



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:15 AM UTC

PDB ID : 9RP2 / pdb_00009rp2
Title : Ensemble refined structure of CotB2 F107A in complex with alendronate
Authors : Helmer, C.P.O.; Loll, B.
Deposited on : 2025-06-23
Resolution : 1.93 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

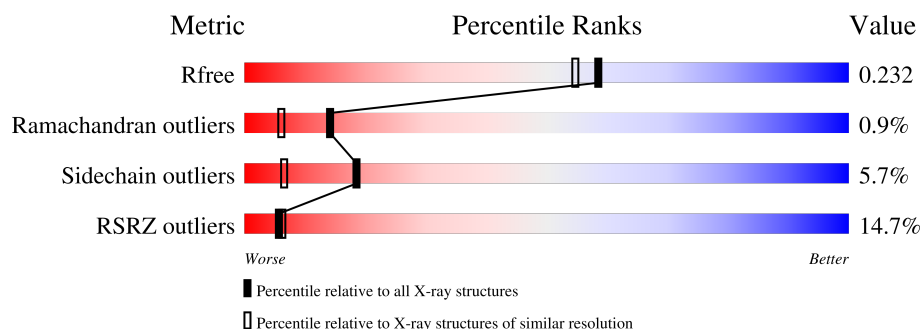
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1452 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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 of 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	318	14% 87% 6% 7%
1	1-B	318	14% 88% 5% 7%
1	10-A	318	87% • • 7%
1	10-B	318	87% 6% 7%
1	11-A	318	86% 6% 7%
1	11-B	318	88% 5% 7%
1	12-A	318	87% 5% 7%

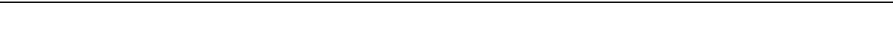
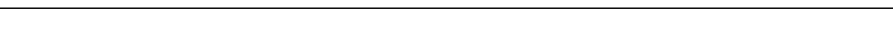
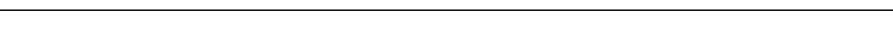
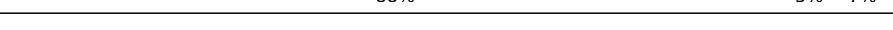
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	12-B	318	 88% 5% 7%
1	13-A	318	 88% 5% 7%
1	13-B	318	 88% 5% 7%
1	14-A	318	 87% 5% 7%
1	14-B	318	 88% 5% 7%
1	15-A	318	 86% 6% 7%
1	15-B	318	 88% 5% 7%
1	16-A	318	 87% 5% 7%
1	16-B	318	 87% 5% 7%
1	17-A	318	 87% 5% 7%
1	17-B	318	 88% 5% 7%
1	18-A	318	 87% 6% 7%
1	18-B	318	 88% 5% 7%
1	19-A	318	 88% 5% 7%
1	19-B	318	 88% 5% 7%
1	2-A	318	 87% 5% 7%
1	2-B	318	 88% 5% 7%
1	20-A	318	 88% 5% 7%
1	20-B	318	 87% 5% 7%
1	21-A	318	 88% 5% 7%
1	21-B	318	 87% 5% 7%
1	22-A	318	 87% 6% 7%
1	22-B	318	 88% 5% 7%
1	23-A	318	 88% 5% 7%
1	23-B	318	 87% 6% 7%

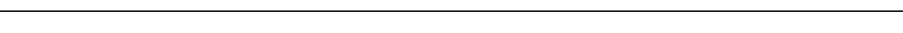
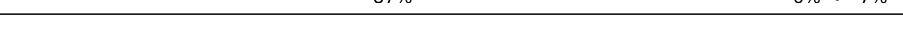
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	24-A	318	 88% 5% 7%
1	24-B	318	 88% 5% 7%
1	25-A	318	 88% 5% 7%
1	25-B	318	 88% 5% 7%
1	26-A	318	 87% 5% 7%
1	26-B	318	 87% 5% 7%
1	27-A	318	 87% 5% 7%
1	27-B	318	 88% 5% 7%
1	28-A	318	 87% 5% 7%
1	28-B	318	 87% 6% 7%
1	29-A	318	 87% 6% 7%
1	29-B	318	 88% 5% 7%
1	3-A	318	 88% 5% 7%
1	3-B	318	 88% 5% 7%
1	30-A	318	 88% 5% 7%
1	30-B	318	 88% 5% 7%
1	31-A	318	 88% 5% 7%
1	31-B	318	 88% 5% 7%
1	32-A	318	 88% 5% 7%
1	32-B	318	 88% 5% 7%
1	33-A	318	 88% 5% 7%
1	33-B	318	 88% 5% 7%
1	34-A	318	 87% 5% 7%
1	34-B	318	 88% 5% 7%
1	35-A	318	 88% 5% 7%

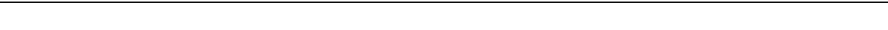
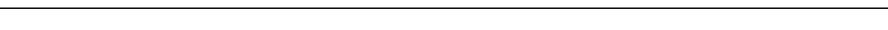
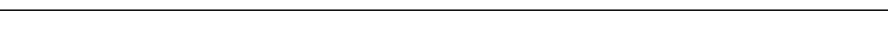
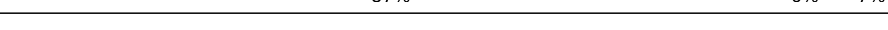
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	35-B	318	 87% 6% • 7%
1	36-A	318	 87% 6% 7%
1	36-B	318	 87% 5% 7%
1	37-A	318	 87% 5% 7%
1	37-B	318	 87% 5% 7%
1	38-A	318	 87% 6% 7%
1	38-B	318	 88% 5% 7%
1	39-A	318	 87% 6% 7%
1	39-B	318	 88% 5% • 7%
1	4-A	318	 88% 5% 7%
1	4-B	318	 87% 6% 7%
1	40-A	318	 87% 5% • 7%
1	40-B	318	 87% 6% • 7%
1	41-A	318	 87% 5% • 7%
1	41-B	318	 87% 6% • 7%
1	42-A	318	 87% 5% 7%
1	42-B	318	 87% 6% 7%
1	43-A	318	 87% 6% 7%
1	43-B	318	 88% • • 7%
1	44-A	318	 87% 6% 7%
1	44-B	318	 87% 5% • 7%
1	45-A	318	 87% 5% 7%
1	45-B	318	 87% 6% 7%
1	46-A	318	 88% • • 7%
1	46-B	318	 88% 5% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	47-A	318	 87% 5% 7%
1	47-B	318	 87% 5% 7%
1	48-A	318	 88% 5% 7%
1	48-B	318	 87% 6% 7%
1	49-A	318	 87% 5% 7%
1	49-B	318	 88% 5% 7%
1	5-A	318	 88% 5% 7%
1	5-B	318	 88% 5% 7%
1	50-A	318	 87% 6% 7%
1	50-B	318	 87% 5% 7%
1	6-A	318	 87% 5% 7%
1	6-B	318	 87% 5% 7%
1	7-A	318	 88% 5% 7%
1	7-B	318	 87% 6% 7%
1	8-A	318	 88% 5% 7%
1	8-B	318	 87% 6% 7%
1	9-A	318	 87% 5% 7%
1	9-B	318	 88% 5% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 261865 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cyclooctat-9-en-7-ol synthase.

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

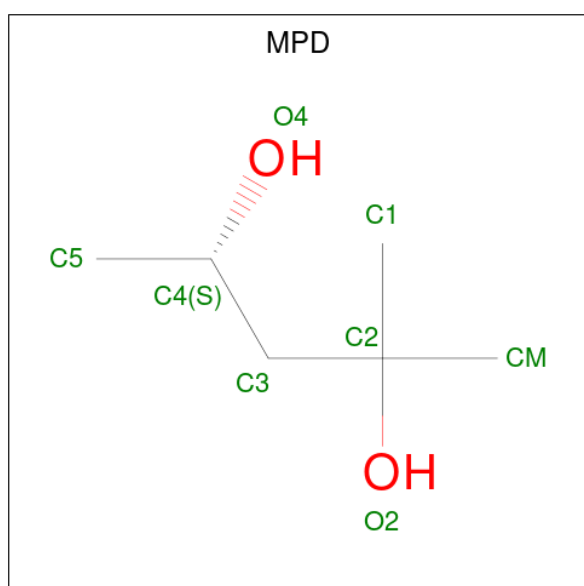
Continued from previous page...

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

There are 24 discrepancies between the modelled and reference sequences:

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

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



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

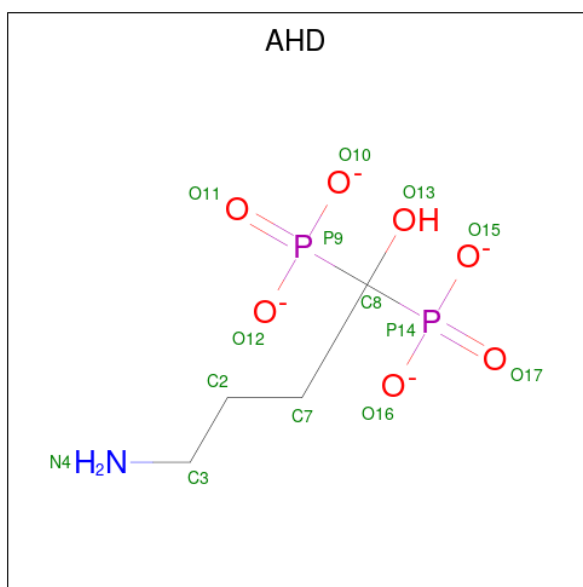
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	20-B	1	Total	C	O	0	0
			8	6	2		
2	21-B	1	Total	C	O	0	0
			8	6	2		
2	22-B	1	Total	C	O	0	0
			8	6	2		
2	23-B	1	Total	C	O	0	0
			8	6	2		
2	24-B	1	Total	C	O	0	0
			8	6	2		
2	25-B	1	Total	C	O	0	0
			8	6	2		
2	26-B	1	Total	C	O	0	0
			8	6	2		
2	27-B	1	Total	C	O	0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

Continued on next page...

Continued from previous page...

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

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



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

- Molecule 6 is water.

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

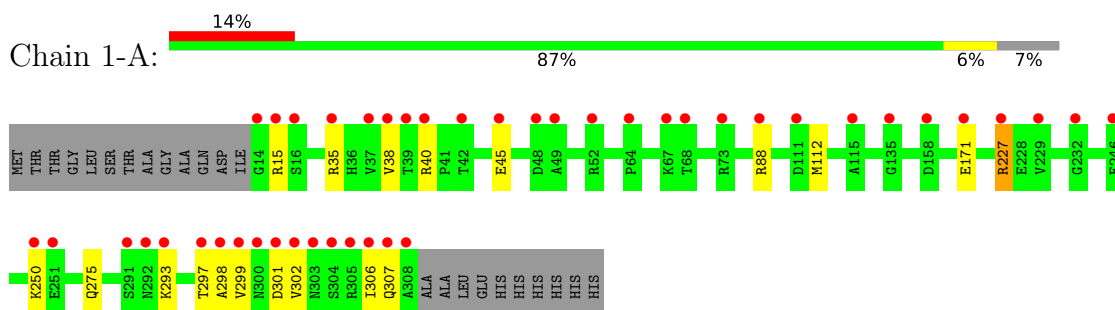
Continued from previous page...

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

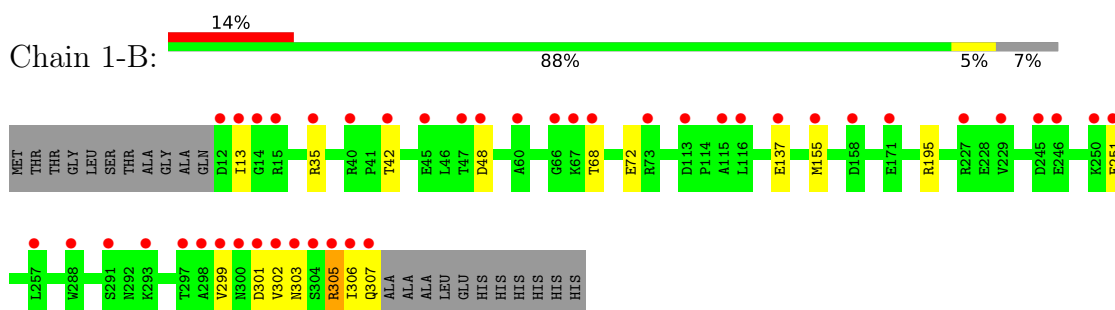
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

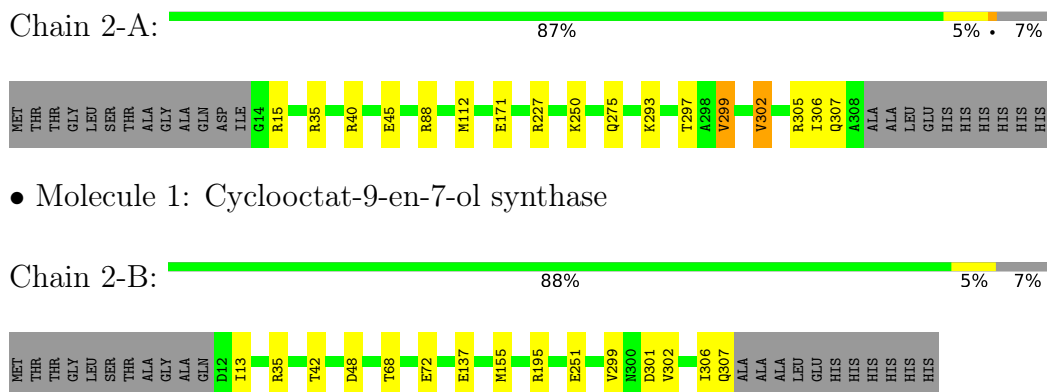
- Molecule 1: Cyclooctat-9-en-7-ol synthase



- Molecule 1: Cyclooctat-9-en-7-ol synthase



- Molecule 1: Cyclooctat-9-en-7-ol synthase



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 3-A:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 3-B:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 4-A:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 4-B:  87% 6% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 5-A:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 5-B:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 6-A:  87% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 6-B:  87% 5% • 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 7-A:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 7-B:  87% 6% • 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 8-A:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 8-B:  87% 6% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 9-A:  87% 5% • 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 9-B:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 10-A:  87% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 10-B:  87% 6% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 11-A:  86% 6% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 11-B:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 12-A:  87% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 12-B:  88% 7% 5%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 13-A:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 13-B:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 14-A:  87% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 14-B:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 15-A:  86% 6% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 15-B:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 16-A:  87% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 16-B:  87% 5% 7%



● Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 17-A:  87% 5% 7%

● Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 17-B:  88% 5% 7%

● Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 18-A:  87% 6% 7%

● Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 18-B:  88% 5% 7%

● Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 19-A:  88% 5% 7%

● Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 19-B:  88% 5% 7%

● Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 20-A:  88% 5% 7%

● Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 20-B:  87% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 21-A:  88% 0% 7%



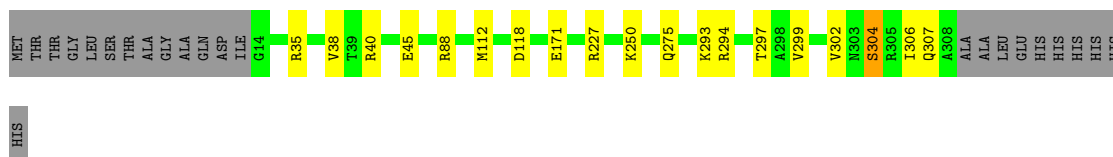
- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 21-B:  87% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 22-A:  87% 6% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 22-B:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 23-A:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 23-B:  87% 6% 7%



• Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 24-A:  88% 5% 7%

• Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 24-B:  88% 5% 7%

• Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 25-A:  88% 5% 7%

• Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 25-B:  88% 5% 7%

• Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 26-A:  87% 5% 7%

• Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 26-B:  87% 5% 7%

• Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 27-A:  87% 5% 7%

• Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 27-B:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 28-A:  87% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 28-B:  87% 6% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 29-A:  87% 6% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 29-B:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 30-A:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 30-B:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

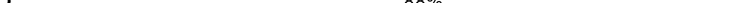
Met	THR	THR	GLY	LEU	SER	THR	ALA	ALA	GLY	GLN	ASP	ILE	GLI4	R35	R40	E45	R88	M112	E171	R227	K250	Q276	K293	T297	A398	V399	V302	I306	Q307	A308	ALA	ALA	LEU	GLI	HIS	HIS	HIS	HIS	HIS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain 31-B: 88% . 7%

[illegible]

- Chain 32-A: 88% 5% 7%

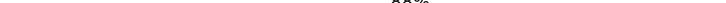
[illegible]

- Chain 32-B:  88% . . 7%

[illegible]

- Chain 33-A:

MET	THR	THR	GLY	LEU	SER	THR	THR	GLY	ALA	ALA	ALA	ALA	GLN	ASP	ILE	GLI4	R35	R40	E45	R88	M112	E171	R227	K250	Q276	K293	T297	Z298	A308	V302	I306	Q307	ALA	ALA	ALA	LEU	GLU	HIS	HIS	HIS	HIS	HIS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain 33-B:  88% 5% 7%

[illegible]

- Chain 34-A: 87% 5% 7%

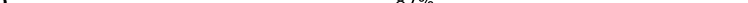
[illegible]

- Molecule 1: Cyclooctat-9-en-7-ol synthase

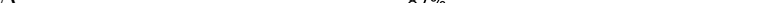
[illegible]

- Chain 35-A: 88% 5% 7%

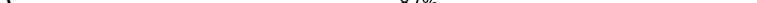
MET	THR	THR	GLY	GLY	SER	THR	THR	ALA	GLY	ALA	ALA	GLN	ASP	ILE	GLI4	R35	R40	E45	R88	M112	E171	R227	K260	Q275	K293	T297	A298	V299	K302	K303	S304	K305	T306	Q307	A308	ALA	ALA	ALA	LEU	LEU	GLU	HTS	HTS	HTS	HTS	HTS	HTS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain 35-B:  87% 6% • 7%

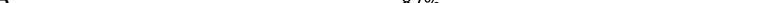
[illegible]

- Chain 36-A:  87% 6% 7%

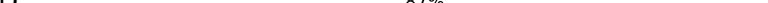
HIS	MET
HIS	THR
	GLY
	LEU
	SER
	THR
	ALA
	GLY
	ALA
	GLN
	ASP
	ILE
	G14
	R35
	V38
	T39
	R40
	E45
	R88
	M112
	P136
	D158
	E171
	R227
	K250
	Q275
	K293
	T297
	A298
	V299
	V302
	N303
	S304
	R305
	I306
	Q307
	A308
	ALA
	ALA
	LEU
	GLU
	HIS
	HIS
	HIS
	HIS

- Chain 36-B:  87% 5% 7%

[illegible]

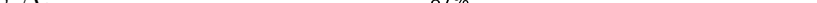
- Chain 37-A:  87% 5% 7%

MET	THR	THR	GLY	LEU	SER	THR	ALA	GLY	ALA	GLN	ASP	ILE	G14	R35	V38	T39	R40	E45	R88	M112	E171	R227	K250	Q276	K293	T297	A298	V299	V302	R306	I306	Q307	A308	A308	LEU	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain 37-B:  87% 5% 7%

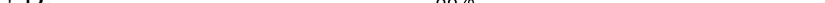
MET	THR	THR	GLY	LEU	SER	THR	ALA	ALA	GLY	ALA	GLN	D12 I13	R35	T42	D48	T68	E72	R88	E137	M155	R195	E251	A298	V299	Z300	D301	V302	R305	I306	Q307	ALA	ALA	ALA	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------------	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 38-A:  87% 6% 7%

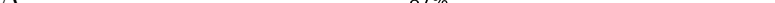


- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 38-B:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 39-A:  87% 6% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 39-B: 88% 5% • 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 40-A: 87% 5% • 7%

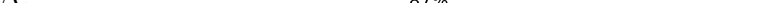


- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 40-B: 87% 6% • 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 41-A:  87% 5% • 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 41-B:  87% 6% • 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 42-A:  87% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 42-B:  87% 6% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 43-A:  87% 6% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 43-B:  88% • • 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 44-A:  87% 6% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 44-B:  87% 5% • 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 45-A:  87% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 45-B:  87% 6% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 46-A:  88% • • 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 46-B:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 47-A:  87% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 47-B:  87% 5% • 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 48-A:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 48-B:  87% 6% 7%



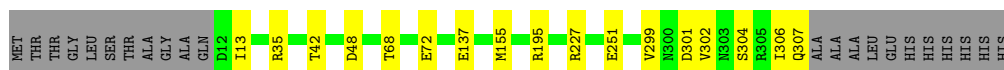
- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 49-A:  87% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 49-B:  88% 5% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 50-A:  87% 6% 7%



- Molecule 1: Cyclooctat-9-en-7-ol synthase

Chain 50-B:  87% 5% 7%



4 Data and refinement statistics

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

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

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: CL, MPD, MG, AHD

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	0.12	0/2460	0.21	0/3336
1	1-B	0.11	0/2471	0.22	0/3351
1	2-A	0.12	0/2460	0.21	0/3336
1	2-B	0.11	0/2471	0.22	0/3351
1	3-A	0.12	0/2460	0.21	0/3336
1	3-B	0.11	0/2471	0.22	0/3351
1	4-A	0.12	0/2460	0.21	0/3336
1	4-B	0.11	0/2471	0.22	0/3351
1	5-A	0.12	0/2460	0.21	0/3336
1	5-B	0.11	0/2471	0.22	0/3351
1	6-A	0.12	0/2460	0.21	0/3336
1	6-B	0.11	0/2471	0.22	0/3351
1	7-A	0.12	0/2460	0.21	0/3336
1	7-B	0.11	0/2471	0.22	0/3351
1	8-A	0.12	0/2460	0.21	0/3336
1	8-B	0.11	0/2471	0.22	0/3351
1	9-A	0.12	0/2460	0.21	0/3336
1	9-B	0.11	0/2471	0.22	0/3351
1	10-A	0.12	0/2460	0.21	0/3336
1	10-B	0.11	0/2471	0.22	0/3351
1	11-A	0.12	0/2460	0.21	0/3336
1	11-B	0.11	0/2471	0.22	0/3351
1	12-A	0.12	0/2460	0.21	0/3336
1	12-B	0.11	0/2471	0.22	0/3351
1	13-A	0.12	0/2460	0.21	0/3336
1	13-B	0.11	0/2471	0.22	0/3351
1	14-A	0.12	0/2460	0.21	0/3336
1	14-B	0.11	0/2471	0.22	0/3351
1	15-A	0.12	0/2460	0.21	0/3336
1	15-B	0.11	0/2471	0.22	0/3351
1	16-A	0.12	0/2460	0.21	0/3336
1	16-B	0.11	0/2471	0.22	0/3351

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	17-A	0.12	0/2460	0.21	0/3336
1	17-B	0.11	0/2471	0.22	0/3351
1	18-A	0.12	0/2460	0.21	0/3336
1	18-B	0.11	0/2471	0.22	0/3351
1	19-A	0.12	0/2460	0.21	0/3336
1	19-B	0.11	0/2471	0.22	0/3351
1	20-A	0.12	0/2460	0.21	0/3336
1	20-B	0.11	0/2471	0.22	0/3351
1	21-A	0.12	0/2460	0.21	0/3336
1	21-B	0.11	0/2471	0.22	0/3351
1	22-A	0.12	0/2460	0.21	0/3336
1	22-B	0.11	0/2471	0.22	0/3351
1	23-A	0.12	0/2460	0.21	0/3336
1	23-B	0.11	0/2471	0.22	0/3351
1	24-A	0.12	0/2460	0.21	0/3336
1	24-B	0.11	0/2471	0.22	0/3351
1	25-A	0.12	0/2460	0.21	0/3336
1	25-B	0.11	0/2471	0.22	0/3351
1	26-A	0.12	0/2460	0.21	0/3336
1	26-B	0.11	0/2471	0.22	0/3351
1	27-A	0.12	0/2460	0.21	0/3336
1	27-B	0.11	0/2471	0.22	0/3351
1	28-A	0.12	0/2460	0.21	0/3336
1	28-B	0.11	0/2471	0.22	0/3351
1	29-A	0.12	0/2460	0.21	0/3336
1	29-B	0.11	0/2471	0.22	0/3351
1	30-A	0.12	0/2460	0.21	0/3336
1	30-B	0.11	0/2471	0.22	0/3351
1	31-A	0.12	0/2460	0.21	0/3336
1	31-B	0.11	0/2471	0.22	0/3351
1	32-A	0.12	0/2460	0.21	0/3336
1	32-B	0.11	0/2471	0.22	0/3351
1	33-A	0.12	0/2460	0.21	0/3336
1	33-B	0.11	0/2471	0.22	0/3351
1	34-A	0.12	0/2460	0.21	0/3336
1	34-B	0.11	0/2471	0.22	0/3351
1	35-A	0.12	0/2460	0.21	0/3336
1	35-B	0.11	0/2471	0.22	0/3351
1	36-A	0.12	0/2460	0.21	0/3336
1	36-B	0.11	0/2471	0.22	0/3351
1	37-A	0.12	0/2460	0.21	0/3336
1	37-B	0.11	0/2471	0.22	0/3351
1	38-A	0.12	0/2460	0.21	0/3336

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	38-B	0.11	0/2471	0.22	0/3351
1	39-A	0.12	0/2460	0.21	0/3336
1	39-B	0.11	0/2471	0.22	0/3351
1	40-A	0.12	0/2460	0.21	0/3336
1	40-B	0.11	0/2471	0.22	0/3351
1	41-A	0.12	0/2460	0.21	0/3336
1	41-B	0.11	0/2471	0.22	0/3351
1	42-A	0.12	0/2460	0.21	0/3336
1	42-B	0.11	0/2471	0.22	0/3351
1	43-A	0.12	0/2460	0.21	0/3336
1	43-B	0.11	0/2471	0.22	0/3351
1	44-A	0.12	0/2460	0.21	0/3336
1	44-B	0.11	0/2471	0.22	0/3351
1	45-A	0.12	0/2460	0.21	0/3336
1	45-B	0.11	0/2471	0.22	0/3351
1	46-A	0.12	0/2460	0.21	0/3336
1	46-B	0.11	0/2471	0.22	0/3351
1	47-A	0.12	0/2460	0.21	0/3336
1	47-B	0.11	0/2471	0.22	0/3351
1	48-A	0.12	0/2460	0.21	0/3336
1	48-B	0.11	0/2471	0.22	0/3351
1	49-A	0.12	0/2460	0.21	0/3336
1	49-B	0.11	0/2471	0.22	0/3351
1	50-A	0.12	0/2460	0.21	0/3336
1	50-B	0.11	0/2471	0.22	0/3351
All	All	0.12	0/246550	0.21	0/334350

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	2
1	1-B	0	1
1	2-A	0	1
1	5-B	0	1
1	6-B	0	2
1	7-A	0	1
1	7-B	0	1
1	9-A	0	1
1	10-A	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	10-B	0	2
1	11-A	0	1
1	12-A	0	1
1	14-A	0	3
1	14-B	0	1
1	15-A	0	3
1	16-A	0	2
1	16-B	0	3
1	17-A	0	1
1	20-A	0	1
1	20-B	0	1
1	21-A	0	2
1	22-A	0	2
1	23-B	0	1
1	24-B	0	1
1	25-A	0	1
1	26-B	0	2
1	27-A	0	2
1	28-A	0	1
1	28-B	0	2
1	29-A	0	1
1	29-B	0	1
1	30-A	0	1
1	30-B	0	1
1	31-B	0	1
1	35-B	0	3
1	36-A	0	1
1	36-B	0	2
1	37-A	0	1
1	37-B	0	3
1	38-A	0	1
1	38-B	0	1
1	39-A	0	2
1	40-A	0	3
1	40-B	0	2
1	41-A	0	2
1	41-B	0	2
1	42-A	0	1
1	42-B	0	1
1	43-A	0	1
1	43-B	0	1
1	44-A	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	44-B	0	3
1	45-B	0	1
1	46-B	0	1
1	47-B	0	2
1	48-A	0	1
1	49-A	0	1
1	49-B	0	1
1	50-B	0	1
All	All	0	88

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 88 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	227	ARG	Sidechain
1	1-A	301	ASP	Peptide
1	1-B	305	ARG	Peptide
1	2-A	305	ARG	Sidechain
1	5-B	303	ASN	Peptide

