



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 31, 2020 – 03:52 PM BST

PDB ID : 4PTH
Title : Ensemble model for Escherichia coli dihydrofolate reductase at 100K
Authors : Keedy, D.A.; van den Bedem, H.; Sivak, D.A.; Petsko, G.A.; Ringe, D.; Wilson, M.A.; Fraser, J.S.
Deposited on : 2014-03-10
Resolution : 0.85 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

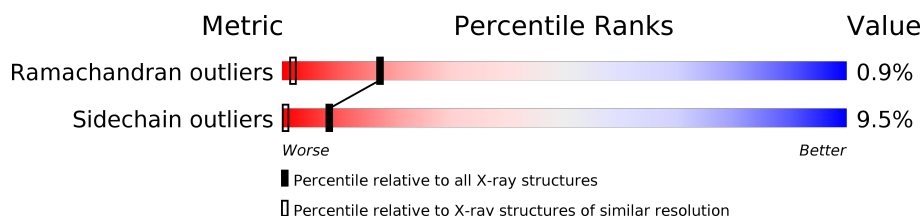
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 0.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	138981	1065 (1.04-0.68)
Sidechain outliers	138945	1066 (1.04-0.68)






















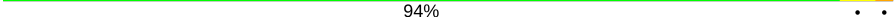



The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1-A	159	88% 9% ..
1	10-A	159	86% 13% .
1	100-A	159	86% 11% .
1	101-A	159	87% 10% .
1	102-A	159	82% 14% .
1	103-A	159	91% 8% .
1	104-A	159	88% 11% .
1	105-A	159	87% 9% .
1	106-A	159	88% 12%


























Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	107-A	159	 86% 11% .
1	108-A	159	 87% 10% .
1	109-A	159	 84% 13% ..
1	11-A	159	 89% 8% .
1	110-A	159	 87% 12% ..
1	111-A	159	 87% 11% ..
1	112-A	159	 87% 9% .
1	113-A	159	 89% 11%
1	114-A	159	 87% 10% .
1	115-A	159	 87% 11% .
1	116-A	159	 85% 12% .
1	117-A	159	 84% 14% .
1	118-A	159	 84% 14% .
1	119-A	159	 87% 9% .
1	12-A	159	 87% 9% .
1	120-A	159	 89% 11% .
1	121-A	159	 87% 11% .
1	122-A	159	 92% 7% .
1	123-A	159	 90% 8% .
1	124-A	159	 92% 6% .
1	125-A	159	 94% . .
1	126-A	159	 92% 7% .
1	127-A	159	 86% 11% .
1	128-A	159	 89% 7% . .
1	129-A	159	 88% 9% .

















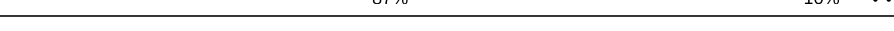

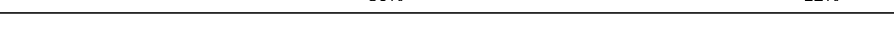
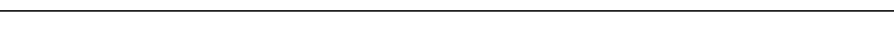
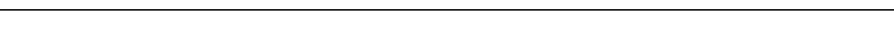
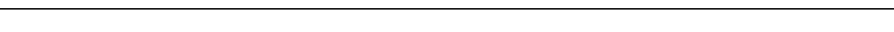
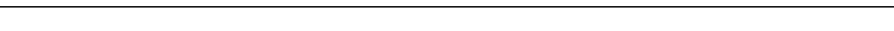
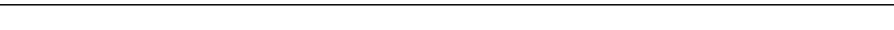

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	13-A	159	 88% 6% 6%
1	130-A	159	 88% 11% .
1	131-A	159	 89% 8% .
1	132-A	159	 90% 8% .
1	133-A	159	 92% 6% .
1	134-A	159	 88% 11% .
1	135-A	159	 89% 10% ..
1	136-A	159	 87% 10% .
1	137-A	159	 88% 10% .
1	138-A	159	 89% 9% .
1	139-A	159	 88% 9% .
1	14-A	159	 90% 8% .
1	140-A	159	 90% 9% .
1	141-A	159	 86% 11% .
1	142-A	159	 87% 10% .
1	143-A	159	 86% 11% ..
1	144-A	159	 85% 10% 5%
1	145-A	159	 84% 14% .
1	146-A	159	 89% 6% .
1	147-A	159	 87% 11% .
1	148-A	159	 89% 8% .
1	149-A	159	 84% 14% .
1	15-A	159	 89% 11% .
1	150-A	159	 87% 8% ..
1	151-A	159	 86% 11% .


























Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	152-A	159	 87% 9% . .
1	153-A	159	 86% 10% .
1	154-A	159	 88% 11% .
1	155-A	159	 86% 11% .
1	156-A	159	 86% 11% .
1	157-A	159	 87% 11% .
1	158-A	159	 86% 13% .
1	159-A	159	 89% 10% .
1	16-A	159	 88% 11% .
1	160-A	159	 88% 11% .
1	161-A	159	 84% 13% . .
1	162-A	159	 84% 15% .
1	163-A	159	 86% 11% .
1	164-A	159	 85% 14% .
1	165-A	159	 84% 14% .
1	166-A	159	 88% 11% .
1	167-A	159	 87% 10% . .
1	168-A	159	 86% 10% .
1	169-A	159	 86% 12% .
1	17-A	159	 89% 8% .
1	170-A	159	 85% 13% .
1	171-A	159	 89% 9% .
1	172-A	159	 86% 13% .
1	173-A	159	 89% 8% .
1	174-A	159	 87% 9% .















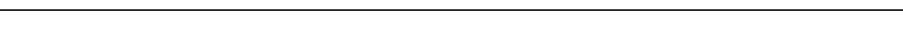




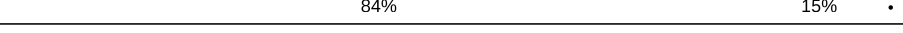





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	175-A	159	 85%12% .
1	176-A	159	 87%10% .
1	177-A	159	 87%9% .
1	178-A	159	 86%9%6%
1	179-A	159	 82%13% . .
1	18-A	159	 86%12% .
1	180-A	159	 83%14% .
1	181-A	159	 83%14% .
1	182-A	159	 86%12% .
1	183-A	159	 83%13% .
1	184-A	159	 86%11% .
1	185-A	159	 86%11% . .
1	186-A	159	 87%9% .
1	187-A	159	 86%9% . .
1	188-A	159	 85%12% . .
1	189-A	159	 87%11% .
1	19-A	159	 89%9% .
1	190-A	159	 87%11% .
1	191-A	159	 86%9%5%
1	192-A	159	 86%13% .
1	193-A	159	 87%13% .
1	194-A	159	 88%11% . .
1	195-A	159	 86%12% .
1	196-A	159	 86%9% . .
1	197-A	159	 87%10% .

















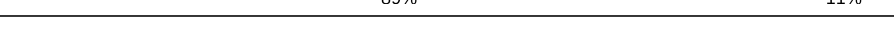

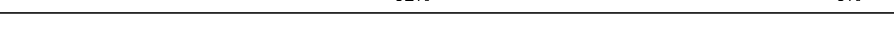
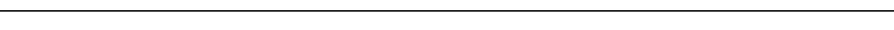
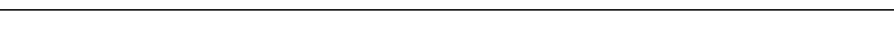
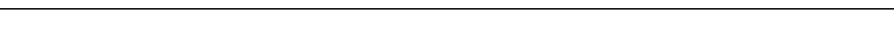
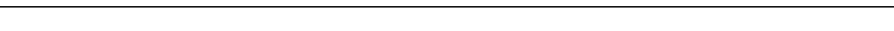
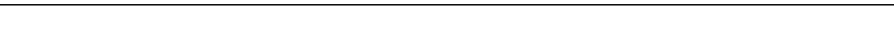

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	198-A	159	 85% 14% .
1	199-A	159	 87% 9% .
1	2-A	159	 85% 13% .
1	20-A	159	 91% 6% .
1	200-A	159	 87% 11% .
1	201-A	159	 86% 14% .
1	202-A	159	 86% 14% .
1	203-A	159	 88% 9% .
1	204-A	159	 86% 11% .
1	205-A	159	 89% 8% .
1	206-A	159	 86% 8% 5% .
1	207-A	159	 87% 9% . .
1	208-A	159	 85% 11% .
1	209-A	159	 84% 13% . .
1	21-A	159	 89% 8% .
1	210-A	159	 85% 13% . .
1	211-A	159	 84% 13% . .
1	212-A	159	 87% 10% .
1	213-A	159	 84% 15% .
1	214-A	159	 84% 13% . .
1	215-A	159	 89% 8% .
1	216-A	159	 87% 10% . .
1	217-A	159	 85% 10% 5%
1	218-A	159	 83% 14% . .
1	219-A	159	 86% 11% .















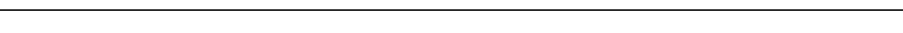




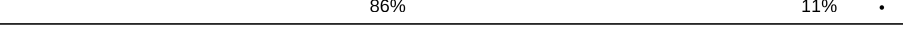





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	22-A	159	 86% 12% .
1	220-A	159	 86% 11% .
1	221-A	159	 86% 9% . .
1	222-A	159	 87% 9% . .
1	223-A	159	 87% 8% . .
1	224-A	159	 91% 6% .
1	225-A	159	 88% 9% .
1	226-A	159	 89% 10% .
1	227-A	159	 87% 10% .
1	228-A	159	 91% 7% .
1	229-A	159	 91% 7% .
1	23-A	159	 91% 8% .
1	230-A	159	 91% . 5%
1	231-A	159	 92% 6% .
1	232-A	159	 90% 9% .
1	233-A	159	 90% 9% . .
1	234-A	159	 89% 11%
1	235-A	159	 91% 9% .
1	236-A	159	 92% 6% .
1	237-A	159	 89% 9% .
1	238-A	159	 87% 13% .
1	239-A	159	 91% 8% .
1	24-A	159	 89% 9% . .
1	240-A	159	 89% 9% .
1	241-A	159	 90% 9% .















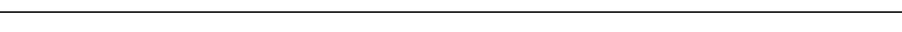

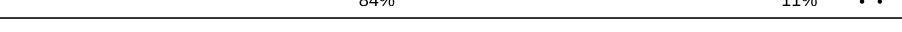

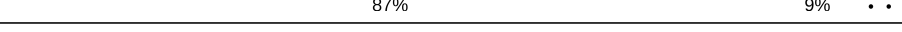






Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	242-A	159	 88% 11% .
1	243-A	159	 90% 8% .
1	244-A	159	 90% 9% .
1	245-A	159	 88% 10% .
1	246-A	159	 83% 17%
1	247-A	159	 87% 11% .
1	248-A	159	 86% 13% .
1	249-A	159	 88% 8% .
1	25-A	159	 89% 8% .
1	250-A	159	 87% 11% .
1	26-A	159	 86% 14%
1	27-A	159	 89% 10% .
1	28-A	159	 84% 13% .
1	29-A	159	 88% 10% .
1	3-A	159	 86% 9% . .
1	30-A	159	 86% 12% .
1	31-A	159	 87% 12% .
1	32-A	159	 89% 9% .
1	33-A	159	 86% 11% .
1	34-A	159	 87% 8% . .
1	35-A	159	 84% 11% . .
1	36-A	159	 88% 9% .
1	37-A	159	 88% 11% .
1	38-A	159	 89% 7% .
1	39-A	159	 87% 11% .















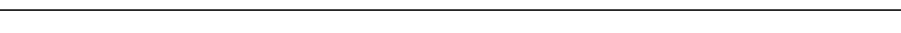




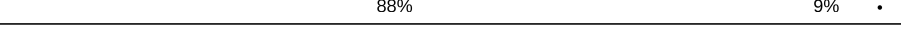





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	4-A	159	 89% 11% .
1	40-A	159	 86% 12% .
1	41-A	159	 83% 13% .
1	42-A	159	 84% 12% .
1	43-A	159	 86% 11% .
1	44-A	159	 89% 8% .
1	45-A	159	 88% 9% .
1	46-A	159	 92% 6% .
1	47-A	159	 87% 9% .
1	48-A	159	 89% 9% ..
1	49-A	159	 87% 11% .
1	5-A	159	 83% 13% .
1	50-A	159	 87% 9% .
1	51-A	159	 86% 11% .
1	52-A	159	 89% 9% ..
1	53-A	159	 84% 11% ..
1	54-A	159	 86% 12% ..
1	55-A	159	 87% 9% ..
1	56-A	159	 86% 10% ..
1	57-A	159	 84% 10% 5% .
1	58-A	159	 86% 10% ..
1	59-A	159	 86% 9% ..
1	6-A	159	 83% 14% .
1	60-A	159	 87% 11% .
1	61-A	159	 87% 9% ..














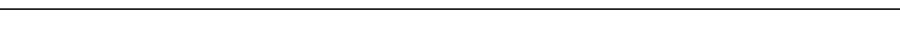

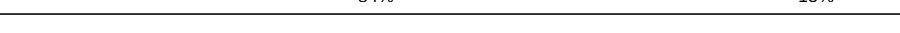
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	62-A	159	 85% 13% .
1	63-A	159	 84% 13% . .
1	64-A	159	 85% 12% .
1	65-A	159	 86% 10% .
1	66-A	159	 87% 7% . .
1	67-A	159	 84% 9% 6% .
1	68-A	159	 86% 11% .
1	69-A	159	 86% 12% .
1	7-A	159	 83% 14% .
1	70-A	159	 87% 9% .
1	71-A	159	 87% 11% .
1	72-A	159	 87% 11% .
1	73-A	159	 86% 10% .
1	74-A	159	 86% 11% .
1	75-A	159	 84% 13% .
1	76-A	159	 85% 13% .
1	77-A	159	 89% 7% .
1	78-A	159	 87% 12% .
1	79-A	159	 88% 9% .
1	8-A	159	 86% 13% .
1	80-A	159	 89% 10% .
1	81-A	159	 86% 11% .
1	82-A	159	 87% 9% .
1	83-A	159	 84% 13% .
1	84-A	159	 87% 11% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	85-A	159	 86% 11% .
1	86-A	159	 86% 11% . .
1	87-A	159	 89% 9% .
1	88-A	159	 85% 11% .
1	89-A	159	 88% 10% .
1	9-A	159	 86% 12% .
1	90-A	159	 87% 9% . .
1	91-A	159	 84% 11% 6%
1	92-A	159	 87% 10% .
1	93-A	159	 89% 9% .
1	94-A	159	 87% 10% .
1	95-A	159	 86% 13% .
1	96-A	159	 87% 11% .
1	97-A	159	 86% 13% .
1	98-A	159	 84% 15% .
1	99-A	159	 89% 9% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 699880 atoms, of which 315750 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 Dihydrofolate reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	2-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	3-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	4-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	5-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	6-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	7-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	8-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	9-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	10-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	11-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	12-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	13-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	14-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	15-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	16-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	18-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	19-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	20-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	21-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	22-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	23-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	24-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	25-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	26-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	27-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	28-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	29-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	30-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	31-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	32-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	33-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	34-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	35-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	36-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	37-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	38-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	39-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	40-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	41-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	42-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	43-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	44-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	45-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	46-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	47-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	48-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	49-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	50-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	51-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	52-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	53-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	54-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	55-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	56-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	57-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	58-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	59-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	60-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	61-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	62-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	63-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	64-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	65-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	66-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	67-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	68-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	69-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	70-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	71-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	72-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	73-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	74-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	75-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	76-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	77-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	78-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	79-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	80-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	81-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	82-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	83-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	84-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	85-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	86-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	87-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	88-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	89-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	90-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	91-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	92-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	93-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	94-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	95-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	96-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	97-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	98-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	99-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	100-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	101-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	102-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	103-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	104-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	105-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	106-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	107-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	108-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	109-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	110-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	111-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	112-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	113-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	114-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	115-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	116-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	117-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	118-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	119-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	120-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	121-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	122-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	123-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	124-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	125-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	126-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	127-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	128-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	129-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	130-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	131-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	132-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	133-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	134-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	135-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	136-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	137-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	138-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	139-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	140-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	141-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	142-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	143-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	144-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	145-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	146-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	147-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	148-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	149-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	150-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	151-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	152-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	153-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	154-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	155-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	156-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	157-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	158-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	159-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	160-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	161-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	162-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	163-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	164-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	165-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	166-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	167-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	168-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	169-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	170-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	171-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	172-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	173-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	174-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	175-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	176-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	177-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	178-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	179-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	180-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	181-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	182-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	183-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	184-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	185-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	186-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	187-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	188-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	189-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	190-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	191-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	192-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	193-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	194-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	195-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	196-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	197-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	198-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	199-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	200-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	201-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	202-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	203-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	204-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	205-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	206-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	207-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	208-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	209-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	210-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	211-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	212-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	213-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	214-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	215-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	216-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	217-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	218-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	219-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	220-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	221-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	222-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	223-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	224-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	225-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	226-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			

Continued on next page...

Continued from previous page...

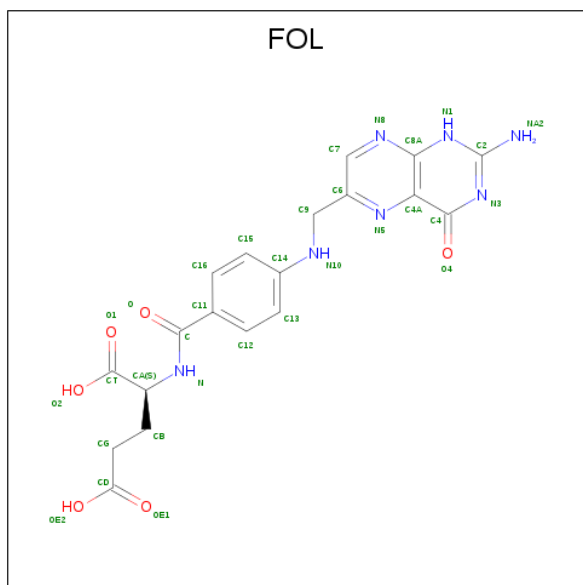
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	227-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	228-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	229-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	230-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	231-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	232-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	233-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	234-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	235-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	236-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	237-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	238-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	239-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	240-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	241-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	242-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	243-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	244-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	245-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	246-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	247-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	248-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	249-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	250-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			

- Molecule 2 is FOLIC ACID (three-letter code: FOL) (formula: $C_{19}H_{19}N_7O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	1-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	2-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	3-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	4-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	5-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	6-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	7-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	8-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	9-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	10-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	11-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	12-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	13-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	14-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	15-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	16-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	17-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	18-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	19-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	20-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	21-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	22-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	23-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	24-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	25-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	26-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	27-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	28-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	29-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	30-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	31-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	32-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	33-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	34-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	35-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	36-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	37-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	38-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	39-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	40-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	41-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	42-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	43-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	44-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	45-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	46-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	47-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	48-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	49-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	50-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	51-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	52-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	53-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	54-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	55-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	56-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	57-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	58-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	59-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	60-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	61-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	62-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	63-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	64-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	65-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	66-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	67-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	68-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	69-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	70-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	71-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	72-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	73-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	74-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	75-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	76-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	77-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	78-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	79-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	80-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	81-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	82-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	83-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	84-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	85-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	86-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	87-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	88-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	89-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	90-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	91-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	92-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	93-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	94-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	95-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	96-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	97-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	98-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	99-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	100-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	101-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	102-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	103-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	104-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	105-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	106-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	107-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	108-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	109-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	110-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	111-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	112-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	113-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	114-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	115-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	116-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	117-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	118-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	119-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	120-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	121-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	122-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	123-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	124-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	125-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	126-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	127-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	128-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	129-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	130-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	131-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	132-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	133-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	134-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	135-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	136-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	137-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	138-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	139-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	140-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	141-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	142-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	143-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	144-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	145-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	146-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	147-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	148-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	149-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	150-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	151-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	152-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	153-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	154-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	155-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	156-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	157-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	158-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	159-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	160-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	161-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	162-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	163-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	164-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	165-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	166-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	167-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	168-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	169-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	170-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	171-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	172-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	173-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	174-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	175-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	176-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	177-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	178-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	179-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	180-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	181-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	182-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	183-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	184-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	185-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	186-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	187-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	188-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	189-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	190-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	191-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	192-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	193-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	194-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	195-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	196-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	197-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	198-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	199-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	200-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	201-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	202-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	203-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	204-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	205-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	206-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	207-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	208-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	209-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	210-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	211-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	212-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	213-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	214-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	215-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	216-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	217-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	218-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

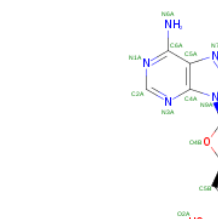
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	219-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	220-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	221-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	222-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	223-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	224-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	225-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	226-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	227-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	228-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	229-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	230-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	231-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	232-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	233-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	234-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	235-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	236-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	237-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	238-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	239-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

Continued on next page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	240-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	241-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	242-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	243-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	244-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	245-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	246-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	247-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	248-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	249-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	250-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

