



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 9, 2025 – 03:03 pm BST

PDB ID : 9RP0 / pdb_00009rp0
Title : Ensemble refined structure of CotB2 in complex with 2-fluoro-3,7,18-dolabellatriene
Authors : Helmer, C.P.O.; Loll, B.
Deposited on : 2025-06-23
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
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

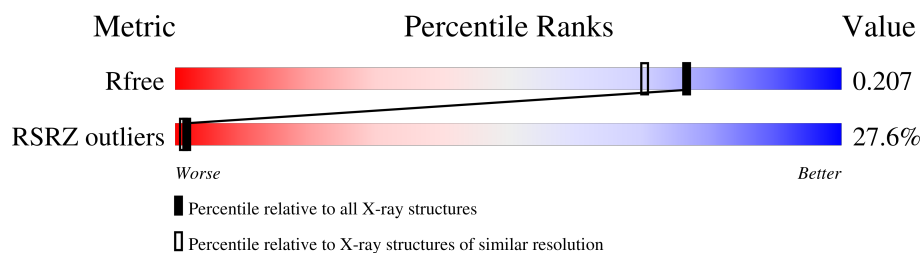
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7108 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EXW	13-A	407	-	X	-	-
4	EXW	16-B	406	-	X	-	-
4	EXW	2-B	406	-	X	-	-
4	EXW	25-A	407	-	X	-	-
4	EXW	28-A	407	-	X	-	-
4	EXW	3-A	407	-	X	-	-
4	EXW	31-A	407	-	X	-	-
4	EXW	33-A	407	-	X	-	-
4	EXW	34-B	406	-	X	-	-
4	EXW	35-A	407	-	X	-	-
4	EXW	37-A	407	-	X	-	-
4	EXW	38-A	407	-	X	-	-
4	EXW	39-B	406	-	X	-	-
4	EXW	40-A	407	-	X	-	-
4	EXW	41-A	407	-	X	-	-
4	EXW	42-B	406	-	X	-	-
4	EXW	43-A	407	-	X	-	-
4	EXW	45-A	407	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EXW	47-B	406	-	X	-	-
4	EXW	49-A	407	-	X	-	-
4	EXW	8-A	407	-	X	-	-
9	K	1-A	413	-	-	-	X
9	K	1-B	410	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 259400 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	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	2-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	3-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	4-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	5-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	6-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	7-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	8-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	9-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	10-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	11-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	12-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	13-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	14-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	15-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	16-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	17-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	18-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	19-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	20-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	21-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	22-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	23-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	24-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	25-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	26-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	27-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	28-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	29-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	30-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	31-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	32-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	33-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	34-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	35-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	36-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	37-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	38-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	39-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	40-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	41-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	42-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	43-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	44-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	45-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	46-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	47-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	48-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	49-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	50-A	294	Total	C	N	O	S	0	0	0
			2404	1528	407	452	17			
1	1-B	300	Total	C	N	O	S	0	0	0
			2443	1551	414	461	17			
1	2-B	300	Total	C	N	O	S	0	0	0
			2443	1551	414	461	17			
1	3-B	300	Total	C	N	O	S	0	0	0
			2443	1551	414	461	17			
1	4-B	300	Total	C	N	O	S	0	0	0
			2443	1551	414	461	17			
1	5-B	300	Total	C	N	O	S	0	0	0
			2443	1551	414	461	17			
1	6-B	300	Total	C	N	O	S	0	0	0
			2443	1551	414	461	17			
1	7-B	300	Total	C	N	O	S	0	0	0
			2443	1551	414	461	17			
1	8-B	300	Total	C	N	O	S	0	0	0
			2443	1551	414	461	17			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	9-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	10-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	11-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	12-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	13-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	14-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	15-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	16-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	17-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	18-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	19-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	20-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	21-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	22-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	23-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	24-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	25-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	26-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	27-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	28-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	29-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	30-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	31-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	32-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	33-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	34-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	35-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	36-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	37-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	38-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	39-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	40-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	41-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	42-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	43-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	44-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	45-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	46-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	47-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	48-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	49-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0
1	50-B	300	Total 2443	C 1551	N 414	O 461	S 17	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1-A	5	Total Mg 5 5	0	0
2	2-A	5	Total Mg 5 5	0	0
2	3-A	5	Total Mg 5 5	0	0
2	4-A	5	Total Mg 5 5	0	0
2	5-A	5	Total Mg 5 5	0	0
2	6-A	5	Total Mg 5 5	0	0
2	7-A	5	Total Mg 5 5	0	0
2	8-A	5	Total Mg 5 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	9-A	5	Total 5	Mg 5	0	0
2	10-A	5	Total 5	Mg 5	0	0
2	11-A	5	Total 5	Mg 5	0	0
2	12-A	5	Total 5	Mg 5	0	0
2	13-A	5	Total 5	Mg 5	0	0
2	14-A	5	Total 5	Mg 5	0	0
2	15-A	5	Total 5	Mg 5	0	0
2	16-A	5	Total 5	Mg 5	0	0
2	17-A	5	Total 5	Mg 5	0	0
2	18-A	5	Total 5	Mg 5	0	0
2	19-A	5	Total 5	Mg 5	0	0
2	20-A	5	Total 5	Mg 5	0	0
2	21-A	5	Total 5	Mg 5	0	0
2	22-A	5	Total 5	Mg 5	0	0
2	23-A	5	Total 5	Mg 5	0	0
2	24-A	5	Total 5	Mg 5	0	0
2	25-A	5	Total 5	Mg 5	0	0
2	26-A	5	Total 5	Mg 5	0	0
2	27-A	5	Total 5	Mg 5	0	0
2	28-A	5	Total 5	Mg 5	0	0
2	29-A	5	Total 5	Mg 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	30-A	5	Total 5	Mg 5	0	0
2	31-A	5	Total 5	Mg 5	0	0
2	32-A	5	Total 5	Mg 5	0	0
2	33-A	5	Total 5	Mg 5	0	0
2	34-A	5	Total 5	Mg 5	0	0
2	35-A	5	Total 5	Mg 5	0	0
2	36-A	5	Total 5	Mg 5	0	0
2	37-A	5	Total 5	Mg 5	0	0
2	38-A	5	Total 5	Mg 5	0	0
2	39-A	5	Total 5	Mg 5	0	0
2	40-A	5	Total 5	Mg 5	0	0
2	41-A	5	Total 5	Mg 5	0	0
2	42-A	5	Total 5	Mg 5	0	0
2	43-A	5	Total 5	Mg 5	0	0
2	44-A	5	Total 5	Mg 5	0	0
2	45-A	5	Total 5	Mg 5	0	0
2	46-A	5	Total 5	Mg 5	0	0
2	47-A	5	Total 5	Mg 5	0	0
2	48-A	5	Total 5	Mg 5	0	0
2	49-A	5	Total 5	Mg 5	0	0
2	50-A	5	Total 5	Mg 5	0	0

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

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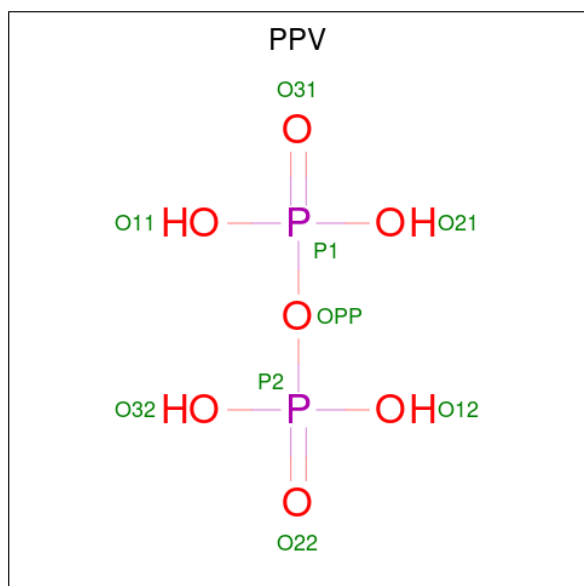
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	22-B	4	Total 4	Mg 4	0	0
2	23-B	4	Total 4	Mg 4	0	0
2	24-B	4	Total 4	Mg 4	0	0
2	25-B	4	Total 4	Mg 4	0	0
2	26-B	4	Total 4	Mg 4	0	0
2	27-B	4	Total 4	Mg 4	0	0
2	28-B	4	Total 4	Mg 4	0	0
2	29-B	4	Total 4	Mg 4	0	0
2	30-B	4	Total 4	Mg 4	0	0
2	31-B	4	Total 4	Mg 4	0	0
2	32-B	4	Total 4	Mg 4	0	0
2	33-B	4	Total 4	Mg 4	0	0
2	34-B	4	Total 4	Mg 4	0	0
2	35-B	4	Total 4	Mg 4	0	0
2	36-B	4	Total 4	Mg 4	0	0
2	37-B	4	Total 4	Mg 4	0	0
2	38-B	4	Total 4	Mg 4	0	0
2	39-B	4	Total 4	Mg 4	0	0
2	40-B	4	Total 4	Mg 4	0	0
2	41-B	4	Total 4	Mg 4	0	0
2	42-B	4	Total 4	Mg 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	43-B	4	Total 4	Mg 4	0	0
2	44-B	4	Total 4	Mg 4	0	0
2	45-B	4	Total 4	Mg 4	0	0
2	46-B	4	Total 4	Mg 4	0	0
2	47-B	4	Total 4	Mg 4	0	0
2	48-B	4	Total 4	Mg 4	0	0
2	49-B	4	Total 4	Mg 4	0	0
2	50-B	4	Total 4	Mg 4	0	0

- Molecule 3 is PYROPHOSPHATE (CCD ID: PPV) (formula: $\text{H}_4\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	1-A	1	Total 9	O 7	P 2	0	0
3	2-A	1	Total 9	O 7	P 2	0	0
3	3-A	1	Total 9	O 7	P 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	4-A	1	Total	O	P	0	0
			9	7	2		
3	5-A	1	Total	O	P	0	0
			9	7	2		
3	6-A	1	Total	O	P	0	0
			9	7	2		
3	7-A	1	Total	O	P	0	0
			9	7	2		
3	8-A	1	Total	O	P	0	0
			9	7	2		
3	9-A	1	Total	O	P	0	0
			9	7	2		
3	10-A	1	Total	O	P	0	0
			9	7	2		
3	11-A	1	Total	O	P	0	0
			9	7	2		
3	12-A	1	Total	O	P	0	0
			9	7	2		
3	13-A	1	Total	O	P	0	0
			9	7	2		
3	14-A	1	Total	O	P	0	0
			9	7	2		
3	15-A	1	Total	O	P	0	0
			9	7	2		
3	16-A	1	Total	O	P	0	0
			9	7	2		
3	17-A	1	Total	O	P	0	0
			9	7	2		
3	18-A	1	Total	O	P	0	0
			9	7	2		
3	19-A	1	Total	O	P	0	0
			9	7	2		
3	20-A	1	Total	O	P	0	0
			9	7	2		
3	21-A	1	Total	O	P	0	0
			9	7	2		
3	22-A	1	Total	O	P	0	0
			9	7	2		
3	23-A	1	Total	O	P	0	0
			9	7	2		
3	24-A	1	Total	O	P	0	0
			9	7	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	25-A	1	Total 9	O 7	P 2	0	0
3	26-A	1	Total 9	O 7	P 2	0	0
3	27-A	1	Total 9	O 7	P 2	0	0
3	28-A	1	Total 9	O 7	P 2	0	0
3	29-A	1	Total 9	O 7	P 2	0	0
3	30-A	1	Total 9	O 7	P 2	0	0
3	31-A	1	Total 9	O 7	P 2	0	0
3	32-A	1	Total 9	O 7	P 2	0	0
3	33-A	1	Total 9	O 7	P 2	0	0
3	34-A	1	Total 9	O 7	P 2	0	0
3	35-A	1	Total 9	O 7	P 2	0	0
3	36-A	1	Total 9	O 7	P 2	0	0
3	37-A	1	Total 9	O 7	P 2	0	0
3	38-A	1	Total 9	O 7	P 2	0	0
3	39-A	1	Total 9	O 7	P 2	0	0
3	40-A	1	Total 9	O 7	P 2	0	0
3	41-A	1	Total 9	O 7	P 2	0	0
3	42-A	1	Total 9	O 7	P 2	0	0
3	43-A	1	Total 9	O 7	P 2	0	0
3	44-A	1	Total 9	O 7	P 2	0	0
3	45-A	1	Total 9	O 7	P 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	46-A	1	Total	O	P	0	0
			9	7	2		
3	47-A	1	Total	O	P	0	0
			9	7	2		
3	48-A	1	Total	O	P	0	0
			9	7	2		
3	49-A	1	Total	O	P	0	0
			9	7	2		
3	50-A	1	Total	O	P	0	0
			9	7	2		
3	1-B	1	Total	O	P	0	0
			9	7	2		
3	2-B	1	Total	O	P	0	0
			9	7	2		
3	3-B	1	Total	O	P	0	0
			9	7	2		
3	4-B	1	Total	O	P	0	0
			9	7	2		
3	5-B	1	Total	O	P	0	0
			9	7	2		
3	6-B	1	Total	O	P	0	0
			9	7	2		
3	7-B	1	Total	O	P	0	0
			9	7	2		
3	8-B	1	Total	O	P	0	0
			9	7	2		
3	9-B	1	Total	O	P	0	0
			9	7	2		
3	10-B	1	Total	O	P	0	0
			9	7	2		
3	11-B	1	Total	O	P	0	0
			9	7	2		
3	12-B	1	Total	O	P	0	0
			9	7	2		
3	13-B	1	Total	O	P	0	0
			9	7	2		
3	14-B	1	Total	O	P	0	0
			9	7	2		
3	15-B	1	Total	O	P	0	0
			9	7	2		
3	16-B	1	Total	O	P	0	0
			9	7	2		

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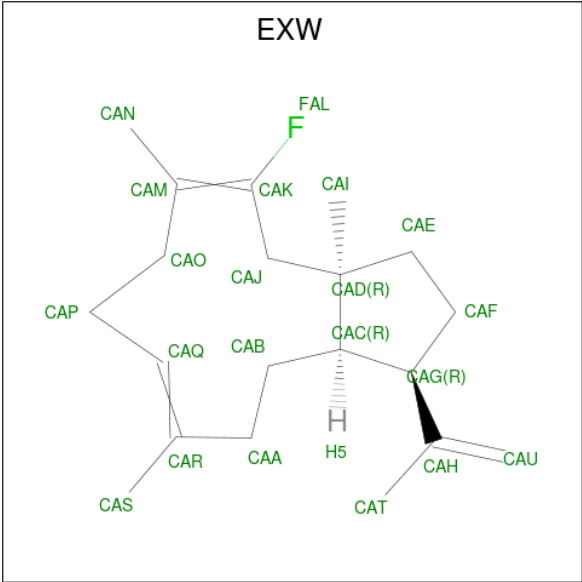
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	17-B	1	Total 9	O 7	P 2	0	0
3	18-B	1	Total 9	O 7	P 2	0	0
3	19-B	1	Total 9	O 7	P 2	0	0
3	20-B	1	Total 9	O 7	P 2	0	0
3	21-B	1	Total 9	O 7	P 2	0	0
3	22-B	1	Total 9	O 7	P 2	0	0
3	23-B	1	Total 9	O 7	P 2	0	0
3	24-B	1	Total 9	O 7	P 2	0	0
3	25-B	1	Total 9	O 7	P 2	0	0
3	26-B	1	Total 9	O 7	P 2	0	0
3	27-B	1	Total 9	O 7	P 2	0	0
3	28-B	1	Total 9	O 7	P 2	0	0
3	29-B	1	Total 9	O 7	P 2	0	0
3	30-B	1	Total 9	O 7	P 2	0	0
3	31-B	1	Total 9	O 7	P 2	0	0
3	32-B	1	Total 9	O 7	P 2	0	0
3	33-B	1	Total 9	O 7	P 2	0	0
3	34-B	1	Total 9	O 7	P 2	0	0
3	35-B	1	Total 9	O 7	P 2	0	0
3	36-B	1	Total 9	O 7	P 2	0	0
3	37-B	1	Total 9	O 7	P 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	38-B	1	Total	O	P	0	0
			9	7	2		
3	39-B	1	Total	O	P	0	0
			9	7	2		
3	40-B	1	Total	O	P	0	0
			9	7	2		
3	41-B	1	Total	O	P	0	0
			9	7	2		
3	42-B	1	Total	O	P	0	0
			9	7	2		
3	43-B	1	Total	O	P	0	0
			9	7	2		
3	44-B	1	Total	O	P	0	0
			9	7	2		
3	45-B	1	Total	O	P	0	0
			9	7	2		
3	46-B	1	Total	O	P	0	0
			9	7	2		
3	47-B	1	Total	O	P	0	0
			9	7	2		
3	48-B	1	Total	O	P	0	0
			9	7	2		
3	49-B	1	Total	O	P	0	0
			9	7	2		
3	50-B	1	Total	O	P	0	0
			9	7	2		

- Molecule 4 is 2-fluoro-3,7,18-dolabellatriene (CCD ID: EXW) (formula: C₂₀H₃₁F).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1-A	1	Total C F 21 20 1	0	0
4	2-A	1	Total C F 21 20 1	0	0
4	3-A	1	Total C F 21 20 1	0	0
4	4-A	1	Total C F 21 20 1	0	0
4	5-A	1	Total C F 21 20 1	0	0
4	6-A	1	Total C F 21 20 1	0	0
4	7-A	1	Total C F 21 20 1	0	0
4	8-A	1	Total C F 21 20 1	0	0
4	9-A	1	Total C F 21 20 1	0	0
4	10-A	1	Total C F 21 20 1	0	0
4	11-A	1	Total C F 21 20 1	0	0
4	12-A	1	Total C F 21 20 1	0	0
4	13-A	1	Total C F 21 20 1	0	0
4	14-A	1	Total C F 21 20 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	15-A	1	Total	C	F	0	0
			21	20	1		
4	16-A	1	Total	C	F	0	0
			21	20	1		
4	17-A	1	Total	C	F	0	0
			21	20	1		
4	18-A	1	Total	C	F	0	0
			21	20	1		
4	19-A	1	Total	C	F	0	0
			21	20	1		
4	20-A	1	Total	C	F	0	0
			21	20	1		
4	21-A	1	Total	C	F	0	0
			21	20	1		
4	22-A	1	Total	C	F	0	0
			21	20	1		
4	23-A	1	Total	C	F	0	0
			21	20	1		
4	24-A	1	Total	C	F	0	0
			21	20	1		
4	25-A	1	Total	C	F	0	0
			21	20	1		
4	26-A	1	Total	C	F	0	0
			21	20	1		
4	27-A	1	Total	C	F	0	0
			21	20	1		
4	28-A	1	Total	C	F	0	0
			21	20	1		
4	29-A	1	Total	C	F	0	0
			21	20	1		
4	30-A	1	Total	C	F	0	0
			21	20	1		
4	31-A	1	Total	C	F	0	0
			21	20	1		
4	32-A	1	Total	C	F	0	0
			21	20	1		
4	33-A	1	Total	C	F	0	0
			21	20	1		
4	34-A	1	Total	C	F	0	0
			21	20	1		
4	35-A	1	Total	C	F	0	0
			21	20	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	36-A	1	Total	C	F	0	0
			21	20	1		
4	37-A	1	Total	C	F	0	0
			21	20	1		
4	38-A	1	Total	C	F	0	0
			21	20	1		
4	39-A	1	Total	C	F	0	0
			21	20	1		
4	40-A	1	Total	C	F	0	0
			21	20	1		
4	41-A	1	Total	C	F	0	0
			21	20	1		
4	42-A	1	Total	C	F	0	0
			21	20	1		
4	43-A	1	Total	C	F	0	0
			21	20	1		
4	44-A	1	Total	C	F	0	0
			21	20	1		
4	45-A	1	Total	C	F	0	0
			21	20	1		
4	46-A	1	Total	C	F	0	0
			21	20	1		
4	47-A	1	Total	C	F	0	0
			21	20	1		
4	48-A	1	Total	C	F	0	0
			21	20	1		
4	49-A	1	Total	C	F	0	0
			21	20	1		
4	50-A	1	Total	C	F	0	0
			21	20	1		
4	1-B	1	Total	C	F	0	0
			21	20	1		
4	2-B	1	Total	C	F	0	0
			21	20	1		
4	3-B	1	Total	C	F	0	0
			21	20	1		
4	4-B	1	Total	C	F	0	0
			21	20	1		
4	5-B	1	Total	C	F	0	0
			21	20	1		
4	6-B	1	Total	C	F	0	0
			21	20	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	7-B	1	Total	C	F	0	0
			21	20	1		
4	8-B	1	Total	C	F	0	0
			21	20	1		
4	9-B	1	Total	C	F	0	0
			21	20	1		
4	10-B	1	Total	C	F	0	0
			21	20	1		
4	11-B	1	Total	C	F	0	0
			21	20	1		
4	12-B	1	Total	C	F	0	0
			21	20	1		
4	13-B	1	Total	C	F	0	0
			21	20	1		
4	14-B	1	Total	C	F	0	0
			21	20	1		
4	15-B	1	Total	C	F	0	0
			21	20	1		
4	16-B	1	Total	C	F	0	0
			21	20	1		
4	17-B	1	Total	C	F	0	0
			21	20	1		
4	18-B	1	Total	C	F	0	0
			21	20	1		
4	19-B	1	Total	C	F	0	0
			21	20	1		
4	20-B	1	Total	C	F	0	0
			21	20	1		
4	21-B	1	Total	C	F	0	0
			21	20	1		
4	22-B	1	Total	C	F	0	0
			21	20	1		
4	23-B	1	Total	C	F	0	0
			21	20	1		
4	24-B	1	Total	C	F	0	0
			21	20	1		
4	25-B	1	Total	C	F	0	0
			21	20	1		
4	26-B	1	Total	C	F	0	0
			21	20	1		
4	27-B	1	Total	C	F	0	0
			21	20	1		

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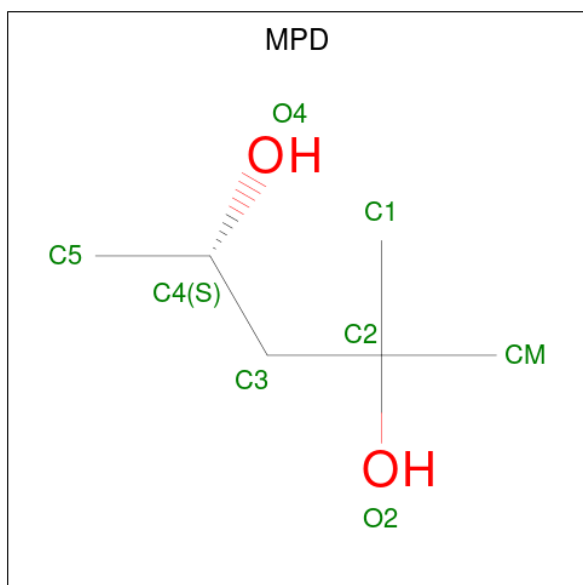
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	28-B	1	Total	C	F	0	0
			21	20	1		
4	29-B	1	Total	C	F	0	0
			21	20	1		
4	30-B	1	Total	C	F	0	0
			21	20	1		
4	31-B	1	Total	C	F	0	0
			21	20	1		
4	32-B	1	Total	C	F	0	0
			21	20	1		
4	33-B	1	Total	C	F	0	0
			21	20	1		
4	34-B	1	Total	C	F	0	0
			21	20	1		
4	35-B	1	Total	C	F	0	0
			21	20	1		
4	36-B	1	Total	C	F	0	0
			21	20	1		
4	37-B	1	Total	C	F	0	0
			21	20	1		
4	38-B	1	Total	C	F	0	0
			21	20	1		
4	39-B	1	Total	C	F	0	0
			21	20	1		
4	40-B	1	Total	C	F	0	0
			21	20	1		
4	41-B	1	Total	C	F	0	0
			21	20	1		
4	42-B	1	Total	C	F	0	0
			21	20	1		
4	43-B	1	Total	C	F	0	0
			21	20	1		
4	44-B	1	Total	C	F	0	0
			21	20	1		
4	45-B	1	Total	C	F	0	0
			21	20	1		
4	46-B	1	Total	C	F	0	0
			21	20	1		
4	47-B	1	Total	C	F	0	0
			21	20	1		
4	48-B	1	Total	C	F	0	0
			21	20	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	49-B	1	Total	C	F	0	0
			21	20	1		
4	50-B	1	Total	C	F	0	0
			21	20	1		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	10-A	1	Total	C	O	0	0
			8	6	2		
5	11-A	1	Total	C	O	0	0
			8	6	2		
5	12-A	1	Total	C	O	0	0
			8	6	2		
5	13-A	1	Total	C	O	0	0
			8	6	2		
5	14-A	1	Total	C	O	0	0
			8	6	2		
5	15-A	1	Total	C	O	0	0
			8	6	2		
5	16-A	1	Total	C	O	0	0
			8	6	2		
5	17-A	1	Total	C	O	0	0
			8	6	2		
5	18-A	1	Total	C	O	0	0
			8	6	2		
5	19-A	1	Total	C	O	0	0
			8	6	2		
5	20-A	1	Total	C	O	0	0
			8	6	2		
5	21-A	1	Total	C	O	0	0
			8	6	2		
5	22-A	1	Total	C	O	0	0
			8	6	2		
5	23-A	1	Total	C	O	0	0
			8	6	2		
5	24-A	1	Total	C	O	0	0
			8	6	2		
5	25-A	1	Total	C	O	0	0
			8	6	2		
5	26-A	1	Total	C	O	0	0
			8	6	2		
5	27-A	1	Total	C	O	0	0
			8	6	2		
5	28-A	1	Total	C	O	0	0
			8	6	2		
5	29-A	1	Total	C	O	0	0
			8	6	2		
5	30-A	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	31-A	1	Total	C	O	0	0
			8	6	2		
5	32-A	1	Total	C	O	0	0
			8	6	2		
5	33-A	1	Total	C	O	0	0
			8	6	2		
5	34-A	1	Total	C	O	0	0
			8	6	2		
5	35-A	1	Total	C	O	0	0
			8	6	2		
5	36-A	1	Total	C	O	0	0
			8	6	2		
5	37-A	1	Total	C	O	0	0
			8	6	2		
5	38-A	1	Total	C	O	0	0
			8	6	2		
5	39-A	1	Total	C	O	0	0
			8	6	2		
5	40-A	1	Total	C	O	0	0
			8	6	2		
5	41-A	1	Total	C	O	0	0
			8	6	2		
5	42-A	1	Total	C	O	0	0
			8	6	2		
5	43-A	1	Total	C	O	0	0
			8	6	2		
5	44-A	1	Total	C	O	0	0
			8	6	2		
5	45-A	1	Total	C	O	0	0
			8	6	2		
5	46-A	1	Total	C	O	0	0
			8	6	2		
5	47-A	1	Total	C	O	0	0
			8	6	2		
5	48-A	1	Total	C	O	0	0
			8	6	2		
5	49-A	1	Total	C	O	0	0
			8	6	2		
5	50-A	1	Total	C	O	0	0
			8	6	2		
5	1-B	1	Total	C	O	0	0
			8	6	2		

