



# wwPDB X-ray Structure Validation Summary Report

May 19, 2014 – 07:21 PM EDT

PDB ID : 4QA9  
Title : Ensemble refinement of an epoxide hydrolase from *Streptomyces carzinostaticus* subsp. *neocarzinostaticus*.  
Authors : Wang, F.; Tan, K.; Bigelow, L.; Clancy, S.; Babnigg, G.; Bingman, C.A.; Yennamalli, R.; Lohman, J.; Ma, M.; Shen, B.; Joachimiak, A.; Phillips Jr., G.N.; Midwest Center for Structural Genomics (MCSG); Enzyme Discovery for Natural Product Biosynthesis (NatPro)  
Deposited on : 2014-05-02  
Resolution : 1.56 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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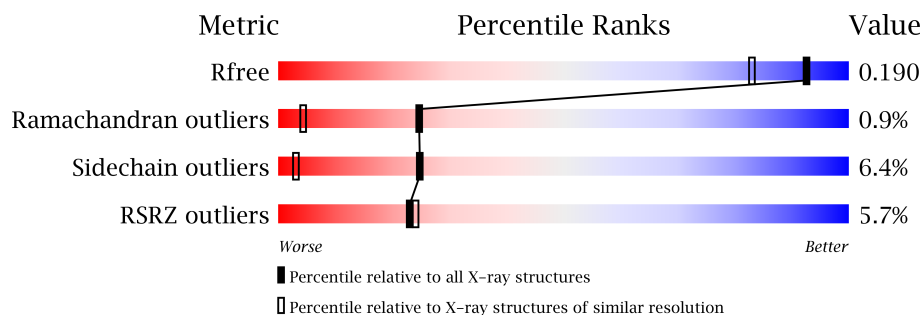
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable22978  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22978

# 1 Overall quality at a glance

The reported resolution of this entry is 1.56 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))
$R_{free}$	66092	1117 (1.58-1.54)
Ramachandran outliers	78287	1212 (1.58-1.54)
Sidechain outliers	78261	1210 (1.58-1.54)
RSRZ outliers	66119	1117 (1.58-1.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	1-A	388	
1	10-A	388	
1	11-A	388	
1	12-A	388	
1	13-A	388	
1	14-A	388	
1	15-A	388	
1	16-A	388	
1	17-A	388	
1	18-A	388	
1	19-A	388	
1	2-A	388	
1	20-A	388	
1	3-A	388	
1	4-A	388	
1	5-A	388	

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Mol	Chain	Length	Quality of chain
1	6-A	388	
1	7-A	388	
1	8-A	388	
1	9-A	388	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	10-A	403	-	X
2	SO4	11-A	403	-	X
2	SO4	12-A	403	-	X
2	SO4	13-A	403	-	X
2	SO4	14-A	403	-	X
2	SO4	15-A	403	-	X
2	SO4	16-A	403	-	X
2	SO4	17-A	403	-	X
2	SO4	18-A	403	-	X
2	SO4	19-A	403	-	X
2	SO4	20-A	403	-	X
3	EDO	10-A	406	-	X
3	EDO	10-A	407	-	X
3	EDO	10-A	408	-	X
3	EDO	10-A	410	-	X
3	EDO	10-A	411	-	X
3	EDO	10-A	412	-	X
3	EDO	10-A	414	-	X
3	EDO	10-A	415	-	X
3	EDO	10-A	416	-	X
3	EDO	11-A	406	-	X
3	EDO	11-A	407	-	X
3	EDO	11-A	408	-	X
3	EDO	11-A	410	-	X
3	EDO	11-A	411	-	X
3	EDO	11-A	412	-	X
3	EDO	11-A	414	-	X
3	EDO	11-A	415	-	X
3	EDO	11-A	416	-	X
3	EDO	12-A	406	-	X
3	EDO	12-A	407	-	X
3	EDO	12-A	408	-	X
3	EDO	12-A	410	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	EDO	12-A	411	-	X
3	EDO	12-A	412	-	X
3	EDO	12-A	414	-	X
3	EDO	12-A	415	-	X
3	EDO	12-A	416	-	X
3	EDO	13-A	406	-	X
3	EDO	13-A	407	-	X
3	EDO	13-A	408	-	X
3	EDO	13-A	410	-	X
3	EDO	13-A	411	-	X
3	EDO	13-A	412	-	X
3	EDO	13-A	414	-	X
3	EDO	13-A	415	-	X
3	EDO	13-A	416	-	X
3	EDO	14-A	406	-	X
3	EDO	14-A	407	-	X
3	EDO	14-A	408	-	X
3	EDO	14-A	410	-	X
3	EDO	14-A	411	-	X
3	EDO	14-A	412	-	X
3	EDO	14-A	414	-	X
3	EDO	14-A	415	-	X
3	EDO	14-A	416	-	X
3	EDO	15-A	406	-	X
3	EDO	15-A	407	-	X
3	EDO	15-A	408	-	X
3	EDO	15-A	410	-	X
3	EDO	15-A	411	-	X
3	EDO	15-A	412	-	X
3	EDO	15-A	414	-	X
3	EDO	15-A	415	-	X
3	EDO	15-A	416	-	X
3	EDO	16-A	406	-	X
3	EDO	16-A	407	-	X
3	EDO	16-A	408	-	X
3	EDO	16-A	410	-	X
3	EDO	16-A	411	-	X
3	EDO	16-A	412	-	X
3	EDO	16-A	414	-	X
3	EDO	16-A	415	-	X
3	EDO	16-A	416	-	X
3	EDO	17-A	406	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	EDO	17-A	407	-	X
3	EDO	17-A	408	-	X
3	EDO	17-A	410	-	X
3	EDO	17-A	411	-	X
3	EDO	17-A	412	-	X
3	EDO	17-A	414	-	X
3	EDO	17-A	415	-	X
3	EDO	17-A	416	-	X
3	EDO	18-A	406	-	X
3	EDO	18-A	407	-	X
3	EDO	18-A	408	-	X
3	EDO	18-A	410	-	X
3	EDO	18-A	411	-	X
3	EDO	18-A	412	-	X
3	EDO	18-A	414	-	X
3	EDO	18-A	415	-	X
3	EDO	18-A	416	-	X
3	EDO	19-A	406	-	X
3	EDO	19-A	407	-	X
3	EDO	19-A	408	-	X
3	EDO	19-A	410	-	X
3	EDO	19-A	411	-	X
3	EDO	19-A	412	-	X
3	EDO	19-A	414	-	X
3	EDO	19-A	415	-	X
3	EDO	19-A	416	-	X
3	EDO	20-A	406	-	X
3	EDO	20-A	407	-	X
3	EDO	20-A	408	-	X
3	EDO	20-A	410	-	X
3	EDO	20-A	411	-	X
3	EDO	20-A	412	-	X
3	EDO	20-A	414	-	X
3	EDO	20-A	415	-	X
3	EDO	20-A	416	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 129042 atoms, of which 61340 are hydrogens and 0 are deuterium.

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 Epoxide hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	388	Total 6046	C 1953	H 2995	N 524	O 563	S 11	0	0	0
1	2-A	388	Total 6046	C 1953	H 2995	N 524	O 563	S 11	0	0	0
1	3-A	388	Total 6046	C 1953	H 2995	N 524	O 563	S 11	0	0	0
1	4-A	388	Total 6046	C 1953	H 2995	N 524	O 563	S 11	0	0	0
1	5-A	388	Total 6046	C 1953	H 2995	N 524	O 563	S 11	0	0	0
1	6-A	388	Total 6046	C 1953	H 2995	N 524	O 563	S 11	0	0	0
1	7-A	388	Total 6046	C 1953	H 2995	N 524	O 563	S 11	0	0	0
1	8-A	388	Total 6046	C 1953	H 2995	N 524	O 563	S 11	0	0	0
1	9-A	388	Total 6046	C 1953	H 2995	N 524	O 563	S 11	0	0	0
1	10-A	388	Total 6046	C 1953	H 2995	N 524	O 563	S 11	0	0	0
1	11-A	388	Total 6046	C 1953	H 2995	N 524	O 563	S 11	0	0	0
1	12-A	388	Total 6046	C 1953	H 2995	N 524	O 563	S 11	0	0	0
1	13-A	388	Total 6046	C 1953	H 2995	N 524	O 563	S 11	0	0	0
1	14-A	388	Total 6046	C 1953	H 2995	N 524	O 563	S 11	0	0	0
1	15-A	388	Total 6046	C 1953	H 2995	N 524	O 563	S 11	0	0	0
1	16-A	388	Total 6046	C 1953	H 2995	N 524	O 563	S 11	0	0	0

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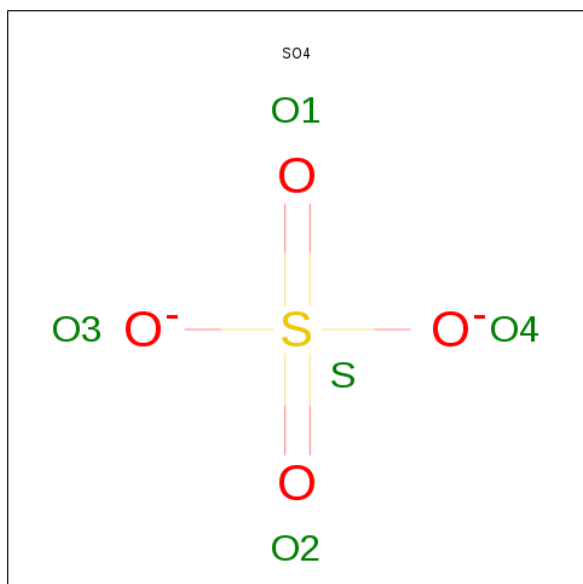
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	388	Total 6046	C 1953	H 2995	N 524	O 563	S 11	0	0	0
1	18-A	388	Total 6046	C 1953	H 2995	N 524	O 563	S 11	0	0	0
1	19-A	388	Total 6046	C 1953	H 2995	N 524	O 563	S 11	0	0	0
1	20-A	388	Total 6046	C 1953	H 2995	N 524	O 563	S 11	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q84HB8
A	-1	ASN	-	EXPRESSION TAG	UNP Q84HB8
A	0	ALA	-	EXPRESSION TAG	UNP Q84HB8

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	1-A	1	Total	O	S	0	0
			5	4	1		
2	2-A	1	Total	O	S	0	0
			5	4	1		
2	3-A	1	Total	O	S	0	0
			5	4	1		
2	4-A	1	Total	O	S	0	0
			5	4	1		

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

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

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

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-A	271	Total	O	0	0
			271	271		
4	2-A	270	Total	O	0	0
			270	270		
4	3-A	288	Total	O	0	0
			288	288		

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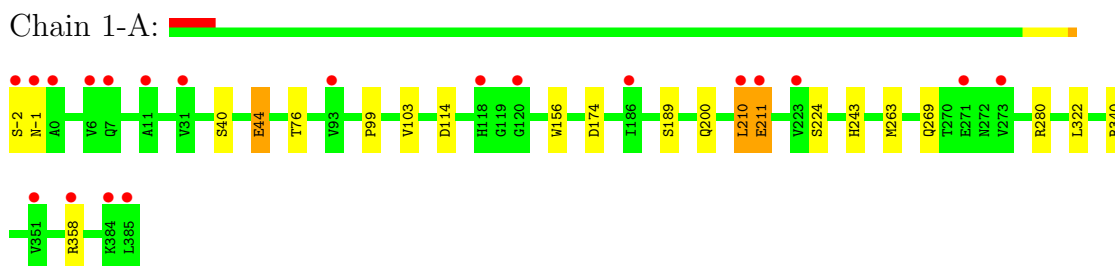
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	4-A	262	Total 262	O 262	0	0
4	5-A	272	Total 272	O 272	0	0
4	6-A	268	Total 268	O 268	0	0
4	7-A	272	Total 272	O 272	0	0
4	8-A	280	Total 280	O 280	0	0
4	9-A	252	Total 252	O 252	0	0
4	10-A	286	Total 286	O 286	0	0
4	11-A	258	Total 258	O 258	0	0
4	12-A	251	Total 251	O 251	0	0
4	13-A	264	Total 264	O 264	0	0
4	14-A	260	Total 260	O 260	0	0
4	15-A	284	Total 284	O 284	0	0
4	16-A	263	Total 263	O 263	0	0
4	17-A	243	Total 243	O 243	0	0
4	18-A	262	Total 262	O 262	0	0
4	19-A	270	Total 270	O 270	0	0
4	20-A	246	Total 246	O 246	0	0



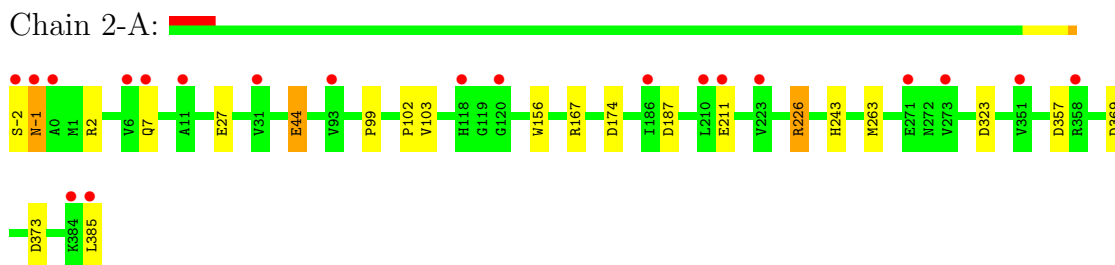
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