- 
- The chemical structure of Naproxen is shown. It consists of a naphthalene ring system. One ring has an amine group (-NH₂) at position 1 and a carboxylic acid group (-COOH) at position 2. The other ring has a carboxylic acid group (-COOH) at position 6 and a carboxylic acid group (-COOH) at position 7. The structure is labeled with 'NAP' and 'NAP'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	1-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	2-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	3-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	4-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	5-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	6-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	7-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	8-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	9-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	10-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	11-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	12-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	13-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	14-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	15-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	16-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	17-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	18-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	19-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	20-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	21-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	22-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	23-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	24-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	25-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	26-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	27-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	28-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	29-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	30-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	31-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	32-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	33-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	34-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	35-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	36-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	37-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	38-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	39-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	40-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	41-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	42-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	43-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	44-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	45-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	46-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	47-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	48-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	49-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	50-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	51-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	52-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	53-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	54-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	55-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	56-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	57-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	58-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	59-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	60-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	61-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	62-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	63-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	64-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	65-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	66-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	67-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	68-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	69-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	70-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	71-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	72-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	73-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	74-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	75-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	76-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	77-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	78-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	79-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	80-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	81-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	82-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	83-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	84-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	85-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	86-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	87-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	88-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	89-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	90-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	91-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	92-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	93-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	94-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	95-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	96-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	97-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	98-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	99-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	100-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	101-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	102-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	103-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	104-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	105-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	106-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	107-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	108-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	109-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	110-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	111-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	112-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	113-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	114-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	115-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	116-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	117-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	118-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	119-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	120-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	121-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	122-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	123-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	124-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	125-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	126-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	127-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	128-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	129-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	130-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	131-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	132-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	133-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	134-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	135-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	136-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	137-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	138-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	139-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	140-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	141-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	142-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	143-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	144-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	145-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	146-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	147-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	148-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	149-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	150-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	151-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	152-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	153-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	154-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	155-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	156-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	157-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	158-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	159-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	160-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	161-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	162-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	163-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	164-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	165-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	166-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	167-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	168-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	169-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	170-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	171-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	172-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	173-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	174-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	175-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	176-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	177-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	178-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	179-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	180-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	181-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	182-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	183-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	184-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	185-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	186-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	187-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	188-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	189-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	190-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	191-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	192-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	193-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	194-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	195-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	196-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	197-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	198-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	199-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	200-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	201-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	202-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	203-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	204-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	205-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	206-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	207-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	208-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	209-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	210-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	211-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	212-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	213-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	214-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	215-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	216-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	217-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	218-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	219-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	220-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	221-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	222-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	223-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	224-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	225-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	226-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	227-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	228-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	229-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	230-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	231-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	232-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	233-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	234-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	235-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	236-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	237-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	238-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	239-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	240-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	241-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	242-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	243-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	244-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	245-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	246-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	247-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	248-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	249-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	250-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	122-A	2	Total	Mn	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	216-A	2	Total 2	Mn 2	0	0
4	110-A	2	Total 2	Mn 2	0	0
4	37-A	2	Total 2	Mn 2	0	0
4	80-A	2	Total 2	Mn 2	0	0
4	94-A	2	Total 2	Mn 2	0	0
4	167-A	2	Total 2	Mn 2	0	0
4	162-A	2	Total 2	Mn 2	0	0
4	60-A	2	Total 2	Mn 2	0	0
4	148-A	2	Total 2	Mn 2	0	0
4	123-A	2	Total 2	Mn 2	0	0
4	44-A	2	Total 2	Mn 2	0	0
4	150-A	2	Total 2	Mn 2	0	0
4	128-A	2	Total 2	Mn 2	0	0
4	135-A	2	Total 2	Mn 2	0	0
4	50-A	2	Total 2	Mn 2	0	0
4	138-A	2	Total 2	Mn 2	0	0
4	177-A	2	Total 2	Mn 2	0	0
4	211-A	2	Total 2	Mn 2	0	0
4	104-A	2	Total 2	Mn 2	0	0
4	225-A	2	Total 2	Mn 2	0	0
4	191-A	2	Total 2	Mn 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	12-A	2	Total 2	Mn 2	0	0
4	188-A	2	Total 2	Mn 2	0	0
4	114-A	2	Total 2	Mn 2	0	0
4	19-A	2	Total 2	Mn 2	0	0
4	165-A	2	Total 2	Mn 2	0	0
4	73-A	2	Total 2	Mn 2	0	0
4	202-A	2	Total 2	Mn 2	0	0
4	1-A	2	Total 2	Mn 2	0	0
4	53-A	2	Total 2	Mn 2	0	0
4	143-A	2	Total 2	Mn 2	0	0
4	230-A	2	Total 2	Mn 2	0	0
4	178-A	2	Total 2	Mn 2	0	0
4	25-A	2	Total 2	Mn 2	0	0
4	131-A	2	Total 2	Mn 2	0	0
4	32-A	2	Total 2	Mn 2	0	0
4	169-A	2	Total 2	Mn 2	0	0
4	93-A	2	Total 2	Mn 2	0	0
4	183-A	2	Total 2	Mn 2	0	0
4	173-A	2	Total 2	Mn 2	0	0
4	172-A	2	Total 2	Mn 2	0	0
4	77-A	2	Total 2	Mn 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	161-A	2	Total 2	Mn 2	0	0
4	58-A	2	Total 2	Mn 2	0	0
4	130-A	2	Total 2	Mn 2	0	0
4	57-A	2	Total 2	Mn 2	0	0
4	186-A	2	Total 2	Mn 2	0	0
4	243-A	2	Total 2	Mn 2	0	0
4	29-A	2	Total 2	Mn 2	0	0
4	212-A	2	Total 2	Mn 2	0	0
4	101-A	2	Total 2	Mn 2	0	0
4	3-A	2	Total 2	Mn 2	0	0
4	194-A	2	Total 2	Mn 2	0	0
4	11-A	2	Total 2	Mn 2	0	0
4	84-A	2	Total 2	Mn 2	0	0
4	98-A	2	Total 2	Mn 2	0	0
4	238-A	2	Total 2	Mn 2	0	0
4	144-A	2	Total 2	Mn 2	0	0
4	235-A	2	Total 2	Mn 2	0	0
4	127-A	2	Total 2	Mn 2	0	0
4	154-A	2	Total 2	Mn 2	0	0
4	224-A	2	Total 2	Mn 2	0	0
4	108-A	2	Total 2	Mn 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	16-A	2	Total 2	Mn 2	0	0
4	65-A	2	Total 2	Mn 2	0	0
4	117-A	2	Total 2	Mn 2	0	0
4	175-A	2	Total 2	Mn 2	0	0
4	209-A	2	Total 2	Mn 2	0	0
4	41-A	2	Total 2	Mn 2	0	0
4	5-A	2	Total 2	Mn 2	0	0
4	8-A	2	Total 2	Mn 2	0	0
4	21-A	2	Total 2	Mn 2	0	0
4	109-A	2	Total 2	Mn 2	0	0
4	217-A	2	Total 2	Mn 2	0	0
4	102-A	2	Total 2	Mn 2	0	0
4	201-A	2	Total 2	Mn 2	0	0
4	113-A	2	Total 2	Mn 2	0	0
4	36-A	2	Total 2	Mn 2	0	0
4	81-A	2	Total 2	Mn 2	0	0
4	221-A	2	Total 2	Mn 2	0	0
4	160-A	2	Total 2	Mn 2	0	0
4	97-A	2	Total 2	Mn 2	0	0
4	187-A	2	Total 2	Mn 2	0	0
4	203-A	2	Total 2	Mn 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	61-A	2	Total 2	Mn 2	0	0
4	149-A	2	Total 2	Mn 2	0	0
4	48-A	2	Total 2	Mn 2	0	0
4	124-A	2	Total 2	Mn 2	0	0
4	45-A	2	Total 2	Mn 2	0	0
4	153-A	2	Total 2	Mn 2	0	0
4	129-A	2	Total 2	Mn 2	0	0
4	134-A	2	Total 2	Mn 2	0	0
4	35-A	2	Total 2	Mn 2	0	0
4	220-A	2	Total 2	Mn 2	0	0
4	227-A	2	Total 2	Mn 2	0	0
4	105-A	2	Total 2	Mn 2	0	0
4	7-A	2	Total 2	Mn 2	0	0
4	190-A	2	Total 2	Mn 2	0	0
4	15-A	2	Total 2	Mn 2	0	0
4	189-A	2	Total 2	Mn 2	0	0
4	88-A	2	Total 2	Mn 2	0	0
4	18-A	2	Total 2	Mn 2	0	0
4	72-A	2	Total 2	Mn 2	0	0
4	206-A	2	Total 2	Mn 2	0	0
4	159-A	2	Total 2	Mn 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	52-A	2	Total 2	Mn 2	0	0
4	140-A	2	Total 2	Mn 2	0	0
4	231-A	2	Total 2	Mn 2	0	0
4	207-A	2	Total 2	Mn 2	0	0
4	26-A	2	Total 2	Mn 2	0	0
4	120-A	2	Total 2	Mn 2	0	0
4	118-A	2	Total 2	Mn 2	0	0
4	89-A	2	Total 2	Mn 2	0	0
4	31-A	2	Total 2	Mn 2	0	0
4	82-A	2	Total 2	Mn 2	0	0
4	229-A	2	Total 2	Mn 2	0	0
4	199-A	2	Total 2	Mn 2	0	0
4	92-A	2	Total 2	Mn 2	0	0
4	180-A	2	Total 2	Mn 2	0	0
4	171-A	2	Total 2	Mn 2	0	0
4	76-A	2	Total 2	Mn 2	0	0
4	46-A	2	Total 2	Mn 2	0	0
4	137-A	2	Total 2	Mn 2	0	0
4	56-A	2	Total 2	Mn 2	0	0
4	242-A	2	Total 2	Mn 2	0	0
4	213-A	2	Total 2	Mn 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	106-A	2	Total 2	Mn 2	0	0
4	185-A	2	Total 2	Mn 2	0	0
4	10-A	2	Total 2	Mn 2	0	0
4	85-A	2	Total 2	Mn 2	0	0
4	218-A	2	Total 2	Mn 2	0	0
4	239-A	2	Total 2	Mn 2	0	0
4	247-A	2	Total 2	Mn 2	0	0
4	145-A	2	Total 2	Mn 2	0	0
4	236-A	2	Total 2	Mn 2	0	0
4	157-A	2	Total 2	Mn 2	0	0
4	226-A	2	Total 2	Mn 2	0	0
4	39-A	2	Total 2	Mn 2	0	0
4	133-A	2	Total 2	Mn 2	0	0
4	91-A	2	Total 2	Mn 2	0	0
4	66-A	2	Total 2	Mn 2	0	0
4	174-A	2	Total 2	Mn 2	0	0
4	208-A	2	Total 2	Mn 2	0	0
4	79-A	2	Total 2	Mn 2	0	0
4	246-A	2	Total 2	Mn 2	0	0
4	55-A	2	Total 2	Mn 2	0	0
4	22-A	2	Total 2	Mn 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	241-A	2	Total 2	Mn 2	0	0
4	214-A	2	Total 2	Mn 2	0	0
4	103-A	2	Total 2	Mn 2	0	0
4	223-A	2	Total 2	Mn 2	0	0
4	112-A	2	Total 2	Mn 2	0	0
4	86-A	2	Total 2	Mn 2	0	0
4	96-A	2	Total 2	Mn 2	0	0
4	184-A	2	Total 2	Mn 2	0	0
4	62-A	2	Total 2	Mn 2	0	0
4	146-A	2	Total 2	Mn 2	0	0
4	49-A	2	Total 2	Mn 2	0	0
4	204-A	2	Total 2	Mn 2	0	0
4	125-A	2	Total 2	Mn 2	0	0
4	42-A	2	Total 2	Mn 2	0	0
4	152-A	2	Total 2	Mn 2	0	0
4	119-A	2	Total 2	Mn 2	0	0
4	34-A	2	Total 2	Mn 2	0	0
4	245-A	2	Total 2	Mn 2	0	0
4	193-A	2	Total 2	Mn 2	0	0
4	14-A	2	Total 2	Mn 2	0	0
4	179-A	2	Total 2	Mn 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	63-A	2	Total 2	Mn 2	0	0
4	68-A	2	Total 2	Mn 2	0	0
4	71-A	2	Total 2	Mn 2	0	0
4	158-A	2	Total 2	Mn 2	0	0
4	141-A	2	Total 2	Mn 2	0	0
4	232-A	2	Total 2	Mn 2	0	0
4	27-A	2	Total 2	Mn 2	0	0
4	163-A	2	Total 2	Mn 2	0	0
4	121-A	2	Total 2	Mn 2	0	0
4	219-A	2	Total 2	Mn 2	0	0
4	111-A	2	Total 2	Mn 2	0	0
4	30-A	2	Total 2	Mn 2	0	0
4	83-A	2	Total 2	Mn 2	0	0
4	228-A	2	Total 2	Mn 2	0	0
4	198-A	2	Total 2	Mn 2	0	0
4	95-A	2	Total 2	Mn 2	0	0
4	2-A	2	Total 2	Mn 2	0	0
4	9-A	2	Total 2	Mn 2	0	0
4	170-A	2	Total 2	Mn 2	0	0
4	244-A	2	Total 2	Mn 2	0	0
4	75-A	2	Total 2	Mn 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	47-A	2	Total 2	Mn 2	0	0
4	151-A	2	Total 2	Mn 2	0	0
4	136-A	2	Total 2	Mn 2	0	0
4	51-A	2	Total 2	Mn 2	0	0
4	250-A	2	Total 2	Mn 2	0	0
4	139-A	2	Total 2	Mn 2	0	0
4	210-A	2	Total 2	Mn 2	0	0
4	107-A	2	Total 2	Mn 2	0	0
4	196-A	2	Total 2	Mn 2	0	0
4	13-A	2	Total 2	Mn 2	0	0
4	115-A	2	Total 2	Mn 2	0	0
4	74-A	2	Total 2	Mn 2	0	0
4	248-A	2	Total 2	Mn 2	0	0
4	142-A	2	Total 2	Mn 2	0	0
4	237-A	2	Total 2	Mn 2	0	0
4	181-A	2	Total 2	Mn 2	0	0
4	24-A	2	Total 2	Mn 2	0	0
4	156-A	2	Total 2	Mn 2	0	0
4	4-A	2	Total 2	Mn 2	0	0
4	38-A	2	Total 2	Mn 2	0	0
4	132-A	2	Total 2	Mn 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	33-A	2	Total 2	Mn 2	0	0
4	116-A	2	Total 2	Mn 2	0	0
4	176-A	2	Total 2	Mn 2	0	0
4	168-A	2	Total 2	Mn 2	0	0
4	164-A	2	Total 2	Mn 2	0	0
4	90-A	2	Total 2	Mn 2	0	0
4	182-A	2	Total 2	Mn 2	0	0
4	67-A	2	Total 2	Mn 2	0	0
4	166-A	2	Total 2	Mn 2	0	0
4	205-A	2	Total 2	Mn 2	0	0
4	78-A	2	Total 2	Mn 2	0	0
4	59-A	2	Total 2	Mn 2	0	0
4	54-A	2	Total 2	Mn 2	0	0
4	23-A	2	Total 2	Mn 2	0	0
4	240-A	2	Total 2	Mn 2	0	0
4	28-A	2	Total 2	Mn 2	0	0
4	215-A	2	Total 2	Mn 2	0	0
4	100-A	2	Total 2	Mn 2	0	0
4	195-A	2	Total 2	Mn 2	0	0
4	200-A	2	Total 2	Mn 2	0	0
4	87-A	2	Total 2	Mn 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	249-A	2	Total 2	Mn 2	0	0
4	99-A	2	Total 2	Mn 2	0	0
4	6-A	2	Total 2	Mn 2	0	0
4	197-A	2	Total 2	Mn 2	0	0
4	147-A	2	Total 2	Mn 2	0	0
4	234-A	2	Total 2	Mn 2	0	0
4	126-A	2	Total 2	Mn 2	0	0
4	43-A	2	Total 2	Mn 2	0	0
4	155-A	2	Total 2	Mn 2	0	0
4	222-A	2	Total 2	Mn 2	0	0
4	192-A	2	Total 2	Mn 2	0	0
4	17-A	2	Total 2	Mn 2	0	0
4	64-A	2	Total 2	Mn 2	0	0
4	69-A	2	Total 2	Mn 2	0	0
4	70-A	2	Total 2	Mn 2	0	0
4	40-A	2	Total 2	Mn 2	0	0
4	233-A	2	Total 2	Mn 2	0	0
4	20-A	2	Total 2	Mn 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1-A	180	Total 180	O 180	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	2-A	171	Total 171	O 171	0	0
5	3-A	185	Total 185	O 185	0	0
5	4-A	189	Total 189	O 189	0	0
5	5-A	176	Total 176	O 176	0	0
5	6-A	189	Total 189	O 189	0	0
5	7-A	179	Total 179	O 179	0	0
5	8-A	196	Total 196	O 196	0	0
5	9-A	198	Total 198	O 198	0	0
5	10-A	197	Total 197	O 197	0	0
5	11-A	199	Total 199	O 199	0	0
5	12-A	191	Total 191	O 191	0	0
5	13-A	176	Total 176	O 176	0	0
5	14-A	191	Total 191	O 191	0	0
5	15-A	197	Total 197	O 197	0	0
5	16-A	183	Total 183	O 183	0	0
5	17-A	177	Total 177	O 177	0	0
5	18-A	170	Total 170	O 170	0	0
5	19-A	173	Total 173	O 173	0	0
5	20-A	179	Total 179	O 179	0	0
5	21-A	185	Total 185	O 185	0	0
5	22-A	195	Total 195	O 195	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	23-A	181	Total 181	O 181	0	0
5	24-A	172	Total 172	O 172	0	0
5	25-A	179	Total 179	O 179	0	0
5	26-A	196	Total 196	O 196	0	0
5	27-A	195	Total 195	O 195	0	0
5	28-A	193	Total 193	O 193	0	0
5	29-A	184	Total 184	O 184	0	0
5	30-A	185	Total 185	O 185	0	0
5	31-A	190	Total 190	O 190	0	0
5	32-A	175	Total 175	O 175	0	0
5	33-A	199	Total 199	O 199	0	0
5	34-A	196	Total 196	O 196	0	0
5	35-A	185	Total 185	O 185	0	0
5	36-A	191	Total 191	O 191	0	0
5	37-A	191	Total 191	O 191	0	0
5	38-A	183	Total 183	O 183	0	0
5	39-A	177	Total 177	O 177	0	0
5	40-A	183	Total 183	O 183	0	0
5	41-A	182	Total 182	O 182	0	0
5	42-A	176	Total 176	O 176	0	0
5	43-A	172	Total 172	O 172	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	44-A	181	Total	O	0	0
			181	181		
5	45-A	194	Total	O	0	0
			194	194		
5	46-A	198	Total	O	0	0
			198	198		
5	47-A	194	Total	O	0	0
			194	194		
5	48-A	177	Total	O	0	0
			177	177		
5	49-A	165	Total	O	0	0
			165	165		
5	50-A	172	Total	O	0	0
			172	172		
5	51-A	171	Total	O	0	0
			171	171		
5	52-A	175	Total	O	0	0
			175	175		
5	53-A	191	Total	O	0	0
			191	191		
5	54-A	185	Total	O	0	0
			185	185		
5	55-A	183	Total	O	0	0
			183	183		
5	56-A	186	Total	O	0	0
			186	186		
5	57-A	187	Total	O	0	0
			187	187		
5	58-A	193	Total	O	0	0
			193	193		
5	59-A	187	Total	O	0	0
			187	187		
5	60-A	178	Total	O	0	0
			178	178		
5	61-A	169	Total	O	0	0
			169	169		
5	62-A	169	Total	O	0	0
			169	169		
5	63-A	179	Total	O	0	0
			179	179		
5	64-A	180	Total	O	0	0
			180	180		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	65-A	189	Total 189	O 189	0	0
5	66-A	194	Total 194	O 194	0	0
5	67-A	170	Total 170	O 170	0	0
5	68-A	174	Total 174	O 174	0	0
5	69-A	193	Total 193	O 193	0	0
5	70-A	199	Total 199	O 199	0	0
5	71-A	176	Total 176	O 176	0	0
5	72-A	172	Total 172	O 172	0	0
5	73-A	175	Total 175	O 175	0	0
5	74-A	185	Total 185	O 185	0	0
5	75-A	186	Total 186	O 186	0	0
5	76-A	183	Total 183	O 183	0	0
5	77-A	192	Total 192	O 192	0	0
5	78-A	192	Total 192	O 192	0	0
5	79-A	178	Total 178	O 178	0	0
5	80-A	181	Total 181	O 181	0	0
5	81-A	178	Total 178	O 178	0	0
5	82-A	188	Total 188	O 188	0	0
5	83-A	189	Total 189	O 189	0	0
5	84-A	189	Total 189	O 189	0	0
5	85-A	179	Total 179	O 179	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	86-A	185	Total 185	O 185	0	0
5	87-A	192	Total 192	O 192	0	0
5	88-A	187	Total 187	O 187	0	0
5	89-A	185	Total 185	O 185	0	0
5	90-A	182	Total 182	O 182	0	0
5	91-A	183	Total 183	O 183	0	0
5	92-A	182	Total 182	O 182	0	0
5	93-A	186	Total 186	O 186	0	0
5	94-A	175	Total 175	O 175	0	0
5	95-A	186	Total 186	O 186	0	0
5	96-A	188	Total 188	O 188	0	0
5	97-A	186	Total 186	O 186	0	0
5	98-A	180	Total 180	O 180	0	0
5	99-A	183	Total 183	O 183	0	0
5	100-A	172	Total 172	O 172	0	0
5	101-A	175	Total 175	O 175	0	0
5	102-A	183	Total 183	O 183	0	0
5	103-A	200	Total 200	O 200	0	0
5	104-A	185	Total 185	O 185	0	0
5	105-A	180	Total 180	O 180	0	0
5	106-A	189	Total 189	O 189	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	107-A	193	Total 193	O 193	0	0
5	108-A	185	Total 185	O 185	0	0
5	109-A	181	Total 181	O 181	0	0
5	110-A	212	Total 212	O 212	0	0
5	111-A	207	Total 207	O 207	0	0
5	112-A	206	Total 206	O 206	0	0
5	113-A	189	Total 189	O 189	0	0
5	114-A	173	Total 173	O 173	0	0
5	115-A	182	Total 182	O 182	0	0
5	116-A	189	Total 189	O 189	0	0
5	117-A	174	Total 174	O 174	0	0
5	118-A	180	Total 180	O 180	0	0
5	119-A	181	Total 181	O 181	0	0
5	120-A	179	Total 179	O 179	0	0
5	121-A	189	Total 189	O 189	0	0
5	122-A	201	Total 201	O 201	0	0
5	123-A	202	Total 202	O 202	0	0
5	124-A	198	Total 198	O 198	0	0
5	125-A	204	Total 204	O 204	0	0
5	126-A	192	Total 192	O 192	0	0
5	127-A	183	Total 183	O 183	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	128-A	184	Total 184	O 184	0	0
5	129-A	186	Total 186	O 186	0	0
5	130-A	196	Total 196	O 196	0	0
5	131-A	176	Total 176	O 176	0	0
5	132-A	187	Total 187	O 187	0	0
5	133-A	183	Total 183	O 183	0	0
5	134-A	182	Total 182	O 182	0	0
5	135-A	193	Total 193	O 193	0	0
5	136-A	185	Total 185	O 185	0	0
5	137-A	185	Total 185	O 185	0	0
5	138-A	181	Total 181	O 181	0	0
5	139-A	167	Total 167	O 167	0	0
5	140-A	173	Total 173	O 173	0	0
5	141-A	186	Total 186	O 186	0	0
5	142-A	206	Total 206	O 206	0	0
5	143-A	187	Total 187	O 187	0	0
5	144-A	178	Total 178	O 178	0	0
5	145-A	171	Total 171	O 171	0	0
5	146-A	174	Total 174	O 174	0	0
5	147-A	171	Total 171	O 171	0	0
5	148-A	176	Total 176	O 176	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	149-A	196	Total 196	O 196	0	0
5	150-A	185	Total 185	O 185	0	0
5	151-A	184	Total 184	O 184	0	0
5	152-A	179	Total 179	O 179	0	0
5	153-A	186	Total 186	O 186	0	0
5	154-A	184	Total 184	O 184	0	0
5	155-A	188	Total 188	O 188	0	0
5	156-A	176	Total 176	O 176	0	0
5	157-A	174	Total 174	O 174	0	0
5	158-A	181	Total 181	O 181	0	0
5	159-A	180	Total 180	O 180	0	0
5	160-A	186	Total 186	O 186	0	0
5	161-A	199	Total 199	O 199	0	0
5	162-A	199	Total 199	O 199	0	0
5	163-A	199	Total 199	O 199	0	0
5	164-A	181	Total 181	O 181	0	0
5	165-A	191	Total 191	O 191	0	0
5	166-A	189	Total 189	O 189	0	0
5	167-A	171	Total 171	O 171	0	0
5	168-A	171	Total 171	O 171	0	0
5	169-A	187	Total 187	O 187	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	170-A	186	Total 186	O 186	0	0
5	171-A	184	Total 184	O 184	0	0
5	172-A	185	Total 185	O 185	0	0
5	173-A	193	Total 193	O 193	0	0
5	174-A	184	Total 184	O 184	0	0
5	175-A	187	Total 187	O 187	0	0
5	176-A	186	Total 186	O 186	0	0
5	177-A	173	Total 173	O 173	0	0
5	178-A	185	Total 185	O 185	0	0
5	179-A	174	Total 174	O 174	0	0
5	180-A	173	Total 173	O 173	0	0
5	181-A	199	Total 199	O 199	0	0
5	182-A	192	Total 192	O 192	0	0
5	183-A	199	Total 199	O 199	0	0
5	184-A	187	Total 187	O 187	0	0
5	185-A	174	Total 174	O 174	0	0
5	186-A	169	Total 169	O 169	0	0
5	187-A	165	Total 165	O 165	0	0
5	188-A	180	Total 180	O 180	0	0
5	189-A	175	Total 175	O 175	0	0
5	190-A	181	Total 181	O 181	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	191-A	192	Total 192	O 192	0	0
5	192-A	191	Total 191	O 191	0	0
5	193-A	190	Total 190	O 190	0	0
5	194-A	193	Total 193	O 193	0	0
5	195-A	194	Total 194	O 194	0	0
5	196-A	186	Total 186	O 186	0	0
5	197-A	167	Total 167	O 167	0	0
5	198-A	174	Total 174	O 174	0	0
5	199-A	184	Total 184	O 184	0	0
5	200-A	190	Total 190	O 190	0	0
5	201-A	189	Total 189	O 189	0	0
5	202-A	171	Total 171	O 171	0	0
5	203-A	185	Total 185	O 185	0	0
5	204-A	188	Total 188	O 188	0	0
5	205-A	185	Total 185	O 185	0	0
5	206-A	186	Total 186	O 186	0	0
5	207-A	199	Total 199	O 199	0	0
5	208-A	186	Total 186	O 186	0	0
5	209-A	179	Total 179	O 179	0	0
5	210-A	179	Total 179	O 179	0	0
5	211-A	176	Total 176	O 176	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	212-A	175	Total 175	O 175	0	0
5	213-A	180	Total 180	O 180	0	0
5	214-A	181	Total 181	O 181	0	0
5	215-A	191	Total 191	O 191	0	0
5	216-A	185	Total 185	O 185	0	0
5	217-A	204	Total 204	O 204	0	0
5	218-A	191	Total 191	O 191	0	0
5	219-A	176	Total 176	O 176	0	0
5	220-A	185	Total 185	O 185	0	0
5	221-A	179	Total 179	O 179	0	0
5	222-A	173	Total 173	O 173	0	0
5	223-A	180	Total 180	O 180	0	0
5	224-A	178	Total 178	O 178	0	0
5	225-A	187	Total 187	O 187	0	0
5	226-A	189	Total 189	O 189	0	0
5	227-A	187	Total 187	O 187	0	0
5	228-A	184	Total 184	O 184	0	0
5	229-A	183	Total 183	O 183	0	0
5	230-A	193	Total 193	O 193	0	0
5	231-A	198	Total 198	O 198	0	0
5	232-A	183	Total 183	O 183	0	0

Continued on next page...

Continued from previous page...


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	233-A	180	Total 180	O 180	0	0
5	234-A	175	Total 175	O 175	0	0
5	235-A	201	Total 201	O 201	0	0
5	236-A	204	Total 204	O 204	0	0
5	237-A	193	Total 193	O 193	0	0
5	238-A	159	Total 159	O 159	0	0
5	239-A	164	Total 164	O 164	0	0
5	240-A	179	Total 179	O 179	0	0
5	241-A	183	Total 183	O 183	0	0
5	242-A	183	Total 183	O 183	0	0
5	243-A	194	Total 194	O 194	0	0
5	244-A	205	Total 205	O 205	0	0
5	245-A	198	Total 198	O 198	0	0
5	246-A	166	Total 166	O 166	0	0
5	247-A	171	Total 171	O 171	0	0
5	248-A	171	Total 171	O 171	0	0
5	249-A	191	Total 191	O 191	0	0
5	250-A	202	Total 202	O 202	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.


Note EDS failed to run properly.

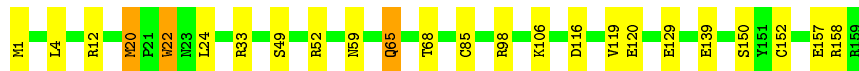
- Molecule 1: Dihydrofolate reductase

Chain 1-A:  88% 9% ..




- Molecule 1: Dihydrofolate reductase

Chain 2-A:  85% 13% .



- Molecule 1: Dihydrofolate reductase

Chain 3-A:  86% 9% ..




- Molecule 1: Dihydrofolate reductase

Chain 4-A:  89% 11% .




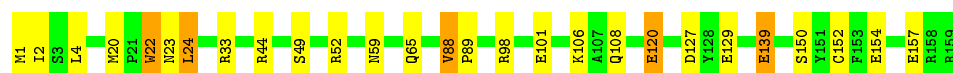
- Molecule 1: Dihydrofolate reductase

Chain 5-A:  83% 13% .




- Molecule 1: Dihydrofolate reductase

Chain 6-A:  83% 14%



- Molecule 1: Dihydrofolate reductase

Chain 7-A:  83% 14%




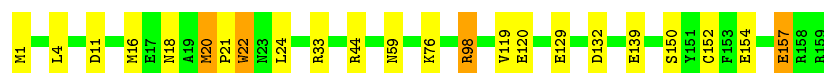
- Molecule 1: Dihydrofolate reductase

Chain 8-A:  86% 13%



- Molecule 1: Dihydrofolate reductase

Chain 9-A:  86% 12%



- Molecule 1: Dihydrofolate reductase

Chain 10-A:  86% 13%



- Molecule 1: Dihydrofolate reductase

Chain 11-A:  89% 8%



- Molecule 1: Dihydrofolate reductase

Chain 12-A:  87% 9%



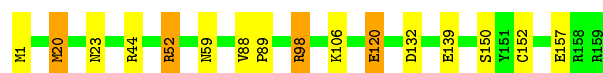
- Molecule 1: Dihydrofolate reductase

Chain 13-A:  88% 6% 6%



- Molecule 1: Dihydrofolate reductase

Chain 14-A:  90% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 15-A:  89% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 16-A:  88% 11% .



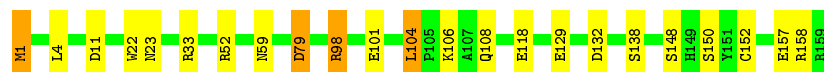
- Molecule 1: Dihydrofolate reductase

Chain 17-A:  89% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 18-A:  86% 12% .



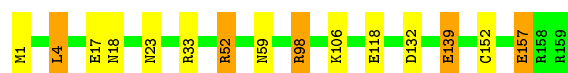
- Molecule 1: Dihydrofolate reductase

Chain 19-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 20-A:  91% 6% •



- Molecule 1: Dihydrofolate reductase

Chain 21-A:  89% 8% •



- Molecule 1: Dihydrofolate reductase

Chain 22-A:  86% 12% •



- Molecule 1: Dihydrofolate reductase

Chain 23-A:  91% 8% •



- Molecule 1: Dihydrofolate reductase

Chain 24-A:  89% 9% ••



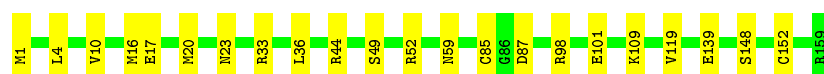
- Molecule 1: Dihydrofolate reductase

Chain 25-A:  89% 8% •



- Molecule 1: Dihydrofolate reductase

Chain 26-A:  86% 14%




- Molecule 1: Dihydrofolate reductase

Chain 27-A:  89% 10% .



- Molecule 1: Dihydrofolate reductase

Chain 28-A:  84% 13% .



- Molecule 1: Dihydrofolate reductase

Chain 29-A:  88% 10% .



- Molecule 1: Dihydrofolate reductase

Chain 30-A:  86% 12% .



- Molecule 1: Dihydrofolate reductase

Chain 31-A:  87% 12% .



- Molecule 1: Dihydrofolate reductase

Chain 32-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 33-A:  86% 11% .




- Molecule 1: Dihydrofolate reductase

Chain 34-A:  87% 8% . .



- Molecule 1: Dihydrofolate reductase

Chain 35-A:  84% 11% . .



- Molecule 1: Dihydrofolate reductase

Chain 36-A:  88% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 37-A:  88% 11% .



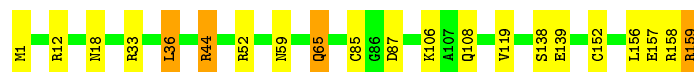
- Molecule 1: Dihydrofolate reductase

Chain 38-A:  89% 7% .



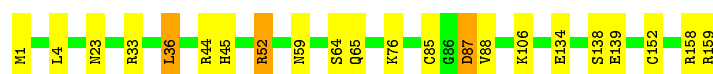
- Molecule 1: Dihydrofolate reductase

Chain 39-A:  87% 11% .




- Molecule 1: Dihydrofolate reductase

Chain 40-A:  86% 12% .




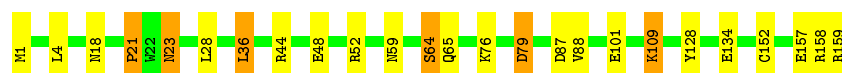
- Molecule 1: Dihydrofolate reductase

Chain 41-A:  83% 13%



- Molecule 1: Dihydrofolate reductase

Chain 42-A:  84% 12%



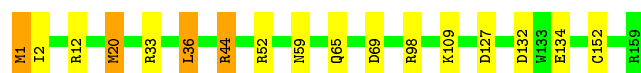
- Molecule 1: Dihydrofolate reductase

Chain 43-A:  86% 11%



- Molecule 1: Dihydrofolate reductase

Chain 44-A:  89% 8%



- Molecule 1: Dihydrofolate reductase

Chain 45-A:  88% 9%



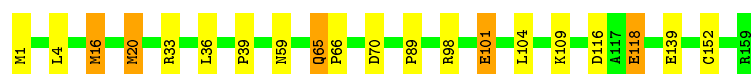
- Molecule 1: Dihydrofolate reductase

Chain 46-A:  92% 6%



- Molecule 1: Dihydrofolate reductase

Chain 47-A:  87% 9%



- Molecule 1: Dihydrofolate reductase

Chain 48-A:  89% 9% ..



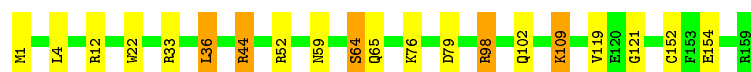
- Molecule 1: Dihydrofolate reductase

Chain 49-A:  87% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 50-A:  87% 9% .



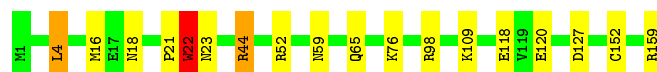
- Molecule 1: Dihydrofolate reductase

Chain 51-A:  86% 11% .



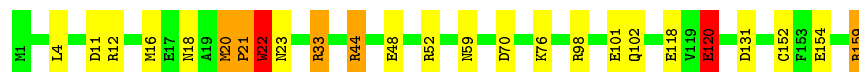
- Molecule 1: Dihydrofolate reductase

Chain 52-A:  89% 9% ..



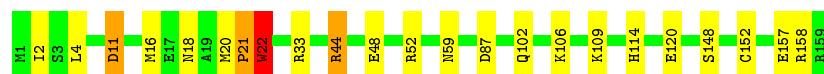
- Molecule 1: Dihydrofolate reductase

Chain 53-A:  84% 11% ..



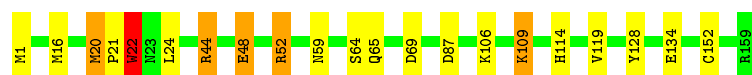
- Molecule 1: Dihydrofolate reductase

Chain 54-A:  86% 12% ..




- Molecule 1: Dihydrofolate reductase

Chain 55-A:  87% 9% . .




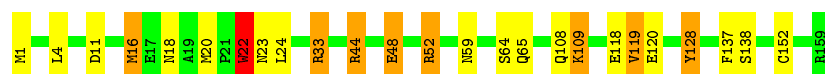
- Molecule 1: Dihydrofolate reductase

Chain 56-A:  86% 10% . .




