



# wwPDB X-ray Structure Validation Summary Report (i)

Feb 27, 2014 – 04:56 AM GMT

PDB ID : 2Q3T  
Title : Ensemble refinement of the protein crystal structure of gene product from Arabidopsis thaliana At3g22680  
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)  
Deposited on : 2007-05-30  
Resolution : 1.60 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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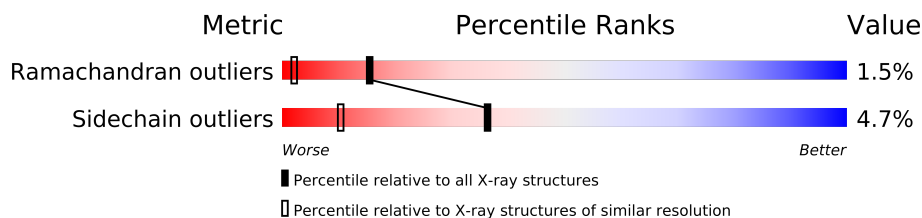
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : **FAILED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	78287	2126 (1.60-1.60)
Sidechain outliers	78261	2125 (1.60-1.60)

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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1-A	157	
1	10-A	157	
1	11-A	157	
1	12-A	157	
1	13-A	157	
1	14-A	157	
1	15-A	157	
1	16-A	157	
1	2-A	157	
1	3-A	157	
1	4-A	157	
1	5-A	157	
1	6-A	157	
1	7-A	157	
1	8-A	157	
1	9-A	157	

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	1-A	300	X	-
2	SO4	11-A	300	X	-
2	SO4	14-A	301	X	-
2	SO4	15-A	301	X	-
2	SO4	2-A	301	X	-
2	SO4	7-A	301	X	-
2	SO4	9-A	301	X	-
3	CPS	1-A	200	X	-
3	CPS	10-A	200	X	-
3	CPS	11-A	200	X	-
3	CPS	12-A	200	X	-
3	CPS	13-A	200	X	-
3	CPS	14-A	200	X	-
3	CPS	15-A	200	X	-
3	CPS	16-A	200	X	-
3	CPS	2-A	200	X	-
3	CPS	3-A	200	X	-
3	CPS	5-A	200	X	-
3	CPS	6-A	200	X	-
3	CPS	7-A	200	X	-
3	CPS	8-A	200	X	-
3	CPS	9-A	200	X	-
4	EDO	1-A	402	X	-
4	EDO	10-A	404	X	-
4	EDO	11-A	403	X	-
4	EDO	12-A	404	X	-
4	EDO	13-A	403	X	-
4	EDO	13-A	404	X	-
4	EDO	14-A	401	X	-
4	EDO	14-A	402	X	-
4	EDO	14-A	403	X	-
4	EDO	15-A	403	X	-
4	EDO	15-A	404	X	-
4	EDO	16-A	403	X	-
4	EDO	3-A	403	X	-
4	EDO	3-A	404	X	-
4	EDO	4-A	402	X	-
4	EDO	4-A	404	X	-
4	EDO	5-A	402	X	-
4	EDO	5-A	404	X	-
4	EDO	8-A	402	X	-
4	EDO	8-A	403	X	-
4	EDO	8-A	404	X	-

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Mol	Type	Chain	Res	Geometry	Electron density
4	EDO	9-A	402	X	-
4	EDO	9-A	404	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19808 atoms, of which 0 are hydrogen 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.

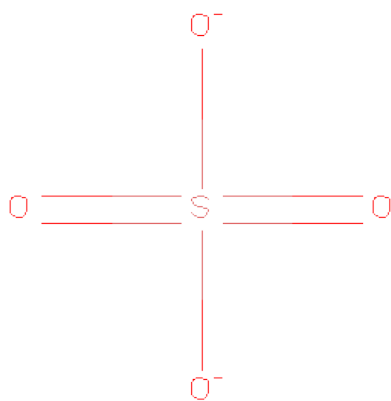
- Molecule 1 is a protein called Protein At3g22680.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	2-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	3-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	4-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	5-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	6-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	7-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	8-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	9-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	10-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	11-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	12-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	13-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	14-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	15-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	16-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP Q9LUJ3

- 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	1-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	2-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	3-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	4-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	5-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	6-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	7-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	8-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	9-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	10-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		

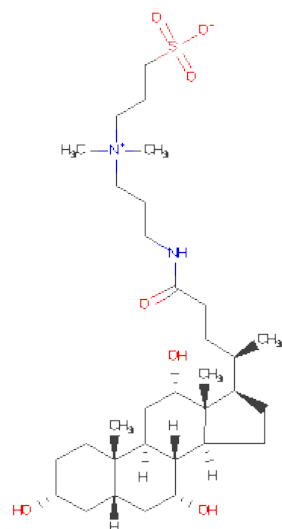
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	11-A	1	Total	O	S	0	0
			5	4	1		
2	11-A	1	Total	O	S	0	0
			5	4	1		
2	12-A	1	Total	O	S	0	0
			5	4	1		
2	12-A	1	Total	O	S	0	0
			5	4	1		
2	12-A	1	Total	O	S	0	0
			5	4	1		
2	13-A	1	Total	O	S	0	0
			5	4	1		
2	13-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	14-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	15-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	16-A	1	Total	O	S	0	0
			5	4	1		
2	16-A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (three-letter code: CPS) (formula: C<sub>32</sub>H<sub>58</sub>N<sub>2</sub>O<sub>7</sub>S).