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	23-B	1	Total	C	O	0	0
			8	6	2		
5	24-B	1	Total	C	O	0	0
			8	6	2		
5	25-B	1	Total	C	O	0	0
			8	6	2		
5	26-B	1	Total	C	O	0	0
			8	6	2		
5	27-B	1	Total	C	O	0	0
			8	6	2		
5	28-B	1	Total	C	O	0	0
			8	6	2		
5	29-B	1	Total	C	O	0	0
			8	6	2		
5	30-B	1	Total	C	O	0	0
			8	6	2		
5	31-B	1	Total	C	O	0	0
			8	6	2		
5	32-B	1	Total	C	O	0	0
			8	6	2		
5	33-B	1	Total	C	O	0	0
			8	6	2		
5	34-B	1	Total	C	O	0	0
			8	6	2		
5	35-B	1	Total	C	O	0	0
			8	6	2		
5	36-B	1	Total	C	O	0	0
			8	6	2		
5	37-B	1	Total	C	O	0	0
			8	6	2		
5	38-B	1	Total	C	O	0	0
			8	6	2		
5	39-B	1	Total	C	O	0	0
			8	6	2		
5	40-B	1	Total	C	O	0	0
			8	6	2		
5	41-B	1	Total	C	O	0	0
			8	6	2		
5	42-B	1	Total	C	O	0	0
			8	6	2		
5	43-B	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	44-B	1	Total	C	O	0	0
			8	6	2		
5	45-B	1	Total	C	O	0	0
			8	6	2		
5	46-B	1	Total	C	O	0	0
			8	6	2		
5	47-B	1	Total	C	O	0	0
			8	6	2		
5	48-B	1	Total	C	O	0	0
			8	6	2		
5	49-B	1	Total	C	O	0	0
			8	6	2		
5	50-B	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	13-A	2	Total 2	Cl 2	0	0
6	14-A	2	Total 2	Cl 2	0	0
6	15-A	2	Total 2	Cl 2	0	0
6	16-A	2	Total 2	Cl 2	0	0
6	17-A	2	Total 2	Cl 2	0	0
6	18-A	2	Total 2	Cl 2	0	0
6	19-A	2	Total 2	Cl 2	0	0
6	20-A	2	Total 2	Cl 2	0	0
6	21-A	2	Total 2	Cl 2	0	0
6	22-A	2	Total 2	Cl 2	0	0
6	23-A	2	Total 2	Cl 2	0	0
6	24-A	2	Total 2	Cl 2	0	0
6	25-A	2	Total 2	Cl 2	0	0
6	26-A	2	Total 2	Cl 2	0	0
6	27-A	2	Total 2	Cl 2	0	0
6	28-A	2	Total 2	Cl 2	0	0
6	29-A	2	Total 2	Cl 2	0	0
6	30-A	2	Total 2	Cl 2	0	0
6	31-A	2	Total 2	Cl 2	0	0
6	32-A	2	Total 2	Cl 2	0	0
6	33-A	2	Total 2	Cl 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	34-A	2	Total 2	Cl 2	0	0
6	35-A	2	Total 2	Cl 2	0	0
6	36-A	2	Total 2	Cl 2	0	0
6	37-A	2	Total 2	Cl 2	0	0
6	38-A	2	Total 2	Cl 2	0	0
6	39-A	2	Total 2	Cl 2	0	0
6	40-A	2	Total 2	Cl 2	0	0
6	41-A	2	Total 2	Cl 2	0	0
6	42-A	2	Total 2	Cl 2	0	0
6	43-A	2	Total 2	Cl 2	0	0
6	44-A	2	Total 2	Cl 2	0	0
6	45-A	2	Total 2	Cl 2	0	0
6	46-A	2	Total 2	Cl 2	0	0
6	47-A	2	Total 2	Cl 2	0	0
6	48-A	2	Total 2	Cl 2	0	0
6	49-A	2	Total 2	Cl 2	0	0
6	50-A	2	Total 2	Cl 2	0	0
6	1-B	1	Total 1	Cl 1	0	0
6	2-B	1	Total 1	Cl 1	0	0
6	3-B	1	Total 1	Cl 1	0	0
6	4-B	1	Total 1	Cl 1	0	0

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

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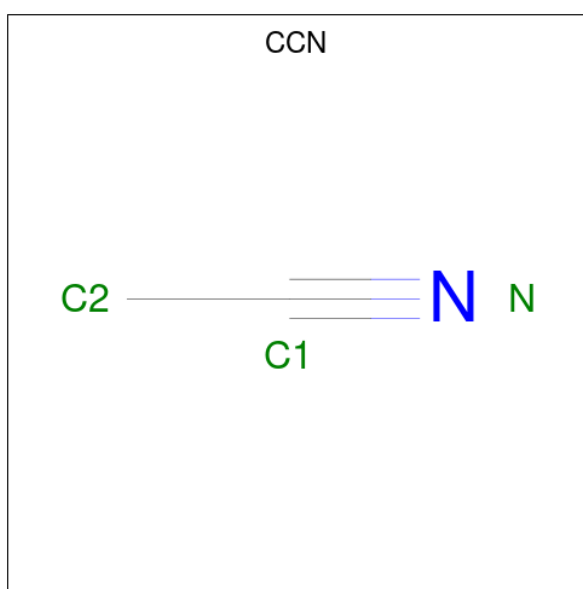
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	26-B	1	Total 1	Cl 1	0	0
6	27-B	1	Total 1	Cl 1	0	0
6	28-B	1	Total 1	Cl 1	0	0
6	29-B	1	Total 1	Cl 1	0	0
6	30-B	1	Total 1	Cl 1	0	0
6	31-B	1	Total 1	Cl 1	0	0
6	32-B	1	Total 1	Cl 1	0	0
6	33-B	1	Total 1	Cl 1	0	0
6	34-B	1	Total 1	Cl 1	0	0
6	35-B	1	Total 1	Cl 1	0	0
6	36-B	1	Total 1	Cl 1	0	0
6	37-B	1	Total 1	Cl 1	0	0
6	38-B	1	Total 1	Cl 1	0	0
6	39-B	1	Total 1	Cl 1	0	0
6	40-B	1	Total 1	Cl 1	0	0
6	41-B	1	Total 1	Cl 1	0	0
6	42-B	1	Total 1	Cl 1	0	0
6	43-B	1	Total 1	Cl 1	0	0
6	44-B	1	Total 1	Cl 1	0	0
6	45-B	1	Total 1	Cl 1	0	0
6	46-B	1	Total 1	Cl 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	47-B	1	Total	Cl	0	0
			1	1		
6	48-B	1	Total	Cl	0	0
			1	1		
6	49-B	1	Total	Cl	0	0
			1	1		
6	50-B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is ACETONITRILE (CCD ID: CCN) (formula: C₂H₃N).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	8-A	1	Total	C	N	0	0
			3	2	1		
7	9-A	1	Total	C	N	0	0
			3	2	1		
7	10-A	1	Total	C	N	0	0
			3	2	1		
7	11-A	1	Total	C	N	0	0
			3	2	1		
7	12-A	1	Total	C	N	0	0
			3	2	1		
7	13-A	1	Total	C	N	0	0
			3	2	1		
7	14-A	1	Total	C	N	0	0
			3	2	1		
7	15-A	1	Total	C	N	0	0
			3	2	1		
7	16-A	1	Total	C	N	0	0
			3	2	1		
7	17-A	1	Total	C	N	0	0
			3	2	1		
7	18-A	1	Total	C	N	0	0
			3	2	1		
7	19-A	1	Total	C	N	0	0
			3	2	1		
7	20-A	1	Total	C	N	0	0
			3	2	1		
7	21-A	1	Total	C	N	0	0
			3	2	1		
7	22-A	1	Total	C	N	0	0
			3	2	1		
7	23-A	1	Total	C	N	0	0
			3	2	1		
7	24-A	1	Total	C	N	0	0
			3	2	1		
7	25-A	1	Total	C	N	0	0
			3	2	1		
7	26-A	1	Total	C	N	0	0
			3	2	1		
7	27-A	1	Total	C	N	0	0
			3	2	1		
7	28-A	1	Total	C	N	0	0
			3	2	1		

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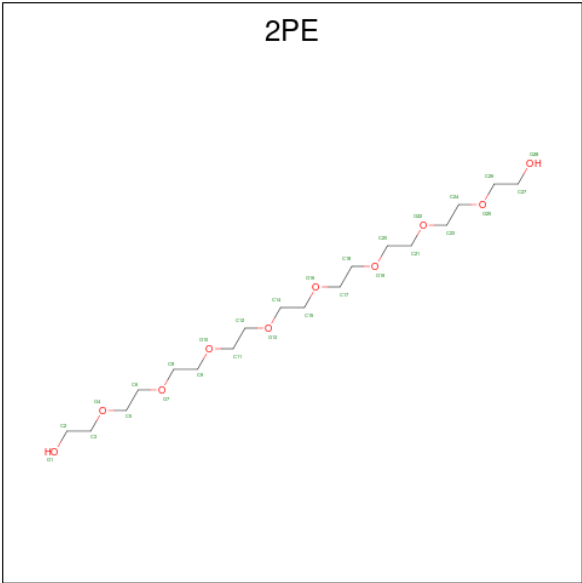
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	29-A	1	Total	C	N	0	0
			3	2	1		
7	30-A	1	Total	C	N	0	0
			3	2	1		
7	31-A	1	Total	C	N	0	0
			3	2	1		
7	32-A	1	Total	C	N	0	0
			3	2	1		
7	33-A	1	Total	C	N	0	0
			3	2	1		
7	34-A	1	Total	C	N	0	0
			3	2	1		
7	35-A	1	Total	C	N	0	0
			3	2	1		
7	36-A	1	Total	C	N	0	0
			3	2	1		
7	37-A	1	Total	C	N	0	0
			3	2	1		
7	38-A	1	Total	C	N	0	0
			3	2	1		
7	39-A	1	Total	C	N	0	0
			3	2	1		
7	40-A	1	Total	C	N	0	0
			3	2	1		
7	41-A	1	Total	C	N	0	0
			3	2	1		
7	42-A	1	Total	C	N	0	0
			3	2	1		
7	43-A	1	Total	C	N	0	0
			3	2	1		
7	44-A	1	Total	C	N	0	0
			3	2	1		
7	45-A	1	Total	C	N	0	0
			3	2	1		
7	46-A	1	Total	C	N	0	0
			3	2	1		
7	47-A	1	Total	C	N	0	0
			3	2	1		
7	48-A	1	Total	C	N	0	0
			3	2	1		
7	49-A	1	Total	C	N	0	0
			3	2	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	50-A	1	Total	C	N	0	0
			3	2	1		

- Molecule 8 is NONAETHYLENE GLYCOL (CCD ID: 2PE) (formula: C₁₈H₃₈O₁₀).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	11-A	1	Total	C	O	0	0
			7	4	3		
8	12-A	1	Total	C	O	0	0
			7	4	3		
8	13-A	1	Total	C	O	0	0
			7	4	3		
8	14-A	1	Total	C	O	0	0
			7	4	3		
8	15-A	1	Total	C	O	0	0
			7	4	3		
8	16-A	1	Total	C	O	0	0
			7	4	3		
8	17-A	1	Total	C	O	0	0
			7	4	3		
8	18-A	1	Total	C	O	0	0
			7	4	3		
8	19-A	1	Total	C	O	0	0
			7	4	3		
8	20-A	1	Total	C	O	0	0
			7	4	3		
8	21-A	1	Total	C	O	0	0
			7	4	3		
8	22-A	1	Total	C	O	0	0
			7	4	3		
8	23-A	1	Total	C	O	0	0
			7	4	3		
8	24-A	1	Total	C	O	0	0
			7	4	3		
8	25-A	1	Total	C	O	0	0
			7	4	3		
8	26-A	1	Total	C	O	0	0
			7	4	3		
8	27-A	1	Total	C	O	0	0
			7	4	3		
8	28-A	1	Total	C	O	0	0
			7	4	3		
8	29-A	1	Total	C	O	0	0
			7	4	3		
8	30-A	1	Total	C	O	0	0
			7	4	3		
8	31-A	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	32-A	1	Total	C	O	0	0
			7	4	3		
8	33-A	1	Total	C	O	0	0
			7	4	3		
8	34-A	1	Total	C	O	0	0
			7	4	3		
8	35-A	1	Total	C	O	0	0
			7	4	3		
8	36-A	1	Total	C	O	0	0
			7	4	3		
8	37-A	1	Total	C	O	0	0
			7	4	3		
8	38-A	1	Total	C	O	0	0
			7	4	3		
8	39-A	1	Total	C	O	0	0
			7	4	3		
8	40-A	1	Total	C	O	0	0
			7	4	3		
8	41-A	1	Total	C	O	0	0
			7	4	3		
8	42-A	1	Total	C	O	0	0
			7	4	3		
8	43-A	1	Total	C	O	0	0
			7	4	3		
8	44-A	1	Total	C	O	0	0
			7	4	3		
8	45-A	1	Total	C	O	0	0
			7	4	3		
8	46-A	1	Total	C	O	0	0
			7	4	3		
8	47-A	1	Total	C	O	0	0
			7	4	3		
8	48-A	1	Total	C	O	0	0
			7	4	3		
8	49-A	1	Total	C	O	0	0
			7	4	3		
8	50-A	1	Total	C	O	0	0
			7	4	3		
8	1-B	1	Total	C	O	0	0
			7	4	3		
8	2-B	1	Total	C	O	0	0
			7	4	3		

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	24-B	1	Total	C	O	0	0
			7	4	3		
8	25-B	1	Total	C	O	0	0
			7	4	3		
8	26-B	1	Total	C	O	0	0
			7	4	3		
8	27-B	1	Total	C	O	0	0
			7	4	3		
8	28-B	1	Total	C	O	0	0
			7	4	3		
8	29-B	1	Total	C	O	0	0
			7	4	3		
8	30-B	1	Total	C	O	0	0
			7	4	3		
8	31-B	1	Total	C	O	0	0
			7	4	3		
8	32-B	1	Total	C	O	0	0
			7	4	3		
8	33-B	1	Total	C	O	0	0
			7	4	3		
8	34-B	1	Total	C	O	0	0
			7	4	3		
8	35-B	1	Total	C	O	0	0
			7	4	3		
8	36-B	1	Total	C	O	0	0
			7	4	3		
8	37-B	1	Total	C	O	0	0
			7	4	3		
8	38-B	1	Total	C	O	0	0
			7	4	3		
8	39-B	1	Total	C	O	0	0
			7	4	3		
8	40-B	1	Total	C	O	0	0
			7	4	3		
8	41-B	1	Total	C	O	0	0
			7	4	3		
8	42-B	1	Total	C	O	0	0
			7	4	3		
8	43-B	1	Total	C	O	0	0
			7	4	3		
8	44-B	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	45-B	1	Total	C	O	0	0
			7	4	3		
8	46-B	1	Total	C	O	0	0
			7	4	3		
8	47-B	1	Total	C	O	0	0
			7	4	3		
8	48-B	1	Total	C	O	0	0
			7	4	3		
8	49-B	1	Total	C	O	0	0
			7	4	3		
8	50-B	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is POTASSIUM ION (CCD ID: K) (formula: K).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	14-A	1	Total K 1 1	0	0
9	15-A	1	Total K 1 1	0	0
9	16-A	1	Total K 1 1	0	0
9	17-A	1	Total K 1 1	0	0
9	18-A	1	Total K 1 1	0	0
9	19-A	1	Total K 1 1	0	0
9	20-A	1	Total K 1 1	0	0
9	21-A	1	Total K 1 1	0	0
9	22-A	1	Total K 1 1	0	0
9	23-A	1	Total K 1 1	0	0
9	24-A	1	Total K 1 1	0	0
9	25-A	1	Total K 1 1	0	0
9	26-A	1	Total K 1 1	0	0
9	27-A	1	Total K 1 1	0	0
9	28-A	1	Total K 1 1	0	0
9	29-A	1	Total K 1 1	0	0
9	30-A	1	Total K 1 1	0	0
9	31-A	1	Total K 1 1	0	0
9	32-A	1	Total K 1 1	0	0
9	33-A	1	Total K 1 1	0	0
9	34-A	1	Total K 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	35-A	1	Total K 1 1	0	0
9	36-A	1	Total K 1 1	0	0
9	37-A	1	Total K 1 1	0	0
9	38-A	1	Total K 1 1	0	0
9	39-A	1	Total K 1 1	0	0
9	40-A	1	Total K 1 1	0	0
9	41-A	1	Total K 1 1	0	0
9	42-A	1	Total K 1 1	0	0
9	43-A	1	Total K 1 1	0	0
9	44-A	1	Total K 1 1	0	0
9	45-A	1	Total K 1 1	0	0
9	46-A	1	Total K 1 1	0	0
9	47-A	1	Total K 1 1	0	0
9	48-A	1	Total K 1 1	0	0
9	49-A	1	Total K 1 1	0	0
9	50-A	1	Total K 1 1	0	0
9	1-B	1	Total K 1 1	0	0
9	2-B	1	Total K 1 1	0	0
9	3-B	1	Total K 1 1	0	0
9	4-B	1	Total K 1 1	0	0
9	5-B	1	Total K 1 1	0	0

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	27-B	1	Total 1	K 1	0	0
9	28-B	1	Total 1	K 1	0	0
9	29-B	1	Total 1	K 1	0	0
9	30-B	1	Total 1	K 1	0	0
9	31-B	1	Total 1	K 1	0	0
9	32-B	1	Total 1	K 1	0	0
9	33-B	1	Total 1	K 1	0	0
9	34-B	1	Total 1	K 1	0	0
9	35-B	1	Total 1	K 1	0	0
9	36-B	1	Total 1	K 1	0	0
9	37-B	1	Total 1	K 1	0	0
9	38-B	1	Total 1	K 1	0	0
9	39-B	1	Total 1	K 1	0	0
9	40-B	1	Total 1	K 1	0	0
9	41-B	1	Total 1	K 1	0	0
9	42-B	1	Total 1	K 1	0	0
9	43-B	1	Total 1	K 1	0	0
9	44-B	1	Total 1	K 1	0	0
9	45-B	1	Total 1	K 1	0	0
9	46-B	1	Total 1	K 1	0	0
9	47-B	1	Total 1	K 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	48-B	1	Total 1	K 1	0	0
9	49-B	1	Total 1	K 1	0	0
9	50-B	1	Total 1	K 1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	1-A	142	Total 142	O 142	0	0
10	2-A	157	Total 157	O 157	0	0
10	3-A	156	Total 156	O 156	0	0
10	4-A	159	Total 159	O 159	0	0
10	5-A	156	Total 156	O 156	0	0
10	6-A	151	Total 151	O 151	0	0
10	7-A	151	Total 151	O 151	0	0
10	8-A	150	Total 150	O 150	0	0
10	9-A	160	Total 160	O 160	0	0
10	10-A	163	Total 163	O 163	0	0
10	11-A	150	Total 150	O 150	0	0
10	12-A	142	Total 142	O 142	0	0
10	13-A	157	Total 157	O 157	0	0
10	14-A	157	Total 157	O 157	0	0
10	15-A	145	Total 145	O 145	0	0
10	16-A	157	Total 157	O 157	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	17-A	169	Total 169	O 169	0	0
10	18-A	153	Total 153	O 153	0	0
10	19-A	146	Total 146	O 146	0	0
10	20-A	145	Total 145	O 145	0	0
10	21-A	154	Total 154	O 154	0	0
10	22-A	153	Total 153	O 153	0	0
10	23-A	153	Total 153	O 153	0	0
10	24-A	162	Total 162	O 162	0	0
10	25-A	164	Total 164	O 164	0	0
10	26-A	151	Total 151	O 151	0	0
10	27-A	156	Total 156	O 156	0	0
10	28-A	142	Total 142	O 142	0	0
10	29-A	157	Total 157	O 157	0	0
10	30-A	151	Total 151	O 151	0	0
10	31-A	154	Total 154	O 154	0	0
10	32-A	157	Total 157	O 157	0	0
10	33-A	159	Total 159	O 159	0	0
10	34-A	158	Total 158	O 158	0	0
10	35-A	156	Total 156	O 156	0	0
10	36-A	152	Total 152	O 152	0	0
10	37-A	154	Total 154	O 154	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	38-A	158	Total 158	O 158	0	0
10	39-A	165	Total 165	O 165	0	0
10	40-A	157	Total 157	O 157	0	0
10	41-A	153	Total 153	O 153	0	0
10	42-A	163	Total 163	O 163	0	0
10	43-A	153	Total 153	O 153	0	0
10	44-A	154	Total 154	O 154	0	0
10	45-A	157	Total 157	O 157	0	0
10	46-A	159	Total 159	O 159	0	0
10	47-A	157	Total 157	O 157	0	0
10	48-A	141	Total 141	O 141	0	0
10	49-A	144	Total 144	O 144	0	0
10	50-A	153	Total 153	O 153	0	0
10	1-B	75	Total 75	O 75	0	0
10	2-B	82	Total 82	O 82	0	0
10	3-B	80	Total 80	O 80	0	0
10	4-B	84	Total 84	O 84	0	0
10	5-B	80	Total 80	O 80	0	0
10	6-B	76	Total 76	O 76	0	0
10	7-B	77	Total 77	O 77	0	0
10	8-B	75	Total 75	O 75	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	9-B	84	Total 84	O 84	0	0
10	10-B	84	Total 84	O 84	0	0
10	11-B	76	Total 76	O 76	0	0
10	12-B	75	Total 75	O 75	0	0
10	13-B	82	Total 82	O 82	0	0
10	14-B	81	Total 81	O 81	0	0
10	15-B	75	Total 75	O 75	0	0
10	16-B	80	Total 80	O 80	0	0
10	17-B	90	Total 90	O 90	0	0
10	18-B	79	Total 79	O 79	0	0
10	19-B	75	Total 75	O 75	0	0
10	20-B	75	Total 75	O 75	0	0
10	21-B	80	Total 80	O 80	0	0
10	22-B	80	Total 80	O 80	0	0
10	23-B	79	Total 79	O 79	0	0
10	24-B	84	Total 84	O 84	0	0
10	25-B	84	Total 84	O 84	0	0
10	26-B	77	Total 77	O 77	0	0
10	27-B	80	Total 80	O 80	0	0
10	28-B	75	Total 75	O 75	0	0
10	29-B	80	Total 80	O 80	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	30-B	77	Total 77	O 77	0	0
10	31-B	80	Total 80	O 80	0	0
10	32-B	80	Total 80	O 80	0	0
10	33-B	82	Total 82	O 82	0	0
10	34-B	82	Total 82	O 82	0	0
10	35-B	80	Total 80	O 80	0	0
10	36-B	78	Total 78	O 78	0	0
10	37-B	80	Total 80	O 80	0	0
10	38-B	82	Total 82	O 82	0	0
10	39-B	86	Total 86	O 86	0	0
10	40-B	82	Total 82	O 82	0	0
10	41-B	80	Total 80	O 80	0	0
10	42-B	84	Total 84	O 84	0	0
10	43-B	78	Total 78	O 78	0	0
10	44-B	80	Total 80	O 80	0	0
10	45-B	80	Total 80	O 80	0	0
10	46-B	82	Total 82	O 82	0	0
10	47-B	80	Total 80	O 80	0	0
10	48-B	75	Total 75	O 75	0	0
10	49-B	75	Total 75	O 75	0	0
10	50-B	80	Total 80	O 80	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, α , β , γ	62.88Å 98.72Å 105.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.42 – 1.80 47.42 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.42-1.80) 99.6 (47.42-1.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.81Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.165 , 0.195 0.181 , 0.207	Depositor DCC
R_{free} test set	2100 reflections (3.42%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.01 , 30.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	259400	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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 64.77 % 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 7.8612e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