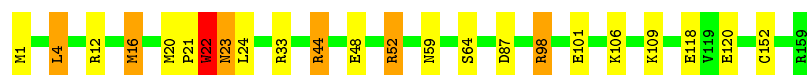
- Molecule 1: Dihydrofolate reductase

Chain 57-A:  84% 10% 5% . .




- Molecule 1: Dihydrofolate reductase

Chain 58-A:  86% 10% . .



- Molecule 1: Dihydrofolate reductase

Chain 59-A:  86% 9% . .



- Molecule 1: Dihydrofolate reductase

Chain 60-A:  87% 11% .




- Molecule 1: Dihydrofolate reductase

Chain 61-A:  87% 9% . .




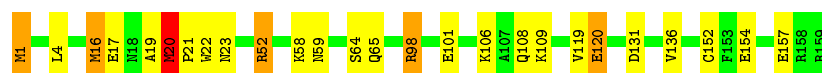
- Molecule 1: Dihydrofolate reductase

Chain 62-A:  85% 13% .




- Molecule 1: Dihydrofolate reductase

Chain 63-A:  84% 13% ..



- Molecule 1: Dihydrofolate reductase

Chain 64-A:  85% 12% .



- Molecule 1: Dihydrofolate reductase

Chain 65-A:  86% 10% .




- Molecule 1: Dihydrofolate reductase

Chain 66-A:  87% 7% ..



- Molecule 1: Dihydrofolate reductase

Chain 67-A:  84% 9% 6% .




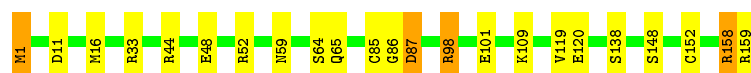
- Molecule 1: Dihydrofolate reductase

Chain 68-A:  86% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 69-A:  86% 12% .



- Molecule 1: Dihydrofolate reductase

Chain 70-A:  87% 9% .



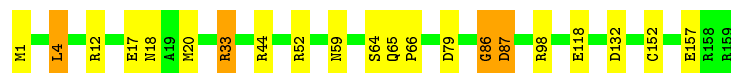
- Molecule 1: Dihydrofolate reductase

Chain 71-A:  87% 11% .




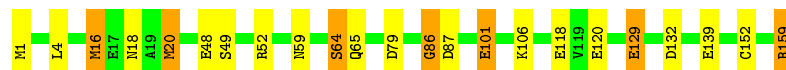
- Molecule 1: Dihydrofolate reductase

Chain 72-A:  87% 11% .




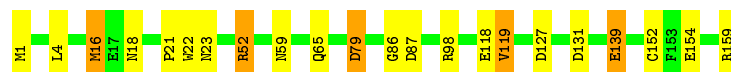
- Molecule 1: Dihydrofolate reductase

Chain 73-A:  86% 10% .




- Molecule 1: Dihydrofolate reductase

Chain 74-A:  86% 11% .




- Molecule 1: Dihydrofolate reductase

Chain 75-A:  84% 13% .



- Molecule 1: Dihydrofolate reductase

Chain 76-A:  85% 13%



- Molecule 1: Dihydrofolate reductase

Chain 77-A:  89% 7%



- Molecule 1: Dihydrofolate reductase

Chain 78-A:  87% 12%



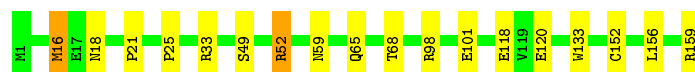
- Molecule 1: Dihydrofolate reductase

Chain 79-A:  88% 9%




- Molecule 1: Dihydrofolate reductase

Chain 80-A:  89% 10%



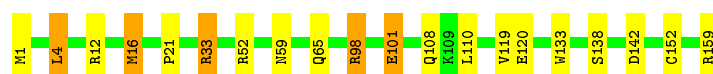
- Molecule 1: Dihydrofolate reductase

Chain 81-A:  86% 11%




- Molecule 1: Dihydrofolate reductase

Chain 82-A:  87% 9%



- Molecule 1: Dihydrofolate reductase

Chain 83-A:  84% 13% •



- Molecule 1: Dihydrofolate reductase

Chain 84-A:  87% 11% •



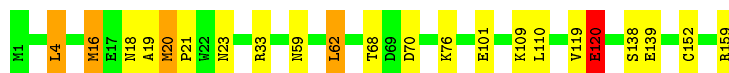
- Molecule 1: Dihydrofolate reductase

Chain 85-A:  86% 11% •



- Molecule 1: Dihydrofolate reductase

Chain 86-A:  86% 11% • •




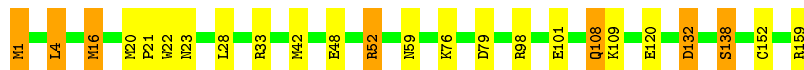
- Molecule 1: Dihydrofolate reductase

Chain 87-A:  89% 9% •



- Molecule 1: Dihydrofolate reductase

Chain 88-A:  85% 11% •



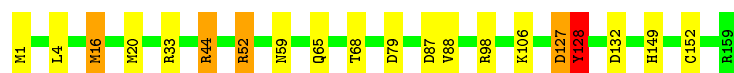
- Molecule 1: Dihydrofolate reductase

Chain 89-A:  88% 10% •




- Molecule 1: Dihydrofolate reductase

Chain 90-A:  87% 9% . .



- Molecule 1: Dihydrofolate reductase

Chain 91-A:  84% 11% 6%



- Molecule 1: Dihydrofolate reductase

Chain 92-A:  87% 10% .



- Molecule 1: Dihydrofolate reductase

Chain 93-A:  89% 9% .



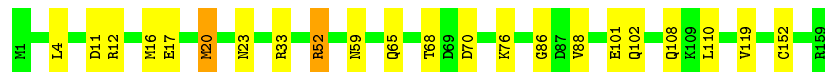
- Molecule 1: Dihydrofolate reductase

Chain 94-A:  87% 10% .



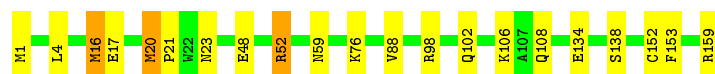
- Molecule 1: Dihydrofolate reductase

Chain 95-A:  86% 13% .




- Molecule 1: Dihydrofolate reductase

Chain 96-A:  87% 11% .




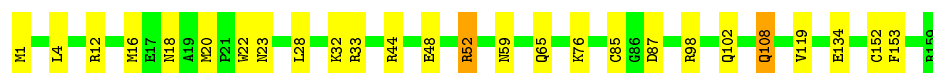
- Molecule 1: Dihydrofolate reductase

Chain 97-A:  86% 13%



- Molecule 1: Dihydrofolate reductase

Chain 98-A:  84% 15%



- Molecule 1: Dihydrofolate reductase

Chain 99-A:  89% 9%



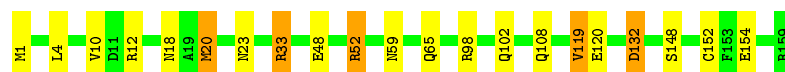
- Molecule 1: Dihydrofolate reductase

Chain 100-A:  86% 11%



- Molecule 1: Dihydrofolate reductase

Chain 101-A:  87% 10%



- Molecule 1: Dihydrofolate reductase

Chain 102-A:  82% 14%



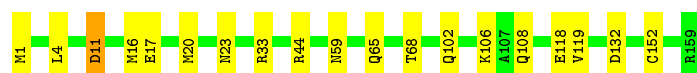
- Molecule 1: Dihydrofolate reductase

Chain 103-A:  91% 8%



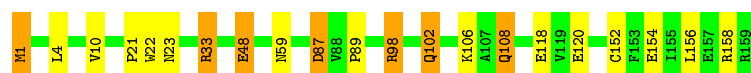
- Molecule 1: Dihydrofolate reductase

Chain 104-A:  88% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 105-A:  87% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 106-A:  88% 12%



- Molecule 1: Dihydrofolate reductase

Chain 107-A:  86% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 108-A:  87% 10% .



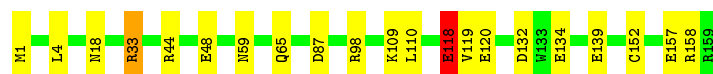
- Molecule 1: Dihydrofolate reductase

Chain 109-A:  84% 13% ..



- Molecule 1: Dihydrofolate reductase

Chain 110-A:  87% 12% ..



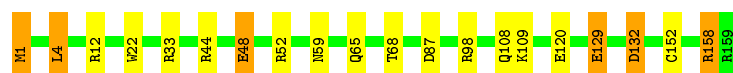
- Molecule 1: Dihydrofolate reductase

Chain 111-A:  87% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 112-A:  87% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 113-A:  89% 11%



- Molecule 1: Dihydrofolate reductase

Chain 114-A:  87% 10% .



- Molecule 1: Dihydrofolate reductase

Chain 115-A:  87% 11% .




- Molecule 1: Dihydrofolate reductase

Chain 116-A:  85% 12% .




- Molecule 1: Dihydrofolate reductase

Chain 117-A:  84% 14% .



- Molecule 1: Dihydrofolate reductase

Chain 118-A:  84% 14% .



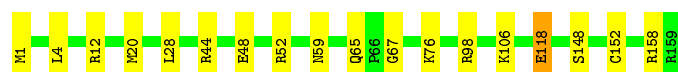
- Molecule 1: Dihydrofolate reductase

Chain 119-A:  87% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 120-A:  89% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 121-A:  87% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 122-A:  92% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 123-A:  90% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 124-A:  92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 125-A:  94% . .



- Molecule 1: Dihydrofolate reductase

Chain 126-A:  92% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 127-A:  86% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 128-A:  89% 7% . .



- Molecule 1: Dihydrofolate reductase

Chain 129-A:  88% 9% .



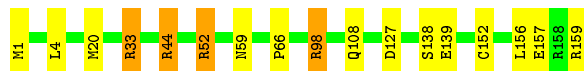
- Molecule 1: Dihydrofolate reductase

Chain 130-A:  88% 11% .




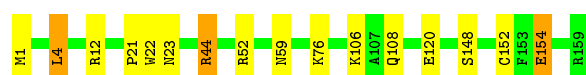
- Molecule 1: Dihydrofolate reductase

Chain 131-A:  89% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 132-A:  90% 8% •



- Molecule 1: Dihydrofolate reductase

Chain 133-A:  92% 6% •



- Molecule 1: Dihydrofolate reductase

Chain 134-A:  88% 11% •



- Molecule 1: Dihydrofolate reductase

Chain 135-A:  89% 10% ••



- Molecule 1: Dihydrofolate reductase

Chain 136-A:  87% 10% •



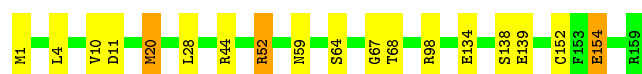
- Molecule 1: Dihydrofolate reductase

Chain 137-A:  88% 10% •



- Molecule 1: Dihydrofolate reductase

Chain 138-A:  89% 9% •



- Molecule 1: Dihydrofolate reductase

Chain 139-A:  88% 9% .



• Molecule 1: Dihydrofolate reductase

Chain 140-A:  90% 9% .



• Molecule 1: Dihydrofolate reductase

Chain 141-A:  86% 11% .



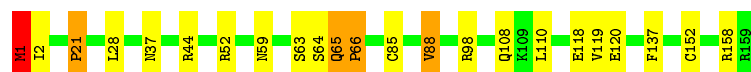
• Molecule 1: Dihydrofolate reductase

Chain 142-A:  87% 10% .



• Molecule 1: Dihydrofolate reductase

Chain 143-A:  86% 11% . .




• Molecule 1: Dihydrofolate reductase

Chain 144-A:  85% 10% 5%




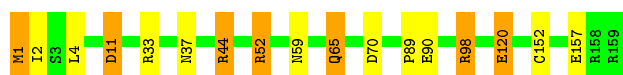
• Molecule 1: Dihydrofolate reductase

Chain 145-A:  84% 14% .



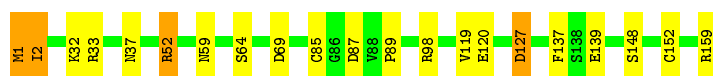
• Molecule 1: Dihydrofolate reductase

Chain 146-A:  89% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 147-A:  87% 11% .



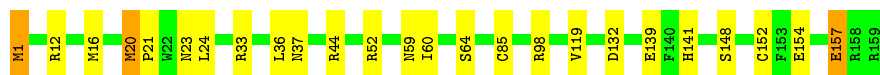
- Molecule 1: Dihydrofolate reductase

Chain 148-A:  89% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 149-A:  84% 14% .



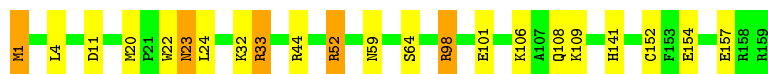
- Molecule 1: Dihydrofolate reductase

Chain 150-A:  87% 8% . .



- Molecule 1: Dihydrofolate reductase

Chain 151-A:  86% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 152-A:  87% 9% . .



- Molecule 1: Dihydrofolate reductase

Chain 153-A:  86% 10% .



- Molecule 1: Dihydrofolate reductase

Chain 154-A:  88% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 155-A:  86% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 156-A:  86% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 157-A:  87% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 158-A:  86% 13% .



- Molecule 1: Dihydrofolate reductase

Chain 159-A:  89% 10% .



- Molecule 1: Dihydrofolate reductase

Chain 160-A:  88% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 161-A:  84% 13% ..



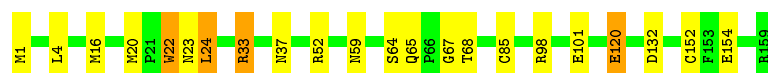
- Molecule 1: Dihydrofolate reductase

Chain 162-A:  84% 15% .



- Molecule 1: Dihydrofolate reductase

Chain 163-A:  86% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 164-A:  85% 14% .



- Molecule 1: Dihydrofolate reductase

Chain 165-A:  84% 14% .



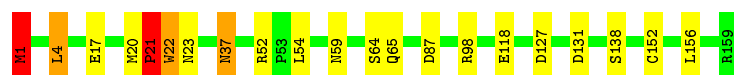
- Molecule 1: Dihydrofolate reductase

Chain 166-A:  88% 11% .



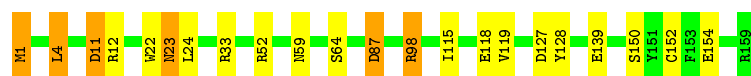
- Molecule 1: Dihydrofolate reductase

Chain 167-A:  87% 10% ..



- Molecule 1: Dihydrofolate reductase

Chain 168-A:  86% 10% .




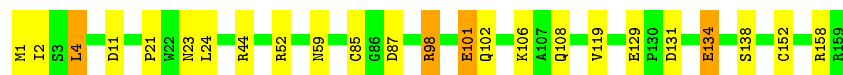
- Molecule 1: Dihydrofolate reductase

Chain 169-A:  86% 12% .



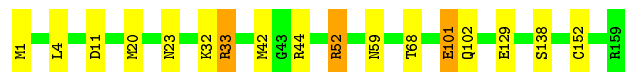
- Molecule 1: Dihydrofolate reductase

Chain 170-A:  85% 13% .



- Molecule 1: Dihydrofolate reductase

Chain 171-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 172-A:  86% 13% .



- Molecule 1: Dihydrofolate reductase

Chain 173-A:  89% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 174-A:  87% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 175-A:  85% 12% .



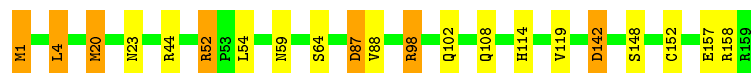
- Molecule 1: Dihydrofolate reductase

Chain 176-A:  87% 10% .



- Molecule 1: Dihydrofolate reductase

Chain 177-A:  87% 9% .




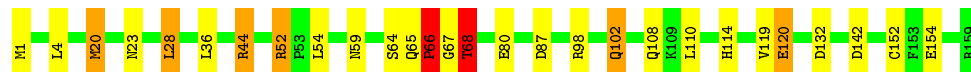
- Molecule 1: Dihydrofolate reductase

Chain 178-A:  86% 9% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 179-A:  82% 13% . .




- Molecule 1: Dihydrofolate reductase

Chain 180-A:  83% 14% .



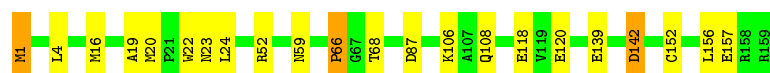
- Molecule 1: Dihydrofolate reductase

Chain 181-A:  83% 14% .




• Molecule 1: Dihydrofolate reductase

Chain 182-A:  86% 12% .



• Molecule 1: Dihydrofolate reductase

Chain 183-A:  83% 13% .



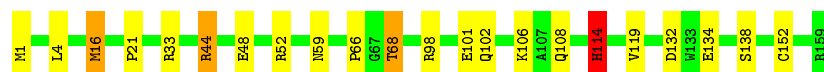
• Molecule 1: Dihydrofolate reductase

Chain 184-A:  86% 11% .



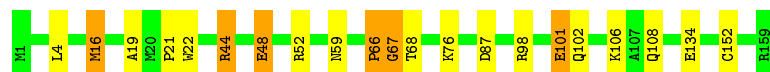
• Molecule 1: Dihydrofolate reductase

Chain 185-A:  86% 11% ..



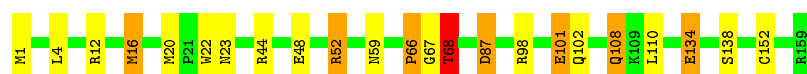
• Molecule 1: Dihydrofolate reductase

Chain 186-A:  87% 9% .




• Molecule 1: Dihydrofolate reductase

Chain 187-A:  86% 9% ..



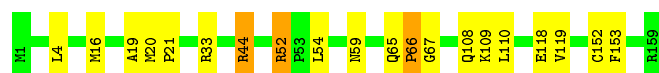
• Molecule 1: Dihydrofolate reductase

Chain 188-A:  85% 12% ..



• Molecule 1: Dihydrofolate reductase

Chain 189-A:  87% 11% .



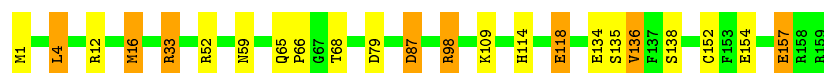
• Molecule 1: Dihydrofolate reductase

Chain 190-A:  87% 11% .



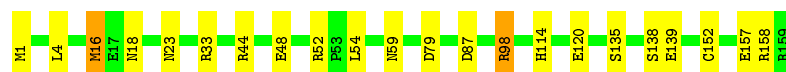
• Molecule 1: Dihydrofolate reductase

Chain 191-A:  86% 9% 5%



• Molecule 1: Dihydrofolate reductase

Chain 192-A:  86% 13% .



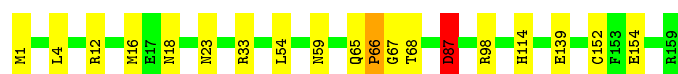
• Molecule 1: Dihydrofolate reductase

Chain 193-A:  87% 13% .



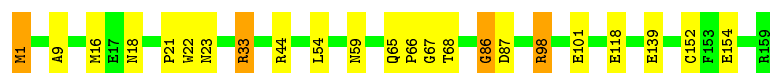
• Molecule 1: Dihydrofolate reductase

Chain 194-A:  88% 11% ..



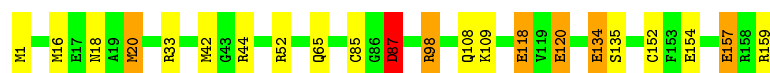
• Molecule 1: Dihydrofolate reductase

Chain 195-A:  86% 12% .



- Molecule 1: Dihydrofolate reductase

Chain 196-A:  86% 9% . .



- Molecule 1: Dihydrofolate reductase

Chain 197-A:  87% 10% .



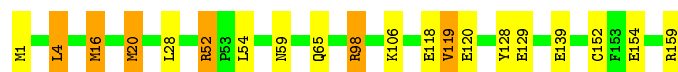
- Molecule 1: Dihydrofolate reductase

Chain 198-A:  85% 14% .



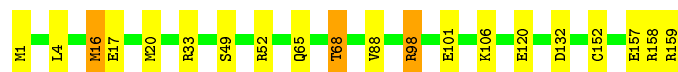
- Molecule 1: Dihydrofolate reductase

Chain 199-A:  87% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 200-A:  87% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 201-A:  86% 14% .



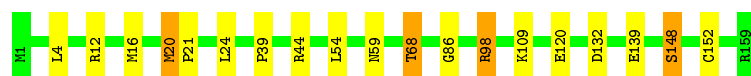
- Molecule 1: Dihydrofolate reductase

Chain 202-A:  86% 14% .



- Molecule 1: Dihydrofolate reductase

Chain 203-A:  88% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 204-A:  86% 11% .



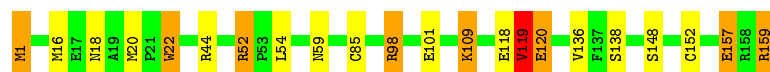
- Molecule 1: Dihydrofolate reductase

Chain 205-A:  89% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 206-A:  86% 8% 5% .



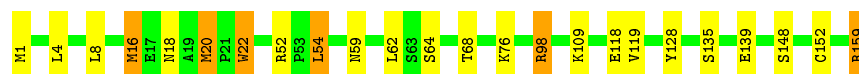
- Molecule 1: Dihydrofolate reductase

Chain 207-A:  87% 9% . .




- Molecule 1: Dihydrofolate reductase

Chain 208-A:  85% 11% .




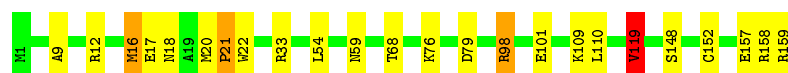
- Molecule 1: Dihydrofolate reductase

Chain 209-A:  84% 13% ..



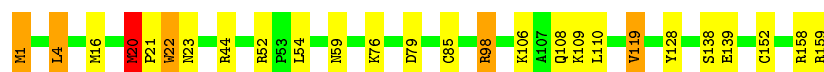
- Molecule 1: Dihydrofolate reductase

Chain 210-A:  85% 13% ..



- Molecule 1: Dihydrofolate reductase

Chain 211-A:  84% 13% ..




- Molecule 1: Dihydrofolate reductase

Chain 212-A:  87% 10% .




- Molecule 1: Dihydrofolate reductase

Chain 213-A:  84% 15% .



- Molecule 1: Dihydrofolate reductase

Chain 214-A:  84% 13% ..



- Molecule 1: Dihydrofolate reductase

Chain 215-A:  89% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 216-A:  87% 10% ..




- Molecule 1: Dihydrofolate reductase

Chain 217-A:  85% 10% 5%



- Molecule 1: Dihydrofolate reductase

Chain 218-A:  83% 14% ..



- Molecule 1: Dihydrofolate reductase

Chain 219-A:  86% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 220-A:  86% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 221-A:  86% 9% ..



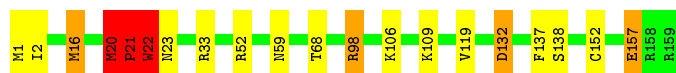
- Molecule 1: Dihydrofolate reductase

Chain 222-A:  87% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 223-A:  87% 8% . .



- Molecule 1: Dihydrofolate reductase

Chain 224-A:  91% 6% .



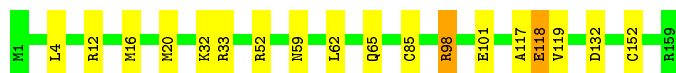
- Molecule 1: Dihydrofolate reductase

Chain 225-A:  88% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 226-A:  89% 10% .



- Molecule 1: Dihydrofolate reductase

Chain 227-A:  87% 10% .



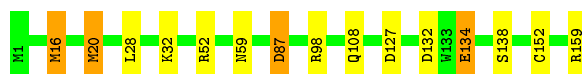
- Molecule 1: Dihydrofolate reductase

Chain 228-A:  91% 7% .



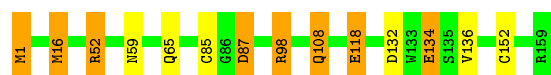
- Molecule 1: Dihydrofolate reductase

Chain 229-A:  91% 7% .



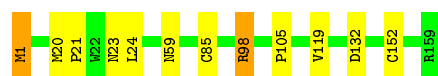
- Molecule 1: Dihydrofolate reductase

Chain 230-A:  91% 5%



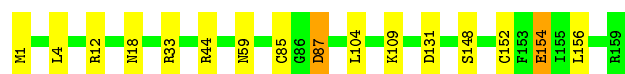
- Molecule 1: Dihydrofolate reductase

Chain 231-A:  92% 6%



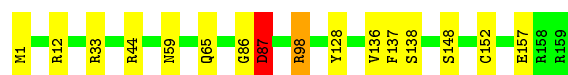
- Molecule 1: Dihydrofolate reductase

Chain 232-A:  90% 9%



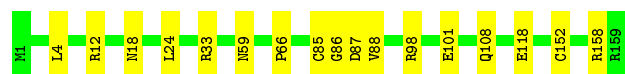
- Molecule 1: Dihydrofolate reductase

Chain 233-A:  90% 9%



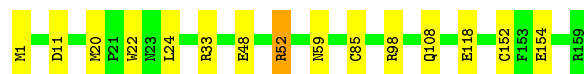
- Molecule 1: Dihydrofolate reductase

Chain 234-A:  89% 11%



- Molecule 1: Dihydrofolate reductase

Chain 235-A:  91% 9%




- Molecule 1: Dihydrofolate reductase

Chain 236-A:  92% 6%



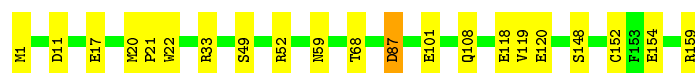
- Molecule 1: Dihydrofolate reductase

Chain 237-A:  89% 9% .



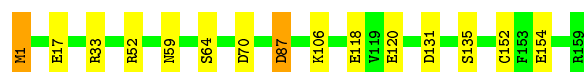
- Molecule 1: Dihydrofolate reductase

Chain 238-A:  87% 13% .



- Molecule 1: Dihydrofolate reductase

Chain 239-A:  91% 8% .



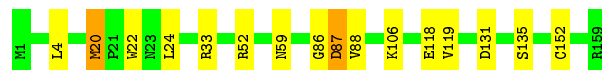
- Molecule 1: Dihydrofolate reductase

Chain 240-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 241-A:  90% 9% .



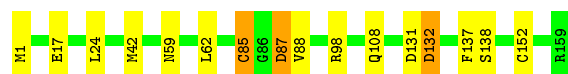
- Molecule 1: Dihydrofolate reductase

Chain 242-A:  88% 11% .



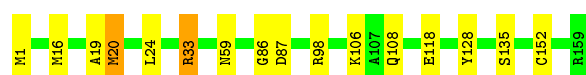
- Molecule 1: Dihydrofolate reductase

Chain 243-A:  90% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 244-A:  90% 9% .




• Molecule 1: Dihydrofolate reductase

Chain 245-A:  88% 10% .



• Molecule 1: Dihydrofolate reductase

Chain 246-A:  83% 17% .



• Molecule 1: Dihydrofolate reductase

Chain 247-A:  87% 11% .



• Molecule 1: Dihydrofolate reductase

Chain 248-A:  86% 13% .



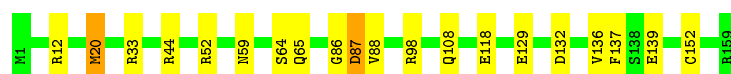
• Molecule 1: Dihydrofolate reductase

Chain 249-A:  88% 8% .



• Molecule 1: Dihydrofolate reductase

Chain 250-A:  87% 11% .