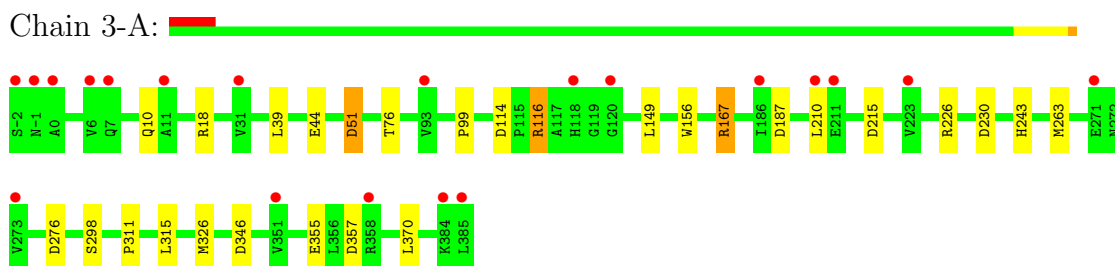
- Molecule 1: Epoxide hydrolase



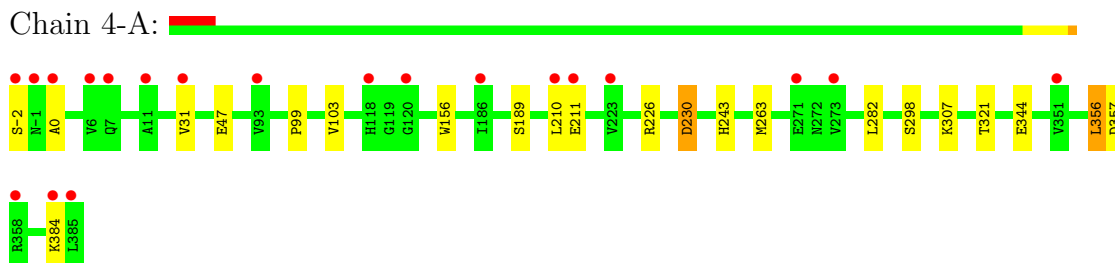
- Molecule 1: Epoxide hydrolase



- Molecule 1: Epoxide hydrolase

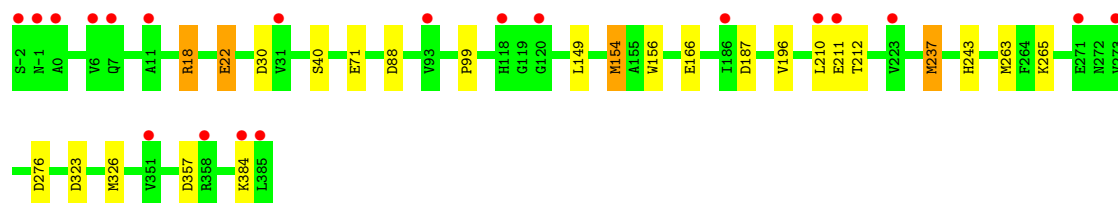


- Molecule 1: Epoxide hydrolase



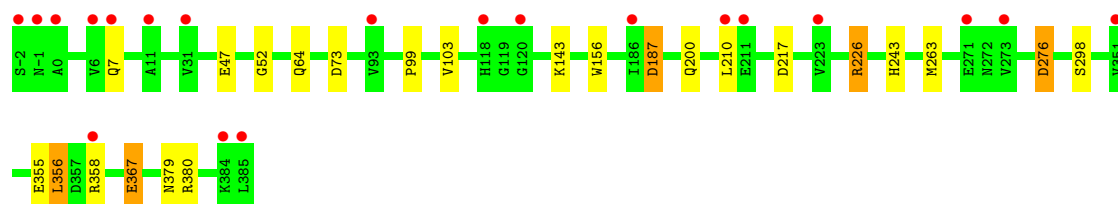
- Molecule 1: Epoxide hydrolase

Chain 5-A:



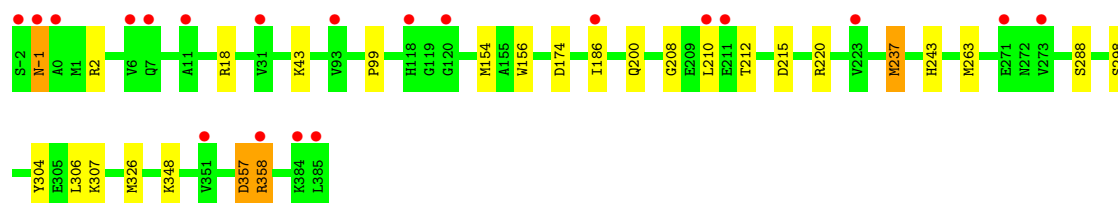
- Molecule 1: Epoxide hydrolase

Chain 6-A:



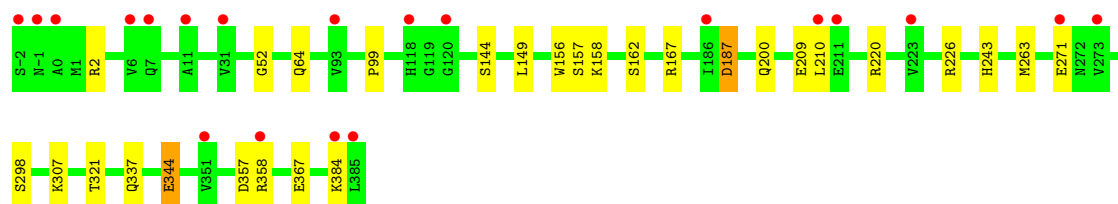
- Molecule 1: Epoxide hydrolase

Chain 7-A:



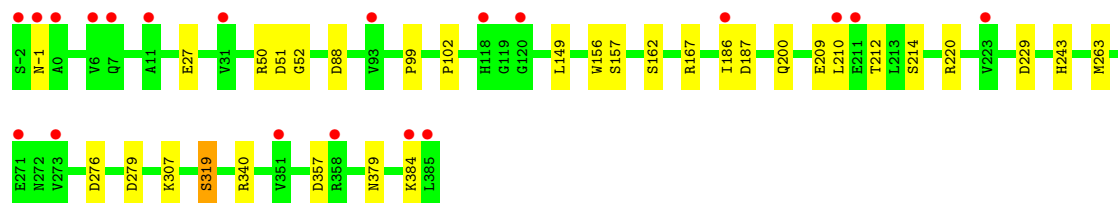
- Molecule 1: Epoxide hydrolase

Chain 8-A:



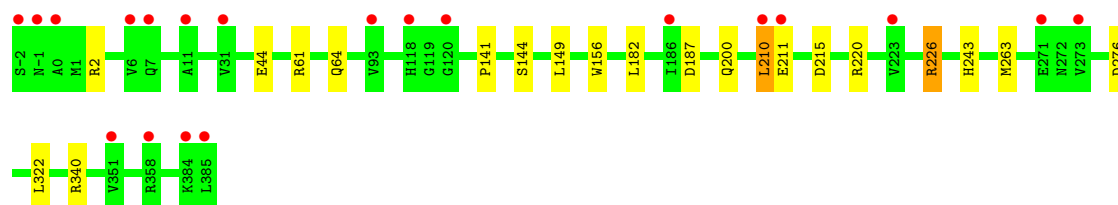
- Molecule 1: Epoxide hydrolase

Chain 9-A:



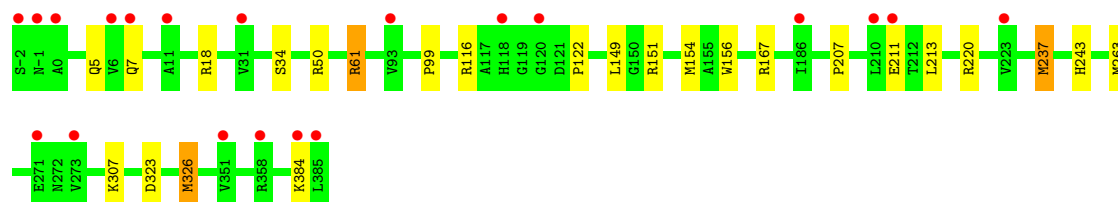
- Molecule 1: Epoxide hydrolase

Chain 10-A:



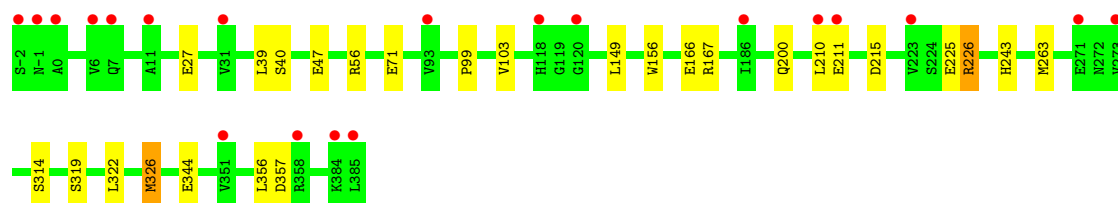
- Molecule 1: Epoxide hydrolase

Chain 11-A:



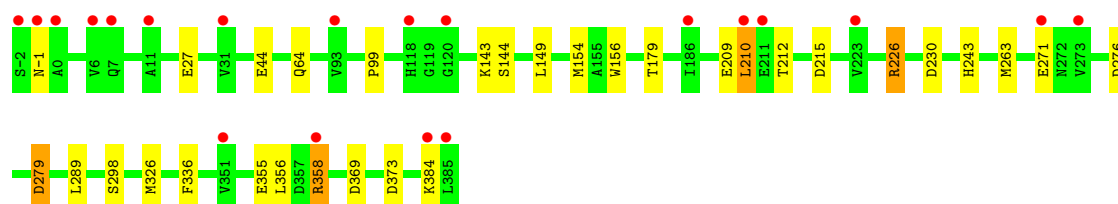
- Molecule 1: Epoxide hydrolase

Chain 12-A:



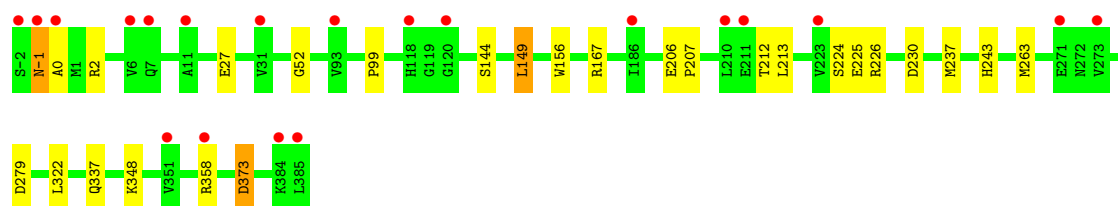
- Molecule 1: Epoxide hydrolase

Chain 13-A:



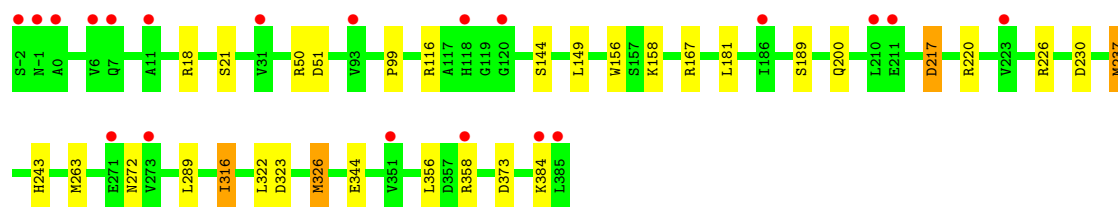
- Molecule 1: Epoxide hydrolase

Chain 14-A:



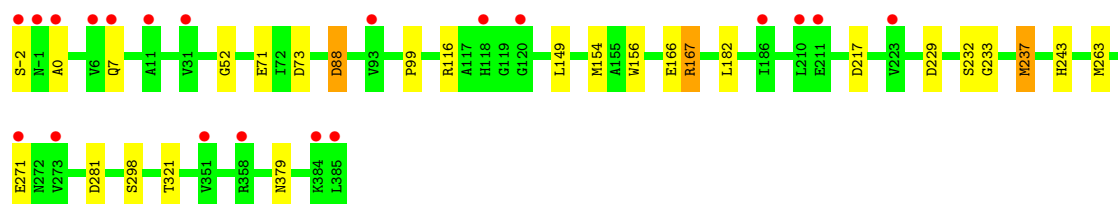
- Molecule 1: Epoxide hydrolase

Chain 15-A:



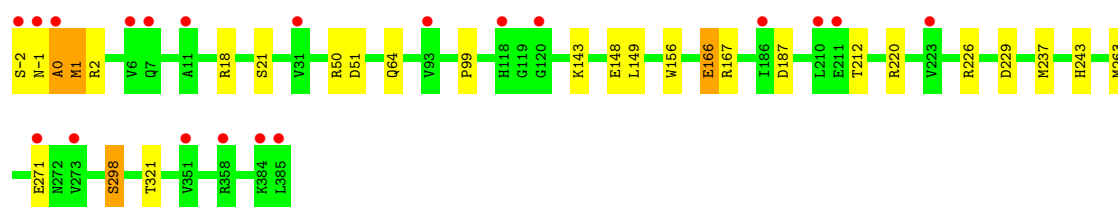
- Molecule 1: Epoxide hydrolase

Chain 16-A:



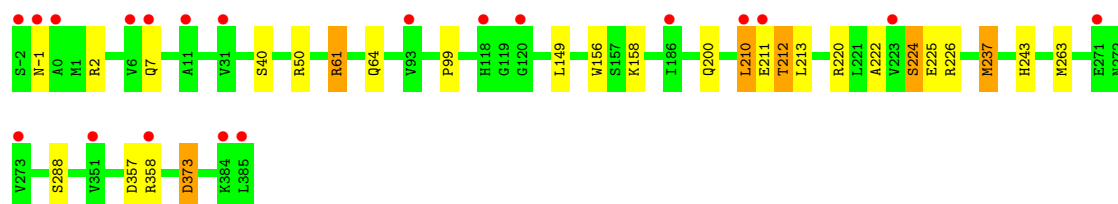
- Molecule 1: Epoxide hydrolase

Chain 17-A:



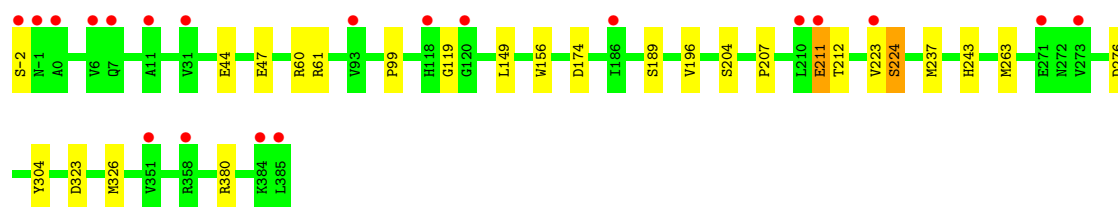
- Molecule 1: Epoxide hydrolase

Chain 18-A:



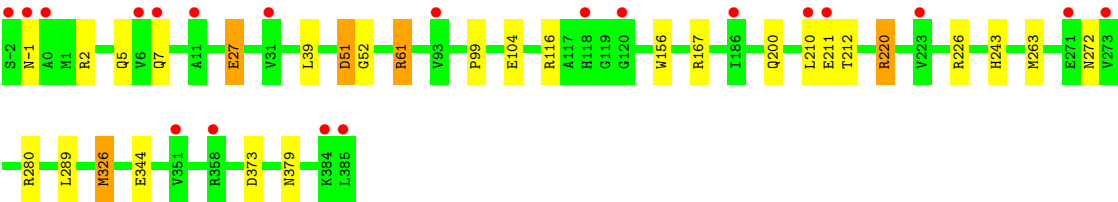
- Molecule 1: Epoxide hydrolase

Chain 19-A:



- Molecule 1: Epoxide hydrolase

Chain 20-A:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.33Å 75.33Å 165.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.82 – 1.56 27.82 – 1.56	Depositor EDS
% Data completeness (in resolution range)	96.4 (27.82-1.56) 96.4 (27.82-1.56)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 1.56Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble.refinement:dev_1420)	Depositor
R, $R_{free}$	0.122 , 0.151 0.168 , 0.190	Depositor DCC
$R_{free}$ test set	3343 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.3	Xtriage
Anisotropy	0.718	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.45 , 322.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 65942 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	129042	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, EDO

