2	MPD	17-B	707	8/8	-	-	17,17,18,18	8
2	MPD	18-B	707	8/8	-	-	17,17,18,18	8
2	MPD	19-B	707	8/8	-	-	17,17,18,18	8
2	MPD	20-B	707	8/8	-	-	17,17,18,18	8
2	MPD	21-B	707	8/8	-	-	17,17,18,18	8
2	MPD	22-B	707	8/8	-	-	17,17,18,18	8
2	MPD	23-B	707	8/8	-	-	17,17,18,18	8
2	MPD	24-B	707	8/8	-	-	17,17,18,18	8
2	MPD	25-B	707	8/8	-	-	17,17,18,18	8
2	MPD	26-B	707	8/8	-	-	17,17,18,18	8
2	MPD	27-B	707	8/8	-	-	17,17,18,18	8
2	MPD	28-B	707	8/8	-	-	17,17,18,18	8
2	MPD	29-B	707	8/8	-	-	17,17,18,18	8
2	MPD	30-B	707	8/8	-	-	17,17,18,18	8
2	MPD	31-B	707	8/8	-	-	17,17,18,18	8
2	MPD	32-B	707	8/8	-	-	17,17,18,18	8
2	MPD	33-B	707	8/8	-	-	17,17,18,18	8
2	MPD	34-B	707	8/8	-	-	17,17,18,18	8
2	MPD	35-B	707	8/8	-	-	17,17,18,18	8
2	MPD	36-B	707	8/8	-	-	17,17,18,18	8
2	MPD	37-B	707	8/8	-	-	17,17,18,18	8
2	MPD	38-B	707	8/8	-	-	17,17,18,18	8
2	MPD	39-B	707	8/8	-	-	17,17,18,18	8
2	MPD	40-B	707	8/8	-	-	17,17,18,18	8
2	MPD	41-B	707	8/8	-	-	17,17,18,18	8
2	MPD	42-B	707	8/8	-	-	17,17,18,18	8
2	MPD	43-B	707	8/8	-	-	17,17,18,18	8
2	MPD	44-B	707	8/8	-	-	17,17,18,18	8
2	MPD	45-B	707	8/8	-	-	17,17,18,18	8
2	MPD	46-B	707	8/8	-	-	17,17,18,18	8
2	MPD	47-B	707	8/8	-	-	17,17,18,18	8
2	MPD	48-B	707	8/8	-	-	17,17,18,18	8
2	MPD	49-B	707	8/8	-	-	17,17,18,18	8
2	MPD	50-B	707	8/8	-	-	17,17,18,18	8

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	1-A	405	1/1	0.75	0.09	19,19,19,19	1
3	AHD	2-A	402	14/14	-	-	17,18,19,19	14
3	AHD	3-A	402	14/14	-	-	17,18,19,19	14
3	AHD	4-A	402	14/14	-	-	17,18,19,19	14
3	AHD	5-A	402	14/14	-	-	17,18,19,19	14
3	AHD	6-A	402	14/14	-	-	17,18,19,19	14
3	AHD	7-A	402	14/14	-	-	17,18,19,19	14
3	AHD	8-A	402	14/14	-	-	17,18,19,19	14
3	AHD	9-A	402	14/14	-	-	17,18,19,19	14
3	AHD	10-A	402	14/14	-	-	17,18,19,19	14
3	AHD	11-A	402	14/14	-	-	17,18,19,19	14
3	AHD	12-A	402	14/14	-	-	17,18,19,19	14
3	AHD	13-A	402	14/14	-	-	17,18,19,19	14
3	AHD	14-A	402	14/14	-	-	17,18,19,19	14
3	AHD	15-A	402	14/14	-	-	17,18,19,19	14
3	AHD	16-A	402	14/14	-	-	17,18,19,19	14
3	AHD	17-A	402	14/14	-	-	17,18,19,19	14
3	AHD	18-A	402	14/14	-	-	17,18,19,19	14
3	AHD	19-A	402	14/14	-	-	17,18,19,19	14
3	AHD	20-A	402	14/14	-	-	17,18,19,19	14
3	AHD	21-A	402	14/14	-	-	17,18,19,19	14
3	AHD	22-A	402	14/14	-	-	17,18,19,19	14
3	AHD	23-A	402	14/14	-	-	17,18,19,19	14
3	AHD	24-A	402	14/14	-	-	17,18,19,19	14
3	AHD	25-A	402	14/14	-	-	17,18,19,19	14
3	AHD	26-A	402	14/14	-	-	17,18,19,19	14
3	AHD	27-A	402	14/14	-	-	17,18,19,19	14
3	AHD	28-A	402	14/14	-	-	17,18,19,19	14
3	AHD	29-A	402	14/14	-	-	17,18,19,19	14
3	AHD	30-A	402	14/14	-	-	17,18,19,19	14
3	AHD	31-A	402	14/14	-	-	17,18,19,19	14