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 1150 ligands modelled in this entry, 700 are monoatomic - leaving 450 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	$\# Z > 2$
8	2PE	44-B	409	-	6,6,27	0.83	0	5,5,26	0.89	0
3	PPV	12-B	405	2	6,8,8	0.98	0	13,13,13	1.25	1 (7%)
4	EXW	46-A	407	-	21,22,22	5.64	12 (57%)	24,32,32	4.31	15 (62%)
5	MPD	46-A	408	-	7,7,7	0.44	0	9,10,10	1.38	1 (11%)
4	EXW	42-B	406	-	21,22,22	5.49	9 (42%)	24,32,32	3.91	18 (75%)
8	2PE	34-A	412	-	6,6,27	0.48	0	5,5,26	1.07	0
3	PPV	46-B	405	2	6,8,8	1.04	0	13,13,13	1.16	2 (15%)
8	2PE	13-B	409	-	6,6,27	0.60	0	5,5,26	0.81	0
8	2PE	40-A	412	-	6,6,27	0.52	0	5,5,26	0.35	0
5	MPD	8-B	407	-	7,7,7	0.35	0	9,10,10	1.21	1 (11%)
3	PPV	8-B	405	2	6,8,8	1.05	0	13,13,13	1.23	2 (15%)
5	MPD	36-B	407	-	7,7,7	0.56	0	9,10,10	1.22	1 (11%)
3	PPV	14-A	406	2	6,8,8	1.02	0	13,13,13	1.13	1 (7%)
8	2PE	21-A	412	-	6,6,27	0.49	0	5,5,26	0.62	0
3	PPV	22-A	406	2	6,8,8	1.01	0	13,13,13	1.20	1 (7%)
5	MPD	9-A	408	-	7,7,7	0.39	0	9,10,10	1.45	2 (22%)
8	2PE	8-A	412	-	6,6,27	0.44	0	5,5,26	0.57	0
8	2PE	9-A	412	-	6,6,27	0.48	0	5,5,26	0.43	0
5	MPD	50-B	407	-	7,7,7	0.31	0	9,10,10	0.76	0
7	CCN	38-A	411	-	2,2,2	0.83	0	1,1,1	0.58	0
4	EXW	33-B	406	-	21,22,22	5.41	10 (47%)	24,32,32	3.78	16 (66%)
3	PPV	32-B	405	2	6,8,8	1.05	0	13,13,13	1.29	2 (15%)
7	CCN	31-A	411	-	2,2,2	0.87	0	1,1,1	0.47	0
3	PPV	30-A	406	2	6,8,8	0.98	0	13,13,13	1.25	1 (7%)
3	PPV	37-B	405	2	6,8,8	1.07	0	13,13,13	1.27	1 (7%)
8	2PE	1-B	409	-	6,6,27	0.50	0	5,5,26	0.27	0
4	EXW	43-A	407	-	21,22,22	6.04	11 (52%)	24,32,32	3.85	20 (83%)
8	2PE	2-A	412	-	6,6,27	0.46	0	5,5,26	0.62	0
4	EXW	29-A	407	-	21,22,22	5.91	9 (42%)	24,32,32	3.46	15 (62%)
3	PPV	39-A	406	2	6,8,8	1.05	0	13,13,13	1.25	1 (7%)
8	2PE	40-B	409	-	6,6,27	0.50	0	5,5,26	0.52	0
4	EXW	25-A	407	-	21,22,22	5.55	11 (52%)	24,32,32	4.76	18 (75%)
4	EXW	45-B	406	-	21,22,22	5.15	10 (47%)	24,32,32	4.19	15 (62%)
8	2PE	7-B	409	-	6,6,27	0.46	0	5,5,26	0.48	0
3	PPV	9-B	405	2	6,8,8	1.00	0	13,13,13	1.26	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	2PE	38-A	412	-	6,6,27	0.49	0	5,5,26	0.46	0
4	EXW	4-A	407	-	21,22,22	5.97	10 (47%)	24,32,32	3.84	15 (62%)
5	MPD	3-A	408	-	7,7,7	0.53	0	9,10,10	0.99	0
5	MPD	2-A	408	-	7,7,7	0.70	0	9,10,10	0.94	1 (11%)
4	EXW	22-B	406	-	21,22,22	5.36	10 (47%)	24,32,32	3.91	16 (66%)
7	CCN	17-A	411	-	2,2,2	0.83	0	1,1,1	0.09	0
8	2PE	27-A	412	-	6,6,27	0.39	0	5,5,26	0.78	0
7	CCN	15-A	411	-	2,2,2	0.90	0	1,1,1	0.54	0
4	EXW	9-B	406	-	21,22,22	5.56	10 (47%)	24,32,32	3.59	14 (58%)
4	EXW	36-A	407	-	21,22,22	5.45	9 (42%)	24,32,32	4.14	15 (62%)
3	PPV	44-B	405	2	6,8,8	1.01	0	13,13,13	1.00	1 (7%)
5	MPD	45-B	407	-	7,7,7	0.45	0	9,10,10	1.49	2 (22%)
4	EXW	15-B	406	-	21,22,22	5.29	11 (52%)	24,32,32	4.54	18 (75%)
4	EXW	50-B	406	-	21,22,22	5.52	8 (38%)	24,32,32	3.14	10 (41%)
4	EXW	23-A	407	-	21,22,22	5.30	9 (42%)	24,32,32	2.69	11 (45%)
8	2PE	31-A	412	-	6,6,27	0.50	0	5,5,26	0.73	0
5	MPD	14-A	408	-	7,7,7	0.65	0	9,10,10	1.06	0
5	MPD	17-A	408	-	7,7,7	0.49	0	9,10,10	1.04	0
4	EXW	28-A	407	-	21,22,22	6.06	13 (61%)	24,32,32	4.03	16 (66%)
7	CCN	4-A	411	-	2,2,2	0.69	0	1,1,1	0.31	0
5	MPD	42-B	407	-	7,7,7	0.42	0	9,10,10	1.77	3 (33%)
3	PPV	18-A	406	2	6,8,8	0.93	0	13,13,13	1.21	1 (7%)
5	MPD	43-B	407	-	7,7,7	0.53	0	9,10,10	1.17	1 (11%)
7	CCN	1-A	411	-	2,2,2	0.82	0	1,1,1	0.53	0
4	EXW	43-B	406	-	21,22,22	5.20	8 (38%)	24,32,32	5.06	16 (66%)
5	MPD	33-B	407	-	7,7,7	0.58	0	9,10,10	0.84	0
5	MPD	12-A	408	-	7,7,7	0.44	0	9,10,10	1.68	2 (22%)
5	MPD	6-B	407	-	7,7,7	0.40	0	9,10,10	1.56	2 (22%)
8	2PE	27-B	409	-	6,6,27	0.52	0	5,5,26	0.47	0
7	CCN	16-A	411	-	2,2,2	0.76	0	1,1,1	0.52	0
3	PPV	25-B	405	2	6,8,8	1.05	0	13,13,13	1.26	1 (7%)
8	2PE	21-B	409	-	6,6,27	0.50	0	5,5,26	0.95	0
3	PPV	8-A	406	2	6,8,8	0.99	0	13,13,13	1.24	1 (7%)
4	EXW	8-B	406	-	21,22,22	5.33	10 (47%)	24,32,32	3.99	14 (58%)
4	EXW	34-A	407	-	21,22,22	5.63	10 (47%)	24,32,32	3.58	14 (58%)
5	MPD	6-A	408	-	7,7,7	0.59	0	9,10,10	0.69	0
7	CCN	29-A	411	-	2,2,2	0.70	0	1,1,1	0.39	0
4	EXW	7-B	406	-	21,22,22	5.10	9 (42%)	24,32,32	3.79	12 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MPD	34-A	408	-	7,7,7	0.50	0	9,10,10	0.59	0
8	2PE	32-B	409	-	6,6,27	0.49	0	5,5,26	0.36	0
5	MPD	37-A	408	-	7,7,7	0.52	0	9,10,10	0.80	0
8	2PE	46-A	412	-	6,6,27	0.50	0	5,5,26	0.36	0
3	PPV	11-B	405	2	6,8,8	1.02	0	13,13,13	1.26	2 (15%)
4	EXW	50-A	407	-	21,22,22	5.82	12 (57%)	24,32,32	3.57	10 (41%)
5	MPD	13-A	408	-	7,7,7	0.49	0	9,10,10	1.33	1 (11%)
8	2PE	4-B	409	-	6,6,27	0.46	0	5,5,26	0.69	0
3	PPV	48-B	405	2	6,8,8	1.05	0	13,13,13	1.22	1 (7%)
3	PPV	42-A	406	2	6,8,8	1.09	0	13,13,13	1.29	2 (15%)
8	2PE	20-B	409	-	6,6,27	0.49	0	5,5,26	0.35	0
4	EXW	7-A	407	-	21,22,22	5.70	11 (52%)	24,32,32	3.40	13 (54%)
5	MPD	7-A	408	-	7,7,7	0.50	0	9,10,10	0.47	0
3	PPV	47-B	405	2	6,8,8	1.08	0	13,13,13	1.32	2 (15%)
3	PPV	29-B	405	2	6,8,8	1.03	0	13,13,13	1.25	1 (7%)
7	CCN	27-A	411	-	2,2,2	0.85	0	1,1,1	0.57	0
4	EXW	22-A	407	-	21,22,22	5.69	11 (52%)	24,32,32	3.31	10 (41%)
3	PPV	7-B	405	2	6,8,8	1.05	0	13,13,13	1.29	2 (15%)
4	EXW	2-A	407	-	21,22,22	5.76	11 (52%)	24,32,32	3.49	13 (54%)
8	2PE	37-A	412	-	6,6,27	0.55	0	5,5,26	0.80	0
3	PPV	10-B	405	2	6,8,8	1.04	0	13,13,13	1.21	1 (7%)
7	CCN	2-A	411	-	2,2,2	0.75	0	1,1,1	0.37	0
8	2PE	16-A	412	-	6,6,27	0.42	0	5,5,26	0.44	0
3	PPV	30-B	405	2	6,8,8	1.06	0	13,13,13	1.37	2 (15%)
8	2PE	29-A	412	-	6,6,27	0.47	0	5,5,26	0.45	0
3	PPV	27-B	405	2	6,8,8	1.04	0	13,13,13	1.30	2 (15%)
3	PPV	33-A	406	2	6,8,8	0.97	0	13,13,13	1.20	1 (7%)
3	PPV	50-A	406	2	6,8,8	1.03	0	13,13,13	1.34	1 (7%)
5	MPD	45-A	408	-	7,7,7	0.68	0	9,10,10	1.05	1 (11%)
5	MPD	20-B	407	-	7,7,7	0.30	0	9,10,10	2.03	1 (11%)
7	CCN	30-A	411	-	2,2,2	0.92	0	1,1,1	0.54	0
8	2PE	35-B	409	-	6,6,27	0.49	0	5,5,26	0.19	0
5	MPD	2-B	407	-	7,7,7	0.40	0	9,10,10	1.39	2 (22%)
3	PPV	16-B	405	2	6,8,8	1.03	0	13,13,13	1.17	2 (15%)
7	CCN	36-A	411	-	2,2,2	0.72	0	1,1,1	0.40	0
4	EXW	14-B	406	-	21,22,22	5.36	9 (42%)	24,32,32	3.75	13 (54%)
5	MPD	17-B	407	-	7,7,7	0.42	0	9,10,10	1.38	2 (22%)
4	EXW	35-B	406	-	21,22,22	5.92	8 (38%)	24,32,32	3.59	13 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MPD	28-B	407	-	7,7,7	0.48	0	9,10,10	1.36	2 (22%)
3	PPV	40-B	405	2	6,8,8	1.03	0	13,13,13	1.25	1 (7%)
4	EXW	30-B	406	-	21,22,22	5.71	9 (42%)	24,32,32	3.45	15 (62%)
5	MPD	15-B	407	-	7,7,7	0.74	0	9,10,10	1.26	2 (22%)
7	CCN	40-A	411	-	2,2,2	0.77	0	1,1,1	0.50	0
5	MPD	31-A	408	-	7,7,7	0.44	0	9,10,10	0.53	0
5	MPD	44-A	408	-	7,7,7	0.62	0	9,10,10	1.04	1 (11%)
4	EXW	6-B	406	-	21,22,22	5.64	9 (42%)	24,32,32	3.64	13 (54%)
7	CCN	50-A	411	-	2,2,2	0.95	0	1,1,1	0.46	0
7	CCN	41-A	411	-	2,2,2	0.69	0	1,1,1	0.47	0
5	MPD	5-B	407	-	7,7,7	0.65	0	9,10,10	1.61	1 (11%)
5	MPD	48-A	408	-	7,7,7	0.64	0	9,10,10	1.53	2 (22%)
8	2PE	4-A	412	-	6,6,27	0.44	0	5,5,26	0.37	0
3	PPV	21-B	405	2	6,8,8	1.03	0	13,13,13	1.24	1 (7%)
4	EXW	9-A	407	-	21,22,22	5.54	9 (42%)	24,32,32	3.35	15 (62%)
8	2PE	13-A	412	-	6,6,27	0.48	0	5,5,26	0.48	0
8	2PE	29-B	409	-	6,6,27	0.51	0	5,5,26	0.25	0
8	2PE	22-B	409	-	6,6,27	0.50	0	5,5,26	0.43	0
5	MPD	27-A	408	-	7,7,7	0.55	0	9,10,10	1.28	1 (11%)
8	2PE	17-B	409	-	6,6,27	0.47	0	5,5,26	0.40	0
7	CCN	32-A	411	-	2,2,2	0.94	0	1,1,1	0.55	0
3	PPV	47-A	406	2	6,8,8	1.11	0	13,13,13	1.29	2 (15%)
5	MPD	21-A	408	-	7,7,7	0.43	0	9,10,10	0.58	0
8	2PE	33-B	409	-	6,6,27	0.50	0	5,5,26	0.39	0
8	2PE	43-A	412	-	6,6,27	0.54	0	5,5,26	0.55	0
5	MPD	26-B	407	-	7,7,7	0.44	0	9,10,10	1.30	2 (22%)
7	CCN	19-A	411	-	2,2,2	0.89	0	1,1,1	0.56	0
5	MPD	7-B	407	-	7,7,7	0.74	0	9,10,10	1.62	2 (22%)
3	PPV	4-B	405	2	6,8,8	1.05	0	13,13,13	1.25	2 (15%)
5	MPD	14-B	407	-	7,7,7	0.40	0	9,10,10	1.50	2 (22%)
7	CCN	34-A	411	-	2,2,2	0.79	0	1,1,1	0.44	0
8	2PE	6-A	412	-	6,6,27	0.53	0	5,5,26	0.39	0
3	PPV	10-A	406	2	6,8,8	1.02	0	13,13,13	1.16	1 (7%)
7	CCN	37-A	411	-	2,2,2	0.93	0	1,1,1	0.53	0
4	EXW	12-B	406	-	21,22,22	5.57	9 (42%)	24,32,32	3.61	10 (41%)
8	2PE	36-A	412	-	6,6,27	0.48	0	5,5,26	0.44	0
8	2PE	39-B	409	-	6,6,27	0.52	0	5,5,26	0.56	0
5	MPD	10-B	407	-	7,7,7	0.43	0	9,10,10	1.04	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	2PE	20-A	412	-	6,6,27	0.51	0	5,5,26	0.29	0
4	EXW	10-B	406	-	21,22,22	5.62	8 (38%)	24,32,32	3.75	15 (62%)
8	2PE	10-A	412	-	6,6,27	0.47	0	5,5,26	0.47	0
8	2PE	25-A	412	-	6,6,27	0.47	0	5,5,26	0.68	0
3	PPV	5-B	405	2	6,8,8	1.04	0	13,13,13	1.18	1 (7%)
3	PPV	28-A	406	2	6,8,8	1.04	0	13,13,13	1.24	1 (7%)
8	2PE	23-A	412	-	6,6,27	0.44	0	5,5,26	0.41	0
8	2PE	50-A	412	-	6,6,27	0.51	0	5,5,26	0.42	0
4	EXW	37-B	406	-	21,22,22	5.52	9 (42%)	24,32,32	3.80	18 (75%)
8	2PE	41-A	412	-	6,6,27	0.42	0	5,5,26	0.58	0
3	PPV	13-A	406	2	6,8,8	0.99	0	13,13,13	1.13	1 (7%)
3	PPV	16-A	406	2	6,8,8	1.01	0	13,13,13	1.27	2 (15%)
5	MPD	39-B	407	-	7,7,7	0.41	0	9,10,10	1.65	2 (22%)
8	2PE	32-A	412	-	6,6,27	0.46	0	5,5,26	0.75	0
5	MPD	19-A	408	-	7,7,7	0.53	0	9,10,10	0.91	1 (11%)
8	2PE	47-B	409	-	6,6,27	0.49	0	5,5,26	0.34	0
4	EXW	45-A	407	-	21,22,22	5.85	10 (47%)	24,32,32	4.72	18 (75%)
4	EXW	32-A	407	-	21,22,22	6.11	11 (52%)	24,32,32	3.63	14 (58%)
8	2PE	36-B	409	-	6,6,27	0.45	0	5,5,26	0.28	0
3	PPV	2-B	405	2	6,8,8	1.02	0	13,13,13	1.20	2 (15%)
5	MPD	12-B	407	-	7,7,7	0.57	0	9,10,10	1.40	1 (11%)
5	MPD	35-A	408	-	7,7,7	0.50	0	9,10,10	0.91	1 (11%)
7	CCN	45-A	411	-	2,2,2	0.95	0	1,1,1	0.47	0
3	PPV	21-A	406	2	6,8,8	0.94	0	13,13,13	1.29	1 (7%)
3	PPV	6-A	406	2	6,8,8	0.95	0	13,13,13	1.18	1 (7%)
5	MPD	18-B	407	-	7,7,7	0.49	0	9,10,10	1.32	1 (11%)
3	PPV	28-B	405	2	6,8,8	1.07	0	13,13,13	1.28	1 (7%)
5	MPD	19-B	407	-	7,7,7	0.47	0	9,10,10	1.77	1 (11%)
8	2PE	50-B	409	-	6,6,27	0.45	0	5,5,26	0.31	0
5	MPD	24-B	407	-	7,7,7	0.50	0	9,10,10	1.15	1 (11%)
5	MPD	22-B	407	-	7,7,7	0.66	0	9,10,10	0.89	0
4	EXW	39-A	407	-	21,22,22	6.01	12 (57%)	24,32,32	3.56	11 (45%)
3	PPV	49-A	406	2	6,8,8	0.99	0	13,13,13	1.37	2 (15%)
5	MPD	1-A	408	-	7,7,7	0.64	0	9,10,10	1.48	1 (11%)
3	PPV	31-B	405	2	6,8,8	1.00	0	13,13,13	1.41	3 (23%)
7	CCN	44-A	411	-	2,2,2	0.89	0	1,1,1	0.56	0
8	2PE	5-B	409	-	6,6,27	0.44	0	5,5,26	0.57	0
8	2PE	22-A	412	-	6,6,27	0.45	0	5,5,26	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PPV	45-B	405	2	6,8,8	1.08	0	13,13,13	1.23	1 (7%)
5	MPD	16-A	408	-	7,7,7	0.51	0	9,10,10	0.57	0
7	CCN	6-A	411	-	2,2,2	0.94	0	1,1,1	0.19	0
5	MPD	40-A	408	-	7,7,7	0.63	0	9,10,10	0.61	0
5	MPD	29-A	408	-	7,7,7	0.38	0	9,10,10	1.22	1 (11%)
5	MPD	3-B	407	-	7,7,7	0.25	0	9,10,10	1.09	1 (11%)
7	CCN	10-A	411	-	2,2,2	0.76	0	1,1,1	0.49	0
3	PPV	41-B	405	2	6,8,8	1.10	0	13,13,13	1.34	2 (15%)
3	PPV	35-A	406	2	6,8,8	0.97	0	13,13,13	1.19	1 (7%)
4	EXW	15-A	407	-	21,22,22	5.76	11 (52%)	24,32,32	4.02	17 (70%)
4	EXW	24-A	407	-	21,22,22	5.79	10 (47%)	24,32,32	3.53	13 (54%)
5	MPD	11-A	408	-	7,7,7	0.58	0	9,10,10	1.00	0
4	EXW	38-B	406	-	21,22,22	5.39	11 (52%)	24,32,32	3.35	14 (58%)
7	CCN	49-A	411	-	2,2,2	0.83	0	1,1,1	0.47	0
8	2PE	49-A	412	-	6,6,27	0.41	0	5,5,26	0.71	0
8	2PE	46-B	409	-	6,6,27	0.51	0	5,5,26	0.87	0
3	PPV	19-A	406	2	6,8,8	0.90	0	13,13,13	1.15	1 (7%)
5	MPD	30-A	408	-	7,7,7	0.56	0	9,10,10	0.74	0
8	2PE	8-B	409	-	6,6,27	0.47	0	5,5,26	0.55	0
8	2PE	9-B	409	-	6,6,27	0.51	0	5,5,26	0.35	0
4	EXW	44-A	407	-	21,22,22	6.19	11 (52%)	24,32,32	4.14	13 (54%)
3	PPV	12-A	406	2	6,8,8	0.96	0	13,13,13	1.20	1 (7%)
5	MPD	46-B	407	-	7,7,7	0.51	0	9,10,10	1.54	1 (11%)
4	EXW	20-A	407	-	21,22,22	5.62	9 (42%)	24,32,32	3.70	14 (58%)
3	PPV	37-A	406	2	6,8,8	0.95	0	13,13,13	1.28	1 (7%)
3	PPV	13-B	405	2	6,8,8	1.05	0	13,13,13	1.20	1 (7%)
7	CCN	25-A	411	-	2,2,2	0.71	0	1,1,1	0.32	0
4	EXW	17-A	407	-	21,22,22	5.31	9 (42%)	24,32,32	3.44	14 (58%)
5	MPD	48-B	407	-	7,7,7	0.36	0	9,10,10	1.52	2 (22%)
4	EXW	8-A	407	-	21,22,22	5.60	10 (47%)	24,32,32	4.06	17 (70%)
3	PPV	26-B	405	2	6,8,8	1.03	0	13,13,13	1.33	2 (15%)
4	EXW	11-B	406	-	21,22,22	5.18	10 (47%)	24,32,32	4.12	16 (66%)
3	PPV	43-B	405	2	6,8,8	0.99	0	13,13,13	1.30	2 (15%)
3	PPV	31-A	406	2	6,8,8	1.01	0	13,13,13	1.30	2 (15%)
3	PPV	5-A	406	2	6,8,8	1.01	0	13,13,13	1.22	2 (15%)
4	EXW	5-A	407	-	21,22,22	5.81	8 (38%)	24,32,32	3.53	13 (54%)
7	CCN	35-A	411	-	2,2,2	0.95	0	1,1,1	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MPD	15-A	408	-	7,7,7	0.52	0	9,10,10	1.18	1 (11%)
5	MPD	50-A	408	-	7,7,7	0.58	0	9,10,10	1.24	1 (11%)
3	PPV	23-B	405	2	6,8,8	1.05	0	13,13,13	1.21	2 (15%)
4	EXW	13-A	407	-	21,22,22	5.96	10 (47%)	24,32,32	4.20	18 (75%)
5	MPD	25-A	408	-	7,7,7	0.47	0	9,10,10	1.18	1 (11%)
7	CCN	5-A	411	-	2,2,2	0.79	0	1,1,1	0.48	0
4	EXW	17-B	406	-	21,22,22	5.35	8 (38%)	24,32,32	4.09	11 (45%)
3	PPV	46-A	406	2	6,8,8	1.05	0	13,13,13	1.26	1 (7%)
4	EXW	42-A	407	-	21,22,22	6.15	11 (52%)	24,32,32	4.51	15 (62%)
3	PPV	3-B	405	2	6,8,8	1.05	0	13,13,13	1.34	2 (15%)
4	EXW	19-A	407	-	21,22,22	5.69	9 (42%)	24,32,32	3.71	16 (66%)
5	MPD	35-B	407	-	7,7,7	0.56	0	9,10,10	1.26	1 (11%)
4	EXW	14-A	407	-	21,22,22	5.48	8 (38%)	24,32,32	3.66	11 (45%)
7	CCN	14-A	411	-	2,2,2	0.86	0	1,1,1	0.50	0
8	2PE	45-A	412	-	6,6,27	0.48	0	5,5,26	0.66	0
5	MPD	4-A	408	-	7,7,7	0.35	0	9,10,10	0.91	0
8	2PE	35-A	412	-	6,6,27	0.43	0	5,5,26	0.48	0
8	2PE	16-B	409	-	6,6,27	0.59	0	5,5,26	0.40	0
4	EXW	28-B	406	-	21,22,22	5.43	9 (42%)	24,32,32	3.57	13 (54%)
5	MPD	8-A	408	-	7,7,7	0.39	0	9,10,10	0.85	1 (11%)
5	MPD	36-A	408	-	7,7,7	0.42	0	9,10,10	1.05	1 (11%)
5	MPD	13-B	407	-	7,7,7	0.56	0	9,10,10	1.10	1 (11%)
3	PPV	6-B	405	2	6,8,8	1.06	0	13,13,13	1.23	2 (15%)
4	EXW	13-B	406	-	21,22,22	5.46	11 (52%)	24,32,32	3.04	9 (37%)
4	EXW	16-B	406	-	21,22,22	5.16	9 (42%)	24,32,32	4.36	20 (83%)
8	2PE	30-B	409	-	6,6,27	0.53	0	5,5,26	0.93	0
4	EXW	40-B	406	-	21,22,22	5.39	9 (42%)	24,32,32	3.84	15 (62%)
3	PPV	49-B	405	2	6,8,8	1.04	0	13,13,13	1.25	1 (7%)
8	2PE	33-A	412	-	6,6,27	0.46	0	5,5,26	0.53	0
3	PPV	29-A	406	2	6,8,8	0.98	0	13,13,13	1.27	2 (15%)
3	PPV	34-B	405	2	6,8,8	1.02	0	13,13,13	1.23	1 (7%)
4	EXW	48-B	406	-	21,22,22	5.16	8 (38%)	24,32,32	3.77	14 (58%)
5	MPD	32-A	408	-	7,7,7	0.25	0	9,10,10	1.21	1 (11%)
4	EXW	26-A	407	-	21,22,22	5.96	10 (47%)	24,32,32	2.94	13 (54%)
4	EXW	12-A	407	-	21,22,22	5.93	9 (42%)	24,32,32	3.45	11 (45%)
5	MPD	23-A	408	-	7,7,7	0.50	0	9,10,10	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EXW	21-B	406	-	21,22,22	4.97	9 (42%)	24,32,32	4.78	16 (66%)
4	EXW	30-A	407	-	21,22,22	5.68	9 (42%)	24,32,32	4.36	12 (50%)
8	2PE	15-A	412	-	6,6,27	0.48	0	5,5,26	0.96	0
7	CCN	18-A	411	-	2,2,2	0.94	0	1,1,1	0.54	0
3	PPV	20-B	405	2	6,8,8	1.06	0	13,13,13	1.03	1 (7%)
3	PPV	3-A	406	2	6,8,8	0.98	0	13,13,13	1.19	2 (15%)
7	CCN	24-A	411	-	2,2,2	0.86	0	1,1,1	0.54	0
3	PPV	17-B	405	2	6,8,8	1.02	0	13,13,13	1.33	1 (7%)
5	MPD	33-A	408	-	7,7,7	0.46	0	9,10,10	2.15	2 (22%)
4	EXW	36-B	406	-	21,22,22	5.62	10 (47%)	24,32,32	4.35	14 (58%)
4	EXW	48-A	407	-	21,22,22	6.31	10 (47%)	24,32,32	3.13	12 (50%)
3	PPV	20-A	406	2	6,8,8	0.99	0	13,13,13	1.17	1 (7%)
5	MPD	16-B	407	-	7,7,7	0.51	0	9,10,10	1.72	3 (33%)
8	2PE	41-B	409	-	6,6,27	0.49	0	5,5,26	1.38	1 (20%)
4	EXW	3-A	407	-	21,22,22	5.41	10 (47%)	24,32,32	3.52	13 (54%)
3	PPV	26-A	406	2	6,8,8	1.01	0	13,13,13	1.24	1 (7%)
8	2PE	25-B	409	-	6,6,27	0.48	0	5,5,26	0.52	0
5	MPD	40-B	407	-	7,7,7	0.39	0	9,10,10	0.85	0
8	2PE	39-A	412	-	6,6,27	0.53	0	5,5,26	0.25	0
5	MPD	47-B	407	-	7,7,7	0.53	0	9,10,10	1.92	2 (22%)
8	2PE	7-A	412	-	6,6,27	0.41	0	5,5,26	0.61	0
3	PPV	17-A	406	2	6,8,8	1.06	0	13,13,13	1.31	1 (7%)
4	EXW	19-B	406	-	21,22,22	5.57	13 (61%)	24,32,32	3.85	16 (66%)
3	PPV	38-B	405	2	6,8,8	1.07	0	13,13,13	1.30	2 (15%)
8	2PE	17-A	412	-	6,6,27	0.47	0	5,5,26	0.44	0
3	PPV	25-A	406	2	6,8,8	1.05	0	13,13,13	1.22	1 (7%)
3	PPV	36-B	405	2	6,8,8	1.10	0	13,13,13	1.25	2 (15%)
3	PPV	23-A	406	2	6,8,8	0.96	0	13,13,13	1.27	1 (7%)
8	2PE	5-A	412	-	6,6,27	0.47	0	5,5,26	0.56	0
7	CCN	12-A	411	-	2,2,2	0.99	0	1,1,1	0.54	0
8	2PE	12-A	412	-	6,6,27	0.55	0	5,5,26	0.75	0
8	2PE	24-A	412	-	6,6,27	0.39	0	5,5,26	0.74	0
5	MPD	27-B	407	-	7,7,7	0.83	0	9,10,10	1.41	1 (11%)
3	PPV	48-A	406	2	6,8,8	0.99	0	13,13,13	1.41	2 (15%)
4	EXW	35-A	407	-	21,22,22	6.05	11 (52%)	24,32,32	3.23	15 (62%)
5	MPD	4-B	407	-	7,7,7	0.52	0	9,10,10	1.59	1 (11%)
4	EXW	4-B	406	-	21,22,22	5.11	9 (42%)	24,32,32	3.50	12 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EXW	1-B	406	-	21,22,22	5.44	9 (42%)	24,32,32	4.26	15 (62%)
5	MPD	22-A	408	-	7,7,7	0.66	0	9,10,10	0.87	0
8	2PE	19-B	409	-	6,6,27	0.51	0	5,5,26	0.84	0
4	EXW	31-B	406	-	21,22,22	5.61	10 (47%)	24,32,32	4.44	14 (58%)
7	CCN	42-A	411	-	2,2,2	0.90	0	1,1,1	0.56	0
7	CCN	48-A	411	-	2,2,2	0.82	0	1,1,1	0.56	0
8	2PE	42-A	412	-	6,6,27	0.53	0	5,5,26	0.35	0
8	2PE	48-A	412	-	6,6,27	0.45	0	5,5,26	0.36	0
7	CCN	26-A	411	-	2,2,2	0.96	0	1,1,1	0.45	0
4	EXW	31-A	407	-	21,22,22	6.49	13 (61%)	24,32,32	4.06	18 (75%)
8	2PE	11-A	412	-	6,6,27	0.50	0	5,5,26	0.63	0
4	EXW	49-A	407	-	21,22,22	6.02	10 (47%)	24,32,32	4.21	18 (75%)
7	CCN	43-A	411	-	2,2,2	0.81	0	1,1,1	0.58	0
8	2PE	18-B	409	-	6,6,27	0.49	0	5,5,26	0.48	0
5	MPD	49-A	408	-	7,7,7	0.59	0	9,10,10	1.21	1 (11%)
8	2PE	14-A	412	-	6,6,27	0.45	0	5,5,26	0.26	0
5	MPD	21-B	407	-	7,7,7	0.45	0	9,10,10	1.49	1 (11%)
5	MPD	9-B	407	-	7,7,7	0.34	0	9,10,10	1.05	1 (11%)
4	EXW	41-B	406	-	21,22,22	5.70	9 (42%)	24,32,32	3.86	13 (54%)
5	MPD	49-B	407	-	7,7,7	0.52	0	9,10,10	1.37	0
3	PPV	27-A	406	2	6,8,8	1.01	0	13,13,13	1.31	2 (15%)
8	2PE	24-B	409	-	6,6,27	0.52	0	5,5,26	0.76	0
3	PPV	1-B	405	2	6,8,8	1.05	0	13,13,13	1.24	1 (7%)
4	EXW	33-A	407	-	21,22,22	5.63	9 (42%)	24,32,32	4.18	19 (79%)
8	2PE	30-A	412	-	6,6,27	0.44	0	5,5,26	0.33	0
5	MPD	32-B	407	-	7,7,7	0.43	0	9,10,10	0.73	0
7	CCN	46-A	411	-	2,2,2	0.70	0	1,1,1	0.51	0
8	2PE	2-B	409	-	6,6,27	0.48	0	5,5,26	0.86	0
4	EXW	32-B	406	-	21,22,22	5.28	10 (47%)	24,32,32	3.94	12 (50%)
7	CCN	8-A	411	-	2,2,2	0.84	0	1,1,1	0.60	0
8	2PE	38-B	409	-	6,6,27	0.46	0	5,5,26	0.49	0
3	PPV	42-B	405	2	6,8,8	1.00	0	13,13,13	1.30	2 (15%)
5	MPD	37-B	407	-	7,7,7	0.35	0	9,10,10	1.65	1 (11%)
3	PPV	22-B	405	2	6,8,8	1.14	0	13,13,13	1.29	1 (7%)
4	EXW	46-B	406	-	21,22,22	4.89	8 (38%)	24,32,32	4.50	15 (62%)
3	PPV	33-B	405	2	6,8,8	1.04	0	13,13,13	1.32	2 (15%)
7	CCN	33-A	411	-	2,2,2	0.91	0	1,1,1	0.31	0
3	PPV	38-A	406	2	6,8,8	0.97	0	13,13,13	1.32	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EXW	6-A	407	-	21,22,22	5.22	10 (47%)	24,32,32	3.60	13 (54%)
8	2PE	42-B	409	-	6,6,27	0.50	0	5,5,26	0.37	0
8	2PE	14-B	409	-	6,6,27	0.53	0	5,5,26	0.27	0
8	2PE	26-A	412	-	6,6,27	0.43	0	5,5,26	0.73	0
3	PPV	40-A	406	2	6,8,8	1.03	0	13,13,13	1.28	1 (7%)
7	CCN	20-A	411	-	2,2,2	0.81	0	1,1,1	0.43	0
3	PPV	50-B	405	2	6,8,8	1.09	0	13,13,13	1.10	1 (7%)
8	2PE	19-A	412	-	6,6,27	0.48	0	5,5,26	0.62	0
4	EXW	26-B	406	-	21,22,22	5.47	10 (47%)	24,32,32	4.20	13 (54%)
7	CCN	13-A	411	-	2,2,2	0.79	0	1,1,1	0.47	0
8	2PE	10-B	409	-	6,6,27	0.51	0	5,5,26	0.38	0
5	MPD	29-B	407	-	7,7,7	0.57	0	9,10,10	0.84	0
4	EXW	47-A	407	-	21,22,22	5.57	12 (57%)	24,32,32	3.63	14 (58%)
4	EXW	18-A	407	-	21,22,22	5.81	9 (42%)	24,32,32	3.74	14 (58%)
8	2PE	34-B	409	-	6,6,27	0.45	0	5,5,26	0.35	0
7	CCN	23-A	411	-	2,2,2	0.79	0	1,1,1	0.45	0
5	MPD	39-A	408	-	7,7,7	0.58	0	9,10,10	0.65	0
7	CCN	28-A	411	-	2,2,2	0.96	0	1,1,1	0.50	0
5	MPD	43-A	408	-	7,7,7	0.57	0	9,10,10	1.32	1 (11%)
7	CCN	3-A	411	-	2,2,2	0.87	0	1,1,1	0.38	0
8	2PE	26-B	409	-	6,6,27	0.41	0	5,5,26	0.37	0
8	2PE	3-A	412	-	6,6,27	0.43	0	5,5,26	0.31	0
3	PPV	4-A	406	2	6,8,8	1.02	0	13,13,13	1.23	1 (7%)
3	PPV	36-A	406	2	6,8,8	0.99	0	13,13,13	1.26	1 (7%)
5	MPD	31-B	407	-	7,7,7	0.31	0	9,10,10	1.18	1 (11%)
5	MPD	44-B	407	-	7,7,7	0.53	0	9,10,10	1.23	0
4	EXW	10-A	407	-	21,22,22	5.54	10 (47%)	24,32,32	3.63	16 (66%)
4	EXW	44-B	406	-	21,22,22	5.53	8 (38%)	24,32,32	3.63	11 (45%)
5	MPD	10-A	408	-	7,7,7	0.44	0	9,10,10	1.55	1 (11%)
4	EXW	1-A	407	-	21,22,22	5.80	10 (47%)	24,32,32	3.80	11 (45%)
5	MPD	18-A	408	-	7,7,7	0.50	0	9,10,10	0.77	0
7	CCN	39-A	411	-	2,2,2	0.89	0	1,1,1	0.55	0
4	EXW	3-B	406	-	21,22,22	5.41	10 (47%)	24,32,32	3.84	13 (54%)
3	PPV	41-A	406	2	6,8,8	1.04	0	13,13,13	1.35	1 (7%)
4	EXW	47-B	406	-	21,22,22	5.74	11 (52%)	24,32,32	4.26	18 (75%)
5	MPD	24-A	408	-	7,7,7	0.74	0	9,10,10	0.97	1 (11%)
3	PPV	11-A	406	2	6,8,8	0.99	0	13,13,13	1.32	2 (15%)
3	PPV	15-B	405	2	6,8,8	1.07	0	13,13,13	1.25	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EXW	40-A	407	-	21,22,22	6.11	11 (52%)	24,32,32	3.53	14 (58%)
4	EXW	20-B	406	-	21,22,22	5.01	8 (38%)	24,32,32	4.28	15 (62%)
3	PPV	32-A	406	2	6,8,8	0.97	0	13,13,13	1.23	1 (7%)
8	2PE	37-B	409	-	6,6,27	0.53	0	5,5,26	0.33	0
7	CCN	7-A	411	-	2,2,2	0.82	0	1,1,1	0.56	0
3	PPV	2-A	406	2	6,8,8	1.03	0	13,13,13	1.02	1 (7%)
5	MPD	5-A	408	-	7,7,7	0.61	0	9,10,10	1.40	1 (11%)
8	2PE	3-B	409	-	6,6,27	0.46	0	5,5,26	0.40	0
5	MPD	47-A	408	-	7,7,7	0.60	0	9,10,10	0.84	0
8	2PE	28-A	412	-	6,6,27	0.48	0	5,5,26	0.48	0
8	2PE	11-B	409	-	6,6,27	0.46	0	5,5,26	0.49	0
4	EXW	25-B	406	-	21,22,22	5.34	8 (38%)	24,32,32	3.00	11 (45%)
3	PPV	45-A	406	2	6,8,8	1.03	0	13,13,13	1.29	2 (15%)
5	MPD	20-A	408	-	7,7,7	0.47	0	9,10,10	1.00	1 (11%)
4	EXW	49-B	406	-	21,22,22	5.34	10 (47%)	24,32,32	3.36	12 (50%)
4	EXW	27-A	407	-	21,22,22	5.95	9 (42%)	24,32,32	3.94	15 (62%)
5	MPD	23-B	407	-	7,7,7	0.21	0	9,10,10	0.56	0
3	PPV	1-A	406	2	6,8,8	1.02	0	13,13,13	1.15	1 (7%)
4	EXW	23-B	406	-	21,22,22	5.29	11 (52%)	24,32,32	3.84	13 (54%)
4	EXW	21-A	407	-	21,22,22	5.19	8 (38%)	24,32,32	3.38	14 (58%)
8	2PE	31-B	409	-	6,6,27	0.51	0	5,5,26	0.53	0
5	MPD	11-B	407	-	7,7,7	0.52	0	9,10,10	1.54	1 (11%)
3	PPV	14-B	405	2	6,8,8	1.07	0	13,13,13	1.23	1 (7%)
3	PPV	35-B	405	2	6,8,8	1.03	0	13,13,13	1.25	1 (7%)
8	2PE	49-B	409	-	6,6,27	0.44	0	5,5,26	0.28	0
8	2PE	12-B	409	-	6,6,27	0.50	0	5,5,26	0.67	0
4	EXW	29-B	406	-	21,22,22	5.74	10 (47%)	24,32,32	3.33	12 (50%)
3	PPV	24-A	406	2	6,8,8	1.00	0	13,13,13	1.18	1 (7%)
5	MPD	41-A	408	-	7,7,7	0.39	0	9,10,10	1.15	1 (11%)
5	MPD	28-A	408	-	7,7,7	0.60	0	9,10,10	0.54	0
8	2PE	28-B	409	-	6,6,27	0.52	0	5,5,26	0.44	0
7	CCN	47-A	411	-	2,2,2	0.91	0	1,1,1	0.53	0
3	PPV	9-A	406	2	6,8,8	0.95	0	13,13,13	1.26	2 (15%)
4	EXW	38-A	407	-	21,22,22	6.04	11 (52%)	24,32,32	4.16	15 (62%)
5	MPD	25-B	407	-	7,7,7	0.36	0	9,10,10	0.58	0
5	MPD	38-A	408	-	7,7,7	0.65	0	9,10,10	0.79	0
7	CCN	22-A	411	-	2,2,2	0.77	0	1,1,1	0.41	0
8	2PE	23-B	409	-	6,6,27	0.44	0	5,5,26	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	2PE	45-B	409	-	6,6,27	0.50	0	5,5,26	0.69	0
3	PPV	15-A	406	2	6,8,8	1.12	0	13,13,13	1.32	1 (7%)
4	EXW	27-B	406	-	21,22,22	5.63	9 (42%)	24,32,32	3.89	15 (62%)
5	MPD	1-B	407	-	7,7,7	0.61	0	9,10,10	1.25	0
8	2PE	43-B	409	-	6,6,27	0.49	0	5,5,26	0.41	0
7	CCN	21-A	411	-	2,2,2	0.94	0	1,1,1	0.52	0
7	CCN	9-A	411	-	2,2,2	0.90	0	1,1,1	0.54	0
3	PPV	34-A	406	2	6,8,8	1.08	0	13,13,13	1.25	1 (7%)
8	2PE	48-B	409	-	6,6,27	0.49	0	5,5,26	0.39	0
5	MPD	38-B	407	-	7,7,7	0.41	0	9,10,10	1.03	1 (11%)
5	MPD	34-B	407	-	7,7,7	0.48	0	9,10,10	1.60	3 (33%)
4	EXW	39-B	406	-	21,22,22	5.12	9 (42%)	24,32,32	4.46	18 (75%)
4	EXW	34-B	406	-	21,22,22	5.71	9 (42%)	24,32,32	3.85	18 (75%)
3	PPV	43-A	406	2	6,8,8	1.09	0	13,13,13	1.29	2 (15%)
3	PPV	44-A	406	2	6,8,8	1.03	0	13,13,13	1.37	3 (23%)
3	PPV	19-B	405	2	6,8,8	1.06	0	13,13,13	1.13	1 (7%)
3	PPV	24-B	405	2	6,8,8	1.15	0	13,13,13	1.32	1 (7%)
8	2PE	6-B	409	-	6,6,27	0.43	0	5,5,26	0.31	0
8	2PE	44-A	412	-	6,6,27	0.45	0	5,5,26	0.59	0
3	PPV	7-A	406	2	6,8,8	0.97	0	13,13,13	1.26	1 (7%)
8	2PE	47-A	412	-	6,6,27	0.53	0	5,5,26	0.32	0
4	EXW	18-B	406	-	21,22,22	5.51	8 (38%)	24,32,32	3.84	12 (50%)
4	EXW	37-A	407	-	21,22,22	6.08	13 (61%)	24,32,32	4.19	15 (62%)
5	MPD	30-B	407	-	7,7,7	0.40	0	9,10,10	1.09	1 (11%)
8	2PE	18-A	412	-	6,6,27	0.46	0	5,5,26	0.62	0
4	EXW	16-A	407	-	21,22,22	6.00	11 (52%)	24,32,32	2.58	10 (41%)
4	EXW	24-B	406	-	21,22,22	5.50	11 (52%)	24,32,32	3.55	13 (54%)
3	PPV	39-B	405	2	6,8,8	1.04	0	13,13,13	1.29	2 (15%)
8	2PE	15-B	409	-	6,6,27	0.50	0	5,5,26	0.28	0
5	MPD	41-B	407	-	7,7,7	0.39	0	9,10,10	0.84	0
4	EXW	2-B	406	-	21,22,22	5.23	8 (38%)	24,32,32	4.37	19 (79%)
4	EXW	11-A	407	-	21,22,22	5.44	9 (42%)	24,32,32	3.39	14 (58%)
7	CCN	11-A	411	-	2,2,2	0.72	0	1,1,1	0.47	0
5	MPD	42-A	408	-	7,7,7	0.39	0	9,10,10	0.69	0
4	EXW	5-B	406	-	21,22,22	5.67	8 (38%)	24,32,32	3.72	13 (54%)
5	MPD	26-A	408	-	7,7,7	0.70	0	9,10,10	0.80	0
3	PPV	18-B	405	2	6,8,8	1.07	0	13,13,13	1.28	1 (7%)
8	2PE	1-A	412	-	6,6,27	0.48	0	5,5,26	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EXW	41-A	407	-	21,22,22	6.32	11 (52%)	24,32,32	4.07	16 (66%)