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	0.65	1/3139 (0.0%)	0.83	2/4275 (0.0%)
1	2-A	0.69	5/3139 (0.2%)	0.82	2/4275 (0.0%)
1	3-A	0.68	1/3139 (0.0%)	0.87	5/4275 (0.1%)
1	4-A	0.65	0/3139	0.83	2/4275 (0.0%)
1	5-A	0.73	3/3139 (0.1%)	0.86	5/4275 (0.1%)
1	6-A	0.67	2/3139 (0.1%)	0.85	6/4275 (0.1%)
1	7-A	0.67	1/3139 (0.0%)	0.88	7/4275 (0.2%)
1	8-A	0.73	3/3139 (0.1%)	0.82	0/4275
1	9-A	0.65	2/3139 (0.1%)	0.88	7/4275 (0.2%)
1	10-A	0.67	0/3139	0.89	5/4275 (0.1%)
1	11-A	0.67	2/3139 (0.1%)	0.85	7/4275 (0.2%)
1	12-A	0.66	2/3139 (0.1%)	0.83	2/4275 (0.0%)
1	13-A	0.71	1/3139 (0.0%)	0.89	9/4275 (0.2%)
1	14-A	0.67	2/3139 (0.1%)	0.86	6/4275 (0.1%)
1	15-A	0.72	3/3139 (0.1%)	0.88	8/4275 (0.2%)
1	16-A	0.66	1/3139 (0.0%)	0.90	8/4275 (0.2%)
1	17-A	0.72	3/3139 (0.1%)	0.86	4/4275 (0.1%)
1	18-A	0.71	3/3139 (0.1%)	0.90	12/4275 (0.3%)
1	19-A	0.65	0/3139	0.86	5/4275 (0.1%)
1	20-A	0.70	4/3139 (0.1%)	0.88	12/4275 (0.3%)
All	All	0.68	39/62780 (0.1%)	0.86	114/85500 (0.1%)

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	2-A	0	1
1	4-A	0	1
1	7-A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	12-A	0	1
1	16-A	0	1
1	17-A	0	1
1	18-A	0	1
1	19-A	0	1
All	All	0	8

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-A	367	GLU	CB-CG	-11.92	1.29	1.52
1	5-A	237	MET	CB-CG	10.58	1.85	1.51
1	16-A	237	MET	CB-CG	10.35	1.84	1.51
1	15-A	344	GLU	CB-CG	10.35	1.71	1.52
1	20-A	344	GLU	CB-CG	8.82	1.69	1.52

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16-A	237	MET	CG-SD-CE	-14.25	77.41	100.20
1	20-A	61	ARG	NE-CZ-NH1	12.29	126.44	120.30
1	10-A	61	ARG	NE-CZ-NH1	12.20	126.40	120.30
1	7-A	237	MET	CG-SD-CE	10.75	117.40	100.20
1	14-A	237	MET	CG-SD-CE	10.57	117.11	100.20

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	12-A	356	LEU	Peptide
1	16-A	232	SER	Peptide
1	2-A	-1	ASN	Peptide
1	4-A	356	LEU	Peptide
1	7-A	-1	ASN	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the



chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	3051	2995	0	0	1
1	2-A	3051	2995	0	0	0
1	3-A	3051	2995	0	0	1
1	4-A	3051	2995	0	0	0
1	5-A	3051	2995	0	0	0
1	6-A	3051	2995	0	0	1
1	7-A	3051	2995	0	0	1
1	8-A	3051	2995	0	0	0
1	9-A	3051	2995	0	0	0
1	10-A	3051	2995	0	0	0
1	11-A	3051	2995	0	0	1
1	12-A	3051	2995	0	0	0
1	13-A	3051	2995	0	0	0
1	14-A	3051	2995	0	0	1
1	15-A	3051	2995	0	0	0
1	16-A	3051	2995	0	0	0
1	17-A	3051	2995	0	0	0
1	18-A	3051	2995	0	0	0
1	19-A	3051	2995	0	0	2
1	20-A	3051	2995	0	0	0
2	1-A	20	0	0	0	0
2	2-A	20	0	0	0	0
2	3-A	20	0	0	0	0
2	4-A	20	0	0	0	0
2	5-A	20	0	0	0	0
2	6-A	20	0	0	0	0
2	7-A	20	0	0	0	0
2	8-A	20	0	0	0	0
2	9-A	20	0	0	0	0
2	10-A	20	0	0	0	0
2	11-A	20	0	0	0	0
2	12-A	20	0	0	0	0
2	13-A	20	0	0	0	0
2	14-A	20	0	0	0	0
2	15-A	20	0	0	0	0
2	16-A	20	0	0	0	0
2	17-A	20	0	0	0	0
2	18-A	20	0	0	0	0
2	19-A	20	0	0	0	0
2	20-A	20	0	0	0	0
3	1-A	48	72	0	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2-A	48	72	0	0	0
3	3-A	48	72	0	0	1
3	4-A	48	72	0	0	0
3	5-A	48	72	0	0	0
3	6-A	48	72	0	0	0
3	7-A	48	72	0	0	0
3	8-A	48	72	0	0	0
3	9-A	48	72	0	0	0
3	10-A	48	72	0	0	0
3	11-A	48	72	0	0	0
3	12-A	48	72	0	0	0
3	13-A	48	72	0	0	0
3	14-A	48	72	0	0	0
3	15-A	48	72	0	0	0
3	16-A	48	72	0	0	0
3	17-A	48	72	0	0	0
3	18-A	48	72	0	0	0
3	19-A	48	72	0	0	1
3	20-A	48	72	0	0	0
4	1-A	271	0	0	0	0
4	2-A	270	0	0	0	0
4	3-A	288	0	0	0	0
4	4-A	262	0	0	0	0
4	5-A	272	0	0	0	0
4	6-A	268	0	0	0	1
4	7-A	272	0	0	0	1
4	8-A	280	0	0	0	0
4	9-A	252	0	0	0	0
4	10-A	286	0	0	0	0
4	11-A	258	0	0	0	1
4	12-A	251	0	0	0	0
4	13-A	264	0	0	0	0
4	14-A	260	0	0	0	1
4	15-A	284	0	0	0	0
4	16-A	263	0	0	0	0
4	17-A	243	0	0	0	0
4	18-A	262	0	0	0	0
4	19-A	270	0	0	0	1
4	20-A	246	0	0	0	0
All	All	67702	61340	0	0	8

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

The worst 5 of 8 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:114:ASP:OD2	3:A:409:EDO:O1[6_544]	1.83	0.37
1:A:34:SER:OG	4:A:563:HOH:O[7_555]	1.88	0.32
1:A:304:TYR:OH	4:A:551:HOH:O[7_555]	1.93	0.27
1:A:298:SER:OG	4:A:508:HOH:O[7_555]	1.97	0.23
1:A:204:SER:O	3:A:416:EDO:O1[6_444]	2.01	0.19

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	386/388 (100%)	367 (95%)	15 (4%)	4 (1%)	22	4
1	2-A	386/388 (100%)	375 (97%)	10 (3%)	1 (0%)	50	21
1	3-A	386/388 (100%)	372 (96%)	12 (3%)	2 (0%)	38	11
1	4-A	386/388 (100%)	367 (95%)	15 (4%)	4 (1%)	22	4
1	5-A	386/388 (100%)	369 (96%)	16 (4%)	1 (0%)	50	21
1	6-A	386/388 (100%)	370 (96%)	13 (3%)	3 (1%)	27	5
1	7-A	386/388 (100%)	365 (95%)	17 (4%)	4 (1%)	22	4
1	8-A	386/388 (100%)	371 (96%)	10 (3%)	5 (1%)	18	2
1	9-A	386/388 (100%)	370 (96%)	12 (3%)	4 (1%)	22	4
1	10-A	386/388 (100%)	369 (96%)	17 (4%)	0	100	100
1	11-A	386/388 (100%)	362 (94%)	20 (5%)	4 (1%)	22	4
1	12-A	386/388 (100%)	366 (95%)	18 (5%)	2 (0%)	38	11
1	13-A	386/388 (100%)	368 (95%)	15 (4%)	3 (1%)	27	5
1	14-A	386/388 (100%)	368 (95%)	12 (3%)	6 (2%)	14	1
1	15-A	386/388 (100%)	370 (96%)	14 (4%)	2 (0%)	38	11
1	16-A	386/388 (100%)	366 (95%)	14 (4%)	6 (2%)	14	1
1	17-A	386/388 (100%)	364 (94%)	17 (4%)	5 (1%)	18	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	18-A	386/388 (100%)	368 (95%)	13 (3%)	5 (1%)	18	2
1	19-A	386/388 (100%)	370 (96%)	12 (3%)	4 (1%)	22	4
1	20-A	386/388 (100%)	369 (96%)	14 (4%)	3 (1%)	27	5
All	All	7720/7760 (100%)	7366 (95%)	286 (4%)	68 (1%)	25	4

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	210	LEU
1	7-A	358	ARG
1	11-A	211	GLU
1	11-A	213	LEU
1	13-A	210	LEU

### 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	322/322 (100%)	305 (95%)	17 (5%)	32	5
1	2-A	322/322 (100%)	304 (94%)	18 (6%)	30	5
1	3-A	322/322 (100%)	298 (92%)	24 (8%)	19	2
1	4-A	322/322 (100%)	305 (95%)	17 (5%)	32	5
1	5-A	322/322 (100%)	302 (94%)	20 (6%)	26	3
1	6-A	322/322 (100%)	303 (94%)	19 (6%)	28	4
1	7-A	322/322 (100%)	303 (94%)	19 (6%)	28	4
1	8-A	322/322 (100%)	298 (92%)	24 (8%)	19	2
1	9-A	322/322 (100%)	298 (92%)	24 (8%)	19	2
1	10-A	322/322 (100%)	302 (94%)	20 (6%)	26	3
1	11-A	322/322 (100%)	304 (94%)	18 (6%)	30	5
1	12-A	322/322 (100%)	300 (93%)	22 (7%)	22	2
1	13-A	322/322 (100%)	294 (91%)	28 (9%)	15	1
1	14-A	322/322 (100%)	305 (95%)	17 (5%)	32	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	15-A	322/322 (100%)	297 (92%)	25 (8%)	18 1
1	16-A	322/322 (100%)	304 (94%)	18 (6%)	30 5
1	17-A	322/322 (100%)	301 (94%)	21 (6%)	24 3
1	18-A	322/322 (100%)	303 (94%)	19 (6%)	28 4
1	19-A	322/322 (100%)	305 (95%)	17 (5%)	32 5
1	20-A	322/322 (100%)	300 (93%)	22 (7%)	22 2
All	All	6440/6440 (100%)	6031 (94%)	409 (6%)	25 3

5 of 409 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	10-A	141	PRO
1	12-A	167	ARG
1	19-A	196	VAL
1	10-A	187	ASP
1	11-A	122	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 148 such sidechains are listed below:

Mol	Chain	Res	Type
1	9-A	361	HIS
1	11-A	202	ASN
1	18-A	379	ASN
1	10-A	5	GLN
1	10-A	286	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