5.2 Too-close contacts

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	2403	0	2319	0	0
1	1-B	2414	0	2330	0	0
1	2-A	2403	0	2319	0	0
1	2-B	2414	0	2330	0	0
1	3-A	2403	0	2320	0	0
1	3-B	2414	0	2330	0	0
1	4-A	2403	0	2320	0	0
1	4-B	2414	0	2330	0	0
1	5-A	2403	0	2320	0	0
1	5-B	2414	0	2330	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6-A	2403	0	2319	0	0
1	6-B	2414	0	2330	0	0
1	7-A	2403	0	2320	0	0
1	7-B	2414	0	2330	0	0
1	8-A	2403	0	2319	0	0
1	8-B	2414	0	2330	0	0
1	9-A	2403	0	2319	0	0
1	9-B	2414	0	2330	0	0
1	10-A	2403	0	2319	0	0
1	10-B	2414	0	2330	0	0
1	11-A	2403	0	2320	0	0
1	11-B	2414	0	2330	0	0
1	12-A	2403	0	2319	0	0
1	12-B	2414	0	2329	0	0
1	13-A	2403	0	2320	0	0
1	13-B	2414	0	2329	0	0
1	14-A	2403	0	2320	0	0
1	14-B	2414	0	2330	0	0
1	15-A	2403	0	2319	0	0
1	15-B	2414	0	2330	0	0
1	16-A	2403	0	2320	0	0
1	16-B	2414	0	2330	0	0
1	17-A	2403	0	2320	0	0
1	17-B	2414	0	2330	0	0
1	18-A	2403	0	2320	0	0
1	18-B	2414	0	2330	0	0
1	19-A	2403	0	2320	0	0
1	19-B	2414	0	2330	0	0
1	20-A	2403	0	2319	0	0
1	20-B	2414	0	2329	0	0
1	21-A	2403	0	2319	0	0
1	21-B	2414	0	2330	0	0
1	22-A	2403	0	2320	0	0
1	22-B	2414	0	2330	0	0
1	23-A	2403	0	2319	0	0
1	23-B	2414	0	2329	0	0
1	24-A	2403	0	2319	0	0
1	24-B	2414	0	2330	0	0
1	25-A	2403	0	2320	0	0
1	25-B	2414	0	2330	0	0
1	26-A	2403	0	2319	0	0
1	26-B	2414	0	2330	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	27-A	2403	0	2319	0	0
1	27-B	2414	0	2329	0	0
1	28-A	2403	0	2320	0	0
1	28-B	2414	0	2330	0	0
1	29-A	2403	0	2320	0	0
1	29-B	2414	0	2330	0	0
1	30-A	2403	0	2320	0	0
1	30-B	2414	0	2330	0	0
1	31-A	2403	0	2320	0	0
1	31-B	2414	0	2330	0	0
1	32-A	2403	0	2319	0	0
1	32-B	2414	0	2330	0	0
1	33-A	2403	0	2319	0	0
1	33-B	2414	0	2330	0	0
1	34-A	2403	0	2320	0	0
1	34-B	2414	0	2330	0	0
1	35-A	2403	0	2319	0	0
1	35-B	2414	0	2330	0	0
1	36-A	2403	0	2320	0	0
1	36-B	2414	0	2330	0	0
1	37-A	2403	0	2319	0	0
1	37-B	2414	0	2330	0	0
1	38-A	2403	0	2320	0	0
1	38-B	2414	0	2330	0	0
1	39-A	2403	0	2319	0	0
1	39-B	2414	0	2330	0	0
1	40-A	2403	0	2320	0	0
1	40-B	2414	0	2329	0	0
1	41-A	2403	0	2319	0	0
1	41-B	2414	0	2330	0	0
1	42-A	2403	0	2320	0	0
1	42-B	2414	0	2330	0	0
1	43-A	2403	0	2320	0	0
1	43-B	2414	0	2330	0	0
1	44-A	2403	0	2319	0	0
1	44-B	2414	0	2330	0	0
1	45-A	2403	0	2320	0	0
1	45-B	2414	0	2330	0	0
1	46-A	2403	0	2320	0	0
1	46-B	2414	0	2330	0	0
1	47-A	2403	0	2320	0	0
1	47-B	2414	0	2330	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	48-A	2403	0	2319	0	0
1	48-B	2414	0	2330	0	0
1	49-A	2403	0	2320	0	0
1	49-B	2414	0	2330	0	0
1	50-A	2403	0	2319	0	0
1	50-B	2414	0	2329	0	0
2	1-A	16	0	28	0	0
2	1-B	16	0	28	0	0
2	2-A	16	0	28	0	0
2	2-B	16	0	28	0	0
2	3-A	16	0	28	0	0
2	3-B	16	0	28	0	0
2	4-A	16	0	28	0	0
2	4-B	16	0	28	0	0
2	5-A	16	0	28	0	0
2	5-B	16	0	28	0	0
2	6-A	16	0	28	0	0
2	6-B	16	0	28	0	0
2	7-A	16	0	28	0	0
2	7-B	16	0	28	0	0
2	8-A	16	0	28	0	0
2	8-B	16	0	28	0	0
2	9-A	16	0	28	0	0
2	9-B	16	0	28	0	0
2	10-A	16	0	28	0	0
2	10-B	16	0	28	0	0
2	11-A	16	0	28	0	0
2	11-B	16	0	28	0	0
2	12-A	16	0	28	0	0
2	12-B	16	0	28	0	0
2	13-A	16	0	28	0	0
2	13-B	16	0	28	0	0
2	14-A	16	0	28	0	0
2	14-B	16	0	28	0	0
2	15-A	16	0	28	0	0
2	15-B	16	0	28	0	0
2	16-A	16	0	28	0	0
2	16-B	16	0	28	0	0
2	17-A	16	0	28	0	0
2	17-B	16	0	28	0	0
2	18-A	16	0	28	0	0
2	18-B	16	0	28	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	19-A	16	0	28	0	0
2	19-B	16	0	28	0	0
2	20-A	16	0	28	0	0
2	20-B	16	0	28	0	0
2	21-A	16	0	28	0	0
2	21-B	16	0	28	0	0
2	22-A	16	0	28	0	0
2	22-B	16	0	28	0	0
2	23-A	16	0	28	0	0
2	23-B	16	0	28	0	0
2	24-A	16	0	28	0	0
2	24-B	16	0	28	0	0
2	25-A	16	0	28	0	0
2	25-B	16	0	28	0	0
2	26-A	16	0	28	0	0
2	26-B	16	0	28	0	0
2	27-A	16	0	28	0	0
2	27-B	16	0	28	0	0
2	28-A	16	0	28	0	0
2	28-B	16	0	28	0	0
2	29-A	16	0	28	0	0
2	29-B	16	0	28	0	0
2	30-A	16	0	28	0	0
2	30-B	16	0	28	0	0
2	31-A	16	0	28	0	0
2	31-B	16	0	28	0	0
2	32-A	16	0	28	0	0
2	32-B	16	0	28	0	0
2	33-A	16	0	28	0	0
2	33-B	16	0	28	0	0
2	34-A	16	0	28	0	0
2	34-B	16	0	28	0	0
2	35-A	16	0	28	0	0
2	35-B	16	0	28	0	0
2	36-A	16	0	28	0	0
2	36-B	16	0	28	0	0
2	37-A	16	0	28	0	0
2	37-B	16	0	28	0	0
2	38-A	16	0	28	0	0
2	38-B	16	0	28	0	0
2	39-A	16	0	28	0	0
2	39-B	16	0	28	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	40-A	16	0	28	0	0
2	40-B	16	0	28	0	0
2	41-A	16	0	28	0	0
2	41-B	16	0	28	0	0
2	42-A	16	0	28	0	0
2	42-B	16	0	28	0	0
2	43-A	16	0	28	0	0
2	43-B	16	0	28	0	0
2	44-A	16	0	28	0	0
2	44-B	16	0	28	0	0
2	45-A	16	0	28	0	0
2	45-B	16	0	28	0	0
2	46-A	16	0	28	0	0
2	46-B	16	0	28	0	0
2	47-A	16	0	28	0	0
2	47-B	16	0	28	0	0
2	48-A	16	0	28	0	0
2	48-B	16	0	28	0	0
2	49-A	16	0	28	0	0
2	49-B	16	0	28	0	0
2	50-A	16	0	28	0	0
2	50-B	16	0	28	0	0
3	1-A	14	0	9	0	0
3	1-B	14	0	9	0	0
3	2-A	14	0	9	0	0
3	2-B	14	0	9	0	0
3	3-A	14	0	9	0	0
3	3-B	14	0	9	0	0
3	4-A	14	0	9	0	0
3	4-B	14	0	9	0	0
3	5-A	14	0	9	0	0
3	5-B	14	0	9	0	0
3	6-A	14	0	9	0	0
3	6-B	14	0	9	0	0
3	7-A	14	0	9	0	0
3	7-B	14	0	9	0	0
3	8-A	14	0	9	0	0
3	8-B	14	0	9	0	0
3	9-A	14	0	9	0	0
3	9-B	14	0	9	0	0
3	10-A	14	0	9	0	0
3	10-B	14	0	9	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	11-A	14	0	9	0	0
3	11-B	14	0	9	0	0
3	12-A	14	0	9	0	0
3	12-B	14	0	9	0	0
3	13-A	14	0	9	0	0
3	13-B	14	0	9	0	0
3	14-A	14	0	9	0	0
3	14-B	14	0	9	0	0
3	15-A	14	0	9	0	0
3	15-B	14	0	9	0	0
3	16-A	14	0	9	0	0
3	16-B	14	0	9	0	0
3	17-A	14	0	9	0	0
3	17-B	14	0	9	0	0
3	18-A	14	0	9	0	0
3	18-B	14	0	9	0	0
3	19-A	14	0	9	0	0
3	19-B	14	0	9	0	0
3	20-A	14	0	9	0	0
3	20-B	14	0	9	0	0
3	21-A	14	0	9	0	0
3	21-B	14	0	9	0	0
3	22-A	14	0	9	0	0
3	22-B	14	0	9	0	0
3	23-A	14	0	9	0	0
3	23-B	14	0	9	0	0
3	24-A	14	0	9	0	0
3	24-B	14	0	9	0	0
3	25-A	14	0	9	0	0
3	25-B	14	0	9	0	0
3	26-A	14	0	9	0	0
3	26-B	14	0	9	0	0
3	27-A	14	0	9	0	0
3	27-B	14	0	9	0	0
3	28-A	14	0	9	0	0
3	28-B	14	0	9	0	0
3	29-A	14	0	9	0	0
3	29-B	14	0	9	0	0
3	30-A	14	0	9	0	0
3	30-B	14	0	9	0	0
3	31-A	14	0	9	0	0
3	31-B	14	0	9	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	32-A	14	0	9	0	0
3	32-B	14	0	9	0	0
3	33-A	14	0	9	0	0
3	33-B	14	0	9	0	0
3	34-A	14	0	9	0	0
3	34-B	14	0	9	0	0
3	35-A	14	0	9	0	0
3	35-B	14	0	9	0	0
3	36-A	14	0	9	0	0
3	36-B	14	0	9	0	0
3	37-A	14	0	9	0	0
3	37-B	14	0	9	0	0
3	38-A	14	0	9	0	0
3	38-B	14	0	9	0	0
3	39-A	14	0	9	0	0
3	39-B	14	0	9	0	0
3	40-A	14	0	9	0	0
3	40-B	14	0	9	0	0
3	41-A	14	0	9	0	0
3	41-B	14	0	9	0	0
3	42-A	14	0	9	0	0
3	42-B	14	0	9	0	0
3	43-A	14	0	9	0	0
3	43-B	14	0	9	0	0
3	44-A	14	0	9	0	0
3	44-B	14	0	9	0	0
3	45-A	14	0	9	0	0
3	45-B	14	0	9	0	0
3	46-A	14	0	9	0	0
3	46-B	14	0	9	0	0
3	47-A	14	0	9	0	0
3	47-B	14	0	9	0	0
3	48-A	14	0	9	0	0
3	48-B	14	0	9	0	0
3	49-A	14	0	9	0	0
3	49-B	14	0	9	0	0
3	50-A	14	0	9	0	0
3	50-B	14	0	9	0	0
4	1-A	3	0	0	0	0
4	1-B	3	0	0	0	0
4	2-A	3	0	0	0	0
4	2-B	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	3-A	3	0	0	0	0
4	3-B	3	0	0	0	0
4	4-A	3	0	0	0	0
4	4-B	3	0	0	0	0
4	5-A	3	0	0	0	0
4	5-B	3	0	0	0	0
4	6-A	3	0	0	0	0
4	6-B	3	0	0	0	0
4	7-A	3	0	0	0	0
4	7-B	3	0	0	0	0
4	8-A	3	0	0	0	0
4	8-B	3	0	0	0	0
4	9-A	3	0	0	0	0
4	9-B	3	0	0	0	0
4	10-A	3	0	0	0	0
4	10-B	3	0	0	0	0
4	11-A	3	0	0	0	0
4	11-B	3	0	0	0	0
4	12-A	3	0	0	0	0
4	12-B	3	0	0	0	0
4	13-A	3	0	0	0	0
4	13-B	3	0	0	0	0
4	14-A	3	0	0	0	0
4	14-B	3	0	0	0	0
4	15-A	3	0	0	0	0
4	15-B	3	0	0	0	0
4	16-A	3	0	0	0	0
4	16-B	3	0	0	0	0
4	17-A	3	0	0	0	0
4	17-B	3	0	0	0	0
4	18-A	3	0	0	0	0
4	18-B	3	0	0	0	0
4	19-A	3	0	0	0	0
4	19-B	3	0	0	0	0
4	20-A	3	0	0	0	0
4	20-B	3	0	0	0	0
4	21-A	3	0	0	0	0
4	21-B	3	0	0	0	0
4	22-A	3	0	0	0	0
4	22-B	3	0	0	0	0
4	23-A	3	0	0	0	0
4	23-B	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	24-A	3	0	0	0	0
4	24-B	3	0	0	0	0
4	25-A	3	0	0	0	0
4	25-B	3	0	0	0	0
4	26-A	3	0	0	0	0
4	26-B	3	0	0	0	0
4	27-A	3	0	0	0	0
4	27-B	3	0	0	0	0
4	28-A	3	0	0	0	0
4	28-B	3	0	0	0	0
4	29-A	3	0	0	0	0
4	29-B	3	0	0	0	0
4	30-A	3	0	0	0	0
4	30-B	3	0	0	0	0
4	31-A	3	0	0	0	0
4	31-B	3	0	0	0	0
4	32-A	3	0	0	0	0
4	32-B	3	0	0	0	0
4	33-A	3	0	0	0	0
4	33-B	3	0	0	0	0
4	34-A	3	0	0	0	0
4	34-B	3	0	0	0	0
4	35-A	3	0	0	0	0
4	35-B	3	0	0	0	0
4	36-A	3	0	0	0	0
4	36-B	3	0	0	0	0
4	37-A	3	0	0	0	0
4	37-B	3	0	0	0	0
4	38-A	3	0	0	0	0
4	38-B	3	0	0	0	0
4	39-A	3	0	0	0	0
4	39-B	3	0	0	0	0
4	40-A	3	0	0	0	0
4	40-B	3	0	0	0	0
4	41-A	3	0	0	0	0
4	41-B	3	0	0	0	0
4	42-A	3	0	0	0	0
4	42-B	3	0	0	0	0
4	43-A	3	0	0	0	0
4	43-B	3	0	0	0	0
4	44-A	3	0	0	0	0
4	44-B	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	45-A	3	0	0	0	0
4	45-B	3	0	0	0	0
4	46-A	3	0	0	0	0
4	46-B	3	0	0	0	0
4	47-A	3	0	0	0	0
4	47-B	3	0	0	0	0
4	48-A	3	0	0	0	0
4	48-B	3	0	0	0	0
4	49-A	3	0	0	0	0
4	49-B	3	0	0	0	0
4	50-A	3	0	0	0	0
4	50-B	3	0	0	0	0
5	1-A	1	0	0	0	0
5	1-B	1	0	0	0	0
5	2-A	1	0	0	0	0
5	2-B	1	0	0	0	0
5	3-A	1	0	0	0	0
5	3-B	1	0	0	0	0
5	4-A	1	0	0	0	0
5	4-B	1	0	0	0	0
5	5-A	1	0	0	0	0
5	5-B	1	0	0	0	0
5	6-A	1	0	0	0	0
5	6-B	1	0	0	0	0
5	7-A	1	0	0	0	0
5	7-B	1	0	0	0	0
5	8-A	1	0	0	0	0
5	8-B	1	0	0	0	0
5	9-A	1	0	0	0	0
5	9-B	1	0	0	0	0
5	10-A	1	0	0	0	0
5	10-B	1	0	0	0	0
5	11-A	1	0	0	0	0
5	11-B	1	0	0	0	0
5	12-A	1	0	0	0	0
5	12-B	1	0	0	0	0
5	13-A	1	0	0	0	0
5	13-B	1	0	0	0	0
5	14-A	1	0	0	0	0