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
8	2PE	44-B	409	-	-	1/4/4/25	-
3	PPV	12-B	405	2	-	0/6/6/6	-
4	EXW	46-A	407	-	-	10/20/40/40	1/2/2/2
5	MPD	46-A	408	-	-	2/5/5/5	-
4	EXW	42-B	406	-	-	12/20/40/40	1/2/2/2
8	2PE	34-A	412	-	-	2/4/4/25	-
3	PPV	46-B	405	2	-	0/6/6/6	-
8	2PE	13-B	409	-	-	4/4/4/25	-
8	2PE	40-A	412	-	-	3/4/4/25	-
5	MPD	8-B	407	-	-	1/5/5/5	-
3	PPV	8-B	405	2	-	0/6/6/6	-
5	MPD	36-B	407	-	-	2/5/5/5	-
3	PPV	14-A	406	2	-	0/6/6/6	-
8	2PE	21-A	412	-	-	3/4/4/25	-
3	PPV	22-A	406	2	-	0/6/6/6	-
5	MPD	9-A	408	-	-	2/5/5/5	-
8	2PE	8-A	412	-	-	3/4/4/25	-
8	2PE	9-A	412	-	-	2/4/4/25	-
5	MPD	50-B	407	-	-	2/5/5/5	-
4	EXW	33-B	406	-	-	9/20/40/40	1/2/2/2
3	PPV	32-B	405	2	-	0/6/6/6	-
3	PPV	30-A	406	2	-	0/6/6/6	-
3	PPV	37-B	405	2	-	0/6/6/6	-
8	2PE	1-B	409	-	-	3/4/4/25	-
4	EXW	43-A	407	-	-	14/20/40/40	1/2/2/2
8	2PE	2-A	412	-	-	2/4/4/25	-
4	EXW	29-A	407	-	-	12/20/40/40	1/2/2/2
3	PPV	39-A	406	2	-	0/6/6/6	-
8	2PE	40-B	409	-	-	3/4/4/25	-
4	EXW	25-A	407	-	-	9/20/40/40	1/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EXW	45-B	406	-	-	9/20/40/40	0/2/2/2
8	2PE	7-B	409	-	-	1/4/4/25	-
3	PPV	9-B	405	2	-	0/6/6/6	-
8	2PE	38-A	412	-	-	3/4/4/25	-
4	EXW	4-A	407	-	-	7/20/40/40	1/2/2/2
5	MPD	3-A	408	-	-	5/5/5/5	-
5	MPD	2-A	408	-	-	3/5/5/5	-
4	EXW	22-B	406	-	-	8/20/40/40	1/2/2/2
8	2PE	27-A	412	-	-	2/4/4/25	-
4	EXW	9-B	406	-	-	7/20/40/40	0/2/2/2
4	EXW	36-A	407	-	-	12/20/40/40	1/2/2/2
3	PPV	44-B	405	2	-	0/6/6/6	-
5	MPD	45-B	407	-	-	2/5/5/5	-
4	EXW	15-B	406	-	-	8/20/40/40	0/2/2/2
4	EXW	50-B	406	-	-	10/20/40/40	1/2/2/2
4	EXW	23-A	407	-	-	13/20/40/40	1/2/2/2
8	2PE	31-A	412	-	-	3/4/4/25	-
5	MPD	14-A	408	-	-	3/5/5/5	-
5	MPD	17-A	408	-	-	3/5/5/5	-
4	EXW	28-A	407	-	-	10/20/40/40	1/2/2/2
5	MPD	42-B	407	-	-	2/5/5/5	-
3	PPV	18-A	406	2	-	0/6/6/6	-
5	MPD	43-B	407	-	-	4/5/5/5	-
4	EXW	43-B	406	-	-	11/20/40/40	1/2/2/2
5	MPD	33-B	407	-	-	4/5/5/5	-
5	MPD	12-A	408	-	-	3/5/5/5	-
5	MPD	6-B	407	-	-	4/5/5/5	-
8	2PE	27-B	409	-	-	2/4/4/25	-
3	PPV	25-B	405	2	-	0/6/6/6	-
8	2PE	21-B	409	-	-	4/4/4/25	-
3	PPV	8-A	406	2	-	0/6/6/6	-
4	EXW	8-B	406	-	-	7/20/40/40	1/2/2/2
4	EXW	34-A	407	-	-	9/20/40/40	0/2/2/2
5	MPD	6-A	408	-	-	3/5/5/5	-
4	EXW	7-B	406	-	-	15/20/40/40	1/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	34-A	408	-	-	1/5/5/5	-
8	2PE	32-B	409	-	-	3/4/4/25	-
5	MPD	37-A	408	-	-	1/5/5/5	-
8	2PE	46-A	412	-	-	1/4/4/25	-
3	PPV	11-B	405	2	-	0/6/6/6	-
4	EXW	50-A	407	-	-	11/20/40/40	0/2/2/2
5	MPD	13-A	408	-	-	3/5/5/5	-
8	2PE	4-B	409	-	-	0/4/4/25	-
3	PPV	48-B	405	2	-	0/6/6/6	-
3	PPV	42-A	406	2	-	0/6/6/6	-
8	2PE	20-B	409	-	-	2/4/4/25	-
4	EXW	7-A	407	-	-	13/20/40/40	1/2/2/2
5	MPD	7-A	408	-	-	2/5/5/5	-
3	PPV	47-B	405	2	-	0/6/6/6	-
3	PPV	29-B	405	2	-	0/6/6/6	-
4	EXW	22-A	407	-	-	10/20/40/40	1/2/2/2
3	PPV	7-B	405	2	-	0/6/6/6	-
4	EXW	2-A	407	-	-	10/20/40/40	1/2/2/2
8	2PE	37-A	412	-	-	1/4/4/25	-
3	PPV	10-B	405	2	-	0/6/6/6	-
8	2PE	16-A	412	-	-	3/4/4/25	-
3	PPV	30-B	405	2	-	0/6/6/6	-
8	2PE	29-A	412	-	-	4/4/4/25	-
3	PPV	27-B	405	2	-	0/6/6/6	-
3	PPV	33-A	406	2	-	0/6/6/6	-
3	PPV	50-A	406	2	-	0/6/6/6	-
5	MPD	45-A	408	-	-	3/5/5/5	-
5	MPD	20-B	407	-	-	1/5/5/5	-
8	2PE	35-B	409	-	-	2/4/4/25	-
5	MPD	2-B	407	-	-	3/5/5/5	-
3	PPV	16-B	405	2	-	0/6/6/6	-
4	EXW	14-B	406	-	-	11/20/40/40	1/2/2/2
5	MPD	17-B	407	-	-	3/5/5/5	-
4	EXW	35-B	406	-	-	11/20/40/40	1/2/2/2
5	MPD	28-B	407	-	-	4/5/5/5	-
3	PPV	40-B	405	2	-	0/6/6/6	-
4	EXW	30-B	406	-	-	10/20/40/40	1/2/2/2
5	MPD	15-B	407	-	-	4/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	31-A	408	-	-	2/5/5/5	-
5	MPD	44-A	408	-	-	3/5/5/5	-
4	EXW	6-B	406	-	-	12/20/40/40	1/2/2/2
5	MPD	5-B	407	-	-	1/5/5/5	-
5	MPD	48-A	408	-	-	0/5/5/5	-
8	2PE	4-A	412	-	-	3/4/4/25	-
3	PPV	21-B	405	2	-	0/6/6/6	-
4	EXW	9-A	407	-	-	9/20/40/40	1/2/2/2
8	2PE	13-A	412	-	-	1/4/4/25	-
8	2PE	29-B	409	-	-	4/4/4/25	-
8	2PE	22-B	409	-	-	2/4/4/25	-
5	MPD	27-A	408	-	-	2/5/5/5	-
8	2PE	17-B	409	-	-	3/4/4/25	-
3	PPV	47-A	406	2	-	0/6/6/6	-
5	MPD	21-A	408	-	-	0/5/5/5	-
8	2PE	33-B	409	-	-	2/4/4/25	-
8	2PE	43-A	412	-	-	2/4/4/25	-
5	MPD	26-B	407	-	-	4/5/5/5	-
5	MPD	7-B	407	-	-	2/5/5/5	-
3	PPV	4-B	405	2	-	0/6/6/6	-
5	MPD	14-B	407	-	-	3/5/5/5	-
8	2PE	6-A	412	-	-	3/4/4/25	-
3	PPV	10-A	406	2	-	0/6/6/6	-
8	2PE	36-A	412	-	-	4/4/4/25	-
4	EXW	12-B	406	-	-	11/20/40/40	0/2/2/2
8	2PE	39-B	409	-	-	2/4/4/25	-
5	MPD	10-B	407	-	-	2/5/5/5	-
8	2PE	20-A	412	-	-	3/4/4/25	-
4	EXW	10-B	406	-	-	11/20/40/40	1/2/2/2
8	2PE	10-A	412	-	-	1/4/4/25	-
8	2PE	25-A	412	-	-	4/4/4/25	-
3	PPV	5-B	405	2	-	0/6/6/6	-
3	PPV	28-A	406	2	-	0/6/6/6	-
8	2PE	23-A	412	-	-	2/4/4/25	-
8	2PE	50-A	412	-	-	4/4/4/25	-
4	EXW	37-B	406	-	-	9/20/40/40	1/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	2PE	41-A	412	-	-	2/4/4/25	-
3	PPV	13-A	406	2	-	0/6/6/6	-
3	PPV	16-A	406	2	-	0/6/6/6	-
5	MPD	39-B	407	-	-	3/5/5/5	-
8	2PE	32-A	412	-	-	4/4/4/25	-
5	MPD	19-A	408	-	-	2/5/5/5	-
8	2PE	47-B	409	-	-	1/4/4/25	-
4	EXW	45-A	407	-	-	13/20/40/40	1/2/2/2
4	EXW	32-A	407	-	-	12/20/40/40	1/2/2/2
8	2PE	36-B	409	-	-	1/4/4/25	-
3	PPV	2-B	405	2	-	0/6/6/6	-
5	MPD	12-B	407	-	-	1/5/5/5	-
5	MPD	35-A	408	-	-	0/5/5/5	-
3	PPV	21-A	406	2	-	0/6/6/6	-
3	PPV	6-A	406	2	-	0/6/6/6	-
5	MPD	18-B	407	-	-	1/5/5/5	-
3	PPV	28-B	405	2	-	0/6/6/6	-
5	MPD	19-B	407	-	-	2/5/5/5	-
8	2PE	50-B	409	-	-	2/4/4/25	-
5	MPD	24-B	407	-	-	4/5/5/5	-
5	MPD	22-B	407	-	-	1/5/5/5	-
4	EXW	39-A	407	-	-	12/20/40/40	1/2/2/2
3	PPV	49-A	406	2	-	0/6/6/6	-
5	MPD	1-A	408	-	-	3/5/5/5	-
3	PPV	31-B	405	2	-	0/6/6/6	-
8	2PE	5-B	409	-	-	3/4/4/25	-
8	2PE	22-A	412	-	-	2/4/4/25	-
3	PPV	45-B	405	2	-	0/6/6/6	-
5	MPD	16-A	408	-	-	3/5/5/5	-
5	MPD	40-A	408	-	-	2/5/5/5	-
5	MPD	29-A	408	-	-	4/5/5/5	-
5	MPD	3-B	407	-	-	2/5/5/5	-
3	PPV	41-B	405	2	-	0/6/6/6	-
3	PPV	35-A	406	2	-	0/6/6/6	-
4	EXW	15-A	407	-	-	8/20/40/40	1/2/2/2
4	EXW	24-A	407	-	-	10/20/40/40	0/2/2/2
5	MPD	11-A	408	-	-	0/5/5/5	-
4	EXW	38-B	406	-	-	9/20/40/40	1/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	2PE	49-A	412	-	-	2/4/4/25	-
8	2PE	46-B	409	-	-	2/4/4/25	-
3	PPV	19-A	406	2	-	0/6/6/6	-
5	MPD	30-A	408	-	-	3/5/5/5	-
8	2PE	8-B	409	-	-	2/4/4/25	-
8	2PE	9-B	409	-	-	3/4/4/25	-
4	EXW	44-A	407	-	-	12/20/40/40	1/2/2/2
3	PPV	12-A	406	2	-	0/6/6/6	-
5	MPD	46-B	407	-	-	5/5/5/5	-
4	EXW	20-A	407	-	-	11/20/40/40	1/2/2/2
3	PPV	37-A	406	2	-	0/6/6/6	-
3	PPV	13-B	405	2	-	0/6/6/6	-
4	EXW	17-A	407	-	-	9/20/40/40	0/2/2/2
5	MPD	48-B	407	-	-	2/5/5/5	-
4	EXW	8-A	407	-	-	11/20/40/40	1/2/2/2
3	PPV	26-B	405	2	-	0/6/6/6	-
4	EXW	11-B	406	-	-	10/20/40/40	1/2/2/2
3	PPV	43-B	405	2	-	0/6/6/6	-
3	PPV	31-A	406	2	-	0/6/6/6	-
3	PPV	5-A	406	2	-	0/6/6/6	-
4	EXW	5-A	407	-	-	9/20/40/40	1/2/2/2
5	MPD	15-A	408	-	-	2/5/5/5	-
5	MPD	50-A	408	-	-	3/5/5/5	-
3	PPV	23-B	405	2	-	0/6/6/6	-
4	EXW	13-A	407	-	-	14/20/40/40	1/2/2/2
5	MPD	25-A	408	-	-	2/5/5/5	-
4	EXW	17-B	406	-	-	10/20/40/40	1/2/2/2
3	PPV	46-A	406	2	-	0/6/6/6	-
4	EXW	42-A	407	-	-	8/20/40/40	1/2/2/2
3	PPV	3-B	405	2	-	0/6/6/6	-
4	EXW	19-A	407	-	-	10/20/40/40	1/2/2/2
5	MPD	35-B	407	-	-	1/5/5/5	-
4	EXW	14-A	407	-	-	9/20/40/40	1/2/2/2
8	2PE	45-A	412	-	-	4/4/4/25	-
5	MPD	4-A	408	-	-	2/5/5/5	-
8	2PE	35-A	412	-	-	4/4/4/25	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	2PE	16-B	409	-	-	2/4/4/25	-
4	EXW	28-B	406	-	-	8/20/40/40	1/2/2/2
5	MPD	8-A	408	-	-	3/5/5/5	-
5	MPD	36-A	408	-	-	0/5/5/5	-
5	MPD	13-B	407	-	-	1/5/5/5	-
3	PPV	6-B	405	2	-	0/6/6/6	-
4	EXW	13-B	406	-	-	9/20/40/40	1/2/2/2
4	EXW	16-B	406	-	-	14/20/40/40	0/2/2/2
8	2PE	30-B	409	-	-	2/4/4/25	-
4	EXW	40-B	406	-	-	7/20/40/40	1/2/2/2
3	PPV	49-B	405	2	-	0/6/6/6	-
8	2PE	33-A	412	-	-	3/4/4/25	-
3	PPV	29-A	406	2	-	0/6/6/6	-
3	PPV	34-B	405	2	-	0/6/6/6	-
4	EXW	48-B	406	-	-	11/20/40/40	1/2/2/2
5	MPD	32-A	408	-	-	4/5/5/5	-
4	EXW	26-A	407	-	-	13/20/40/40	1/2/2/2
4	EXW	12-A	407	-	-	9/20/40/40	1/2/2/2
5	MPD	23-A	408	-	-	3/5/5/5	-
4	EXW	21-B	406	-	-	12/20/40/40	1/2/2/2
4	EXW	30-A	407	-	-	9/20/40/40	1/2/2/2
8	2PE	15-A	412	-	-	2/4/4/25	-
3	PPV	20-B	405	2	-	0/6/6/6	-
3	PPV	3-A	406	2	-	0/6/6/6	-
3	PPV	17-B	405	2	-	0/6/6/6	-
5	MPD	33-A	408	-	-	2/5/5/5	-
4	EXW	36-B	406	-	-	11/20/40/40	1/2/2/2
4	EXW	48-A	407	-	-	13/20/40/40	1/2/2/2
3	PPV	20-A	406	2	-	0/6/6/6	-
5	MPD	16-B	407	-	-	2/5/5/5	-
8	2PE	41-B	409	-	-	1/4/4/25	-
4	EXW	3-A	407	-	-	15/20/40/40	1/2/2/2
3	PPV	26-A	406	2	-	0/6/6/6	-
8	2PE	25-B	409	-	-	3/4/4/25	-
5	MPD	40-B	407	-	-	1/5/5/5	-
8	2PE	39-A	412	-	-	1/4/4/25	-
5	MPD	47-B	407	-	-	1/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	2PE	7-A	412	-	-	3/4/4/25	-
3	PPV	17-A	406	2	-	0/6/6/6	-
4	EXW	19-B	406	-	-	9/20/40/40	0/2/2/2
3	PPV	38-B	405	2	-	0/6/6/6	-
8	2PE	17-A	412	-	-	3/4/4/25	-
3	PPV	25-A	406	2	-	0/6/6/6	-
3	PPV	36-B	405	2	-	0/6/6/6	-
3	PPV	23-A	406	2	-	0/6/6/6	-
8	2PE	5-A	412	-	-	2/4/4/25	-
8	2PE	12-A	412	-	-	3/4/4/25	-
8	2PE	24-A	412	-	-	3/4/4/25	-
5	MPD	27-B	407	-	-	5/5/5/5	-
3	PPV	48-A	406	2	-	0/6/6/6	-
4	EXW	35-A	407	-	-	15/20/40/40	1/2/2/2
5	MPD	4-B	407	-	-	3/5/5/5	-
4	EXW	4-B	406	-	-	11/20/40/40	1/2/2/2
4	EXW	1-B	406	-	-	8/20/40/40	0/2/2/2
5	MPD	22-A	408	-	-	3/5/5/5	-
8	2PE	19-B	409	-	-	3/4/4/25	-
4	EXW	31-B	406	-	-	12/20/40/40	1/2/2/2
8	2PE	42-A	412	-	-	1/4/4/25	-
8	2PE	48-A	412	-	-	2/4/4/25	-
4	EXW	31-A	407	-	-	12/20/40/40	1/2/2/2
8	2PE	11-A	412	-	-	4/4/4/25	-
4	EXW	49-A	407	-	-	12/20/40/40	1/2/2/2
8	2PE	18-B	409	-	-	3/4/4/25	-
5	MPD	49-A	408	-	-	2/5/5/5	-
8	2PE	14-A	412	-	-	2/4/4/25	-
5	MPD	21-B	407	-	-	3/5/5/5	-
5	MPD	9-B	407	-	-	1/5/5/5	-
4	EXW	41-B	406	-	-	11/20/40/40	0/2/2/2
5	MPD	49-B	407	-	-	4/5/5/5	-
3	PPV	27-A	406	2	-	0/6/6/6	-
8	2PE	24-B	409	-	-	3/4/4/25	-
3	PPV	1-B	405	2	-	0/6/6/6	-
4	EXW	33-A	407	-	-	14/20/40/40	1/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	2PE	30-A	412	-	-	1/4/4/25	-
5	MPD	32-B	407	-	-	2/5/5/5	-
8	2PE	2-B	409	-	-	2/4/4/25	-
4	EXW	32-B	406	-	-	9/20/40/40	1/2/2/2
8	2PE	38-B	409	-	-	4/4/4/25	-
3	PPV	42-B	405	2	-	0/6/6/6	-
5	MPD	37-B	407	-	-	2/5/5/5	-
3	PPV	22-B	405	2	-	0/6/6/6	-
4	EXW	46-B	406	-	-	11/20/40/40	1/2/2/2
3	PPV	33-B	405	2	-	0/6/6/6	-
3	PPV	38-A	406	2	-	0/6/6/6	-
4	EXW	6-A	407	-	-	11/20/40/40	1/2/2/2
8	2PE	42-B	409	-	-	1/4/4/25	-
8	2PE	14-B	409	-	-	1/4/4/25	-
8	2PE	26-A	412	-	-	3/4/4/25	-
3	PPV	40-A	406	2	-	0/6/6/6	-
3	PPV	50-B	405	2	-	0/6/6/6	-
8	2PE	19-A	412	-	-	2/4/4/25	-
4	EXW	26-B	406	-	-	11/20/40/40	1/2/2/2
8	2PE	10-B	409	-	-	2/4/4/25	-
5	MPD	29-B	407	-	-	2/5/5/5	-
4	EXW	47-A	407	-	-	9/20/40/40	0/2/2/2
4	EXW	18-A	407	-	-	11/20/40/40	1/2/2/2
8	2PE	34-B	409	-	-	3/4/4/25	-
5	MPD	39-A	408	-	-	3/5/5/5	-
5	MPD	43-A	408	-	-	1/5/5/5	-
8	2PE	26-B	409	-	-	2/4/4/25	-
8	2PE	3-A	412	-	-	4/4/4/25	-
3	PPV	4-A	406	2	-	0/6/6/6	-
3	PPV	36-A	406	2	-	0/6/6/6	-
5	MPD	31-B	407	-	-	1/5/5/5	-
5	MPD	44-B	407	-	-	2/5/5/5	-
4	EXW	10-A	407	-	-	9/20/40/40	1/2/2/2
4	EXW	44-B	406	-	-	8/20/40/40	1/2/2/2
5	MPD	10-A	408	-	-	2/5/5/5	-
4	EXW	1-A	407	-	-	14/20/40/40	1/2/2/2
5	MPD	18-A	408	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EXW	3-B	406	-	-	9/20/40/40	1/2/2/2
3	PPV	41-A	406	2	-	0/6/6/6	-
4	EXW	47-B	406	-	-	10/20/40/40	1/2/2/2
5	MPD	24-A	408	-	-	0/5/5/5	-
3	PPV	11-A	406	2	-	0/6/6/6	-
3	PPV	15-B	405	2	-	0/6/6/6	-
4	EXW	40-A	407	-	-	13/20/40/40	1/2/2/2
4	EXW	20-B	406	-	-	11/20/40/40	1/2/2/2
3	PPV	32-A	406	2	-	0/6/6/6	-
8	2PE	37-B	409	-	-	3/4/4/25	-
3	PPV	2-A	406	2	-	0/6/6/6	-
5	MPD	5-A	408	-	-	2/5/5/5	-
8	2PE	3-B	409	-	-	0/4/4/25	-
5	MPD	47-A	408	-	-	0/5/5/5	-
8	2PE	28-A	412	-	-	2/4/4/25	-
8	2PE	11-B	409	-	-	0/4/4/25	-
4	EXW	25-B	406	-	-	12/20/40/40	1/2/2/2
3	PPV	45-A	406	2	-	0/6/6/6	-
5	MPD	20-A	408	-	-	1/5/5/5	-
4	EXW	49-B	406	-	-	9/20/40/40	1/2/2/2
4	EXW	27-A	407	-	-	13/20/40/40	1/2/2/2
5	MPD	23-B	407	-	-	1/5/5/5	-
3	PPV	1-A	406	2	-	0/6/6/6	-
4	EXW	23-B	406	-	-	10/20/40/40	1/2/2/2
4	EXW	21-A	407	-	-	10/20/40/40	1/2/2/2
8	2PE	31-B	409	-	-	2/4/4/25	-
5	MPD	11-B	407	-	-	2/5/5/5	-
3	PPV	14-B	405	2	-	0/6/6/6	-
3	PPV	35-B	405	2	-	0/6/6/6	-
8	2PE	49-B	409	-	-	3/4/4/25	-
8	2PE	12-B	409	-	-	2/4/4/25	-
4	EXW	29-B	406	-	-	9/20/40/40	1/2/2/2
3	PPV	24-A	406	2	-	0/6/6/6	-
5	MPD	41-A	408	-	-	1/5/5/5	-
5	MPD	28-A	408	-	-	0/5/5/5	-
8	2PE	28-B	409	-	-	2/4/4/25	-
3	PPV	9-A	406	2	-	0/6/6/6	-
4	EXW	38-A	407	-	-	12/20/40/40	1/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	25-B	407	-	-	3/5/5/5	-
5	MPD	38-A	408	-	-	1/5/5/5	-
8	2PE	23-B	409	-	-	3/4/4/25	-
8	2PE	45-B	409	-	-	1/4/4/25	-
3	PPV	15-A	406	2	-	0/6/6/6	-
4	EXW	27-B	406	-	-	8/20/40/40	1/2/2/2
5	MPD	1-B	407	-	-	5/5/5/5	-
8	2PE	43-B	409	-	-	3/4/4/25	-
8	2PE	48-B	409	-	-	1/4/4/25	-
3	PPV	34-A	406	2	-	0/6/6/6	-
5	MPD	38-B	407	-	-	4/5/5/5	-
5	MPD	34-B	407	-	-	3/5/5/5	-
4	EXW	39-B	406	-	-	12/20/40/40	0/2/2/2
4	EXW	34-B	406	-	-	14/20/40/40	1/2/2/2
3	PPV	43-A	406	2	-	0/6/6/6	-
3	PPV	44-A	406	2	-	0/6/6/6	-
3	PPV	19-B	405	2	-	0/6/6/6	-
3	PPV	24-B	405	2	-	0/6/6/6	-
8	2PE	6-B	409	-	-	2/4/4/25	-
8	2PE	44-A	412	-	-	3/4/4/25	-
3	PPV	7-A	406	2	-	0/6/6/6	-
8	2PE	47-A	412	-	-	2/4/4/25	-
4	EXW	18-B	406	-	-	9/20/40/40	0/2/2/2
4	EXW	37-A	407	-	-	14/20/40/40	1/2/2/2
5	MPD	30-B	407	-	-	2/5/5/5	-
8	2PE	18-A	412	-	-	3/4/4/25	-
4	EXW	16-A	407	-	-	12/20/40/40	1/2/2/2
4	EXW	24-B	406	-	-	9/20/40/40	1/2/2/2
3	PPV	39-B	405	2	-	0/6/6/6	-
8	2PE	15-B	409	-	-	2/4/4/25	-
5	MPD	41-B	407	-	-	3/5/5/5	-
4	EXW	2-B	406	-	-	13/20/40/40	0/2/2/2
4	EXW	11-A	407	-	-	10/20/40/40	1/2/2/2
5	MPD	42-A	408	-	-	1/5/5/5	-
4	EXW	5-B	406	-	-	9/20/40/40	1/2/2/2
5	MPD	26-A	408	-	-	1/5/5/5	-
3	PPV	18-B	405	2	-	0/6/6/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	2PE	1-A	412	-	-	2/4/4/25	-
4	EXW	41-A	407	-	-	13/20/40/40	1/2/2/2

