



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 06:33 PM UTC

PDB ID : 2Q3T / pdb_00002q3t
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 X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

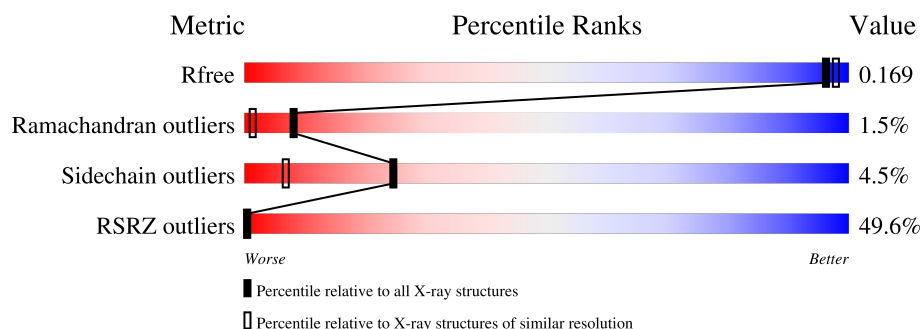
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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))
R_{free}	180053	4673 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	157	38% 56%19%•23%
1	10-A	157	56%20%••23%
1	11-A	157	57%17%••23%
1	12-A	157	59%17%•23%
1	13-A	157	54%21%•23%
1	14-A	157	53%22%•23%

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Mol	Chain	Length	Quality of chain
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, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	1-A	300	-	X	-	-
2	SO4	10-A	301	-	X	-	-
2	SO4	11-A	300	-	X	-	-
2	SO4	13-A	301	-	X	-	-
2	SO4	14-A	300	-	X	-	-
2	SO4	14-A	301	-	X	-	-
2	SO4	15-A	301	-	X	-	-
2	SO4	16-A	300	-	X	-	-
2	SO4	2-A	301	-	X	-	-
2	SO4	7-A	301	-	X	-	-
2	SO4	8-A	301	-	X	-	-
2	SO4	9-A	301	-	X	-	-
3	CPS	1-A	200	X	X	-	-
3	CPS	10-A	200	X	X	-	-
3	CPS	11-A	200	X	X	-	-
3	CPS	12-A	200	X	X	-	-
3	CPS	13-A	200	X	X	-	-
3	CPS	14-A	200	X	X	-	-
3	CPS	15-A	200	X	X	-	-
3	CPS	16-A	200	X	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CPS	2-A	200	X	X	-	-
3	CPS	3-A	200	X	X	-	-
3	CPS	4-A	200	X	X	-	-
3	CPS	5-A	200	X	X	-	-
3	CPS	6-A	200	X	X	-	-
3	CPS	7-A	200	X	X	-	-
3	CPS	8-A	200	X	X	-	-
3	CPS	9-A	200	X	X	-	-
4	EDO	1-A	402	-	X	-	-
4	EDO	1-A	403	-	X	-	-
4	EDO	1-A	404	-	X	-	-
4	EDO	10-A	402	-	X	-	-
4	EDO	10-A	404	-	X	-	-
4	EDO	11-A	403	-	X	-	-
4	EDO	11-A	404	-	X	-	-
4	EDO	12-A	402	-	X	-	-
4	EDO	12-A	403	-	X	-	-
4	EDO	12-A	404	-	X	-	-
4	EDO	13-A	402	-	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	14-A	404	-	X	-	-
4	EDO	15-A	402	-	X	-	-
4	EDO	15-A	403	-	X	-	-
4	EDO	15-A	404	-	X	-	-
4	EDO	16-A	403	-	X	-	-
4	EDO	16-A	404	-	X	-	-
4	EDO	2-A	401	-	X	-	-
4	EDO	2-A	402	-	X	-	-
4	EDO	2-A	403	-	X	-	-
4	EDO	2-A	404	-	X	-	-
4	EDO	3-A	403	-	X	-	-
4	EDO	3-A	404	-	X	-	-
4	EDO	4-A	402	-	X	-	-
4	EDO	4-A	403	-	X	-	-
4	EDO	4-A	404	-	X	-	-
4	EDO	5-A	402	-	X	-	-
4	EDO	5-A	403	-	X	-	-
4	EDO	5-A	404	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	6-A	401	-	X	-	-
4	EDO	6-A	402	-	X	-	-
4	EDO	6-A	403	-	X	-	-
4	EDO	6-A	404	-	X	-	-
4	EDO	7-A	403	-	X	-	-
4	EDO	7-A	404	-	X	-	-
4	EDO	8-A	402	-	X	-	-
4	EDO	8-A	403	-	X	-	-
4	EDO	8-A	404	-	X	-	-
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 hydrogens and 0 are deuteriums.

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

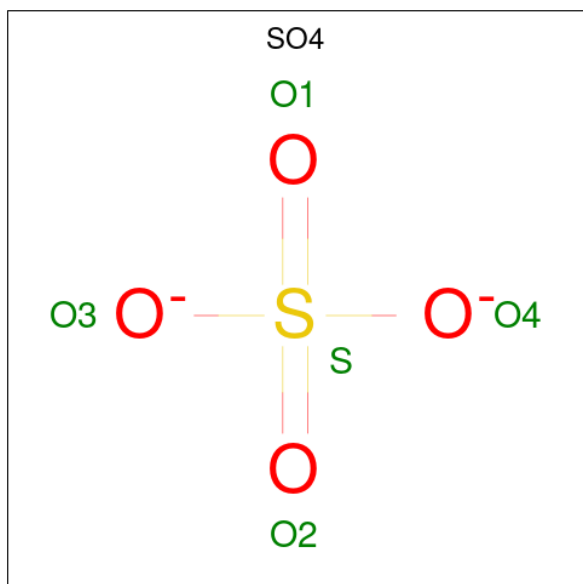
- Molecule 1 is a protein called Protein At3g22680.