3	AHD	32-A	402	14/14	-	-	17,18,19,19	14
3	AHD	33-A	402	14/14	-	-	17,18,19,19	14
3	AHD	34-A	402	14/14	-	-	17,18,19,19	14
3	AHD	35-A	402	14/14	-	-	17,18,19,19	14
3	AHD	36-A	402	14/14	-	-	17,18,19,19	14
3	AHD	37-A	402	14/14	-	-	17,18,19,19	14
3	AHD	38-A	402	14/14	-	-	17,18,19,19	14
3	AHD	39-A	402	14/14	-	-	17,18,19,19	14
3	AHD	40-A	402	14/14	-	-	17,18,19,19	14
3	AHD	41-A	402	14/14	-	-	17,18,19,19	14
3	AHD	42-A	402	14/14	-	-	17,18,19,19	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	AHD	43-A	402	14/14	-	-	17,18,19,19	14
3	AHD	44-A	402	14/14	-	-	17,18,19,19	14
3	AHD	45-A	402	14/14	-	-	17,18,19,19	14
3	AHD	46-A	402	14/14	-	-	17,18,19,19	14
3	AHD	47-A	402	14/14	-	-	17,18,19,19	14
3	AHD	48-A	402	14/14	-	-	17,18,19,19	14
3	AHD	49-A	402	14/14	-	-	17,18,19,19	14
3	AHD	50-A	402	14/14	-	-	17,18,19,19	14
4	MG	1-B	703	1/1	0.75	0.12	19,19,19,19	1
3	AHD	2-B	706	14/14	-	-	18,19,20,20	14
3	AHD	3-B	706	14/14	-	-	18,19,20,20	14
3	AHD	4-B	706	14/14	-	-	18,19,20,20	14
3	AHD	5-B	706	14/14	-	-	18,19,20,20	14
3	AHD	6-B	706	14/14	-	-	18,19,20,20	14
3	AHD	7-B	706	14/14	-	-	18,19,20,20	14
3	AHD	8-B	706	14/14	-	-	18,19,20,20	14
3	AHD	9-B	706	14/14	-	-	18,19,20,20	14
3	AHD	10-B	706	14/14	-	-	18,19,20,20	14
3	AHD	11-B	706	14/14	-	-	18,19,20,20	14
3	AHD	12-B	706	14/14	-	-	18,19,20,20	14
3	AHD	13-B	706	14/14	-	-	18,19,20,20	14
3	AHD	14-B	706	14/14	-	-	18,19,20,20	14
3	AHD	15-B	706	14/14	-	-	18,19,20,20	14
3	AHD	16-B	706	14/14	-	-	18,19,20,20	14
3	AHD	17-B	706	14/14	-	-	18,19,20,20	14
3	AHD	18-B	706	14/14	-	-	18,19,20,20	14
3	AHD	19-B	706	14/14	-	-	18,19,20,20	14
3	AHD	20-B	706	14/14	-	-	18,19,20,20	14
3	AHD	21-B	706	14/14	-	-	18,19,20,20	14
3	AHD	22-B	706	14/14	-	-	18,19,20,20	14
3	AHD	23-B	706	14/14	-	-	18,19,20,20	14
3	AHD	24-B	706	14/14	-	-	18,19,20,20	14
3	AHD	25-B	706	14/14	-	-	18,19,20,20	14
3	AHD	26-B	706	14/14	-	-	18,19,20,20	14
3	AHD	27-B	706	14/14	-	-	18,19,20,20	14
3	AHD	28-B	706	14/14	-	-	18,19,20,20	14
3	AHD	29-B	706	14/14	-	-	18,19,20,20	14
3	AHD	30-B	706	14/14	-	-	18,19,20,20	14
3	AHD	31-B	706	14/14	-	-	18,19,20,20	14
3	AHD	32-B	706	14/14	-	-	18,19,20,20	14
3	AHD	33-B	706	14/14	-	-	18,19,20,20	14
3	AHD	34-B	706	14/14	-	-	18,19,20,20	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	AHD	35-B	706	14/14	-	-	18,19,20,20	14
3	AHD	36-B	706	14/14	-	-	18,19,20,20	14
3	AHD	37-B	706	14/14	-	-	18,19,20,20	14
3	AHD	38-B	706	14/14	-	-	18,19,20,20	14
3	AHD	39-B	706	14/14	-	-	18,19,20,20	14
3	AHD	40-B	706	14/14	-	-	18,19,20,20	14
3	AHD	41-B	706	14/14	-	-	18,19,20,20	14
3	AHD	42-B	706	14/14	-	-	18,19,20,20	14