320 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	1-A	401	-	4,4,4	0.48	0	6,6,6	1.18	1 (16%)
2	SO4	1-A	402	-	4,4,4	0.55	0	6,6,6	1.36	1 (16%)
2	SO4	1-A	403	-	4,4,4	0.21	0	6,6,6	0.48	0
2	SO4	1-A	404	-	4,4,4	0.65	0	6,6,6	0.47	0
3	EDO	1-A	405	-	3,3,3	0.43	0	2,2,2	0.86	0
3	EDO	1-A	406	-	3,3,3	0.33	0	2,2,2	0.81	0
3	EDO	1-A	407	-	3,3,3	0.55	0	2,2,2	0.89	0
3	EDO	1-A	408	-	3,3,3	0.25	0	2,2,2	0.91	0
3	EDO	1-A	409	-	3,3,3	0.74	0	2,2,2	0.29	0
3	EDO	1-A	410	-	3,3,3	0.89	0	2,2,2	0.45	0
3	EDO	1-A	411	-	3,3,3	0.47	0	2,2,2	0.96	0
3	EDO	1-A	412	-	3,3,3	0.50	0	2,2,2	1.38	0
3	EDO	1-A	413	-	3,3,3	0.76	0	2,2,2	0.30	0
3	EDO	1-A	414	-	3,3,3	0.70	0	2,2,2	1.20	0
3	EDO	1-A	415	-	3,3,3	0.83	0	2,2,2	0.89	0
3	EDO	1-A	416	-	3,3,3	0.64	0	2,2,2	0.07	0
2	SO4	10-A	401	-	4,4,4	0.27	0	6,6,6	1.03	0
2	SO4	10-A	402	-	4,4,4	0.84	0	6,6,6	0.68	0
2	SO4	10-A	403	-	4,4,4	0.38	0	6,6,6	0.68	0
2	SO4	10-A	404	-	4,4,4	0.22	0	6,6,6	0.52	0
3	EDO	10-A	405	-	3,3,3	0.35	0	2,2,2	0.91	0
3	EDO	10-A	406	-	3,3,3	0.54	0	2,2,2	1.02	0
3	EDO	10-A	407	-	3,3,3	0.81	0	2,2,2	0.32	0
3	EDO	10-A	408	-	3,3,3	0.27	0	2,2,2	1.52	0
3	EDO	10-A	409	-	3,3,3	0.56	0	2,2,2	0.56	0
3	EDO	10-A	410	-	3,3,3	0.50	0	2,2,2	0.65	0
3	EDO	10-A	411	-	3,3,3	0.65	0	2,2,2	0.15	0
3	EDO	10-A	412	-	3,3,3	0.45	0	2,2,2	0.16	0
3	EDO	10-A	413	-	3,3,3	0.43	0	2,2,2	0.39	0
3	EDO	10-A	414	-	3,3,3	0.46	0	2,2,2	0.58	0
3	EDO	10-A	415	-	3,3,3	0.25	0	2,2,2	0.90	0
3	EDO	10-A	416	-	3,3,3	0.89	0	2,2,2	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	11-A	401	-	4,4,4	0.56	0	6,6,6	0.22	0
2	SO4	11-A	402	-	4,4,4	0.24	0	6,6,6	0.80	0
2	SO4	11-A	403	-	4,4,4	0.56	0	6,6,6	0.27	0
2	SO4	11-A	404	-	4,4,4	0.76	0	6,6,6	0.51	0
3	EDO	11-A	405	-	3,3,3	0.49	0	2,2,2	0.29	0
3	EDO	11-A	406	-	3,3,3	0.54	0	2,2,2	0.76	0
3	EDO	11-A	407	-	3,3,3	0.99	0	2,2,2	0.34	0
3	EDO	11-A	408	-	3,3,3	0.33	0	2,2,2	0.49	0
3	EDO	11-A	409	-	3,3,3	0.73	0	2,2,2	0.12	0
3	EDO	11-A	410	-	3,3,3	0.24	0	2,2,2	1.73	1 (50%)
3	EDO	11-A	411	-	3,3,3	0.51	0	2,2,2	0.70	0
3	EDO	11-A	412	-	3,3,3	0.59	0	2,2,2	0.42	0
3	EDO	11-A	413	-	3,3,3	0.51	0	2,2,2	0.25	0
3	EDO	11-A	414	-	3,3,3	0.35	0	2,2,2	1.32	0
3	EDO	11-A	415	-	3,3,3	0.60	0	2,2,2	0.05	0
3	EDO	11-A	416	-	3,3,3	0.95	0	2,2,2	0.62	0
2	SO4	12-A	401	-	4,4,4	0.31	0	6,6,6	1.06	1 (16%)
2	SO4	12-A	402	-	4,4,4	0.39	0	6,6,6	0.52	0
2	SO4	12-A	403	-	4,4,4	0.40	0	6,6,6	0.94	1 (16%)
2	SO4	12-A	404	-	4,4,4	0.32	0	6,6,6	0.71	0
3	EDO	12-A	405	-	3,3,3	0.60	0	2,2,2	0.09	0
3	EDO	12-A	406	-	3,3,3	0.44	0	2,2,2	0.84	0
3	EDO	12-A	407	-	3,3,3	0.94	0	2,2,2	0.42	0
3	EDO	12-A	408	-	3,3,3	0.39	0	2,2,2	0.67	0
3	EDO	12-A	409	-	3,3,3	0.46	0	2,2,2	0.69	0
3	EDO	12-A	410	-	3,3,3	0.38	0	2,2,2	1.55	1 (50%)
3	EDO	12-A	411	-	3,3,3	0.54	0	2,2,2	0.99	0
3	EDO	12-A	412	-	3,3,3	0.46	0	2,2,2	1.32	0
3	EDO	12-A	413	-	3,3,3	0.24	0	2,2,2	0.32	0
3	EDO	12-A	414	-	3,3,3	0.45	0	2,2,2	1.34	0
3	EDO	12-A	415	-	3,3,3	0.56	0	2,2,2	0.71	0
3	EDO	12-A	416	-	3,3,3	0.55	0	2,2,2	0.13	0
2	SO4	13-A	401	-	4,4,4	0.44	0	6,6,6	1.01	1 (16%)
2	SO4	13-A	402	-	4,4,4	0.21	0	6,6,6	0.47	0
2	SO4	13-A	403	-	4,4,4	0.33	0	6,6,6	0.33	0
2	SO4	13-A	404	-	4,4,4	0.33	0	6,6,6	0.66	0
3	EDO	13-A	405	-	3,3,3	0.59	0	2,2,2	0.78	0
3	EDO	13-A	406	-	3,3,3	0.22	0	2,2,2	2.03	1 (50%)
3	EDO	13-A	407	-	3,3,3	0.71	0	2,2,2	0.38	0
3	EDO	13-A	408	-	3,3,3	0.69	0	2,2,2	0.97	0
3	EDO	13-A	409	-	3,3,3	0.71	0	2,2,2	0.73	0
3	EDO	13-A	410	-	3,3,3	0.42	0	2,2,2	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	13-A	411	-	3,3,3	0.67	0	2,2,2	0.29	0
3	EDO	13-A	412	-	3,3,3	0.47	0	2,2,2	0.46	0
3	EDO	13-A	413	-	3,3,3	0.76	0	2,2,2	0.83	0
3	EDO	13-A	414	-	3,3,3	0.48	0	2,2,2	1.03	0
3	EDO	13-A	415	-	3,3,3	0.44	0	2,2,2	1.23	0
3	EDO	13-A	416	-	3,3,3	0.56	0	2,2,2	0.69	0
2	SO4	14-A	401	-	4,4,4	0.71	0	6,6,6	0.79	0
2	SO4	14-A	402	-	4,4,4	0.81	0	6,6,6	0.62	0
2	SO4	14-A	403	-	4,4,4	0.37	0	6,6,6	0.93	0
2	SO4	14-A	404	-	4,4,4	0.59	0	6,6,6	1.98	2 (33%)
3	EDO	14-A	405	-	3,3,3	0.68	0	2,2,2	0.75	0
3	EDO	14-A	406	-	3,3,3	0.69	0	2,2,2	0.31	0
3	EDO	14-A	407	-	3,3,3	0.70	0	2,2,2	0.68	0
3	EDO	14-A	408	-	3,3,3	0.39	0	2,2,2	0.76	0
3	EDO	14-A	409	-	3,3,3	0.63	0	2,2,2	0.26	0
3	EDO	14-A	410	-	3,3,3	0.83	0	2,2,2	0.40	0
3	EDO	14-A	411	-	3,3,3	0.66	0	2,2,2	0.11	0
3	EDO	14-A	412	-	3,3,3	0.32	0	2,2,2	0.64	0
3	EDO	14-A	413	-	3,3,3	0.41	0	2,2,2	0.74	0
3	EDO	14-A	414	-	3,3,3	0.86	0	2,2,2	1.22	0
3	EDO	14-A	415	-	3,3,3	0.80	0	2,2,2	0.78	0
3	EDO	14-A	416	-	3,3,3	1.08	0	2,2,2	0.81	0
2	SO4	15-A	401	-	4,4,4	0.48	0	6,6,6	0.71	0
2	SO4	15-A	402	-	4,4,4	0.31	0	6,6,6	0.36	0
2	SO4	15-A	403	-	4,4,4	0.26	0	6,6,6	0.35	0
2	SO4	15-A	404	-	4,4,4	1.12	0	6,6,6	0.78	0
3	EDO	15-A	405	-	3,3,3	1.04	0	2,2,2	0.99	0
3	EDO	15-A	406	-	3,3,3	0.50	0	2,2,2	0.31	0
3	EDO	15-A	407	-	3,3,3	0.60	0	2,2,2	0.58	0
3	EDO	15-A	408	-	3,3,3	0.81	0	2,2,2	0.23	0
3	EDO	15-A	409	-	3,3,3	0.67	0	2,2,2	0.49	0
3	EDO	15-A	410	-	3,3,3	0.45	0	2,2,2	1.38	0
3	EDO	15-A	411	-	3,3,3	0.36	0	2,2,2	1.46	1 (50%)
3	EDO	15-A	412	-	3,3,3	0.82	0	2,2,2	0.22	0
3	EDO	15-A	413	-	3,3,3	0.33	0	2,2,2	0.89	0
3	EDO	15-A	414	-	3,3,3	0.46	0	2,2,2	1.23	0
3	EDO	15-A	415	-	3,3,3	0.38	0	2,2,2	0.35	0
3	EDO	15-A	416	-	3,3,3	0.71	0	2,2,2	0.73	0
2	SO4	16-A	401	-	4,4,4	0.52	0	6,6,6	0.44	0
2	SO4	16-A	402	-	4,4,4	0.54	0	6,6,6	0.97	0
2	SO4	16-A	403	-	4,4,4	0.50	0	6,6,6	0.56	0
2	SO4	16-A	404	-	4,4,4	0.79	0	6,6,6	1.27	1 (16%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	16-A	405	-	3,3,3	0.39	0	2,2,2	0.90	0
3	EDO	16-A	406	-	3,3,3	0.89	0	2,2,2	1.28	0
3	EDO	16-A	407	-	3,3,3	0.46	0	2,2,2	1.17	0
3	EDO	16-A	408	-	3,3,3	0.46	0	2,2,2	0.83	0
3	EDO	16-A	409	-	3,3,3	0.64	0	2,2,2	0.02	0
3	EDO	16-A	410	-	3,3,3	0.46	0	2,2,2	0.93	0
3	EDO	16-A	411	-	3,3,3	0.31	0	2,2,2	1.36	0
3	EDO	16-A	412	-	3,3,3	0.79	0	2,2,2	0.11	0
3	EDO	16-A	413	-	3,3,3	0.52	0	2,2,2	0.54	0
3	EDO	16-A	414	-	3,3,3	0.33	0	2,2,2	0.91	0
3	EDO	16-A	415	-	3,3,3	0.56	0	2,2,2	0.36	0
3	EDO	16-A	416	-	3,3,3	0.62	0	2,2,2	0.21	0
2	SO4	17-A	401	-	4,4,4	0.48	0	6,6,6	0.36	0
2	SO4	17-A	402	-	4,4,4	0.30	0	6,6,6	0.55	0
2	SO4	17-A	403	-	4,4,4	0.21	0	6,6,6	0.31	0
2	SO4	17-A	404	-	4,4,4	0.87	0	6,6,6	0.70	0
3	EDO	17-A	405	-	3,3,3	0.45	0	2,2,2	0.24	0
3	EDO	17-A	406	-	3,3,3	0.15	0	2,2,2	1.24	0
3	EDO	17-A	407	-	3,3,3	0.69	0	2,2,2	0.63	0
3	EDO	17-A	408	-	3,3,3	0.80	0	2,2,2	0.21	0
3	EDO	17-A	409	-	3,3,3	0.41	0	2,2,2	0.49	0
3	EDO	17-A	410	-	3,3,3	0.23	0	2,2,2	1.01	0
3	EDO	17-A	411	-	3,3,3	0.67	0	2,2,2	0.97	0
3	EDO	17-A	412	-	3,3,3	0.70	0	2,2,2	0.12	0
3	EDO	17-A	413	-	3,3,3	0.47	0	2,2,2	1.17	0
3	EDO	17-A	414	-	3,3,3	0.42	0	2,2,2	1.01	0
3	EDO	17-A	415	-	3,3,3	1.12	0	2,2,2	0.86	0
3	EDO	17-A	416	-	3,3,3	0.64	0	2,2,2	0.36	0
2	SO4	18-A	401	-	4,4,4	0.76	0	6,6,6	0.95	0
2	SO4	18-A	402	-	4,4,4	0.36	0	6,6,6	0.70	0
2	SO4	18-A	403	-	4,4,4	0.38	0	6,6,6	0.79	0
2	SO4	18-A	404	-	4,4,4	0.41	0	6,6,6	1.19	1 (16%)
3	EDO	18-A	405	-	3,3,3	0.58	0	2,2,2	1.04	0
3	EDO	18-A	406	-	3,3,3	1.22	0	2,2,2	0.88	0
3	EDO	18-A	407	-	3,3,3	0.45	0	2,2,2	0.50	0
3	EDO	18-A	408	-	3,3,3	0.40	0	2,2,2	0.81	0
3	EDO	18-A	409	-	3,3,3	0.69	0	2,2,2	0.34	0
3	EDO	18-A	410	-	3,3,3	0.81	0	2,2,2	0.04	0
3	EDO	18-A	411	-	3,3,3	0.54	0	2,2,2	0.15	0
3	EDO	18-A	412	-	3,3,3	0.64	0	2,2,2	0.59	0
3	EDO	18-A	413	-	3,3,3	0.51	0	2,2,2	0.45	0
3	EDO	18-A	414	-	3,3,3	0.39	0	2,2,2	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	18-A	415	-	3,3,3	1.11	0	2,2,2	2.00	1 (50%)
3	EDO	18-A	416	-	3,3,3	0.82	0	2,2,2	1.26	0
2	SO4	19-A	401	-	4,4,4	0.47	0	6,6,6	0.59	0
2	SO4	19-A	402	-	4,4,4	0.44	0	6,6,6	0.79	0
2	SO4	19-A	403	-	4,4,4	0.31	0	6,6,6	1.33	1 (16%)
2	SO4	19-A	404	-	4,4,4	0.63	0	6,6,6	0.65	0
3	EDO	19-A	405	-	3,3,3	0.65	0	2,2,2	0.50	0
3	EDO	19-A	406	-	3,3,3	0.44	0	2,2,2	0.47	0
3	EDO	19-A	407	-	3,3,3	0.55	0	2,2,2	1.12	0
3	EDO	19-A	408	-	3,3,3	0.90	0	2,2,2	0.75	0
3	EDO	19-A	409	-	3,3,3	0.23	0	2,2,2	0.89	0
3	EDO	19-A	410	-	3,3,3	0.58	0	2,2,2	1.12	0
3	EDO	19-A	411	-	3,3,3	0.44	0	2,2,2	0.41	0
3	EDO	19-A	412	-	3,3,3	0.70	0	2,2,2	0.74	0
3	EDO	19-A	413	-	3,3,3	0.49	0	2,2,2	0.59	0
3	EDO	19-A	414	-	3,3,3	0.84	0	2,2,2	1.17	0
3	EDO	19-A	415	-	3,3,3	0.58	0	2,2,2	0.71	0
3	EDO	19-A	416	-	3,3,3	0.62	0	2,2,2	0.71	0
2	SO4	2-A	401	-	4,4,4	0.68	0	6,6,6	0.59	0
2	SO4	2-A	402	-	4,4,4	0.57	0	6,6,6	0.74	0
2	SO4	2-A	403	-	4,4,4	0.56	0	6,6,6	1.05	1 (16%)
2	SO4	2-A	404	-	4,4,4	0.12	0	6,6,6	0.68	0
3	EDO	2-A	405	-	3,3,3	0.52	0	2,2,2	0.18	0
3	EDO	2-A	406	-	3,3,3	0.24	0	2,2,2	1.23	0
3	EDO	2-A	407	-	3,3,3	0.72	0	2,2,2	0.20	0
3	EDO	2-A	408	-	3,3,3	0.64	0	2,2,2	0.21	0
3	EDO	2-A	409	-	3,3,3	0.63	0	2,2,2	0.10	0
3	EDO	2-A	410	-	3,3,3	0.72	0	2,2,2	0.29	0
3	EDO	2-A	411	-	3,3,3	0.76	0	2,2,2	0.65	0
3	EDO	2-A	412	-	3,3,3	0.50	0	2,2,2	0.56	0
3	EDO	2-A	413	-	3,3,3	0.70	0	2,2,2	0.20	0
3	EDO	2-A	414	-	3,3,3	0.38	0	2,2,2	1.22	0
3	EDO	2-A	415	-	3,3,3	0.54	0	2,2,2	0.36	0
3	EDO	2-A	416	-	3,3,3	0.41	0	2,2,2	0.23	0
2	SO4	20-A	401	-	4,4,4	0.51	0	6,6,6	1.19	1 (16%)
2	SO4	20-A	402	-	4,4,4	0.28	0	6,6,6	0.66	0
2	SO4	20-A	403	-	4,4,4	0.32	0	6,6,6	0.45	0
2	SO4	20-A	404	-	4,4,4	0.44	0	6,6,6	0.50	0
3	EDO	20-A	405	-	3,3,3	0.50	0	2,2,2	0.91	0
3	EDO	20-A	406	-	3,3,3	0.65	0	2,2,2	0.43	0
3	EDO	20-A	407	-	3,3,3	0.84	0	2,2,2	0.11	0
3	EDO	20-A	408	-	3,3,3	0.40	0	2,2,2	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	20-A	409	-	3,3,3	0.71	0	2,2,2	1.25	0
3	EDO	20-A	410	-	3,3,3	0.45	0	2,2,2	0.81	0
3	EDO	20-A	411	-	3,3,3	0.40	0	2,2,2	0.82	0
3	EDO	20-A	412	-	3,3,3	0.67	0	2,2,2	0.22	0
3	EDO	20-A	413	-	3,3,3	0.51	0	2,2,2	0.82	0
3	EDO	20-A	414	-	3,3,3	0.99	0	2,2,2	2.04	1 (50%)
3	EDO	20-A	415	-	3,3,3	0.60	0	2,2,2	0.40	0
3	EDO	20-A	416	-	3,3,3	1.81	1 (33%)	2,2,2	2.27	1 (50%)
2	SO4	3-A	401	-	4,4,4	0.53	0	6,6,6	0.48	0
2	SO4	3-A	402	-	4,4,4	0.08	0	6,6,6	0.59	0
2	SO4	3-A	403	-	4,4,4	0.50	0	6,6,6	0.50	0
2	SO4	3-A	404	-	4,4,4	0.45	0	6,6,6	1.20	1 (16%)
3	EDO	3-A	405	-	3,3,3	0.49	0	2,2,2	1.10	0
3	EDO	3-A	406	-	3,3,3	0.58	0	2,2,2	1.37	0
3	EDO	3-A	407	-	3,3,3	0.67	0	2,2,2	1.46	0
3	EDO	3-A	408	-	3,3,3	0.47	0	2,2,2	0.39	0
3	EDO	3-A	409	-	3,3,3	0.45	0	2,2,2	0.66	0
3	EDO	3-A	410	-	3,3,3	0.52	0	2,2,2	0.99	0
3	EDO	3-A	411	-	3,3,3	0.55	0	2,2,2	0.82	0
3	EDO	3-A	412	-	3,3,3	0.46	0	2,2,2	1.03	0
3	EDO	3-A	413	-	3,3,3	0.78	0	2,2,2	0.12	0
3	EDO	3-A	414	-	3,3,3	0.52	0	2,2,2	1.22	0
3	EDO	3-A	415	-	3,3,3	0.88	0	2,2,2	1.24	0
3	EDO	3-A	416	-	3,3,3	0.69	0	2,2,2	0.69	0
2	SO4	4-A	401	-	4,4,4	0.22	0	6,6,6	0.60	0
2	SO4	4-A	402	-	4,4,4	0.31	0	6,6,6	0.65	0
2	SO4	4-A	403	-	4,4,4	0.26	0	6,6,6	0.49	0
2	SO4	4-A	404	-	4,4,4	0.35	0	6,6,6	0.92	0
3	EDO	4-A	405	-	3,3,3	1.41	1 (33%)	2,2,2	0.34	0
3	EDO	4-A	406	-	3,3,3	0.82	0	2,2,2	0.07	0
3	EDO	4-A	407	-	3,3,3	0.35	0	2,2,2	0.25	0
3	EDO	4-A	408	-	3,3,3	0.70	0	2,2,2	0.30	0
3	EDO	4-A	409	-	3,3,3	0.49	0	2,2,2	0.41	0
3	EDO	4-A	410	-	3,3,3	0.96	0	2,2,2	0.39	0
3	EDO	4-A	411	-	3,3,3	0.33	0	2,2,2	1.31	0
3	EDO	4-A	412	-	3,3,3	0.54	0	2,2,2	0.72	0
3	EDO	4-A	413	-	3,3,3	0.52	0	2,2,2	0.60	0
3	EDO	4-A	414	-	3,3,3	0.94	0	2,2,2	1.82	1 (50%)
3	EDO	4-A	415	-	3,3,3	0.48	0	2,2,2	0.26	0
3	EDO	4-A	416	-	3,3,3	0.56	0	2,2,2	0.38	0
2	SO4	5-A	401	-	4,4,4	0.38	0	6,6,6	0.77	0
2	SO4	5-A	402	-	4,4,4	0.41	0	6,6,6	1.36	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	5-A	403	-	4,4,4	0.42	0	6,6,6	1.19	1 (16%)
2	SO4	5-A	404	-	4,4,4	0.89	0	6,6,6	1.20	1 (16%)
3	EDO	5-A	405	-	3,3,3	0.51	0	2,2,2	1.00	0
3	EDO	5-A	406	-	3,3,3	0.67	0	2,2,2	0.81	0
3	EDO	5-A	407	-	3,3,3	0.48	0	2,2,2	0.30	0
3	EDO	5-A	408	-	3,3,3	0.29	0	2,2,2	0.83	0
3	EDO	5-A	409	-	3,3,3	0.31	0	2,2,2	0.26	0
3	EDO	5-A	410	-	3,3,3	0.75	0	2,2,2	0.28	0
3	EDO	5-A	411	-	3,3,3	0.44	0	2,2,2	0.03	0
3	EDO	5-A	412	-	3,3,3	1.05	0	2,2,2	0.87	0
3	EDO	5-A	413	-	3,3,3	0.58	0	2,2,2	0.68	0
3	EDO	5-A	414	-	3,3,3	0.48	0	2,2,2	1.11	0
3	EDO	5-A	415	-	3,3,3	0.86	0	2,2,2	0.14	0
3	EDO	5-A	416	-	3,3,3	0.59	0	2,2,2	0.52	0
2	SO4	6-A	401	-	4,4,4	0.78	0	6,6,6	0.71	0
2	SO4	6-A	402	-	4,4,4	0.54	0	6,6,6	0.25	0
2	SO4	6-A	403	-	4,4,4	0.32	0	6,6,6	0.73	0
2	SO4	6-A	404	-	4,4,4	0.48	0	6,6,6	1.22	1 (16%)
3	EDO	6-A	405	-	3,3,3	0.42	0	2,2,2	0.68	0
3	EDO	6-A	406	-	3,3,3	0.40	0	2,2,2	1.02	0
3	EDO	6-A	407	-	3,3,3	0.61	0	2,2,2	0.16	0
3	EDO	6-A	408	-	3,3,3	0.59	0	2,2,2	0.61	0
3	EDO	6-A	409	-	3,3,3	0.34	0	2,2,2	0.96	0
3	EDO	6-A	410	-	3,3,3	0.81	0	2,2,2	0.29	0
3	EDO	6-A	411	-	3,3,3	0.65	0	2,2,2	0.87	0
3	EDO	6-A	412	-	3,3,3	0.41	0	2,2,2	0.48	0
3	EDO	6-A	413	-	3,3,3	0.51	0	2,2,2	1.29	0
3	EDO	6-A	414	-	3,3,3	0.44	0	2,2,2	0.94	0
3	EDO	6-A	415	-	3,3,3	0.59	0	2,2,2	0.47	0
3	EDO	6-A	416	-	3,3,3	0.60	0	2,2,2	0.51	0
2	SO4	7-A	401	-	4,4,4	0.16	0	6,6,6	0.70	0
2	SO4	7-A	402	-	4,4,4	0.17	0	6,6,6	0.49	0
2	SO4	7-A	403	-	4,4,4	0.52	0	6,6,6	1.30	1 (16%)
2	SO4	7-A	404	-	4,4,4	0.34	0	6,6,6	0.57	0
3	EDO	7-A	405	-	3,3,3	0.44	0	2,2,2	0.62	0
3	EDO	7-A	406	-	3,3,3	0.30	0	2,2,2	0.90	0
3	EDO	7-A	407	-	3,3,3	0.59	0	2,2,2	0.64	0
3	EDO	7-A	408	-	3,3,3	0.94	0	2,2,2	0.81	0
3	EDO	7-A	409	-	3,3,3	0.76	0	2,2,2	0.28	0
3	EDO	7-A	410	-	3,3,3	0.36	0	2,2,2	0.58	0
3	EDO	7-A	411	-	3,3,3	0.55	0	2,2,2	0.40	0
3	EDO	7-A	412	-	3,3,3	0.56	0	2,2,2	1.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	7-A	413	-	3,3,3	0.48	0	2,2,2	0.72	0
3	EDO	7-A	414	-	3,3,3	0.40	0	2,2,2	0.78	0
3	EDO	7-A	415	-	3,3,3	0.89	0	2,2,2	0.15	0
3	EDO	7-A	416	-	3,3,3	0.79	0	2,2,2	0.05	0
2	SO4	8-A	401	-	4,4,4	0.74	0	6,6,6	0.81	0
2	SO4	8-A	402	-	4,4,4	0.16	0	6,6,6	0.59	0
2	SO4	8-A	403	-	4,4,4	0.26	0	6,6,6	0.89	0
2	SO4	8-A	404	-	4,4,4	0.28	0	6,6,6	0.62	0
3	EDO	8-A	405	-	3,3,3	0.87	0	2,2,2	0.63	0
3	EDO	8-A	406	-	3,3,3	0.55	0	2,2,2	0.39	0
3	EDO	8-A	407	-	3,3,3	0.73	0	2,2,2	0.06	0
3	EDO	8-A	408	-	3,3,3	0.38	0	2,2,2	0.90	0
3	EDO	8-A	409	-	3,3,3	0.55	0	2,2,2	0.36	0
3	EDO	8-A	410	-	3,3,3	0.73	0	2,2,2	0.74	0
3	EDO	8-A	411	-	3,3,3	0.61	0	2,2,2	0.50	0
3	EDO	8-A	412	-	3,3,3	0.72	0	2,2,2	0.51	0
3	EDO	8-A	413	-	3,3,3	0.33	0	2,2,2	0.69	0
3	EDO	8-A	414	-	3,3,3	0.44	0	2,2,2	0.23	0
3	EDO	8-A	415	-	3,3,3	0.82	0	2,2,2	0.50	0
3	EDO	8-A	416	-	3,3,3	0.76	0	2,2,2	0.13	0