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 (CCD ID: SO4) (formula: O₄S).



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		
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		

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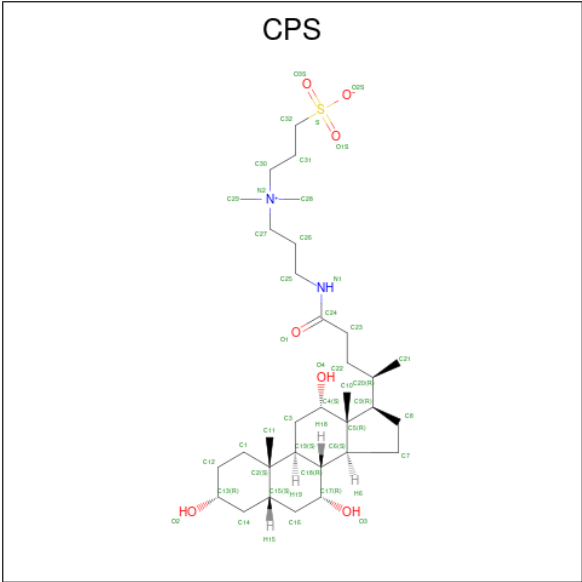
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	11-A	1	Total	O	S	0	0
			5	4	1		
2	12-A	1	Total	O	S	0	0
			5	4	1		
2	13-A	1	Total	O	S	0	0
			5	4	1		
2	14-A	1	Total	O	S	0	0
			5	4	1		
2	15-A	1	Total	O	S	0	0
			5	4	1		
2	16-A	1	Total	O	S	0	0
			5	4	1		
2	1-A	1	Total	O	S	0	0
			5	4	1		
2	2-A	1	Total	O	S	0	0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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	16-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		
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		

- Molecule 3 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (CCD ID: CPS) (formula: C₃₂H₅₈N₂O₇S).



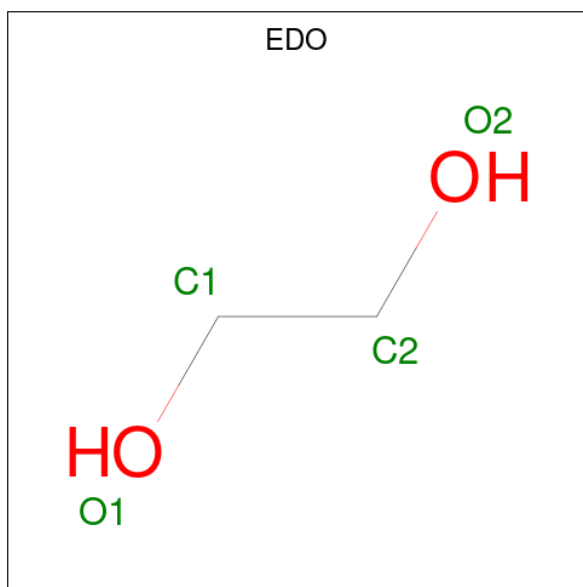
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	1-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	2-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	3-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	4-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	5-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	6-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	7-A	1	Total	C	N	O	0	0
			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 (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	10-A	1	Total	C	O	0	0
			4	2	2		
4	11-A	1	Total	C	O	0	0
			4	2	2		
4	12-A	1	Total	C	O	0	0
			4	2	2		
4	13-A	1	Total	C	O	0	0
			4	2	2		
4	14-A	1	Total	C	O	0	0
			4	2	2		
4	15-A	1	Total	C	O	0	0
			4	2	2		
4	16-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	3-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	6-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	9-A	1	Total	C	O	0	0
			4	2	2		
4	10-A	1	Total	C	O	0	0
			4	2	2		
4	11-A	1	Total	C	O	0	0
			4	2	2		
4	12-A	1	Total	C	O	0	0
			4	2	2		
4	13-A	1	Total	C	O	0	0
			4	2	2		
4	14-A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	15-A	1	Total	C	O	0	0
			4	2	2		
4	16-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	3-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	6-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	9-A	1	Total	C	O	0	0
			4	2	2		
4	10-A	1	Total	C	O	0	0
			4	2	2		
4	11-A	1	Total	C	O	0	0
			4	2	2		
4	12-A	1	Total	C	O	0	0
			4	2	2		
4	13-A	1	Total	C	O	0	0
			4	2	2		
4	14-A	1	Total	C	O	0	0
			4	2	2		
4	15-A	1	Total	C	O	0	0
			4	2	2		
4	16-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	3-A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	4-A	1	Total C O 4 2 2	0	0
4	5-A	1	Total C O 4 2 2	0	0
4	6-A	1	Total C O 4 2 2	0	0
4	7-A	1	Total C O 4 2 2	0	0
4	8-A	1	Total C O 4 2 2	0	0
4	9-A	1	Total C O 4 2 2	0	0
4	10-A	1	Total C O 4 2 2	0	0
4	11-A	1	Total C O 4 2 2	0	0
4	12-A	1	Total C O 4 2 2	0	0
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	15-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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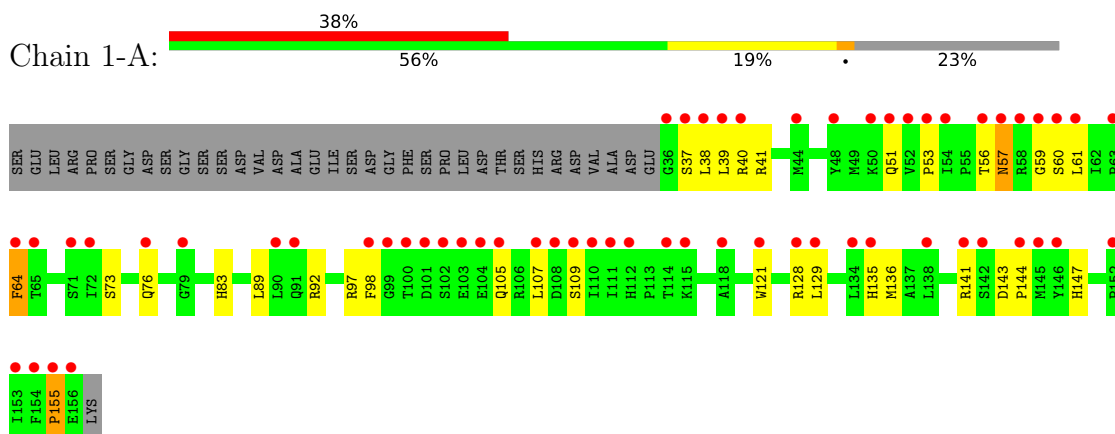
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	7-A	172	Total 172	O 172	0	0
5	8-A	172	Total 172	O 172	0	0
5	9-A	172	Total 172	O 172	0	0
5	10-A	172	Total 172	O 172	0	0
5	11-A	172	Total 172	O 172	0	0
5	12-A	172	Total 172	O 172	0	0
5	13-A	172	Total 172	O 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