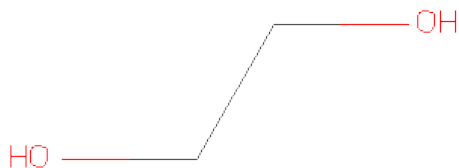
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	1-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	2-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	3-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	4-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	5-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	6-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	7-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	8-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	9-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	10-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	11-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	12-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	13-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	14-A	1	Total	C	N	O	0	0
			32	27	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	15-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	16-A	1	Total	C	N	O	0	0
			32	27	1	4		

- Molecule 4 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
4	1-A	1	Total	C	O	0	0
			4	2	2		
4	1-A	1	Total	C	O	0	0
			4	2	2		
4	1-A	1	Total	C	O	0	0
			4	2	2		
4	1-A	1	Total	C	O	0	0
			4	2	2		
4	2-A	1	Total	C	O	0	0
			4	2	2		
4	2-A	1	Total	C	O	0	0
			4	2	2		
4	2-A	1	Total	C	O	0	0
			4	2	2		
4	2-A	1	Total	C	O	0	0
			4	2	2		
4	3-A	1	Total	C	O	0	0
			4	2	2		

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	8-A	1	Total 4	C 2	O 2	0	0
4	8-A	1	Total 4	C 2	O 2	0	0
4	9-A	1	Total 4	C 2	O 2	0	0
4	9-A	1	Total 4	C 2	O 2	0	0
4	9-A	1	Total 4	C 2	O 2	0	0
4	9-A	1	Total 4	C 2	O 2	0	0
4	10-A	1	Total 4	C 2	O 2	0	0
4	10-A	1	Total 4	C 2	O 2	0	0
4	10-A	1	Total 4	C 2	O 2	0	0
4	10-A	1	Total 4	C 2	O 2	0	0
4	11-A	1	Total 4	C 2	O 2	0	0
4	11-A	1	Total 4	C 2	O 2	0	0
4	11-A	1	Total 4	C 2	O 2	0	0
4	11-A	1	Total 4	C 2	O 2	0	0
4	12-A	1	Total 4	C 2	O 2	0	0
4	12-A	1	Total 4	C 2	O 2	0	0
4	12-A	1	Total 4	C 2	O 2	0	0
4	12-A	1	Total 4	C 2	O 2	0	0
4	13-A	1	Total 4	C 2	O 2	0	0
4	13-A	1	Total 4	C 2	O 2	0	0
4	13-A	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	13-A	1	Total C O 4 2 2	0	0
4	14-A	1	Total C O 4 2 2	0	0
4	14-A	1	Total C O 4 2 2	0	0
4	14-A	1	Total C O 4 2 2	0	0
4	14-A	1	Total C O 4 2 2	0	0
4	15-A	1	Total C O 4 2 2	0	0
4	15-A	1	Total C O 4 2 2	0	0
4	15-A	1	Total C O 4 2 2	0	0
4	15-A	1	Total C O 4 2 2	0	0
4	16-A	1	Total C O 4 2 2	0	0
4	16-A	1	Total C O 4 2 2	0	0
4	16-A	1	Total C O 4 2 2	0	0
4	16-A	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	1-A	172	Total O 172 172	0	0
5	2-A	172	Total O 172 172	0	0
5	3-A	172	Total O 172 172	0	0
5	4-A	172	Total O 172 172	0	0
5	5-A	172	Total O 172 172	0	0
5	6-A	172	Total O 172 172	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	7-A	172	Total 172	O 172	0	0
5	8-A	172	Total 172	O 172	0	0
5	9-A	172	Total 172	O 172	0	0
5	10-A	172	Total 172	O 172	0	0
5	11-A	172	Total 172	O 172	0	0
5	12-A	172	Total 172	O 172	0	0
5	13-A	172	Total 172	O 172	0	0
5	14-A	172	Total 172	O 172	0	0
5	15-A	172	Total 172	O 172	0	0
5	16-A	172	Total 172	O 172	0	0

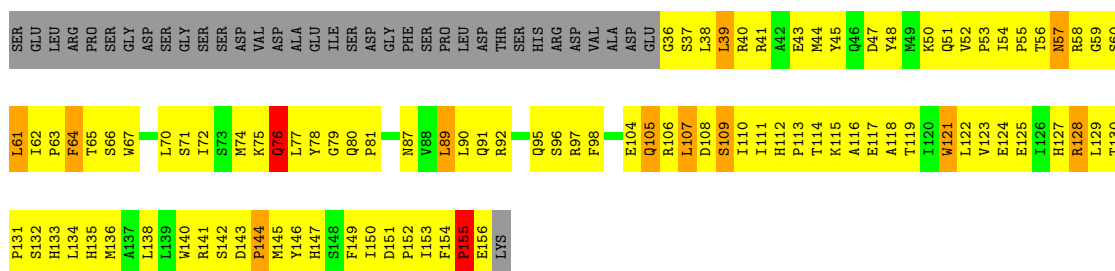
### 3 Residue-property plots

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.

Note EDS failed to run properly.

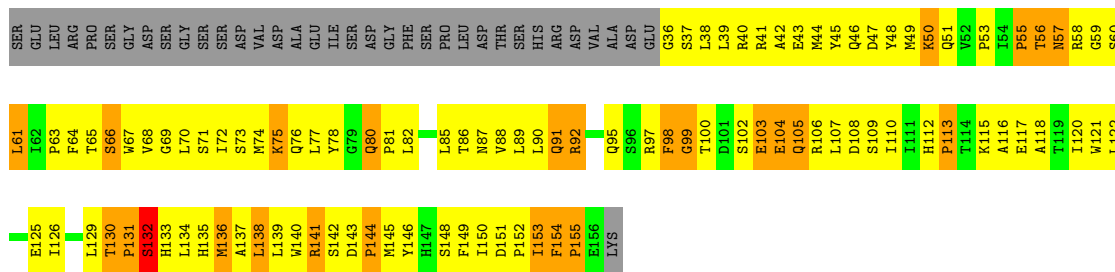
#### • Molecule 1: Protein At3g22680

Chain 1-A:



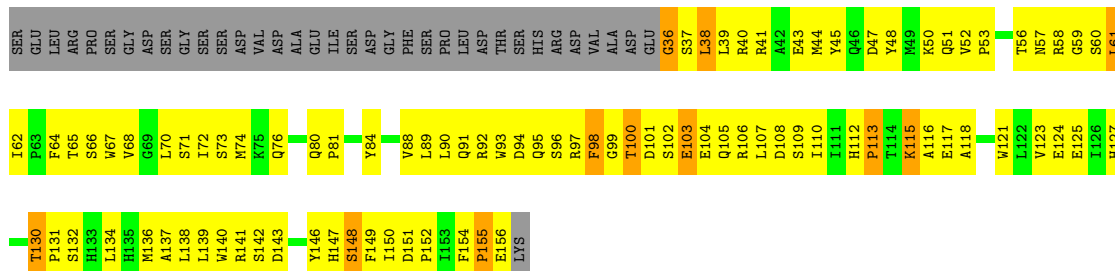
#### • Molecule 1: Protein At3g22680

Chain 2-A:



#### • Molecule 1: Protein At3g22680

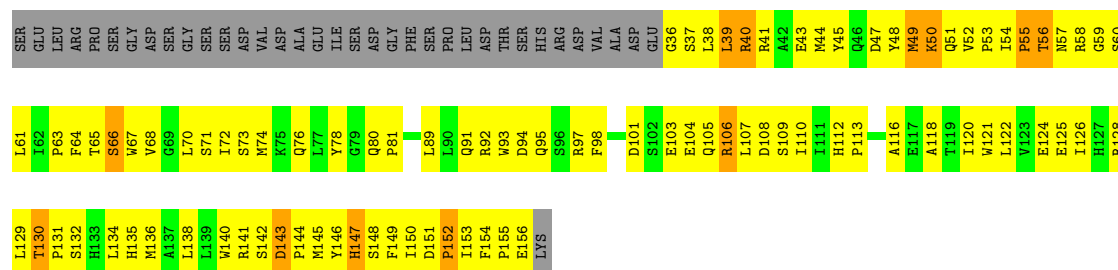
Chain 3-A:



#### • Molecule 1: Protein At3g22680

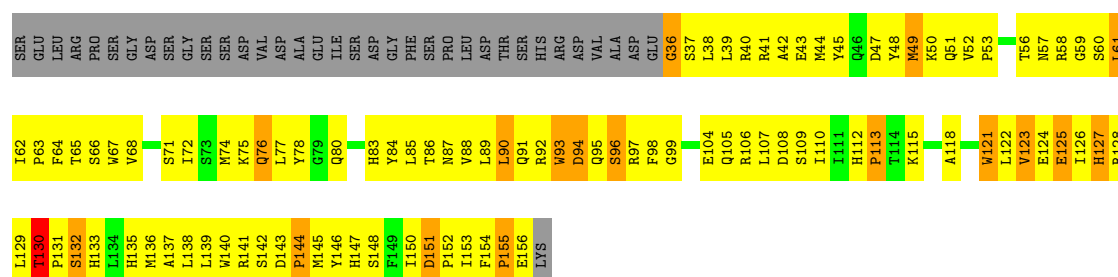






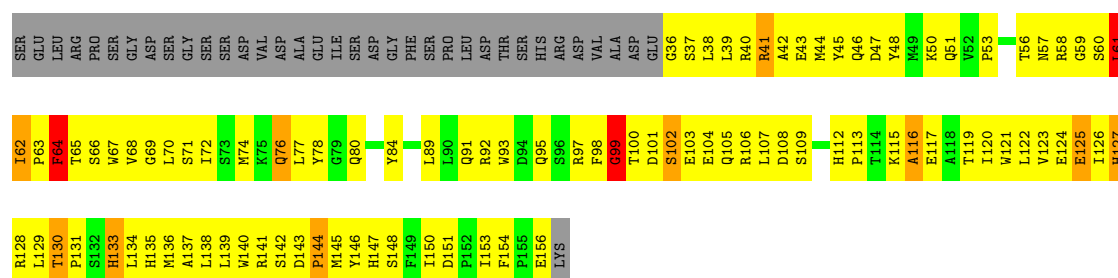
• Molecule 1: Protein At3g22680

Chain 9-A:



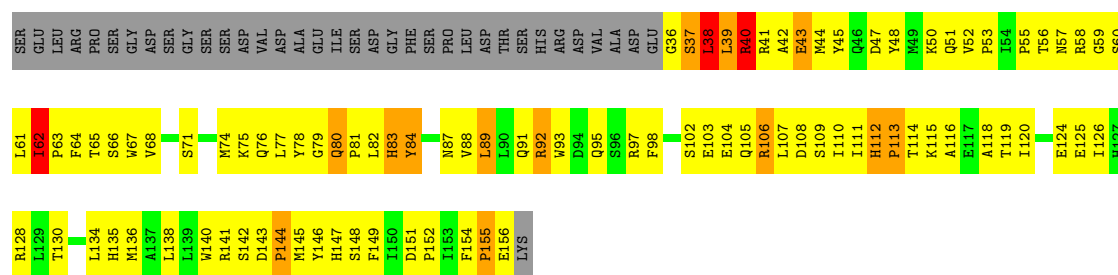
• Molecule 1: Protein At3g22680

Chain 10-A:



• Molecule 1: Protein At3g22680

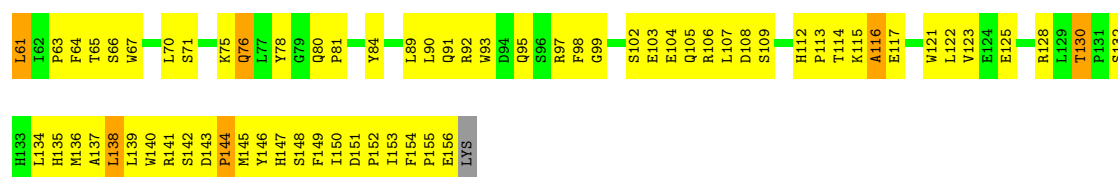
Chain 11-A:



• Molecule 1: Protein At3g22680

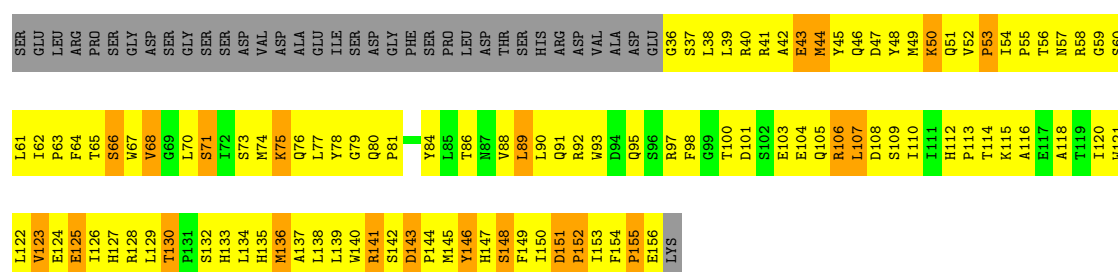
Chain 12-A:





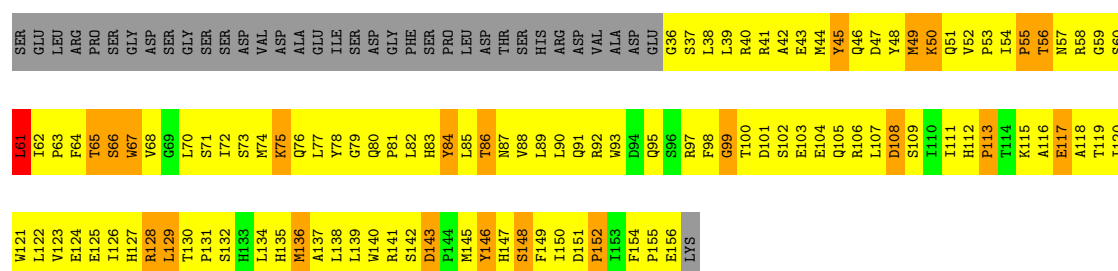
• Molecule 1: Protein At3g22680

Chain 13-A:



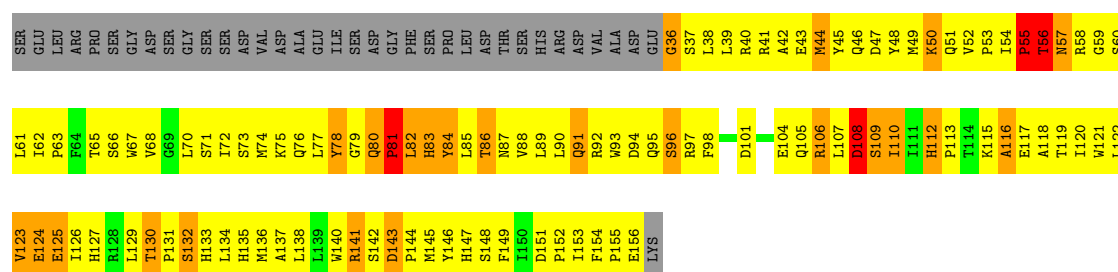
• Molecule 1: Protein At3g22680

Chain 14-A:



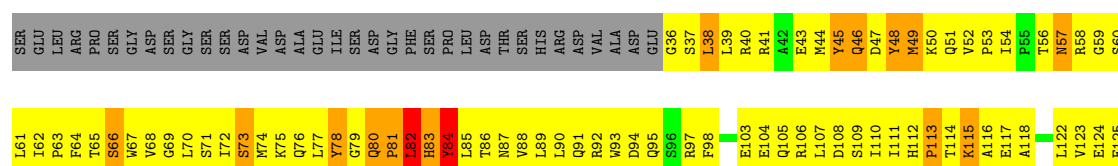
• Molecule 1: Protein At3g22680

Chain 15-A:



• Molecule 1: Protein At3g22680

Chain 16-A:



I126	H127	R128	L129	T130	P131	S132	H133	L134	M135	M136	A137	L138	L139	W140	R141	S142	D143	P144	M145	Y146	H147	S148	F149	I150	D151	P152	I153	F154	P155	E156	LYS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----

## 4 Data and refinement statistics i

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.45Å 83.45Å 60.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.03 – 1.60	Depositor
% Data completeness (in resolution range)	99.9 (31.03-1.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.43 (at 1.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.139 , 0.170	Depositor
Wilson B-factor (Å <sup>2</sup> )	18.0	Xtriage
Anisotropy	0.019	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 32203 reflections	Xtriage
Total number of atoms	19808	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.97% 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: CPS, 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	4.50	189/1034 (18.3%)	3.79	147/1407 (10.4%)
1	2-A	4.69	207/1034 (20.0%)	3.87	188/1407 (13.4%)
1	3-A	4.13	142/1034 (13.7%)	3.38	132/1407 (9.4%)
1	4-A	4.59	179/1034 (17.3%)	3.79	163/1407 (11.6%)
1	5-A	4.18	159/1034 (15.4%)	3.83	138/1407 (9.8%)
1	6-A	3.79	135/1034 (13.1%)	3.37	122/1407 (8.7%)
1	7-A	4.00	151/1034 (14.6%)	3.40	123/1407 (8.7%)
1	8-A	4.47	190/1034 (18.4%)	3.61	155/1407 (11.0%)
1	9-A	4.83	213/1034 (20.6%)	3.87	182/1407 (12.9%)
1	10-A	4.80	201/1034 (19.4%)	3.91	178/1407 (12.7%)
1	11-A	4.73	194/1034 (18.8%)	3.86	149/1407 (10.6%)
1	12-A	3.70	132/1034 (12.8%)	3.21	115/1407 (8.2%)
1	13-A	5.17	237/1034 (22.9%)	4.26	209/1407 (14.9%)
1	14-A	5.92	268/1034 (25.9%)	4.61	246/1407 (17.5%)
1	15-A	5.89	293/1034 (28.3%)	4.79	270/1407 (19.2%)
1	16-A	6.21	303/1034 (29.3%)	5.01	264/1407 (18.8%)
All	All	4.78	3193/16544 (19.3%)	3.94	2781/22512 (12.4%)

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	10
1	2-A	0	16
1	3-A	0	5
1	4-A	0	15
1	5-A	0	4
1	6-A	0	6
1	7-A	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	8-A	0	6
1	9-A	0	8
1	10-A	0	8
1	11-A	0	10
1	12-A	0	5
1	13-A	0	14
1	14-A	0	17
1	15-A	0	21
1	16-A	0	18
All	All	0	168

The worst 5 of 3193 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	14-A	45	TYR	CD2-CE2	48.45	2.12	1.39
1	14-A	124	GLU	CD-OE1	42.84	1.72	1.25
1	16-A	93	TRP	CG-CD1	37.28	1.89	1.36
1	11-A	78	TYR	CD1-CE1	36.76	1.94	1.39
1	15-A	49	MET	CG-SD	36.34	2.75	1.81

The worst 5 of 2781 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16-A	143	ASP	CB-CG-OD1	-59.30	64.92	118.30
1	11-A	40	ARG	NE-CZ-NH1	40.59	140.59	120.30
1	13-A	92	ARG	NE-CZ-NH1	38.80	139.70	120.30
1	5-A	92	ARG	NE-CZ-NH2	-38.57	101.01	120.30
1	7-A	92	ARG	NE-CZ-NH2	-37.16	101.72	120.30

There are no chirality outliers.