2	SO4	9-A	401	-	4,4,4	0.64	0	6,6,6	0.86	0
2	SO4	9-A	402	-	4,4,4	0.22	0	6,6,6	0.57	0
2	SO4	9-A	403	-	4,4,4	0.29	0	6,6,6	1.21	1 (16%)
2	SO4	9-A	404	-	4,4,4	0.48	0	6,6,6	1.25	1 (16%)
3	EDO	9-A	405	-	3,3,3	0.46	0	2,2,2	0.32	0
3	EDO	9-A	406	-	3,3,3	0.44	0	2,2,2	1.73	1 (50%)
3	EDO	9-A	407	-	3,3,3	0.62	0	2,2,2	0.62	0
3	EDO	9-A	408	-	3,3,3	0.60	0	2,2,2	0.47	0
3	EDO	9-A	409	-	3,3,3	0.47	0	2,2,2	0.88	0
3	EDO	9-A	410	-	3,3,3	0.54	0	2,2,2	1.35	0
3	EDO	9-A	411	-	3,3,3	0.75	0	2,2,2	0.42	0
3	EDO	9-A	412	-	3,3,3	0.56	0	2,2,2	0.33	0
3	EDO	9-A	413	-	3,3,3	0.55	0	2,2,2	0.98	0
3	EDO	9-A	414	-	3,3,3	0.63	0	2,2,2	0.80	0
3	EDO	9-A	415	-	3,3,3	0.61	0	2,2,2	0.17	0
3	EDO	9-A	416	-	3,3,3	0.97	0	2,2,2	0.32	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	SO4	1-A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	1-A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	1-A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	1-A	404	-	-	0/0/0/0	0/0/0/0
3	EDO	1-A	405	-	-	0/1/1/1	0/0/0/0
3	EDO	1-A	406	-	-	0/1/1/1	0/0/0/0
3	EDO	1-A	407	-	-	0/1/1/1	0/0/0/0
3	EDO	1-A	408	-	-	0/1/1/1	0/0/0/0
3	EDO	1-A	409	-	-	0/1/1/1	0/0/0/0
3	EDO	1-A	410	-	-	0/1/1/1	0/0/0/0
3	EDO	1-A	411	-	-	0/1/1/1	0/0/0/0
3	EDO	1-A	412	-	-	0/1/1/1	0/0/0/0
3	EDO	1-A	413	-	-	0/1/1/1	0/0/0/0
3	EDO	1-A	414	-	-	0/1/1/1	0/0/0/0
3	EDO	1-A	415	-	-	0/1/1/1	0/0/0/0
3	EDO	1-A	416	-	-	0/1/1/1	0/0/0/0
2	SO4	10-A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	10-A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	10-A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	10-A	404	-	-	0/0/0/0	0/0/0/0
3	EDO	10-A	405	-	-	0/1/1/1	0/0/0/0
3	EDO	10-A	406	-	-	0/1/1/1	0/0/0/0
3	EDO	10-A	407	-	-	0/1/1/1	0/0/0/0
3	EDO	10-A	408	-	-	0/1/1/1	0/0/0/0
3	EDO	10-A	409	-	-	0/1/1/1	0/0/0/0
3	EDO	10-A	410	-	-	0/1/1/1	0/0/0/0
3	EDO	10-A	411	-	-	0/1/1/1	0/0/0/0
3	EDO	10-A	412	-	-	0/1/1/1	0/0/0/0
3	EDO	10-A	413	-	-	0/1/1/1	0/0/0/0
3	EDO	10-A	414	-	-	0/1/1/1	0/0/0/0
3	EDO	10-A	415	-	-	0/1/1/1	0/0/0/0
3	EDO	10-A	416	-	-	0/1/1/1	0/0/0/0
2	SO4	11-A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	11-A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	11-A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	11-A	404	-	-	0/0/0/0	0/0/0/0
3	EDO	11-A	405	-	-	0/1/1/1	0/0/0/0
3	EDO	11-A	406	-	-	0/1/1/1	0/0/0/0
3	EDO	11-A	407	-	-	0/1/1/1	0/0/0/0
3	EDO	11-A	408	-	-	0/1/1/1	0/0/0/0
3	EDO	11-A	409	-	-	0/1/1/1	0/0/0/0
3	EDO	11-A	410	-	-	0/1/1/1	0/0/0/0
3	EDO	11-A	411	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	11-A	412	-	-	0/1/1/1	0/0/0/0
3	EDO	11-A	413	-	-	0/1/1/1	0/0/0/0
3	EDO	11-A	414	-	-	0/1/1/1	0/0/0/0
3	EDO	11-A	415	-	-	0/1/1/1	0/0/0/0
3	EDO	11-A	416	-	-	0/1/1/1	0/0/0/0
2	SO4	12-A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	12-A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	12-A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	12-A	404	-	-	0/0/0/0	0/0/0/0
3	EDO	12-A	405	-	-	0/1/1/1	0/0/0/0
3	EDO	12-A	406	-	-	0/1/1/1	0/0/0/0
3	EDO	12-A	407	-	-	0/1/1/1	0/0/0/0
3	EDO	12-A	408	-	-	0/1/1/1	0/0/0/0
3	EDO	12-A	409	-	-	0/1/1/1	0/0/0/0
3	EDO	12-A	410	-	-	0/1/1/1	0/0/0/0
3	EDO	12-A	411	-	-	0/1/1/1	0/0/0/0
3	EDO	12-A	412	-	-	0/1/1/1	0/0/0/0
3	EDO	12-A	413	-	-	0/1/1/1	0/0/0/0
3	EDO	12-A	414	-	-	0/1/1/1	0/0/0/0
3	EDO	12-A	415	-	-	0/1/1/1	0/0/0/0
3	EDO	12-A	416	-	-	0/1/1/1	0/0/0/0
2	SO4	13-A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	13-A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	13-A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	13-A	404	-	-	0/0/0/0	0/0/0/0
3	EDO	13-A	405	-	-	0/1/1/1	0/0/0/0
3	EDO	13-A	406	-	-	0/1/1/1	0/0/0/0
3	EDO	13-A	407	-	-	0/1/1/1	0/0/0/0
3	EDO	13-A	408	-	-	0/1/1/1	0/0/0/0
3	EDO	13-A	409	-	-	0/1/1/1	0/0/0/0
3	EDO	13-A	410	-	-	0/1/1/1	0/0/0/0
3	EDO	13-A	411	-	-	0/1/1/1	0/0/0/0
3	EDO	13-A	412	-	-	0/1/1/1	0/0/0/0
3	EDO	13-A	413	-	-	0/1/1/1	0/0/0/0
3	EDO	13-A	414	-	-	0/1/1/1	0/0/0/0
3	EDO	13-A	415	-	-	0/1/1/1	0/0/0/0
3	EDO	13-A	416	-	-	0/1/1/1	0/0/0/0
2	SO4	14-A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	14-A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	14-A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	14-A	404	-	-	0/0/0/0	0/0/0/0
3	EDO	14-A	405	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	14-A	406	-	-	0/1/1/1	0/0/0/0
3	EDO	14-A	407	-	-	0/1/1/1	0/0/0/0
3	EDO	14-A	408	-	-	0/1/1/1	0/0/0/0
3	EDO	14-A	409	-	-	0/1/1/1	0/0/0/0
3	EDO	14-A	410	-	-	0/1/1/1	0/0/0/0
3	EDO	14-A	411	-	-	0/1/1/1	0/0/0/0
3	EDO	14-A	412	-	-	0/1/1/1	0/0/0/0
3	EDO	14-A	413	-	-	0/1/1/1	0/0/0/0
3	EDO	14-A	414	-	-	0/1/1/1	0/0/0/0
3	EDO	14-A	415	-	-	0/1/1/1	0/0/0/0
3	EDO	14-A	416	-	-	0/1/1/1	0/0/0/0
2	SO4	15-A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	15-A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	15-A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	15-A	404	-	-	0/0/0/0	0/0/0/0
3	EDO	15-A	405	-	-	0/1/1/1	0/0/0/0
3	EDO	15-A	406	-	-	0/1/1/1	0/0/0/0
3	EDO	15-A	407	-	-	0/1/1/1	0/0/0/0
3	EDO	15-A	408	-	-	0/1/1/1	0/0/0/0
3	EDO	15-A	409	-	-	0/1/1/1	0/0/0/0
3	EDO	15-A	410	-	-	0/1/1/1	0/0/0/0
3	EDO	15-A	411	-	-	0/1/1/1	0/0/0/0
3	EDO	15-A	412	-	-	0/1/1/1	0/0/0/0
3	EDO	15-A	413	-	-	0/1/1/1	0/0/0/0
3	EDO	15-A	414	-	-	0/1/1/1	0/0/0/0
3	EDO	15-A	415	-	-	0/1/1/1	0/0/0/0
3	EDO	15-A	416	-	-	0/1/1/1	0/0/0/0
2	SO4	16-A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	16-A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	16-A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	16-A	404	-	-	0/0/0/0	0/0/0/0
3	EDO	16-A	405	-	-	0/1/1/1	0/0/0/0
3	EDO	16-A	406	-	-	0/1/1/1	0/0/0/0
3	EDO	16-A	407	-	-	0/1/1/1	0/0/0/0
3	EDO	16-A	408	-	-	0/1/1/1	0/0/0/0
3	EDO	16-A	409	-	-	0/1/1/1	0/0/0/0
3	EDO	16-A	410	-	-	0/1/1/1	0/0/0/0
3	EDO	16-A	411	-	-	0/1/1/1	0/0/0/0
3	EDO	16-A	412	-	-	0/1/1/1	0/0/0/0
3	EDO	16-A	413	-	-	0/1/1/1	0/0/0/0
3	EDO	16-A	414	-	-	0/1/1/1	0/0/0/0
3	EDO	16-A	415	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	16-A	416	-	-	0/1/1/1	0/0/0/0
2	SO4	17-A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	17-A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	17-A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	17-A	404	-	-	0/0/0/0	0/0/0/0
3	EDO	17-A	405	-	-	0/1/1/1	0/0/0/0
3	EDO	17-A	406	-	-	0/1/1/1	0/0/0/0
3	EDO	17-A	407	-	-	0/1/1/1	0/0/0/0
3	EDO	17-A	408	-	-	0/1/1/1	0/0/0/0
3	EDO	17-A	409	-	-	0/1/1/1	0/0/0/0
3	EDO	17-A	410	-	-	0/1/1/1	0/0/0/0
3	EDO	17-A	411	-	-	0/1/1/1	0/0/0/0
3	EDO	17-A	412	-	-	0/1/1/1	0/0/0/0
3	EDO	17-A	413	-	-	0/1/1/1	0/0/0/0
3	EDO	17-A	414	-	-	0/1/1/1	0/0/0/0
3	EDO	17-A	415	-	-	0/1/1/1	0/0/0/0
3	EDO	17-A	416	-	-	0/1/1/1	0/0/0/0
2	SO4	18-A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	18-A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	18-A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	18-A	404	-	-	0/0/0/0	0/0/0/0
3	EDO	18-A	405	-	-	0/1/1/1	0/0/0/0
3	EDO	18-A	406	-	-	0/1/1/1	0/0/0/0
3	EDO	18-A	407	-	-	0/1/1/1	0/0/0/0
3	EDO	18-A	408	-	-	0/1/1/1	0/0/0/0
3	EDO	18-A	409	-	-	0/1/1/1	0/0/0/0
3	EDO	18-A	410	-	-	0/1/1/1	0/0/0/0
3	EDO	18-A	411	-	-	0/1/1/1	0/0/0/0
3	EDO	18-A	412	-	-	0/1/1/1	0/0/0/0
3	EDO	18-A	413	-	-	0/1/1/1	0/0/0/0
3	EDO	18-A	414	-	-	0/1/1/1	0/0/0/0
3	EDO	18-A	415	-	-	0/1/1/1	0/0/0/0
3	EDO	18-A	416	-	-	0/1/1/1	0/0/0/0
2	SO4	19-A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	19-A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	19-A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	19-A	404	-	-	0/0/0/0	0/0/0/0
3	EDO	19-A	405	-	-	0/1/1/1	0/0/0/0
3	EDO	19-A	406	-	-	0/1/1/1	0/0/0/0
3	EDO	19-A	407	-	-	0/1/1/1	0/0/0/0
3	EDO	19-A	408	-	-	0/1/1/1	0/0/0/0
3	EDO	19-A	409	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	19-A	410	-	-	0/1/1/1	0/0/0/0
3	EDO	19-A	411	-	-	0/1/1/1	0/0/0/0
3	EDO	19-A	412	-	-	0/1/1/1	0/0/0/0
3	EDO	19-A	413	-	-	0/1/1/1	0/0/0/0
3	EDO	19-A	414	-	-	0/1/1/1	0/0/0/0
3	EDO	19-A	415	-	-	0/1/1/1	0/0/0/0
3	EDO	19-A	416	-	-	0/1/1/1	0/0/0/0
2	SO4	2-A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	2-A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	2-A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	2-A	404	-	-	0/0/0/0	0/0/0/0
3	EDO	2-A	405	-	-	0/1/1/1	0/0/0/0
3	EDO	2-A	406	-	-	0/1/1/1	0/0/0/0
3	EDO	2-A	407	-	-	0/1/1/1	0/0/0/0
3	EDO	2-A	408	-	-	0/1/1/1	0/0/0/0
3	EDO	2-A	409	-	-	0/1/1/1	0/0/0/0
3	EDO	2-A	410	-	-	0/1/1/1	0/0/0/0
3	EDO	2-A	411	-	-	0/1/1/1	0/0/0/0
3	EDO	2-A	412	-	-	0/1/1/1	0/0/0/0
3	EDO	2-A	413	-	-	0/1/1/1	0/0/0/0
3	EDO	2-A	414	-	-	0/1/1/1	0/0/0/0
3	EDO	2-A	415	-	-	0/1/1/1	0/0/0/0
3	EDO	2-A	416	-	-	0/1/1/1	0/0/0/0
2	SO4	20-A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	20-A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	20-A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	20-A	404	-	-	0/0/0/0	0/0/0/0
3	EDO	20-A	405	-	-	0/1/1/1	0/0/0/0
3	EDO	20-A	406	-	-	0/1/1/1	0/0/0/0
3	EDO	20-A	407	-	-	0/1/1/1	0/0/0/0
3	EDO	20-A	408	-	-	0/1/1/1	0/0/0/0
3	EDO	20-A	409	-	-	0/1/1/1	0/0/0/0
3	EDO	20-A	410	-	-	0/1/1/1	0/0/0/0
3	EDO	20-A	411	-	-	0/1/1/1	0/0/0/0
3	EDO	20-A	412	-	-	0/1/1/1	0/0/0/0
3	EDO	20-A	413	-	-	0/1/1/1	0/0/0/0
3	EDO	20-A	414	-	-	0/1/1/1	0/0/0/0
3	EDO	20-A	415	-	-	0/1/1/1	0/0/0/0
3	EDO	20-A	416	-	-	0/1/1/1	0/0/0/0
2	SO4	3-A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	3-A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	3-A	403	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	3-A	404	-	-	0/0/0/0	0/0/0/0
3	EDO	3-A	405	-	-	0/1/1/1	0/0/0/0
3	EDO	3-A	406	-	-	0/1/1/1	0/0/0/0
3	EDO	3-A	407	-	-	0/1/1/1	0/0/0/0
3	EDO	3-A	408	-	-	0/1/1/1	0/0/0/0
3	EDO	3-A	409	-	-	0/1/1/1	0/0/0/0
3	EDO	3-A	410	-	-	0/1/1/1	0/0/0/0
3	EDO	3-A	411	-	-	0/1/1/1	0/0/0/0
3	EDO	3-A	412	-	-	0/1/1/1	0/0/0/0
3	EDO	3-A	413	-	-	0/1/1/1	0/0/0/0
3	EDO	3-A	414	-	-	0/1/1/1	0/0/0/0
3	EDO	3-A	415	-	-	0/1/1/1	0/0/0/0
3	EDO	3-A	416	-	-	0/1/1/1	0/0/0/0
2	SO4	4-A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	4-A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	4-A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	4-A	404	-	-	0/0/0/0	0/0/0/0
3	EDO	4-A	405	-	-	0/1/1/1	0/0/0/0
3	EDO	4-A	406	-	-	0/1/1/1	0/0/0/0
3	EDO	4-A	407	-	-	0/1/1/1	0/0/0/0
3	EDO	4-A	408	-	-	0/1/1/1	0/0/0/0
3	EDO	4-A	409	-	-	0/1/1/1	0/0/0/0
3	EDO	4-A	410	-	-	0/1/1/1	0/0/0/0
3	EDO	4-A	411	-	-	0/1/1/1	0/0/0/0
3	EDO	4-A	412	-	-	0/1/1/1	0/0/0/0
3	EDO	4-A	413	-	-	0/1/1/1	0/0/0/0
3	EDO	4-A	414	-	-	0/1/1/1	0/0/0/0
3	EDO	4-A	415	-	-	0/1/1/1	0/0/0/0
3	EDO	4-A	416	-	-	0/1/1/1	0/0/0/0
2	SO4	5-A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	5-A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	5-A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	5-A	404	-	-	0/0/0/0	0/0/0/0
3	EDO	5-A	405	-	-	0/1/1/1	0/0/0/0
3	EDO	5-A	406	-	-	0/1/1/1	0/0/0/0
3	EDO	5-A	407	-	-	0/1/1/1	0/0/0/0
3	EDO	5-A	408	-	-	0/1/1/1	0/0/0/0
3	EDO	5-A	409	-	-	0/1/1/1	0/0/0/0
3	EDO	5-A	410	-	-	0/1/1/1	0/0/0/0
3	EDO	5-A	411	-	-	0/1/1/1	0/0/0/0
3	EDO	5-A	412	-	-	0/1/1/1	0/0/0/0
3	EDO	5-A	413	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	5-A	414	-	-	0/1/1/1	0/0/0/0
3	EDO	5-A	415	-	-	0/1/1/1	0/0/0/0
3	EDO	5-A	416	-	-	0/1/1/1	0/0/0/0
2	SO4	6-A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	6-A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	6-A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	6-A	404	-	-	0/0/0/0	0/0/0/0
3	EDO	6-A	405	-	-	0/1/1/1	0/0/0/0
3	EDO	6-A	406	-	-	0/1/1/1	0/0/0/0
3	EDO	6-A	407	-	-	0/1/1/1	0/0/0/0
3	EDO	6-A	408	-	-	0/1/1/1	0/0/0/0
3	EDO	6-A	409	-	-	0/1/1/1	0/0/0/0
3	EDO	6-A	410	-	-	0/1/1/1	0/0/0/0
3	EDO	6-A	411	-	-	0/1/1/1	0/0/0/0
3	EDO	6-A	412	-	-	0/1/1/1	0/0/0/0
3	EDO	6-A	413	-	-	0/1/1/1	0/0/0/0
3	EDO	6-A	414	-	-	0/1/1/1	0/0/0/0
3	EDO	6-A	415	-	-	0/1/1/1	0/0/0/0
3	EDO	6-A	416	-	-	0/1/1/1	0/0/0/0
2	SO4	7-A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	7-A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	7-A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	7-A	404	-	-	0/0/0/0	0/0/0/0
3	EDO	7-A	405	-	-	0/1/1/1	0/0/0/0
3	EDO	7-A	406	-	-	0/1/1/1	0/0/0/0
3	EDO	7-A	407	-	-	0/1/1/1	0/0/0/0
3	EDO	7-A	408	-	-	0/1/1/1	0/0/0/0
3	EDO	7-A	409	-	-	0/1/1/1	0/0/0/0
3	EDO	7-A	410	-	-	0/1/1/1	0/0/0/0
3	EDO	7-A	411	-	-	0/1/1/1	0/0/0/0
3	EDO	7-A	412	-	-	0/1/1/1	0/0/0/0
3	EDO	7-A	413	-	-	0/1/1/1	0/0/0/0
3	EDO	7-A	414	-	-	0/1/1/1	0/0/0/0
3	EDO	7-A	415	-	-	0/1/1/1	0/0/0/0
3	EDO	7-A	416	-	-	0/1/1/1	0/0/0/0
2	SO4	8-A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	8-A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	8-A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	8-A	404	-	-	0/0/0/0	0/0/0/0
3	EDO	8-A	405	-	-	0/1/1/1	0/0/0/0
3	EDO	8-A	406	-	-	0/1/1/1	0/0/0/0
3	EDO	8-A	407	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	8-A	408	-	-	0/1/1/1	0/0/0/0
3	EDO	8-A	409	-	-	0/1/1/1	0/0/0/0
3	EDO	8-A	410	-	-	0/1/1/1	0/0/0/0
3	EDO	8-A	411	-	-	0/1/1/1	0/0/0/0
3	EDO	8-A	412	-	-	0/1/1/1	0/0/0/0
3	EDO	8-A	413	-	-	0/1/1/1	0/0/0/0
3	EDO	8-A	414	-	-	0/1/1/1	0/0/0/0
3	EDO	8-A	415	-	-	0/1/1/1	0/0/0/0
3	EDO	8-A	416	-	-	0/1/1/1	0/0/0/0
2	SO4	9-A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	9-A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	9-A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	9-A	404	-	-	0/0/0/0	0/0/0/0
3	EDO	9-A	405	-	-	0/1/1/1	0/0/0/0
3	EDO	9-A	406	-	-	0/1/1/1	0/0/0/0
3	EDO	9-A	407	-	-	0/1/1/1	0/0/0/0
3	EDO	9-A	408	-	-	0/1/1/1	0/0/0/0
3	EDO	9-A	409	-	-	0/1/1/1	0/0/0/0
3	EDO	9-A	410	-	-	0/1/1/1	0/0/0/0
3	EDO	9-A	411	-	-	0/1/1/1	0/0/0/0
3	EDO	9-A	412	-	-	0/1/1/1	0/0/0/0
3	EDO	9-A	413	-	-	0/1/1/1	0/0/0/0
3	EDO	9-A	414	-	-	0/1/1/1	0/0/0/0
3	EDO	9-A	415	-	-	0/1/1/1	0/0/0/0
3	EDO	9-A	416	-	-	0/1/1/1	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	20-A	416	EDO	O1-C1	2.36	1.54	1.42
3	4-A	405	EDO	O2-C2	2.18	1.53	1.42