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	33.96Å 44.82Å 98.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 0.85	Depositor
% Data completeness (in resolution range)	98.0 (49.00-0.85)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 0.85Å)	Xtriage
Refinement program	PHENIX 1.8.4-1496	Depositor
R, R_{free}	0.126 , 0.144	Depositor
Wilson B-factor (Å ²)	7.7	Xtriage
Anisotropy	0.182	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	699880	wwPDB-VP
Average B, all atoms (Å ²)	6.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FOL, CSD, NAP, MN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1-A	0.96	3/1296 (0.2%)	1.08	7/1762 (0.4%)
1	2-A	1.15	9/1296 (0.7%)	1.11	8/1762 (0.5%)
1	3-A	1.30	5/1296 (0.4%)	1.16	8/1762 (0.5%)
1	4-A	0.98	6/1296 (0.5%)	1.27	7/1762 (0.4%)
1	5-A	0.93	4/1296 (0.3%)	1.18	17/1762 (1.0%)
1	6-A	1.05	9/1296 (0.7%)	1.20	15/1762 (0.9%)
1	7-A	0.90	4/1296 (0.3%)	1.10	8/1762 (0.5%)
1	8-A	0.93	5/1296 (0.4%)	1.11	7/1762 (0.4%)
1	9-A	0.90	1/1296 (0.1%)	1.14	11/1762 (0.6%)
1	10-A	0.87	2/1296 (0.2%)	1.09	9/1762 (0.5%)
1	11-A	0.92	6/1296 (0.5%)	1.15	11/1762 (0.6%)
1	12-A	0.93	5/1296 (0.4%)	1.13	13/1762 (0.7%)
1	13-A	1.13	10/1296 (0.8%)	1.35	11/1762 (0.6%)
1	14-A	0.88	2/1296 (0.2%)	1.34	13/1762 (0.7%)
1	15-A	0.85	1/1296 (0.1%)	1.05	7/1762 (0.4%)
1	16-A	0.79	0/1296	1.09	7/1762 (0.4%)
1	17-A	0.90	4/1296 (0.3%)	1.07	5/1762 (0.3%)
1	18-A	0.92	4/1296 (0.3%)	1.10	11/1762 (0.6%)
1	19-A	0.77	1/1296 (0.1%)	1.00	7/1762 (0.4%)
1	20-A	0.85	4/1296 (0.3%)	1.03	3/1762 (0.2%)
1	21-A	0.87	3/1296 (0.2%)	1.04	8/1762 (0.5%)
1	22-A	0.91	4/1296 (0.3%)	1.16	10/1762 (0.6%)
1	23-A	0.92	4/1296 (0.3%)	1.15	8/1762 (0.5%)
1	24-A	0.86	2/1296 (0.2%)	1.08	9/1762 (0.5%)
1	25-A	0.90	6/1296 (0.5%)	1.08	9/1762 (0.5%)
1	26-A	0.92	5/1296 (0.4%)	1.03	2/1762 (0.1%)
1	27-A	0.87	3/1296 (0.2%)	1.01	2/1762 (0.1%)
1	28-A	0.88	2/1296 (0.2%)	1.17	10/1762 (0.6%)
1	29-A	0.87	3/1296 (0.2%)	1.14	9/1762 (0.5%)
1	30-A	0.84	1/1296 (0.1%)	1.14	10/1762 (0.6%)
1	31-A	0.87	4/1296 (0.3%)	1.11	9/1762 (0.5%)
1	32-A	0.81	2/1296 (0.2%)	1.08	5/1762 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	33-A	0.93	4/1296 (0.3%)	1.12	12/1762 (0.7%)
1	34-A	0.87	5/1296 (0.4%)	1.08	6/1762 (0.3%)
1	35-A	0.89	4/1296 (0.3%)	1.12	9/1762 (0.5%)
1	36-A	0.82	0/1296	1.03	9/1762 (0.5%)
1	37-A	0.90	1/1296 (0.1%)	1.08	7/1762 (0.4%)
1	38-A	0.86	1/1296 (0.1%)	1.09	8/1762 (0.5%)
1	39-A	0.89	3/1296 (0.2%)	1.13	7/1762 (0.4%)
1	40-A	0.93	5/1296 (0.4%)	1.18	11/1762 (0.6%)
1	41-A	0.87	3/1296 (0.2%)	1.26	12/1762 (0.7%)
1	42-A	0.92	3/1296 (0.2%)	1.15	14/1762 (0.8%)
1	43-A	0.83	2/1296 (0.2%)	1.22	14/1762 (0.8%)
1	44-A	0.80	1/1296 (0.1%)	1.20	11/1762 (0.6%)
1	45-A	0.92	4/1296 (0.3%)	1.15	9/1762 (0.5%)
1	46-A	0.90	2/1296 (0.2%)	1.11	8/1762 (0.5%)
1	47-A	0.94	2/1296 (0.2%)	1.13	10/1762 (0.6%)
1	48-A	0.86	0/1296	1.11	8/1762 (0.5%)
1	49-A	0.96	3/1296 (0.2%)	1.08	5/1762 (0.3%)
1	50-A	0.96	5/1296 (0.4%)	1.19	10/1762 (0.6%)
1	51-A	0.88	2/1296 (0.2%)	1.17	12/1762 (0.7%)
1	52-A	0.90	2/1296 (0.2%)	1.35	11/1762 (0.6%)
1	53-A	1.02	8/1296 (0.6%)	1.21	16/1762 (0.9%)
1	54-A	0.90	1/1296 (0.1%)	1.38	16/1762 (0.9%)
1	55-A	1.01	6/1296 (0.5%)	1.17	12/1762 (0.7%)
1	56-A	1.01	6/1296 (0.5%)	1.20	10/1762 (0.6%)
1	57-A	1.07	8/1296 (0.6%)	1.23	13/1762 (0.7%)
1	58-A	1.11	8/1296 (0.6%)	1.27	20/1762 (1.1%)
1	59-A	0.96	5/1296 (0.4%)	1.13	11/1762 (0.6%)
1	60-A	0.90	4/1296 (0.3%)	1.13	9/1762 (0.5%)
1	61-A	1.00	6/1296 (0.5%)	1.15	12/1762 (0.7%)
1	62-A	0.93	4/1296 (0.3%)	1.14	10/1762 (0.6%)
1	63-A	0.99	4/1296 (0.3%)	1.14	12/1762 (0.7%)
1	64-A	0.88	3/1296 (0.2%)	1.16	11/1762 (0.6%)
1	65-A	0.91	3/1296 (0.2%)	1.11	8/1762 (0.5%)
1	66-A	1.04	4/1296 (0.3%)	1.23	14/1762 (0.8%)
1	67-A	1.08	9/1296 (0.7%)	1.29	13/1762 (0.7%)
1	68-A	0.92	1/1296 (0.1%)	1.14	13/1762 (0.7%)
1	69-A	0.90	4/1296 (0.3%)	1.12	8/1762 (0.5%)
1	70-A	1.04	7/1296 (0.5%)	1.14	12/1762 (0.7%)
1	71-A	0.88	4/1296 (0.3%)	1.16	9/1762 (0.5%)
1	72-A	0.80	1/1296 (0.1%)	1.02	6/1762 (0.3%)
1	73-A	0.94	8/1296 (0.6%)	1.14	7/1762 (0.4%)
1	74-A	1.00	5/1296 (0.4%)	1.16	13/1762 (0.7%)
1	75-A	0.89	2/1296 (0.2%)	1.28	15/1762 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	76-A	0.94	5/1296 (0.4%)	1.11	9/1762 (0.5%)
1	77-A	0.81	2/1296 (0.2%)	1.11	13/1762 (0.7%)
1	78-A	0.81	0/1296	1.10	7/1762 (0.4%)
1	79-A	0.87	2/1296 (0.2%)	1.15	8/1762 (0.5%)
1	80-A	0.84	3/1296 (0.2%)	1.05	4/1762 (0.2%)
1	81-A	0.97	5/1296 (0.4%)	1.16	10/1762 (0.6%)
1	82-A	0.92	4/1296 (0.3%)	1.17	10/1762 (0.6%)
1	83-A	0.94	3/1296 (0.2%)	1.17	14/1762 (0.8%)
1	84-A	0.78	0/1296	1.06	6/1762 (0.3%)
1	85-A	0.90	5/1296 (0.4%)	1.19	11/1762 (0.6%)
1	86-A	0.84	1/1296 (0.1%)	1.10	8/1762 (0.5%)
1	87-A	0.87	4/1296 (0.3%)	1.23	9/1762 (0.5%)
1	88-A	0.91	6/1296 (0.5%)	1.30	23/1762 (1.3%)
1	89-A	0.84	2/1296 (0.2%)	1.09	8/1762 (0.5%)
1	90-A	0.87	3/1296 (0.2%)	1.15	15/1762 (0.9%)
1	91-A	0.91	5/1296 (0.4%)	1.20	14/1762 (0.8%)
1	92-A	0.86	0/1296	1.28	10/1762 (0.6%)
1	93-A	0.89	3/1296 (0.2%)	1.18	8/1762 (0.5%)
1	94-A	1.03	4/1296 (0.3%)	1.28	9/1762 (0.5%)
1	95-A	0.86	3/1296 (0.2%)	1.03	7/1762 (0.4%)
1	96-A	0.85	2/1296 (0.2%)	1.18	9/1762 (0.5%)
1	97-A	0.91	4/1296 (0.3%)	1.08	9/1762 (0.5%)
1	98-A	0.87	4/1296 (0.3%)	1.21	11/1762 (0.6%)
1	99-A	0.86	2/1296 (0.2%)	1.17	9/1762 (0.5%)
1	100-A	0.83	2/1296 (0.2%)	1.22	11/1762 (0.6%)
1	101-A	0.95	5/1296 (0.4%)	1.16	8/1762 (0.5%)
1	102-A	0.95	8/1296 (0.6%)	1.14	14/1762 (0.8%)
1	103-A	0.78	1/1296 (0.1%)	1.01	3/1762 (0.2%)
1	104-A	0.88	3/1296 (0.2%)	1.02	4/1762 (0.2%)
1	105-A	0.91	5/1296 (0.4%)	1.12	9/1762 (0.5%)
1	106-A	0.91	4/1296 (0.3%)	1.08	7/1762 (0.4%)
1	107-A	0.90	3/1296 (0.2%)	1.14	7/1762 (0.4%)
1	108-A	0.92	3/1296 (0.2%)	1.14	7/1762 (0.4%)
1	109-A	0.93	7/1296 (0.5%)	1.19	9/1762 (0.5%)
1	110-A	0.86	2/1296 (0.2%)	1.14	12/1762 (0.7%)
1	111-A	0.91	1/1296 (0.1%)	1.28	13/1762 (0.7%)
1	112-A	0.84	3/1296 (0.2%)	1.06	8/1762 (0.5%)
1	113-A	0.89	2/1296 (0.2%)	1.02	4/1762 (0.2%)
1	114-A	0.86	4/1296 (0.3%)	1.04	7/1762 (0.4%)
1	115-A	0.83	0/1296	1.17	12/1762 (0.7%)
1	116-A	0.97	6/1296 (0.5%)	1.13	12/1762 (0.7%)
1	117-A	0.88	4/1296 (0.3%)	1.03	3/1762 (0.2%)
1	118-A	0.89	4/1296 (0.3%)	1.06	10/1762 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	119-A	0.88	2/1296 (0.2%)	1.11	12/1762 (0.7%)
1	120-A	0.92	3/1296 (0.2%)	1.22	10/1762 (0.6%)
1	121-A	0.94	4/1296 (0.3%)	1.13	8/1762 (0.5%)
1	122-A	0.81	1/1296 (0.1%)	1.06	7/1762 (0.4%)
1	123-A	0.83	0/1296	1.12	12/1762 (0.7%)
1	124-A	0.82	2/1296 (0.2%)	1.07	9/1762 (0.5%)
1	125-A	0.78	1/1296 (0.1%)	1.06	5/1762 (0.3%)
1	126-A	0.76	0/1296	1.03	7/1762 (0.4%)
1	127-A	0.83	4/1296 (0.3%)	1.08	5/1762 (0.3%)
1	128-A	0.90	3/1296 (0.2%)	1.15	14/1762 (0.8%)
1	129-A	0.85	2/1296 (0.2%)	1.10	11/1762 (0.6%)
1	130-A	0.85	3/1296 (0.2%)	1.00	5/1762 (0.3%)
1	131-A	0.88	3/1296 (0.2%)	1.10	9/1762 (0.5%)
1	132-A	0.85	4/1296 (0.3%)	1.12	7/1762 (0.4%)
1	133-A	0.88	4/1296 (0.3%)	1.07	4/1762 (0.2%)
1	134-A	0.86	4/1296 (0.3%)	1.07	7/1762 (0.4%)
1	135-A	0.85	2/1296 (0.2%)	1.01	5/1762 (0.3%)
1	136-A	0.90	3/1296 (0.2%)	1.09	9/1762 (0.5%)
1	137-A	0.87	2/1296 (0.2%)	1.14	8/1762 (0.5%)
1	138-A	0.78	3/1296 (0.2%)	1.10	7/1762 (0.4%)
1	139-A	0.84	3/1296 (0.2%)	1.08	7/1762 (0.4%)
1	140-A	0.90	3/1296 (0.2%)	1.04	3/1762 (0.2%)
1	141-A	0.84	2/1296 (0.2%)	1.16	10/1762 (0.6%)
1	142-A	0.90	1/1296 (0.1%)	1.10	7/1762 (0.4%)
1	143-A	0.83	2/1296 (0.2%)	1.17	14/1762 (0.8%)
1	144-A	0.84	3/1296 (0.2%)	1.15	11/1762 (0.6%)
1	145-A	0.82	0/1296	1.02	5/1762 (0.3%)
1	146-A	0.84	3/1296 (0.2%)	1.13	11/1762 (0.6%)
1	147-A	0.91	4/1296 (0.3%)	1.12	8/1762 (0.5%)
1	148-A	0.91	2/1296 (0.2%)	1.13	7/1762 (0.4%)
1	149-A	0.92	7/1296 (0.5%)	1.13	12/1762 (0.7%)
1	150-A	0.87	3/1296 (0.2%)	1.09	10/1762 (0.6%)
1	151-A	0.97	4/1296 (0.3%)	1.11	6/1762 (0.3%)
1	152-A	0.98	4/1296 (0.3%)	1.16	10/1762 (0.6%)
1	153-A	0.95	5/1296 (0.4%)	1.11	10/1762 (0.6%)
1	154-A	0.80	0/1296	1.14	10/1762 (0.6%)
1	155-A	0.90	5/1296 (0.4%)	1.14	12/1762 (0.7%)
1	156-A	0.98	6/1296 (0.5%)	1.14	9/1762 (0.5%)
1	157-A	0.90	2/1296 (0.2%)	1.06	6/1762 (0.3%)
1	158-A	0.89	4/1296 (0.3%)	1.09	9/1762 (0.5%)
1	159-A	0.85	3/1296 (0.2%)	1.01	5/1762 (0.3%)
1	160-A	0.92	5/1296 (0.4%)	1.08	7/1762 (0.4%)
1	161-A	0.95	5/1296 (0.4%)	1.07	8/1762 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	162-A	0.81	2/1296 (0.2%)	1.06	6/1762 (0.3%)
1	163-A	1.01	8/1296 (0.6%)	1.13	8/1762 (0.5%)
1	164-A	0.89	4/1296 (0.3%)	1.08	10/1762 (0.6%)
1	165-A	0.95	7/1296 (0.5%)	1.12	13/1762 (0.7%)
1	166-A	0.84	1/1296 (0.1%)	1.13	8/1762 (0.5%)
1	167-A	0.96	5/1296 (0.4%)	1.08	12/1762 (0.7%)
1	168-A	0.86	3/1296 (0.2%)	1.13	13/1762 (0.7%)
1	169-A	0.90	3/1296 (0.2%)	1.15	11/1762 (0.6%)
1	170-A	1.01	6/1296 (0.5%)	1.09	9/1762 (0.5%)
1	171-A	0.85	2/1296 (0.2%)	1.13	9/1762 (0.5%)
1	172-A	0.91	4/1296 (0.3%)	1.10	9/1762 (0.5%)
1	173-A	0.94	4/1296 (0.3%)	1.23	9/1762 (0.5%)
1	174-A	0.86	3/1296 (0.2%)	1.10	9/1762 (0.5%)
1	175-A	0.90	4/1296 (0.3%)	1.11	8/1762 (0.5%)
1	176-A	0.87	6/1296 (0.5%)	1.17	7/1762 (0.4%)
1	177-A	0.88	2/1296 (0.2%)	1.20	14/1762 (0.8%)
1	178-A	0.83	1/1296 (0.1%)	1.12	14/1762 (0.8%)
1	179-A	0.94	5/1296 (0.4%)	1.10	9/1762 (0.5%)
1	180-A	0.93	5/1296 (0.4%)	1.12	12/1762 (0.7%)
1	181-A	0.89	3/1296 (0.2%)	1.21	13/1762 (0.7%)
1	182-A	0.85	1/1296 (0.1%)	1.15	10/1762 (0.6%)
1	183-A	0.95	4/1296 (0.3%)	1.27	15/1762 (0.9%)
1	184-A	0.98	7/1296 (0.5%)	1.20	11/1762 (0.6%)
1	185-A	0.84	1/1296 (0.1%)	1.16	10/1762 (0.6%)
1	186-A	0.97	7/1296 (0.5%)	1.26	12/1762 (0.7%)
1	187-A	0.89	3/1296 (0.2%)	1.22	17/1762 (1.0%)
1	188-A	0.92	3/1296 (0.2%)	1.21	12/1762 (0.7%)
1	189-A	0.87	3/1296 (0.2%)	1.17	7/1762 (0.4%)
1	190-A	0.92	4/1296 (0.3%)	1.12	9/1762 (0.5%)
1	191-A	0.90	3/1296 (0.2%)	1.38	16/1762 (0.9%)
1	192-A	0.86	3/1296 (0.2%)	1.14	10/1762 (0.6%)
1	193-A	0.84	3/1296 (0.2%)	1.01	4/1762 (0.2%)
1	194-A	0.87	3/1296 (0.2%)	1.12	10/1762 (0.6%)
1	195-A	0.89	3/1296 (0.2%)	1.13	9/1762 (0.5%)
1	196-A	0.99	8/1296 (0.6%)	1.20	13/1762 (0.7%)
1	197-A	0.95	5/1296 (0.4%)	1.18	18/1762 (1.0%)
1	198-A	0.84	3/1296 (0.2%)	1.11	9/1762 (0.5%)
1	199-A	0.93	2/1296 (0.2%)	1.31	13/1762 (0.7%)
1	200-A	0.93	5/1296 (0.4%)	1.15	10/1762 (0.6%)
1	201-A	0.86	1/1296 (0.1%)	1.27	8/1762 (0.5%)
1	202-A	0.86	1/1296 (0.1%)	1.05	7/1762 (0.4%)
1	203-A	0.85	2/1296 (0.2%)	1.13	11/1762 (0.6%)
1	204-A	0.91	5/1296 (0.4%)	1.18	10/1762 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	205-A	0.83	3/1296 (0.2%)	1.15	9/1762 (0.5%)
1	206-A	1.04	7/1296 (0.5%)	1.19	12/1762 (0.7%)
1	207-A	0.91	6/1296 (0.5%)	1.13	11/1762 (0.6%)
1	208-A	0.97	5/1296 (0.4%)	1.18	12/1762 (0.7%)
1	209-A	0.92	4/1296 (0.3%)	1.27	17/1762 (1.0%)
1	210-A	1.02	8/1296 (0.6%)	1.19	15/1762 (0.9%)
1	211-A	0.90	5/1296 (0.4%)	1.10	9/1762 (0.5%)
1	212-A	0.82	1/1296 (0.1%)	1.11	11/1762 (0.6%)
1	213-A	0.94	4/1296 (0.3%)	1.21	14/1762 (0.8%)
1	214-A	0.92	5/1296 (0.4%)	1.19	18/1762 (1.0%)
1	215-A	0.84	1/1296 (0.1%)	1.11	8/1762 (0.5%)
1	216-A	0.85	1/1296 (0.1%)	1.31	13/1762 (0.7%)
1	217-A	0.88	4/1296 (0.3%)	1.23	13/1762 (0.7%)
1	218-A	0.94	5/1296 (0.4%)	1.18	8/1762 (0.5%)
1	219-A	0.91	5/1296 (0.4%)	1.19	13/1762 (0.7%)
1	220-A	0.86	0/1296	1.16	8/1762 (0.5%)
1	221-A	0.96	5/1296 (0.4%)	1.08	8/1762 (0.5%)
1	222-A	0.89	1/1296 (0.1%)	1.23	11/1762 (0.6%)
1	223-A	0.87	1/1296 (0.1%)	1.16	10/1762 (0.6%)
1	224-A	0.93	5/1296 (0.4%)	1.20	10/1762 (0.6%)
1	225-A	0.97	4/1296 (0.3%)	1.17	11/1762 (0.6%)
1	226-A	1.00	8/1296 (0.6%)	1.17	12/1762 (0.7%)
1	227-A	0.93	5/1296 (0.4%)	1.10	8/1762 (0.5%)
1	228-A	0.84	2/1296 (0.2%)	1.03	4/1762 (0.2%)
1	229-A	0.89	2/1296 (0.2%)	1.08	8/1762 (0.5%)
1	230-A	0.88	3/1296 (0.2%)	1.05	6/1762 (0.3%)
1	231-A	0.85	2/1296 (0.2%)	1.09	6/1762 (0.3%)
1	232-A	0.83	2/1296 (0.2%)	1.07	8/1762 (0.5%)
1	233-A	0.87	4/1296 (0.3%)	1.11	9/1762 (0.5%)
1	234-A	0.87	3/1296 (0.2%)	1.05	1/1762 (0.1%)
1	235-A	0.96	6/1296 (0.5%)	1.08	11/1762 (0.6%)
1	236-A	0.85	1/1296 (0.1%)	1.04	6/1762 (0.3%)
1	237-A	0.84	3/1296 (0.2%)	1.06	7/1762 (0.4%)
1	238-A	0.89	4/1296 (0.3%)	1.16	10/1762 (0.6%)
1	239-A	0.87	2/1296 (0.2%)	1.01	7/1762 (0.4%)
1	240-A	0.80	3/1296 (0.2%)	1.12	13/1762 (0.7%)
1	241-A	0.86	1/1296 (0.1%)	1.03	7/1762 (0.4%)
1	242-A	0.91	3/1296 (0.2%)	1.06	6/1762 (0.3%)
1	243-A	0.88	1/1296 (0.1%)	1.12	12/1762 (0.7%)
1	244-A	0.82	2/1296 (0.2%)	1.11	9/1762 (0.5%)
1	245-A	0.84	2/1296 (0.2%)	1.04	7/1762 (0.4%)
1	246-A	0.87	3/1296 (0.2%)	1.19	13/1762 (0.7%)
1	247-A	0.83	1/1296 (0.1%)	1.11	10/1762 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	248-A	0.83	3/1296 (0.2%)	1.09	9/1762 (0.5%)
1	249-A	0.88	3/1296 (0.2%)	1.12	10/1762 (0.6%)
1	250-A	0.91	4/1296 (0.3%)	1.18	10/1762 (0.6%)
All	All	0.90	863/324000 (0.3%)	1.14	2402/440500 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	1
1	3-A	0	1
1	7-A	0	1
1	16-A	0	1
1	18-A	0	1
1	19-A	0	1
1	21-A	0	1
1	24-A	0	1
1	28-A	0	2
1	31-A	0	1
1	35-A	0	1
1	36-A	0	3
1	41-A	0	1
1	42-A	0	2
1	48-A	0	1
1	51-A	0	1
1	52-A	0	1
1	53-A	0	4
1	54-A	0	1
1	55-A	0	1
1	56-A	0	3
1	57-A	0	2
1	58-A	0	2
1	59-A	0	3
1	60-A	0	2
1	61-A	0	3
1	62-A	0	2
1	63-A	0	3
1	64-A	0	2
1	65-A	0	1
1	66-A	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	67-A	0	4
1	69-A	0	1
1	72-A	0	1
1	73-A	0	1
1	74-A	0	1
1	91-A	0	2
1	92-A	0	1
1	98-A	0	1
1	100-A	0	1
1	106-A	0	1
1	109-A	0	3
1	110-A	0	1
1	115-A	0	2
1	117-A	0	1
1	119-A	0	1
1	127-A	0	1
1	128-A	0	1
1	129-A	0	1
1	130-A	0	1
1	135-A	0	1
1	136-A	0	1
1	138-A	0	1
1	141-A	0	3
1	142-A	0	2
1	143-A	0	2
1	144-A	0	3
1	145-A	0	1
1	146-A	0	1
1	148-A	0	1
1	149-A	0	1
1	150-A	0	1
1	151-A	0	1
1	152-A	0	1
1	155-A	0	1
1	156-A	0	1
1	157-A	0	2
1	162-A	0	1
1	163-A	0	2
1	164-A	0	2
1	165-A	0	1
1	167-A	0	2
1	169-A	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	175-A	0	1
1	176-A	0	1
1	177-A	0	1
1	178-A	0	1
1	179-A	0	2
1	182-A	0	1
1	183-A	0	1
1	184-A	0	1
1	185-A	0	1
1	186-A	0	2
1	187-A	0	2
1	188-A	0	1
1	189-A	0	1
1	190-A	0	1
1	193-A	0	1
1	195-A	0	2
1	201-A	0	1
1	207-A	0	1
1	209-A	0	2
1	210-A	0	1
1	211-A	0	3
1	212-A	0	1
1	213-A	0	3
1	214-A	0	2
1	216-A	0	1
1	217-A	0	1
1	218-A	0	2
1	221-A	0	2
1	222-A	0	1
1	223-A	0	2
1	226-A	0	1
1	227-A	0	1
1	230-A	0	1
1	233-A	0	2
1	234-A	0	1
1	243-A	0	1
1	244-A	0	2
1	249-A	0	1
All	All	0	165

The worst 5 of 863 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3-A	22	TRP	CB-CG	31.13	2.06	1.50
1	2-A	22	TRP	CB-CG	22.03	1.89	1.50
1	58-A	22	TRP	CB-CG	-19.51	1.15	1.50
1	57-A	22	TRP	CB-CG	-17.50	1.18	1.50
1	13-A	101	GLU	CB-CG	15.44	1.81	1.52

The worst 5 of 2402 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	94-A	16	MET	CG-SD-CE	-25.71	59.06	100.20
1	201-A	159	ARG	NE-CZ-NH2	-21.78	109.41	120.30
1	13-A	52	ARG	NE-CZ-NH1	21.45	131.02	120.30
1	191-A	52	ARG	NE-CZ-NH1	21.14	130.87	120.30
1	52-A	52	ARG	NE-CZ-NH1	21.10	130.85	120.30

There are no chirality outliers.