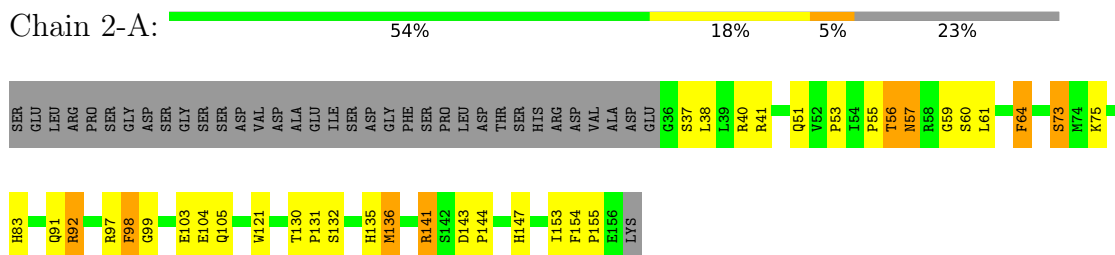
3 Residue-property plots [i](#)

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

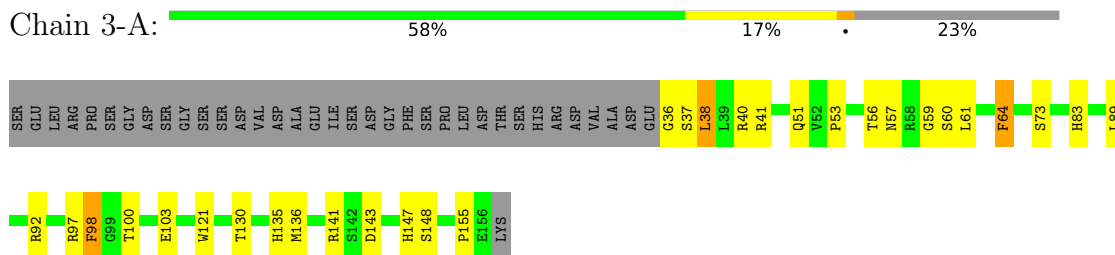
- Molecule 1: Protein At3g22680



- Molecule 1: Protein At3g22680

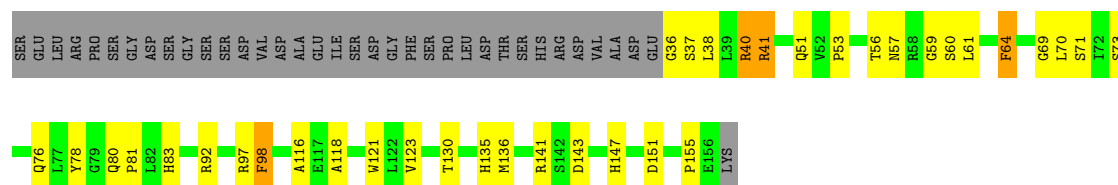


- Molecule 1: Protein At3g22680

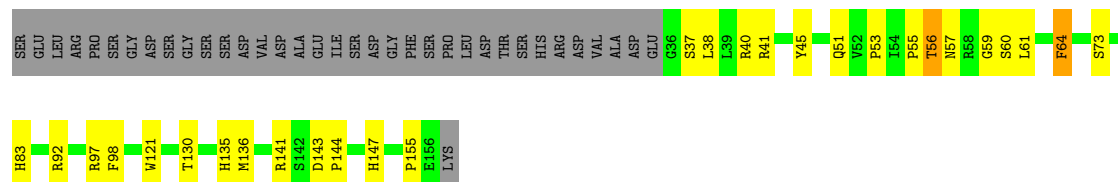


- Molecule 1: Protein At3g22680

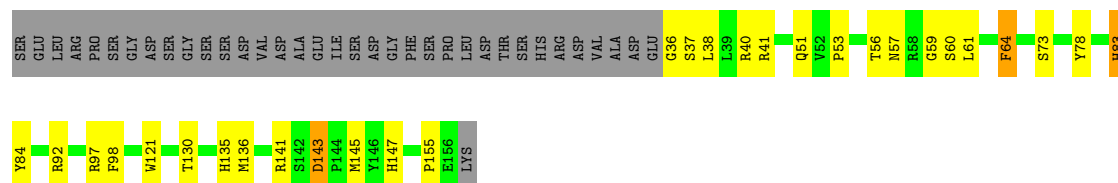




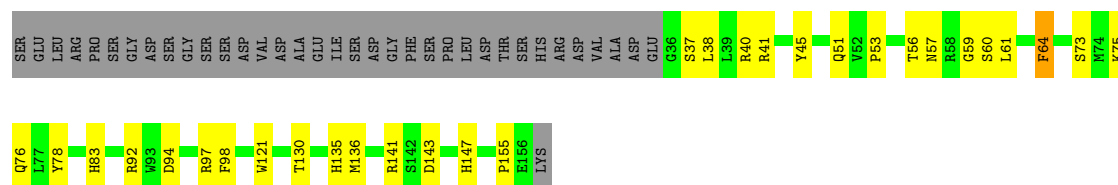
• Molecule 1: Protein At3g22680



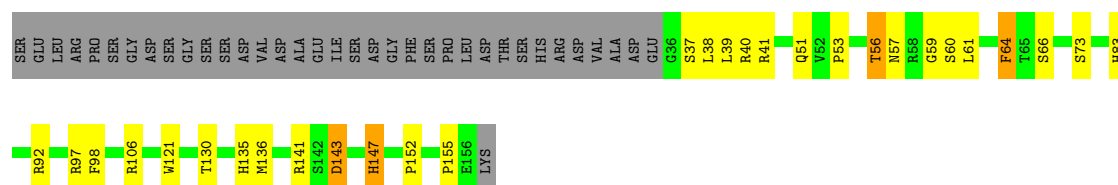
• Molecule 1: Protein At3g22680



• Molecule 1: Protein At3g22680

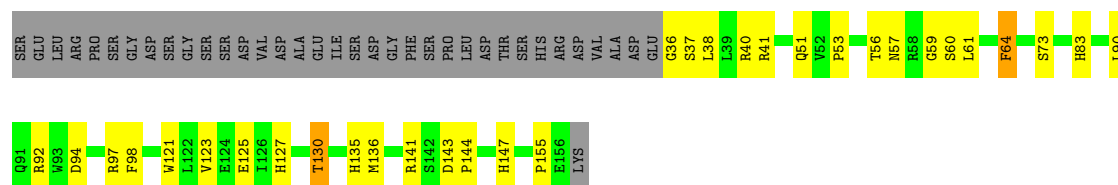


• Molecule 1: Protein At3g22680

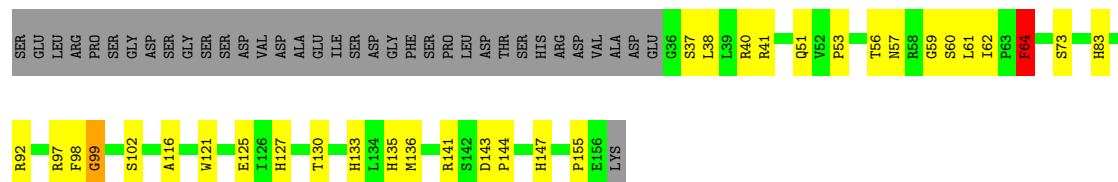


• Molecule 1: Protein At3g22680

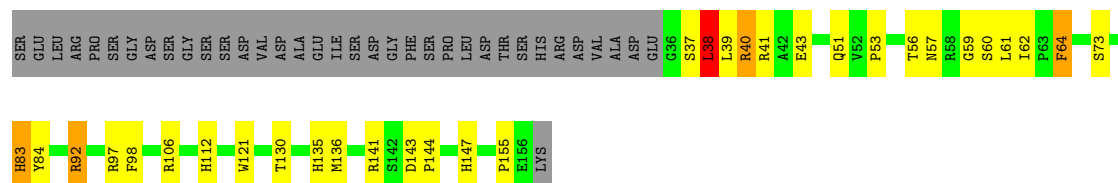




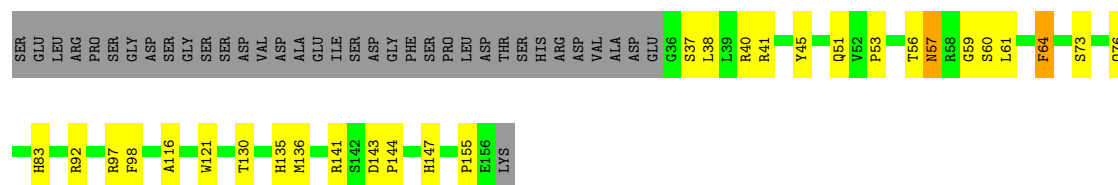
• Molecule 1: Protein At3g22680



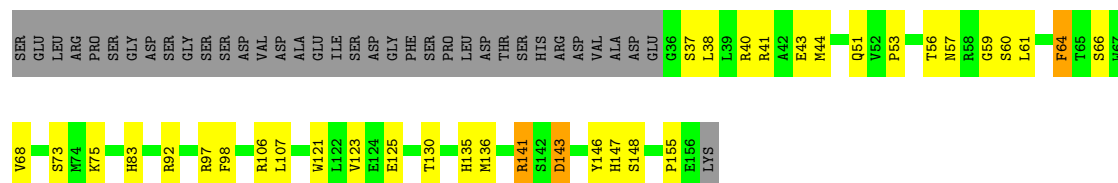
• Molecule 1: Protein At3g22680



• Molecule 1: Protein At3g22680



• Molecule 1: Protein At3g22680



• Molecule 1: Protein At3g22680



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	83.45Å 83.45Å 60.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.03 – 1.60 31.03 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.03-1.60) 100.0 (31.03-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.43 (at 1.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.139 , 0.170 0.139 , 0.169	Depositor DCC
R_{free} test set	1633 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.03 , 64.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	19808	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.32	18/1034 (1.7%)	0.98	7/1407 (0.5%)
1	2-A	1.32	18/1034 (1.7%)	0.98	7/1407 (0.5%)
1	3-A	1.32	18/1034 (1.7%)	0.98	7/1407 (0.5%)
1	4-A	1.32	18/1034 (1.7%)	0.98	7/1407 (0.5%)
1	5-A	1.32	18/1034 (1.7%)	0.98	7/1407 (0.5%)
1	6-A	1.32	18/1034 (1.7%)	0.98	7/1407 (0.5%)
1	7-A	1.32	18/1034 (1.7%)	0.98	7/1407 (0.5%)
1	8-A	1.32	18/1034 (1.7%)	0.98	7/1407 (0.5%)
1	9-A	1.32	18/1034 (1.7%)	0.98	7/1407 (0.5%)
1	10-A	1.32	18/1034 (1.7%)	0.98	7/1407 (0.5%)
1	11-A	1.32	18/1034 (1.7%)	0.98	7/1407 (0.5%)
1	12-A	1.32	18/1034 (1.7%)	0.98	7/1407 (0.5%)
1	13-A	1.32	18/1034 (1.7%)	0.98	7/1407 (0.5%)
1	14-A	1.32	18/1034 (1.7%)	0.98	7/1407 (0.5%)
1	15-A	1.32	18/1034 (1.7%)	0.98	7/1407 (0.5%)
1	16-A	1.32	18/1034 (1.7%)	0.98	7/1407 (0.5%)
All	All	1.32	288/16544 (1.7%)	0.98	112/22512 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	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 288 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-A	40	ARG	CA-CB	9.09	1.67	1.53