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	14-A	404	SO4	O2-S-O1	3.64	121.20	109.50
2	1-A	402	SO4	O2-S-O1	-3.27	99.01	109.50
2	14-A	404	SO4	O4-S-O3	-3.16	95.83	109.05
2	7-A	403	SO4	O2-S-O1	3.09	119.44	109.50
2	19-A	403	SO4	O2-S-O1	2.80	118.48	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	1-A	388/388 (100%)	0.02	20 (5%)	26	27	14, 18, 23, 27	388 (100%)
1	2-A	388/388 (100%)	0.02	20 (5%)	26	27	14, 18, 23, 27	388 (100%)
1	3-A	388/388 (100%)	0.02	20 (5%)	26	27	14, 18, 23, 27	388 (100%)
1	4-A	388/388 (100%)	0.02	20 (5%)	26	27	14, 18, 23, 27	388 (100%)
1	5-A	388/388 (100%)	0.02	20 (5%)	26	27	14, 18, 23, 27	388 (100%)
1	6-A	388/388 (100%)	0.02	20 (5%)	26	27	14, 18, 23, 27	388 (100%)
1	7-A	388/388 (100%)	0.02	20 (5%)	26	27	14, 18, 23, 27	388 (100%)
1	8-A	388/388 (100%)	0.02	20 (5%)	26	27	14, 18, 23, 27	388 (100%)
1	9-A	388/388 (100%)	0.02	20 (5%)	26	27	14, 18, 23, 27	388 (100%)
1	10-A	388/388 (100%)	0.02	20 (5%)	26	27	14, 18, 23, 27	388 (100%)
1	11-A	388/388 (100%)	0.02	20 (5%)	26	27	14, 18, 23, 27	388 (100%)
1	12-A	388/388 (100%)	0.02	20 (5%)	26	27	14, 18, 23, 27	388 (100%)
1	13-A	388/388 (100%)	0.02	20 (5%)	26	27	14, 18, 23, 27	388 (100%)
1	14-A	388/388 (100%)	0.02	20 (5%)	26	27	14, 18, 23, 27	388 (100%)
1	15-A	388/388 (100%)	0.02	20 (5%)	26	27	14, 18, 23, 27	388 (100%)
1	16-A	388/388 (100%)	0.02	20 (5%)	26	27	14, 18, 23, 27	388 (100%)
1	17-A	388/388 (100%)	0.02	20 (5%)	26	27	14, 18, 23, 27	388 (100%)
1	18-A	388/388 (100%)	0.02	20 (5%)	26	27	14, 18, 23, 27	388 (100%)
1	19-A	388/388 (100%)	0.02	20 (5%)	26	27	14, 18, 23, 27	388 (100%)
1	20-A	388/388 (100%)	0.02	20 (5%)	26	27	14, 18, 23, 27	388 (100%)
All	All	7760/7760 (100%)	0.02	400 (5%)	23	27	14, 18, 23, 27	7760 (100%)