The worst 5 of 978 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	44-A	407	EXW	CAM-CAK	20.31	1.57	1.32
4	41-A	407	EXW	CAM-CAK	20.00	1.57	1.32
4	16-A	407	EXW	CAM-CAK	19.49	1.56	1.32
4	37-A	407	EXW	CAM-CAK	19.08	1.55	1.32
4	29-B	406	EXW	CAM-CAK	19.07	1.55	1.32

The worst 5 of 1657 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	44-A	407	EXW	CAN-CAM-CAO	-12.22	89.01	115.33
4	46-A	407	EXW	CAA-CAB-CAC	12.20	144.47	114.43
4	45-A	407	EXW	CAT-CAH-CAU	-11.85	92.87	121.38
4	47-B	406	EXW	CAS-CAR-CAQ	-11.41	94.42	123.68
4	30-A	407	EXW	CAA-CAB-CAC	11.32	142.31	114.43

There are no chirality outliers.

5 of 1524 torsion outliers are listed below:

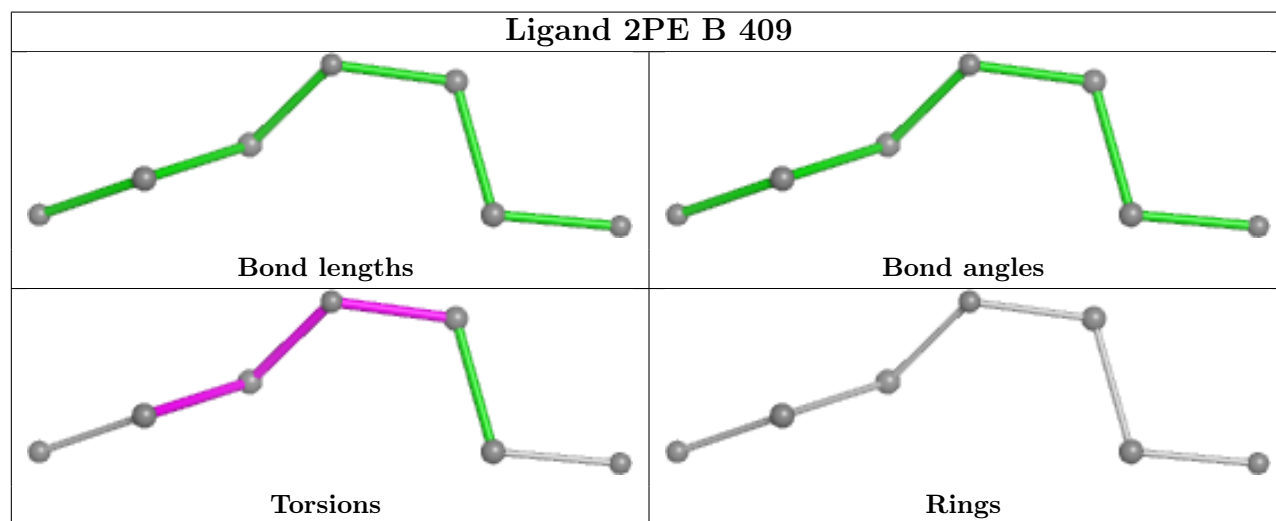
Mol	Chain	Res	Type	Atoms
4	1-A	407	EXW	CAA-CAB-CAC-CAG
4	1-A	407	EXW	CAC-CAD-CAJ-CAK
4	1-A	407	EXW	CAE-CAD-CAJ-CAK
4	1-A	407	EXW	CAI-CAD-CAJ-CAK
4	1-A	407	EXW	CAD-CAJ-CAK-CAM

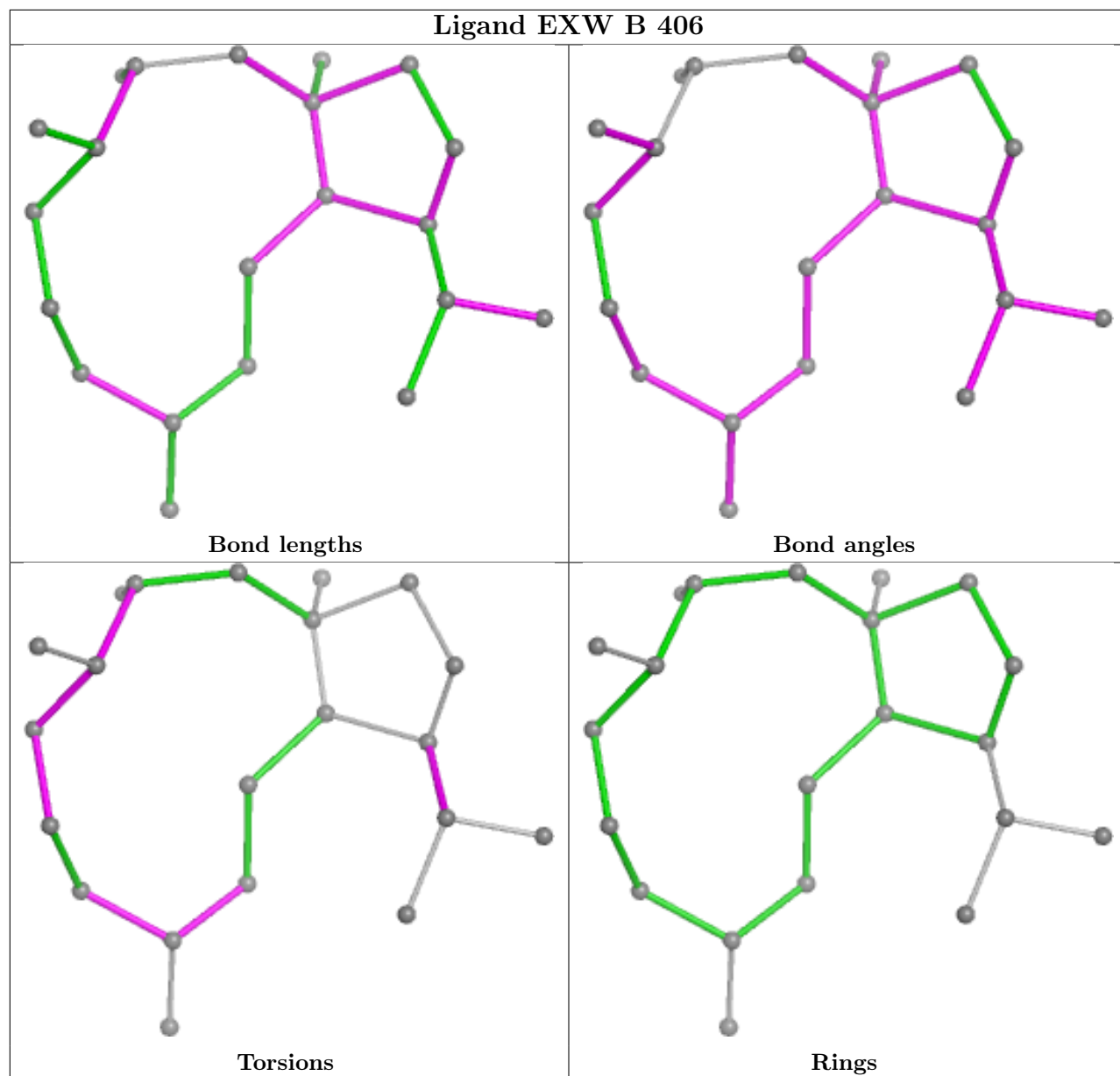
5 of 84 ring outliers are listed below:

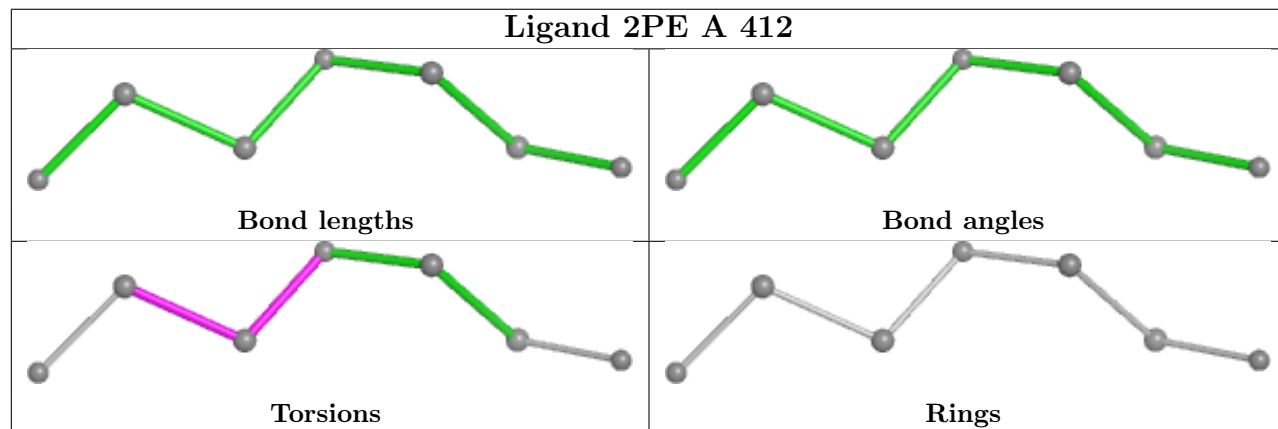
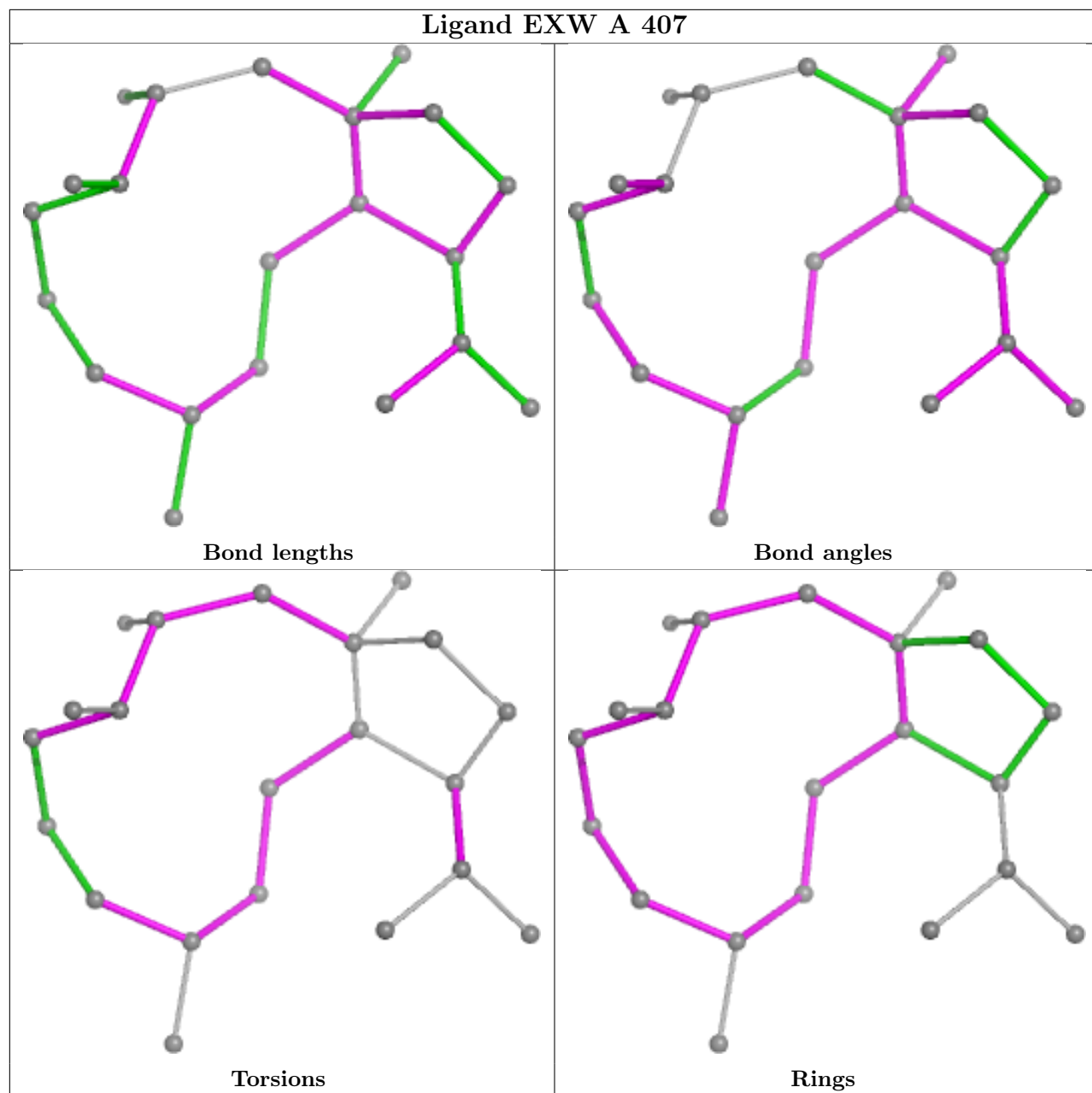
Mol	Chain	Res	Type	Atoms
4	21-A	407	EXW	CAA-CAB-CAC-CAD-CAJ-CAK-CAM-CAO-CAP-CAQ-CAR
4	37-B	406	EXW	CAA-CAB-CAC-CAD-CAJ-CAK-CAM-CAO-CAP-CAQ-CAR
4	27-B	406	EXW	CAA-CAB-CAC-CAD-CAJ-CAK-CAM-CAO-CAP-CAQ-CAR
4	48-B	406	EXW	CAA-CAB-CAC-CAD-CAJ-CAK-CAM-CAO-CAP-CAQ-CAR
4	14-B	406	EXW	CAA-CAB-CAC-CAD-CAJ-CAK-CAM-CAO-CAP-CAQ-CAR

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	294/318 (92%)	1.44	68 (23%) 2 2	0, 0, 1, 1	294 (100%)
1	1-B	300/318 (94%)	1.74	96 (32%) 1 1	0, 1, 1, 1	300 (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 ²)	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 ²)	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	594/31800 (1%)	1.59	164 (27%) 2 1	0, 0, 1, 1	594 (100%)

The worst 5 of 164 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	297	THR	10.4
1	1-A	297	THR	9.9
1	1-A	49	ALA	8.3
1	1-B	10	ALA	8.3
1	1-B	298	ALA	8.2