5 of 168 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	105	GLN	Mainchain
1	1-A	39	LEU	Mainchain
1	1-A	57	ASN	Mainchain
1	1-A	76	GLN	Mainchain
1	1-A	89	LEU	Mainchain

## 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	1003	0	985	0	2
1	2-A	1003	0	985	0	0
1	3-A	1003	0	986	0	0
1	4-A	1003	0	986	0	1
1	5-A	1003	0	985	0	1
1	6-A	1003	0	986	0	1
1	7-A	1003	0	985	0	0
1	8-A	1003	0	985	0	0
1	9-A	1003	0	986	0	4
1	10-A	1003	0	986	0	2
1	11-A	1003	0	986	0	2
1	12-A	1003	0	986	0	0
1	13-A	1003	0	986	0	0
1	14-A	1003	0	986	0	0
1	15-A	1003	0	984	0	0
1	16-A	1003	0	986	0	0
2	1-A	15	0	0	0	0
2	2-A	15	0	0	0	0
2	3-A	15	0	0	0	0
2	4-A	15	0	0	0	0
2	5-A	15	0	0	0	0
2	6-A	15	0	0	0	0
2	7-A	15	0	0	0	0
2	8-A	15	0	0	0	0
2	9-A	15	0	0	0	0
2	10-A	15	0	0	0	0
2	11-A	15	0	0	0	0
2	12-A	15	0	0	0	0
2	13-A	15	0	0	0	0
2	14-A	15	0	0	0	0
2	15-A	15	0	0	0	0
2	16-A	15	0	0	0	0
3	1-A	32	0	33	0	2
3	2-A	32	0	33	0	0
3	3-A	32	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	4-A	32	0	38	0	0
3	5-A	32	0	28	0	2
3	6-A	32	0	31	0	1
3	7-A	32	0	30	0	0
3	8-A	32	0	38	0	0
3	9-A	32	0	39	0	0
3	10-A	32	0	28	0	0
3	11-A	32	0	34	0	1
3	12-A	32	0	29	0	0
3	13-A	32	0	37	0	0
3	14-A	32	0	23	0	0
3	15-A	32	0	38	0	0
3	16-A	32	0	27	0	0
4	1-A	16	0	23	0	0
4	2-A	16	0	22	0	0
4	3-A	16	0	22	0	0
4	4-A	16	0	22	0	0
4	5-A	16	0	22	0	1
4	6-A	16	0	23	0	0
4	7-A	16	0	22	0	0
4	8-A	16	0	22	0	0
4	9-A	16	0	22	0	0
4	10-A	16	0	22	0	0
4	11-A	16	0	23	0	0
4	12-A	16	0	22	0	0
4	13-A	16	0	22	0	1
4	14-A	16	0	23	0	1
4	15-A	16	0	22	0	1
4	16-A	16	0	23	0	0
5	1-A	172	0	0	0	0
5	2-A	172	0	0	0	0
5	3-A	172	0	0	0	0
5	4-A	172	0	0	0	0
5	5-A	172	0	0	0	0
5	6-A	172	0	0	0	0
5	7-A	172	0	0	0	0
5	8-A	172	0	0	0	0
5	9-A	172	0	0	0	3
5	10-A	172	0	0	0	1
5	11-A	172	0	0	0	1
5	12-A	172	0	0	0	0
5	13-A	172	0	0	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	14-A	172	0	0	0	1
5	15-A	172	0	0	0	1
5	16-A	172	0	0	0	0
All	All	19808	0	16631	0	17

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 17 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:76:GLN:OE1	3:A:200:CPS:O3[2_655]	1.59	0.61
1:A:76:GLN:NE2	5:A:569:HOH:O[2_655]	1.90	0.30
1:A:73:SER:OG	3:A:200:CPS:O2[2_655]	1.93	0.27
4:A:403:EDO:O1	5:A:547:HOH:O[2_655]	1.99	0.21
1:A:76:GLN:OE1	5:A:525:HOH:O[2_655]	2.00	0.20

## 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	119/157 (76%)	114 (96%)	4 (3%)	1 (1%)	27	7
1	2-A	119/157 (76%)	107 (90%)	8 (7%)	4 (3%)	6	0
1	3-A	119/157 (76%)	111 (93%)	5 (4%)	3 (2%)	9	1
1	4-A	119/157 (76%)	114 (96%)	4 (3%)	1 (1%)	27	7
1	5-A	119/157 (76%)	117 (98%)	1 (1%)	1 (1%)	27	7
1	6-A	119/157 (76%)	116 (98%)	2 (2%)	1 (1%)	27	7
1	7-A	119/157 (76%)	117 (98%)	1 (1%)	1 (1%)	27	7
1	8-A	119/157 (76%)	116 (98%)	1 (1%)	2 (2%)	14	2
1	9-A	119/157 (76%)	114 (96%)	4 (3%)	1 (1%)	27	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	10-A	119/157 (76%)	114 (96%)	2 (2%)	3 (2%)	9	1
1	11-A	119/157 (76%)	110 (92%)	6 (5%)	3 (2%)	9	1
1	12-A	119/157 (76%)	117 (98%)	1 (1%)	1 (1%)	27	7
1	13-A	119/157 (76%)	113 (95%)	5 (4%)	1 (1%)	27	7
1	14-A	119/157 (76%)	116 (98%)	3 (2%)	0	100	100
1	15-A	119/157 (76%)	106 (89%)	10 (8%)	3 (2%)	9	1
1	16-A	119/157 (76%)	113 (95%)	3 (2%)	3 (2%)	9	1
All	All	1904/2512 (76%)	1815 (95%)	60 (3%)	29 (2%)	15	2

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2-A	132	SER
1	3-A	103	GLU
1	10-A	102	SER
1	11-A	83	HIS
1	15-A	83	HIS