5	14-B	1	0	0	0	0
5	15-A	1	0	0	0	0
5	15-B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	16-A	1	0	0	0	0
5	16-B	1	0	0	0	0
5	17-A	1	0	0	0	0
5	17-B	1	0	0	0	0
5	18-A	1	0	0	0	0
5	18-B	1	0	0	0	0
5	19-A	1	0	0	0	0
5	19-B	1	0	0	0	0
5	20-A	1	0	0	0	0
5	20-B	1	0	0	0	0
5	21-A	1	0	0	0	0
5	21-B	1	0	0	0	0
5	22-A	1	0	0	0	0
5	22-B	1	0	0	0	0
5	23-A	1	0	0	0	0
5	23-B	1	0	0	0	0
5	24-A	1	0	0	0	0
5	24-B	1	0	0	0	0
5	25-A	1	0	0	0	0
5	25-B	1	0	0	0	0
5	26-A	1	0	0	0	0
5	26-B	1	0	0	0	0
5	27-A	1	0	0	0	0
5	27-B	1	0	0	0	0
5	28-A	1	0	0	0	0
5	28-B	1	0	0	0	0
5	29-A	1	0	0	0	0
5	29-B	1	0	0	0	0
5	30-A	1	0	0	0	0
5	30-B	1	0	0	0	0
5	31-A	1	0	0	0	0
5	31-B	1	0	0	0	0
5	32-A	1	0	0	0	0
5	32-B	1	0	0	0	0
5	33-A	1	0	0	0	0
5	33-B	1	0	0	0	0
5	34-A	1	0	0	0	0
5	34-B	1	0	0	0	0
5	35-A	1	0	0	0	0
5	35-B	1	0	0	0	0
5	36-A	1	0	0	0	0
5	36-B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	37-A	1	0	0	0	0
5	37-B	1	0	0	0	0
5	38-A	1	0	0	0	0
5	38-B	1	0	0	0	0
5	39-A	1	0	0	0	0
5	39-B	1	0	0	0	0
5	40-A	1	0	0	0	0
5	40-B	1	0	0	0	0
5	41-A	1	0	0	0	0
5	41-B	1	0	0	0	0
5	42-A	1	0	0	0	0
5	42-B	1	0	0	0	0
5	43-A	1	0	0	0	0
5	43-B	1	0	0	0	0
5	44-A	1	0	0	0	0
5	44-B	1	0	0	0	0
5	45-A	1	0	0	0	0
5	45-B	1	0	0	0	0
5	46-A	1	0	0	0	0
5	46-B	1	0	0	0	0
5	47-A	1	0	0	0	0
5	47-B	1	0	0	0	0
5	48-A	1	0	0	0	0
5	48-B	1	0	0	0	0
5	49-A	1	0	0	0	0
5	49-B	1	0	0	0	0
5	50-A	1	0	0	0	0
5	50-B	1	0	0	0	0
6	1-A	232	0	0	0	0
6	1-B	121	0	0	0	0
6	2-A	241	0	0	0	0
6	2-B	124	0	0	0	0
6	3-A	242	0	0	0	0
6	3-B	126	0	0	0	0
6	4-A	221	0	0	0	0
6	4-B	116	0	0	0	0
6	5-A	236	0	0	0	0
6	5-B	122	0	0	0	0
6	6-A	239	0	0	0	0
6	6-B	124	0	0	0	0
6	7-A	228	0	0	0	0
6	7-B	120	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	8-A	226	0	0	0	0
6	8-B	119	0	0	0	0
6	9-A	229	0	0	0	0
6	9-B	120	0	0	0	0
6	10-A	234	0	0	0	0
6	10-B	121	0	0	0	0
6	11-A	236	0	0	0	0
6	11-B	122	0	0	0	0
6	12-A	221	0	0	0	0
6	12-B	117	0	0	0	0
6	13-A	221	0	0	0	0
6	13-B	116	0	0	0	0
6	14-A	229	0	0	0	0
6	14-B	120	0	0	0	0
6	15-A	230	0	0	0	0
6	15-B	120	0	0	0	0
6	16-A	246	0	0	0	0
6	16-B	129	0	0	0	0
6	17-A	229	0	0	0	0
6	17-B	120	0	0	0	0
6	18-A	234	0	0	0	0
6	18-B	121	0	0	0	0
6	19-A	231	0	0	0	0
6	19-B	121	0	0	0	0
6	20-A	226	0	0	0	0
6	20-B	119	0	0	0	0
6	21-A	227	0	0	0	0
6	21-B	120	0	0	0	0
6	22-A	238	0	0	0	0
6	22-B	122	0	0	0	0
6	23-A	236	0	0	0	0
6	23-B	122	0	0	0	0
6	24-A	221	0	0	0	0
6	24-B	118	0	0	0	0
6	25-A	230	0	0	0	0
6	25-B	120	0	0	0	0
6	26-A	230	0	0	0	0
6	26-B	120	0	0	0	0
6	27-A	236	0	0	0	0
6	27-B	121	0	0	0	0
6	28-A	222	0	0	0	0
6	28-B	118	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	29-A	222	0	0	0	0
6	29-B	118	0	0	0	0
6	30-A	227	0	0	0	0
6	30-B	120	0	0	0	0
6	31-A	211	0	0	0	0
6	31-B	113	0	0	0	0
6	32-A	227	0	0	0	0
6	32-B	120	0	0	0	0
6	33-A	224	0	0	0	0
6	33-B	119	0	0	0	0
6	34-A	240	0	0	0	0
6	34-B	124	0	0	0	0
6	35-A	231	0	0	0	0
6	35-B	120	0	0	0	0
6	36-A	225	0	0	0	0
6	36-B	119	0	0	0	0
6	37-A	221	0	0	0	0
6	37-B	116	0	0	0	0
6	38-A	225	0	0	0	0
6	38-B	119	0	0	0	0
6	39-A	235	0	0	0	0
6	39-B	121	0	0	0	0
6	40-A	226	0	0	0	0
6	40-B	119	0	0	0	0
6	41-A	226	0	0	0	0
6	41-B	120	0	0	0	0
6	42-A	229	0	0	0	0
6	42-B	120	0	0	0	0
6	43-A	241	0	0	0	0
6	43-B	125	0	0	0	0
6	44-A	250	0	0	0	0
6	44-B	129	0	0	0	0
6	45-A	253	0	0	0	0
6	45-B	130	0	0	0	0
6	46-A	240	0	0	0	0
6	46-B	124	0	0	0	0
6	47-A	224	0	0	0	0
6	47-B	119	0	0	0	0
6	48-A	226	0	0	0	0
6	48-B	119	0	0	0	0
6	49-A	250	0	0	0	0
6	49-B	129	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	50-A	242	0	0	0	0
6	50-B	127	0	0	0	0
All	All	261865	0	236170	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	293/318 (92%)	283 (97%)	7 (2%)	3 (1%)	12	5
1	1-B	294/318 (92%)	283 (96%)	9 (3%)	2 (1%)	18	9
1	2-A	293/318 (92%)	283 (97%)	7 (2%)	3 (1%)	12	5
1	2-B	294/318 (92%)	284 (97%)	10 (3%)	0	100	100
1	3-A	293/318 (92%)	284 (97%)	8 (3%)	1 (0%)	36	30
1	3-B	294/318 (92%)	286 (97%)	8 (3%)	0	100	100
1	4-A	293/318 (92%)	280 (96%)	12 (4%)	1 (0%)	36	30
1	4-B	294/318 (92%)	282 (96%)	8 (3%)	4 (1%)	9	2
1	5-A	293/318 (92%)	286 (98%)	7 (2%)	0	100	100
1	5-B	294/318 (92%)	285 (97%)	8 (3%)	1 (0%)	36	30
1	6-A	293/318 (92%)	278 (95%)	11 (4%)	4 (1%)	9	2
1	6-B	294/318 (92%)	284 (97%)	5 (2%)	5 (2%)	7	1
1	7-A	293/318 (92%)	283 (97%)	9 (3%)	1 (0%)	36	30
1	7-B	294/318 (92%)	279 (95%)	9 (3%)	6 (2%)	6	1
1	8-A	293/318 (92%)	282 (96%)	10 (3%)	1 (0%)	36	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8-B	294/318 (92%)	280 (95%)	8 (3%)	6 (2%)	6	1
1	9-A	293/318 (92%)	277 (94%)	13 (4%)	3 (1%)	12	5
1	9-B	294/318 (92%)	285 (97%)	7 (2%)	2 (1%)	18	9
1	10-A	293/318 (92%)	281 (96%)	8 (3%)	4 (1%)	9	2
1	10-B	294/318 (92%)	289 (98%)	4 (1%)	1 (0%)	36	30
1	11-A	293/318 (92%)	279 (95%)	9 (3%)	5 (2%)	7	1
1	11-B	294/318 (92%)	290 (99%)	3 (1%)	1 (0%)	36	30
1	12-A	293/318 (92%)	283 (97%)	9 (3%)	1 (0%)	36	30
1	12-B	294/318 (92%)	284 (97%)	9 (3%)	1 (0%)	36	30
1	13-A	293/318 (92%)	282 (96%)	10 (3%)	1 (0%)	36	30
1	13-B	294/318 (92%)	285 (97%)	7 (2%)	2 (1%)	18	9
1	14-A	293/318 (92%)	284 (97%)	6 (2%)	3 (1%)	12	5
1	14-B	294/318 (92%)	284 (97%)	8 (3%)	2 (1%)	18	9
1	15-A	293/318 (92%)	284 (97%)	5 (2%)	4 (1%)	9	2
1	15-B	294/318 (92%)	280 (95%)	11 (4%)	3 (1%)	12	5
1	16-A	293/318 (92%)	275 (94%)	14 (5%)	4 (1%)	9	2
1	16-B	294/318 (92%)	282 (96%)	5 (2%)	7 (2%)	4	0
1	17-A	293/318 (92%)	281 (96%)	10 (3%)	2 (1%)	18	9
1	17-B	294/318 (92%)	280 (95%)	12 (4%)	2 (1%)	18	9
1	18-A	293/318 (92%)	285 (97%)	5 (2%)	3 (1%)	12	5
1	18-B	294/318 (92%)	282 (96%)	9 (3%)	3 (1%)	12	5
1	19-A	293/318 (92%)	280 (96%)	11 (4%)	2 (1%)	18	9
1	19-B	294/318 (92%)	284 (97%)	8 (3%)	2 (1%)	18	9
1	20-A	293/318 (92%)	279 (95%)	11 (4%)	3 (1%)	12	5
1	20-B	294/318 (92%)	284 (97%)	7 (2%)	3 (1%)	12	5
1	21-A	293/318 (92%)	285 (97%)	6 (2%)	2 (1%)	18	9
1	21-B	294/318 (92%)	282 (96%)	8 (3%)	4 (1%)	9	2
1	22-A	293/318 (92%)	281 (96%)	9 (3%)	3 (1%)	12	5
1	22-B	294/318 (92%)	284 (97%)	7 (2%)	3 (1%)	12	5
1	23-A	293/318 (92%)	281 (96%)	10 (3%)	2 (1%)	18	9
1	23-B	294/318 (92%)	281 (96%)	9 (3%)	4 (1%)	9	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	24-A	293/318 (92%)	281 (96%)	10 (3%)	2 (1%)	18	9
1	24-B	294/318 (92%)	280 (95%)	11 (4%)	3 (1%)	12	5
1	25-A	293/318 (92%)	282 (96%)	10 (3%)	1 (0%)	36	30
1	25-B	294/318 (92%)	282 (96%)	8 (3%)	4 (1%)	9	2
1	26-A	293/318 (92%)	281 (96%)	9 (3%)	3 (1%)	12	5
1	26-B	294/318 (92%)	281 (96%)	9 (3%)	4 (1%)	9	2
1	27-A	293/318 (92%)	283 (97%)	7 (2%)	3 (1%)	12	5
1	27-B	294/318 (92%)	283 (96%)	9 (3%)	2 (1%)	18	9
1	28-A	293/318 (92%)	277 (94%)	14 (5%)	2 (1%)	18	9
1	28-B	294/318 (92%)	284 (97%)	7 (2%)	3 (1%)	12	5
1	29-A	293/318 (92%)	282 (96%)	9 (3%)	2 (1%)	18	9
1	29-B	294/318 (92%)	285 (97%)	9 (3%)	0	100	100
1	30-A	293/318 (92%)	283 (97%)	9 (3%)	1 (0%)	36	30
1	30-B	294/318 (92%)	282 (96%)	11 (4%)	1 (0%)	36	30
1	31-A	293/318 (92%)	280 (96%)	13 (4%)	0	100	100
1	31-B	294/318 (92%)	288 (98%)	6 (2%)	0	100	100
1	32-A	293/318 (92%)	282 (96%)	9 (3%)	2 (1%)	18	9
1	32-B	294/318 (92%)	283 (96%)	9 (3%)	2 (1%)	18	9
1	33-A	293/318 (92%)	281 (96%)	11 (4%)	1 (0%)	36	30
1	33-B	294/318 (92%)	283 (96%)	8 (3%)	3 (1%)	12	5
1	34-A	293/318 (92%)	282 (96%)	9 (3%)	2 (1%)	18	9
1	34-B	294/318 (92%)	282 (96%)	11 (4%)	1 (0%)	36	30
1	35-A	293/318 (92%)	285 (97%)	7 (2%)	1 (0%)	36	30
1	35-B	294/318 (92%)	282 (96%)	8 (3%)	4 (1%)	9	2
1	36-A	293/318 (92%)	281 (96%)	9 (3%)	3 (1%)	12	5
1	36-B	294/318 (92%)	285 (97%)	7 (2%)	2 (1%)	18	9
1	37-A	293/318 (92%)	275 (94%)	16 (6%)	2 (1%)	18	9
1	37-B	294/318 (92%)	284 (97%)	9 (3%)	1 (0%)	36	30
1	38-A	293/318 (92%)	282 (96%)	8 (3%)	3 (1%)	12	5
1	38-B	294/318 (92%)	286 (97%)	8 (3%)	0	100	100
1	39-A	293/318 (92%)	278 (95%)	12 (4%)	3 (1%)	12	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	39-B	294/318 (92%)	281 (96%)	9 (3%)	4 (1%)	9	2
1	40-A	293/318 (92%)	276 (94%)	12 (4%)	5 (2%)	7	1
1	40-B	294/318 (92%)	281 (96%)	8 (3%)	5 (2%)	7	1
1	41-A	293/318 (92%)	281 (96%)	9 (3%)	3 (1%)	12	5
1	41-B	294/318 (92%)	280 (95%)	9 (3%)	5 (2%)	7	1
1	42-A	293/318 (92%)	279 (95%)	12 (4%)	2 (1%)	18	9
1	42-B	294/318 (92%)	279 (95%)	11 (4%)	4 (1%)	9	2
1	43-A	293/318 (92%)	280 (96%)	11 (4%)	2 (1%)	18	9
1	43-B	294/318 (92%)	281 (96%)	9 (3%)	4 (1%)	9	2
1	44-A	293/318 (92%)	282 (96%)	8 (3%)	3 (1%)	12	5
1	44-B	294/318 (92%)	284 (97%)	7 (2%)	3 (1%)	12	5
1	45-A	293/318 (92%)	284 (97%)	7 (2%)	2 (1%)	18	9
1	45-B	294/318 (92%)	281 (96%)	10 (3%)	3 (1%)	12	5
1	46-A	293/318 (92%)	279 (95%)	11 (4%)	3 (1%)	12	5
1	46-B	294/318 (92%)	279 (95%)	14 (5%)	1 (0%)	36	30
1	47-A	293/318 (92%)	282 (96%)	7 (2%)	4 (1%)	9	2
1	47-B	294/318 (92%)	278 (95%)	13 (4%)	3 (1%)	12	5
1	48-A	293/318 (92%)	284 (97%)	8 (3%)	1 (0%)	36	30
1	48-B	294/318 (92%)	281 (96%)	10 (3%)	3 (1%)	12	5
1	49-A	293/318 (92%)	281 (96%)	7 (2%)	5 (2%)	7	1
1	49-B	294/318 (92%)	286 (97%)	7 (2%)	1 (0%)	36	30
1	50-A	293/318 (92%)	281 (96%)	9 (3%)	3 (1%)	12	5
1	50-B	294/318 (92%)	279 (95%)	12 (4%)	3 (1%)	12	5
All	All	29350/31800 (92%)	28199 (96%)	898 (3%)	253 (1%)	14	6