5 of 165 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	19	ALA	Peptide
1	16-A	19	ALA	Peptide
1	18-A	1	MET	Peptide
1	3-A	21	PRO	Peptide
1	7-A	21	PRO	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	1270	1221	1221	0	0
1	2-A	1270	1221	1222	0	0
1	3-A	1270	1221	1221	0	0
1	4-A	1270	1221	1221	0	0
1	5-A	1270	1221	1220	0	0
1	6-A	1270	1221	1221	0	0
1	7-A	1270	1221	1221	0	0
1	8-A	1270	1221	1221	0	0
1	9-A	1270	1221	1221	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	10-A	1270	1221	1221	0	0
1	11-A	1270	1221	1221	0	0
1	12-A	1270	1221	1221	0	0
1	13-A	1270	1221	1221	0	0
1	14-A	1270	1221	1222	0	0
1	15-A	1270	1221	1221	0	0
1	16-A	1270	1221	1221	0	0
1	17-A	1270	1221	1220	0	0
1	18-A	1270	1221	1221	0	0
1	19-A	1270	1221	1221	0	0
1	20-A	1270	1221	1221	0	0
1	21-A	1270	1221	1221	0	0
1	22-A	1270	1221	1221	0	0
1	23-A	1270	1221	1221	0	0
1	24-A	1270	1221	1221	0	0
1	25-A	1270	1221	1221	0	0
1	26-A	1270	1221	1221	0	0
1	27-A	1270	1221	1221	0	0
1	28-A	1270	1221	1221	0	0
1	29-A	1270	1221	1221	0	0
1	30-A	1270	1221	1221	0	0
1	31-A	1270	1221	1221	0	0
1	32-A	1270	1221	1221	0	0
1	33-A	1270	1221	1221	0	0
1	34-A	1270	1221	1221	0	0
1	35-A	1270	1221	1221	0	0
1	36-A	1270	1221	1221	0	0
1	37-A	1270	1221	1221	0	0
1	38-A	1270	1221	1221	0	0
1	39-A	1270	1221	1221	0	0
1	40-A	1270	1221	1221	0	0
1	41-A	1270	1221	1221	0	0
1	42-A	1270	1221	1221	0	0
1	43-A	1270	1221	1222	0	0
1	44-A	1270	1221	1221	0	0
1	45-A	1270	1221	1221	0	0
1	46-A	1270	1221	1221	0	0
1	47-A	1270	1221	1221	0	0
1	48-A	1270	1221	1221	0	0
1	49-A	1270	1221	1220	0	0
1	50-A	1270	1221	1220	0	0
1	51-A	1270	1221	1221	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	52-A	1270	1221	1221	0	0
1	53-A	1270	1221	1221	0	0
1	54-A	1270	1221	1221	0	0
1	55-A	1270	1221	1221	0	0
1	56-A	1270	1221	1221	0	0
1	57-A	1270	1221	1221	0	0
1	58-A	1270	1221	1221	0	0
1	59-A	1270	1221	1221	0	0
1	60-A	1270	1221	1221	0	0
1	61-A	1270	1221	1220	0	0
1	62-A	1270	1221	1221	0	0
1	63-A	1270	1221	1221	0	0
1	64-A	1270	1221	1221	0	0
1	65-A	1270	1221	1221	0	0
1	66-A	1270	1221	1220	0	0
1	67-A	1270	1221	1221	0	0
1	68-A	1270	1221	1221	0	0
1	69-A	1270	1221	1221	0	0
1	70-A	1270	1221	1221	0	0
1	71-A	1270	1221	1221	0	0
1	72-A	1270	1221	1221	0	0
1	73-A	1270	1221	1221	0	0
1	74-A	1270	1221	1221	0	0
1	75-A	1270	1221	1221	0	0
1	76-A	1270	1221	1221	0	0
1	77-A	1270	1221	1221	0	0
1	78-A	1270	1221	1221	0	0
1	79-A	1270	1221	1221	0	0
1	80-A	1270	1221	1220	0	0
1	81-A	1270	1221	1221	0	0
1	82-A	1270	1221	1221	0	0
1	83-A	1270	1221	1222	0	0
1	84-A	1270	1221	1221	0	0
1	85-A	1270	1221	1221	0	0
1	86-A	1270	1221	1221	0	0
1	87-A	1270	1221	1221	0	0
1	88-A	1270	1221	1221	0	0
1	89-A	1270	1221	1221	0	0
1	90-A	1270	1221	1221	0	0
1	91-A	1270	1221	1221	0	0
1	92-A	1270	1221	1221	0	0
1	93-A	1270	1221	1221	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	94-A	1270	1221	1221	0	0
1	95-A	1270	1221	1221	0	0
1	96-A	1270	1221	1221	0	0
1	97-A	1270	1221	1220	0	0
1	98-A	1270	1221	1221	0	0
1	99-A	1270	1221	1221	0	0
1	100-A	1270	1221	1221	0	0
1	101-A	1270	1221	1221	0	0
1	102-A	1270	1221	1221	0	0
1	103-A	1270	1221	1221	0	0
1	104-A	1270	1221	1221	0	0
1	105-A	1270	1221	1221	0	0
1	106-A	1270	1221	1221	0	0
1	107-A	1270	1221	1221	0	0
1	108-A	1270	1221	1221	0	0
1	109-A	1270	1221	1221	0	0
1	110-A	1270	1221	1221	0	0
1	111-A	1270	1221	1221	0	0
1	112-A	1270	1221	1221	0	0
1	113-A	1270	1221	1221	0	0
1	114-A	1270	1221	1221	0	0
1	115-A	1270	1221	1221	0	0
1	116-A	1270	1221	1221	0	0
1	117-A	1270	1221	1221	0	0
1	118-A	1270	1221	1221	0	0
1	119-A	1270	1221	1221	0	0
1	120-A	1270	1221	1220	0	0
1	121-A	1270	1221	1221	0	0
1	122-A	1270	1221	1221	0	0
1	123-A	1270	1221	1221	0	0
1	124-A	1270	1221	1221	0	0
1	125-A	1270	1221	1221	0	0
1	126-A	1270	1221	1221	0	0
1	127-A	1270	1221	1221	0	0
1	128-A	1270	1221	1221	0	0
1	129-A	1270	1221	1221	0	0
1	130-A	1270	1221	1221	0	0
1	131-A	1270	1221	1221	0	0
1	132-A	1270	1221	1221	0	0
1	133-A	1270	1221	1221	0	0
1	134-A	1270	1221	1221	0	0
1	135-A	1270	1221	1221	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	136-A	1270	1221	1221	0	0
1	137-A	1270	1221	1220	0	0
1	138-A	1270	1221	1221	0	0
1	139-A	1270	1221	1221	0	0
1	140-A	1270	1221	1221	0	0
1	141-A	1270	1221	1221	0	0
1	142-A	1270	1221	1221	0	0
1	143-A	1270	1221	1222	0	0
1	144-A	1270	1221	1221	0	0
1	145-A	1270	1221	1221	0	0
1	146-A	1270	1221	1221	0	0
1	147-A	1270	1221	1221	0	0
1	148-A	1270	1221	1221	0	0
1	149-A	1270	1221	1220	0	0
1	150-A	1270	1221	1220	0	0
1	151-A	1270	1221	1221	0	0
1	152-A	1270	1221	1220	0	0
1	153-A	1270	1221	1221	0	0
1	154-A	1270	1221	1221	0	0
1	155-A	1270	1221	1221	0	0
1	156-A	1270	1221	1221	0	0
1	157-A	1270	1221	1221	0	0
1	158-A	1270	1221	1221	0	0
1	159-A	1270	1221	1221	0	0
1	160-A	1270	1221	1221	0	0
1	161-A	1270	1221	1221	0	0
1	162-A	1270	1221	1221	0	0
1	163-A	1270	1221	1221	0	0
1	164-A	1270	1221	1222	0	0
1	165-A	1270	1221	1222	0	0
1	166-A	1270	1221	1221	0	0
1	167-A	1270	1221	1221	0	0
1	168-A	1270	1221	1221	0	0
1	169-A	1270	1221	1221	0	0
1	170-A	1270	1221	1221	0	0
1	171-A	1270	1221	1221	0	0
1	172-A	1270	1221	1221	0	0
1	173-A	1270	1221	1221	0	0
1	174-A	1270	1221	1221	0	0
1	175-A	1270	1221	1221	0	0
1	176-A	1270	1221	1221	0	0
1	177-A	1270	1221	1220	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	178-A	1270	1221	1221	0	0
1	179-A	1270	1221	1221	0	0
1	180-A	1270	1221	1221	0	0
1	181-A	1270	1221	1221	0	0
1	182-A	1270	1221	1222	0	0
1	183-A	1270	1221	1221	0	0
1	184-A	1270	1221	1222	0	0
1	185-A	1270	1221	1221	0	0
1	186-A	1270	1221	1221	0	0
1	187-A	1270	1221	1219	0	0
1	188-A	1270	1221	1220	0	0
1	189-A	1270	1221	1221	0	0
1	190-A	1270	1221	1221	0	0
1	191-A	1270	1221	1221	0	0
1	192-A	1270	1221	1221	0	0
1	193-A	1270	1221	1221	0	0
1	194-A	1270	1221	1221	0	0
1	195-A	1270	1221	1221	0	0
1	196-A	1270	1221	1221	0	0
1	197-A	1270	1221	1221	0	0
1	198-A	1270	1221	1221	0	0
1	199-A	1270	1221	1221	0	0
1	200-A	1270	1221	1221	0	0
1	201-A	1270	1221	1220	0	0
1	202-A	1270	1221	1222	0	0
1	203-A	1270	1221	1221	0	0
1	204-A	1270	1221	1221	0	0
1	205-A	1270	1221	1222	0	0
1	206-A	1270	1221	1221	0	0
1	207-A	1270	1221	1220	0	0
1	208-A	1270	1221	1221	0	0
1	209-A	1270	1221	1220	0	0
1	210-A	1270	1221	1220	0	0
1	211-A	1270	1221	1221	0	0
1	212-A	1270	1221	1220	0	0
1	213-A	1270	1221	1221	0	0
1	214-A	1270	1221	1221	0	0
1	215-A	1270	1221	1221	0	0
1	216-A	1270	1221	1221	0	0
1	217-A	1270	1221	1221	0	0
1	218-A	1270	1221	1221	0	0
1	219-A	1270	1221	1221	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	220-A	1270	1221	1222	0	0
1	221-A	1270	1221	1221	0	0
1	222-A	1270	1221	1222	0	0
1	223-A	1270	1221	1221	0	0
1	224-A	1270	1221	1221	0	0
1	225-A	1270	1221	1222	0	0
1	226-A	1270	1221	1221	0	0
1	227-A	1270	1221	1221	0	0
1	228-A	1270	1221	1220	0	0
1	229-A	1270	1221	1221	0	0
1	230-A	1270	1221	1221	0	0
1	231-A	1270	1221	1221	0	0
1	232-A	1270	1221	1221	0	0
1	233-A	1270	1221	1221	0	0
1	234-A	1270	1221	1221	0	0
1	235-A	1270	1221	1221	0	0
1	236-A	1270	1221	1219	0	0
1	237-A	1270	1221	1220	0	0
1	238-A	1270	1221	1220	0	0
1	239-A	1270	1221	1220	0	0
1	240-A	1270	1221	1221	0	0
1	241-A	1270	1221	1222	0	0
1	242-A	1270	1221	1220	0	0
1	243-A	1270	1221	1221	0	0
1	244-A	1270	1221	1221	0	0
1	245-A	1270	1221	1221	0	0
1	246-A	1270	1221	1221	0	0
1	247-A	1270	1221	1221	0	0
1	248-A	1270	1221	1220	0	0
1	249-A	1270	1221	1221	0	0
1	250-A	1270	1221	1221	0	0
2	1-A	32	17	17	0	0
2	2-A	32	17	17	0	0
2	3-A	32	17	17	0	0
2	4-A	32	17	17	0	0
2	5-A	32	17	17	0	0
2	6-A	32	17	17	0	0
2	7-A	32	17	17	0	0
2	8-A	32	17	17	0	0
2	9-A	32	17	17	0	0
2	10-A	32	17	17	0	0
2	11-A	32	17	17	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	12-A	32	17	17	0	0
2	13-A	32	17	17	0	0
2	14-A	32	17	17	0	0
2	15-A	32	17	17	0	0
2	16-A	32	17	17	0	0
2	17-A	32	17	17	0	0
2	18-A	32	17	17	0	0
2	19-A	32	17	17	0	0
2	20-A	32	17	17	0	0
2	21-A	32	17	17	0	0
2	22-A	32	17	17	0	0
2	23-A	32	17	17	0	0
2	24-A	32	17	17	0	0
2	25-A	32	17	17	0	0
2	26-A	32	17	17	0	0
2	27-A	32	17	17	0	0
2	28-A	32	17	17	0	0
2	29-A	32	17	17	0	0
2	30-A	32	17	17	0	0
2	31-A	32	17	17	0	0
2	32-A	32	17	17	0	0
2	33-A	32	17	17	0	0
2	34-A	32	17	17	0	0
2	35-A	32	17	17	0	0
2	36-A	32	17	17	0	0
2	37-A	32	17	17	0	0
2	38-A	32	17	17	0	0
2	39-A	32	17	17	0	0
2	40-A	32	17	17	0	0
2	41-A	32	17	17	0	0
2	42-A	32	17	17	0	0
2	43-A	32	17	17	0	0
2	44-A	32	17	17	0	0
2	45-A	32	17	17	0	0
2	46-A	32	17	17	0	0
2	47-A	32	17	17	0	0
2	48-A	32	17	17	0	0
2	49-A	32	17	17	0	0
2	50-A	32	17	17	0	0
2	51-A	32	17	17	0	0
2	52-A	32	17	17	0	0
2	53-A	32	17	17	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	54-A	32	17	17	0	0
2	55-A	32	17	17	0	0
2	56-A	32	17	17	0	0
2	57-A	32	17	17	0	0
2	58-A	32	17	17	0	0
2	59-A	32	17	17	0	0
2	60-A	32	17	17	0	0
2	61-A	32	17	17	0	0
2	62-A	32	17	17	0	0
2	63-A	32	17	17	0	0
2	64-A	32	17	17	0	0
2	65-A	32	17	17	0	0
2	66-A	32	17	17	0	0
2	67-A	32	17	17	0	0
2	68-A	32	17	17	0	0
2	69-A	32	17	17	0	0
2	70-A	32	17	17	0	0
2	71-A	32	17	17	0	0
2	72-A	32	17	17	0	0
2	73-A	32	17	17	0	0
2	74-A	32	17	17	0	0
2	75-A	32	17	17	0	0
2	76-A	32	17	17	0	0
2	77-A	32	17	17	0	0
2	78-A	32	17	17	0	0
2	79-A	32	17	17	0	0
2	80-A	32	17	17	0	0
2	81-A	32	17	17	0	0
2	82-A	32	17	17	0	0
2	83-A	32	17	17	0	0
2	84-A	32	17	17	0	0
2	85-A	32	17	17	0	0
2	86-A	32	17	17	0	0
2	87-A	32	17	17	0	0
2	88-A	32	17	17	0	0
2	89-A	32	17	17	0	0
2	90-A	32	17	17	0	0
2	91-A	32	17	17	0	0
2	92-A	32	17	17	0	0
2	93-A	32	17	17	0	0
2	94-A	32	17	17	0	0
2	95-A	32	17	17	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	96-A	32	17	17	0	0
2	97-A	32	17	17	0	0
2	98-A	32	17	17	0	0
2	99-A	32	17	17	0	0
2	100-A	32	17	17	0	0
2	101-A	32	17	17	0	0
2	102-A	32	17	17	0	0
2	103-A	32	17	17	0	0
2	104-A	32	17	17	0	0
2	105-A	32	17	17	0	0
2	106-A	32	17	17	0	0
2	107-A	32	17	17	0	0
2	108-A	32	17	17	0	0
2	109-A	32	17	17	0	0
2	110-A	32	17	17	0	0
2	111-A	32	17	17	0	0
2	112-A	32	17	17	0	0
2	113-A	32	17	17	0	0
2	114-A	32	17	17	0	0
2	115-A	32	17	17	0	0
2	116-A	32	17	17	0	0
2	117-A	32	17	17	0	0
2	118-A	32	17	17	0	0
2	119-A	32	17	17	0	0
2	120-A	32	17	17	0	0
2	121-A	32	17	17	0	0
2	122-A	32	17	17	0	0
2	123-A	32	17	17	0	0
2	124-A	32	17	17	0	0
2	125-A	32	17	17	0	0
2	126-A	32	17	17	0	0
2	127-A	32	17	17	0	0
2	128-A	32	17	17	0	0
2	129-A	32	17	17	0	0
2	130-A	32	17	17	0	0
2	131-A	32	17	17	0	0
2	132-A	32	17	17	0	0
2	133-A	32	17	17	0	0
2	134-A	32	17	17	0	0
2	135-A	32	17	17	0	0
2	136-A	32	17	17	0	0
2	137-A	32	17	17	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	138-A	32	17	17	0	0
2	139-A	32	17	17	0	0
2	140-A	32	17	17	0	0
2	141-A	32	17	17	0	0
2	142-A	32	17	17	0	0
2	143-A	32	17	17	0	0
2	144-A	32	17	17	0	0
2	145-A	32	17	17	0	0
2	146-A	32	17	17	0	0
2	147-A	32	17	17	0	0
2	148-A	32	17	17	0	0
2	149-A	32	17	17	0	0
2	150-A	32	17	17	0	0
2	151-A	32	17	17	0	0
2	152-A	32	17	17	0	0
2	153-A	32	17	17	0	0
2	154-A	32	17	17	0	0
2	155-A	32	17	17	0	0
2	156-A	32	17	17	0	0
2	157-A	32	17	17	0	0
2	158-A	32	17	17	0	0
2	159-A	32	17	17	0	0
2	160-A	32	17	17	0	0
2	161-A	32	17	17	0	0
2	162-A	32	17	17	0	0
2	163-A	32	17	17	0	0
2	164-A	32	17	17	0	0
2	165-A	32	17	17	0	0
2	166-A	32	17	17	0	0
2	167-A	32	17	17	0	0
2	168-A	32	17	17	0	0
2	169-A	32	17	17	0	0
2	170-A	32	17	17	0	0
2	171-A	32	17	17	0	0
2	172-A	32	17	17	0	0
2	173-A	32	17	17	0	0
2	174-A	32	17	17	0	0
2	175-A	32	17	17	0	0
2	176-A	32	17	17	0	0
2	177-A	32	17	17	0	0
2	178-A	32	17	17	0	0
2	179-A	32	17	17	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	180-A	32	17	17	0	0
2	181-A	32	17	17	0	0
2	182-A	32	17	17	0	0
2	183-A	32	17	17	0	0
2	184-A	32	17	17	0	0
2	185-A	32	17	17	0	0
2	186-A	32	17	17	0	0
2	187-A	32	17	17	0	0
2	188-A	32	17	17	0	0
2	189-A	32	17	17	0	0
2	190-A	32	17	17	0	0
2	191-A	32	17	17	0	0
2	192-A	32	17	17	0	0
2	193-A	32	17	17	0	0
2	194-A	32	17	17	0	0
2	195-A	32	17	17	0	0
2	196-A	32	17	17	0	0
2	197-A	32	17	17	0	0
2	198-A	32	17	17	0	0
2	199-A	32	17	17	0	0
2	200-A	32	17	17	0	0
2	201-A	32	17	17	0	0
2	202-A	32	17	17	0	0
2	203-A	32	17	17	0	0
2	204-A	32	17	17	0	0
2	205-A	32	17	17	0	0
2	206-A	32	17	17	0	0
2	207-A	32	17	17	0	0
2	208-A	32	17	17	0	0
2	209-A	32	17	17	0	0
2	210-A	32	17	17	0	0
2	211-A	32	17	17	0	0
2	212-A	32	17	17	0	0
2	213-A	32	17	17	0	0
2	214-A	32	17	17	0	0
2	215-A	32	17	17	0	0
2	216-A	32	17	17	0	0
2	217-A	32	17	17	0	0
2	218-A	32	17	17	0	0
2	219-A	32	17	17	0	0
2	220-A	32	17	17	0	0
2	221-A	32	17	17	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	222-A	32	17	17	0	0
2	223-A	32	17	17	0	0
2	224-A	32	17	17	0	0
2	225-A	32	17	17	0	0
2	226-A	32	17	17	0	0
2	227-A	32	17	17	0	0
2	228-A	32	17	17	0	0
2	229-A	32	17	17	0	0
2	230-A	32	17	17	0	0
2	231-A	32	17	17	0	0
2	232-A	32	17	17	0	0
2	233-A	32	17	17	0	0
2	234-A	32	17	17	0	0
2	235-A	32	17	17	0	0
2	236-A	32	17	17	0	0
2	237-A	32	17	17	0	0
2	238-A	32	17	17	0	0
2	239-A	32	17	17	0	0
2	240-A	32	17	17	0	0
2	241-A	32	17	17	0	0
2	242-A	32	17	17	0	0
2	243-A	32	17	17	0	0
2	244-A	32	17	17	0	0
2	245-A	32	17	17	0	0
2	246-A	32	17	17	0	0
2	247-A	32	17	17	0	0
2	248-A	32	17	17	0	0
2	249-A	32	17	17	0	0
2	250-A	32	17	17	0	0
3	1-A	48	25	25	0	0
3	2-A	48	25	25	0	0
3	3-A	48	25	25	0	0
3	4-A	48	25	25	0	0
3	5-A	48	25	25	0	0
3	6-A	48	25	25	0	0
3	7-A	48	25	25	0	0
3	8-A	48	25	25	0	0
3	9-A	48	25	25	0	0
3	10-A	48	25	25	0	0
3	11-A	48	25	25	0	0
3	12-A	48	25	25	0	0
3	13-A	48	25	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	14-A	48	25	25	0	0
3	15-A	48	25	25	0	0
3	16-A	48	25	25	0	0
3	17-A	48	25	25	0	0
3	18-A	48	25	25	0	0
3	19-A	48	25	25	0	0
3	20-A	48	25	25	0	0
3	21-A	48	25	25	0	0
3	22-A	48	25	24	0	0
3	23-A	48	25	25	0	0
3	24-A	48	25	25	0	0
3	25-A	48	25	25	0	0
3	26-A	48	25	25	0	0
3	27-A	48	25	25	0	0
3	28-A	48	25	25	0	0
3	29-A	48	25	25	0	0
3	30-A	48	25	25	0	0
3	31-A	48	25	25	0	0
3	32-A	48	25	25	0	0
3	33-A	48	25	25	0	0
3	34-A	48	25	25	0	0
3	35-A	48	25	25	0	0
3	36-A	48	25	25	0	0
3	37-A	48	25	25	0	0
3	38-A	48	25	25	0	0
3	39-A	48	25	25	0	0
3	40-A	48	25	25	0	0
3	41-A	48	25	25	0	0
3	42-A	48	25	25	0	0
3	43-A	48	25	25	0	0
3	44-A	48	25	25	0	0
3	45-A	48	25	25	0	0
3	46-A	48	25	25	0	0
3	47-A	48	25	25	0	0
3	48-A	48	25	25	0	0
3	49-A	48	25	25	0	0
3	50-A	48	25	25	0	0
3	51-A	48	25	25	0	0
3	52-A	48	25	25	0	0
3	53-A	48	25	25	0	0
3	54-A	48	25	25	0	0
3	55-A	48	25	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	56-A	48	25	25	0	0
3	57-A	48	25	25	0	0
3	58-A	48	25	25	0	0
3	59-A	48	25	25	0	0
3	60-A	48	25	25	0	0
3	61-A	48	25	25	0	0
3	62-A	48	25	25	0	0
3	63-A	48	25	25	0	0
3	64-A	48	25	25	0	0
3	65-A	48	25	25	0	0
3	66-A	48	25	25	0	0
3	67-A	48	25	25	0	0
3	68-A	48	25	25	0	0
3	69-A	48	25	25	0	0
3	70-A	48	25	25	0	0
3	71-A	48	25	25	0	0
3	72-A	48	25	25	0	0
3	73-A	48	25	25	0	0
3	74-A	48	25	25	0	0
3	75-A	48	25	25	0	0
3	76-A	48	25	25	0	0
3	77-A	48	25	25	0	0
3	78-A	48	25	25	0	0
3	79-A	48	25	25	0	0
3	80-A	48	25	25	0	0
3	81-A	48	25	25	0	0
3	82-A	48	25	25	0	0
3	83-A	48	25	25	0	0
3	84-A	48	25	25	0	0
3	85-A	48	25	25	0	0
3	86-A	48	25	25	0	0
3	87-A	48	25	25	0	0
3	88-A	48	25	25	0	0
3	89-A	48	25	25	0	0
3	90-A	48	25	25	0	0
3	91-A	48	25	25	0	0
3	92-A	48	25	25	0	0
3	93-A	48	25	25	0	0
3	94-A	48	25	25	0	0
3	95-A	48	25	25	0	0
3	96-A	48	25	25	0	0
3	97-A	48	25	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	98-A	48	25	25	0	0
3	99-A	48	25	25	0	0
3	100-A	48	25	25	0	0
3	101-A	48	25	25	0	0
3	102-A	48	25	25	0	0
3	103-A	48	25	25	0	0
3	104-A	48	25	25	0	0
3	105-A	48	25	25	0	0
3	106-A	48	25	25	0	0
3	107-A	48	25	25	0	0
3	108-A	48	25	25	0	0
3	109-A	48	25	25	0	0
3	110-A	48	25	25	0	0
3	111-A	48	25	25	0	0
3	112-A	48	25	25	0	0
3	113-A	48	25	25	0	0
3	114-A	48	25	25	0	0
3	115-A	48	25	25	0	0
3	116-A	48	25	25	0	0
3	117-A	48	25	25	0	0
3	118-A	48	25	25	0	0
3	119-A	48	25	25	0	0
3	120-A	48	25	25	0	0
3	121-A	48	25	25	0	0
3	122-A	48	25	25	0	0
3	123-A	48	25	25	0	0
3	124-A	48	25	25	0	0
3	125-A	48	25	25	0	0
3	126-A	48	25	25	0	0
3	127-A	48	25	25	0	0
3	128-A	48	25	25	0	0
3	129-A	48	25	25	0	0
3	130-A	48	25	25	0	0
3	131-A	48	25	25	0	0
3	132-A	48	25	25	0	0
3	133-A	48	25	25	0	0
3	134-A	48	25	25	0	0
3	135-A	48	25	25	0	0
3	136-A	48	25	25	0	0
3	137-A	48	25	25	0	0
3	138-A	48	25	25	0	0
3	139-A	48	25	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	140-A	48	25	25	0	0
3	141-A	48	25	25	0	0
3	142-A	48	25	25	0	0
3	143-A	48	25	25	0	0
3	144-A	48	25	25	0	0
3	145-A	48	25	25	0	0
3	146-A	48	25	25	0	0
3	147-A	48	25	25	0	0
3	148-A	48	25	25	0	0
3	149-A	48	25	25	0	0
3	150-A	48	25	25	0	0
3	151-A	48	25	25	0	0
3	152-A	48	25	25	0	0
3	153-A	48	25	25	0	0
3	154-A	48	25	25	0	0
3	155-A	48	25	25	0	0
3	156-A	48	25	25	0	0
3	157-A	48	25	25	0	0
3	158-A	48	25	25	0	0
3	159-A	48	25	25	0	0
3	160-A	48	25	25	0	0
3	161-A	48	25	25	0	0
3	162-A	48	25	25	0	0
3	163-A	48	25	25	0	0
3	164-A	48	25	25	0	0
3	165-A	48	25	25	0	0
3	166-A	48	25	25	0	0
3	167-A	48	25	24	0	0
3	168-A	48	25	25	0	0
3	169-A	48	25	25	0	0
3	170-A	48	25	24	0	0
3	171-A	48	25	25	0	0
3	172-A	48	25	25	0	0
3	173-A	48	25	25	0	0
3	174-A	48	25	25	0	0
3	175-A	48	25	25	0	0
3	176-A	48	25	25	0	0
3	177-A	48	25	25	0	0
3	178-A	48	25	25	0	0
3	179-A	48	25	25	0	0
3	180-A	48	25	25	0	0
3	181-A	48	25	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	182-A	48	25	25	0	0
3	183-A	48	25	25	0	0
3	184-A	48	25	25	0	0
3	185-A	48	25	25	0	0
3	186-A	48	25	25	0	0
3	187-A	48	25	25	0	0
3	188-A	48	25	25	0	0
3	189-A	48	25	25	0	0
3	190-A	48	25	25	0	0
3	191-A	48	25	25	0	0
3	192-A	48	25	25	0	0
3	193-A	48	25	25	0	0
3	194-A	48	25	25	0	0
3	195-A	48	25	25	0	0
3	196-A	48	25	25	0	0
3	197-A	48	25	25	0	0
3	198-A	48	25	25	0	0
3	199-A	48	25	25	0	0
3	200-A	48	25	25	0	0
3	201-A	48	25	25	0	0
3	202-A	48	25	25	0	0
3	203-A	48	25	25	0	0
3	204-A	48	25	25	0	0
3	205-A	48	25	25	0	0
3	206-A	48	25	25	0	0
3	207-A	48	25	24	0	0
3	208-A	48	25	25	0	0
3	209-A	48	25	25	0	0
3	210-A	48	25	25	0	0
3	211-A	48	25	25	0	0
3	212-A	48	25	25	0	0
3	213-A	48	25	25	0	0
3	214-A	48	25	25	0	0
3	215-A	48	25	25	0	0
3	216-A	48	25	25	0	0
3	217-A	48	25	25	0	0
3	218-A	48	25	25	0	0
3	219-A	48	25	25	0	0
3	220-A	48	25	25	0	0
3	221-A	48	25	25	0	0
3	222-A	48	25	25	0	0
3	223-A	48	25	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	224-A	48	25	25	0	0
3	225-A	48	25	25	0	0
3	226-A	48	25	25	0	0
3	227-A	48	25	25	0	0
3	228-A	48	25	25	0	0
3	229-A	48	25	25	0	0
3	230-A	48	25	25	0	0
3	231-A	48	25	25	0	0
3	232-A	48	25	25	0	0
3	233-A	48	25	25	0	0
3	234-A	48	25	25	0	0
3	235-A	48	25	25	0	0
3	236-A	48	25	25	0	0
3	237-A	48	25	25	0	0
3	238-A	48	25	25	0	0
3	239-A	48	25	24	0	0
3	240-A	48	25	25	0	0
3	241-A	48	25	25	0	0
3	242-A	48	25	25	0	0
3	243-A	48	25	25	0	0
3	244-A	48	25	25	0	0
3	245-A	48	25	25	0	0
3	246-A	48	25	25	0	0
3	247-A	48	25	25	0	0
3	248-A	48	25	25	0	0
3	249-A	48	25	25	0	0
3	250-A	48	25	25	0	0
4	1-A	2	0	0	0	0
4	2-A	2	0	0	0	0
4	3-A	2	0	0	0	0
4	4-A	2	0	0	0	0
4	5-A	2	0	0	0	0
4	6-A	2	0	0	0	0
4	7-A	2	0	0	0	0
4	8-A	2	0	0	0	0
4	9-A	2	0	0	0	0
4	10-A	2	0	0	0	0
4	11-A	2	0	0	0	0
4	12-A	2	0	0	0	0
4	13-A	2	0	0	0	0
4	14-A	2	0	0	0	0
4	15-A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	16-A	2	0	0	0	0
4	17-A	2	0	0	0	0
4	18-A	2	0	0	0	0
4	19-A	2	0	0	0	0
4	20-A	2	0	0	0	0
4	21-A	2	0	0	0	0
4	22-A	2	0	0	0	0
4	23-A	2	0	0	0	0
4	24-A	2	0	0	0	0
4	25-A	2	0	0	0	0
4	26-A	2	0	0	0	0
4	27-A	2	0	0	0	0
4	28-A	2	0	0	0	0
4	29-A	2	0	0	0	0
4	30-A	2	0	0	0	0
4	31-A	2	0	0	0	0
4	32-A	2	0	0	0	0
4	33-A	2	0	0	0	0
4	34-A	2	0	0	0	0
4	35-A	2	0	0	0	0
4	36-A	2	0	0	0	0
4	37-A	2	0	0	0	0
4	38-A	2	0	0	0	0
4	39-A	2	0	0	0	0
4	40-A	2	0	0	0	0
4	41-A	2	0	0	0	0
4	42-A	2	0	0	0	0
4	43-A	2	0	0	0	0
4	44-A	2	0	0	0	0
4	45-A	2	0	0	0	0
4	46-A	2	0	0	0	0
4	47-A	2	0	0	0	0
4	48-A	2	0	0	0	0
4	49-A	2	0	0	0	0
4	50-A	2	0	0	0	0
4	51-A	2	0	0	0	0
4	52-A	2	0	0	0	0
4	53-A	2	0	0	0	0
4	54-A	2	0	0	0	0
4	55-A	2	0	0	0	0
4	56-A	2	0	0	0	0
4	57-A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	58-A	2	0	0	0	0
4	59-A	2	0	0	0	0
4	60-A	2	0	0	0	0
4	61-A	2	0	0	0	0
4	62-A	2	0	0	0	0
4	63-A	2	0	0	0	0
4	64-A	2	0	0	0	0
4	65-A	2	0	0	0	0
4	66-A	2	0	0	0	0
4	67-A	2	0	0	0	0
4	68-A	2	0	0	0	0
4	69-A	2	0	0	0	0
4	70-A	2	0	0	0	0
4	71-A	2	0	0	0	0
4	72-A	2	0	0	0	0
4	73-A	2	0	0	0	0
4	74-A	2	0	0	0	0
4	75-A	2	0	0	0	0
4	76-A	2	0	0	0	0
4	77-A	2	0	0	0	0
4	78-A	2	0	0	0	0
4	79-A	2	0	0	0	0
4	80-A	2	0	0	0	0
4	81-A	2	0	0	0	0
4	82-A	2	0	0	0	0
4	83-A	2	0	0	0	0
4	84-A	2	0	0	0	0
4	85-A	2	0	0	0	0
4	86-A	2	0	0	0	0
4	87-A	2	0	0	0	0
4	88-A	2	0	0	0	0
4	89-A	2	0	0	0	0
4	90-A	2	0	0	0	0
4	91-A	2	0	0	0	0
4	92-A	2	0	0	0	0
4	93-A	2	0	0	0	0
4	94-A	2	0	0	0	0
4	95-A	2	0	0	0	0
4	96-A	2	0	0	0	0
4	97-A	2	0	0	0	0
4	98-A	2	0	0	0	0
4	99-A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	100-A	2	0	0	0	0
4	101-A	2	0	0	0	0
4	102-A	2	0	0	0	0
4	103-A	2	0	0	0	0
4	104-A	2	0	0	0	0
4	105-A	2	0	0	0	0
4	106-A	2	0	0	0	0
4	107-A	2	0	0	0	0
4	108-A	2	0	0	0	0
4	109-A	2	0	0	0	0
4	110-A	2	0	0	0	0
4	111-A	2	0	0	0	0
4	112-A	2	0	0	0	0
4	113-A	2	0	0	0	0
4	114-A	2	0	0	0	0
4	115-A	2	0	0	0	0
4	116-A	2	0	0	0	0
4	117-A	2	0	0	0	0
4	118-A	2	0	0	0	0
4	119-A	2	0	0	0	0
4	120-A	2	0	0	0	0
4	121-A	2	0	0	0	0
4	122-A	2	0	0	0	0
4	123-A	2	0	0	0	0
4	124-A	2	0	0	0	0
4	125-A	2	0	0	0	0
4	126-A	2	0	0	0	0
4	127-A	2	0	0	0	0
4	128-A	2	0	0	0	0
4	129-A	2	0	0	0	0
4	130-A	2	0	0	0	0
4	131-A	2	0	0	0	0
4	132-A	2	0	0	0	0
4	133-A	2	0	0	0	0
4	134-A	2	0	0	0	0
4	135-A	2	0	0	0	0
4	136-A	2	0	0	0	0
4	137-A	2	0	0	0	0
4	138-A	2	0	0	0	0
4	139-A	2	0	0	0	0
4	140-A	2	0	0	0	0
4	141-A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	142-A	2	0	0	0	0
4	143-A	2	0	0	0	0
4	144-A	2	0	0	0	0
4	145-A	2	0	0	0	0
4	146-A	2	0	0	0	0
4	147-A	2	0	0	0	0
4	148-A	2	0	0	0	0
4	149-A	2	0	0	0	0
4	150-A	2	0	0	0	0
4	151-A	2	0	0	0	0
4	152-A	2	0	0	0	0
4	153-A	2	0	0	0	0
4	154-A	2	0	0	0	0
4	155-A	2	0	0	0	0
4	156-A	2	0	0	0	0
4	157-A	2	0	0	0	0
4	158-A	2	0	0	0	0
4	159-A	2	0	0	0	0
4	160-A	2	0	0	0	0
4	161-A	2	0	0	0	0
4	162-A	2	0	0	0	0
4	163-A	2	0	0	0	0
4	164-A	2	0	0	0	0
4	165-A	2	0	0	0	0
4	166-A	2	0	0	0	0
4	167-A	2	0	0	0	0
4	168-A	2	0	0	0	0
4	169-A	2	0	0	0	0
4	170-A	2	0	0	0	0
4	171-A	2	0	0	0	0
4	172-A	2	0	0	0	0
4	173-A	2	0	0	0	0
4	174-A	2	0	0	0	0
4	175-A	2	0	0	0	0
4	176-A	2	0	0	0	0
4	177-A	2	0	0	0	0
4	178-A	2	0	0	0	0
4	179-A	2	0	0	0	0
4	180-A	2	0	0	0	0
4	181-A	2	0	0	0	0
4	182-A	2	0	0	0	0
4	183-A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	184-A	2	0	0	0	0
4	185-A	2	0	0	0	0
4	186-A	2	0	0	0	0
4	187-A	2	0	0	0	0
4	188-A	2	0	0	0	0
4	189-A	2	0	0	0	0
4	190-A	2	0	0	0	0
4	191-A	2	0	0	0	0
4	192-A	2	0	0	0	0
4	193-A	2	0	0	0	0
4	194-A	2	0	0	0	0
4	195-A	2	0	0	0	0
4	196-A	2	0	0	0	0
4	197-A	2	0	0	0	0
4	198-A	2	0	0	0	0
4	199-A	2	0	0	0	0
4	200-A	2	0	0	0	0
4	201-A	2	0	0	0	0
4	202-A	2	0	0	0	0
4	203-A	2	0	0	0	0
4	204-A	2	0	0	0	0
4	205-A	2	0	0	0	0
4	206-A	2	0	0	0	0
4	207-A	2	0	0	0	0
4	208-A	2	0	0	0	0
4	209-A	2	0	0	0	0
4	210-A	2	0	0	0	0
4	211-A	2	0	0	0	0
4	212-A	2	0	0	0	0
4	213-A	2	0	0	0	0
4	214-A	2	0	0	0	0
4	215-A	2	0	0	0	0
4	216-A	2	0	0	0	0
4	217-A	2	0	0	0	0
4	218-A	2	0	0	0	0
4	219-A	2	0	0	0	0
4	220-A	2	0	0	0	0
4	221-A	2	0	0	0	0
4	222-A	2	0	0	0	0
4	223-A	2	0	0	0	0
4	224-A	2	0	0	0	0
4	225-A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	226-A	2	0	0	0	0
4	227-A	2	0	0	0	0
4	228-A	2	0	0	0	0
4	229-A	2	0	0	0	0
4	230-A	2	0	0	0	0
4	231-A	2	0	0	0	0
4	232-A	2	0	0	0	0
4	233-A	2	0	0	0	0
4	234-A	2	0	0	0	0
4	235-A	2	0	0	0	0
4	236-A	2	0	0	0	0
4	237-A	2	0	0	0	0
4	238-A	2	0	0	0	0
4	239-A	2	0	0	0	0
4	240-A	2	0	0	0	0
4	241-A	2	0	0	0	0
4	242-A	2	0	0	0	0
4	243-A	2	0	0	0	0
4	244-A	2	0	0	0	0
4	245-A	2	0	0	0	0
4	246-A	2	0	0	0	0
4	247-A	2	0	0	0	0
4	248-A	2	0	0	0	0
4	249-A	2	0	0	0	0
4	250-A	2	0	0	0	0
5	1-A	180	0	0	0	0
5	2-A	171	0	0	0	0
5	3-A	185	0	0	0	0
5	4-A	189	0	0	0	0
5	5-A	176	0	0	0	0
5	6-A	189	0	0	0	0
5	7-A	179	0	0	0	0
5	8-A	196	0	0	0	0
5	9-A	198	0	0	0	0
5	10-A	197	0	0	0	0
5	11-A	199	0	0	0	0
5	12-A	191	0	0	0	0
5	13-A	176	0	0	0	0
5	14-A	191	0	0	0	0
5	15-A	197	0	0	0	0
5	16-A	183	0	0	0	0
5	17-A	177	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	18-A	170	0	0	0	0
5	19-A	173	0	0	0	0
5	20-A	179	0	0	0	0
5	21-A	185	0	0	0	0
5	22-A	195	0	0	0	0
5	23-A	181	0	0	0	0
5	24-A	172	0	0	0	0
5	25-A	179	0	0	0	0
5	26-A	196	0	0	0	0
5	27-A	195	0	0	0	0
5	28-A	193	0	0	0	0
5	29-A	184	0	0	0	0
5	30-A	185	0	0	0	0
5	31-A	190	0	0	0	0
5	32-A	175	0	0	0	0
5	33-A	199	0	0	0	0
5	34-A	196	0	0	0	0
5	35-A	185	0	0	0	0
5	36-A	191	0	0	0	0
5	37-A	191	0	0	0	0
5	38-A	183	0	0	0	0
5	39-A	177	0	0	0	0
5	40-A	183	0	0	0	0
5	41-A	182	0	0	0	0
5	42-A	176	0	0	0	0
5	43-A	172	0	0	0	0
5	44-A	181	0	0	0	0
5	45-A	194	0	0	0	0
5	46-A	198	0	0	0	0
5	47-A	194	0	0	0	0
5	48-A	177	0	0	0	0
5	49-A	165	0	0	0	0
5	50-A	172	0	0	0	0
5	51-A	171	0	0	0	0
5	52-A	175	0	0	0	0
5	53-A	191	0	0	0	0
5	54-A	185	0	0	0	0
5	55-A	183	0	0	0	0
5	56-A	186	0	0	0	0
5	57-A	187	0	0	0	0
5	58-A	193	0	0	0	0
5	59-A	187	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	60-A	178	0	0	0	0
5	61-A	169	0	0	0	0
5	62-A	169	0	0	0	0
5	63-A	179	0	0	0	0
5	64-A	180	0	0	0	0
5	65-A	189	0	0	0	0
5	66-A	194	0	0	0	0
5	67-A	170	0	0	0	0
5	68-A	174	0	0	0	0
5	69-A	193	0	0	0	0
5	70-A	199	0	0	0	0
5	71-A	176	0	0	0	0
5	72-A	172	0	0	0	0
5	73-A	175	0	0	0	0
5	74-A	185	0	0	0	0
5	75-A	186	0	0	0	0
5	76-A	183	0	0	0	0
5	77-A	192	0	0	0	0
5	78-A	192	0	0	0	0
5	79-A	178	0	0	0	0
5	80-A	181	0	0	0	0
5	81-A	178	0	0	0	0
5	82-A	188	0	0	0	0
5	83-A	189	0	0	0	0
5	84-A	189	0	0	0	0
5	85-A	179	0	0	0	0
5	86-A	185	0	0	0	0
5	87-A	192	0	0	0	0
5	88-A	187	0	0	0	0
5	89-A	185	0	0	0	0
5	90-A	182	0	0	0	0
5	91-A	183	0	0	0	0
5	92-A	182	0	0	0	0
5	93-A	186	0	0	0	0
5	94-A	175	0	0	0	0
5	95-A	186	0	0	0	0
5	96-A	188	0	0	0	0
5	97-A	186	0	0	0	0
5	98-A	180	0	0	0	0
5	99-A	183	0	0	0	0
5	100-A	172	0	0	0	0
5	101-A	175	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	102-A	183	0	0	0	0
5	103-A	200	0	0	0	0
5	104-A	185	0	0	0	0
5	105-A	180	0	0	0	0
5	106-A	189	0	0	0	0
5	107-A	193	0	0	0	0
5	108-A	185	0	0	0	0
5	109-A	181	0	0	0	0
5	110-A	212	0	0	0	0
5	111-A	207	0	0	0	0
5	112-A	206	0	0	0	0
5	113-A	189	0	0	0	0
5	114-A	173	0	0	0	0
5	115-A	182	0	0	0	0
5	116-A	189	0	0	0	0
5	117-A	174	0	0	0	0
5	118-A	180	0	0	0	0
5	119-A	181	0	0	0	0
5	120-A	179	0	0	0	0
5	121-A	189	0	0	0	0
5	122-A	201	0	0	0	0
5	123-A	202	0	0	0	0
5	124-A	198	0	0	0	0
5	125-A	204	0	0	0	0
5	126-A	192	0	0	0	0
5	127-A	183	0	0	0	0
5	128-A	184	0	0	0	0
5	129-A	186	0	0	0	0
5	130-A	196	0	0	0	0
5	131-A	176	0	0	0	0
5	132-A	187	0	0	0	0
5	133-A	183	0	0	0	0
5	134-A	182	0	0	0	0
5	135-A	193	0	0	0	0
5	136-A	185	0	0	0	0
5	137-A	185	0	0	0	0
5	138-A	181	0	0	0	0
5	139-A	167	0	0	0	0
5	140-A	173	0	0	0	0
5	141-A	186	0	0	0	0
5	142-A	206	0	0	0	0
5	143-A	187	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	144-A	178	0	0	0	0
5	145-A	171	0	0	0	0
5	146-A	174	0	0	0	0
5	147-A	171	0	0	0	0
5	148-A	176	0	0	0	0
5	149-A	196	0	0	0	0
5	150-A	185	0	0	0	0
5	151-A	184	0	0	0	0
5	152-A	179	0	0	0	0
5	153-A	186	0	0	0	0
5	154-A	184	0	0	0	0
5	155-A	188	0	0	0	0
5	156-A	176	0	0	0	0
5	157-A	174	0	0	0	0
5	158-A	181	0	0	0	0
5	159-A	180	0	0	0	0
5	160-A	186	0	0	0	0
5	161-A	199	0	0	0	0
5	162-A	199	0	0	0	0
5	163-A	199	0	0	0	0
5	164-A	181	0	0	0	0
5	165-A	191	0	0	0	0
5	166-A	189	0	0	0	0
5	167-A	171	0	0	0	0
5	168-A	171	0	0	0	0
5	169-A	187	0	0	0	0
5	170-A	186	0	0	0	0
5	171-A	184	0	0	0	0
5	172-A	185	0	0	0	0
5	173-A	193	0	0	0	0
5	174-A	184	0	0	0	0
5	175-A	187	0	0	0	0
5	176-A	186	0	0	0	0
5	177-A	173	0	0	0	0
5	178-A	185	0	0	0	0
5	179-A	174	0	0	0	0
5	180-A	173	0	0	0	0
5	181-A	199	0	0	0	0
5	182-A	192	0	0	0	0
5	183-A	199	0	0	0	0
5	184-A	187	0	0	0	0
5	185-A	174	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	186-A	169	0	0	0	0
5	187-A	165	0	0	0	0
5	188-A	180	0	0	0	0
5	189-A	175	0	0	0	0
5	190-A	181	0	0	0	0
5	191-A	192	0	0	0	0
5	192-A	191	0	0	0	0
5	193-A	190	0	0	0	0
5	194-A	193	0	0	0	0
5	195-A	194	0	0	0	0
5	196-A	186	0	0	0	0
5	197-A	167	0	0	0	0
5	198-A	174	0	0	0	0
5	199-A	184	0	0	0	0
5	200-A	190	0	0	0	0
5	201-A	189	0	0	0	0
5	202-A	171	0	0	0	0
5	203-A	185	0	0	0	0
5	204-A	188	0	0	0	0
5	205-A	185	0	0	0	0
5	206-A	186	0	0	0	0
5	207-A	199	0	0	0	0
5	208-A	186	0	0	0	0
5	209-A	179	0	0	0	0
5	210-A	179	0	0	0	0
5	211-A	176	0	0	0	0
5	212-A	175	0	0	0	0
5	213-A	180	0	0	0	0
5	214-A	181	0	0	0	0
5	215-A	191	0	0	0	0
5	216-A	185	0	0	0	0
5	217-A	204	0	0	0	0
5	218-A	191	0	0	0	0
5	219-A	176	0	0	0	0
5	220-A	185	0	0	0	0
5	221-A	179	0	0	0	0
5	222-A	173	0	0	0	0
5	223-A	180	0	0	0	0
5	224-A	178	0	0	0	0
5	225-A	187	0	0	0	0
5	226-A	189	0	0	0	0
5	227-A	187	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	228-A	184	0	0	0	0
5	229-A	183	0	0	0	0
5	230-A	193	0	0	0	0
5	231-A	198	0	0	0	0
5	232-A	183	0	0	0	0
5	233-A	180	0	0	0	0
5	234-A	175	0	0	0	0
5	235-A	201	0	0	0	0
5	236-A	204	0	0	0	0
5	237-A	193	0	0	0	0
5	238-A	159	0	0	0	0
5	239-A	164	0	0	0	0
5	240-A	179	0	0	0	0
5	241-A	183	0	0	0	0
5	242-A	183	0	0	0	0
5	243-A	194	0	0	0	0
5	244-A	205	0	0	0	0
5	245-A	198	0	0	0	0
5	246-A	166	0	0	0	0
5	247-A	171	0	0	0	0
5	248-A	171	0	0	0	0
5	249-A	191	0	0	0	0
5	250-A	202	0	0	0	0
All	All	384130	315750	315730	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	156/159 (98%)	150 (96%)	5 (3%)	1 (1%)	25	5
1	2-A	156/159 (98%)	150 (96%)	6 (4%)	0	100	100
1	3-A	156/159 (98%)	148 (95%)	5 (3%)	3 (2%)	8	0
1	4-A	156/159 (98%)	147 (94%)	7 (4%)	2 (1%)	12	1
1	5-A	156/159 (98%)	152 (97%)	3 (2%)	1 (1%)	25	5
1	6-A	156/159 (98%)	153 (98%)	3 (2%)	0	100	100
1	7-A	156/159 (98%)	149 (96%)	6 (4%)	1 (1%)	25	5
1	8-A	156/159 (98%)	152 (97%)	3 (2%)	1 (1%)	25	5
1	9-A	156/159 (98%)	149 (96%)	7 (4%)	0	100	100
1	10-A	156/159 (98%)	154 (99%)	2 (1%)	0	100	100
1	11-A	156/159 (98%)	149 (96%)	7 (4%)	0	100	100
1	12-A	156/159 (98%)	152 (97%)	4 (3%)	0	100	100
1	13-A	156/159 (98%)	150 (96%)	6 (4%)	0	100	100
1	14-A	156/159 (98%)	153 (98%)	3 (2%)	0	100	100
1	15-A	156/159 (98%)	152 (97%)	4 (3%)	0	100	100
1	16-A	156/159 (98%)	154 (99%)	1 (1%)	1 (1%)	25	5
1	17-A	156/159 (98%)	149 (96%)	6 (4%)	1 (1%)	25	5
1	18-A	156/159 (98%)	152 (97%)	3 (2%)	1 (1%)	25	5
1	19-A	156/159 (98%)	150 (96%)	5 (3%)	1 (1%)	25	5
1	20-A	156/159 (98%)	153 (98%)	3 (2%)	0	100	100
1	21-A	156/159 (98%)	147 (94%)	8 (5%)	1 (1%)	25	5
1	22-A	156/159 (98%)	151 (97%)	3 (2%)	2 (1%)	12	1
1	23-A	156/159 (98%)	151 (97%)	5 (3%)	0	100	100
1	24-A	156/159 (98%)	153 (98%)	2 (1%)	1 (1%)	25	5
1	25-A	156/159 (98%)	150 (96%)	6 (4%)	0	100	100
1	26-A	156/159 (98%)	152 (97%)	3 (2%)	1 (1%)	25	5
1	27-A	156/159 (98%)	153 (98%)	2 (1%)	1 (1%)	25	5
1	28-A	156/159 (98%)	147 (94%)	7 (4%)	2 (1%)	12	1
1	29-A	156/159 (98%)	150 (96%)	6 (4%)	0	100	100
1	30-A	156/159 (98%)	149 (96%)	5 (3%)	2 (1%)	12	1
1	31-A	156/159 (98%)	149 (96%)	7 (4%)	0	100	100
1	32-A	156/159 (98%)	148 (95%)	7 (4%)	1 (1%)	25	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	33-A	156/159 (98%)	147 (94%)	7 (4%)	2 (1%)	12	1
1	34-A	156/159 (98%)	149 (96%)	4 (3%)	3 (2%)	8	0
1	35-A	156/159 (98%)	147 (94%)	4 (3%)	5 (3%)	4	0
1	36-A	156/159 (98%)	150 (96%)	5 (3%)	1 (1%)	25	5
1	37-A	156/159 (98%)	149 (96%)	6 (4%)	1 (1%)	25	5
1	38-A	156/159 (98%)	149 (96%)	4 (3%)	3 (2%)	8	0
1	39-A	156/159 (98%)	150 (96%)	6 (4%)	0	100	100
1	40-A	156/159 (98%)	149 (96%)	7 (4%)	0	100	100
1	41-A	156/159 (98%)	149 (96%)	6 (4%)	1 (1%)	25	5
1	42-A	156/159 (98%)	152 (97%)	2 (1%)	2 (1%)	12	1
1	43-A	156/159 (98%)	148 (95%)	7 (4%)	1 (1%)	25	5
1	44-A	156/159 (98%)	153 (98%)	2 (1%)	1 (1%)	25	5
1	45-A	156/159 (98%)	149 (96%)	6 (4%)	1 (1%)	25	5
1	46-A	156/159 (98%)	154 (99%)	1 (1%)	1 (1%)	25	5
1	47-A	156/159 (98%)	153 (98%)	3 (2%)	0	100	100
1	48-A	156/159 (98%)	147 (94%)	6 (4%)	3 (2%)	8	0
1	49-A	156/159 (98%)	149 (96%)	4 (3%)	3 (2%)	8	0
1	50-A	156/159 (98%)	146 (94%)	9 (6%)	1 (1%)	25	5
1	51-A	156/159 (98%)	149 (96%)	6 (4%)	1 (1%)	25	5
1	52-A	156/159 (98%)	149 (96%)	7 (4%)	0	100	100
1	53-A	156/159 (98%)	151 (97%)	3 (2%)	2 (1%)	12	1
1	54-A	156/159 (98%)	152 (97%)	2 (1%)	2 (1%)	12	1
1	55-A	156/159 (98%)	151 (97%)	4 (3%)	1 (1%)	25	5
1	56-A	156/159 (98%)	147 (94%)	7 (4%)	2 (1%)	12	1
1	57-A	156/159 (98%)	147 (94%)	6 (4%)	3 (2%)	8	0
1	58-A	156/159 (98%)	150 (96%)	5 (3%)	1 (1%)	25	5
1	59-A	156/159 (98%)	149 (96%)	4 (3%)	3 (2%)	8	0
1	60-A	156/159 (98%)	151 (97%)	2 (1%)	3 (2%)	8	0
1	61-A	156/159 (98%)	150 (96%)	5 (3%)	1 (1%)	25	5
1	62-A	156/159 (98%)	150 (96%)	6 (4%)	0	100	100
1	63-A	156/159 (98%)	148 (95%)	6 (4%)	2 (1%)	12	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	64-A	156/159 (98%)	149 (96%)	6 (4%)	1 (1%)	25	5
1	65-A	156/159 (98%)	148 (95%)	7 (4%)	1 (1%)	25	5
1	66-A	156/159 (98%)	148 (95%)	6 (4%)	2 (1%)	12	1
1	67-A	156/159 (98%)	149 (96%)	3 (2%)	4 (3%)	5	0
1	68-A	156/159 (98%)	153 (98%)	3 (2%)	0	100	100
1	69-A	156/159 (98%)	151 (97%)	4 (3%)	1 (1%)	25	5
1	70-A	156/159 (98%)	152 (97%)	3 (2%)	1 (1%)	25	5
1	71-A	156/159 (98%)	149 (96%)	5 (3%)	2 (1%)	12	1
1	72-A	156/159 (98%)	146 (94%)	6 (4%)	4 (3%)	5	0
1	73-A	156/159 (98%)	150 (96%)	4 (3%)	2 (1%)	12	1
1	74-A	156/159 (98%)	151 (97%)	2 (1%)	3 (2%)	8	0
1	75-A	156/159 (98%)	150 (96%)	3 (2%)	3 (2%)	8	0
1	76-A	156/159 (98%)	150 (96%)	3 (2%)	3 (2%)	8	0
1	77-A	156/159 (98%)	151 (97%)	3 (2%)	2 (1%)	12	1
1	78-A	156/159 (98%)	148 (95%)	7 (4%)	1 (1%)	25	5
1	79-A	156/159 (98%)	152 (97%)	4 (3%)	0	100	100
1	80-A	156/159 (98%)	150 (96%)	6 (4%)	0	100	100
1	81-A	156/159 (98%)	149 (96%)	7 (4%)	0	100	100
1	82-A	156/159 (98%)	152 (97%)	4 (3%)	0	100	100
1	83-A	156/159 (98%)	150 (96%)	4 (3%)	2 (1%)	12	1
1	84-A	156/159 (98%)	150 (96%)	6 (4%)	0	100	100
1	85-A	156/159 (98%)	147 (94%)	8 (5%)	1 (1%)	25	5
1	86-A	156/159 (98%)	147 (94%)	6 (4%)	3 (2%)	8	0
1	87-A	156/159 (98%)	152 (97%)	3 (2%)	1 (1%)	25	5
1	88-A	156/159 (98%)	154 (99%)	1 (1%)	1 (1%)	25	5
1	89-A	156/159 (98%)	151 (97%)	5 (3%)	0	100	100
1	90-A	156/159 (98%)	148 (95%)	6 (4%)	2 (1%)	12	1
1	91-A	156/159 (98%)	152 (97%)	3 (2%)	1 (1%)	25	5
1	92-A	156/159 (98%)	146 (94%)	5 (3%)	5 (3%)	4	0
1	93-A	156/159 (98%)	149 (96%)	5 (3%)	2 (1%)	12	1
1	94-A	156/159 (98%)	152 (97%)	2 (1%)	2 (1%)	12	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	95-A	156/159 (98%)	150 (96%)	5 (3%)	1 (1%)	25	5
1	96-A	156/159 (98%)	149 (96%)	6 (4%)	1 (1%)	25	5
1	97-A	156/159 (98%)	152 (97%)	2 (1%)	2 (1%)	12	1
1	98-A	156/159 (98%)	149 (96%)	7 (4%)	0	100	100
1	99-A	156/159 (98%)	151 (97%)	4 (3%)	1 (1%)	25	5
1	100-A	156/159 (98%)	151 (97%)	5 (3%)	0	100	100
1	101-A	156/159 (98%)	149 (96%)	7 (4%)	0	100	100
1	102-A	156/159 (98%)	148 (95%)	7 (4%)	1 (1%)	25	5
1	103-A	156/159 (98%)	151 (97%)	5 (3%)	0	100	100
1	104-A	156/159 (98%)	149 (96%)	7 (4%)	0	100	100
1	105-A	156/159 (98%)	149 (96%)	6 (4%)	1 (1%)	25	5
1	106-A	156/159 (98%)	147 (94%)	9 (6%)	0	100	100
1	107-A	156/159 (98%)	153 (98%)	2 (1%)	1 (1%)	25	5
1	108-A	156/159 (98%)	152 (97%)	4 (3%)	0	100	100
1	109-A	156/159 (98%)	152 (97%)	1 (1%)	3 (2%)	8	0
1	110-A	156/159 (98%)	148 (95%)	7 (4%)	1 (1%)	25	5
1	111-A	156/159 (98%)	148 (95%)	7 (4%)	1 (1%)	25	5
1	112-A	156/159 (98%)	151 (97%)	5 (3%)	0	100	100
1	113-A	156/159 (98%)	154 (99%)	2 (1%)	0	100	100
1	114-A	156/159 (98%)	152 (97%)	4 (3%)	0	100	100
1	115-A	156/159 (98%)	150 (96%)	5 (3%)	1 (1%)	25	5
1	116-A	156/159 (98%)	151 (97%)	5 (3%)	0	100	100
1	117-A	156/159 (98%)	148 (95%)	5 (3%)	3 (2%)	8	0
1	118-A	156/159 (98%)	147 (94%)	4 (3%)	5 (3%)	4	0
1	119-A	156/159 (98%)	148 (95%)	6 (4%)	2 (1%)	12	1
1	120-A	156/159 (98%)	150 (96%)	4 (3%)	2 (1%)	12	1
1	121-A	156/159 (98%)	152 (97%)	4 (3%)	0	100	100
1	122-A	156/159 (98%)	151 (97%)	4 (3%)	1 (1%)	25	5
1	123-A	156/159 (98%)	151 (97%)	4 (3%)	1 (1%)	25	5
1	124-A	156/159 (98%)	151 (97%)	4 (3%)	1 (1%)	25	5
1	125-A	156/159 (98%)	152 (97%)	3 (2%)	1 (1%)	25	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	126-A	156/159 (98%)	152 (97%)	4 (3%)	0	100	100
1	127-A	156/159 (98%)	149 (96%)	7 (4%)	0	100	100
1	128-A	156/159 (98%)	152 (97%)	4 (3%)	0	100	100
1	129-A	156/159 (98%)	150 (96%)	5 (3%)	1 (1%)	25	5
1	130-A	156/159 (98%)	150 (96%)	6 (4%)	0	100	100
1	131-A	156/159 (98%)	153 (98%)	2 (1%)	1 (1%)	25	5
1	132-A	156/159 (98%)	151 (97%)	5 (3%)	0	100	100
1	133-A	156/159 (98%)	153 (98%)	3 (2%)	0	100	100
1	134-A	156/159 (98%)	153 (98%)	1 (1%)	2 (1%)	12	1
1	135-A	156/159 (98%)	152 (97%)	2 (1%)	2 (1%)	12	1
1	136-A	156/159 (98%)	151 (97%)	4 (3%)	1 (1%)	25	5
1	137-A	156/159 (98%)	151 (97%)	5 (3%)	0	100	100
1	138-A	156/159 (98%)	148 (95%)	7 (4%)	1 (1%)	25	5
1	139-A	156/159 (98%)	151 (97%)	4 (3%)	1 (1%)	25	5
1	140-A	156/159 (98%)	150 (96%)	4 (3%)	2 (1%)	12	1
1	141-A	156/159 (98%)	146 (94%)	7 (4%)	3 (2%)	8	0
1	142-A	156/159 (98%)	149 (96%)	6 (4%)	1 (1%)	25	5
1	143-A	156/159 (98%)	143 (92%)	11 (7%)	2 (1%)	12	1
1	144-A	156/159 (98%)	147 (94%)	6 (4%)	3 (2%)	8	0
1	145-A	156/159 (98%)	147 (94%)	5 (3%)	4 (3%)	5	0
1	146-A	156/159 (98%)	148 (95%)	5 (3%)	3 (2%)	8	0
1	147-A	156/159 (98%)	150 (96%)	4 (3%)	2 (1%)	12	1
1	148-A	156/159 (98%)	147 (94%)	8 (5%)	1 (1%)	25	5
1	149-A	156/159 (98%)	149 (96%)	6 (4%)	1 (1%)	25	5
1	150-A	156/159 (98%)	151 (97%)	4 (3%)	1 (1%)	25	5
1	151-A	156/159 (98%)	147 (94%)	7 (4%)	2 (1%)	12	1
1	152-A	156/159 (98%)	150 (96%)	4 (3%)	2 (1%)	12	1
1	153-A	156/159 (98%)	149 (96%)	5 (3%)	2 (1%)	12	1
1	154-A	156/159 (98%)	150 (96%)	4 (3%)	2 (1%)	12	1
1	155-A	156/159 (98%)	150 (96%)	3 (2%)	3 (2%)	8	0
1	156-A	156/159 (98%)	146 (94%)	9 (6%)	1 (1%)	25	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	157-A	156/159 (98%)	150 (96%)	6 (4%)	0	100	100
1	158-A	156/159 (98%)	149 (96%)	6 (4%)	1 (1%)	25	5
1	159-A	156/159 (98%)	149 (96%)	4 (3%)	3 (2%)	8	0
1	160-A	156/159 (98%)	148 (95%)	6 (4%)	2 (1%)	12	1
1	161-A	156/159 (98%)	144 (92%)	9 (6%)	3 (2%)	8	0
1	162-A	156/159 (98%)	146 (94%)	6 (4%)	4 (3%)	5	0
1	163-A	156/159 (98%)	149 (96%)	6 (4%)	1 (1%)	25	5
1	164-A	156/159 (98%)	149 (96%)	6 (4%)	1 (1%)	25	5
1	165-A	156/159 (98%)	151 (97%)	4 (3%)	1 (1%)	25	5
1	166-A	156/159 (98%)	151 (97%)	4 (3%)	1 (1%)	25	5
1	167-A	156/159 (98%)	148 (95%)	7 (4%)	1 (1%)	25	5
1	168-A	156/159 (98%)	150 (96%)	4 (3%)	2 (1%)	12	1
1	169-A	156/159 (98%)	149 (96%)	6 (4%)	1 (1%)	25	5
1	170-A	156/159 (98%)	148 (95%)	6 (4%)	2 (1%)	12	1
1	171-A	156/159 (98%)	152 (97%)	4 (3%)	0	100	100
1	172-A	156/159 (98%)	151 (97%)	5 (3%)	0	100	100
1	173-A	156/159 (98%)	151 (97%)	5 (3%)	0	100	100
1	174-A	156/159 (98%)	151 (97%)	5 (3%)	0	100	100
1	175-A	156/159 (98%)	151 (97%)	5 (3%)	0	100	100
1	176-A	156/159 (98%)	153 (98%)	3 (2%)	0	100	100
1	177-A	156/159 (98%)	150 (96%)	6 (4%)	0	100	100
1	178-A	156/159 (98%)	147 (94%)	6 (4%)	3 (2%)	8	0
1	179-A	156/159 (98%)	147 (94%)	6 (4%)	3 (2%)	8	0
1	180-A	156/159 (98%)	146 (94%)	9 (6%)	1 (1%)	25	5
1	181-A	156/159 (98%)	150 (96%)	5 (3%)	1 (1%)	25	5
1	182-A	156/159 (98%)	148 (95%)	4 (3%)	4 (3%)	5	0
1	183-A	156/159 (98%)	144 (92%)	8 (5%)	4 (3%)	5	0
1	184-A	156/159 (98%)	154 (99%)	1 (1%)	1 (1%)	25	5
1	185-A	156/159 (98%)	152 (97%)	1 (1%)	3 (2%)	8	0
1	186-A	156/159 (98%)	149 (96%)	4 (3%)	3 (2%)	8	0
1	187-A	156/159 (98%)	150 (96%)	4 (3%)	2 (1%)	12	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	188-A	156/159 (98%)	150 (96%)	4 (3%)	2 (1%)	12	1
1	189-A	156/159 (98%)	152 (97%)	1 (1%)	3 (2%)	8	0
1	190-A	156/159 (98%)	151 (97%)	3 (2%)	2 (1%)	12	1
1	191-A	156/159 (98%)	150 (96%)	5 (3%)	1 (1%)	25	5
1	192-A	156/159 (98%)	148 (95%)	8 (5%)	0	100	100
1	193-A	156/159 (98%)	150 (96%)	4 (3%)	2 (1%)	12	1
1	194-A	156/159 (98%)	149 (96%)	4 (3%)	3 (2%)	8	0
1	195-A	156/159 (98%)	148 (95%)	5 (3%)	3 (2%)	8	0
1	196-A	156/159 (98%)	150 (96%)	5 (3%)	1 (1%)	25	5
1	197-A	156/159 (98%)	153 (98%)	3 (2%)	0	100	100
1	198-A	156/159 (98%)	152 (97%)	4 (3%)	0	100	100
1	199-A	156/159 (98%)	152 (97%)	4 (3%)	0	100	100
1	200-A	156/159 (98%)	149 (96%)	7 (4%)	0	100	100
1	201-A	156/159 (98%)	150 (96%)	5 (3%)	1 (1%)	25	5
1	202-A	156/159 (98%)	151 (97%)	5 (3%)	0	100	100
1	203-A	156/159 (98%)	150 (96%)	3 (2%)	3 (2%)	8	0
1	204-A	156/159 (98%)	148 (95%)	8 (5%)	0	100	100
1	205-A	156/159 (98%)	150 (96%)	4 (3%)	2 (1%)	12	1
1	206-A	156/159 (98%)	154 (99%)	1 (1%)	1 (1%)	25	5
1	207-A	156/159 (98%)	151 (97%)	3 (2%)	2 (1%)	12	1
1	208-A	156/159 (98%)	153 (98%)	2 (1%)	1 (1%)	25	5
1	209-A	156/159 (98%)	152 (97%)	3 (2%)	1 (1%)	25	5
1	210-A	156/159 (98%)	148 (95%)	6 (4%)	2 (1%)	12	1
1	211-A	156/159 (98%)	147 (94%)	6 (4%)	3 (2%)	8	0
1	212-A	156/159 (98%)	152 (97%)	3 (2%)	1 (1%)	25	5
1	213-A	156/159 (98%)	148 (95%)	6 (4%)	2 (1%)	12	1
1	214-A	156/159 (98%)	148 (95%)	7 (4%)	1 (1%)	25	5
1	215-A	156/159 (98%)	147 (94%)	7 (4%)	2 (1%)	12	1
1	216-A	156/159 (98%)	142 (91%)	7 (4%)	7 (4%)	2	0
1	217-A	156/159 (98%)	145 (93%)	7 (4%)	4 (3%)	5	0
1	218-A	156/159 (98%)	145 (93%)	5 (3%)	6 (4%)	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	219-A	156/159 (98%)	146 (94%)	7 (4%)	3 (2%)	8	0
1	220-A	156/159 (98%)	148 (95%)	3 (2%)	5 (3%)	4	0
1	221-A	156/159 (98%)	145 (93%)	8 (5%)	3 (2%)	8	0
1	222-A	156/159 (98%)	148 (95%)	5 (3%)	3 (2%)	8	0
1	223-A	156/159 (98%)	148 (95%)	4 (3%)	4 (3%)	5	0
1	224-A	156/159 (98%)	149 (96%)	6 (4%)	1 (1%)	25	5
1	225-A	156/159 (98%)	149 (96%)	2 (1%)	5 (3%)	4	0
1	226-A	156/159 (98%)	150 (96%)	6 (4%)	0	100	100
1	227-A	156/159 (98%)	153 (98%)	3 (2%)	0	100	100
1	228-A	156/159 (98%)	154 (99%)	2 (1%)	0	100	100
1	229-A	156/159 (98%)	150 (96%)	6 (4%)	0	100	100
1	230-A	156/159 (98%)	152 (97%)	3 (2%)	1 (1%)	25	5
1	231-A	156/159 (98%)	151 (97%)	4 (3%)	1 (1%)	25	5
1	232-A	156/159 (98%)	150 (96%)	6 (4%)	0	100	100
1	233-A	156/159 (98%)	153 (98%)	2 (1%)	1 (1%)	25	5
1	234-A	156/159 (98%)	144 (92%)	12 (8%)	0	100	100
1	235-A	156/159 (98%)	152 (97%)	4 (3%)	0	100	100
1	236-A	156/159 (98%)	152 (97%)	4 (3%)	0	100	100
1	237-A	156/159 (98%)	152 (97%)	3 (2%)	1 (1%)	25	5
1	238-A	156/159 (98%)	149 (96%)	5 (3%)	2 (1%)	12	1
1	239-A	156/159 (98%)	151 (97%)	5 (3%)	0	100	100
1	240-A	156/159 (98%)	147 (94%)	6 (4%)	3 (2%)	8	0
1	241-A	156/159 (98%)	146 (94%)	7 (4%)	3 (2%)	8	0
1	242-A	156/159 (98%)	152 (97%)	2 (1%)	2 (1%)	12	1
1	243-A	156/159 (98%)	151 (97%)	5 (3%)	0	100	100
1	244-A	156/159 (98%)	150 (96%)	6 (4%)	0	100	100
1	245-A	156/159 (98%)	148 (95%)	5 (3%)	3 (2%)	8	0
1	246-A	156/159 (98%)	150 (96%)	4 (3%)	2 (1%)	12	1
1	247-A	156/159 (98%)	152 (97%)	3 (2%)	1 (1%)	25	5
1	248-A	156/159 (98%)	151 (97%)	4 (3%)	1 (1%)	25	5
1	249-A	156/159 (98%)	149 (96%)	6 (4%)	1 (1%)	25	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	250-A	156/159 (98%)	149 (96%)	5 (3%)	2 (1%)	12	1
All	All	39000/39750 (98%)	37442 (96%)	1208 (3%)	350 (1%)	17	2