### 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	112/143 (78%)	108 (96%)	4 (4%)	47	17
1	2-A	112/143 (78%)	104 (93%)	8 (7%)	21	4
1	3-A	112/143 (78%)	108 (96%)	4 (4%)	47	17
1	4-A	112/143 (78%)	105 (94%)	7 (6%)	25	5
1	5-A	112/143 (78%)	107 (96%)	5 (4%)	38	11
1	6-A	112/143 (78%)	109 (97%)	3 (3%)	57	26
1	7-A	112/143 (78%)	110 (98%)	2 (2%)	71	44
1	8-A	112/143 (78%)	108 (96%)	4 (4%)	47	17
1	9-A	112/143 (78%)	106 (95%)	6 (5%)	31	7
1	10-A	112/143 (78%)	109 (97%)	3 (3%)	57	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	11-A	112/143 (78%)	107 (96%)	5 (4%)	38	11
1	12-A	112/143 (78%)	110 (98%)	2 (2%)	71	44
1	13-A	112/143 (78%)	104 (93%)	8 (7%)	21	4
1	14-A	112/143 (78%)	105 (94%)	7 (6%)	25	5
1	15-A	112/143 (78%)	103 (92%)	9 (8%)	17	2
1	16-A	112/143 (78%)	104 (93%)	8 (7%)	21	4
All	All	1792/2288 (78%)	1707 (95%)	85 (5%)	36	10

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	9-A	61	LEU
1	11-A	80	GLN
1	16-A	66	SER
1	9-A	113	PRO
1	10-A	61	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	11-A	87	ASN
1	11-A	95	GLN
1	15-A	80	GLN
1	9-A	105	GLN
1	13-A	135	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 ⓘ