5 of 253 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	15	ARG
1	4-B	298	ALA
1	5-B	297	THR
1	6-A	303	ASN
1	6-B	304	SER

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	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	1-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	2-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	2-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	3-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	3-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	4-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	4-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	5-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	5-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	6-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	6-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	7-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	7-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	8-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	8-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	9-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	9-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	10-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	10-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	11-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	11-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	12-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	12-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	13-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	13-B	265/280 (95%)	250 (94%)	15 (6%)	18	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	14-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	14-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	15-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	15-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	16-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	16-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	17-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	17-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	18-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	18-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	19-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	19-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	20-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	20-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	21-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	21-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	22-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	22-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	23-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	23-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	24-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	24-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	25-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	25-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	26-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	26-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	27-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	27-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	28-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	28-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	29-A	263/280 (94%)	248 (94%)	15 (6%)	18	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	29-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	30-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	30-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	31-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	31-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	32-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	32-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	33-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	33-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	34-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	34-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	35-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	35-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	36-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	36-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	37-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	37-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	38-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	38-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	39-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	39-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	40-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	40-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	41-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	41-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	42-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	42-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	43-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	43-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	44-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	44-B	265/280 (95%)	250 (94%)	15 (6%)	18	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	45-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	45-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	46-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	46-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	47-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	47-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	48-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	48-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	49-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	49-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
1	50-A	263/280 (94%)	248 (94%)	15 (6%)	18	6
1	50-B	265/280 (95%)	250 (94%)	15 (6%)	18	6
All	All	26400/28000 (94%)	24900 (94%)	1500 (6%)	18	6

5 of 1500 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	31-B	301	ASP
1	39-A	227	ARG
1	32-B	195	ARG
1	31-B	299	VAL
1	35-B	72	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 314 such sidechains are listed below:

Mol	Chain	Res	Type
1	39-B	285	ASN
1	47-B	285	ASN
1	40-B	285	ASN
1	44-A	300	ASN
1	49-A	202	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MPD	27-B	707	-	7,7,7	0.36	0	9,10,10	0.74	0
2	MPD	16-A	401	-	7,7,7	0.42	0	9,10,10	0.91	0
2	MPD	5-A	401	-	7,7,7	0.43	0	9,10,10	0.90	0
3	AHD	46-B	706	4	13,13,13	1.53	2 (15%)	19,21,21	1.47	2 (10%)
2	MPD	43-A	403	-	7,7,7	0.42	0	9,10,10	0.55	0
3	AHD	18-B	706	4	13,13,13	1.63	4 (30%)	19,21,21	1.46	3 (15%)
2	MPD	42-B	707	-	7,7,7	0.34	0	9,10,10	0.81	0
2	MPD	5-B	701	-	7,7,7	0.76	0	9,10,10	0.78	0
3	AHD	48-A	402	4	13,13,13	1.56	3 (23%)	19,21,21	1.84	4 (21%)
2	MPD	39-A	403	-	7,7,7	0.72	0	9,10,10	1.22	1 (11%)
2	MPD	3-A	403	-	7,7,7	0.32	0	9,10,10	0.71	0
2	MPD	34-A	401	-	7,7,7	0.63	0	9,10,10	1.81	2 (22%)
2	MPD	23-B	701	-	7,7,7	0.60	0	9,10,10	1.16	0
2	MPD	31-B	707	-	7,7,7	0.62	0	9,10,10	0.97	0
2	MPD	26-A	403	-	7,7,7	0.35	0	9,10,10	0.69	0
2	MPD	18-A	401	-	7,7,7	0.28	0	9,10,10	0.75	0
2	MPD	36-A	401	-	7,7,7	0.41	0	9,10,10	0.78	0
2	MPD	40-A	403	-	7,7,7	0.65	0	9,10,10	0.85	0
2	MPD	3-A	401	-	7,7,7	0.38	0	9,10,10	0.73	0
3	AHD	31-B	706	4	13,13,13	1.40	3 (23%)	19,21,21	1.62	4 (21%)
2	MPD	9-B	707	-	7,7,7	0.40	0	9,10,10	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MPD	27-A	403	-	7,7,7	0.27	0	9,10,10	0.73	0
2	MPD	38-B	707	-	7,7,7	0.41	0	9,10,10	0.87	0
3	AHD	7-B	706	4	13,13,13	1.50	3 (23%)	19,21,21	1.59	3 (15%)
2	MPD	21-A	401	-	7,7,7	0.58	0	9,10,10	0.82	0
2	MPD	19-A	403	-	7,7,7	0.37	0	9,10,10	0.38	0
3	AHD	41-A	402	4	13,13,13	1.66	3 (23%)	19,21,21	1.60	2 (10%)
2	MPD	28-A	403	-	7,7,7	0.57	0	9,10,10	0.40	0
3	AHD	13-B	706	4	13,13,13	1.72	5 (38%)	19,21,21	1.55	4 (21%)
2	MPD	28-B	707	-	7,7,7	0.48	0	9,10,10	0.94	0
2	MPD	33-A	403	-	7,7,7	0.34	0	9,10,10	0.79	1 (11%)
3	AHD	6-A	402	4	13,13,13	1.59	2 (15%)	19,21,21	1.61	4 (21%)
3	AHD	26-B	706	4	13,13,13	1.62	3 (23%)	19,21,21	1.70	3 (15%)
2	MPD	8-B	701	-	7,7,7	0.39	0	9,10,10	0.91	1 (11%)
3	AHD	21-A	402	4	13,13,13	1.45	2 (15%)	19,21,21	1.56	5 (26%)
2	MPD	42-A	401	-	7,7,7	0.34	0	9,10,10	0.44	0
2	MPD	10-A	401	-	7,7,7	0.46	0	9,10,10	1.71	2 (22%)
2	MPD	23-A	401	-	7,7,7	0.49	0	9,10,10	0.68	0
2	MPD	7-A	403	-	7,7,7	0.35	0	9,10,10	0.77	0
2	MPD	17-A	403	-	7,7,7	0.52	0	9,10,10	1.47	1 (11%)
2	MPD	7-B	701	-	7,7,7	0.63	0	9,10,10	1.58	2 (22%)
2	MPD	7-B	707	-	7,7,7	0.46	0	9,10,10	2.62	2 (22%)
2	MPD	41-B	707	-	7,7,7	0.41	0	9,10,10	0.89	0
3	AHD	38-A	402	4	13,13,13	1.53	3 (23%)	19,21,21	1.75	5 (26%)
3	AHD	17-A	402	4	13,13,13	1.53	3 (23%)	19,21,21	1.69	4 (21%)
2	MPD	36-B	701	-	7,7,7	0.67	0	9,10,10	1.21	0
3	AHD	19-A	402	4	13,13,13	1.65	2 (15%)	19,21,21	1.33	2 (10%)
3	AHD	4-B	706	4	13,13,13	1.65	2 (15%)	19,21,21	1.30	4 (21%)
3	AHD	1-B	706	4	13,13,13	1.43	2 (15%)	19,21,21	1.48	2 (10%)
2	MPD	29-A	401	-	7,7,7	0.42	0	9,10,10	0.77	0
2	MPD	2-B	707	-	7,7,7	0.53	0	9,10,10	0.38	0
3	AHD	22-A	402	4	13,13,13	1.51	4 (30%)	19,21,21	1.70	6 (31%)
3	AHD	37-B	706	4	13,13,13	1.53	4 (30%)	19,21,21	1.58	4 (21%)
3	AHD	21-B	706	4	13,13,13	1.56	3 (23%)	19,21,21	1.61	1 (5%)
2	MPD	1-A	401	-	7,7,7	0.44	0	9,10,10	0.77	0
2	MPD	15-A	401	-	7,7,7	0.33	0	9,10,10	0.84	0
2	MPD	39-B	701	-	7,7,7	0.39	0	9,10,10	0.83	0
2	MPD	10-A	403	-	7,7,7	0.29	0	9,10,10	0.57	0
2	MPD	17-B	707	-	7,7,7	0.56	0	9,10,10	1.30	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AHD	15-A	402	4	13,13,13	1.45	1 (7%)	19,21,21	1.53	3 (15%)
2	MPD	6-A	401	-	7,7,7	0.53	0	9,10,10	1.35	2 (22%)
2	MPD	50-A	401	-	7,7,7	0.63	0	9,10,10	0.66	0
2	MPD	45-A	403	-	7,7,7	0.34	0	9,10,10	0.86	0
3	AHD	29-B	706	4	13,13,13	1.69	3 (23%)	19,21,21	1.90	6 (31%)
2	MPD	44-B	701	-	7,7,7	0.32	0	9,10,10	0.88	0
2	MPD	18-B	707	-	7,7,7	0.28	0	9,10,10	1.06	1 (11%)
3	AHD	14-A	402	4	13,13,13	1.63	2 (15%)	19,21,21	2.00	9 (47%)
3	AHD	23-B	706	4	13,13,13	1.58	4 (30%)	19,21,21	1.72	3 (15%)
2	MPD	11-B	701	-	7,7,7	0.32	0	9,10,10	1.24	2 (22%)
2	MPD	47-B	707	-	7,7,7	0.33	0	9,10,10	0.93	0
2	MPD	48-A	401	-	7,7,7	0.38	0	9,10,10	0.72	0
3	AHD	36-A	402	4	13,13,13	1.82	4 (30%)	19,21,21	1.76	5 (26%)
2	MPD	22-B	701	-	7,7,7	0.25	0	9,10,10	1.22	1 (11%)
2	MPD	49-B	701	-	7,7,7	0.55	0	9,10,10	1.30	1 (11%)
2	MPD	28-B	701	-	7,7,7	0.54	0	9,10,10	0.85	1 (11%)
2	MPD	6-B	707	-	7,7,7	0.53	0	9,10,10	1.16	1 (11%)
2	MPD	30-A	403	-	7,7,7	0.40	0	9,10,10	0.67	0
3	AHD	39-A	402	4	13,13,13	1.48	2 (15%)	19,21,21	1.38	3 (15%)
2	MPD	50-A	403	-	7,7,7	0.34	0	9,10,10	0.66	0
2	MPD	25-A	401	-	7,7,7	0.54	0	9,10,10	0.73	0
3	AHD	44-A	402	4	13,13,13	1.66	1 (7%)	19,21,21	1.74	3 (15%)
2	MPD	5-B	707	-	7,7,7	0.33	0	9,10,10	1.22	1 (11%)
2	MPD	26-A	401	-	7,7,7	0.38	0	9,10,10	1.23	1 (11%)
2	MPD	2-A	403	-	7,7,7	0.34	0	9,10,10	1.72	2 (22%)
2	MPD	11-A	403	-	7,7,7	0.60	0	9,10,10	0.80	0
2	MPD	13-A	403	-	7,7,7	0.25	0	9,10,10	1.05	1 (11%)
2	MPD	47-A	403	-	7,7,7	0.22	0	9,10,10	0.57	0
2	MPD	16-B	701	-	7,7,7	0.53	0	9,10,10	1.10	1 (11%)
2	MPD	1-B	707	-	7,7,7	0.49	0	9,10,10	0.59	0
2	MPD	46-A	403	-	7,7,7	0.30	0	9,10,10	0.69	0
2	MPD	2-A	401	-	7,7,7	0.32	0	9,10,10	0.75	0
2	MPD	10-B	701	-	7,7,7	0.27	0	9,10,10	1.19	1 (11%)
2	MPD	7-A	401	-	7,7,7	0.37	0	9,10,10	0.92	0
2	MPD	41-B	701	-	7,7,7	0.48	0	9,10,10	0.77	0
2	MPD	10-B	707	-	7,7,7	0.40	0	9,10,10	0.85	0
2	MPD	23-B	707	-	7,7,7	0.54	0	9,10,10	0.52	0
2	MPD	33-A	401	-	7,7,7	0.33	0	9,10,10	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MPD	37-A	401	-	7,7,7	0.35	0	9,10,10	0.72	0
2	MPD	45-B	701	-	7,7,7	0.45	0	9,10,10	1.25	1 (11%)
2	MPD	39-B	707	-	7,7,7	0.34	0	9,10,10	1.08	1 (11%)
3	AHD	1-A	402	4	13,13,13	1.47	2 (15%)	19,21,21	1.71	3 (15%)
2	MPD	3-B	707	-	7,7,7	0.49	0	9,10,10	0.55	0
3	AHD	43-A	402	4	13,13,13	1.57	4 (30%)	19,21,21	1.74	5 (26%)
3	AHD	17-B	706	4	13,13,13	1.62	2 (15%)	19,21,21	1.55	3 (15%)
2	MPD	23-A	403	-	7,7,7	0.33	0	9,10,10	0.96	1 (11%)
2	MPD	43-B	701	-	7,7,7	0.49	0	9,10,10	1.03	1 (11%)
3	AHD	35-B	706	4	13,13,13	1.54	3 (23%)	19,21,21	1.51	2 (10%)
2	MPD	14-B	707	-	7,7,7	0.41	0	9,10,10	0.77	0
2	MPD	34-A	403	-	7,7,7	0.33	0	9,10,10	0.54	0
3	AHD	43-B	706	4	13,13,13	1.59	2 (15%)	19,21,21	1.43	2 (10%)
2	MPD	13-A	401	-	7,7,7	0.47	0	9,10,10	1.57	2 (22%)
2	MPD	42-B	701	-	7,7,7	0.49	0	9,10,10	0.68	0
2	MPD	32-A	401	-	7,7,7	0.48	0	9,10,10	0.54	0
2	MPD	42-A	403	-	7,7,7	0.44	0	9,10,10	0.70	0
2	MPD	46-B	707	-	7,7,7	0.48	0	9,10,10	0.53	0
2	MPD	37-B	701	-	7,7,7	0.70	0	9,10,10	0.81	0
3	AHD	29-A	402	4	13,13,13	1.75	3 (23%)	19,21,21	1.69	4 (21%)
2	MPD	13-B	707	-	7,7,7	0.40	0	9,10,10	0.84	0
2	MPD	13-B	701	-	7,7,7	0.62	0	9,10,10	1.14	1 (11%)
3	AHD	16-B	706	4	13,13,13	1.56	3 (23%)	19,21,21	1.65	4 (21%)
2	MPD	45-B	707	-	7,7,7	0.62	0	9,10,10	1.07	1 (11%)
2	MPD	48-B	707	-	7,7,7	0.34	0	9,10,10	0.82	0
2	MPD	31-B	701	-	7,7,7	0.58	0	9,10,10	0.74	0
2	MPD	41-A	403	-	7,7,7	0.36	0	9,10,10	0.71	0
2	MPD	46-B	701	-	7,7,7	1.00	0	9,10,10	1.95	3 (33%)
2	MPD	27-B	701	-	7,7,7	0.63	0	9,10,10	1.18	0
3	AHD	5-A	402	4	13,13,13	1.49	2 (15%)	19,21,21	1.81	5 (26%)
2	MPD	14-A	403	-	7,7,7	0.31	0	9,10,10	0.42	0
2	MPD	32-B	701	-	7,7,7	0.37	0	9,10,10	1.28	0
2	MPD	4-A	401	-	7,7,7	0.33	0	9,10,10	0.96	0
3	AHD	25-A	402	4	13,13,13	1.77	4 (30%)	19,21,21	1.74	4 (21%)
2	MPD	14-A	401	-	7,7,7	0.56	0	9,10,10	0.63	0
2	MPD	15-A	403	-	7,7,7	0.42	0	9,10,10	0.49	0
3	AHD	40-B	706	4	13,13,13	1.71	4 (30%)	19,21,21	1.70	5 (26%)
2	MPD	44-A	401	-	7,7,7	0.38	0	9,10,10	1.53	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MPD	38-A	403	-	7,7,7	0.27	0	9,10,10	0.60	0
3	AHD	31-A	402	4	13,13,13	1.80	4 (30%)	19,21,21	1.26	1 (5%)
3	AHD	19-B	706	4	13,13,13	1.80	4 (30%)	19,21,21	1.61	2 (10%)
3	AHD	33-A	402	4	13,13,13	1.55	2 (15%)	19,21,21	1.38	2 (10%)
2	MPD	12-B	707	-	7,7,7	0.46	0	9,10,10	0.78	0
3	AHD	22-B	706	4	13,13,13	1.66	2 (15%)	19,21,21	0.81	0
2	MPD	20-A	403	-	7,7,7	0.31	0	9,10,10	0.65	0
2	MPD	15-B	701	-	7,7,7	0.38	0	9,10,10	1.19	1 (11%)
2	MPD	4-B	701	-	7,7,7	0.75	0	9,10,10	1.10	1 (11%)
3	AHD	2-B	706	4	13,13,13	1.54	3 (23%)	19,21,21	1.45	4 (21%)
3	AHD	47-B	706	4	13,13,13	1.53	3 (23%)	19,21,21	1.49	4 (21%)
2	MPD	30-B	707	-	7,7,7	0.35	0	9,10,10	1.02	0
2	MPD	22-B	707	-	7,7,7	0.46	0	9,10,10	0.46	0
3	AHD	33-B	706	4	13,13,13	1.69	3 (23%)	19,21,21	1.46	3 (15%)
2	MPD	8-B	707	-	7,7,7	0.50	0	9,10,10	1.07	0
2	MPD	2-B	701	-	7,7,7	0.65	0	9,10,10	1.10	1 (11%)
2	MPD	43-B	707	-	7,7,7	0.35	0	9,10,10	1.07	0
2	MPD	21-B	701	-	7,7,7	0.56	0	9,10,10	0.77	0
2	MPD	11-B	707	-	7,7,7	0.38	0	9,10,10	0.70	0
3	AHD	20-A	402	4	13,13,13	1.45	2 (15%)	19,21,21	1.76	3 (15%)
2	MPD	17-B	701	-	7,7,7	0.51	0	9,10,10	0.86	0
3	AHD	10-A	402	4	13,13,13	1.51	2 (15%)	19,21,21	1.66	2 (10%)
2	MPD	27-A	401	-	7,7,7	0.26	0	9,10,10	1.11	0
2	MPD	24-A	401	-	7,7,7	0.50	0	9,10,10	0.76	0
2	MPD	19-A	401	-	7,7,7	0.47	0	9,10,10	0.83	0
2	MPD	9-B	701	-	7,7,7	0.58	0	9,10,10	0.64	0
2	MPD	38-B	701	-	7,7,7	0.26	0	9,10,10	0.95	0
3	AHD	27-B	706	4	13,13,13	1.63	3 (23%)	19,21,21	1.24	2 (10%)
2	MPD	1-A	403	-	7,7,7	0.69	0	9,10,10	0.71	0
2	MPD	34-B	701	-	7,7,7	0.79	0	9,10,10	0.62	0
2	MPD	4-A	403	-	7,7,7	0.22	0	9,10,10	0.72	0
2	MPD	6-A	403	-	7,7,7	0.31	0	9,10,10	0.74	0
3	AHD	49-A	402	4	13,13,13	1.56	2 (15%)	19,21,21	1.27	2 (10%)
3	AHD	32-A	402	4	13,13,13	1.53	3 (23%)	19,21,21	2.27	7 (36%)
2	MPD	35-A	401	-	7,7,7	0.66	0	9,10,10	0.96	0
2	MPD	48-B	701	-	7,7,7	0.55	0	9,10,10	0.81	0
3	AHD	6-B	706	4	13,13,13	1.54	3 (23%)	19,21,21	1.25	2 (10%)
3	AHD	39-B	706	4	13,13,13	1.50	2 (15%)	19,21,21	1.39	2 (10%)
3	AHD	3-B	706	4	13,13,13	1.66	4 (30%)	19,21,21	1.42	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AHD	9-A	402	4	13,13,13	1.74	2 (15%)	19,21,21	1.82	4 (21%)
2	MPD	12-A	403	-	7,7,7	0.84	1 (14%)	9,10,10	0.79	0
2	MPD	21-A	403	-	7,7,7	0.43	0	9,10,10	0.77	0
2	MPD	36-A	403	-	7,7,7	0.33	0	9,10,10	0.87	0
3	AHD	24-A	402	4	13,13,13	1.60	3 (23%)	19,21,21	1.69	4 (21%)
2	MPD	9-A	403	-	7,7,7	0.43	0	9,10,10	0.81	0
3	AHD	42-A	402	4	13,13,13	1.52	4 (30%)	19,21,21	1.63	5 (26%)
3	AHD	14-B	706	4	13,13,13	1.61	2 (15%)	19,21,21	1.26	3 (15%)
2	MPD	17-A	401	-	7,7,7	0.60	0	9,10,10	0.80	0
2	MPD	12-B	701	-	7,7,7	0.68	0	9,10,10	1.08	0
2	MPD	44-B	707	-	7,7,7	0.47	0	9,10,10	0.67	0
2	MPD	21-B	707	-	7,7,7	0.53	0	9,10,10	0.70	0
2	MPD	30-B	701	-	7,7,7	0.61	0	9,10,10	1.61	1 (11%)
2	MPD	20-B	701	-	7,7,7	0.54	0	9,10,10	0.85	0
3	AHD	5-B	706	4	13,13,13	1.77	4 (30%)	19,21,21	1.47	3 (15%)
3	AHD	28-B	706	4	13,13,13	1.50	4 (30%)	19,21,21	1.24	2 (10%)
3	AHD	7-A	402	4	13,13,13	1.83	4 (30%)	19,21,21	1.34	4 (21%)
2	MPD	25-B	707	-	7,7,7	0.46	0	9,10,10	0.48	0
3	AHD	27-A	402	4	13,13,13	1.49	2 (15%)	19,21,21	1.56	2 (10%)
3	AHD	50-A	402	4	13,13,13	1.46	2 (15%)	19,21,21	1.56	3 (15%)
3	AHD	49-B	706	4	13,13,13	1.59	2 (15%)	19,21,21	1.39	3 (15%)
2	MPD	35-B	701	-	7,7,7	0.41	0	9,10,10	1.04	0
2	MPD	50-B	701	-	7,7,7	0.52	0	9,10,10	0.73	0
2	MPD	41-A	401	-	7,7,7	0.50	0	9,10,10	0.71	0
2	MPD	9-A	401	-	7,7,7	0.30	0	9,10,10	1.13	1 (11%)
2	MPD	50-B	707	-	7,7,7	0.47	0	9,10,10	0.86	0
2	MPD	22-A	401	-	7,7,7	0.34	0	9,10,10	1.03	1 (11%)
2	MPD	24-A	403	-	7,7,7	0.37	0	9,10,10	0.47	0
2	MPD	34-B	707	-	7,7,7	0.62	0	9,10,10	1.55	2 (22%)
2	MPD	45-A	401	-	7,7,7	0.51	0	9,10,10	0.82	0
3	AHD	28-A	402	4	13,13,13	1.53	1 (7%)	19,21,21	1.60	4 (21%)
3	AHD	45-A	402	4	13,13,13	1.64	1 (7%)	19,21,21	1.58	3 (15%)
3	AHD	10-B	706	4	13,13,13	1.45	2 (15%)	19,21,21	1.47	2 (10%)
3	AHD	41-B	706	4	13,13,13	1.46	2 (15%)	19,21,21	1.49	2 (10%)
3	AHD	18-A	402	4	13,13,13	1.37	1 (7%)	19,21,21	1.54	4 (21%)
2	MPD	25-B	701	-	7,7,7	0.38	0	9,10,10	0.58	0
3	AHD	45-B	706	4	13,13,13	1.45	1 (7%)	19,21,21	1.52	1 (5%)
2	MPD	16-B	707	-	7,7,7	0.50	0	9,10,10	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MPD	18-A	403	-	7,7,7	0.49	0	9,10,10	0.66	0
2	MPD	29-B	707	-	7,7,7	0.38	0	9,10,10	0.67	0
3	AHD	35-A	402	4	13,13,13	1.64	4 (30%)	19,21,21	1.80	5 (26%)
3	AHD	48-B	706	4	13,13,13	1.62	2 (15%)	19,21,21	1.73	2 (10%)
3	AHD	16-A	402	4	13,13,13	1.55	2 (15%)	19,21,21	1.65	4 (21%)
3	AHD	24-B	706	4	13,13,13	1.52	2 (15%)	19,21,21	1.73	3 (15%)
2	MPD	39-A	401	-	7,7,7	0.27	0	9,10,10	1.02	0
2	MPD	40-B	701	-	7,7,7	0.60	0	9,10,10	1.38	1 (11%)
2	MPD	24-B	701	-	7,7,7	0.71	0	9,10,10	0.72	0
2	MPD	47-A	401	-	7,7,7	0.33	0	9,10,10	0.75	0
3	AHD	38-B	706	4	13,13,13	1.47	3 (23%)	19,21,21	1.65	4 (21%)
2	MPD	43-A	401	-	7,7,7	0.42	0	9,10,10	0.65	0
2	MPD	1-B	701	-	7,7,7	0.58	0	9,10,10	0.88	0
2	MPD	37-A	403	-	7,7,7	0.41	0	9,10,10	0.70	0
2	MPD	32-A	403	-	7,7,7	0.62	0	9,10,10	1.25	1 (11%)
2	MPD	19-B	701	-	7,7,7	0.79	0	9,10,10	0.76	0
2	MPD	19-B	707	-	7,7,7	0.25	0	9,10,10	1.14	1 (11%)
3	AHD	4-A	402	4	13,13,13	1.52	2 (15%)	19,21,21	1.58	2 (10%)
2	MPD	20-B	707	-	7,7,7	0.43	0	9,10,10	1.11	1 (11%)
2	MPD	32-B	707	-	7,7,7	0.39	0	9,10,10	0.77	0
2	MPD	12-A	401	-	7,7,7	0.84	0	9,10,10	1.45	2 (22%)
3	AHD	42-B	706	4	13,13,13	1.49	3 (23%)	19,21,21	1.32	2 (10%)
2	MPD	33-B	701	-	7,7,7	0.70	0	9,10,10	0.89	0
3	AHD	25-B	706	4	13,13,13	1.49	3 (23%)	19,21,21	1.46	3 (15%)
2	MPD	36-B	707	-	7,7,7	0.34	0	9,10,10	1.00	0
2	MPD	49-B	707	-	7,7,7	0.40	0	9,10,10	1.02	0
3	AHD	13-A	402	4	13,13,13	1.82	2 (15%)	19,21,21	1.75	4 (21%)
3	AHD	2-A	402	4	13,13,13	1.57	1 (7%)	19,21,21	1.76	6 (31%)
2	MPD	14-B	701	-	7,7,7	0.53	0	9,10,10	1.89	2 (22%)
3	AHD	15-B	706	4	13,13,13	1.53	3 (23%)	19,21,21	1.56	3 (15%)
2	MPD	44-A	403	-	7,7,7	0.35	0	9,10,10	1.32	1 (11%)
2	MPD	29-A	403	-	7,7,7	0.17	0	9,10,10	0.67	0
2	MPD	24-B	707	-	7,7,7	0.51	0	9,10,10	0.76	0
3	AHD	46-A	402	4	13,13,13	1.72	2 (15%)	19,21,21	1.82	6 (31%)
3	AHD	12-A	402	4	13,13,13	1.62	1 (7%)	19,21,21	1.39	4 (21%)
2	MPD	26-B	707	-	7,7,7	0.47	0	9,10,10	1.10	1 (11%)
2	MPD	49-A	403	-	7,7,7	0.48	0	9,10,10	0.50	0
2	MPD	26-B	701	-	7,7,7	0.72	0	9,10,10	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AHD	8-A	402	4	13,13,13	1.46	3 (23%)	19,21,21	1.47	2 (10%)
2	MPD	40-B	707	-	7,7,7	0.36	0	9,10,10	0.78	0
2	MPD	3-B	701	-	7,7,7	0.52	0	9,10,10	1.18	1 (11%)
3	AHD	23-A	402	4	13,13,13	1.51	2 (15%)	19,21,21	1.23	4 (21%)
2	MPD	38-A	401	-	7,7,7	0.46	0	9,10,10	0.86	0
2	MPD	48-A	403	-	7,7,7	0.57	0	9,10,10	0.79	0
2	MPD	31-A	401	-	7,7,7	0.45	0	9,10,10	0.58	0
2	MPD	30-A	401	-	7,7,7	0.39	0	9,10,10	0.87	0
2	MPD	35-A	403	-	7,7,7	0.33	0	9,10,10	0.70	0
2	MPD	25-A	403	-	7,7,7	0.38	0	9,10,10	0.73	0
3	AHD	34-B	706	4	13,13,13	1.47	3 (23%)	19,21,21	1.88	3 (15%)
2	MPD	20-A	401	-	7,7,7	0.40	0	9,10,10	1.08	0
2	MPD	47-B	701	-	7,7,7	0.63	0	9,10,10	0.88	1 (11%)
3	AHD	3-A	402	4	13,13,13	1.82	3 (23%)	19,21,21	1.72	3 (15%)
3	AHD	8-B	706	4	13,13,13	1.56	2 (15%)	19,21,21	1.33	2 (10%)
2	MPD	8-A	403	-	7,7,7	0.26	0	9,10,10	0.64	0
2	MPD	35-B	707	-	7,7,7	0.32	0	9,10,10	0.96	0
3	AHD	26-A	402	4	13,13,13	1.47	1 (7%)	19,21,21	1.46	4 (21%)
2	MPD	46-A	401	-	7,7,7	0.31	0	9,10,10	0.79	0
2	MPD	40-A	401	-	7,7,7	0.51	0	9,10,10	0.60	0
2	MPD	29-B	701	-	7,7,7	0.45	0	9,10,10	0.87	0
3	AHD	34-A	402	4	13,13,13	1.66	4 (30%)	19,21,21	1.79	4 (21%)
3	AHD	47-A	402	4	13,13,13	1.56	2 (15%)	19,21,21	1.41	3 (15%)
3	AHD	36-B	706	4	13,13,13	1.56	3 (23%)	19,21,21	1.51	5 (26%)
2	MPD	8-A	401	-	7,7,7	0.53	0	9,10,10	0.53	0
2	MPD	18-B	701	-	7,7,7	0.57	0	9,10,10	0.95	0
3	AHD	37-A	402	4	13,13,13	1.66	3 (23%)	19,21,21	1.73	4 (21%)
3	AHD	12-B	706	4	13,13,13	1.58	3 (23%)	19,21,21	1.38	3 (15%)
2	MPD	11-A	401	-	7,7,7	0.40	0	9,10,10	0.78	0
3	AHD	40-A	402	4	13,13,13	1.59	2 (15%)	19,21,21	1.82	4 (21%)
3	AHD	9-B	706	4	13,13,13	1.44	2 (15%)	19,21,21	1.44	1 (5%)
3	AHD	30-B	706	4	13,13,13	1.46	3 (23%)	19,21,21	1.44	4 (21%)
2	MPD	15-B	707	-	7,7,7	0.41	0	9,10,10	0.69	0
2	MPD	49-A	401	-	7,7,7	0.64	0	9,10,10	1.30	1 (11%)
2	MPD	4-B	707	-	7,7,7	0.37	0	9,10,10	0.73	0
2	MPD	6-B	701	-	7,7,7	0.30	0	9,10,10	0.94	0
2	MPD	31-A	403	-	7,7,7	0.52	0	9,10,10	0.90	0
3	AHD	11-B	706	4	13,13,13	1.46	2 (15%)	19,21,21	1.71	3 (15%)
2	MPD	37-B	707	-	7,7,7	0.40	0	9,10,10	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AHD	20-B	706	4	13,13,13	1.48	4 (30%)	19,21,21	1.45	4 (21%)
3	AHD	32-B	706	4	13,13,13	1.63	3 (23%)	19,21,21	1.69	4 (21%)
3	AHD	44-B	706	4	13,13,13	1.58	3 (23%)	19,21,21	1.53	3 (15%)
2	MPD	28-A	401	-	7,7,7	0.34	0	9,10,10	0.56	0
3	AHD	30-A	402	4	13,13,13	1.51	1 (7%)	19,21,21	1.68	5 (26%)
3	AHD	50-B	706	4	13,13,13	1.58	3 (23%)	19,21,21	1.51	3 (15%)
2	MPD	5-A	403	-	7,7,7	0.58	0	9,10,10	0.65	0
2	MPD	16-A	403	-	7,7,7	0.42	0	9,10,10	0.58	0
3	AHD	11-A	402	4	13,13,13	1.52	1 (7%)	19,21,21	1.21	1 (5%)
2	MPD	22-A	403	-	7,7,7	0.39	0	9,10,10	0.96	0
2	MPD	33-B	707	-	7,7,7	0.39	0	9,10,10	0.62	0