The worst 5 of 400 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	-2	SER	17.5
1	2-A	-2	SER	17.5
1	3-A	-2	SER	17.5
1	4-A	-2	SER	17.5
1	5-A	-2	SER	17.5

## 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	EDO	10-A	416	4/4	0.49	23.14	18,19,20,20	10
3	EDO	13-A	416	4/4	0.49	22.73	19,19,20,20	10
3	EDO	10-A	407	4/4	0.28	22.43	16,16,17,17	10
3	EDO	18-A	416	4/4	0.49	22.26	18,18,19,20	10
3	EDO	11-A	416	4/4	0.49	22.26	18,19,19,20	10
3	EDO	19-A	407	4/4	0.28	21.99	16,16,17,17	10
3	EDO	14-A	407	4/4	0.28	21.87	16,16,17,17	10
3	EDO	11-A	407	4/4	0.28	21.54	16,17,17,17	10
3	EDO	13-A	407	4/4	0.28	21.50	16,16,17,17	10
3	EDO	15-A	407	4/4	0.28	20.51	16,16,17,17	10
3	EDO	17-A	407	4/4	0.28	20.17	16,16,17,17	10
3	EDO	16-A	407	4/4	0.28	20.09	16,16,17,17	10
3	EDO	17-A	416	4/4	0.49	19.83	18,19,19,19	10
3	EDO	20-A	407	4/4	0.28	17.85	16,17,17,17	10
3	EDO	19-A	416	4/4	0.49	17.45	18,19,20,20	10
3	EDO	12-A	407	4/4	0.28	16.97	16,16,17,18	10
2	SO4	15-A	403	5/5	0.55	15.21	26,26,27,28	5

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	18-A	403	5/5	0.55	14.45	25,25,26,27	5
3	EDO	18-A	407	4/4	0.28	14.04	16,16,17,17	10
3	EDO	14-A	416	4/4	0.49	13.86	19,19,20,20	10
2	SO4	12-A	403	5/5	0.55	13.56	25,25,26,26	5
3	EDO	11-A	411	4/4	0.17	13.54	14,14,14,14	10
2	SO4	10-A	403	5/5	0.55	13.39	25,26,27,27	5
3	EDO	20-A	416	4/4	0.49	13.35	18,19,20,20	10
3	EDO	15-A	416	4/4	0.49	12.99	19,19,20,20	10
3	EDO	12-A	416	4/4	0.49	12.90	18,19,19,20	10
2	SO4	20-A	403	5/5	0.55	11.90	25,26,27,27	5
3	EDO	16-A	416	4/4	0.49	11.86	20,20,21,22	10
2	SO4	14-A	403	5/5	0.55	11.21	25,26,26,27	5
2	SO4	16-A	403	5/5	0.55	11.21	25,25,26,26	5
3	EDO	17-A	415	4/4	0.24	9.46	16,17,18,18	10
3	EDO	12-A	415	4/4	0.24	8.97	16,16,17,17	10
3	EDO	11-A	415	4/4	0.24	8.89	16,17,17,18	10
3	EDO	20-A	415	4/4	0.24	8.39	16,17,17,17	10
3	EDO	13-A	415	4/4	0.24	8.31	16,17,18,18	10
3	EDO	15-A	415	4/4	0.24	8.30	16,17,17,18	10
3	EDO	18-A	415	4/4	0.24	8.30	16,16,17,17	10
3	EDO	14-A	415	4/4	0.24	8.28	15,16,17,17	10
3	EDO	19-A	414	4/4	0.17	8.23	13,14,14,14	10
3	EDO	13-A	414	4/4	0.17	8.17	14,14,14,14	10
3	EDO	16-A	414	4/4	0.17	8.13	14,14,14,14	10
3	EDO	18-A	414	4/4	0.17	8.02	14,14,14,14	10
3	EDO	12-A	414	4/4	0.17	8.02	13,14,14,14	10
3	EDO	17-A	414	4/4	0.17	8.02	14,14,14,14	10
3	EDO	11-A	414	4/4	0.17	7.97	14,14,14,14	10
3	EDO	10-A	414	4/4	0.17	7.85	14,14,14,14	10
3	EDO	14-A	411	4/4	0.17	7.85	14,14,14,14	10
3	EDO	18-A	411	4/4	0.17	7.76	14,14,14,14	10
3	EDO	10-A	415	4/4	0.24	7.67	16,17,17,17	10
3	EDO	14-A	414	4/4	0.17	7.65	14,14,14,14	10
2	SO4	17-A	403	5/5	0.55	7.57	23,24,25,25	5
3	EDO	15-A	414	4/4	0.17	7.57	13,14,14,14	10
3	EDO	20-A	414	4/4	0.17	7.49	14,14,14,14	10
2	SO4	19-A	403	5/5	0.55	7.08	22,23,23,24	5
2	SO4	13-A	403	5/5	0.55	7.08	24,24,25,25	5
3	EDO	16-A	415	4/4	0.24	6.82	16,17,17,18	10
3	EDO	18-A	406	4/4	0.15	6.73	13,14,14,14	10
2	SO4	11-A	403	5/5	0.55	6.65	24,26,26,27	5

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	19-A	406	4/4	0.15	6.63	13,13,13,13	10
3	EDO	10-A	411	4/4	0.17	6.11	14,14,14,14	10
3	EDO	19-A	415	4/4	0.24	6.03	17,17,18,18	10
3	EDO	20-A	411	4/4	0.17	5.29	14,14,14,14	10
3	EDO	11-A	406	4/4	0.15	5.26	13,14,14,14	10
3	EDO	15-A	406	4/4	0.15	5.07	13,13,14,14	10
3	EDO	13-A	406	4/4	0.15	5.07	13,14,14,14	10
3	EDO	12-A	411	4/4	0.17	4.90	14,14,14,14	10
3	EDO	15-A	412	4/4	0.21	4.84	19,20,21,21	10
3	EDO	17-A	406	4/4	0.15	4.74	13,13,14,14	10
3	EDO	12-A	406	4/4	0.15	4.71	13,14,14,14	10
3	EDO	17-A	408	4/4	0.24	4.67	15,16,17,17	10
3	EDO	19-A	408	4/4	0.24	4.61	15,16,17,17	10
3	EDO	12-A	408	4/4	0.24	4.48	15,16,16,17	10
3	EDO	20-A	408	4/4	0.24	4.44	16,16,16,16	10
3	EDO	13-A	411	4/4	0.17	4.41	14,14,14,14	10
3	EDO	18-A	408	4/4	0.24	4.41	15,16,16,16	10
3	EDO	10-A	408	4/4	0.24	4.32	15,16,16,17	10
3	EDO	15-A	411	4/4	0.17	4.28	14,14,14,14	10
3	EDO	16-A	408	4/4	0.24	4.26	15,16,17,17	10
3	EDO	14-A	408	4/4	0.24	4.20	15,16,16,17	10
3	EDO	14-A	406	4/4	0.15	4.17	14,14,14,14	10
3	EDO	13-A	408	4/4	0.24	4.12	16,16,16,16	10
3	EDO	11-A	408	4/4	0.24	4.03	15,16,16,17	10
3	EDO	19-A	411	4/4	0.17	3.93	14,14,14,14	10
3	EDO	15-A	408	4/4	0.24	3.89	15,16,16,16	10
3	EDO	17-A	411	4/4	0.17	3.88	14,14,14,14	10
3	EDO	10-A	406	4/4	0.15	3.19	13,14,14,14	10
3	EDO	18-A	412	4/4	0.21	2.88	19,20,21,21	10
3	EDO	16-A	412	4/4	0.21	2.88	18,19,20,21	10
3	EDO	14-A	412	4/4	0.21	2.87	19,20,21,21	10
3	EDO	19-A	412	4/4	0.21	2.85	20,20,21,21	10
3	EDO	12-A	412	4/4	0.21	2.85	19,20,21,21	10
3	EDO	11-A	412	4/4	0.21	2.83	20,20,21,21	10
3	EDO	13-A	412	4/4	0.21	2.82	19,19,21,21	10
3	EDO	20-A	412	4/4	0.21	2.81	20,20,21,21	10
3	EDO	17-A	412	4/4	0.21	2.76	19,20,21,21	10
3	EDO	10-A	412	4/4	0.21	2.75	19,20,20,20	10
3	EDO	14-A	410	4/4	0.17	2.74	14,14,14,14	10
3	EDO	16-A	411	4/4	0.17	2.73	14,14,14,14	10
3	EDO	10-A	410	4/4	0.17	2.61	14,15,15,15	10

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	18-A	410	4/4	0.17	2.60	14,15,15,15	10
3	EDO	17-A	410	4/4	0.17	2.60	14,15,15,15	10
3	EDO	16-A	410	4/4	0.17	2.58	14,15,15,15	10
3	EDO	13-A	410	4/4	0.17	2.55	14,14,15,15	10
3	EDO	11-A	410	4/4	0.17	2.50	14,14,15,15	10
3	EDO	20-A	410	4/4	0.17	2.49	14,15,15,15	10
3	EDO	19-A	410	4/4	0.17	2.46	14,14,15,15	10
3	EDO	12-A	410	4/4	0.17	2.45	14,14,15,15	10
3	EDO	15-A	410	4/4	0.17	2.36	14,15,15,15	10
3	EDO	16-A	406	4/4	0.15	2.26	14,14,14,14	10
3	EDO	20-A	406	4/4	0.15	2.22	14,14,14,14	10
2	SO4	18-A	402	5/5	0.36	1.88	19,20,20,20	5
2	SO4	16-A	402	5/5	0.36	1.64	20,20,21,22	5
3	EDO	10-A	413	4/4	0.11	1.24	18,19,19,20	10
2	SO4	12-A	404	5/5	0.12	1.22	18,19,20,20	5
2	SO4	20-A	404	5/5	0.12	1.20	18,19,19,19	5
2	SO4	13-A	404	5/5	0.12	1.20	18,18,19,19	5
3	EDO	15-A	413	4/4	0.11	1.11	17,18,19,19	10
3	EDO	14-A	413	4/4	0.11	1.08	17,18,19,19	10
2	SO4	11-A	404	5/5	0.12	1.07	17,18,18,19	5
3	EDO	19-A	413	4/4	0.11	1.03	17,18,19,19	10
3	EDO	18-A	413	4/4	0.11	1.02	17,18,18,19	10
3	EDO	17-A	413	4/4	0.11	1.00	17,18,19,19	10
2	SO4	14-A	404	5/5	0.12	1.00	18,18,19,19	5
3	EDO	16-A	413	4/4	0.11	0.98	18,19,20,20	10
3	EDO	12-A	413	4/4	0.11	0.97	17,18,18,18	10
3	EDO	13-A	413	4/4	0.11	0.94	18,18,19,20	10
3	EDO	20-A	413	4/4	0.11	0.94	17,17,18,18	10
3	EDO	11-A	413	4/4	0.11	0.91	18,18,19,19	10
2	SO4	17-A	404	5/5	0.12	0.88	18,19,19,19	5
2	SO4	15-A	402	5/5	0.36	0.80	19,20,20,20	5
2	SO4	10-A	404	5/5	0.12	0.72	19,19,20,20	5
2	SO4	15-A	404	5/5	0.12	0.69	17,17,18,18	5
3	EDO	20-A	409	4/4	0.10	0.68	18,18,19,20	10
3	EDO	18-A	409	4/4	0.10	0.64	18,18,19,19	10
3	EDO	12-A	409	4/4	0.10	0.64	18,19,19,19	10
3	EDO	15-A	409	4/4	0.10	0.57	18,19,19,19	10
3	EDO	19-A	409	4/4	0.10	0.56	18,19,20,20	10
3	EDO	13-A	409	4/4	0.10	0.56	18,18,19,19	10
3	EDO	16-A	409	4/4	0.10	0.56	18,19,19,19	10
3	EDO	14-A	409	4/4	0.10	0.55	18,18,19,19	10
3	EDO	10-A	409	4/4	0.10	0.55	18,19,19,20	10