1	2-A	40	ARG	CA-CB	9.09	1.67	1.53
1	3-A	40	ARG	CA-CB	9.09	1.67	1.53
1	4-A	40	ARG	CA-CB	9.09	1.67	1.53
1	5-A	40	ARG	CA-CB	9.09	1.67	1.53

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	41	ARG	NE-CZ-NH1	7.30	128.80	121.50
1	2-A	41	ARG	NE-CZ-NH1	7.30	128.80	121.50
1	3-A	41	ARG	NE-CZ-NH1	7.30	128.80	121.50
1	4-A	41	ARG	NE-CZ-NH1	7.30	128.80	121.50
1	5-A	41	ARG	NE-CZ-NH1	7.30	128.80	121.50

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 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	1003	0	985	0	0
1	2-A	1003	0	986	0	0
1	3-A	1003	0	986	0	0
1	4-A	1003	0	986	0	0
1	5-A	1003	0	985	0	0
1	6-A	1003	0	986	0	0
1	7-A	1003	0	986	0	0
1	8-A	1003	0	986	0	0
1	9-A	1003	0	986	0	0
1	10-A	1003	0	986	0	0
1	11-A	1003	0	986	0	0
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	986	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	0
3	2-A	32	0	33	0	0
3	3-A	32	0	19	0	0
3	4-A	32	0	38	0	0
3	5-A	32	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	6-A	32	0	31	0	0
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	0
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	0
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	0
4	14-A	16	0	23	0	0
4	15-A	16	0	22	0	0
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	0
5	10-A	172	0	0	0	0
5	11-A	172	0	0	0	0
5	12-A	172	0	0	0	0
5	13-A	172	0	0	0	0
5	14-A	172	0	0	0	0
5	15-A	172	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	16-A	172	0	0	0	0
All	All	19808	0	16636	0	0

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

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	119/157 (76%)	114 (96%)	4 (3%)	1 (1%)	16	5
1	2-A	119/157 (76%)	107 (90%)	8 (7%)	4 (3%)	3	0
1	3-A	119/157 (76%)	111 (93%)	5 (4%)	3 (2%)	4	0
1	4-A	119/157 (76%)	114 (96%)	4 (3%)	1 (1%)	16	5
1	5-A	119/157 (76%)	117 (98%)	1 (1%)	1 (1%)	16	5
1	6-A	119/157 (76%)	116 (98%)	2 (2%)	1 (1%)	16	5
1	7-A	119/157 (76%)	117 (98%)	1 (1%)	1 (1%)	16	5
1	8-A	119/157 (76%)	116 (98%)	1 (1%)	2 (2%)	7	1
1	9-A	119/157 (76%)	114 (96%)	4 (3%)	1 (1%)	16	5
1	10-A	119/157 (76%)	114 (96%)	2 (2%)	3 (2%)	4	0
1	11-A	119/157 (76%)	110 (92%)	6 (5%)	3 (2%)	4	0
1	12-A	119/157 (76%)	117 (98%)	1 (1%)	1 (1%)	16	5
1	13-A	119/157 (76%)	113 (95%)	5 (4%)	1 (1%)	16	5
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%)	4	0
1	16-A	119/157 (76%)	113 (95%)	3 (2%)	3 (2%)	4	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1904/2512 (76%)	1815 (95%)	60 (3%)	29 (2%)	8 1