3	AHD	43-B	706	14/14	-	-	18,19,20,20	14
3	AHD	44-B	706	14/14	-	-	18,19,20,20	14
3	AHD	45-B	706	14/14	-	-	18,19,20,20	14
3	AHD	46-B	706	14/14	-	-	18,19,20,20	14
3	AHD	47-B	706	14/14	-	-	18,19,20,20	14
3	AHD	48-B	706	14/14	-	-	18,19,20,20	14
3	AHD	49-B	706	14/14	-	-	18,19,20,20	14
3	AHD	50-B	706	14/14	-	-	18,19,20,20	14
5	CL	1-A	407	1/1	0.81	0.14	19,19,19,19	1
4	MG	2-A	404	1/1	-	-	18,18,18,18	1
4	MG	3-A	404	1/1	-	-	18,18,18,18	1
4	MG	4-A	404	1/1	-	-	18,18,18,18	1
4	MG	5-A	404	1/1	-	-	18,18,18,18	1
4	MG	6-A	404	1/1	-	-	18,18,18,18	1
4	MG	7-A	404	1/1	-	-	18,18,18,18	1
4	MG	8-A	404	1/1	-	-	18,18,18,18	1
4	MG	9-A	404	1/1	-	-	18,18,18,18	1
4	MG	10-A	404	1/1	-	-	18,18,18,18	1
4	MG	11-A	404	1/1	-	-	18,18,18,18	1
4	MG	12-A	404	1/1	-	-	18,18,18,18	1
4	MG	13-A	404	1/1	-	-	18,18,18,18	1
4	MG	14-A	404	1/1	-	-	18,18,18,18	1
4	MG	15-A	404	1/1	-	-	18,18,18,18	1
4	MG	16-A	404	1/1	-	-	18,18,18,18	1
4	MG	17-A	404	1/1	-	-	18,18,18,18	1
4	MG	18-A	404	1/1	-	-	18,18,18,18	1
4	MG	19-A	404	1/1	-	-	18,18,18,18	1
4	MG	20-A	404	1/1	-	-	18,18,18,18	1
4	MG	21-A	404	1/1	-	-	18,18,18,18	1
4	MG	22-A	404	1/1	-	-	18,18,18,18	1
4	MG	23-A	404	1/1	-	-	18,18,18,18	1
4	MG	24-A	404	1/1	-	-	18,18,18,18	1
4	MG	25-A	404	1/1	-	-	18,18,18,18	1
4	MG	26-A	404	1/1	-	-	18,18,18,18	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	27-A	404	1/1	-	-	18,18,18,18	1
4	MG	28-A	404	1/1	-	-	18,18,18,18	1
4	MG	29-A	404	1/1	-	-	18,18,18,18	1
4	MG	30-A	404	1/1	-	-	18,18,18,18	1
4	MG	31-A	404	1/1	-	-	18,18,18,18	1
4	MG	32-A	404	1/1	-	-	18,18,18,18	1
4	MG	33-A	404	1/1	-	-	18,18,18,18	1
4	MG	34-A	404	1/1	-	-	18,18,18,18	1
4	MG	35-A	404	1/1	-	-	18,18,18,18	1
4	MG	36-A	404	1/1	-	-	18,18,18,18	1
4	MG	37-A	404	1/1	-	-	18,18,18,18	1
4	MG	38-A	404	1/1	-	-	18,18,18,18	1
4	MG	39-A	404	1/1	-	-	18,18,18,18	1
4	MG	40-A	404	1/1	-	-	18,18,18,18	1
4	MG	41-A	404	1/1	-	-	18,18,18,18	1
4	MG	42-A	404	1/1	-	-	18,18,18,18	1
4	MG	43-A	404	1/1	-	-	18,18,18,18	1
4	MG	44-A	404	1/1	-	-	18,18,18,18	1
4	MG	45-A	404	1/1	-	-	18,18,18,18	1
4	MG	46-A	404	1/1	-	-	18,18,18,18	1
4	MG	47-A	404	1/1	-	-	18,18,18,18	1
4	MG	48-A	404	1/1	-	-	18,18,18,18	1
4	MG	49-A	404	1/1	-	-	18,18,18,18	1
4	MG	50-A	404	1/1	-	-	18,18,18,18	1
5	CL	1-B	705	1/1	0.89	0.11	20,20,20,20	1
4	MG	2-A	405	1/1	-	-	19,19,19,19	1
4	MG	3-A	405	1/1	-	-	19,19,19,19	1
4	MG	4-A	405	1/1	-	-	19,19,19,19	1
4	MG	5-A	405	1/1	-	-	19,19,19,19	1
4	MG	6-A	405	1/1	-	-	19,19,19,19	1
4	MG	7-A	405	1/1	-	-	19,19,19,19	1
4	MG	8-A	405	1/1	-	-	19,19,19,19	1
4	MG	9-A	405	1/1	-	-	19,19,19,19	1
4	MG	10-A	405	1/1	-	-	19,19,19,19	1