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	K	1-A	413	1/1	0.50	0.66	22,22,22,22	1
2	MG	2-A	401	1/1	-	-	22,22,22,22	1
2	MG	3-A	401	1/1	-	-	22,22,22,22	1
2	MG	4-A	401	1/1	-	-	22,22,22,22	1
2	MG	5-A	401	1/1	-	-	22,22,22,22	1
2	MG	6-A	401	1/1	-	-	22,22,22,22	1
2	MG	7-A	401	1/1	-	-	22,22,22,22	1
2	MG	8-A	401	1/1	-	-	22,22,22,22	1
2	MG	9-A	401	1/1	-	-	22,22,22,22	1
2	MG	10-A	401	1/1	-	-	22,22,22,22	1
2	MG	11-A	401	1/1	-	-	22,22,22,22	1
2	MG	12-A	401	1/1	-	-	22,22,22,22	1
2	MG	13-A	401	1/1	-	-	22,22,22,22	1
2	MG	14-A	401	1/1	-	-	22,22,22,22	1
2	MG	15-A	401	1/1	-	-	22,22,22,22	1
2	MG	16-A	401	1/1	-	-	22,22,22,22	1
2	MG	17-A	401	1/1	-	-	22,22,22,22	1
2	MG	18-A	401	1/1	-	-	22,22,22,22	1
2	MG	19-A	401	1/1	-	-	22,22,22,22	1
2	MG	20-A	401	1/1	-	-	22,22,22,22	1
2	MG	21-A	401	1/1	-	-	22,22,22,22	1
2	MG	22-A	401	1/1	-	-	22,22,22,22	1
2	MG	23-A	401	1/1	-	-	22,22,22,22	1
2	MG	24-A	401	1/1	-	-	22,22,22,22	1
2	MG	25-A	401	1/1	-	-	22,22,22,22	1
2	MG	26-A	401	1/1	-	-	22,22,22,22	1
2	MG	27-A	401	1/1	-	-	22,22,22,22	1
2	MG	28-A	401	1/1	-	-	22,22,22,22	1
2	MG	29-A	401	1/1	-	-	22,22,22,22	1
2	MG	30-A	401	1/1	-	-	22,22,22,22	1
2	MG	31-A	401	1/1	-	-	22,22,22,22	1
2	MG	32-A	401	1/1	-	-	22,22,22,22	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	33-A	401	1/1	-	-	22,22,22,22	1
2	MG	34-A	401	1/1	-	-	22,22,22,22	1
2	MG	35-A	401	1/1	-	-	22,22,22,22	1
2	MG	36-A	401	1/1	-	-	22,22,22,22	1
2	MG	37-A	401	1/1	-	-	22,22,22,22	1
2	MG	38-A	401	1/1	-	-	22,22,22,22	1
2	MG	39-A	401	1/1	-	-	22,22,22,22	1
2	MG	40-A	401	1/1	-	-	22,22,22,22	1
2	MG	41-A	401	1/1	-	-	22,22,22,22	1
2	MG	42-A	401	1/1	-	-	22,22,22,22	1
2	MG	43-A	401	1/1	-	-	22,22,22,22	1
2	MG	44-A	401	1/1	-	-	22,22,22,22	1
2	MG	45-A	401	1/1	-	-	22,22,22,22	1
2	MG	46-A	401	1/1	-	-	22,22,22,22	1
2	MG	47-A	401	1/1	-	-	22,22,22,22	1
2	MG	48-A	401	1/1	-	-	22,22,22,22	1
2	MG	49-A	401	1/1	-	-	22,22,22,22	1
2	MG	50-A	401	1/1	-	-	22,22,22,22	1
4	EXW	1-A	407	21/21	0.52	0.28	21,21,22,22	21
2	MG	2-A	402	1/1	-	-	22,22,22,22	1
2	MG	3-A	402	1/1	-	-	22,22,22,22	1
2	MG	4-A	402	1/1	-	-	22,22,22,22	1
2	MG	5-A	402	1/1	-	-	22,22,22,22	1
2	MG	6-A	402	1/1	-	-	22,22,22,22	1
2	MG	7-A	402	1/1	-	-	22,22,22,22	1
2	MG	8-A	402	1/1	-	-	22,22,22,22	1
2	MG	9-A	402	1/1	-	-	22,22,22,22	1
2	MG	10-A	402	1/1	-	-	22,22,22,22	1
2	MG	11-A	402	1/1	-	-	22,22,22,22	1
2	MG	12-A	402	1/1	-	-	22,22,22,22	1
2	MG	13-A	402	1/1	-	-	22,22,22,22	1
2	MG	14-A	402	1/1	-	-	22,22,22,22	1
2	MG	15-A	402	1/1	-	-	22,22,22,22	1
2	MG	16-A	402	1/1	-	-	22,22,22,22	1
2	MG	17-A	402	1/1	-	-	22,22,22,22	1
2	MG	18-A	402	1/1	-	-	22,22,22,22	1
2	MG	19-A	402	1/1	-	-	22,22,22,22	1
2	MG	20-A	402	1/1	-	-	22,22,22,22	1
2	MG	21-A	402	1/1	-	-	22,22,22,22	1
2	MG	22-A	402	1/1	-	-	22,22,22,22	1
2	MG	23-A	402	1/1	-	-	22,22,22,22	1
2	MG	24-A	402	1/1	-	-	22,22,22,22	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	25-A	402	1/1	-	-	22,22,22,22	1
2	MG	26-A	402	1/1	-	-	22,22,22,22	1
2	MG	27-A	402	1/1	-	-	22,22,22,22	1
2	MG	28-A	402	1/1	-	-	22,22,22,22	1
2	MG	29-A	402	1/1	-	-	22,22,22,22	1
2	MG	30-A	402	1/1	-	-	22,22,22,22	1
2	MG	31-A	402	1/1	-	-	22,22,22,22	1
2	MG	32-A	402	1/1	-	-	22,22,22,22	1
2	MG	33-A	402	1/1	-	-	22,22,22,22	1
2	MG	34-A	402	1/1	-	-	22,22,22,22	1
2	MG	35-A	402	1/1	-	-	22,22,22,22	1
2	MG	36-A	402	1/1	-	-	22,22,22,22	1
2	MG	37-A	402	1/1	-	-	22,22,22,22	1
2	MG	38-A	402	1/1	-	-	22,22,22,22	1
2	MG	39-A	402	1/1	-	-	22,22,22,22	1
2	MG	40-A	402	1/1	-	-	22,22,22,22	1
2	MG	41-A	402	1/1	-	-	22,22,22,22	1
2	MG	42-A	402	1/1	-	-	22,22,22,22	1
2	MG	43-A	402	1/1	-	-	22,22,22,22	1
2	MG	44-A	402	1/1	-	-	22,22,22,22	1
2	MG	45-A	402	1/1	-	-	22,22,22,22	1
2	MG	46-A	402	1/1	-	-	22,22,22,22	1
2	MG	47-A	402	1/1	-	-	22,22,22,22	1
2	MG	48-A	402	1/1	-	-	22,22,22,22	1
2	MG	49-A	402	1/1	-	-	22,22,22,22	1
2	MG	50-A	402	1/1	-	-	22,22,22,22	1
4	EXW	1-B	406	21/21	0.56	0.26	21,22,23,23	21
2	MG	2-A	403	1/1	-	-	22,22,22,22	1
2	MG	3-A	403	1/1	-	-	22,22,22,22	1
2	MG	4-A	403	1/1	-	-	22,22,22,22	1
2	MG	5-A	403	1/1	-	-	22,22,22,22	1
2	MG	6-A	403	1/1	-	-	22,22,22,22	1
2	MG	7-A	403	1/1	-	-	22,22,22,22	1
2	MG	8-A	403	1/1	-	-	22,22,22,22	1
2	MG	9-A	403	1/1	-	-	22,22,22,22	1
2	MG	10-A	403	1/1	-	-	22,22,22,22	1
2	MG	11-A	403	1/1	-	-	22,22,22,22	1
2	MG	12-A	403	1/1	-	-	22,22,22,22	1
2	MG	13-A	403	1/1	-	-	22,22,22,22	1
2	MG	14-A	403	1/1	-	-	22,22,22,22	1
2	MG	15-A	403	1/1	-	-	22,22,22,22	1
2	MG	16-A	403	1/1	-	-	22,22,22,22	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	17-A	403	1/1	-	-	22,22,22,22	1
2	MG	18-A	403	1/1	-	-	22,22,22,22	1
2	MG	19-A	403	1/1	-	-	22,22,22,22	1
2	MG	20-A	403	1/1	-	-	22,22,22,22	1
2	MG	21-A	403	1/1	-	-	22,22,22,22	1
2	MG	22-A	403	1/1	-	-	22,22,22,22	1
2	MG	23-A	403	1/1	-	-	22,22,22,22	1
2	MG	24-A	403	1/1	-	-	22,22,22,22	1
2	MG	25-A	403	1/1	-	-	22,22,22,22	1
2	MG	26-A	403	1/1	-	-	22,22,22,22	1
2	MG	27-A	403	1/1	-	-	22,22,22,22	1
2	MG	28-A	403	1/1	-	-	22,22,22,22	1
2	MG	29-A	403	1/1	-	-	22,22,22,22	1
2	MG	30-A	403	1/1	-	-	22,22,22,22	1
2	MG	31-A	403	1/1	-	-	22,22,22,22	1
2	MG	32-A	403	1/1	-	-	22,22,22,22	1
2	MG	33-A	403	1/1	-	-	22,22,22,22	1
2	MG	34-A	403	1/1	-	-	22,22,22,22	1
2	MG	35-A	403	1/1	-	-	22,22,22,22	1
2	MG	36-A	403	1/1	-	-	22,22,22,22	1
2	MG	37-A	403	1/1	-	-	22,22,22,22	1
2	MG	38-A	403	1/1	-	-	22,22,22,22	1
2	MG	39-A	403	1/1	-	-	22,22,22,22	1
2	MG	40-A	403	1/1	-	-	22,22,22,22	1
2	MG	41-A	403	1/1	-	-	22,22,22,22	1
2	MG	42-A	403	1/1	-	-	22,22,22,22	1
2	MG	43-A	403	1/1	-	-	22,22,22,22	1
2	MG	44-A	403	1/1	-	-	22,22,22,22	1
2	MG	45-A	403	1/1	-	-	22,22,22,22	1
2	MG	46-A	403	1/1	-	-	22,22,22,22	1
2	MG	47-A	403	1/1	-	-	22,22,22,22	1
2	MG	48-A	403	1/1	-	-	22,22,22,22	1
2	MG	49-A	403	1/1	-	-	22,22,22,22	1
2	MG	50-A	403	1/1	-	-	22,22,22,22	1
2	MG	1-B	404	1/1	0.57	0.22	28,28,28,28	1
2	MG	2-A	404	1/1	-	-	27,27,27,27	1
2	MG	3-A	404	1/1	-	-	27,27,27,27	1
2	MG	4-A	404	1/1	-	-	27,27,27,27	1
2	MG	5-A	404	1/1	-	-	27,27,27,27	1
2	MG	6-A	404	1/1	-	-	27,27,27,27	1
2	MG	7-A	404	1/1	-	-	27,27,27,27	1
2	MG	8-A	404	1/1	-	-	27,27,27,27	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	9-A	404	1/1	-	-	27,27,27,27	1
2	MG	10-A	404	1/1	-	-	27,27,27,27	1
2	MG	11-A	404	1/1	-	-	27,27,27,27	1
2	MG	12-A	404	1/1	-	-	27,27,27,27	1
2	MG	13-A	404	1/1	-	-	27,27,27,27	1
2	MG	14-A	404	1/1	-	-	27,27,27,27	1
2	MG	15-A	404	1/1	-	-	27,27,27,27	1
2	MG	16-A	404	1/1	-	-	27,27,27,27	1
2	MG	17-A	404	1/1	-	-	27,27,27,27	1
2	MG	18-A	404	1/1	-	-	27,27,27,27	1
2	MG	19-A	404	1/1	-	-	27,27,27,27	1
2	MG	20-A	404	1/1	-	-	27,27,27,27	1
2	MG	21-A	404	1/1	-	-	27,27,27,27	1
2	MG	22-A	404	1/1	-	-	27,27,27,27	1
2	MG	23-A	404	1/1	-	-	27,27,27,27	1
2	MG	24-A	404	1/1	-	-	27,27,27,27	1
2	MG	25-A	404	1/1	-	-	27,27,27,27	1
2	MG	26-A	404	1/1	-	-	27,27,27,27	1
2	MG	27-A	404	1/1	-	-	27,27,27,27	1
2	MG	28-A	404	1/1	-	-	27,27,27,27	1
2	MG	29-A	404	1/1	-	-	27,27,27,27	1
2	MG	30-A	404	1/1	-	-	27,27,27,27	1
2	MG	31-A	404	1/1	-	-	27,27,27,27	1
2	MG	32-A	404	1/1	-	-	27,27,27,27	1
2	MG	33-A	404	1/1	-	-	27,27,27,27	1
2	MG	34-A	404	1/1	-	-	27,27,27,27	1
2	MG	35-A	404	1/1	-	-	27,27,27,27	1
2	MG	36-A	404	1/1	-	-	27,27,27,27	1
2	MG	37-A	404	1/1	-	-	27,27,27,27	1
2	MG	38-A	404	1/1	-	-	27,27,27,27	1
2	MG	39-A	404	1/1	-	-	27,27,27,27	1
2	MG	40-A	404	1/1	-	-	27,27,27,27	1
2	MG	41-A	404	1/1	-	-	27,27,27,27	1
2	MG	42-A	404	1/1	-	-	27,27,27,27	1
2	MG	43-A	404	1/1	-	-	27,27,27,27	1
2	MG	44-A	404	1/1	-	-	27,27,27,27	1
2	MG	45-A	404	1/1	-	-	27,27,27,27	1
2	MG	46-A	404	1/1	-	-	27,27,27,27	1
2	MG	47-A	404	1/1	-	-	27,27,27,27	1
2	MG	48-A	404	1/1	-	-	27,27,27,27	1
2	MG	49-A	404	1/1	-	-	27,27,27,27	1
2	MG	50-A	404	1/1	-	-	27,27,27,27	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MPD	1-A	408	8/8	0.58	0.23	20,20,20,20	8
2	MG	2-A	405	1/1	-	-	29,29,29,29	1
2	MG	3-A	405	1/1	-	-	29,29,29,29	1
2	MG	4-A	405	1/1	-	-	29,29,29,29	1
2	MG	5-A	405	1/1	-	-	29,29,29,29	1
2	MG	6-A	405	1/1	-	-	29,29,29,29	1
2	MG	7-A	405	1/1	-	-	29,29,29,29	1
2	MG	8-A	405	1/1	-	-	29,29,29,29	1
2	MG	9-A	405	1/1	-	-	29,29,29,29	1
2	MG	10-A	405	1/1	-	-	29,29,29,29	1
2	MG	11-A	405	1/1	-	-	29,29,29,29	1
2	MG	12-A	405	1/1	-	-	29,29,29,29	1
2	MG	13-A	405	1/1	-	-	29,29,29,29	1
2	MG	14-A	405	1/1	-	-	29,29,29,29	1
2	MG	15-A	405	1/1	-	-	29,29,29,29	1
2	MG	16-A	405	1/1	-	-	29,29,29,29	1
2	MG	17-A	405	1/1	-	-	29,29,29,29	1
2	MG	18-A	405	1/1	-	-	29,29,29,29	1
2	MG	19-A	405	1/1	-	-	29,29,29,29	1
2	MG	20-A	405	1/1	-	-	29,29,29,29	1
2	MG	21-A	405	1/1	-	-	29,29,29,29	1
2	MG	22-A	405	1/1	-	-	29,29,29,29	1
2	MG	23-A	405	1/1	-	-	29,29,29,29	1
2	MG	24-A	405	1/1	-	-	29,29,29,29	1
2	MG	25-A	405	1/1	-	-	29,29,29,29	1
2	MG	26-A	405	1/1	-	-	29,29,29,29	1
2	MG	27-A	405	1/1	-	-	29,29,29,29	1
2	MG	28-A	405	1/1	-	-	29,29,29,29	1
2	MG	29-A	405	1/1	-	-	29,29,29,29	1
2	MG	30-A	405	1/1	-	-	29,29,29,29	1
2	MG	31-A	405	1/1	-	-	29,29,29,29	1
2	MG	32-A	405	1/1	-	-	29,29,29,29	1
2	MG	33-A	405	1/1	-	-	29,29,29,29	1
2	MG	34-A	405	1/1	-	-	29,29,29,29	1
2	MG	35-A	405	1/1	-	-	29,29,29,29	1
2	MG	36-A	405	1/1	-	-	29,29,29,29	1
2	MG	37-A	405	1/1	-	-	29,29,29,29	1
2	MG	38-A	405	1/1	-	-	29,29,29,29	1
2	MG	39-A	405	1/1	-	-	29,29,29,29	1
2	MG	40-A	405	1/1	-	-	29,29,29,29	1
2	MG	41-A	405	1/1	-	-	29,29,29,29	1
2	MG	42-A	405	1/1	-	-	29,29,29,29	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	43-A	405	1/1	-	-	29,29,29,29	1
2	MG	44-A	405	1/1	-	-	29,29,29,29	1
2	MG	45-A	405	1/1	-	-	29,29,29,29	1
2	MG	46-A	405	1/1	-	-	29,29,29,29	1
2	MG	47-A	405	1/1	-	-	29,29,29,29	1
2	MG	48-A	405	1/1	-	-	29,29,29,29	1
2	MG	49-A	405	1/1	-	-	29,29,29,29	1
2	MG	50-A	405	1/1	-	-	29,29,29,29	1
8	2PE	1-B	409	7/28	0.59	0.23	24,25,26,27	7
2	MG	2-B	401	1/1	-	-	23,23,23,23	1
2	MG	3-B	401	1/1	-	-	23,23,23,23	1
2	MG	4-B	401	1/1	-	-	23,23,23,23	1
2	MG	5-B	401	1/1	-	-	23,23,23,23	1
2	MG	6-B	401	1/1	-	-	23,23,23,23	1
2	MG	7-B	401	1/1	-	-	23,23,23,23	1
2	MG	8-B	401	1/1	-	-	23,23,23,23	1
2	MG	9-B	401	1/1	-	-	23,23,23,23	1
2	MG	10-B	401	1/1	-	-	23,23,23,23	1
2	MG	11-B	401	1/1	-	-	23,23,23,23	1
2	MG	12-B	401	1/1	-	-	23,23,23,23	1
2	MG	13-B	401	1/1	-	-	23,23,23,23	1
2	MG	14-B	401	1/1	-	-	23,23,23,23	1
2	MG	15-B	401	1/1	-	-	23,23,23,23	1
2	MG	16-B	401	1/1	-	-	23,23,23,23	1
2	MG	17-B	401	1/1	-	-	23,23,23,23	1
2	MG	18-B	401	1/1	-	-	23,23,23,23	1
2	MG	19-B	401	1/1	-	-	23,23,23,23	1
2	MG	20-B	401	1/1	-	-	23,23,23,23	1
2	MG	21-B	401	1/1	-	-	23,23,23,23	1
2	MG	22-B	401	1/1	-	-	23,23,23,23	1
2	MG	23-B	401	1/1	-	-	23,23,23,23	1
2	MG	24-B	401	1/1	-	-	23,23,23,23	1
2	MG	25-B	401	1/1	-	-	23,23,23,23	1
2	MG	26-B	401	1/1	-	-	23,23,23,23	1
2	MG	27-B	401	1/1	-	-	23,23,23,23	1
2	MG	28-B	401	1/1	-	-	23,23,23,23	1
2	MG	29-B	401	1/1	-	-	23,23,23,23	1
2	MG	30-B	401	1/1	-	-	23,23,23,23	1
2	MG	31-B	401	1/1	-	-	23,23,23,23	1
2	MG	32-B	401	1/1	-	-	23,23,23,23	1
2	MG	33-B	401	1/1	-	-	23,23,23,23	1
2	MG	34-B	401	1/1	-	-	23,23,23,23	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	35-B	401	1/1	-	-	23,23,23,23	1
2	MG	36-B	401	1/1	-	-	23,23,23,23	1
2	MG	37-B	401	1/1	-	-	23,23,23,23	1
2	MG	38-B	401	1/1	-	-	23,23,23,23	1
2	MG	39-B	401	1/1	-	-	23,23,23,23	1
2	MG	40-B	401	1/1	-	-	23,23,23,23	1
2	MG	41-B	401	1/1	-	-	23,23,23,23	1
2	MG	42-B	401	1/1	-	-	23,23,23,23	1
2	MG	43-B	401	1/1	-	-	23,23,23,23	1
2	MG	44-B	401	1/1	-	-	23,23,23,23	1
2	MG	45-B	401	1/1	-	-	23,23,23,23	1
2	MG	46-B	401	1/1	-	-	23,23,23,23	1
2	MG	47-B	401	1/1	-	-	23,23,23,23	1
2	MG	48-B	401	1/1	-	-	23,23,23,23	1
2	MG	49-B	401	1/1	-	-	23,23,23,23	1
2	MG	50-B	401	1/1	-	-	23,23,23,23	1
2	MG	1-A	404	1/1	0.59	0.32	27,27,27,27	1
2	MG	2-B	402	1/1	-	-	22,22,22,22	1
2	MG	3-B	402	1/1	-	-	22,22,22,22	1
2	MG	4-B	402	1/1	-	-	22,22,22,22	1
2	MG	5-B	402	1/1	-	-	22,22,22,22	1
2	MG	6-B	402	1/1	-	-	22,22,22,22	1
2	MG	7-B	402	1/1	-	-	22,22,22,22	1
2	MG	8-B	402	1/1	-	-	22,22,22,22	1
2	MG	9-B	402	1/1	-	-	22,22,22,22	1
2	MG	10-B	402	1/1	-	-	22,22,22,22	1
2	MG	11-B	402	1/1	-	-	22,22,22,22	1
2	MG	12-B	402	1/1	-	-	22,22,22,22	1
2	MG	13-B	402	1/1	-	-	22,22,22,22	1
2	MG	14-B	402	1/1	-	-	22,22,22,22	1
2	MG	15-B	402	1/1	-	-	22,22,22,22	1
2	MG	16-B	402	1/1	-	-	22,22,22,22	1
2	MG	17-B	402	1/1	-	-	22,22,22,22	1
2	MG	18-B	402	1/1	-	-	22,22,22,22	1
2	MG	19-B	402	1/1	-	-	22,22,22,22	1
2	MG	20-B	402	1/1	-	-	22,22,22,22	1
2	MG	21-B	402	1/1	-	-	22,22,22,22	1
2	MG	22-B	402	1/1	-	-	22,22,22,22	1
2	MG	23-B	402	1/1	-	-	22,22,22,22	1
2	MG	24-B	402	1/1	-	-	22,22,22,22	1
2	MG	25-B	402	1/1	-	-	22,22,22,22	1
2	MG	26-B	402	1/1	-	-	22,22,22,22	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	27-B	402	1/1	-	-	22,22,22,22	1
2	MG	28-B	402	1/1	-	-	22,22,22,22	1
2	MG	29-B	402	1/1	-	-	22,22,22,22	1
2	MG	30-B	402	1/1	-	-	22,22,22,22	1
2	MG	31-B	402	1/1	-	-	22,22,22,22	1
2	MG	32-B	402	1/1	-	-	22,22,22,22	1
2	MG	33-B	402	1/1	-	-	22,22,22,22	1
2	MG	34-B	402	1/1	-	-	22,22,22,22	1
2	MG	35-B	402	1/1	-	-	22,22,22,22	1
2	MG	36-B	402	1/1	-	-	22,22,22,22	1
2	MG	37-B	402	1/1	-	-	22,22,22,22	1
2	MG	38-B	402	1/1	-	-	22,22,22,22	1
2	MG	39-B	402	1/1	-	-	22,22,22,22	1
2	MG	40-B	402	1/1	-	-	22,22,22,22	1
2	MG	41-B	402	1/1	-	-	22,22,22,22	1
2	MG	42-B	402	1/1	-	-	22,22,22,22	1
2	MG	43-B	402	1/1	-	-	22,22,22,22	1
2	MG	44-B	402	1/1	-	-	22,22,22,22	1
2	MG	45-B	402	1/1	-	-	22,22,22,22	1
2	MG	46-B	402	1/1	-	-	22,22,22,22	1
2	MG	47-B	402	1/1	-	-	22,22,22,22	1
2	MG	48-B	402	1/1	-	-	22,22,22,22	1
2	MG	49-B	402	1/1	-	-	22,22,22,22	1
2	MG	50-B	402	1/1	-	-	22,22,22,22	1
9	K	1-B	410	1/1	0.60	0.42	22,22,22,22	1
2	MG	2-B	403	1/1	-	-	23,23,23,23	1
2	MG	3-B	403	1/1	-	-	23,23,23,23	1
2	MG	4-B	403	1/1	-	-	23,23,23,23	1
2	MG	5-B	403	1/1	-	-	23,23,23,23	1
2	MG	6-B	403	1/1	-	-	23,23,23,23	1
2	MG	7-B	403	1/1	-	-	23,23,23,23	1
2	MG	8-B	403	1/1	-	-	23,23,23,23	1
2	MG	9-B	403	1/1	-	-	23,23,23,23	1
2	MG	10-B	403	1/1	-	-	23,23,23,23	1
2	MG	11-B	403	1/1	-	-	23,23,23,23	1
2	MG	12-B	403	1/1	-	-	23,23,23,23	1
2	MG	13-B	403	1/1	-	-	23,23,23,23	1
2	MG	14-B	403	1/1	-	-	23,23,23,23	1
2	MG	15-B	403	1/1	-	-	23,23,23,23	1
2	MG	16-B	403	1/1	-	-	23,23,23,23	1
2	MG	17-B	403	1/1	-	-	23,23,23,23	1
2	MG	18-B	403	1/1	-	-	23,23,23,23	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	19-B	403	1/1	-	-	23,23,23,23	1
2	MG	20-B	403	1/1	-	-	23,23,23,23	1
2	MG	21-B	403	1/1	-	-	23,23,23,23	1
2	MG	22-B	403	1/1	-	-	23,23,23,23	1
2	MG	23-B	403	1/1	-	-	23,23,23,23	1
2	MG	24-B	403	1/1	-	-	23,23,23,23	1
2	MG	25-B	403	1/1	-	-	23,23,23,23	1
2	MG	26-B	403	1/1	-	-	23,23,23,23	1
2	MG	27-B	403	1/1	-	-	23,23,23,23	1
2	MG	28-B	403	1/1	-	-	23,23,23,23	1
2	MG	29-B	403	1/1	-	-	23,23,23,23	1
2	MG	30-B	403	1/1	-	-	23,23,23,23	1
2	MG	31-B	403	1/1	-	-	23,23,23,23	1
2	MG	32-B	403	1/1	-	-	23,23,23,23	1
2	MG	33-B	403	1/1	-	-	23,23,23,23	1
2	MG	34-B	403	1/1	-	-	23,23,23,23	1
2	MG	35-B	403	1/1	-	-	23,23,23,23	1
2	MG	36-B	403	1/1	-	-	23,23,23,23	1
2	MG	37-B	403	1/1	-	-	23,23,23,23	1
2	MG	38-B	403	1/1	-	-	23,23,23,23	1
2	MG	39-B	403	1/1	-	-	23,23,23,23	1
2	MG	40-B	403	1/1	-	-	23,23,23,23	1
2	MG	41-B	403	1/1	-	-	23,23,23,23	1
2	MG	42-B	403	1/1	-	-	23,23,23,23	1
2	MG	43-B	403	1/1	-	-	23,23,23,23	1
2	MG	44-B	403	1/1	-	-	23,23,23,23	1
2	MG	45-B	403	1/1	-	-	23,23,23,23	1
2	MG	46-B	403	1/1	-	-	23,23,23,23	1
2	MG	47-B	403	1/1	-	-	23,23,23,23	1
2	MG	48-B	403	1/1	-	-	23,23,23,23	1
2	MG	49-B	403	1/1	-	-	23,23,23,23	1
2	MG	50-B	403	1/1	-	-	23,23,23,23	1
8	2PE	1-A	412	7/28	0.63	0.20	24,25,26,26	7
2	MG	2-B	404	1/1	-	-	28,28,28,28	1
2	MG	3-B	404	1/1	-	-	28,28,28,28	1
2	MG	4-B	404	1/1	-	-	28,28,28,28	1
2	MG	5-B	404	1/1	-	-	28,28,28,28	1
2	MG	6-B	404	1/1	-	-	28,28,28,28	1
2	MG	7-B	404	1/1	-	-	28,28,28,28	1
2	MG	8-B	404	1/1	-	-	28,28,28,28	1
2	MG	9-B	404	1/1	-	-	28,28,28,28	1
2	MG	10-B	404	1/1	-	-	28,28,28,28	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	11-B	404	1/1	-	-	28,28,28,28	1
2	MG	12-B	404	1/1	-	-	28,28,28,28	1
2	MG	13-B	404	1/1	-	-	28,28,28,28	1
2	MG	14-B	404	1/1	-	-	28,28,28,28	1
2	MG	15-B	404	1/1	-	-	28,28,28,28	1
2	MG	16-B	404	1/1	-	-	28,28,28,28	1
2	MG	17-B	404	1/1	-	-	28,28,28,28	1
2	MG	18-B	404	1/1	-	-	28,28,28,28	1
2	MG	19-B	404	1/1	-	-	28,28,28,28	1
2	MG	20-B	404	1/1	-	-	28,28,28,28	1
2	MG	21-B	404	1/1	-	-	28,28,28,28	1
2	MG	22-B	404	1/1	-	-	28,28,28,28	1
2	MG	23-B	404	1/1	-	-	28,28,28,28	1
2	MG	24-B	404	1/1	-	-	28,28,28,28	1
2	MG	25-B	404	1/1	-	-	28,28,28,28	1
2	MG	26-B	404	1/1	-	-	28,28,28,28	1
2	MG	27-B	404	1/1	-	-	28,28,28,28	1
2	MG	28-B	404	1/1	-	-	28,28,28,28	1
2	MG	29-B	404	1/1	-	-	28,28,28,28	1
2	MG	30-B	404	1/1	-	-	28,28,28,28	1
2	MG	31-B	404	1/1	-	-	28,28,28,28	1
2	MG	32-B	404	1/1	-	-	28,28,28,28	1
2	MG	33-B	404	1/1	-	-	28,28,28,28	1
2	MG	34-B	404	1/1	-	-	28,28,28,28	1
2	MG	35-B	404	1/1	-	-	28,28,28,28	1
2	MG	36-B	404	1/1	-	-	28,28,28,28	1
2	MG	37-B	404	1/1	-	-	28,28,28,28	1
2	MG	38-B	404	1/1	-	-	28,28,28,28	1
2	MG	39-B	404	1/1	-	-	28,28,28,28	1
2	MG	40-B	404	1/1	-	-	28,28,28,28	1
2	MG	41-B	404	1/1	-	-	28,28,28,28	1
2	MG	42-B	404	1/1	-	-	28,28,28,28	1
2	MG	43-B	404	1/1	-	-	28,28,28,28	1
2	MG	44-B	404	1/1	-	-	28,28,28,28	1
2	MG	45-B	404	1/1	-	-	28,28,28,28	1
2	MG	46-B	404	1/1	-	-	28,28,28,28	1
2	MG	47-B	404	1/1	-	-	28,28,28,28	1
2	MG	48-B	404	1/1	-	-	28,28,28,28	1
2	MG	49-B	404	1/1	-	-	28,28,28,28	1
2	MG	50-B	404	1/1	-	-	28,28,28,28	1
6	CL	1-B	408	1/1	0.64	0.27	26,26,26,26	1
3	PPV	2-A	406	9/9	-	-	21,22,22,22	9