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%)	107 (96%)	5 (4%)	24 7
1	2-A	112/143 (78%)	107 (96%)	5 (4%)	24 7
1	3-A	112/143 (78%)	107 (96%)	5 (4%)	24 7
1	4-A	112/143 (78%)	107 (96%)	5 (4%)	24 7
1	5-A	112/143 (78%)	107 (96%)	5 (4%)	24 7
1	6-A	112/143 (78%)	107 (96%)	5 (4%)	24 7
1	7-A	112/143 (78%)	107 (96%)	5 (4%)	24 7
1	8-A	112/143 (78%)	107 (96%)	5 (4%)	24 7
1	9-A	112/143 (78%)	107 (96%)	5 (4%)	24 7
1	10-A	112/143 (78%)	107 (96%)	5 (4%)	24 7
1	11-A	112/143 (78%)	107 (96%)	5 (4%)	24 7
1	12-A	112/143 (78%)	107 (96%)	5 (4%)	24 7
1	13-A	112/143 (78%)	107 (96%)	5 (4%)	24 7
1	14-A	112/143 (78%)	107 (96%)	5 (4%)	24 7
1	15-A	112/143 (78%)	107 (96%)	5 (4%)	24 7
1	16-A	112/143 (78%)	107 (96%)	5 (4%)	24 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1792/2288 (78%)	1712 (96%)	80 (4%)	24 7