4	MG	11-A	405	1/1	-	-	19,19,19,19	1
4	MG	12-A	405	1/1	-	-	19,19,19,19	1
4	MG	13-A	405	1/1	-	-	19,19,19,19	1
4	MG	14-A	405	1/1	-	-	19,19,19,19	1
4	MG	15-A	405	1/1	-	-	19,19,19,19	1
4	MG	16-A	405	1/1	-	-	19,19,19,19	1
4	MG	17-A	405	1/1	-	-	19,19,19,19	1
4	MG	18-A	405	1/1	-	-	19,19,19,19	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	19-A	405	1/1	-	-	19,19,19,19	1
4	MG	20-A	405	1/1	-	-	19,19,19,19	1
4	MG	21-A	405	1/1	-	-	19,19,19,19	1
4	MG	22-A	405	1/1	-	-	19,19,19,19	1
4	MG	23-A	405	1/1	-	-	19,19,19,19	1
4	MG	24-A	405	1/1	-	-	19,19,19,19	1
4	MG	25-A	405	1/1	-	-	19,19,19,19	1
4	MG	26-A	405	1/1	-	-	19,19,19,19	1
4	MG	27-A	405	1/1	-	-	19,19,19,19	1
4	MG	28-A	405	1/1	-	-	19,19,19,19	1
4	MG	29-A	405	1/1	-	-	19,19,19,19	1
4	MG	30-A	405	1/1	-	-	19,19,19,19	1
4	MG	31-A	405	1/1	-	-	19,19,19,19	1
4	MG	32-A	405	1/1	-	-	19,19,19,19	1
4	MG	33-A	405	1/1	-	-	19,19,19,19	1
4	MG	34-A	405	1/1	-	-	19,19,19,19	1
4	MG	35-A	405	1/1	-	-	19,19,19,19	1
4	MG	36-A	405	1/1	-	-	19,19,19,19	1
4	MG	37-A	405	1/1	-	-	19,19,19,19	1
4	MG	38-A	405	1/1	-	-	19,19,19,19	1
4	MG	39-A	405	1/1	-	-	19,19,19,19	1
4	MG	40-A	405	1/1	-	-	19,19,19,19	1
4	MG	41-A	405	1/1	-	-	19,19,19,19	1
4	MG	42-A	405	1/1	-	-	19,19,19,19	1
4	MG	43-A	405	1/1	-	-	19,19,19,19	1
4	MG	44-A	405	1/1	-	-	19,19,19,19	1
4	MG	45-A	405	1/1	-	-	19,19,19,19	1
4	MG	46-A	405	1/1	-	-	19,19,19,19	1
4	MG	47-A	405	1/1	-	-	19,19,19,19	1
4	MG	48-A	405	1/1	-	-	19,19,19,19	1
4	MG	49-A	405	1/1	-	-	19,19,19,19	1
4	MG	50-A	405	1/1	-	-	19,19,19,19	1
4	MG	1-B	702	1/1	0.90	0.06	20,20,20,20	1
4	MG	2-A	406	1/1	-	-	18,18,18,18	1
4	MG	3-A	406	1/1	-	-	18,18,18,18	1
4	MG	4-A	406	1/1	-	-	18,18,18,18	1
4	MG	5-A	406	1/1	-	-	18,18,18,18	1
4	MG	6-A	406	1/1	-	-	18,18,18,18	1
4	MG	7-A	406	1/1	-	-	18,18,18,18	1
4	MG	8-A	406	1/1	-	-	18,18,18,18	1
4	MG	9-A	406	1/1	-	-	18,18,18,18	1
4	MG	10-A	406	1/1	-	-	18,18,18,18	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	11-A	406	1/1	-	-	18,18,18,18	1
4	MG	12-A	406	1/1	-	-	18,18,18,18	1
4	MG	13-A	406	1/1	-	-	18,18,18,18	1
4	MG	14-A	406	1/1	-	-	18,18,18,18	1
4	MG	15-A	406	1/1	-	-	18,18,18,18	1
4	MG	16-A	406	1/1	-	-	18,18,18,18	1
4	MG	17-A	406	1/1	-	-	18,18,18,18	1
4	MG	18-A	406	1/1	-	-	18,18,18,18	1
4	MG	19-A	406	1/1	-	-	18,18,18,18	1
4	MG	20-A	406	1/1	-	-	18,18,18,18	1
4	MG	21-A	406	1/1	-	-	18,18,18,18	1
4	MG	22-A	406	1/1	-	-	18,18,18,18	1
4	MG	23-A	406	1/1	-	-	18,18,18,18	1
4	MG	24-A	406	1/1	-	-	18,18,18,18	1
4	MG	25-A	406	1/1	-	-	18,18,18,18	1
4	MG	26-A	406	1/1	-	-	18,18,18,18	1
4	MG	27-A	406	1/1	-	-	18,18,18,18	1
4	MG	28-A	406	1/1	-	-	18,18,18,18	1