128 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$
3	CPS	1-A	200	-	35,35,45	18.98	30 (85%)	54,54,70	10.89	48 (88%)
2	SO4	1-A	300	-	4,4,4	4.07	4 (100%)	6,6,6	1.76	2 (33%)
2	SO4	1-A	301	-	4,4,4	2.94	1 (25%)	6,6,6	0.78	0
2	SO4	1-A	302	-	4,4,4	0.65	0	6,6,6	0.40	0
4	EDO	1-A	401	-	3,3,3	2.14	1 (33%)	2,2,2	0.60	0
4	EDO	1-A	402	-	3,3,3	2.82	2 (66%)	2,2,2	2.11	1 (50%)
4	EDO	1-A	403	-	3,3,3	2.83	2 (66%)	2,2,2	0.92	0
4	EDO	1-A	404	-	3,3,3	4.86	2 (66%)	2,2,2	1.19	0
3	CPS	10-A	200	-	35,35,45	19.64	34 (97%)	54,54,70	11.84	44 (81%)
2	SO4	10-A	300	-	4,4,4	1.14	0	6,6,6	0.91	0
2	SO4	10-A	301	-	4,4,4	6.44	3 (75%)	6,6,6	2.38	1 (16%)
2	SO4	10-A	302	-	4,4,4	1.43	1 (25%)	6,6,6	0.53	0
4	EDO	10-A	401	-	3,3,3	1.55	1 (33%)	2,2,2	0.34	0
4	EDO	10-A	402	-	3,3,3	2.42	2 (66%)	2,2,2	1.15	0
4	EDO	10-A	403	-	3,3,3	2.87	2 (66%)	2,2,2	1.39	0
4	EDO	10-A	404	-	3,3,3	3.07	2 (66%)	2,2,2	2.08	1 (50%)
3	CPS	11-A	200	-	35,35,45	16.56	31 (88%)	54,54,70	10.03	45 (83%)
2	SO4	11-A	300	-	4,4,4	9.66	3 (75%)	6,6,6	5.31	6 (100%)
2	SO4	11-A	301	-	4,4,4	2.33	2 (50%)	6,6,6	1.75	2 (33%)
2	SO4	11-A	302	-	4,4,4	0.71	0	6,6,6	0.33	0
4	EDO	11-A	401	-	3,3,3	1.54	1 (33%)	2,2,2	1.31	0
4	EDO	11-A	402	-	3,3,3	2.40	2 (66%)	2,2,2	1.43	0
4	EDO	11-A	403	-	3,3,3	3.59	2 (66%)	2,2,2	2.07	1 (50%)
4	EDO	11-A	404	-	3,3,3	3.44	2 (66%)	2,2,2	1.72	0
3	CPS	12-A	200	-	35,35,45	14.10	28 (80%)	54,54,70	10.13	44 (81%)
2	SO4	12-A	300	-	4,4,4	0.66	0	6,6,6	0.73	0
2	SO4	12-A	301	-	4,4,4	4.81	3 (75%)	6,6,6	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	12-A	302	-	4,4,4	0.55	0	6,6,6	0.34	0
4	EDO	12-A	401	-	3,3,3	1.54	1 (33%)	2,2,2	0.94	0
4	EDO	12-A	402	-	3,3,3	2.55	2 (66%)	2,2,2	1.16	0
4	EDO	12-A	403	-	3,3,3	2.88	2 (66%)	2,2,2	0.84	0
4	EDO	12-A	404	-	3,3,3	4.66	3 (100%)	2,2,2	0.68	0
3	CPS	13-A	200	-	35,35,45	21.72	31 (88%)	54,54,70	18.58	40 (74%)
2	SO4	13-A	300	-	4,4,4	2.81	2 (50%)	6,6,6	0.78	0
2	SO4	13-A	301	-	4,4,4	4.91	2 (50%)	6,6,6	2.41	1 (16%)
2	SO4	13-A	302	-	4,4,4	0.72	0	6,6,6	0.44	0
4	EDO	13-A	401	-	3,3,3	2.84	1 (33%)	2,2,2	0.72	0
4	EDO	13-A	402	-	3,3,3	5.01	2 (66%)	2,2,2	0.90	0
4	EDO	13-A	403	-	3,3,3	5.06	3 (100%)	2,2,2	1.97	1 (50%)
4	EDO	13-A	404	-	3,3,3	8.27	3 (100%)	2,2,2	1.14	0
3	CPS	14-A	200	-	35,35,45	23.57	30 (85%)	54,54,70	13.75	42 (77%)
2	SO4	14-A	300	-	4,4,4	7.30	2 (50%)	6,6,6	1.77	2 (33%)
2	SO4	14-A	301	-	4,4,4	4.18	3 (75%)	6,6,6	3.29	3 (50%)
2	SO4	14-A	302	-	4,4,4	0.50	0	6,6,6	0.23	0
4	EDO	14-A	401	-	3,3,3	4.05	3 (100%)	2,2,2	0.56	0
4	EDO	14-A	402	-	3,3,3	2.72	3 (100%)	2,2,2	1.23	0
4	EDO	14-A	403	-	3,3,3	4.50	3 (100%)	2,2,2	2.35	1 (50%)
4	EDO	14-A	404	-	3,3,3	7.56	2 (66%)	2,2,2	0.89	0
3	CPS	15-A	200	-	35,35,45	23.59	34 (97%)	54,54,70	17.80	40 (74%)
2	SO4	15-A	300	-	4,4,4	2.84	2 (50%)	6,6,6	0.75	0
2	SO4	15-A	301	-	4,4,4	5.10	4 (100%)	6,6,6	4.46	3 (50%)
2	SO4	15-A	302	-	4,4,4	2.35	1 (25%)	6,6,6	0.31	0
4	EDO	15-A	401	-	3,3,3	3.10	1 (33%)	2,2,2	0.91	0
4	EDO	15-A	402	-	3,3,3	4.34	2 (66%)	2,2,2	0.67	0
4	EDO	15-A	403	-	3,3,3	4.86	3 (100%)	2,2,2	1.98	1 (50%)
4	EDO	15-A	404	-	3,3,3	7.76	3 (100%)	2,2,2	0.73	0
3	CPS	16-A	200	-	35,35,45	20.27	29 (82%)	54,54,70	10.10	42 (77%)
2	SO4	16-A	300	-	4,4,4	6.96	2 (50%)	6,6,6	1.90	1 (16%)
2	SO4	16-A	301	-	4,4,4	4.42	2 (50%)	6,6,6	0.90	0
2	SO4	16-A	302	-	4,4,4	1.07	1 (25%)	6,6,6	0.34	0
4	EDO	16-A	401	-	3,3,3	1.92	1 (33%)	2,2,2	1.65	1 (50%)
4	EDO	16-A	402	-	3,3,3	1.35	0	2,2,2	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	16-A	403	-	3,3,3	3.08	3 (100%)	2,2,2	2.79	2 (100%)
4	EDO	16-A	404	-	3,3,3	8.09	2 (66%)	2,2,2	1.83	0
3	CPS	2-A	200	-	35,35,45	21.42	30 (85%)	54,54,70	10.55	41 (75%)
2	SO4	2-A	300	-	4,4,4	0.80	0	6,6,6	0.82	0
2	SO4	2-A	301	-	4,4,4	9.58	4 (100%)	6,6,6	1.36	1 (16%)
2	SO4	2-A	302	-	4,4,4	1.36	1 (25%)	6,6,6	0.96	0
4	EDO	2-A	401	-	3,3,3	2.81	2 (66%)	2,2,2	0.86	0
4	EDO	2-A	402	-	3,3,3	2.33	2 (66%)	2,2,2	0.55	0
4	EDO	2-A	403	-	3,3,3	4.48	2 (66%)	2,2,2	0.80	0
4	EDO	2-A	404	-	3,3,3	4.91	2 (66%)	2,2,2	0.95	0
3	CPS	3-A	200	-	35,35,45	37.76	30 (85%)	54,54,70	18.21	47 (87%)
2	SO4	3-A	300	-	4,4,4	2.53	2 (50%)	6,6,6	0.75	0
2	SO4	3-A	301	-	4,4,4	4.22	2 (50%)	6,6,6	0.78	0
2	SO4	3-A	302	-	4,4,4	0.51	0	6,6,6	0.26	0
4	EDO	3-A	401	-	3,3,3	1.48	1 (33%)	2,2,2	0.72	0
4	EDO	3-A	402	-	3,3,3	2.42	2 (66%)	2,2,2	1.57	0
4	EDO	3-A	403	-	3,3,3	2.82	1 (33%)	2,2,2	2.69	2 (100%)
4	EDO	3-A	404	-	3,3,3	3.99	3 (100%)	2,2,2	0.73	0
3	CPS	4-A	200	-	35,35,45	19.19	29 (82%)	54,54,70	9.15	40 (74%)
2	SO4	4-A	300	-	4,4,4	1.28	0	6,6,6	0.83	0
2	SO4	4-A	301	-	4,4,4	4.17	2 (50%)	6,6,6	0.66	0
2	SO4	4-A	302	-	4,4,4	0.75	0	6,6,6	0.36	0
4	EDO	4-A	401	-	3,3,3	1.85	1 (33%)	2,2,2	0.23	0
4	EDO	4-A	402	-	3,3,3	2.43	3 (100%)	2,2,2	0.81	0
4	EDO	4-A	403	-	3,3,3	4.52	2 (66%)	2,2,2	0.56	0
4	EDO	4-A	404	-	3,3,3	5.28	3 (100%)	2,2,2	1.07	0
3	CPS	5-A	200	-	35,35,45	20.17	32 (91%)	54,54,70	12.02	49 (90%)
2	SO4	5-A	300	-	4,4,4	1.69	1 (25%)	6,6,6	0.85	0
2	SO4	5-A	301	-	4,4,4	2.72	1 (25%)	6,6,6	0.97	0
2	SO4	5-A	302	-	4,4,4	1.98	1 (25%)	6,6,6	0.33	0
4	EDO	5-A	401	-	3,3,3	1.03	0	2,2,2	0.91	0
4	EDO	5-A	402	-	3,3,3	2.98	2 (66%)	2,2,2	2.35	2 (100%)
4	EDO	5-A	403	-	3,3,3	3.36	2 (66%)	2,2,2	0.72	0
4	EDO	5-A	404	-	3,3,3	3.83	2 (66%)	2,2,2	1.96	1 (50%)
3	CPS	6-A	200	-	35,35,45	13.79	29 (82%)	54,54,70	8.71	42 (77%)
2	SO4	6-A	300	-	4,4,4	1.38	0	6,6,6	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	6-A	301	-	4,4,4	2.27	2 (50%)	6,6,6	1.31	1 (16%)
2	SO4	6-A	302	-	4,4,4	0.56	0	6,6,6	0.33	0
4	EDO	6-A	401	-	3,3,3	1.42	1 (33%)	2,2,2	2.14	1 (50%)
4	EDO	6-A	402	-	3,3,3	2.33	2 (66%)	2,2,2	0.29	0
4	EDO	6-A	403	-	3,3,3	3.99	2 (66%)	2,2,2	1.06	0
4	EDO	6-A	404	-	3,3,3	2.81	1 (33%)	2,2,2	1.62	0
3	CPS	7-A	200	-	35,35,45	17.58	31 (88%)	54,54,70	10.21	43 (79%)
2	SO4	7-A	300	-	4,4,4	0.50	0	6,6,6	0.76	0
2	SO4	7-A	301	-	4,4,4	7.69	3 (75%)	6,6,6	3.48	2 (33%)
2	SO4	7-A	302	-	4,4,4	0.59	0	6,6,6	0.34	0
4	EDO	7-A	401	-	3,3,3	1.01	0	2,2,2	0.68	0
4	EDO	7-A	402	-	3,3,3	2.44	2 (66%)	2,2,2	1.40	0
4	EDO	7-A	403	-	3,3,3	2.88	2 (66%)	2,2,2	0.87	0
4	EDO	7-A	404	-	3,3,3	2.92	2 (66%)	2,2,2	1.17	0
3	CPS	8-A	200	-	35,35,45	26.79	32 (91%)	54,54,70	13.86	41 (75%)
2	SO4	8-A	300	-	4,4,4	2.91	2 (50%)	6,6,6	1.20	1 (16%)
2	SO4	8-A	301	-	4,4,4	5.41	3 (75%)	6,6,6	2.61	1 (16%)
2	SO4	8-A	302	-	4,4,4	0.94	0	6,6,6	0.52	0
4	EDO	8-A	401	-	3,3,3	1.35	0	2,2,2	0.75	0
4	EDO	8-A	402	-	3,3,3	2.44	3 (100%)	2,2,2	0.90	0
4	EDO	8-A	403	-	3,3,3	2.98	3 (100%)	2,2,2	2.53	2 (100%)
4	EDO	8-A	404	-	3,3,3	3.72	3 (100%)	2,2,2	0.75	0
3	CPS	9-A	200	-	35,35,45	21.27	31 (88%)	54,54,70	16.31	46 (85%)
2	SO4	9-A	300	-	4,4,4	2.64	2 (50%)	6,6,6	1.27	1 (16%)
2	SO4	9-A	301	-	4,4,4	5.58	3 (75%)	6,6,6	3.33	3 (50%)
2	SO4	9-A	302	-	4,4,4	0.72	0	6,6,6	0.29	0
4	EDO	9-A	401	-	3,3,3	1.26	0	2,2,2	0.70	0
4	EDO	9-A	402	-	3,3,3	2.49	3 (100%)	2,2,2	1.11	0
4	EDO	9-A	403	-	3,3,3	2.59	2 (66%)	2,2,2	1.10	0
4	EDO	9-A	404	-	3,3,3	3.52	2 (66%)	2,2,2	2.09	1 (50%)