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	12-A	64	PHE
1	15-A	61	LEU
1	12-A	155	PRO
1	14-A	38	LEU
1	16-A	38	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	14-A	105	GLN
1	15-A	95	GLN
1	15-A	105	GLN
1	15-A	80	GLN
1	6-A	105	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides 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	$\# Z > 2$
2	SO4	6-A	301	-	4,4,4	0.94	0	6,6,6	1.41	1 (16%)
2	SO4	4-A	302	-	4,4,4	0.39	0	6,6,6	0.38	0
2	SO4	1-A	300	-	4,4,4	1.98	2 (50%)	6,6,6	1.98	2 (33%)
2	SO4	4-A	301	-	4,4,4	1.98	2 (50%)	6,6,6	0.49	0
2	SO4	2-A	302	-	4,4,4	0.54	0	6,6,6	0.83	0
4	EDO	9-A	402	-	3,3,3	2.37	3 (100%)	2,2,2	1.05	0
4	EDO	10-A	404	-	3,3,3	2.81	2 (66%)	2,2,2	1.95	1 (50%)
2	SO4	2-A	301	-	4,4,4	4.78	3 (75%)	6,6,6	1.35	1 (16%)
4	EDO	7-A	403	-	3,3,3	2.81	2 (66%)	2,2,2	0.77	0
2	SO4	1-A	301	-	4,4,4	1.33	1 (25%)	6,6,6	0.88	0
3	CPS	1-A	200	-	35,35,45	20.47	30 (85%)	54,54,70	11.15	48 (88%)
2	SO4	15-A	302	-	4,4,4	1.05	0	6,6,6	0.44	0
4	EDO	12-A	401	-	3,3,3	1.49	1 (33%)	2,2,2	0.88	0
4	EDO	8-A	404	-	3,3,3	3.57	3 (100%)	2,2,2	0.71	0
4	EDO	16-A	404	-	3,3,3	8.17	2 (66%)	2,2,2	1.71	0
3	CPS	16-A	200	-	35,35,45	18.79	29 (82%)	54,54,70	10.40	42 (77%)
4	EDO	5-A	404	-	3,3,3	3.69	2 (66%)	2,2,2	1.83	1 (50%)
2	SO4	9-A	300	-	4,4,4	1.49	1 (25%)	6,6,6	1.80	2 (33%)
4	EDO	10-A	403	-	3,3,3	2.96	2 (66%)	2,2,2	1.27	0
2	SO4	10-A	301	-	4,4,4	3.76	2 (50%)	6,6,6	1.80	2 (33%)
4	EDO	6-A	403	-	3,3,3	4.15	2 (66%)	2,2,2	1.00	0
2	SO4	12-A	301	-	4,4,4	2.32	2 (50%)	6,6,6	0.44	0
4	EDO	10-A	402	-	3,3,3	2.31	3 (100%)	2,2,2	1.09	0
2	SO4	2-A	300	-	4,4,4	0.31	0	6,6,6	0.78	0
2	SO4	14-A	301	-	4,4,4	1.77	1 (25%)	6,6,6	4.56	4 (66%)
3	CPS	9-A	200	-	35,35,45	21.06	31 (88%)	54,54,70	16.08	46 (85%)
4	EDO	11-A	402	-	3,3,3	2.32	2 (66%)	2,2,2	1.35	0
4	EDO	11-A	404	-	3,3,3	3.23	2 (66%)	2,2,2	1.61	0
4	EDO	14-A	403	-	3,3,3	4.65	2 (66%)	2,2,2	2.16	1 (50%)
2	SO4	6-A	300	-	4,4,4	0.54	0	6,6,6	0.82	0
4	EDO	6-A	401	-	3,3,3	1.16	1 (33%)	2,2,2	2.00	1 (50%)
2	SO4	16-A	301	-	4,4,4	2.00	2 (50%)	6,6,6	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	14-A	404	-	3,3,3	7.56	2 (66%)	2,2,2	0.81	0
4	EDO	12-A	404	-	3,3,3	4.63	3 (100%)	2,2,2	0.63	0
3	CPS	6-A	200	-	35,35,45	14.58	28 (80%)	54,54,70	8.72	41 (75%)
4	EDO	7-A	401	-	3,3,3	0.86	0	2,2,2	0.65	0
2	SO4	7-A	300	-	4,4,4	0.22	0	6,6,6	0.80	0
3	CPS	3-A	200	-	35,35,45	36.93	30 (85%)	54,54,70	18.50	47 (87%)
2	SO4	7-A	302	-	4,4,4	0.47	0	6,6,6	0.46	0
4	EDO	9-A	403	-	3,3,3	2.67	2 (66%)	2,2,2	0.99	0
2	SO4	7-A	301	-	4,4,4	3.41	3 (75%)	6,6,6	2.68	4 (66%)
4	EDO	13-A	401	-	3,3,3	2.96	1 (33%)	2,2,2	0.69	0