4	MG	29-A	406	1/1	-	-	18,18,18,18	1
4	MG	30-A	406	1/1	-	-	18,18,18,18	1
4	MG	31-A	406	1/1	-	-	18,18,18,18	1
4	MG	32-A	406	1/1	-	-	18,18,18,18	1
4	MG	33-A	406	1/1	-	-	18,18,18,18	1
4	MG	34-A	406	1/1	-	-	18,18,18,18	1
4	MG	35-A	406	1/1	-	-	18,18,18,18	1
4	MG	36-A	406	1/1	-	-	18,18,18,18	1
4	MG	37-A	406	1/1	-	-	18,18,18,18	1
4	MG	38-A	406	1/1	-	-	18,18,18,18	1
4	MG	39-A	406	1/1	-	-	18,18,18,18	1
4	MG	40-A	406	1/1	-	-	18,18,18,18	1
4	MG	41-A	406	1/1	-	-	18,18,18,18	1
4	MG	42-A	406	1/1	-	-	18,18,18,18	1
4	MG	43-A	406	1/1	-	-	18,18,18,18	1
4	MG	44-A	406	1/1	-	-	18,18,18,18	1
4	MG	45-A	406	1/1	-	-	18,18,18,18	1
4	MG	46-A	406	1/1	-	-	18,18,18,18	1
4	MG	47-A	406	1/1	-	-	18,18,18,18	1
4	MG	48-A	406	1/1	-	-	18,18,18,18	1
4	MG	49-A	406	1/1	-	-	18,18,18,18	1
4	MG	50-A	406	1/1	-	-	18,18,18,18	1
4	MG	1-A	406	1/1	0.91	0.05	18,18,18,18	1
4	MG	2-B	702	1/1	-	-	20,20,20,20	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	3-B	702	1/1	-	-	20,20,20,20	1
4	MG	4-B	702	1/1	-	-	20,20,20,20	1
4	MG	5-B	702	1/1	-	-	20,20,20,20	1
4	MG	6-B	702	1/1	-	-	20,20,20,20	1
4	MG	7-B	702	1/1	-	-	20,20,20,20	1
4	MG	8-B	702	1/1	-	-	20,20,20,20	1
4	MG	9-B	702	1/1	-	-	20,20,20,20	1
4	MG	10-B	702	1/1	-	-	20,20,20,20	1
4	MG	11-B	702	1/1	-	-	20,20,20,20	1
4	MG	12-B	702	1/1	-	-	20,20,20,20	1
4	MG	13-B	702	1/1	-	-	20,20,20,20	1
4	MG	14-B	702	1/1	-	-	20,20,20,20	1
4	MG	15-B	702	1/1	-	-	20,20,20,20	1
4	MG	16-B	702	1/1	-	-	20,20,20,20	1
4	MG	17-B	702	1/1	-	-	20,20,20,20	1
4	MG	18-B	702	1/1	-	-	20,20,20,20	1
4	MG	19-B	702	1/1	-	-	20,20,20,20	1
4	MG	20-B	702	1/1	-	-	20,20,20,20	1
4	MG	21-B	702	1/1	-	-	20,20,20,20	1
4	MG	22-B	702	1/1	-	-	20,20,20,20	1
4	MG	23-B	702	1/1	-	-	20,20,20,20	1
4	MG	24-B	702	1/1	-	-	20,20,20,20	1
4	MG	25-B	702	1/1	-	-	20,20,20,20	1
4	MG	26-B	702	1/1	-	-	20,20,20,20	1
4	MG	27-B	702	1/1	-	-	20,20,20,20	1
4	MG	28-B	702	1/1	-	-	20,20,20,20	1
4	MG	29-B	702	1/1	-	-	20,20,20,20	1
4	MG	30-B	702	1/1	-	-	20,20,20,20	1
4	MG	31-B	702	1/1	-	-	20,20,20,20	1
4	MG	32-B	702	1/1	-	-	20,20,20,20	1
4	MG	33-B	702	1/1	-	-	20,20,20,20	1
4	MG	34-B	702	1/1	-	-	20,20,20,20	1
4	MG	35-B	702	1/1	-	-	20,20,20,20	1
4	MG	36-B	702	1/1	-	-	20,20,20,20	1
4	MG	37-B	702	1/1	-	-	20,20,20,20	1
4	MG	38-B	702	1/1	-	-	20,20,20,20	1
4	MG	39-B	702	1/1	-	-	20,20,20,20	1
4	MG	40-B	702	1/1	-	-	20,20,20,20	1
4	MG	41-B	702	1/1	-	-	20,20,20,20	1
4	MG	42-B	702	1/1	-	-	20,20,20,20	1
4	MG	43-B	702	1/1	-	-	20,20,20,20	1
4	MG	44-B	702	1/1	-	-	20,20,20,20	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	45-B	702	1/1	-	-	20,20,20,20	1
4	MG	46-B	702	1/1	-	-	20,20,20,20	1