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	MPD	27-B	707	-	-	1/5/5/5	-
2	MPD	16-A	401	-	-	4/5/5/5	-
2	MPD	5-A	401	-	-	5/5/5/5	-
3	AHD	46-B	706	4	-	4/23/23/23	-
2	MPD	43-A	403	-	-	1/5/5/5	-
3	AHD	18-B	706	4	-	4/23/23/23	-
2	MPD	42-B	707	-	-	1/5/5/5	-
2	MPD	5-B	701	-	-	4/5/5/5	-
3	AHD	48-A	402	4	-	4/23/23/23	-
2	MPD	39-A	403	-	-	3/5/5/5	-
2	MPD	3-A	403	-	-	1/5/5/5	-
2	MPD	34-A	401	-	-	4/5/5/5	-
2	MPD	23-B	701	-	-	3/5/5/5	-
2	MPD	31-B	707	-	-	0/5/5/5	-
2	MPD	26-A	403	-	-	0/5/5/5	-
2	MPD	18-A	401	-	-	4/5/5/5	-
2	MPD	36-A	401	-	-	5/5/5/5	-
2	MPD	40-A	403	-	-	2/5/5/5	-
2	MPD	3-A	401	-	-	5/5/5/5	-
3	AHD	31-B	706	4	-	4/23/23/23	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	9-B	707	-	-	3/5/5/5	-
2	MPD	27-A	403	-	-	0/5/5/5	-
2	MPD	38-B	707	-	-	3/5/5/5	-
3	AHD	7-B	706	4	-	0/23/23/23	-
2	MPD	21-A	401	-	-	0/5/5/5	-
2	MPD	19-A	403	-	-	1/5/5/5	-
3	AHD	41-A	402	4	-	4/23/23/23	-
2	MPD	28-A	403	-	-	4/5/5/5	-
3	AHD	13-B	706	4	-	3/23/23/23	-
2	MPD	28-B	707	-	-	0/5/5/5	-
2	MPD	33-A	403	-	-	0/5/5/5	-
3	AHD	6-A	402	4	-	4/23/23/23	-
3	AHD	26-B	706	4	-	3/23/23/23	-
2	MPD	8-B	701	-	-	2/5/5/5	-
3	AHD	21-A	402	4	-	0/23/23/23	-
2	MPD	42-A	401	-	-	5/5/5/5	-
2	MPD	10-A	401	-	-	5/5/5/5	-
2	MPD	23-A	401	-	-	5/5/5/5	-
2	MPD	7-A	403	-	-	0/5/5/5	-
2	MPD	17-A	403	-	-	1/5/5/5	-
2	MPD	7-B	701	-	-	1/5/5/5	-
2	MPD	7-B	707	-	-	0/5/5/5	-
2	MPD	41-B	707	-	-	0/5/5/5	-
3	AHD	38-A	402	4	-	3/23/23/23	-
3	AHD	17-A	402	4	-	4/23/23/23	-
2	MPD	36-B	701	-	-	2/5/5/5	-
3	AHD	19-A	402	4	-	2/23/23/23	-
3	AHD	4-B	706	4	-	4/23/23/23	-
3	AHD	1-B	706	4	-	4/23/23/23	-
2	MPD	29-A	401	-	-	2/5/5/5	-
2	MPD	2-B	707	-	-	0/5/5/5	-
3	AHD	22-A	402	4	-	3/23/23/23	-
3	AHD	37-B	706	4	-	4/23/23/23	-
3	AHD	21-B	706	4	-	1/23/23/23	-
2	MPD	1-A	401	-	-	3/5/5/5	-
2	MPD	15-A	401	-	-	3/5/5/5	-
2	MPD	39-B	701	-	-	3/5/5/5	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	10-A	403	-	-	2/5/5/5	-
2	MPD	17-B	707	-	-	3/5/5/5	-
3	AHD	15-A	402	4	-	1/23/23/23	-
2	MPD	6-A	401	-	-	4/5/5/5	-
2	MPD	50-A	401	-	-	4/5/5/5	-
2	MPD	45-A	403	-	-	2/5/5/5	-
3	AHD	29-B	706	4	-	4/23/23/23	-
2	MPD	44-B	701	-	-	2/5/5/5	-
2	MPD	18-B	707	-	-	1/5/5/5	-
3	AHD	14-A	402	4	-	3/23/23/23	-
3	AHD	23-B	706	4	-	4/23/23/23	-
2	MPD	11-B	701	-	-	3/5/5/5	-
2	MPD	47-B	707	-	-	2/5/5/5	-
2	MPD	48-A	401	-	-	5/5/5/5	-
3	AHD	36-A	402	4	-	3/23/23/23	-
2	MPD	22-B	701	-	-	2/5/5/5	-
2	MPD	49-B	701	-	-	0/5/5/5	-
2	MPD	28-B	701	-	-	1/5/5/5	-
2	MPD	6-B	707	-	-	1/5/5/5	-
2	MPD	30-A	403	-	-	0/5/5/5	-
3	AHD	39-A	402	4	-	3/23/23/23	-
2	MPD	50-A	403	-	-	0/5/5/5	-
2	MPD	25-A	401	-	-	2/5/5/5	-
3	AHD	44-A	402	4	-	1/23/23/23	-
2	MPD	5-B	707	-	-	3/5/5/5	-
2	MPD	26-A	401	-	-	5/5/5/5	-
2	MPD	2-A	403	-	-	0/5/5/5	-
2	MPD	11-A	403	-	-	1/5/5/5	-
2	MPD	13-A	403	-	-	0/5/5/5	-
2	MPD	47-A	403	-	-	0/5/5/5	-
2	MPD	16-B	701	-	-	2/5/5/5	-
2	MPD	1-B	707	-	-	2/5/5/5	-
2	MPD	46-A	403	-	-	1/5/5/5	-
2	MPD	2-A	401	-	-	5/5/5/5	-
2	MPD	10-B	701	-	-	4/5/5/5	-
2	MPD	7-A	401	-	-	4/5/5/5	-
2	MPD	41-B	701	-	-	4/5/5/5	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	10-B	707	-	-	0/5/5/5	-
2	MPD	23-B	707	-	-	0/5/5/5	-
2	MPD	33-A	401	-	-	4/5/5/5	-
2	MPD	37-A	401	-	-	2/5/5/5	-
2	MPD	45-B	701	-	-	2/5/5/5	-
2	MPD	39-B	707	-	-	0/5/5/5	-
3	AHD	1-A	402	4	-	5/23/23/23	-
2	MPD	3-B	707	-	-	0/5/5/5	-
3	AHD	43-A	402	4	-	0/23/23/23	-
3	AHD	17-B	706	4	-	3/23/23/23	-
2	MPD	23-A	403	-	-	0/5/5/5	-
2	MPD	43-B	701	-	-	3/5/5/5	-
3	AHD	35-B	706	4	-	1/23/23/23	-
2	MPD	14-B	707	-	-	0/5/5/5	-
2	MPD	34-A	403	-	-	2/5/5/5	-
3	AHD	43-B	706	4	-	4/23/23/23	-
2	MPD	13-A	401	-	-	3/5/5/5	-
2	MPD	42-B	701	-	-	1/5/5/5	-
2	MPD	32-A	401	-	-	5/5/5/5	-
2	MPD	42-A	403	-	-	1/5/5/5	-
2	MPD	46-B	707	-	-	1/5/5/5	-
2	MPD	37-B	701	-	-	4/5/5/5	-
3	AHD	29-A	402	4	-	0/23/23/23	-
2	MPD	13-B	707	-	-	3/5/5/5	-
2	MPD	13-B	701	-	-	3/5/5/5	-
3	AHD	16-B	706	4	-	2/23/23/23	-
2	MPD	45-B	707	-	-	0/5/5/5	-
2	MPD	48-B	707	-	-	0/5/5/5	-
2	MPD	31-B	701	-	-	2/5/5/5	-
2	MPD	41-A	403	-	-	0/5/5/5	-
2	MPD	46-B	701	-	-	3/5/5/5	-
2	MPD	27-B	701	-	-	4/5/5/5	-
3	AHD	5-A	402	4	-	6/23/23/23	-
2	MPD	14-A	403	-	-	0/5/5/5	-
2	MPD	32-B	701	-	-	2/5/5/5	-
2	MPD	4-A	401	-	-	5/5/5/5	-
3	AHD	25-A	402	4	-	5/23/23/23	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	14-A	401	-	-	5/5/5/5	-
2	MPD	15-A	403	-	-	0/5/5/5	-
3	AHD	40-B	706	4	-	0/23/23/23	-
2	MPD	44-A	401	-	-	5/5/5/5	-
2	MPD	38-A	403	-	-	0/5/5/5	-
3	AHD	31-A	402	4	-	4/23/23/23	-
3	AHD	19-B	706	4	-	1/23/23/23	-
3	AHD	33-A	402	4	-	1/23/23/23	-
2	MPD	12-B	707	-	-	1/5/5/5	-
3	AHD	22-B	706	4	-	4/23/23/23	-
2	MPD	20-A	403	-	-	1/5/5/5	-
2	MPD	15-B	701	-	-	5/5/5/5	-
2	MPD	4-B	701	-	-	3/5/5/5	-
3	AHD	2-B	706	4	-	1/23/23/23	-
3	AHD	47-B	706	4	-	4/23/23/23	-
2	MPD	30-B	707	-	-	0/5/5/5	-
2	MPD	22-B	707	-	-	1/5/5/5	-
3	AHD	33-B	706	4	-	4/23/23/23	-
2	MPD	8-B	707	-	-	0/5/5/5	-
2	MPD	2-B	701	-	-	3/5/5/5	-
2	MPD	43-B	707	-	-	0/5/5/5	-
2	MPD	21-B	701	-	-	4/5/5/5	-
2	MPD	11-B	707	-	-	0/5/5/5	-
3	AHD	20-A	402	4	-	4/23/23/23	-
2	MPD	17-B	701	-	-	1/5/5/5	-
3	AHD	10-A	402	4	-	2/23/23/23	-
2	MPD	27-A	401	-	-	5/5/5/5	-
2	MPD	24-A	401	-	-	4/5/5/5	-
2	MPD	19-A	401	-	-	4/5/5/5	-
2	MPD	9-B	701	-	-	2/5/5/5	-
2	MPD	38-B	701	-	-	2/5/5/5	-
3	AHD	27-B	706	4	-	4/23/23/23	-
2	MPD	1-A	403	-	-	3/5/5/5	-
2	MPD	34-B	701	-	-	2/5/5/5	-
2	MPD	4-A	403	-	-	3/5/5/5	-
2	MPD	6-A	403	-	-	0/5/5/5	-
3	AHD	49-A	402	4	-	4/23/23/23	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AHD	32-A	402	4	-	4/23/23/23	-
2	MPD	35-A	401	-	-	5/5/5/5	-
2	MPD	48-B	701	-	-	4/5/5/5	-
3	AHD	6-B	706	4	-	4/23/23/23	-
3	AHD	39-B	706	4	-	4/23/23/23	-
3	AHD	3-B	706	4	-	3/23/23/23	-
3	AHD	9-A	402	4	-	4/23/23/23	-
2	MPD	12-A	403	-	-	3/5/5/5	-
2	MPD	21-A	403	-	-	4/5/5/5	-
2	MPD	36-A	403	-	-	2/5/5/5	-
3	AHD	24-A	402	4	-	4/23/23/23	-
2	MPD	9-A	403	-	-	0/5/5/5	-
3	AHD	42-A	402	4	-	2/23/23/23	-
3	AHD	14-B	706	4	-	4/23/23/23	-
2	MPD	17-A	401	-	-	4/5/5/5	-
2	MPD	12-B	701	-	-	3/5/5/5	-
2	MPD	44-B	707	-	-	0/5/5/5	-
2	MPD	21-B	707	-	-	2/5/5/5	-
2	MPD	30-B	701	-	-	4/5/5/5	-
2	MPD	20-B	701	-	-	2/5/5/5	-
3	AHD	5-B	706	4	-	0/23/23/23	-
3	AHD	28-B	706	4	-	3/23/23/23	-
3	AHD	7-A	402	4	-	2/23/23/23	-
2	MPD	25-B	707	-	-	0/5/5/5	-
3	AHD	27-A	402	4	-	3/23/23/23	-
3	AHD	50-A	402	4	-	3/23/23/23	-
3	AHD	49-B	706	4	-	2/23/23/23	-
2	MPD	35-B	701	-	-	2/5/5/5	-
2	MPD	50-B	701	-	-	1/5/5/5	-
2	MPD	41-A	401	-	-	5/5/5/5	-
2	MPD	9-A	401	-	-	5/5/5/5	-
2	MPD	50-B	707	-	-	0/5/5/5	-
2	MPD	22-A	401	-	-	2/5/5/5	-
2	MPD	24-A	403	-	-	0/5/5/5	-
2	MPD	34-B	707	-	-	0/5/5/5	-
2	MPD	45-A	401	-	-	3/5/5/5	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AHD	28-A	402	4	-	3/23/23/23	-
3	AHD	45-A	402	4	-	3/23/23/23	-
3	AHD	10-B	706	4	-	1/23/23/23	-
3	AHD	41-B	706	4	-	5/23/23/23	-
3	AHD	18-A	402	4	-	3/23/23/23	-
2	MPD	25-B	701	-	-	1/5/5/5	-
3	AHD	45-B	706	4	-	3/23/23/23	-
2	MPD	16-B	707	-	-	0/5/5/5	-
2	MPD	18-A	403	-	-	0/5/5/5	-
2	MPD	29-B	707	-	-	0/5/5/5	-
3	AHD	35-A	402	4	-	9/23/23/23	-
3	AHD	48-B	706	4	-	1/23/23/23	-
3	AHD	16-A	402	4	-	2/23/23/23	-
3	AHD	24-B	706	4	-	4/23/23/23	-
2	MPD	39-A	401	-	-	2/5/5/5	-
2	MPD	40-B	701	-	-	3/5/5/5	-
2	MPD	24-B	701	-	-	4/5/5/5	-
2	MPD	47-A	401	-	-	2/5/5/5	-
3	AHD	38-B	706	4	-	4/23/23/23	-
2	MPD	43-A	401	-	-	4/5/5/5	-
2	MPD	1-B	701	-	-	3/5/5/5	-
2	MPD	37-A	403	-	-	2/5/5/5	-
2	MPD	32-A	403	-	-	3/5/5/5	-
2	MPD	19-B	701	-	-	1/5/5/5	-
2	MPD	19-B	707	-	-	1/5/5/5	-
3	AHD	4-A	402	4	-	3/23/23/23	-
2	MPD	20-B	707	-	-	0/5/5/5	-
2	MPD	32-B	707	-	-	1/5/5/5	-
2	MPD	12-A	401	-	-	4/5/5/5	-
3	AHD	42-B	706	4	-	0/23/23/23	-
2	MPD	33-B	701	-	-	4/5/5/5	-
3	AHD	25-B	706	4	-	1/23/23/23	-
2	MPD	36-B	707	-	-	0/5/5/5	-
2	MPD	49-B	707	-	-	0/5/5/5	-
3	AHD	13-A	402	4	-	4/23/23/23	-
3	AHD	2-A	402	4	-	4/23/23/23	-
2	MPD	14-B	701	-	-	4/5/5/5	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AHD	15-B	706	4	-	3/23/23/23	-
2	MPD	44-A	403	-	-	0/5/5/5	-
2	MPD	29-A	403	-	-	0/5/5/5	-
2	MPD	24-B	707	-	-	0/5/5/5	-
3	AHD	46-A	402	4	-	3/23/23/23	-
3	AHD	12-A	402	4	-	1/23/23/23	-
2	MPD	26-B	707	-	-	3/5/5/5	-
2	MPD	49-A	403	-	-	3/5/5/5	-
2	MPD	26-B	701	-	-	1/5/5/5	-
3	AHD	8-A	402	4	-	4/23/23/23	-
2	MPD	40-B	707	-	-	0/5/5/5	-
2	MPD	3-B	701	-	-	1/5/5/5	-
3	AHD	23-A	402	4	-	3/23/23/23	-
2	MPD	38-A	401	-	-	5/5/5/5	-
2	MPD	48-A	403	-	-	0/5/5/5	-
2	MPD	31-A	401	-	-	2/5/5/5	-
2	MPD	30-A	401	-	-	2/5/5/5	-
2	MPD	35-A	403	-	-	0/5/5/5	-
2	MPD	25-A	403	-	-	0/5/5/5	-
3	AHD	34-B	706	4	-	1/23/23/23	-
2	MPD	20-A	401	-	-	2/5/5/5	-
2	MPD	47-B	701	-	-	4/5/5/5	-
3	AHD	3-A	402	4	-	3/23/23/23	-
3	AHD	8-B	706	4	-	3/23/23/23	-
2	MPD	8-A	403	-	-	0/5/5/5	-
2	MPD	35-B	707	-	-	0/5/5/5	-
3	AHD	26-A	402	4	-	3/23/23/23	-
2	MPD	46-A	401	-	-	3/5/5/5	-
2	MPD	40-A	401	-	-	4/5/5/5	-
2	MPD	29-B	701	-	-	0/5/5/5	-
3	AHD	34-A	402	4	-	4/23/23/23	-
3	AHD	47-A	402	4	-	4/23/23/23	-
3	AHD	36-B	706	4	-	1/23/23/23	-
2	MPD	8-A	401	-	-	5/5/5/5	-
2	MPD	18-B	701	-	-	0/5/5/5	-
3	AHD	37-A	402	4	-	5/23/23/23	-
3	AHD	12-B	706	4	-	4/23/23/23	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	11-A	401	-	-	3/5/5/5	-
3	AHD	40-A	402	4	-	3/23/23/23	-
3	AHD	9-B	706	4	-	4/23/23/23	-
3	AHD	30-B	706	4	-	3/23/23/23	-
2	MPD	15-B	707	-	-	0/5/5/5	-
2	MPD	49-A	401	-	-	4/5/5/5	-
2	MPD	4-B	707	-	-	3/5/5/5	-
2	MPD	6-B	701	-	-	4/5/5/5	-
2	MPD	31-A	403	-	-	2/5/5/5	-
3	AHD	11-B	706	4	-	4/23/23/23	-
2	MPD	37-B	707	-	-	0/5/5/5	-
3	AHD	20-B	706	4	-	4/23/23/23	-
3	AHD	32-B	706	4	-	4/23/23/23	-
3	AHD	44-B	706	4	-	4/23/23/23	-
2	MPD	28-A	401	-	-	4/5/5/5	-
3	AHD	30-A	402	4	-	4/23/23/23	-
3	AHD	50-B	706	4	-	1/23/23/23	-
2	MPD	5-A	403	-	-	4/5/5/5	-
2	MPD	16-A	403	-	-	0/5/5/5	-
3	AHD	11-A	402	4	-	3/23/23/23	-
2	MPD	22-A	403	-	-	0/5/5/5	-
2	MPD	33-B	707	-	-	0/5/5/5	-