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PPV	3-A	406	9/9	-	-	21,22,22,22	9
3	PPV	4-A	406	9/9	-	-	21,22,22,22	9
3	PPV	5-A	406	9/9	-	-	21,22,22,22	9
3	PPV	6-A	406	9/9	-	-	21,22,22,22	9
3	PPV	7-A	406	9/9	-	-	21,22,22,22	9
3	PPV	8-A	406	9/9	-	-	21,22,22,22	9
3	PPV	9-A	406	9/9	-	-	21,22,22,22	9
3	PPV	10-A	406	9/9	-	-	21,22,22,22	9
3	PPV	11-A	406	9/9	-	-	21,22,22,22	9
3	PPV	12-A	406	9/9	-	-	21,22,22,22	9
3	PPV	13-A	406	9/9	-	-	21,22,22,22	9
3	PPV	14-A	406	9/9	-	-	21,22,22,22	9
3	PPV	15-A	406	9/9	-	-	21,22,22,22	9
3	PPV	16-A	406	9/9	-	-	21,22,22,22	9
3	PPV	17-A	406	9/9	-	-	21,22,22,22	9
3	PPV	18-A	406	9/9	-	-	21,22,22,22	9
3	PPV	19-A	406	9/9	-	-	21,22,22,22	9
3	PPV	20-A	406	9/9	-	-	21,22,22,22	9
3	PPV	21-A	406	9/9	-	-	21,22,22,22	9
3	PPV	22-A	406	9/9	-	-	21,22,22,22	9
3	PPV	23-A	406	9/9	-	-	21,22,22,22	9
3	PPV	24-A	406	9/9	-	-	21,22,22,22	9
3	PPV	25-A	406	9/9	-	-	21,22,22,22	9
3	PPV	26-A	406	9/9	-	-	21,22,22,22	9
3	PPV	27-A	406	9/9	-	-	21,22,22,22	9
3	PPV	28-A	406	9/9	-	-	21,22,22,22	9
3	PPV	29-A	406	9/9	-	-	21,22,22,22	9
3	PPV	30-A	406	9/9	-	-	21,22,22,22	9
3	PPV	31-A	406	9/9	-	-	21,22,22,22	9
3	PPV	32-A	406	9/9	-	-	21,22,22,22	9
3	PPV	33-A	406	9/9	-	-	21,22,22,22	9
3	PPV	34-A	406	9/9	-	-	21,22,22,22	9
3	PPV	35-A	406	9/9	-	-	21,22,22,22	9
3	PPV	36-A	406	9/9	-	-	21,22,22,22	9
3	PPV	37-A	406	9/9	-	-	21,22,22,22	9
3	PPV	38-A	406	9/9	-	-	21,22,22,22	9
3	PPV	39-A	406	9/9	-	-	21,22,22,22	9
3	PPV	40-A	406	9/9	-	-	21,22,22,22	9
3	PPV	41-A	406	9/9	-	-	21,22,22,22	9
3	PPV	42-A	406	9/9	-	-	21,22,22,22	9
3	PPV	43-A	406	9/9	-	-	21,22,22,22	9
3	PPV	44-A	406	9/9	-	-	21,22,22,22	9

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PPV	45-A	406	9/9	-	-	21,22,22,22	9
3	PPV	46-A	406	9/9	-	-	21,22,22,22	9
3	PPV	47-A	406	9/9	-	-	21,22,22,22	9
3	PPV	48-A	406	9/9	-	-	21,22,22,22	9
3	PPV	49-A	406	9/9	-	-	21,22,22,22	9
3	PPV	50-A	406	9/9	-	-	21,22,22,22	9
7	CCN	1-A	411	3/3	0.64	0.20	22,22,22,22	3
3	PPV	2-B	405	9/9	-	-	22,23,23,23	9
3	PPV	3-B	405	9/9	-	-	22,23,23,23	9
3	PPV	4-B	405	9/9	-	-	22,23,23,23	9
3	PPV	5-B	405	9/9	-	-	22,23,23,23	9
3	PPV	6-B	405	9/9	-	-	22,23,23,23	9
3	PPV	7-B	405	9/9	-	-	22,23,23,23	9
3	PPV	8-B	405	9/9	-	-	22,23,23,23	9
3	PPV	9-B	405	9/9	-	-	22,23,23,23	9
3	PPV	10-B	405	9/9	-	-	22,23,23,23	9
3	PPV	11-B	405	9/9	-	-	22,23,23,23	9
3	PPV	12-B	405	9/9	-	-	22,23,23,23	9
3	PPV	13-B	405	9/9	-	-	22,23,23,23	9
3	PPV	14-B	405	9/9	-	-	22,23,23,23	9
3	PPV	15-B	405	9/9	-	-	22,23,23,23	9
3	PPV	16-B	405	9/9	-	-	22,23,23,23	9
3	PPV	17-B	405	9/9	-	-	22,23,23,23	9
3	PPV	18-B	405	9/9	-	-	22,23,23,23	9
3	PPV	19-B	405	9/9	-	-	22,23,23,23	9
3	PPV	20-B	405	9/9	-	-	22,23,23,23	9
3	PPV	21-B	405	9/9	-	-	22,23,23,23	9
3	PPV	22-B	405	9/9	-	-	22,23,23,23	9
3	PPV	23-B	405	9/9	-	-	22,23,23,23	9
3	PPV	24-B	405	9/9	-	-	22,23,23,23	9
3	PPV	25-B	405	9/9	-	-	22,23,23,23	9
3	PPV	26-B	405	9/9	-	-	22,23,23,23	9
3	PPV	27-B	405	9/9	-	-	22,23,23,23	9
3	PPV	28-B	405	9/9	-	-	22,23,23,23	9
3	PPV	29-B	405	9/9	-	-	22,23,23,23	9
3	PPV	30-B	405	9/9	-	-	22,23,23,23	9
3	PPV	31-B	405	9/9	-	-	22,23,23,23	9
3	PPV	32-B	405	9/9	-	-	22,23,23,23	9
3	PPV	33-B	405	9/9	-	-	22,23,23,23	9
3	PPV	34-B	405	9/9	-	-	22,23,23,23	9
3	PPV	35-B	405	9/9	-	-	22,23,23,23	9
3	PPV	36-B	405	9/9	-	-	22,23,23,23	9

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PPV	37-B	405	9/9	-	-	22,23,23,23	9
3	PPV	38-B	405	9/9	-	-	22,23,23,23	9
3	PPV	39-B	405	9/9	-	-	22,23,23,23	9
3	PPV	40-B	405	9/9	-	-	22,23,23,23	9
3	PPV	41-B	405	9/9	-	-	22,23,23,23	9
3	PPV	42-B	405	9/9	-	-	22,23,23,23	9
3	PPV	43-B	405	9/9	-	-	22,23,23,23	9
3	PPV	44-B	405	9/9	-	-	22,23,23,23	9
3	PPV	45-B	405	9/9	-	-	22,23,23,23	9
3	PPV	46-B	405	9/9	-	-	22,23,23,23	9
3	PPV	47-B	405	9/9	-	-	22,23,23,23	9
3	PPV	48-B	405	9/9	-	-	22,23,23,23	9
3	PPV	49-B	405	9/9	-	-	22,23,23,23	9
3	PPV	50-B	405	9/9	-	-	22,23,23,23	9
2	MG	1-A	405	1/1	0.66	0.24	29,29,29,29	1
4	EXW	2-A	407	21/21	-	-	21,21,22,22	21
4	EXW	3-A	407	21/21	-	-	21,21,22,22	21
4	EXW	4-A	407	21/21	-	-	21,21,22,22	21
4	EXW	5-A	407	21/21	-	-	21,21,22,22	21
4	EXW	6-A	407	21/21	-	-	21,21,22,22	21
4	EXW	7-A	407	21/21	-	-	21,21,22,22	21
4	EXW	8-A	407	21/21	-	-	21,21,22,22	21
4	EXW	9-A	407	21/21	-	-	21,21,22,22	21
4	EXW	10-A	407	21/21	-	-	21,21,22,22	21
4	EXW	11-A	407	21/21	-	-	21,21,22,22	21
4	EXW	12-A	407	21/21	-	-	21,21,22,22	21
4	EXW	13-A	407	21/21	-	-	21,21,22,22	21
4	EXW	14-A	407	21/21	-	-	21,21,22,22	21
4	EXW	15-A	407	21/21	-	-	21,21,22,22	21
4	EXW	16-A	407	21/21	-	-	21,21,22,22	21
4	EXW	17-A	407	21/21	-	-	21,21,22,22	21
4	EXW	18-A	407	21/21	-	-	21,21,22,22	21
4	EXW	19-A	407	21/21	-	-	21,21,22,22	21
4	EXW	20-A	407	21/21	-	-	21,21,22,22	21
4	EXW	21-A	407	21/21	-	-	21,21,22,22	21
4	EXW	22-A	407	21/21	-	-	21,21,22,22	21
4	EXW	23-A	407	21/21	-	-	21,21,22,22	21
4	EXW	24-A	407	21/21	-	-	21,21,22,22	21
4	EXW	25-A	407	21/21	-	-	21,21,22,22	21
4	EXW	26-A	407	21/21	-	-	21,21,22,22	21
4	EXW	27-A	407	21/21	-	-	21,21,22,22	21
4	EXW	28-A	407	21/21	-	-	21,21,22,22	21

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EXW	29-A	407	21/21	-	-	21,21,22,22	21
4	EXW	30-A	407	21/21	-	-	21,21,22,22	21
4	EXW	31-A	407	21/21	-	-	21,21,22,22	21
4	EXW	32-A	407	21/21	-	-	21,21,22,22	21
4	EXW	33-A	407	21/21	-	-	21,21,22,22	21
4	EXW	34-A	407	21/21	-	-	21,21,22,22	21
4	EXW	35-A	407	21/21	-	-	21,21,22,22	21
4	EXW	36-A	407	21/21	-	-	21,21,22,22	21
4	EXW	37-A	407	21/21	-	-	21,21,22,22	21
4	EXW	38-A	407	21/21	-	-	21,21,22,22	21
4	EXW	39-A	407	21/21	-	-	21,21,22,22	21
4	EXW	40-A	407	21/21	-	-	21,21,22,22	21
4	EXW	41-A	407	21/21	-	-	21,21,22,22	21
4	EXW	42-A	407	21/21	-	-	21,21,22,22	21
4	EXW	43-A	407	21/21	-	-	21,21,22,22	21
4	EXW	44-A	407	21/21	-	-	21,21,22,22	21
4	EXW	45-A	407	21/21	-	-	21,21,22,22	21
4	EXW	46-A	407	21/21	-	-	21,21,22,22	21
4	EXW	47-A	407	21/21	-	-	21,21,22,22	21
4	EXW	48-A	407	21/21	-	-	21,21,22,22	21
4	EXW	49-A	407	21/21	-	-	21,21,22,22	21
4	EXW	50-A	407	21/21	-	-	21,21,22,22	21
5	MPD	1-B	407	8/8	0.72	0.22	19,19,20,20	8
4	EXW	2-B	406	21/21	-	-	21,22,23,23	21
4	EXW	3-B	406	21/21	-	-	21,22,23,23	21
4	EXW	4-B	406	21/21	-	-	21,22,23,23	21
4	EXW	5-B	406	21/21	-	-	21,22,23,23	21
4	EXW	6-B	406	21/21	-	-	21,22,23,23	21
4	EXW	7-B	406	21/21	-	-	21,22,23,23	21
4	EXW	8-B	406	21/21	-	-	21,22,23,23	21
4	EXW	9-B	406	21/21	-	-	21,22,23,23	21
4	EXW	10-B	406	21/21	-	-	21,22,23,23	21
4	EXW	11-B	406	21/21	-	-	21,22,23,23	21
4	EXW	12-B	406	21/21	-	-	21,22,23,23	21
4	EXW	13-B	406	21/21	-	-	21,22,23,23	21
4	EXW	14-B	406	21/21	-	-	21,22,23,23	21
4	EXW	15-B	406	21/21	-	-	21,22,23,23	21
4	EXW	16-B	406	21/21	-	-	21,22,23,23	21
4	EXW	17-B	406	21/21	-	-	21,22,23,23	21
4	EXW	18-B	406	21/21	-	-	21,22,23,23	21
4	EXW	19-B	406	21/21	-	-	21,22,23,23	21
4	EXW	20-B	406	21/21	-	-	21,22,23,23	21

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EXW	21-B	406	21/21	-	-	21,22,23,23	21
4	EXW	22-B	406	21/21	-	-	21,22,23,23	21
4	EXW	23-B	406	21/21	-	-	21,22,23,23	21
4	EXW	24-B	406	21/21	-	-	21,22,23,23	21
4	EXW	25-B	406	21/21	-	-	21,22,23,23	21
4	EXW	26-B	406	21/21	-	-	21,22,23,23	21
4	EXW	27-B	406	21/21	-	-	21,22,23,23	21
4	EXW	28-B	406	21/21	-	-	21,22,23,23	21
4	EXW	29-B	406	21/21	-	-	21,22,23,23	21
4	EXW	30-B	406	21/21	-	-	21,22,23,23	21
4	EXW	31-B	406	21/21	-	-	21,22,23,23	21
4	EXW	32-B	406	21/21	-	-	21,22,23,23	21
4	EXW	33-B	406	21/21	-	-	21,22,23,23	21
4	EXW	34-B	406	21/21	-	-	21,22,23,23	21
4	EXW	35-B	406	21/21	-	-	21,22,23,23	21
4	EXW	36-B	406	21/21	-	-	21,22,23,23	21
4	EXW	37-B	406	21/21	-	-	21,22,23,23	21
4	EXW	38-B	406	21/21	-	-	21,22,23,23	21
4	EXW	39-B	406	21/21	-	-	21,22,23,23	21
4	EXW	40-B	406	21/21	-	-	21,22,23,23	21
4	EXW	41-B	406	21/21	-	-	21,22,23,23	21
4	EXW	42-B	406	21/21	-	-	21,22,23,23	21
4	EXW	43-B	406	21/21	-	-	21,22,23,23	21
4	EXW	44-B	406	21/21	-	-	21,22,23,23	21
4	EXW	45-B	406	21/21	-	-	21,22,23,23	21
4	EXW	46-B	406	21/21	-	-	21,22,23,23	21
4	EXW	47-B	406	21/21	-	-	21,22,23,23	21
4	EXW	48-B	406	21/21	-	-	21,22,23,23	21
4	EXW	49-B	406	21/21	-	-	21,22,23,23	21
4	EXW	50-B	406	21/21	-	-	21,22,23,23	21
6	CL	1-A	409	1/1	0.93	0.08	26,26,26,26	1
5	MPD	2-A	408	8/8	-	-	20,20,20,20	8
5	MPD	3-A	408	8/8	-	-	20,20,20,20	8
5	MPD	4-A	408	8/8	-	-	20,20,20,20	8
5	MPD	5-A	408	8/8	-	-	20,20,20,20	8
5	MPD	6-A	408	8/8	-	-	20,20,20,20	8
5	MPD	7-A	408	8/8	-	-	20,20,20,20	8
5	MPD	8-A	408	8/8	-	-	20,20,20,20	8
5	MPD	9-A	408	8/8	-	-	20,20,20,20	8
5	MPD	10-A	408	8/8	-	-	20,20,20,20	8
5	MPD	11-A	408	8/8	-	-	20,20,20,20	8
5	MPD	12-A	408	8/8	-	-	20,20,20,20	8

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MPD	13-A	408	8/8	-	-	20,20,20,20	8
5	MPD	14-A	408	8/8	-	-	20,20,20,20	8
5	MPD	15-A	408	8/8	-	-	20,20,20,20	8
5	MPD	16-A	408	8/8	-	-	20,20,20,20	8
5	MPD	17-A	408	8/8	-	-	20,20,20,20	8
5	MPD	18-A	408	8/8	-	-	20,20,20,20	8
5	MPD	19-A	408	8/8	-	-	20,20,20,20	8
5	MPD	20-A	408	8/8	-	-	20,20,20,20	8
5	MPD	21-A	408	8/8	-	-	20,20,20,20	8
5	MPD	22-A	408	8/8	-	-	20,20,20,20	8
5	MPD	23-A	408	8/8	-	-	20,20,20,20	8
5	MPD	24-A	408	8/8	-	-	20,20,20,20	8
5	MPD	25-A	408	8/8	-	-	20,20,20,20	8
5	MPD	26-A	408	8/8	-	-	20,20,20,20	8
5	MPD	27-A	408	8/8	-	-	20,20,20,20	8
5	MPD	28-A	408	8/8	-	-	20,20,20,20	8
5	MPD	29-A	408	8/8	-	-	20,20,20,20	8
5	MPD	30-A	408	8/8	-	-	20,20,20,20	8
5	MPD	31-A	408	8/8	-	-	20,20,20,20	8
5	MPD	32-A	408	8/8	-	-	20,20,20,20	8
5	MPD	33-A	408	8/8	-	-	20,20,20,20	8
5	MPD	34-A	408	8/8	-	-	20,20,20,20	8
5	MPD	35-A	408	8/8	-	-	20,20,20,20	8
5	MPD	36-A	408	8/8	-	-	20,20,20,20	8
5	MPD	37-A	408	8/8	-	-	20,20,20,20	8
5	MPD	38-A	408	8/8	-	-	20,20,20,20	8
5	MPD	39-A	408	8/8	-	-	20,20,20,20	8
5	MPD	40-A	408	8/8	-	-	20,20,20,20	8
5	MPD	41-A	408	8/8	-	-	20,20,20,20	8
5	MPD	42-A	408	8/8	-	-	20,20,20,20	8
5	MPD	43-A	408	8/8	-	-	20,20,20,20	8
5	MPD	44-A	408	8/8	-	-	20,20,20,20	8
5	MPD	45-A	408	8/8	-	-	20,20,20,20	8
5	MPD	46-A	408	8/8	-	-	20,20,20,20	8
5	MPD	47-A	408	8/8	-	-	20,20,20,20	8
5	MPD	48-A	408	8/8	-	-	20,20,20,20	8
5	MPD	49-A	408	8/8	-	-	20,20,20,20	8
5	MPD	50-A	408	8/8	-	-	20,20,20,20	8
2	MG	1-A	401	1/1	0.95	0.05	22,22,22,22	1
5	MPD	2-B	407	8/8	-	-	19,19,20,20	8
5	MPD	3-B	407	8/8	-	-	19,19,20,20	8
5	MPD	4-B	407	8/8	-	-	19,19,20,20	8

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MPD	5-B	407	8/8	-	-	19,19,20,20	8
5	MPD	6-B	407	8/8	-	-	19,19,20,20	8
5	MPD	7-B	407	8/8	-	-	19,19,20,20	8
5	MPD	8-B	407	8/8	-	-	19,19,20,20	8
5	MPD	9-B	407	8/8	-	-	19,19,20,20	8
5	MPD	10-B	407	8/8	-	-	19,19,20,20	8
5	MPD	11-B	407	8/8	-	-	19,19,20,20	8
5	MPD	12-B	407	8/8	-	-	19,19,20,20	8
5	MPD	13-B	407	8/8	-	-	19,19,20,20	8
5	MPD	14-B	407	8/8	-	-	19,19,20,20	8
5	MPD	15-B	407	8/8	-	-	19,19,20,20	8
5	MPD	16-B	407	8/8	-	-	19,19,20,20	8
5	MPD	17-B	407	8/8	-	-	19,19,20,20	8
5	MPD	18-B	407	8/8	-	-	19,19,20,20	8
5	MPD	19-B	407	8/8	-	-	19,19,20,20	8
5	MPD	20-B	407	8/8	-	-	19,19,20,20	8
5	MPD	21-B	407	8/8	-	-	19,19,20,20	8
5	MPD	22-B	407	8/8	-	-	19,19,20,20	8
5	MPD	23-B	407	8/8	-	-	19,19,20,20	8
5	MPD	24-B	407	8/8	-	-	19,19,20,20	8
5	MPD	25-B	407	8/8	-	-	19,19,20,20	8
5	MPD	26-B	407	8/8	-	-	19,19,20,20	8
5	MPD	27-B	407	8/8	-	-	19,19,20,20	8
5	MPD	28-B	407	8/8	-	-	19,19,20,20	8
5	MPD	29-B	407	8/8	-	-	19,19,20,20	8
5	MPD	30-B	407	8/8	-	-	19,19,20,20	8
5	MPD	31-B	407	8/8	-	-	19,19,20,20	8
5	MPD	32-B	407	8/8	-	-	19,19,20,20	8
5	MPD	33-B	407	8/8	-	-	19,19,20,20	8
5	MPD	34-B	407	8/8	-	-	19,19,20,20	8
5	MPD	35-B	407	8/8	-	-	19,19,20,20	8
5	MPD	36-B	407	8/8	-	-	19,19,20,20	8
5	MPD	37-B	407	8/8	-	-	19,19,20,20	8
5	MPD	38-B	407	8/8	-	-	19,19,20,20	8
5	MPD	39-B	407	8/8	-	-	19,19,20,20	8
5	MPD	40-B	407	8/8	-	-	19,19,20,20	8
5	MPD	41-B	407	8/8	-	-	19,19,20,20	8
5	MPD	42-B	407	8/8	-	-	19,19,20,20	8
5	MPD	43-B	407	8/8	-	-	19,19,20,20	8
5	MPD	44-B	407	8/8	-	-	19,19,20,20	8
5	MPD	45-B	407	8/8	-	-	19,19,20,20	8
5	MPD	46-B	407	8/8	-	-	19,19,20,20	8