5 of 350 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	3-A	21	PRO
1	3-A	22	TRP
1	24-A	21	PRO
1	28-A	86	GLY
1	32-A	88	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	2-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	3-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	4-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	5-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	6-A	135/135 (100%)	116 (86%)	19 (14%)	3	0
1	7-A	135/135 (100%)	115 (85%)	20 (15%)	3	0
1	8-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	9-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	10-A	135/135 (100%)	117 (87%)	18 (13%)	4	0
1	11-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	12-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	13-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	14-A	135/135 (100%)	127 (94%)	8 (6%)	19	2
1	15-A	135/135 (100%)	123 (91%)	12 (9%)	9	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	16-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	17-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	18-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	19-A	135/135 (100%)	126 (93%)	9 (7%)	16	1
1	20-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	21-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	22-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	23-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	24-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	25-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	26-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	27-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	28-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	29-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	30-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	31-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	32-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	33-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	34-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	35-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	36-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	37-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	38-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	39-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	40-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	41-A	135/135 (100%)	116 (86%)	19 (14%)	3	0
1	42-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	43-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	44-A	135/135 (100%)	126 (93%)	9 (7%)	16	1
1	45-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	46-A	135/135 (100%)	127 (94%)	8 (6%)	19	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	47-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	48-A	135/135 (100%)	125 (93%)	10 (7%)	13	1
1	49-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	50-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	51-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	52-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	53-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	54-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	55-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	56-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	57-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	58-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	59-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	60-A	135/135 (100%)	125 (93%)	10 (7%)	13	1
1	61-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	62-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	63-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	64-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	65-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	66-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	67-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	68-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	69-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	70-A	135/135 (100%)	125 (93%)	10 (7%)	13	1
1	71-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	72-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	73-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	74-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	75-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	76-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	77-A	135/135 (100%)	125 (93%)	10 (7%)	13	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	78-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	79-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	80-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	81-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	82-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	83-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	84-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	85-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	86-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	87-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	88-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	89-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	90-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	91-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	92-A	135/135 (100%)	125 (93%)	10 (7%)	13	1
1	93-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	94-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	95-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	96-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	97-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	98-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	99-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	100-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	101-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	102-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	103-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	104-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	105-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	106-A	135/135 (100%)	126 (93%)	9 (7%)	16	1
1	107-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	108-A	135/135 (100%)	120 (89%)	15 (11%)	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	109-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	110-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	111-A	135/135 (100%)	125 (93%)	10 (7%)	13	1
1	112-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	113-A	135/135 (100%)	125 (93%)	10 (7%)	13	1
1	114-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	115-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	116-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	117-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	118-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	119-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	120-A	135/135 (100%)	127 (94%)	8 (6%)	19	2
1	121-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	122-A	135/135 (100%)	127 (94%)	8 (6%)	19	2
1	123-A	135/135 (100%)	127 (94%)	8 (6%)	19	2
1	124-A	135/135 (100%)	127 (94%)	8 (6%)	19	2
1	125-A	135/135 (100%)	130 (96%)	5 (4%)	34	6
1	126-A	135/135 (100%)	125 (93%)	10 (7%)	13	1
1	127-A	135/135 (100%)	117 (87%)	18 (13%)	4	0
1	128-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	129-A	135/135 (100%)	125 (93%)	10 (7%)	13	1
1	130-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	131-A	135/135 (100%)	125 (93%)	10 (7%)	13	1
1	132-A	135/135 (100%)	126 (93%)	9 (7%)	16	1
1	133-A	135/135 (100%)	129 (96%)	6 (4%)	28	4
1	134-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	135-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	136-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	137-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	138-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	139-A	135/135 (100%)	121 (90%)	14 (10%)	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	140-A	135/135 (100%)	125 (93%)	10 (7%)	13	1
1	141-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	142-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	143-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	144-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	145-A	135/135 (100%)	116 (86%)	19 (14%)	3	0
1	146-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	147-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	148-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	149-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	150-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	151-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	152-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	153-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	154-A	135/135 (100%)	125 (93%)	10 (7%)	13	1
1	155-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	156-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	157-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	158-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	159-A	135/135 (100%)	125 (93%)	10 (7%)	13	1
1	160-A	135/135 (100%)	127 (94%)	8 (6%)	19	2
1	161-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	162-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	163-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	164-A	135/135 (100%)	125 (93%)	10 (7%)	13	1
1	165-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	166-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	167-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	168-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	169-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	170-A	135/135 (100%)	122 (90%)	13 (10%)	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	171-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	172-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	173-A	135/135 (100%)	125 (93%)	10 (7%)	13	1
1	174-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	175-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	176-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	177-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	178-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	179-A	135/135 (100%)	116 (86%)	19 (14%)	3	0
1	180-A	135/135 (100%)	117 (87%)	18 (13%)	4	0
1	181-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	182-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	183-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	184-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	185-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	186-A	135/135 (100%)	125 (93%)	10 (7%)	13	1
1	187-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	188-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	189-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	190-A	135/135 (100%)	126 (93%)	9 (7%)	16	1
1	191-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	192-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	193-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	194-A	135/135 (100%)	127 (94%)	8 (6%)	19	2
1	195-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	196-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	197-A	135/135 (100%)	126 (93%)	9 (7%)	16	1
1	198-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	199-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	200-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	201-A	135/135 (100%)	119 (88%)	16 (12%)	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	202-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	203-A	135/135 (100%)	125 (93%)	10 (7%)	13	1
1	204-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	205-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	206-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	207-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	208-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	209-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	210-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	211-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	212-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	213-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	214-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	215-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	216-A	135/135 (100%)	123 (91%)	12 (9%)	9	1
1	217-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	218-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	219-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	220-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	221-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	222-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	223-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	224-A	135/135 (100%)	126 (93%)	9 (7%)	16	1
1	225-A	135/135 (100%)	125 (93%)	10 (7%)	13	1
1	226-A	135/135 (100%)	128 (95%)	7 (5%)	23	3
1	227-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	228-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	229-A	135/135 (100%)	125 (93%)	10 (7%)	13	1
1	230-A	135/135 (100%)	124 (92%)	11 (8%)	11	1
1	231-A	135/135 (100%)	128 (95%)	7 (5%)	23	3
1	232-A	135/135 (100%)	127 (94%)	8 (6%)	19	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	233-A	135/135 (100%)	128 (95%)	7 (5%)	23 3
1	234-A	135/135 (100%)	124 (92%)	11 (8%)	11 1
1	235-A	135/135 (100%)	130 (96%)	5 (4%)	34 6
1	236-A	135/135 (100%)	126 (93%)	9 (7%)	16 1
1	237-A	135/135 (100%)	125 (93%)	10 (7%)	13 1
1	238-A	135/135 (100%)	123 (91%)	12 (9%)	9 1
1	239-A	135/135 (100%)	125 (93%)	10 (7%)	13 1
1	240-A	135/135 (100%)	131 (97%)	4 (3%)	41 9
1	241-A	135/135 (100%)	127 (94%)	8 (6%)	19 2
1	242-A	135/135 (100%)	125 (93%)	10 (7%)	13 1
1	243-A	135/135 (100%)	129 (96%)	6 (4%)	28 4
1	244-A	135/135 (100%)	128 (95%)	7 (5%)	23 3
1	245-A	135/135 (100%)	125 (93%)	10 (7%)	13 1
1	246-A	135/135 (100%)	121 (90%)	14 (10%)	7 0
1	247-A	135/135 (100%)	123 (91%)	12 (9%)	9 1
1	248-A	135/135 (100%)	123 (91%)	12 (9%)	9 1
1	249-A	135/135 (100%)	122 (90%)	13 (10%)	8 0
1	250-A	135/135 (100%)	126 (93%)	9 (7%)	16 1
All	All	33750/33750 (100%)	30533 (90%)	3217 (10%)	8 0