4	EDO	8-A	402	-	3,3,3	2.33	3 (100%)	2,2,2	0.86	0
4	EDO	5-A	403	-	3,3,3	3.50	2 (66%)	2,2,2	0.65	0
4	EDO	12-A	402	-	3,3,3	2.44	3 (100%)	2,2,2	1.10	0
4	EDO	4-A	402	-	3,3,3	2.31	3 (100%)	2,2,2	0.77	0
2	SO4	9-A	302	-	4,4,4	0.42	0	6,6,6	0.32	0
4	EDO	8-A	401	-	3,3,3	1.40	0	2,2,2	0.72	0
4	EDO	2-A	402	-	3,3,3	2.23	3 (100%)	2,2,2	0.54	0
4	EDO	9-A	404	-	3,3,3	3.33	2 (66%)	2,2,2	1.95	1 (50%)
3	CPS	10-A	200	-	35,35,45	20.94	33 (94%)	54,54,70	12.03	43 (79%)
4	EDO	13-A	402	-	3,3,3	5.09	2 (66%)	2,2,2	0.84	0
2	SO4	1-A	302	-	4,4,4	0.52	0	6,6,6	0.52	0
4	EDO	10-A	401	-	3,3,3	1.36	0	2,2,2	0.33	0
4	EDO	8-A	403	-	3,3,3	3.02	2 (66%)	2,2,2	2.33	2 (100%)
2	SO4	11-A	301	-	4,4,4	1.03	0	6,6,6	1.58	1 (16%)
4	EDO	3-A	403	-	3,3,3	2.85	1 (33%)	2,2,2	2.47	2 (100%)
2	SO4	3-A	300	-	4,4,4	1.04	0	6,6,6	0.90	0
2	SO4	16-A	302	-	4,4,4	0.52	0	6,6,6	0.38	0
2	SO4	8-A	302	-	4,4,4	0.78	0	6,6,6	0.82	0
4	EDO	9-A	401	-	3,3,3	1.08	0	2,2,2	0.65	0
2	SO4	11-A	300	-	4,4,4	5.30	2 (50%)	6,6,6	5.19	6 (100%)
2	SO4	15-A	300	-	4,4,4	1.17	0	6,6,6	0.98	0
2	SO4	14-A	300	-	4,4,4	3.07	1 (25%)	6,6,6	1.70	3 (50%)
4	EDO	1-A	402	-	3,3,3	2.73	2 (66%)	2,2,2	1.97	1 (50%)
4	EDO	1-A	404	-	3,3,3	4.81	2 (66%)	2,2,2	1.12	0
4	EDO	11-A	403	-	3,3,3	3.72	2 (66%)	2,2,2	1.91	1 (50%)
2	SO4	9-A	301	-	4,4,4	2.62	2 (50%)	6,6,6	3.01	4 (66%)
2	SO4	15-A	301	-	4,4,4	2.45	3 (75%)	6,6,6	3.27	4 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CPS	13-A	200	-	35,35,45	22.36	30 (85%)	54,54,70	18.53	38 (70%)
3	CPS	12-A	200	-	35,35,45	14.28	28 (80%)	54,54,70	10.20	43 (79%)
4	EDO	15-A	402	-	3,3,3	4.39	2 (66%)	2,2,2	0.62	0
4	EDO	7-A	404	-	3,3,3	2.63	2 (66%)	2,2,2	1.11	0
3	CPS	4-A	200	-	35,35,45	19.51	28 (80%)	54,54,70	9.44	40 (74%)
2	SO4	3-A	302	-	4,4,4	0.43	0	6,6,6	0.34	0
2	SO4	12-A	300	-	4,4,4	0.25	0	6,6,6	0.78	0
3	CPS	2-A	200	-	35,35,45	23.06	28 (80%)	54,54,70	10.57	42 (77%)
4	EDO	13-A	403	-	3,3,3	5.23	3 (100%)	2,2,2	1.84	1 (50%)
2	SO4	4-A	300	-	4,4,4	0.50	0	6,6,6	0.85	0
4	EDO	4-A	401	-	3,3,3	1.66	1 (33%)	2,2,2	0.20	0
2	SO4	5-A	301	-	4,4,4	1.28	0	6,6,6	1.05	0
2	SO4	12-A	302	-	4,4,4	0.45	0	6,6,6	0.42	0
3	CPS	8-A	200	-	35,35,45	27.49	32 (91%)	54,54,70	13.82	40 (74%)
2	SO4	8-A	301	-	4,4,4	2.96	3 (75%)	6,6,6	1.59	2 (33%)
2	SO4	10-A	300	-	4,4,4	0.62	0	6,6,6	0.99	0
4	EDO	11-A	401	-	3,3,3	1.31	1 (33%)	2,2,2	1.24	0
4	EDO	15-A	403	-	3,3,3	5.00	3 (100%)	2,2,2	1.84	1 (50%)
2	SO4	13-A	300	-	4,4,4	1.16	0	6,6,6	1.03	0
2	SO4	16-A	300	-	4,4,4	2.91	1 (25%)	6,6,6	1.78	3 (50%)
4	EDO	4-A	403	-	3,3,3	4.73	2 (66%)	2,2,2	0.55	0
2	SO4	10-A	302	-	4,4,4	0.65	0	6,6,6	0.55	0
4	EDO	15-A	404	-	3,3,3	7.80	3 (100%)	2,2,2	0.66	0