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CPS	1-A	200	-	5/5/12/15	0/13/78/90	0/0/4/4
2	SO4	1-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	1-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	1-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	1-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	1-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	1-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	1-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	10-A	200	-	4/4/12/15	0/13/78/90	0/0/4/4
2	SO4	10-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	10-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	10-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	10-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	10-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	10-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	10-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	11-A	200	-	5/5/12/15	0/13/78/90	0/0/4/4
2	SO4	11-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	11-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	11-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	11-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	11-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	11-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	11-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	12-A	200	-	5/5/12/15	0/13/78/90	0/0/4/4
2	SO4	12-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	12-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	12-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	12-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	12-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	12-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	12-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	13-A	200	-	5/5/12/15	0/13/78/90	0/0/4/4
2	SO4	13-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	13-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	13-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	13-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	13-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	13-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	13-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	14-A	200	-	5/5/12/15	0/13/78/90	0/0/4/4
2	SO4	14-A	300	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	14-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	14-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	14-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	14-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	14-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	14-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	15-A	200	-	4/4/12/15	0/13/78/90	0/0/4/4
2	SO4	15-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	15-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	15-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	15-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	15-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	15-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	15-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	16-A	200	-	5/5/12/15	0/13/78/90	0/0/4/4
2	SO4	16-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	16-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	16-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	16-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	16-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	16-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	16-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	2-A	200	-	5/5/12/15	0/13/78/90	0/0/4/4
2	SO4	2-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	2-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	2-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	2-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	2-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	2-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	2-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	3-A	200	-	7/7/12/15	0/13/78/90	0/0/4/4
2	SO4	3-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	3-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	3-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	3-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	3-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	3-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	3-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	4-A	200	-	4/4/12/15	0/13/78/90	0/0/4/4
2	SO4	4-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	4-A	301	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	4-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	4-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	4-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	4-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	4-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	5-A	200	-	4/4/12/15	0/13/78/90	0/0/4/4
2	SO4	5-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	5-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	5-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	5-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	5-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	5-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	5-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	6-A	200	-	8/8/12/15	0/13/78/90	0/0/4/4
2	SO4	6-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	6-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	6-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	6-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	6-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	6-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	6-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	7-A	200	-	5/5/12/15	0/13/78/90	0/0/4/4
2	SO4	7-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	7-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	7-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	7-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	7-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	7-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	7-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	8-A	200	-	5/5/12/15	0/13/78/90	0/0/4/4
2	SO4	8-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	8-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	8-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	8-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	8-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	8-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	8-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	9-A	200	-	3/3/12/15	0/13/78/90	0/0/4/4
2	SO4	9-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	9-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	9-A	302	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	9-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	9-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	9-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	9-A	404	-	-	0/1/1/1	0/0/0/0

The worst 5 of 680 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-A	200	CPS	C18-C17	157.14	4.19	1.53
3	3-A	200	CPS	C12-C13	93.99	4.25	1.51
3	8-A	200	CPS	C5-C9	84.77	3.01	1.55
3	3-A	200	CPS	C27-C26	-78.71	1.23	1.55
3	2-A	200	CPS	C3-C4	71.59	2.82	1.53

The worst 5 of 743 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-A	200	CPS	C14-C13-C12	-54.95	40.34	110.54
3	8-A	200	CPS	C8-C9-C5	-49.92	53.61	103.58
3	13-A	200	CPS	C7-C6-C5	-46.58	56.95	103.58
3	5-A	200	CPS	C7-C6-C5	-43.99	59.55	103.58
3	15-A	200	CPS	C6-C5-C4	-43.91	66.77	107.40

5 of 79 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	10-A	200	CPS	C18
3	10-A	200	CPS	C6
3	10-A	200	CPS	C19
3	10-A	200	CPS	C20
3	4-A	200	CPS	C18

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 ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.