5 of 3217 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	107-A	1	MET
1	136-A	68	THR
1	225-A	32	LYS
1	109-A	118	GLU
1	120-A	59	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

250 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	CSD	35-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	240-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	39-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	134-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	115-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	190-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	149-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	142-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	58-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	49-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	103-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	196-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	107-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	238-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	218-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	214-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	6-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	18-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	140-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	67-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	221-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	104-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	109-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	33-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	154-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	62-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	66-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	89-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	151-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	186-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	136-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	93-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	127-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	28-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	158-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	141-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	77-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	139-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	212-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	106-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	159-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	68-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	184-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	172-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	233-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	73-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	76-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	152-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	210-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	20-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	10-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	122-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	156-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	230-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	8-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	229-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	197-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	169-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	13-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	112-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	51-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	60-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	150-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	2-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	209-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	23-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	90-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	239-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	11-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	161-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	105-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	137-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	132-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	193-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	145-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	128-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	138-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	248-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	59-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	162-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	246-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	19-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	213-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	206-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	249-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	87-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	45-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	216-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	143-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	5-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	40-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	38-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	110-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	242-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	17-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	120-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	80-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	92-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	199-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	147-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	83-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	231-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	124-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	121-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	148-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	215-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	82-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	4-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	144-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	200-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	146-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	185-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	50-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	84-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	130-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	108-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	211-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	71-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	207-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	21-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	27-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	72-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	178-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	37-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	48-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	100-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	217-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	227-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	14-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	163-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	111-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	114-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	102-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	54-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	81-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	182-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	43-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	52-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	25-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	79-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	123-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	198-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	131-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	95-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	135-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	183-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	12-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	65-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	26-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	228-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	194-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	189-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	245-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	175-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	219-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	160-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	195-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	166-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	3-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	205-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	176-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	24-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	179-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	57-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	85-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	241-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	244-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	177-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	203-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	96-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	47-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	101-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	36-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	41-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	34-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	86-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	171-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	116-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	204-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	94-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	119-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	126-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	56-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	201-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	220-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	53-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	167-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	9-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	125-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	97-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	208-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	22-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	133-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	225-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	237-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	226-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	129-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	181-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	44-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	78-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	64-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	61-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	91-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	153-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	191-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	32-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	174-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	1-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	29-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	222-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	15-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	74-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	55-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	88-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	165-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	113-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	247-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	70-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	42-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	164-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	99-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	236-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	192-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	155-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	202-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	250-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	180-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	16-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	235-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	7-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	118-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	31-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	170-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	168-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	98-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	234-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	187-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	117-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	157-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	224-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	223-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	188-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	232-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	63-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	46-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	75-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	173-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	243-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	30-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)
1	CSD	69-A	152	1	3,7,8	1.03	0	1,8,10	5.48	1 (100%)

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
1	CSD	35-A	152	1	-	1/2/6/8	-
1	CSD	240-A	152	1	-	1/2/6/8	-
1	CSD	39-A	152	1	-	1/2/6/8	-
1	CSD	134-A	152	1	-	1/2/6/8	-
1	CSD	115-A	152	1	-	1/2/6/8	-
1	CSD	190-A	152	1	-	1/2/6/8	-
1	CSD	149-A	152	1	-	1/2/6/8	-
1	CSD	142-A	152	1	-	1/2/6/8	-
1	CSD	58-A	152	1	-	1/2/6/8	-
1	CSD	49-A	152	1	-	1/2/6/8	-
1	CSD	103-A	152	1	-	1/2/6/8	-
1	CSD	196-A	152	1	-	1/2/6/8	-
1	CSD	107-A	152	1	-	1/2/6/8	-
1	CSD	238-A	152	1	-	1/2/6/8	-
1	CSD	218-A	152	1	-	1/2/6/8	-
1	CSD	214-A	152	1	-	1/2/6/8	-
1	CSD	6-A	152	1	-	1/2/6/8	-
1	CSD	18-A	152	1	-	1/2/6/8	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	140-A	152	1	-	1/2/6/8	-
1	CSD	67-A	152	1	-	1/2/6/8	-
1	CSD	221-A	152	1	-	1/2/6/8	-
1	CSD	104-A	152	1	-	1/2/6/8	-
1	CSD	109-A	152	1	-	1/2/6/8	-
1	CSD	33-A	152	1	-	1/2/6/8	-
1	CSD	154-A	152	1	-	1/2/6/8	-
1	CSD	62-A	152	1	-	1/2/6/8	-
1	CSD	66-A	152	1	-	1/2/6/8	-
1	CSD	89-A	152	1	-	1/2/6/8	-
1	CSD	151-A	152	1	-	1/2/6/8	-
1	CSD	186-A	152	1	-	1/2/6/8	-
1	CSD	136-A	152	1	-	1/2/6/8	-
1	CSD	93-A	152	1	-	1/2/6/8	-
1	CSD	127-A	152	1	-	1/2/6/8	-
1	CSD	28-A	152	1	-	1/2/6/8	-
1	CSD	158-A	152	1	-	1/2/6/8	-
1	CSD	141-A	152	1	-	1/2/6/8	-
1	CSD	77-A	152	1	-	1/2/6/8	-
1	CSD	139-A	152	1	-	1/2/6/8	-
1	CSD	212-A	152	1	-	1/2/6/8	-
1	CSD	106-A	152	1	-	1/2/6/8	-
1	CSD	159-A	152	1	-	1/2/6/8	-
1	CSD	68-A	152	1	-	1/2/6/8	-
1	CSD	184-A	152	1	-	1/2/6/8	-
1	CSD	172-A	152	1	-	1/2/6/8	-
1	CSD	233-A	152	1	-	1/2/6/8	-
1	CSD	73-A	152	1	-	1/2/6/8	-
1	CSD	76-A	152	1	-	1/2/6/8	-
1	CSD	152-A	152	1	-	1/2/6/8	-
1	CSD	210-A	152	1	-	1/2/6/8	-
1	CSD	20-A	152	1	-	1/2/6/8	-
1	CSD	10-A	152	1	-	1/2/6/8	-
1	CSD	122-A	152	1	-	1/2/6/8	-
1	CSD	156-A	152	1	-	1/2/6/8	-
1	CSD	230-A	152	1	-	1/2/6/8	-
1	CSD	8-A	152	1	-	1/2/6/8	-
1	CSD	229-A	152	1	-	1/2/6/8	-
1	CSD	197-A	152	1	-	1/2/6/8	-
1	CSD	169-A	152	1	-	1/2/6/8	-
1	CSD	13-A	152	1	-	1/2/6/8	-
1	CSD	112-A	152	1	-	1/2/6/8	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	51-A	152	1	-	1/2/6/8	-
1	CSD	60-A	152	1	-	1/2/6/8	-
1	CSD	150-A	152	1	-	1/2/6/8	-
1	CSD	2-A	152	1	-	1/2/6/8	-
1	CSD	209-A	152	1	-	1/2/6/8	-
1	CSD	23-A	152	1	-	1/2/6/8	-
1	CSD	90-A	152	1	-	1/2/6/8	-
1	CSD	239-A	152	1	-	1/2/6/8	-
1	CSD	11-A	152	1	-	1/2/6/8	-
1	CSD	161-A	152	1	-	1/2/6/8	-
1	CSD	105-A	152	1	-	1/2/6/8	-
1	CSD	137-A	152	1	-	1/2/6/8	-
1	CSD	132-A	152	1	-	1/2/6/8	-
1	CSD	193-A	152	1	-	1/2/6/8	-
1	CSD	145-A	152	1	-	1/2/6/8	-
1	CSD	128-A	152	1	-	1/2/6/8	-
1	CSD	138-A	152	1	-	1/2/6/8	-
1	CSD	248-A	152	1	-	1/2/6/8	-
1	CSD	59-A	152	1	-	1/2/6/8	-
1	CSD	162-A	152	1	-	1/2/6/8	-
1	CSD	246-A	152	1	-	1/2/6/8	-
1	CSD	19-A	152	1	-	1/2/6/8	-
1	CSD	213-A	152	1	-	1/2/6/8	-
1	CSD	206-A	152	1	-	1/2/6/8	-
1	CSD	249-A	152	1	-	1/2/6/8	-
1	CSD	87-A	152	1	-	1/2/6/8	-
1	CSD	45-A	152	1	-	1/2/6/8	-
1	CSD	216-A	152	1	-	1/2/6/8	-
1	CSD	143-A	152	1	-	1/2/6/8	-
1	CSD	5-A	152	1	-	1/2/6/8	-
1	CSD	40-A	152	1	-	1/2/6/8	-
1	CSD	38-A	152	1	-	1/2/6/8	-
1	CSD	110-A	152	1	-	1/2/6/8	-
1	CSD	242-A	152	1	-	1/2/6/8	-
1	CSD	17-A	152	1	-	1/2/6/8	-
1	CSD	120-A	152	1	-	1/2/6/8	-
1	CSD	80-A	152	1	-	1/2/6/8	-
1	CSD	92-A	152	1	-	1/2/6/8	-
1	CSD	199-A	152	1	-	1/2/6/8	-
1	CSD	147-A	152	1	-	1/2/6/8	-
1	CSD	83-A	152	1	-	1/2/6/8	-
1	CSD	231-A	152	1	-	1/2/6/8	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	124-A	152	1	-	1/2/6/8	-
1	CSD	121-A	152	1	-	1/2/6/8	-
1	CSD	148-A	152	1	-	1/2/6/8	-
1	CSD	215-A	152	1	-	1/2/6/8	-
1	CSD	82-A	152	1	-	1/2/6/8	-
1	CSD	4-A	152	1	-	1/2/6/8	-
1	CSD	144-A	152	1	-	1/2/6/8	-
1	CSD	200-A	152	1	-	1/2/6/8	-
1	CSD	146-A	152	1	-	1/2/6/8	-
1	CSD	185-A	152	1	-	1/2/6/8	-
1	CSD	50-A	152	1	-	1/2/6/8	-
1	CSD	84-A	152	1	-	1/2/6/8	-
1	CSD	130-A	152	1	-	1/2/6/8	-
1	CSD	108-A	152	1	-	1/2/6/8	-
1	CSD	211-A	152	1	-	1/2/6/8	-
1	CSD	71-A	152	1	-	1/2/6/8	-
1	CSD	207-A	152	1	-	1/2/6/8	-
1	CSD	21-A	152	1	-	1/2/6/8	-
1	CSD	27-A	152	1	-	1/2/6/8	-
1	CSD	72-A	152	1	-	1/2/6/8	-
1	CSD	178-A	152	1	-	1/2/6/8	-
1	CSD	37-A	152	1	-	1/2/6/8	-
1	CSD	48-A	152	1	-	1/2/6/8	-
1	CSD	100-A	152	1	-	1/2/6/8	-
1	CSD	217-A	152	1	-	1/2/6/8	-
1	CSD	227-A	152	1	-	1/2/6/8	-
1	CSD	14-A	152	1	-	1/2/6/8	-
1	CSD	163-A	152	1	-	1/2/6/8	-
1	CSD	111-A	152	1	-	1/2/6/8	-
1	CSD	114-A	152	1	-	1/2/6/8	-
1	CSD	102-A	152	1	-	1/2/6/8	-
1	CSD	54-A	152	1	-	1/2/6/8	-
1	CSD	81-A	152	1	-	1/2/6/8	-
1	CSD	182-A	152	1	-	1/2/6/8	-
1	CSD	43-A	152	1	-	1/2/6/8	-
1	CSD	52-A	152	1	-	1/2/6/8	-
1	CSD	25-A	152	1	-	1/2/6/8	-
1	CSD	79-A	152	1	-	1/2/6/8	-
1	CSD	123-A	152	1	-	1/2/6/8	-
1	CSD	198-A	152	1	-	1/2/6/8	-
1	CSD	131-A	152	1	-	1/2/6/8	-
1	CSD	95-A	152	1	-	1/2/6/8	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	135-A	152	1	-	1/2/6/8	-
1	CSD	183-A	152	1	-	1/2/6/8	-
1	CSD	12-A	152	1	-	1/2/6/8	-
1	CSD	65-A	152	1	-	1/2/6/8	-
1	CSD	26-A	152	1	-	1/2/6/8	-
1	CSD	228-A	152	1	-	1/2/6/8	-
1	CSD	194-A	152	1	-	1/2/6/8	-
1	CSD	189-A	152	1	-	1/2/6/8	-
1	CSD	245-A	152	1	-	1/2/6/8	-
1	CSD	175-A	152	1	-	1/2/6/8	-
1	CSD	219-A	152	1	-	1/2/6/8	-
1	CSD	160-A	152	1	-	1/2/6/8	-
1	CSD	195-A	152	1	-	1/2/6/8	-
1	CSD	166-A	152	1	-	1/2/6/8	-
1	CSD	3-A	152	1	-	1/2/6/8	-
1	CSD	205-A	152	1	-	1/2/6/8	-
1	CSD	176-A	152	1	-	1/2/6/8	-
1	CSD	24-A	152	1	-	1/2/6/8	-
1	CSD	179-A	152	1	-	1/2/6/8	-
1	CSD	57-A	152	1	-	1/2/6/8	-
1	CSD	85-A	152	1	-	1/2/6/8	-
1	CSD	241-A	152	1	-	1/2/6/8	-
1	CSD	244-A	152	1	-	1/2/6/8	-
1	CSD	177-A	152	1	-	1/2/6/8	-
1	CSD	203-A	152	1	-	1/2/6/8	-
1	CSD	96-A	152	1	-	1/2/6/8	-
1	CSD	47-A	152	1	-	1/2/6/8	-
1	CSD	101-A	152	1	-	1/2/6/8	-
1	CSD	36-A	152	1	-	1/2/6/8	-
1	CSD	41-A	152	1	-	1/2/6/8	-
1	CSD	34-A	152	1	-	1/2/6/8	-
1	CSD	86-A	152	1	-	1/2/6/8	-
1	CSD	171-A	152	1	-	1/2/6/8	-
1	CSD	116-A	152	1	-	1/2/6/8	-
1	CSD	204-A	152	1	-	1/2/6/8	-
1	CSD	94-A	152	1	-	1/2/6/8	-
1	CSD	119-A	152	1	-	1/2/6/8	-
1	CSD	126-A	152	1	-	1/2/6/8	-
1	CSD	56-A	152	1	-	1/2/6/8	-
1	CSD	201-A	152	1	-	1/2/6/8	-
1	CSD	220-A	152	1	-	1/2/6/8	-
1	CSD	53-A	152	1	-	1/2/6/8	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	167-A	152	1	-	1/2/6/8	-
1	CSD	9-A	152	1	-	1/2/6/8	-
1	CSD	125-A	152	1	-	1/2/6/8	-
1	CSD	97-A	152	1	-	1/2/6/8	-
1	CSD	208-A	152	1	-	1/2/6/8	-
1	CSD	22-A	152	1	-	1/2/6/8	-
1	CSD	133-A	152	1	-	1/2/6/8	-
1	CSD	225-A	152	1	-	1/2/6/8	-
1	CSD	237-A	152	1	-	1/2/6/8	-
1	CSD	226-A	152	1	-	1/2/6/8	-
1	CSD	129-A	152	1	-	1/2/6/8	-
1	CSD	181-A	152	1	-	1/2/6/8	-
1	CSD	44-A	152	1	-	1/2/6/8	-
1	CSD	78-A	152	1	-	1/2/6/8	-
1	CSD	64-A	152	1	-	1/2/6/8	-
1	CSD	61-A	152	1	-	1/2/6/8	-
1	CSD	91-A	152	1	-	1/2/6/8	-
1	CSD	153-A	152	1	-	1/2/6/8	-
1	CSD	191-A	152	1	-	1/2/6/8	-
1	CSD	32-A	152	1	-	1/2/6/8	-
1	CSD	174-A	152	1	-	1/2/6/8	-
1	CSD	1-A	152	1	-	1/2/6/8	-
1	CSD	29-A	152	1	-	1/2/6/8	-
1	CSD	222-A	152	1	-	1/2/6/8	-
1	CSD	15-A	152	1	-	1/2/6/8	-
1	CSD	74-A	152	1	-	1/2/6/8	-
1	CSD	55-A	152	1	-	1/2/6/8	-
1	CSD	88-A	152	1	-	1/2/6/8	-
1	CSD	165-A	152	1	-	1/2/6/8	-
1	CSD	113-A	152	1	-	1/2/6/8	-
1	CSD	247-A	152	1	-	1/2/6/8	-
1	CSD	70-A	152	1	-	1/2/6/8	-
1	CSD	42-A	152	1	-	1/2/6/8	-
1	CSD	164-A	152	1	-	1/2/6/8	-
1	CSD	99-A	152	1	-	1/2/6/8	-
1	CSD	236-A	152	1	-	1/2/6/8	-
1	CSD	192-A	152	1	-	1/2/6/8	-
1	CSD	155-A	152	1	-	1/2/6/8	-
1	CSD	202-A	152	1	-	1/2/6/8	-
1	CSD	250-A	152	1	-	1/2/6/8	-
1	CSD	180-A	152	1	-	1/2/6/8	-
1	CSD	16-A	152	1	-	1/2/6/8	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	235-A	152	1	-	1/2/6/8	-
1	CSD	7-A	152	1	-	1/2/6/8	-
1	CSD	118-A	152	1	-	1/2/6/8	-
1	CSD	31-A	152	1	-	1/2/6/8	-
1	CSD	170-A	152	1	-	1/2/6/8	-
1	CSD	168-A	152	1	-	1/2/6/8	-
1	CSD	98-A	152	1	-	1/2/6/8	-
1	CSD	234-A	152	1	-	1/2/6/8	-
1	CSD	187-A	152	1	-	1/2/6/8	-
1	CSD	117-A	152	1	-	1/2/6/8	-
1	CSD	157-A	152	1	-	1/2/6/8	-
1	CSD	224-A	152	1	-	1/2/6/8	-
1	CSD	223-A	152	1	-	1/2/6/8	-
1	CSD	188-A	152	1	-	1/2/6/8	-
1	CSD	232-A	152	1	-	1/2/6/8	-
1	CSD	63-A	152	1	-	1/2/6/8	-
1	CSD	46-A	152	1	-	1/2/6/8	-
1	CSD	75-A	152	1	-	1/2/6/8	-
1	CSD	173-A	152	1	-	1/2/6/8	-
1	CSD	243-A	152	1	-	1/2/6/8	-
1	CSD	30-A	152	1	-	1/2/6/8	-
1	CSD	69-A	152	1	-	1/2/6/8	-