4	MG	47-B	702	1/1	-	-	20,20,20,20	1
4	MG	48-B	702	1/1	-	-	20,20,20,20	1
4	MG	49-B	702	1/1	-	-	20,20,20,20	1
4	MG	50-B	702	1/1	-	-	20,20,20,20	1
4	MG	1-A	404	1/1	0.93	0.07	18,18,18,18	1
4	MG	2-B	703	1/1	-	-	19,19,19,19	1
4	MG	3-B	703	1/1	-	-	19,19,19,19	1
4	MG	4-B	703	1/1	-	-	19,19,19,19	1
4	MG	5-B	703	1/1	-	-	19,19,19,19	1
4	MG	6-B	703	1/1	-	-	19,19,19,19	1
4	MG	7-B	703	1/1	-	-	19,19,19,19	1
4	MG	8-B	703	1/1	-	-	19,19,19,19	1
4	MG	9-B	703	1/1	-	-	19,19,19,19	1
4	MG	10-B	703	1/1	-	-	19,19,19,19	1
4	MG	11-B	703	1/1	-	-	19,19,19,19	1
4	MG	12-B	703	1/1	-	-	19,19,19,19	1
4	MG	13-B	703	1/1	-	-	19,19,19,19	1
4	MG	14-B	703	1/1	-	-	19,19,19,19	1
4	MG	15-B	703	1/1	-	-	19,19,19,19	1
4	MG	16-B	703	1/1	-	-	19,19,19,19	1
4	MG	17-B	703	1/1	-	-	19,19,19,19	1
4	MG	18-B	703	1/1	-	-	19,19,19,19	1
4	MG	19-B	703	1/1	-	-	19,19,19,19	1
4	MG	20-B	703	1/1	-	-	19,19,19,19	1
4	MG	21-B	703	1/1	-	-	19,19,19,19	1
4	MG	22-B	703	1/1	-	-	19,19,19,19	1
4	MG	23-B	703	1/1	-	-	19,19,19,19	1
4	MG	24-B	703	1/1	-	-	19,19,19,19	1
4	MG	25-B	703	1/1	-	-	19,19,19,19	1
4	MG	26-B	703	1/1	-	-	19,19,19,19	1
4	MG	27-B	703	1/1	-	-	19,19,19,19	1
4	MG	28-B	703	1/1	-	-	19,19,19,19	1
4	MG	29-B	703	1/1	-	-	19,19,19,19	1
4	MG	30-B	703	1/1	-	-	19,19,19,19	1
4	MG	31-B	703	1/1	-	-	19,19,19,19	1
4	MG	32-B	703	1/1	-	-	19,19,19,19	1
4	MG	33-B	703	1/1	-	-	19,19,19,19	1
4	MG	34-B	703	1/1	-	-	19,19,19,19	1
4	MG	35-B	703	1/1	-	-	19,19,19,19	1
4	MG	36-B	703	1/1	-	-	19,19,19,19	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	37-B	703	1/1	-	-	19,19,19,19	1
4	MG	38-B	703	1/1	-	-	19,19,19,19	1
4	MG	39-B	703	1/1	-	-	19,19,19,19	1
4	MG	40-B	703	1/1	-	-	19,19,19,19	1
4	MG	41-B	703	1/1	-	-	19,19,19,19	1
4	MG	42-B	703	1/1	-	-	19,19,19,19	1
4	MG	43-B	703	1/1	-	-	19,19,19,19	1
4	MG	44-B	703	1/1	-	-	19,19,19,19	1
4	MG	45-B	703	1/1	-	-	19,19,19,19	1
4	MG	46-B	703	1/1	-	-	19,19,19,19	1
4	MG	47-B	703	1/1	-	-	19,19,19,19	1
4	MG	48-B	703	1/1	-	-	19,19,19,19	1
4	MG	49-B	703	1/1	-	-	19,19,19,19	1
4	MG	50-B	703	1/1	-	-	19,19,19,19	1
3	AHD	1-B	706	14/14	0.94	0.10	18,19,20,20	14
4	MG	2-B	704	1/1	-	-	19,19,19,19	1
4	MG	3-B	704	1/1	-	-	19,19,19,19	1
4	MG	4-B	704	1/1	-	-	19,19,19,19	1
4	MG	5-B	704	1/1	-	-	19,19,19,19	1
4	MG	6-B	704	1/1	-	-	19,19,19,19	1
4	MG	7-B	704	1/1	-	-	19,19,19,19	1
4	MG	8-B	704	1/1	-	-	19,19,19,19	1
4	MG	9-B	704	1/1	-	-	19,19,19,19	1
4	MG	10-B	704	1/1	-	-	19,19,19,19	1
4	MG	11-B	704	1/1	-	-	19,19,19,19	1
4	MG	12-B	704	1/1	-	-	19,19,19,19	1
4	MG	13-B	704	1/1	-	-	19,19,19,19	1
4	MG	14-B	704	1/1	-	-	19,19,19,19	1
4	MG	15-B	704	1/1	-	-	19,19,19,19	1