The worst 5 of 262 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	46-A	402	AHD	O13-C8	-4.92	1.38	1.44
3	12-A	402	AHD	O13-C8	-4.46	1.39	1.44
3	37-A	402	AHD	O13-C8	-4.23	1.39	1.44
3	9-A	402	AHD	O13-C8	-4.20	1.39	1.44
3	33-A	402	AHD	O13-C8	-4.19	1.39	1.44

The worst 5 of 397 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	32-A	402	AHD	C2-C7-C8	-6.42	104.86	116.02
2	7-B	707	MPD	CM-C2-C1	-6.07	97.02	110.63
3	34-B	706	AHD	C2-C7-C8	-6.02	105.57	116.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	21-B	706	AHD	C2-C7-C8	-5.83	105.89	116.02
3	29-B	706	AHD	C2-C7-C8	-5.62	106.26	116.02

There are no chirality outliers.

5 of 705 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1-A	401	MPD	C2-C3-C4-O4
2	1-A	401	MPD	C2-C3-C4-C5
2	2-A	401	MPD	C2-C3-C4-O4
2	2-A	401	MPD	C2-C3-C4-C5
2	3-A	401	MPD	C2-C3-C4-O4

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	295/318 (92%)	1.16	44 (14%) 5 6	0, 0, 1, 1	295 (100%)
1	1-B	296/318 (93%)	1.15	43 (14%) 6 6	0, 0, 1, 1	296 (100%)
1	2-A	0/318	-	-	-	-
1	2-B	0/318	-	-	-	-
1	3-A	0/318	-	-	-	-
1	3-B	0/318	-	-	-	-
1	4-A	0/318	-	-	-	-
1	4-B	0/318	-	-	-	-
1	5-A	0/318	-	-	-	-
1	5-B	0/318	-	-	-	-
1	6-A	0/318	-	-	-	-
1	6-B	0/318	-	-	-	-
1	7-A	0/318	-	-	-	-
1	7-B	0/318	-	-	-	-
1	8-A	0/318	-	-	-	-
1	8-B	0/318	-	-	-	-
1	9-A	0/318	-	-	-	-
1	9-B	0/318	-	-	-	-
1	10-A	0/318	-	-	-	-
1	10-B	0/318	-	-	-	-
1	11-A	0/318	-	-	-	-
1	11-B	0/318	-	-	-	-
1	12-A	0/318	-	-	-	-
1	12-B	0/318	-	-	-	-
1	13-A	0/318	-	-	-	-
1	13-B	0/318	-	-	-	-
1	14-A	0/318	-	-	-	-
1	14-B	0/318	-	-	-	-
1	15-A	0/318	-	-	-	-
1	15-B	0/318	-	-	-	-
1	16-A	0/318	-	-	-	-
1	16-B	0/318	-	-	-	-

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	38-A	0/318	-	-	-	-
1	38-B	0/318	-	-	-	-
1	39-A	0/318	-	-	-	-
1	39-B	0/318	-	-	-	-
1	40-A	0/318	-	-	-	-
1	40-B	0/318	-	-	-	-
1	41-A	0/318	-	-	-	-
1	41-B	0/318	-	-	-	-
1	42-A	0/318	-	-	-	-
1	42-B	0/318	-	-	-	-
1	43-A	0/318	-	-	-	-
1	43-B	0/318	-	-	-	-
1	44-A	0/318	-	-	-	-
1	44-B	0/318	-	-	-	-
1	45-A	0/318	-	-	-	-
1	45-B	0/318	-	-	-	-
1	46-A	0/318	-	-	-	-
1	46-B	0/318	-	-	-	-
1	47-A	0/318	-	-	-	-
1	47-B	0/318	-	-	-	-
1	48-A	0/318	-	-	-	-
1	48-B	0/318	-	-	-	-
1	49-A	0/318	-	-	-	-
1	49-B	0/318	-	-	-	-
1	50-A	0/318	-	-	-	-
1	50-B	0/318	-	-	-	-
All	All	591/31800 (1%)	1.16	87 (14%) 6 6	0, 0, 1, 1	591 (100%)

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	303	ASN	14.6
1	1-A	308	ALA	13.8
1	1-B	306	ILE	13.0
1	1-A	306	ILE	12.5
1	1-A	298	ALA	11.9

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

6.5 Other polymers ⓘ

There are no such residues in this entry.