There are no bond length outliers.

The worst 5 of 250 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	35-A	152	CSD	OD1-SG-CB	5.48	115.96	105.54
1	240-A	152	CSD	OD1-SG-CB	5.48	115.96	105.54
1	39-A	152	CSD	OD1-SG-CB	5.48	115.96	105.54
1	134-A	152	CSD	OD1-SG-CB	5.48	115.96	105.54
1	115-A	152	CSD	OD1-SG-CB	5.48	115.96	105.54

There are no chirality outliers.

5 of 250 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	35-A	152	CSD	CA-CB-SG-OD1
1	240-A	152	CSD	CA-CB-SG-OD1
1	39-A	152	CSD	CA-CB-SG-OD1
1	134-A	152	CSD	CA-CB-SG-OD1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	115-A	152	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1000 ligands modelled in this entry, 500 are monoatomic - leaving 500 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
2	FOL	141-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	240-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	174-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	110-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	185-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	165-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	230-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	129-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	10-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	12-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	114-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	195-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	85-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	1-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	89-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	30-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	66-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	113-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	2-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	240-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	193-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	69-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	118-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	7-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	162-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	39-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	101-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	9-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	95-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	108-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	41-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	116-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	37-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	64-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	46-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	64-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	191-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	1-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	63-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	209-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	230-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	113-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	20-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	171-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	92-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	42-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	43-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	210-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	179-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	197-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	49-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	25-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	76-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	79-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	106-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	108-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	192-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	71-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	191-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	25-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	152-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	40-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	148-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	86-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	165-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	94-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	146-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	161-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	28-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	145-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	158-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	190-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	93-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	148-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	135-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	48-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	232-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	245-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	99-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	72-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	33-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	35-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	95-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	30-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	23-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	97-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	158-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	13-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	220-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	45-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	229-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	221-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	50-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	43-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	20-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	91-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	146-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	38-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	149-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	26-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	205-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	53-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	119-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	11-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	150-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	47-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	203-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	96-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	169-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	176-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	247-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	181-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	56-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	231-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	104-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	37-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	189-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	167-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	150-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	80-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	159-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	139-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	206-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	83-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	51-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	54-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	153-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	29-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	243-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	111-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	128-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	194-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	186-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	228-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	179-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	93-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	197-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	123-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	32-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	185-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	203-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	56-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	59-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	216-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	124-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	154-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	177-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	187-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	194-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	7-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	175-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	38-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	223-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	247-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	126-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	145-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	237-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	183-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	136-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	215-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	198-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	107-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	61-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	31-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	102-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	67-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	170-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	67-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	117-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	117-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	152-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	211-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	66-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	159-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	118-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	228-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	105-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	155-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	130-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	104-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	18-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	36-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	71-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	85-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	226-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	222-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	222-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	210-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	212-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	16-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	164-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	151-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	182-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	237-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	187-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	121-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	127-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	186-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	239-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	157-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	78-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	235-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	3-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	172-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	140-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	168-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	198-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	221-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	242-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	96-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	123-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	14-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	17-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	102-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	80-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	21-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	125-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	97-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	81-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	214-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	60-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	188-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	227-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	173-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	248-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	201-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	188-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	134-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	26-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	174-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	76-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	147-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	242-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	149-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	58-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	136-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	18-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	220-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	19-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	53-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	218-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	83-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	244-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	44-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	127-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	199-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	12-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	206-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	122-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	196-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	243-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	115-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	90-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	231-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	47-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	81-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	17-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	98-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	116-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	35-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	153-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	27-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	131-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	52-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	225-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	110-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	6-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	144-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	120-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	73-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	105-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	143-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	23-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	180-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	87-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	34-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	98-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	68-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	70-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	48-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	250-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	218-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	160-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	219-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	202-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	172-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	9-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	169-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	133-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	207-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	170-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	128-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	16-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	248-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	143-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	178-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	70-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	14-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	167-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	168-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	125-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	234-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	106-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	3-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	241-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	49-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	234-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	190-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	61-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	74-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	236-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	200-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	59-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	250-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	72-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	115-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	119-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	90-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	161-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	94-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	238-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	227-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	171-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	166-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	173-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	11-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	217-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	215-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	68-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	160-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	207-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	27-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	4-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	114-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	139-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	134-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	8-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	122-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	166-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	60-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	137-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	65-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	164-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	154-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	107-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	41-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	155-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	137-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	208-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	42-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	182-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	130-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	200-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	21-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	86-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	22-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	34-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	246-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	120-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	50-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	163-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	82-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	196-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	181-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	180-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	52-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	205-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	73-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	192-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	82-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	78-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	92-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	22-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	132-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	109-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	44-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	141-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	24-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	15-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	55-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	63-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	79-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	238-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	233-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	6-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	213-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	226-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	57-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	4-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	62-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	183-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	156-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	84-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	101-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	29-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	77-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	36-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	204-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	176-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	51-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	217-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	178-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	58-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	236-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	32-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	214-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	133-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	140-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	229-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	103-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	103-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	157-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	199-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	232-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	138-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	244-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	100-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	88-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	88-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	100-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	74-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	65-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	54-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	224-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	99-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	245-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	10-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	55-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	249-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	235-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	87-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	189-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	39-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	184-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	195-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	249-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	8-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	147-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	175-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	19-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	138-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	111-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	239-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	129-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	201-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	45-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	91-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	112-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	233-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	31-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	225-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	211-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	131-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	62-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	46-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	28-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	213-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	241-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	15-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	177-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	202-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	223-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	216-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	121-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	209-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	163-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	212-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	40-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	208-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	75-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	33-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	162-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	126-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	132-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	89-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	2-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	84-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	5-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	142-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	57-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	156-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	5-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	109-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	144-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	77-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	204-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	135-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	124-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	69-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	151-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	184-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	142-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	219-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	13-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	224-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
2	FOL	246-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
2	FOL	112-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.57	18 (50%)
3	NAP	193-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	75-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)
3	NAP	24-A	202	-	45,52,52	2.54	8 (17%)	56,80,80	1.22	7 (12%)

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
2	FOL	141-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	240-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	174-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	110-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	185-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	165-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	230-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	129-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	10-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	12-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	114-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	195-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	85-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	1-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	89-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	30-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	66-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	113-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	2-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	240-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	193-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	69-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	118-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	7-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	162-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	39-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	101-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	9-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	95-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	108-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	41-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	116-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	37-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	64-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	46-A	201	-	-	2/16/22/22	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	64-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	191-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	1-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	63-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	209-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	230-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	113-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	20-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	171-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	92-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	42-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	43-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	210-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	179-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	197-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	49-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	25-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	76-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	79-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	106-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	108-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	192-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	71-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	191-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	25-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	152-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	40-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	148-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	86-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	165-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	94-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	146-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	161-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	28-A	202	-	-	4/31/67/67	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	145-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	158-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	190-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	93-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	148-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	135-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	48-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	232-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	245-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	99-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	72-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	33-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	35-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	95-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	30-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	23-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	97-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	158-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	13-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	220-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	45-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	229-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	221-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	50-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	43-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	20-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	91-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	146-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	38-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	149-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	26-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	205-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	53-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	119-A	202	-	-	4/31/67/67	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	11-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	150-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	47-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	203-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	96-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	169-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	176-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	247-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	181-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	56-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	231-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	104-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	37-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	189-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	167-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	150-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	80-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	159-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	139-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	206-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	83-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	51-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	54-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	153-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	29-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	243-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	111-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	128-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	194-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	186-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	228-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	179-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	93-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	197-A	201	-	-	2/16/22/22	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	123-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	32-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	185-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	203-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	56-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	59-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	216-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	124-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	154-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	177-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	187-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	194-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	7-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	175-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	38-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	223-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	247-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	126-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	145-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	237-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	183-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	136-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	215-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	198-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	107-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	61-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	31-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	102-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	67-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	170-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	67-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	117-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	117-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	152-A	201	-	-	2/16/22/22	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	211-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	66-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	159-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	118-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	228-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	105-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	155-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	130-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	104-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	18-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	36-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	71-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	85-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	226-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	222-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	222-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	210-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	212-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	16-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	164-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	151-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	182-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	237-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	187-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	121-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	127-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	186-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	239-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	157-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	78-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	235-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	3-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	172-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	140-A	201	-	-	2/16/22/22	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	168-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	198-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	221-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	242-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	96-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	123-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	14-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	17-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	102-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	80-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	21-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	125-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	97-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	81-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	214-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	60-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	188-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	227-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	173-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	248-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	201-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	188-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	134-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	26-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	174-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	76-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	147-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	242-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	149-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	58-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	136-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	18-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	220-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	19-A	201	-	-	2/16/22/22	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	53-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	218-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	83-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	244-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	44-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	127-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	199-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	12-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	206-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	122-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	196-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	243-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	115-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	90-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	231-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	47-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	81-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	17-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	98-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	116-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	35-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	153-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	27-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	131-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	52-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	225-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	110-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	6-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	144-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	120-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	73-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	105-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	143-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	23-A	202	-	-	4/31/67/67	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	180-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	87-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	34-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	98-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	68-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	70-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	48-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	250-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	218-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	160-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	219-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	202-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	172-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	9-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	169-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	133-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	207-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	170-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	128-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	16-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	248-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	143-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	178-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	70-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	14-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	167-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	168-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	125-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	234-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	106-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	3-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	241-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	49-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	234-A	201	-	-	2/16/22/22	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	190-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	61-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	74-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	236-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	200-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	59-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	250-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	72-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	115-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	119-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	90-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	161-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	94-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	238-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	227-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	171-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	166-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	173-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	11-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	217-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	215-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	68-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	160-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	207-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	27-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	4-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	114-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	139-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	134-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	8-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	122-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	166-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	60-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	137-A	202	-	-	4/31/67/67	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	65-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	164-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	154-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	107-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	41-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	155-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	137-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	208-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	42-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	182-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	130-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	200-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	21-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	86-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	22-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	34-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	246-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	120-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	50-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	163-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	82-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	196-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	181-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	180-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	52-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	205-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	73-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	192-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	82-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	78-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	92-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	22-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	132-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	109-A	201	-	-	2/16/22/22	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	44-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	141-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	24-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	15-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	55-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	63-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	79-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	238-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	233-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	6-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	213-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	226-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	57-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	4-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	62-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	183-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	156-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	84-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	101-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	29-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	77-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	36-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	204-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	176-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	51-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	217-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	178-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	58-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	236-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	32-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	214-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	133-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	140-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	229-A	201	-	-	2/16/22/22	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	103-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	103-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	157-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	199-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	232-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	138-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	244-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	100-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	88-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	88-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	100-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	74-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	65-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	54-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	224-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	99-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	245-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	10-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	55-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	249-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	235-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	87-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	189-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	39-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	184-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	195-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	249-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	8-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	147-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	175-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	19-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	138-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	111-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	239-A	202	-	-	4/31/67/67	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	129-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	201-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	45-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	91-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	112-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	233-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	31-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	225-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	211-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	131-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	62-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	46-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	28-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	213-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	241-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	15-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	177-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	202-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	223-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	216-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	121-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	209-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	163-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	212-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	40-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	208-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	75-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	33-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	162-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	126-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	132-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	89-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	2-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	84-A	202	-	-	4/31/67/67	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	5-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	142-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	57-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	156-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	5-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	109-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	144-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	77-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	204-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	135-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	124-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	69-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	151-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	184-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	142-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	219-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	13-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	224-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	246-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	112-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	193-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	75-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	24-A	202	-	-	4/31/67/67	0/5/5/5

The worst 5 of 3250 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	110-A	202	NAP	C2D-C1D	-9.27	1.39	1.53
3	165-A	202	NAP	C2D-C1D	-9.27	1.39	1.53
3	10-A	202	NAP	C2D-C1D	-9.27	1.39	1.53
3	195-A	202	NAP	C2D-C1D	-9.27	1.39	1.53
3	66-A	202	NAP	C2D-C1D	-9.27	1.39	1.53

The worst 5 of 6250 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	141-A	201	FOL	C4-C4A-C8A	-4.96	116.67	119.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	240-A	201	FOL	C4-C4A-C8A	-4.96	116.67	119.95
2	174-A	201	FOL	C4-C4A-C8A	-4.96	116.67	119.95
2	185-A	201	FOL	C4-C4A-C8A	-4.96	116.67	119.95
2	230-A	201	FOL	C4-C4A-C8A	-4.96	116.67	119.95

There are no chirality outliers.

5 of 1500 torsion outliers are listed below:

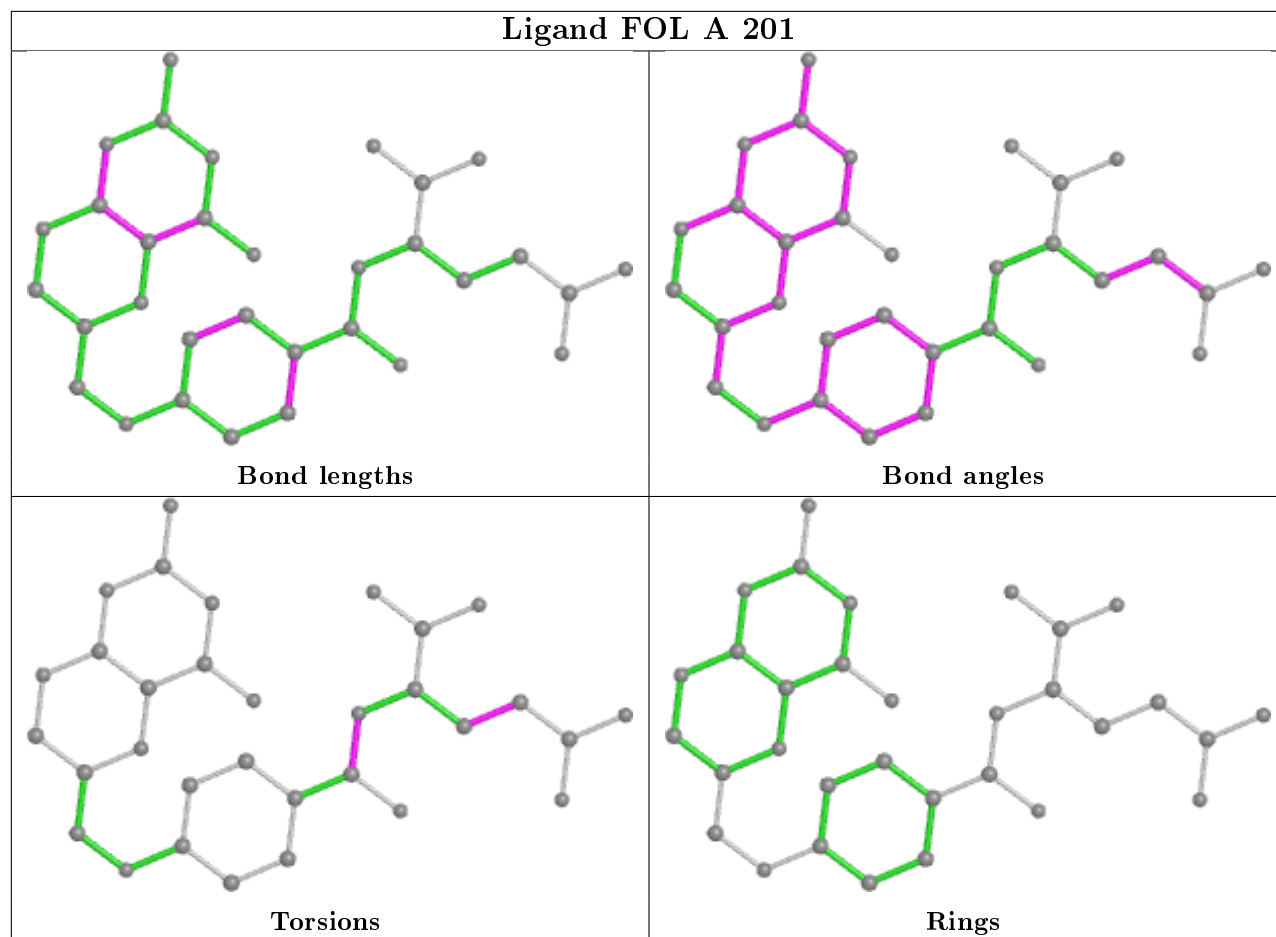
Mol	Chain	Res	Type	Atoms
3	110-A	202	NAP	C2B-O2B-P2B-O3X
3	110-A	202	NAP	O4D-C1D-N1N-C6N
3	165-A	202	NAP	C2B-O2B-P2B-O3X
3	165-A	202	NAP	O4D-C1D-N1N-C6N
3	10-A	202	NAP	C2B-O2B-P2B-O3X

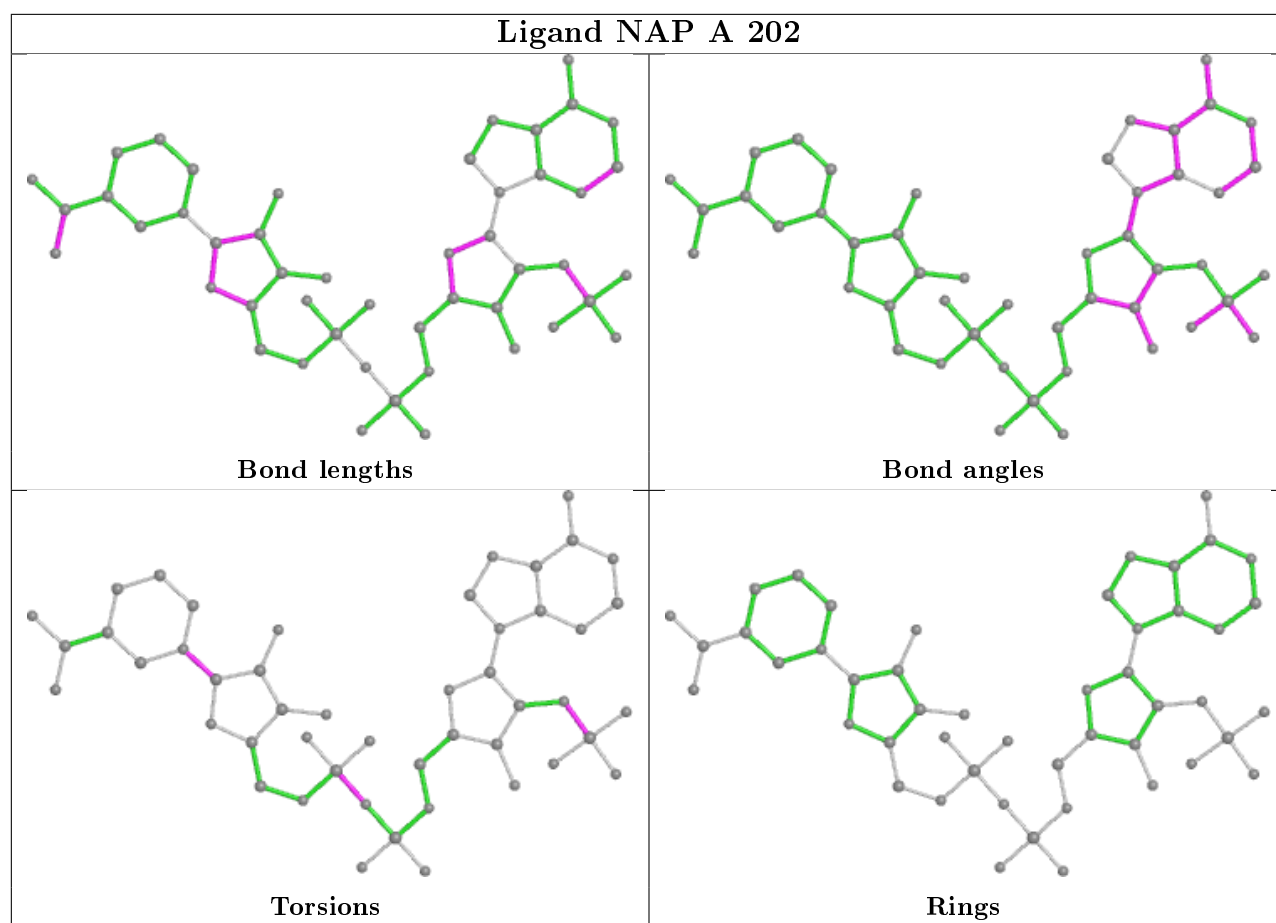
There are no ring outliers.

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.

Ligand FOL A 201





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

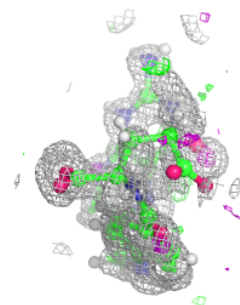
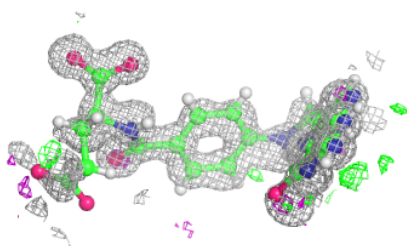
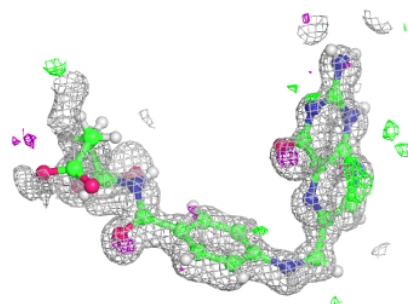
6.4 Ligands ⓘ

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

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.

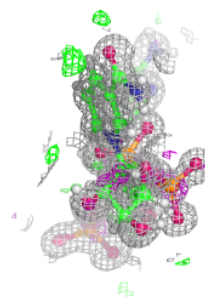
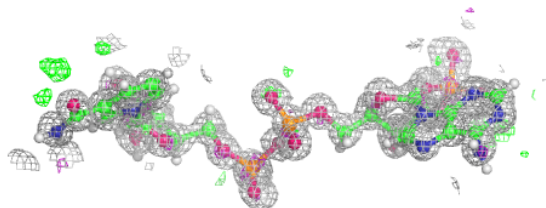
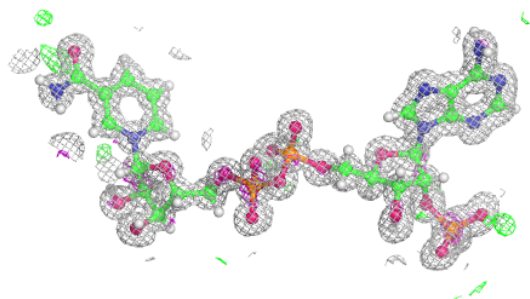
Electron density around FOL A 201:

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



Electron density around NAP A 202:

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



6.5 Other polymers ⓘ

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