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	17-A	409	4/4	0.10	0.53	18,19,20,20	10
3	EDO	11-A	409	4/4	0.10	0.52	18,19,20,20	10
2	SO4	16-A	404	5/5	0.12	0.47	19,19,19,20	5
2	SO4	20-A	402	5/5	0.36	0.28	20,21,22,22	5
2	SO4	14-A	402	5/5	0.36	0.27	20,20,20,21	5
2	SO4	10-A	402	5/5	0.36	0.27	20,20,20,21	5
2	SO4	19-A	402	5/5	0.36	0.27	21,21,22,22	5
2	SO4	12-A	402	5/5	0.36	0.24	20,20,20,21	5
2	SO4	13-A	402	5/5	0.36	0.23	21,22,22,23	5
2	SO4	11-A	402	5/5	0.36	0.19	20,21,21,21	5
3	EDO	16-A	405	4/4	0.07	0.19	17,17,18,18	10
3	EDO	13-A	405	4/4	0.07	0.19	17,17,18,18	10
3	EDO	14-A	405	4/4	0.07	0.19	17,17,18,18	10
3	EDO	18-A	405	4/4	0.07	0.18	17,17,18,18	10
3	EDO	15-A	405	4/4	0.07	0.18	17,17,18,18	10
3	EDO	12-A	405	4/4	0.07	0.18	17,17,18,18	10
3	EDO	20-A	405	4/4	0.07	0.15	17,17,18,18	10
3	EDO	11-A	405	4/4	0.07	0.15	16,17,18,18	10
3	EDO	10-A	405	4/4	0.07	0.14	16,17,18,18	10
3	EDO	19-A	405	4/4	0.07	0.12	17,18,18,18	10
3	EDO	17-A	405	4/4	0.07	0.11	17,17,18,18	10
2	SO4	17-A	402	5/5	0.36	-0.06	20,21,21,21	5
2	SO4	19-A	404	5/5	0.12	-0.69	21,22,22,23	5
2	SO4	17-A	401	5/5	0.08	-1.14	23,23,23,24	5
2	SO4	16-A	401	5/5	0.08	-1.17	22,22,23,24	5
2	SO4	11-A	401	5/5	0.08	-1.17	22,23,24,24	5
2	SO4	19-A	401	5/5	0.08	-1.18	23,23,24,25	5
2	SO4	18-A	401	5/5	0.08	-1.18	23,23,24,25	5
2	SO4	20-A	401	5/5	0.08	-1.21	23,23,24,24	5
2	SO4	10-A	401	5/5	0.08	-1.21	23,24,24,25	5
2	SO4	15-A	401	5/5	0.08	-1.22	23,23,24,24	5
2	SO4	14-A	401	5/5	0.08	-1.23	23,23,24,24	5
2	SO4	18-A	404	5/5	0.12	-1.33	21,22,22,22	5
2	SO4	12-A	401	5/5	0.08	-1.39	21,22,23,23	5
2	SO4	13-A	401	5/5	0.08	-2.55	23,24,24,25	5
3	EDO	5-A	413	4/4	0.11	-	18,19,19,20	10
2	SO4	8-A	403	5/5	0.55	-	28,29,30,30	5
3	EDO	8-A	407	4/4	0.28	-	16,17,17,17	10
3	EDO	2-A	413	4/4	0.11	-	18,19,20,20	10
2	SO4	4-A	404	5/5	0.12	-	20,20,21,21	5
3	EDO	5-A	408	4/4	0.24	-	15,16,16,17	10
2	SO4	3-A	403	5/5	0.55	-	27,28,29,29	5

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	9-A	406	4/4	0.15	-	13,14,14,14	10
3	EDO	2-A	414	4/4	0.17	-	14,14,14,14	10
2	SO4	7-A	403	5/5	0.55	-	24,25,26,26	5
2	SO4	7-A	404	5/5	0.12	-	18,19,19,19	5
3	EDO	3-A	413	4/4	0.11	-	18,19,20,20	10
3	EDO	8-A	405	4/4	0.07	-	17,17,18,18	10
2	SO4	7-A	402	5/5	0.36	-	20,21,22,22	5
3	EDO	6-A	414	4/4	0.17	-	14,14,14,14	10
3	EDO	9-A	413	4/4	0.11	-	17,18,19,19	10
3	EDO	9-A	408	4/4	0.24	-	15,16,16,17	10
3	EDO	3-A	406	4/4	0.15	-	13,14,14,14	10
3	EDO	4-A	410	4/4	0.17	-	14,14,15,15	10
3	EDO	3-A	407	4/4	0.28	-	16,17,17,18	10
3	EDO	1-A	414	4/4	0.17	-	14,14,14,14	10
3	EDO	1-A	411	4/4	0.17	-	14,14,14,14	10
2	SO4	6-A	401	5/5	0.08	-	22,23,24,24	5
3	EDO	8-A	411	4/4	0.17	-	14,14,14,14	10
3	EDO	5-A	405	4/4	0.07	-	17,17,18,18	10
3	EDO	3-A	415	4/4	0.24	-	16,16,17,17	10
2	SO4	1-A	403	5/5	0.55	-	23,25,25,25	5
3	EDO	9-A	412	4/4	0.21	-	19,19,21,21	10
3	EDO	8-A	415	4/4	0.24	-	16,17,18,18	10
2	SO4	8-A	401	5/5	0.08	-	22,23,24,24	5
3	EDO	5-A	410	4/4	0.17	-	14,15,15,15	10
3	EDO	6-A	410	4/4	0.17	-	14,15,15,15	10
2	SO4	3-A	401	5/5	0.08	-	23,23,23,24	5
3	EDO	3-A	414	4/4	0.17	-	14,14,14,14	10
3	EDO	9-A	405	4/4	0.07	-	17,17,18,18	10
2	SO4	3-A	404	5/5	0.12	-	18,19,19,19	5
3	EDO	2-A	409	4/4	0.10	-	18,19,19,19	10
3	EDO	9-A	407	4/4	0.28	-	16,16,17,17	10
3	EDO	7-A	411	4/4	0.17	-	14,14,14,14	10
3	EDO	6-A	408	4/4	0.24	-	16,16,16,16	10
3	EDO	5-A	409	4/4	0.10	-	17,18,19,20	10
3	EDO	9-A	409	4/4	0.10	-	18,19,20,20	10
3	EDO	4-A	407	4/4	0.28	-	16,17,17,18	10
3	EDO	1-A	410	4/4	0.17	-	15,15,15,16	10
3	EDO	2-A	406	4/4	0.15	-	13,14,14,14	10
3	EDO	8-A	409	4/4	0.10	-	18,19,19,19	10
3	EDO	5-A	414	4/4	0.17	-	14,14,14,14	10
3	EDO	1-A	405	4/4	0.07	-	17,17,18,18	10
2	SO4	4-A	401	5/5	0.08	-	23,24,24,25	5

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	9-A	410	4/4	0.17	-	15,15,15,15	10
3	EDO	1-A	409	4/4	0.10	-	18,19,20,20	10
3	EDO	1-A	413	4/4	0.11	-	18,19,20,20	10
3	EDO	1-A	416	4/4	0.49	-	20,20,21,22	10
3	EDO	4-A	405	4/4	0.07	-	17,17,18,18	10
3	EDO	9-A	414	4/4	0.17	-	14,14,14,14	10
3	EDO	7-A	416	4/4	0.49	-	19,19,20,20	10
3	EDO	8-A	408	4/4	0.24	-	15,16,16,16	10
3	EDO	7-A	408	4/4	0.24	-	16,16,16,17	10
3	EDO	6-A	407	4/4	0.28	-	16,16,17,17	10
3	EDO	4-A	416	4/4	0.49	-	19,19,20,20	10
3	EDO	1-A	406	4/4	0.15	-	13,13,14,14	10
3	EDO	9-A	415	4/4	0.24	-	16,17,18,18	10
3	EDO	9-A	416	4/4	0.49	-	19,19,20,20	10
3	EDO	4-A	414	4/4	0.17	-	13,14,14,14	10
2	SO4	9-A	403	5/5	0.55	-	23,24,25,25	5
2	SO4	3-A	402	5/5	0.36	-	20,20,21,21	5
3	EDO	4-A	412	4/4	0.21	-	19,20,21,21	10
3	EDO	2-A	410	4/4	0.17	-	14,15,15,15	10
2	SO4	4-A	402	5/5	0.36	-	21,21,21,22	5
3	EDO	2-A	416	4/4	0.49	-	19,19,21,21	10
2	SO4	4-A	403	5/5	0.55	-	26,26,27,28	5
3	EDO	5-A	407	4/4	0.28	-	16,16,17,17	10
3	EDO	6-A	412	4/4	0.21	-	19,20,20,21	10
3	EDO	2-A	405	4/4	0.07	-	17,17,17,18	10
3	EDO	6-A	413	4/4	0.11	-	17,18,19,19	10
3	EDO	7-A	412	4/4	0.21	-	18,19,20,20	10
3	EDO	1-A	412	4/4	0.21	-	19,20,20,20	10
3	EDO	3-A	405	4/4	0.07	-	17,17,18,18	10
3	EDO	7-A	414	4/4	0.17	-	14,14,14,14	10
2	SO4	1-A	402	5/5	0.36	-	20,20,21,21	5
3	EDO	8-A	416	4/4	0.49	-	18,19,20,20	10
3	EDO	8-A	413	4/4	0.11	-	17,18,19,19	10
3	EDO	3-A	411	4/4	0.17	-	14,14,14,14	10
3	EDO	6-A	415	4/4	0.24	-	16,16,17,18	10
3	EDO	4-A	409	4/4	0.10	-	18,18,19,19	10
3	EDO	8-A	406	4/4	0.15	-	14,14,14,14	10
3	EDO	5-A	415	4/4	0.24	-	16,17,17,18	10
3	EDO	1-A	408	4/4	0.24	-	16,16,16,17	10
3	EDO	3-A	410	4/4	0.17	-	14,14,15,15	10
3	EDO	8-A	412	4/4	0.21	-	19,20,21,21	10
2	SO4	8-A	404	5/5	0.12	-	20,20,20,21	5

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	7-A	401	5/5	0.08	-	23,23,23,24	5
2	SO4	2-A	401	5/5	0.08	-	23,23,24,24	5
2	SO4	6-A	403	5/5	0.55	-	25,25,26,27	5
3	EDO	6-A	406	4/4	0.15	-	13,13,14,14	10
2	SO4	2-A	402	5/5	0.36	-	21,22,22,23	5
3	EDO	5-A	406	4/4	0.15	-	13,14,14,14	10
3	EDO	6-A	405	4/4	0.07	-	17,17,18,18	10
2	SO4	1-A	404	5/5	0.12	-	18,18,18,19	5
3	EDO	4-A	415	4/4	0.24	-	16,17,18,18	10
3	EDO	2-A	415	4/4	0.24	-	16,17,17,17	10
3	EDO	8-A	414	4/4	0.17	-	13,14,14,14	10
3	EDO	4-A	413	4/4	0.11	-	17,18,19,19	10
3	EDO	4-A	408	4/4	0.24	-	16,17,18,18	10
2	SO4	5-A	404	5/5	0.12	-	17,17,18,18	5
3	EDO	3-A	409	4/4	0.10	-	18,19,20,20	10
2	SO4	6-A	402	5/5	0.36	-	20,20,21,21	5
3	EDO	2-A	408	4/4	0.24	-	15,16,16,16	10
2	SO4	8-A	402	5/5	0.36	-	22,22,23,24	5
3	EDO	2-A	412	4/4	0.21	-	19,19,20,21	10
2	SO4	9-A	402	5/5	0.36	-	20,20,21,21	5
3	EDO	5-A	412	4/4	0.21	-	19,20,21,21	10
3	EDO	6-A	411	4/4	0.17	-	14,14,14,14	10
3	EDO	8-A	410	4/4	0.17	-	14,14,15,15	10
3	EDO	5-A	411	4/4	0.17	-	14,14,14,14	10
3	EDO	7-A	415	4/4	0.24	-	17,17,18,18	10
3	EDO	3-A	416	4/4	0.49	-	19,20,20,21	10
2	SO4	1-A	401	5/5	0.08	-	25,25,26,26	5
3	EDO	1-A	415	4/4	0.24	-	16,16,17,17	10
3	EDO	1-A	407	4/4	0.28	-	16,16,17,17	10
3	EDO	3-A	408	4/4	0.24	-	16,16,17,17	10
3	EDO	7-A	409	4/4	0.10	-	18,19,20,20	10
3	EDO	7-A	407	4/4	0.28	-	15,16,16,17	10
2	SO4	5-A	402	5/5	0.36	-	20,20,21,21	5
3	EDO	7-A	410	4/4	0.17	-	14,15,15,15	10
3	EDO	9-A	411	4/4	0.17	-	14,14,14,14	10
3	EDO	7-A	405	4/4	0.07	-	17,17,18,18	10
3	EDO	4-A	411	4/4	0.17	-	14,14,14,14	10
3	EDO	7-A	406	4/4	0.15	-	13,14,14,14	10
3	EDO	6-A	409	4/4	0.10	-	18,19,19,20	10
2	SO4	5-A	403	5/5	0.55	-	24,25,25,25	5
2	SO4	9-A	401	5/5	0.08	-	23,24,24,25	5
3	EDO	7-A	413	4/4	0.11	-	17,18,19,19	10

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	2-A	411	4/4	0.17	-	14,14,14,14	10
3	EDO	6-A	416	4/4	0.49	-	18,19,20,20	10
3	EDO	5-A	416	4/4	0.49	-	18,19,19,20	10
2	SO4	6-A	404	5/5	0.12	-	20,20,21,21	5
3	EDO	2-A	407	4/4	0.28	-	16,16,17,17	10
2	SO4	5-A	401	5/5	0.08	-	23,23,23,24	5
3	EDO	3-A	412	4/4	0.21	-	19,20,20,21	10
2	SO4	2-A	404	5/5	0.12	-	18,19,20,20	5
2	SO4	2-A	403	5/5	0.55	-	25,25,25,26	5
3	EDO	4-A	406	4/4	0.15	-	13,14,14,14	10
2	SO4	9-A	404	5/5	0.12	-	18,18,19,19	5

## 6.5 Other polymers

There are no such residues in this entry.