4	MG	16-B	704	1/1	-	-	19,19,19,19	1
4	MG	17-B	704	1/1	-	-	19,19,19,19	1
4	MG	18-B	704	1/1	-	-	19,19,19,19	1
4	MG	19-B	704	1/1	-	-	19,19,19,19	1
4	MG	20-B	704	1/1	-	-	19,19,19,19	1
4	MG	21-B	704	1/1	-	-	19,19,19,19	1
4	MG	22-B	704	1/1	-	-	19,19,19,19	1
4	MG	23-B	704	1/1	-	-	19,19,19,19	1
4	MG	24-B	704	1/1	-	-	19,19,19,19	1
4	MG	25-B	704	1/1	-	-	19,19,19,19	1
4	MG	26-B	704	1/1	-	-	19,19,19,19	1
4	MG	27-B	704	1/1	-	-	19,19,19,19	1
4	MG	28-B	704	1/1	-	-	19,19,19,19	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	29-B	704	1/1	-	-	19,19,19,19	1
4	MG	30-B	704	1/1	-	-	19,19,19,19	1
4	MG	31-B	704	1/1	-	-	19,19,19,19	1
4	MG	32-B	704	1/1	-	-	19,19,19,19	1
4	MG	33-B	704	1/1	-	-	19,19,19,19	1
4	MG	34-B	704	1/1	-	-	19,19,19,19	1
4	MG	35-B	704	1/1	-	-	19,19,19,19	1
4	MG	36-B	704	1/1	-	-	19,19,19,19	1
4	MG	37-B	704	1/1	-	-	19,19,19,19	1
4	MG	38-B	704	1/1	-	-	19,19,19,19	1
4	MG	39-B	704	1/1	-	-	19,19,19,19	1
4	MG	40-B	704	1/1	-	-	19,19,19,19	1
4	MG	41-B	704	1/1	-	-	19,19,19,19	1
4	MG	42-B	704	1/1	-	-	19,19,19,19	1
4	MG	43-B	704	1/1	-	-	19,19,19,19	1
4	MG	44-B	704	1/1	-	-	19,19,19,19	1
4	MG	45-B	704	1/1	-	-	19,19,19,19	1
4	MG	46-B	704	1/1	-	-	19,19,19,19	1
4	MG	47-B	704	1/1	-	-	19,19,19,19	1
4	MG	48-B	704	1/1	-	-	19,19,19,19	1
4	MG	49-B	704	1/1	-	-	19,19,19,19	1
4	MG	50-B	704	1/1	-	-	19,19,19,19	1
3	AHD	1-A	402	14/14	0.94	0.10	17,18,19,19	14
5	CL	2-A	407	1/1	-	-	19,19,19,19	1
5	CL	3-A	407	1/1	-	-	19,19,19,19	1
5	CL	4-A	407	1/1	-	-	19,19,19,19	1
5	CL	5-A	407	1/1	-	-	19,19,19,19	1
5	CL	6-A	407	1/1	-	-	19,19,19,19	1
5	CL	7-A	407	1/1	-	-	19,19,19,19	1
5	CL	8-A	407	1/1	-	-	19,19,19,19	1
5	CL	9-A	407	1/1	-	-	19,19,19,19	1
5	CL	10-A	407	1/1	-	-	19,19,19,19	1
5	CL	11-A	407	1/1	-	-	19,19,19,19	1
5	CL	12-A	407	1/1	-	-	19,19,19,19	1
5	CL	13-A	407	1/1	-	-	19,19,19,19	1
5	CL	14-A	407	1/1	-	-	19,19,19,19	1
5	CL	15-A	407	1/1	-	-	19,19,19,19	1
5	CL	16-A	407	1/1	-	-	19,19,19,19	1
5	CL	17-A	407	1/1	-	-	19,19,19,19	1
5	CL	18-A	407	1/1	-	-	19,19,19,19	1
5	CL	19-A	407	1/1	-	-	19,19,19,19	1
5	CL	20-A	407	1/1	-	-	19,19,19,19	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CL	21-A	407	1/1	-	-	19,19,19,19	1
5	CL	22-A	407	1/1	-	-	19,19,19,19	1
5	CL	23-A	407	1/1	-	-	19,19,19,19	1
5	CL	24-A	407	1/1	-	-	19,19,19,19	1
5	CL	25-A	407	1/1	-	-	19,19,19,19	1
5	CL	26-A	407	1/1	-	-	19,19,19,19	1
5	CL	27-A	407	1/1	-	-	19,19,19,19	1
5	CL	28-A	407	1/1	-	-	19,19,19,19	1
5	CL	29-A	407	1/1	-	-	19,19,19,19	1
5	CL	30-A	407	1/1	-	-	19,19,19,19	1
5	CL	31-A	407	1/1	-	-	19,19,19,19	1
5	CL	32-A	407	1/1	-	-	19,19,19,19	1
5	CL	33-A	407	1/1	-	-	19,19,19,19	1