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MPD	47-B	407	8/8	-	-	19,19,20,20	8
5	MPD	48-B	407	8/8	-	-	19,19,20,20	8
5	MPD	49-B	407	8/8	-	-	19,19,20,20	8
5	MPD	50-B	407	8/8	-	-	19,19,20,20	8
2	MG	1-A	403	1/1	0.95	0.07	22,22,22,22	1
6	CL	2-A	409	1/1	-	-	26,26,26,26	1
6	CL	3-A	409	1/1	-	-	26,26,26,26	1
6	CL	4-A	409	1/1	-	-	26,26,26,26	1
6	CL	5-A	409	1/1	-	-	26,26,26,26	1
6	CL	6-A	409	1/1	-	-	26,26,26,26	1
6	CL	7-A	409	1/1	-	-	26,26,26,26	1
6	CL	8-A	409	1/1	-	-	26,26,26,26	1
6	CL	9-A	409	1/1	-	-	26,26,26,26	1
6	CL	10-A	409	1/1	-	-	26,26,26,26	1
6	CL	11-A	409	1/1	-	-	26,26,26,26	1
6	CL	12-A	409	1/1	-	-	26,26,26,26	1
6	CL	13-A	409	1/1	-	-	26,26,26,26	1
6	CL	14-A	409	1/1	-	-	26,26,26,26	1
6	CL	15-A	409	1/1	-	-	26,26,26,26	1
6	CL	16-A	409	1/1	-	-	26,26,26,26	1
6	CL	17-A	409	1/1	-	-	26,26,26,26	1
6	CL	18-A	409	1/1	-	-	26,26,26,26	1
6	CL	19-A	409	1/1	-	-	26,26,26,26	1
6	CL	20-A	409	1/1	-	-	26,26,26,26	1
6	CL	21-A	409	1/1	-	-	26,26,26,26	1
6	CL	22-A	409	1/1	-	-	26,26,26,26	1
6	CL	23-A	409	1/1	-	-	26,26,26,26	1
6	CL	24-A	409	1/1	-	-	26,26,26,26	1
6	CL	25-A	409	1/1	-	-	26,26,26,26	1
6	CL	26-A	409	1/1	-	-	26,26,26,26	1
6	CL	27-A	409	1/1	-	-	26,26,26,26	1
6	CL	28-A	409	1/1	-	-	26,26,26,26	1
6	CL	29-A	409	1/1	-	-	26,26,26,26	1
6	CL	30-A	409	1/1	-	-	26,26,26,26	1
6	CL	31-A	409	1/1	-	-	26,26,26,26	1
6	CL	32-A	409	1/1	-	-	26,26,26,26	1
6	CL	33-A	409	1/1	-	-	26,26,26,26	1
6	CL	34-A	409	1/1	-	-	26,26,26,26	1
6	CL	35-A	409	1/1	-	-	26,26,26,26	1
6	CL	36-A	409	1/1	-	-	26,26,26,26	1
6	CL	37-A	409	1/1	-	-	26,26,26,26	1
6	CL	38-A	409	1/1	-	-	26,26,26,26	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	CL	39-A	409	1/1	-	-	26,26,26,26	1
6	CL	40-A	409	1/1	-	-	26,26,26,26	1
6	CL	41-A	409	1/1	-	-	26,26,26,26	1
6	CL	42-A	409	1/1	-	-	26,26,26,26	1
6	CL	43-A	409	1/1	-	-	26,26,26,26	1
6	CL	44-A	409	1/1	-	-	26,26,26,26	1
6	CL	45-A	409	1/1	-	-	26,26,26,26	1
6	CL	46-A	409	1/1	-	-	26,26,26,26	1
6	CL	47-A	409	1/1	-	-	26,26,26,26	1
6	CL	48-A	409	1/1	-	-	26,26,26,26	1
6	CL	49-A	409	1/1	-	-	26,26,26,26	1
6	CL	50-A	409	1/1	-	-	26,26,26,26	1
2	MG	1-A	402	1/1	0.97	0.05	22,22,22,22	1
6	CL	2-A	410	1/1	-	-	20,20,20,20	1
6	CL	3-A	410	1/1	-	-	20,20,20,20	1
6	CL	4-A	410	1/1	-	-	20,20,20,20	1
6	CL	5-A	410	1/1	-	-	20,20,20,20	1
6	CL	6-A	410	1/1	-	-	20,20,20,20	1
6	CL	7-A	410	1/1	-	-	20,20,20,20	1
6	CL	8-A	410	1/1	-	-	20,20,20,20	1
6	CL	9-A	410	1/1	-	-	20,20,20,20	1
6	CL	10-A	410	1/1	-	-	20,20,20,20	1
6	CL	11-A	410	1/1	-	-	20,20,20,20	1
6	CL	12-A	410	1/1	-	-	20,20,20,20	1
6	CL	13-A	410	1/1	-	-	20,20,20,20	1
6	CL	14-A	410	1/1	-	-	20,20,20,20	1
6	CL	15-A	410	1/1	-	-	20,20,20,20	1
6	CL	16-A	410	1/1	-	-	20,20,20,20	1
6	CL	17-A	410	1/1	-	-	20,20,20,20	1
6	CL	18-A	410	1/1	-	-	20,20,20,20	1
6	CL	19-A	410	1/1	-	-	20,20,20,20	1
6	CL	20-A	410	1/1	-	-	20,20,20,20	1
6	CL	21-A	410	1/1	-	-	20,20,20,20	1
6	CL	22-A	410	1/1	-	-	20,20,20,20	1
6	CL	23-A	410	1/1	-	-	20,20,20,20	1
6	CL	24-A	410	1/1	-	-	20,20,20,20	1
6	CL	25-A	410	1/1	-	-	20,20,20,20	1
6	CL	26-A	410	1/1	-	-	20,20,20,20	1
6	CL	27-A	410	1/1	-	-	20,20,20,20	1
6	CL	28-A	410	1/1	-	-	20,20,20,20	1
6	CL	29-A	410	1/1	-	-	20,20,20,20	1
6	CL	30-A	410	1/1	-	-	20,20,20,20	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	CL	31-A	410	1/1	-	-	20,20,20,20	1
6	CL	32-A	410	1/1	-	-	20,20,20,20	1
6	CL	33-A	410	1/1	-	-	20,20,20,20	1
6	CL	34-A	410	1/1	-	-	20,20,20,20	1
6	CL	35-A	410	1/1	-	-	20,20,20,20	1
6	CL	36-A	410	1/1	-	-	20,20,20,20	1
6	CL	37-A	410	1/1	-	-	20,20,20,20	1
6	CL	38-A	410	1/1	-	-	20,20,20,20	1
6	CL	39-A	410	1/1	-	-	20,20,20,20	1
6	CL	40-A	410	1/1	-	-	20,20,20,20	1
6	CL	41-A	410	1/1	-	-	20,20,20,20	1
6	CL	42-A	410	1/1	-	-	20,20,20,20	1
6	CL	43-A	410	1/1	-	-	20,20,20,20	1
6	CL	44-A	410	1/1	-	-	20,20,20,20	1
6	CL	45-A	410	1/1	-	-	20,20,20,20	1
6	CL	46-A	410	1/1	-	-	20,20,20,20	1
6	CL	47-A	410	1/1	-	-	20,20,20,20	1
6	CL	48-A	410	1/1	-	-	20,20,20,20	1
6	CL	49-A	410	1/1	-	-	20,20,20,20	1
6	CL	50-A	410	1/1	-	-	20,20,20,20	1
6	CL	1-A	410	1/1	0.97	0.04	20,20,20,20	1
6	CL	2-B	408	1/1	-	-	26,26,26,26	1
6	CL	3-B	408	1/1	-	-	26,26,26,26	1
6	CL	4-B	408	1/1	-	-	26,26,26,26	1
6	CL	5-B	408	1/1	-	-	26,26,26,26	1
6	CL	6-B	408	1/1	-	-	26,26,26,26	1
6	CL	7-B	408	1/1	-	-	26,26,26,26	1
6	CL	8-B	408	1/1	-	-	26,26,26,26	1
6	CL	9-B	408	1/1	-	-	26,26,26,26	1
6	CL	10-B	408	1/1	-	-	26,26,26,26	1
6	CL	11-B	408	1/1	-	-	26,26,26,26	1
6	CL	12-B	408	1/1	-	-	26,26,26,26	1
6	CL	13-B	408	1/1	-	-	26,26,26,26	1
6	CL	14-B	408	1/1	-	-	26,26,26,26	1
6	CL	15-B	408	1/1	-	-	26,26,26,26	1
6	CL	16-B	408	1/1	-	-	26,26,26,26	1
6	CL	17-B	408	1/1	-	-	26,26,26,26	1
6	CL	18-B	408	1/1	-	-	26,26,26,26	1
6	CL	19-B	408	1/1	-	-	26,26,26,26	1
6	CL	20-B	408	1/1	-	-	26,26,26,26	1
6	CL	21-B	408	1/1	-	-	26,26,26,26	1
6	CL	22-B	408	1/1	-	-	26,26,26,26	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	CL	23-B	408	1/1	-	-	26,26,26,26	1
6	CL	24-B	408	1/1	-	-	26,26,26,26	1
6	CL	25-B	408	1/1	-	-	26,26,26,26	1
6	CL	26-B	408	1/1	-	-	26,26,26,26	1
6	CL	27-B	408	1/1	-	-	26,26,26,26	1
6	CL	28-B	408	1/1	-	-	26,26,26,26	1
6	CL	29-B	408	1/1	-	-	26,26,26,26	1
6	CL	30-B	408	1/1	-	-	26,26,26,26	1
6	CL	31-B	408	1/1	-	-	26,26,26,26	1
6	CL	32-B	408	1/1	-	-	26,26,26,26	1
6	CL	33-B	408	1/1	-	-	26,26,26,26	1
6	CL	34-B	408	1/1	-	-	26,26,26,26	1
6	CL	35-B	408	1/1	-	-	26,26,26,26	1
6	CL	36-B	408	1/1	-	-	26,26,26,26	1
6	CL	37-B	408	1/1	-	-	26,26,26,26	1
6	CL	38-B	408	1/1	-	-	26,26,26,26	1
6	CL	39-B	408	1/1	-	-	26,26,26,26	1
6	CL	40-B	408	1/1	-	-	26,26,26,26	1
6	CL	41-B	408	1/1	-	-	26,26,26,26	1
6	CL	42-B	408	1/1	-	-	26,26,26,26	1
6	CL	43-B	408	1/1	-	-	26,26,26,26	1
6	CL	44-B	408	1/1	-	-	26,26,26,26	1
6	CL	45-B	408	1/1	-	-	26,26,26,26	1
6	CL	46-B	408	1/1	-	-	26,26,26,26	1
6	CL	47-B	408	1/1	-	-	26,26,26,26	1
6	CL	48-B	408	1/1	-	-	26,26,26,26	1
6	CL	49-B	408	1/1	-	-	26,26,26,26	1
6	CL	50-B	408	1/1	-	-	26,26,26,26	1
3	PPV	1-B	405	9/9	0.97	0.07	22,23,23,23	9
7	CCN	2-A	411	3/3	-	-	22,22,22,22	3
7	CCN	3-A	411	3/3	-	-	22,22,22,22	3
7	CCN	4-A	411	3/3	-	-	22,22,22,22	3
7	CCN	5-A	411	3/3	-	-	22,22,22,22	3
7	CCN	6-A	411	3/3	-	-	22,22,22,22	3
7	CCN	7-A	411	3/3	-	-	22,22,22,22	3
7	CCN	8-A	411	3/3	-	-	22,22,22,22	3
7	CCN	9-A	411	3/3	-	-	22,22,22,22	3
7	CCN	10-A	411	3/3	-	-	22,22,22,22	3
7	CCN	11-A	411	3/3	-	-	22,22,22,22	3
7	CCN	12-A	411	3/3	-	-	22,22,22,22	3
7	CCN	13-A	411	3/3	-	-	22,22,22,22	3
7	CCN	14-A	411	3/3	-	-	22,22,22,22	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	CCN	15-A	411	3/3	-	-	22,22,22,22	3
7	CCN	16-A	411	3/3	-	-	22,22,22,22	3
7	CCN	17-A	411	3/3	-	-	22,22,22,22	3
7	CCN	18-A	411	3/3	-	-	22,22,22,22	3
7	CCN	19-A	411	3/3	-	-	22,22,22,22	3
7	CCN	20-A	411	3/3	-	-	22,22,22,22	3
7	CCN	21-A	411	3/3	-	-	22,22,22,22	3
7	CCN	22-A	411	3/3	-	-	22,22,22,22	3
7	CCN	23-A	411	3/3	-	-	22,22,22,22	3
7	CCN	24-A	411	3/3	-	-	22,22,22,22	3
7	CCN	25-A	411	3/3	-	-	22,22,22,22	3
7	CCN	26-A	411	3/3	-	-	22,22,22,22	3
7	CCN	27-A	411	3/3	-	-	22,22,22,22	3
7	CCN	28-A	411	3/3	-	-	22,22,22,22	3
7	CCN	29-A	411	3/3	-	-	22,22,22,22	3
7	CCN	30-A	411	3/3	-	-	22,22,22,22	3
7	CCN	31-A	411	3/3	-	-	22,22,22,22	3
7	CCN	32-A	411	3/3	-	-	22,22,22,22	3
7	CCN	33-A	411	3/3	-	-	22,22,22,22	3
7	CCN	34-A	411	3/3	-	-	22,22,22,22	3
7	CCN	35-A	411	3/3	-	-	22,22,22,22	3
7	CCN	36-A	411	3/3	-	-	22,22,22,22	3
7	CCN	37-A	411	3/3	-	-	22,22,22,22	3
7	CCN	38-A	411	3/3	-	-	22,22,22,22	3
7	CCN	39-A	411	3/3	-	-	22,22,22,22	3
7	CCN	40-A	411	3/3	-	-	22,22,22,22	3
7	CCN	41-A	411	3/3	-	-	22,22,22,22	3
7	CCN	42-A	411	3/3	-	-	22,22,22,22	3
7	CCN	43-A	411	3/3	-	-	22,22,22,22	3
7	CCN	44-A	411	3/3	-	-	22,22,22,22	3
7	CCN	45-A	411	3/3	-	-	22,22,22,22	3
7	CCN	46-A	411	3/3	-	-	22,22,22,22	3
7	CCN	47-A	411	3/3	-	-	22,22,22,22	3
7	CCN	48-A	411	3/3	-	-	22,22,22,22	3
7	CCN	49-A	411	3/3	-	-	22,22,22,22	3
7	CCN	50-A	411	3/3	-	-	22,22,22,22	3
2	MG	1-B	402	1/1	0.97	0.07	22,22,22,22	1
8	2PE	2-A	412	7/28	-	-	24,25,26,26	7
8	2PE	3-A	412	7/28	-	-	24,25,26,26	7
8	2PE	4-A	412	7/28	-	-	24,25,26,26	7
8	2PE	5-A	412	7/28	-	-	24,25,26,26	7
8	2PE	6-A	412	7/28	-	-	24,25,26,26	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	2PE	7-A	412	7/28	-	-	24,25,26,26	7
8	2PE	8-A	412	7/28	-	-	24,25,26,26	7
8	2PE	9-A	412	7/28	-	-	24,25,26,26	7
8	2PE	10-A	412	7/28	-	-	24,25,26,26	7
8	2PE	11-A	412	7/28	-	-	24,25,26,26	7
8	2PE	12-A	412	7/28	-	-	24,25,26,26	7
8	2PE	13-A	412	7/28	-	-	24,25,26,26	7
8	2PE	14-A	412	7/28	-	-	24,25,26,26	7
8	2PE	15-A	412	7/28	-	-	24,25,26,26	7
8	2PE	16-A	412	7/28	-	-	24,25,26,26	7
8	2PE	17-A	412	7/28	-	-	24,25,26,26	7
8	2PE	18-A	412	7/28	-	-	24,25,26,26	7
8	2PE	19-A	412	7/28	-	-	24,25,26,26	7
8	2PE	20-A	412	7/28	-	-	24,25,26,26	7
8	2PE	21-A	412	7/28	-	-	24,25,26,26	7
8	2PE	22-A	412	7/28	-	-	24,25,26,26	7
8	2PE	23-A	412	7/28	-	-	24,25,26,26	7
8	2PE	24-A	412	7/28	-	-	24,25,26,26	7
8	2PE	25-A	412	7/28	-	-	24,25,26,26	7
8	2PE	26-A	412	7/28	-	-	24,25,26,26	7
8	2PE	27-A	412	7/28	-	-	24,25,26,26	7
8	2PE	28-A	412	7/28	-	-	24,25,26,26	7
8	2PE	29-A	412	7/28	-	-	24,25,26,26	7
8	2PE	30-A	412	7/28	-	-	24,25,26,26	7
8	2PE	31-A	412	7/28	-	-	24,25,26,26	7
8	2PE	32-A	412	7/28	-	-	24,25,26,26	7
8	2PE	33-A	412	7/28	-	-	24,25,26,26	7
8	2PE	34-A	412	7/28	-	-	24,25,26,26	7
8	2PE	35-A	412	7/28	-	-	24,25,26,26	7
8	2PE	36-A	412	7/28	-	-	24,25,26,26	7
8	2PE	37-A	412	7/28	-	-	24,25,26,26	7
8	2PE	38-A	412	7/28	-	-	24,25,26,26	7
8	2PE	39-A	412	7/28	-	-	24,25,26,26	7
8	2PE	40-A	412	7/28	-	-	24,25,26,26	7
8	2PE	41-A	412	7/28	-	-	24,25,26,26	7
8	2PE	42-A	412	7/28	-	-	24,25,26,26	7
8	2PE	43-A	412	7/28	-	-	24,25,26,26	7
8	2PE	44-A	412	7/28	-	-	24,25,26,26	7
8	2PE	45-A	412	7/28	-	-	24,25,26,26	7
8	2PE	46-A	412	7/28	-	-	24,25,26,26	7
8	2PE	47-A	412	7/28	-	-	24,25,26,26	7
8	2PE	48-A	412	7/28	-	-	24,25,26,26	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	2PE	49-A	412	7/28	-	-	24,25,26,26	7
8	2PE	50-A	412	7/28	-	-	24,25,26,26	7
2	MG	1-B	401	1/1	0.98	0.03	23,23,23,23	1
8	2PE	2-B	409	7/28	-	-	24,25,26,27	7
8	2PE	3-B	409	7/28	-	-	24,25,26,27	7
8	2PE	4-B	409	7/28	-	-	24,25,26,27	7
8	2PE	5-B	409	7/28	-	-	24,25,26,27	7
8	2PE	6-B	409	7/28	-	-	24,25,26,27	7
8	2PE	7-B	409	7/28	-	-	24,25,26,27	7
8	2PE	8-B	409	7/28	-	-	24,25,26,27	7
8	2PE	9-B	409	7/28	-	-	24,25,26,27	7
8	2PE	10-B	409	7/28	-	-	24,25,26,27	7
8	2PE	11-B	409	7/28	-	-	24,25,26,27	7
8	2PE	12-B	409	7/28	-	-	24,25,26,27	7
8	2PE	13-B	409	7/28	-	-	24,25,26,27	7
8	2PE	14-B	409	7/28	-	-	24,25,26,27	7
8	2PE	15-B	409	7/28	-	-	24,25,26,27	7
8	2PE	16-B	409	7/28	-	-	24,25,26,27	7
8	2PE	17-B	409	7/28	-	-	24,25,26,27	7
8	2PE	18-B	409	7/28	-	-	24,25,26,27	7
8	2PE	19-B	409	7/28	-	-	24,25,26,27	7
8	2PE	20-B	409	7/28	-	-	24,25,26,27	7
8	2PE	21-B	409	7/28	-	-	24,25,26,27	7
8	2PE	22-B	409	7/28	-	-	24,25,26,27	7
8	2PE	23-B	409	7/28	-	-	24,25,26,27	7
8	2PE	24-B	409	7/28	-	-	24,25,26,27	7
8	2PE	25-B	409	7/28	-	-	24,25,26,27	7
8	2PE	26-B	409	7/28	-	-	24,25,26,27	7
8	2PE	27-B	409	7/28	-	-	24,25,26,27	7
8	2PE	28-B	409	7/28	-	-	24,25,26,27	7
8	2PE	29-B	409	7/28	-	-	24,25,26,27	7
8	2PE	30-B	409	7/28	-	-	24,25,26,27	7
8	2PE	31-B	409	7/28	-	-	24,25,26,27	7
8	2PE	32-B	409	7/28	-	-	24,25,26,27	7
8	2PE	33-B	409	7/28	-	-	24,25,26,27	7
8	2PE	34-B	409	7/28	-	-	24,25,26,27	7
8	2PE	35-B	409	7/28	-	-	24,25,26,27	7
8	2PE	36-B	409	7/28	-	-	24,25,26,27	7
8	2PE	37-B	409	7/28	-	-	24,25,26,27	7
8	2PE	38-B	409	7/28	-	-	24,25,26,27	7
8	2PE	39-B	409	7/28	-	-	24,25,26,27	7
8	2PE	40-B	409	7/28	-	-	24,25,26,27	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	2PE	41-B	409	7/28	-	-	24,25,26,27	7
8	2PE	42-B	409	7/28	-	-	24,25,26,27	7
8	2PE	43-B	409	7/28	-	-	24,25,26,27	7
8	2PE	44-B	409	7/28	-	-	24,25,26,27	7
8	2PE	45-B	409	7/28	-	-	24,25,26,27	7
8	2PE	46-B	409	7/28	-	-	24,25,26,27	7
8	2PE	47-B	409	7/28	-	-	24,25,26,27	7
8	2PE	48-B	409	7/28	-	-	24,25,26,27	7
8	2PE	49-B	409	7/28	-	-	24,25,26,27	7
8	2PE	50-B	409	7/28	-	-	24,25,26,27	7
3	PPV	1-A	406	9/9	0.98	0.05	21,22,22,22	9
9	K	2-A	413	1/1	-	-	22,22,22,22	1
9	K	3-A	413	1/1	-	-	22,22,22,22	1
9	K	4-A	413	1/1	-	-	22,22,22,22	1
9	K	5-A	413	1/1	-	-	22,22,22,22	1
9	K	6-A	413	1/1	-	-	22,22,22,22	1
9	K	7-A	413	1/1	-	-	22,22,22,22	1
9	K	8-A	413	1/1	-	-	22,22,22,22	1
9	K	9-A	413	1/1	-	-	22,22,22,22	1
9	K	10-A	413	1/1	-	-	22,22,22,22	1
9	K	11-A	413	1/1	-	-	22,22,22,22	1
9	K	12-A	413	1/1	-	-	22,22,22,22	1
9	K	13-A	413	1/1	-	-	22,22,22,22	1
9	K	14-A	413	1/1	-	-	22,22,22,22	1
9	K	15-A	413	1/1	-	-	22,22,22,22	1
9	K	16-A	413	1/1	-	-	22,22,22,22	1
9	K	17-A	413	1/1	-	-	22,22,22,22	1
9	K	18-A	413	1/1	-	-	22,22,22,22	1
9	K	19-A	413	1/1	-	-	22,22,22,22	1
9	K	20-A	413	1/1	-	-	22,22,22,22	1
9	K	21-A	413	1/1	-	-	22,22,22,22	1
9	K	22-A	413	1/1	-	-	22,22,22,22	1
9	K	23-A	413	1/1	-	-	22,22,22,22	1
9	K	24-A	413	1/1	-	-	22,22,22,22	1
9	K	25-A	413	1/1	-	-	22,22,22,22	1
9	K	26-A	413	1/1	-	-	22,22,22,22	1
9	K	27-A	413	1/1	-	-	22,22,22,22	1
9	K	28-A	413	1/1	-	-	22,22,22,22	1
9	K	29-A	413	1/1	-	-	22,22,22,22	1
9	K	30-A	413	1/1	-	-	22,22,22,22	1
9	K	31-A	413	1/1	-	-	22,22,22,22	1
9	K	32-A	413	1/1	-	-	22,22,22,22	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	K	33-A	413	1/1	-	-	22,22,22,22	1
9	K	34-A	413	1/1	-	-	22,22,22,22	1
9	K	35-A	413	1/1	-	-	22,22,22,22	1
9	K	36-A	413	1/1	-	-	22,22,22,22	1
9	K	37-A	413	1/1	-	-	22,22,22,22	1
9	K	38-A	413	1/1	-	-	22,22,22,22	1
9	K	39-A	413	1/1	-	-	22,22,22,22	1
9	K	40-A	413	1/1	-	-	22,22,22,22	1
9	K	41-A	413	1/1	-	-	22,22,22,22	1
9	K	42-A	413	1/1	-	-	22,22,22,22	1
9	K	43-A	413	1/1	-	-	22,22,22,22	1
9	K	44-A	413	1/1	-	-	22,22,22,22	1
9	K	45-A	413	1/1	-	-	22,22,22,22	1
9	K	46-A	413	1/1	-	-	22,22,22,22	1
9	K	47-A	413	1/1	-	-	22,22,22,22	1
9	K	48-A	413	1/1	-	-	22,22,22,22	1
9	K	49-A	413	1/1	-	-	22,22,22,22	1
9	K	50-A	413	1/1	-	-	22,22,22,22	1
2	MG	1-B	403	1/1	0.98	0.06	23,23,23,23	1
9	K	2-B	410	1/1	-	-	22,22,22,22	1
9	K	3-B	410	1/1	-	-	22,22,22,22	1
9	K	4-B	410	1/1	-	-	22,22,22,22	1
9	K	5-B	410	1/1	-	-	22,22,22,22	1
9	K	6-B	410	1/1	-	-	22,22,22,22	1
9	K	7-B	410	1/1	-	-	22,22,22,22	1
9	K	8-B	410	1/1	-	-	22,22,22,22	1
9	K	9-B	410	1/1	-	-	22,22,22,22	1
9	K	10-B	410	1/1	-	-	22,22,22,22	1
9	K	11-B	410	1/1	-	-	22,22,22,22	1
9	K	12-B	410	1/1	-	-	22,22,22,22	1
9	K	13-B	410	1/1	-	-	22,22,22,22	1
9	K	14-B	410	1/1	-	-	22,22,22,22	1
9	K	15-B	410	1/1	-	-	22,22,22,22	1
9	K	16-B	410	1/1	-	-	22,22,22,22	1
9	K	17-B	410	1/1	-	-	22,22,22,22	1
9	K	18-B	410	1/1	-	-	22,22,22,22	1
9	K	19-B	410	1/1	-	-	22,22,22,22	1
9	K	20-B	410	1/1	-	-	22,22,22,22	1
9	K	21-B	410	1/1	-	-	22,22,22,22	1
9	K	22-B	410	1/1	-	-	22,22,22,22	1
9	K	23-B	410	1/1	-	-	22,22,22,22	1
9	K	24-B	410	1/1	-	-	22,22,22,22	1

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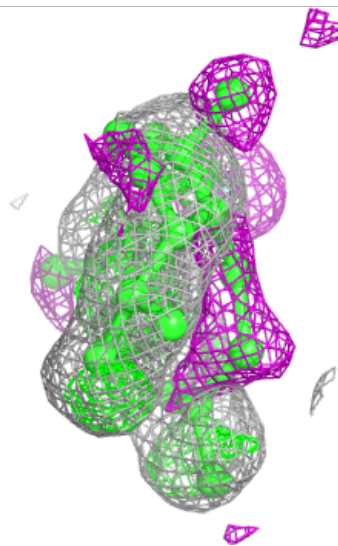
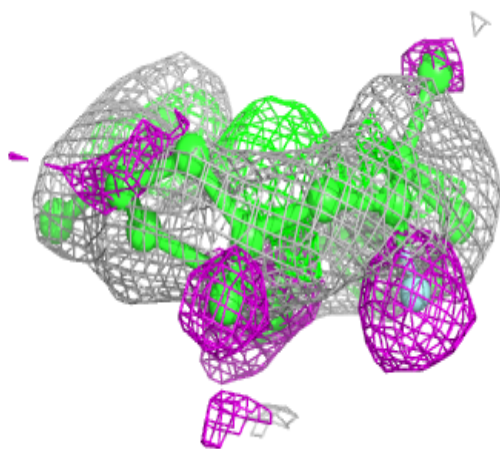
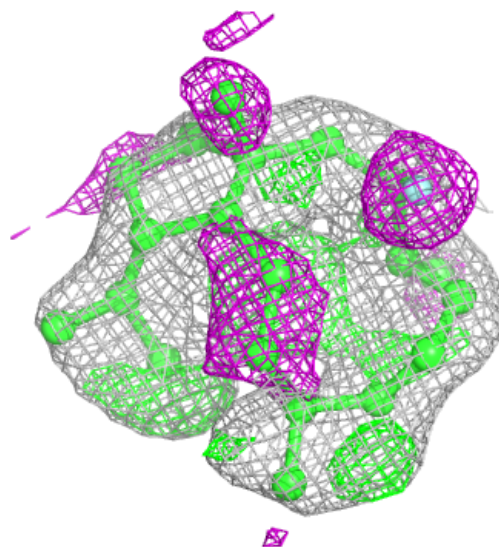
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	K	25-B	410	1/1	-	-	22,22,22,22	1
9	K	26-B	410	1/1	-	-	22,22,22,22	1
9	K	27-B	410	1/1	-	-	22,22,22,22	1
9	K	28-B	410	1/1	-	-	22,22,22,22	1
9	K	29-B	410	1/1	-	-	22,22,22,22	1
9	K	30-B	410	1/1	-	-	22,22,22,22	1
9	K	31-B	410	1/1	-	-	22,22,22,22	1
9	K	32-B	410	1/1	-	-	22,22,22,22	1
9	K	33-B	410	1/1	-	-	22,22,22,22	1
9	K	34-B	410	1/1	-	-	22,22,22,22	1
9	K	35-B	410	1/1	-	-	22,22,22,22	1
9	K	36-B	410	1/1	-	-	22,22,22,22	1
9	K	37-B	410	1/1	-	-	22,22,22,22	1
9	K	38-B	410	1/1	-	-	22,22,22,22	1
9	K	39-B	410	1/1	-	-	22,22,22,22	1
9	K	40-B	410	1/1	-	-	22,22,22,22	1
9	K	41-B	410	1/1	-	-	22,22,22,22	1
9	K	42-B	410	1/1	-	-	22,22,22,22	1
9	K	43-B	410	1/1	-	-	22,22,22,22	1
9	K	44-B	410	1/1	-	-	22,22,22,22	1
9	K	45-B	410	1/1	-	-	22,22,22,22	1
9	K	46-B	410	1/1	-	-	22,22,22,22	1
9	K	47-B	410	1/1	-	-	22,22,22,22	1
9	K	48-B	410	1/1	-	-	22,22,22,22	1
9	K	49-B	410	1/1	-	-	22,22,22,22	1
9	K	50-B	410	1/1	-	-	22,22,22,22	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

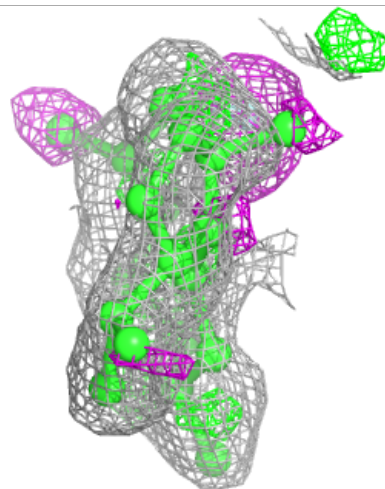
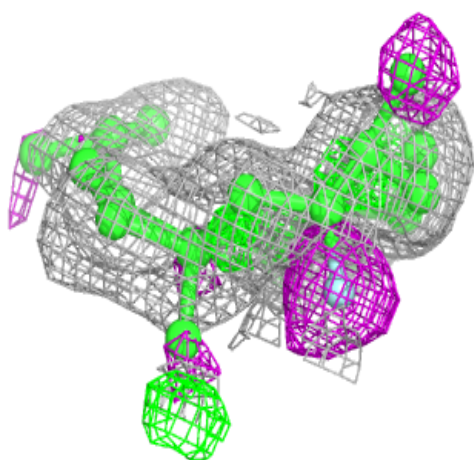
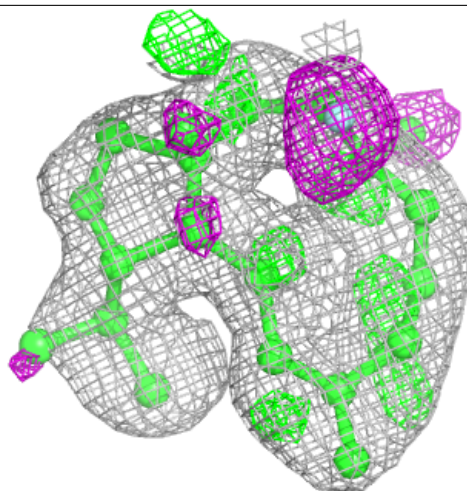
Electron density around EXW A 407:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



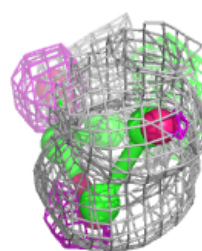
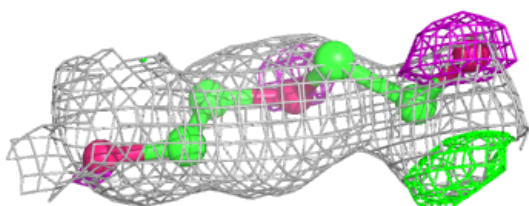
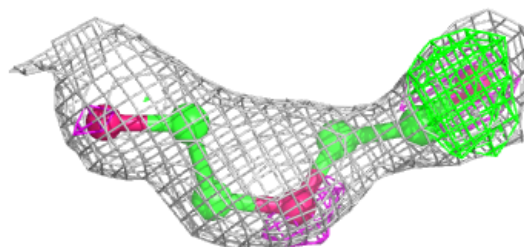
Electron density around EXW B 406:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

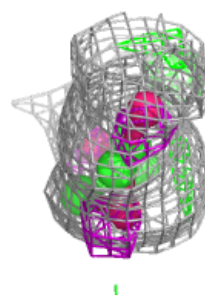
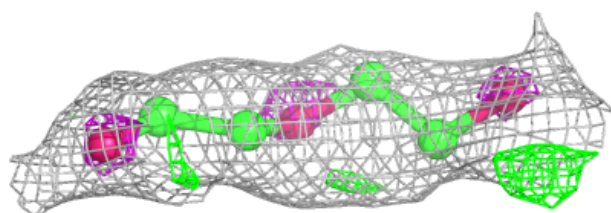
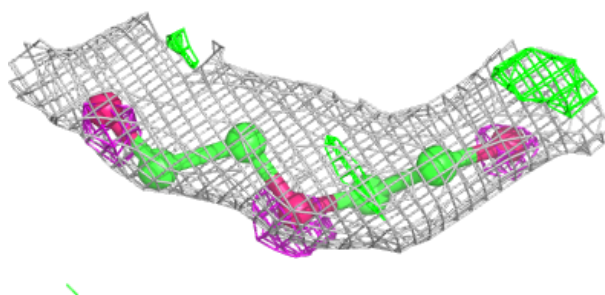


Electron density around 2PE B 409:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 2PE A 412:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



5.5 Other polymers [i](#)

There are no such residues in this entry.