5	CL	34-A	407	1/1	-	-	19,19,19,19	1
5	CL	35-A	407	1/1	-	-	19,19,19,19	1
5	CL	36-A	407	1/1	-	-	19,19,19,19	1
5	CL	37-A	407	1/1	-	-	19,19,19,19	1
5	CL	38-A	407	1/1	-	-	19,19,19,19	1
5	CL	39-A	407	1/1	-	-	19,19,19,19	1
5	CL	40-A	407	1/1	-	-	19,19,19,19	1
5	CL	41-A	407	1/1	-	-	19,19,19,19	1
5	CL	42-A	407	1/1	-	-	19,19,19,19	1
5	CL	43-A	407	1/1	-	-	19,19,19,19	1
5	CL	44-A	407	1/1	-	-	19,19,19,19	1
5	CL	45-A	407	1/1	-	-	19,19,19,19	1
5	CL	46-A	407	1/1	-	-	19,19,19,19	1
5	CL	47-A	407	1/1	-	-	19,19,19,19	1
5	CL	48-A	407	1/1	-	-	19,19,19,19	1
5	CL	49-A	407	1/1	-	-	19,19,19,19	1
5	CL	50-A	407	1/1	-	-	19,19,19,19	1
4	MG	1-B	704	1/1	0.99	0.05	19,19,19,19	1
5	CL	2-B	705	1/1	-	-	20,20,20,20	1
5	CL	3-B	705	1/1	-	-	20,20,20,20	1
5	CL	4-B	705	1/1	-	-	20,20,20,20	1
5	CL	5-B	705	1/1	-	-	20,20,20,20	1
5	CL	6-B	705	1/1	-	-	20,20,20,20	1
5	CL	7-B	705	1/1	-	-	20,20,20,20	1
5	CL	8-B	705	1/1	-	-	20,20,20,20	1
5	CL	9-B	705	1/1	-	-	20,20,20,20	1
5	CL	10-B	705	1/1	-	-	20,20,20,20	1
5	CL	11-B	705	1/1	-	-	20,20,20,20	1
5	CL	12-B	705	1/1	-	-	20,20,20,20	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CL	13-B	705	1/1	-	-	20,20,20,20	1
5	CL	14-B	705	1/1	-	-	20,20,20,20	1
5	CL	15-B	705	1/1	-	-	20,20,20,20	1
5	CL	16-B	705	1/1	-	-	20,20,20,20	1
5	CL	17-B	705	1/1	-	-	20,20,20,20	1
5	CL	18-B	705	1/1	-	-	20,20,20,20	1
5	CL	19-B	705	1/1	-	-	20,20,20,20	1
5	CL	20-B	705	1/1	-	-	20,20,20,20	1
5	CL	21-B	705	1/1	-	-	20,20,20,20	1
5	CL	22-B	705	1/1	-	-	20,20,20,20	1
5	CL	23-B	705	1/1	-	-	20,20,20,20	1
5	CL	24-B	705	1/1	-	-	20,20,20,20	1
5	CL	25-B	705	1/1	-	-	20,20,20,20	1
5	CL	26-B	705	1/1	-	-	20,20,20,20	1
5	CL	27-B	705	1/1	-	-	20,20,20,20	1
5	CL	28-B	705	1/1	-	-	20,20,20,20	1
5	CL	29-B	705	1/1	-	-	20,20,20,20	1
5	CL	30-B	705	1/1	-	-	20,20,20,20	1
5	CL	31-B	705	1/1	-	-	20,20,20,20	1
5	CL	32-B	705	1/1	-	-	20,20,20,20	1
5	CL	33-B	705	1/1	-	-	20,20,20,20	1
5	CL	34-B	705	1/1	-	-	20,20,20,20	1
5	CL	35-B	705	1/1	-	-	20,20,20,20	1
5	CL	36-B	705	1/1	-	-	20,20,20,20	1
5	CL	37-B	705	1/1	-	-	20,20,20,20	1
5	CL	38-B	705	1/1	-	-	20,20,20,20	1
5	CL	39-B	705	1/1	-	-	20,20,20,20	1
5	CL	40-B	705	1/1	-	-	20,20,20,20	1
5	CL	41-B	705	1/1	-	-	20,20,20,20	1
5	CL	42-B	705	1/1	-	-	20,20,20,20	1
5	CL	43-B	705	1/1	-	-	20,20,20,20	1
5	CL	44-B	705	1/1	-	-	20,20,20,20	1
5	CL	45-B	705	1/1	-	-	20,20,20,20	1
5	CL	46-B	705	1/1	-	-	20,20,20,20	1
5	CL	47-B	705	1/1	-	-	20,20,20,20	1
5	CL	48-B	705	1/1	-	-	20,20,20,20	1
5	CL	49-B	705	1/1	-	-	20,20,20,20	1
5	CL	50-B	705	1/1	-	-	20,20,20,20	1

## 5.5 Other polymers ⓘ

There are no such residues in this entry.