2	SO4	6-A	302	-	4,4,4	0.46	0	6,6,6	0.44	0
2	SO4	5-A	300	-	4,4,4	0.90	0	6,6,6	1.09	1 (16%)
4	EDO	5-A	401	-	3,3,3	0.88	0	2,2,2	0.87	0
4	EDO	1-A	401	-	3,3,3	1.99	2 (66%)	2,2,2	0.57	0
4	EDO	2-A	403	-	3,3,3	4.68	2 (66%)	2,2,2	0.77	0
4	EDO	3-A	402	-	3,3,3	2.33	2 (66%)	2,2,2	1.48	0
4	EDO	3-A	404	-	3,3,3	3.88	3 (100%)	2,2,2	0.69	0
2	SO4	8-A	300	-	4,4,4	1.30	1 (25%)	6,6,6	1.40	0
3	CPS	11-A	200	-	35,35,45	16.52	29 (82%)	54,54,70	9.84	43 (79%)
4	EDO	13-A	404	-	3,3,3	8.31	3 (100%)	2,2,2	1.06	0
3	CPS	5-A	200	-	35,35,45	21.49	31 (88%)	54,54,70	12.09	48 (88%)
3	CPS	14-A	200	-	35,35,45	24.70	30 (85%)	54,54,70	13.74	41 (75%)
4	EDO	3-A	401	-	3,3,3	1.28	0	2,2,2	0.68	0
4	EDO	14-A	401	-	3,3,3	4.05	3 (100%)	2,2,2	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	16-A	402	-	3,3,3	1.27	0	2,2,2	0.94	0
4	EDO	5-A	402	-	3,3,3	2.89	3 (100%)	2,2,2	2.19	1 (50%)
4	EDO	14-A	402	-	3,3,3	2.71	2 (66%)	2,2,2	1.16	0
4	EDO	1-A	403	-	3,3,3	2.84	2 (66%)	2,2,2	0.81	0
4	EDO	4-A	404	-	3,3,3	5.30	3 (100%)	2,2,2	0.98	0
4	EDO	12-A	403	-	3,3,3	2.87	2 (66%)	2,2,2	0.74	0
4	EDO	2-A	404	-	3,3,3	4.86	2 (66%)	2,2,2	0.87	0
4	EDO	2-A	401	-	3,3,3	2.51	2 (66%)	2,2,2	0.80	0
2	SO4	3-A	301	-	4,4,4	1.98	2 (50%)	6,6,6	0.55	0
4	EDO	16-A	401	-	3,3,3	1.75	1 (33%)	2,2,2	1.53	1 (50%)
3	CPS	15-A	200	-	35,35,45	25.37	32 (91%)	54,54,70	17.64	40 (74%)
4	EDO	6-A	404	-	3,3,3	2.46	2 (66%)	2,2,2	1.52	0
4	EDO	15-A	401	-	3,3,3	3.23	1 (33%)	2,2,2	0.86	0
2	SO4	13-A	301	-	4,4,4	2.95	2 (50%)	6,6,6	2.17	3 (50%)
2	SO4	11-A	302	-	4,4,4	0.40	0	6,6,6	0.36	0
2	SO4	13-A	302	-	4,4,4	0.51	0	6,6,6	0.56	0
4	EDO	16-A	403	-	3,3,3	3.12	2 (66%)	2,2,2	2.56	2 (100%)
3	CPS	7-A	200	-	35,35,45	17.11	30 (85%)	54,54,70	10.25	43 (79%)
4	EDO	6-A	402	-	3,3,3	2.22	2 (66%)	2,2,2	0.30	0
2	SO4	5-A	302	-	4,4,4	0.88	0	6,6,6	0.39	0
2	SO4	14-A	302	-	4,4,4	0.33	0	6,6,6	0.33	0
4	EDO	7-A	402	-	3,3,3	2.34	2 (66%)	2,2,2	1.32	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
4	EDO	9-A	402	-	-	0/1/1/1	-
4	EDO	10-A	404	-	-	1/1/1/1	-
4	EDO	7-A	403	-	-	1/1/1/1	-
3	CPS	1-A	200	-	5/5/12/15	5/13/78/90	0/4/4/4
4	EDO	12-A	401	-	-	0/1/1/1	-
4	EDO	8-A	404	-	-	1/1/1/1	-
4	EDO	16-A	404	-	-	1/1/1/1	-
3	CPS	16-A	200	-	5/5/12/15	4/13/78/90	0/4/4/4
4	EDO	5-A	404	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	10-A	403	-	-	0/1/1/1	-
4	EDO	6-A	403	-	-	1/1/1/1	-
4	EDO	10-A	402	-	-	0/1/1/1	-
3	CPS	9-A	200	-	3/3/12/15	2/13/78/90	0/4/4/4
4	EDO	11-A	402	-	-	0/1/1/1	-
4	EDO	11-A	404	-	-	1/1/1/1	-
4	EDO	14-A	403	-	-	0/1/1/1	-
4	EDO	6-A	401	-	-	1/1/1/1	-
4	EDO	14-A	404	-	-	1/1/1/1	-
4	EDO	12-A	404	-	-	1/1/1/1	-
3	CPS	6-A	200	-	8/8/12/15	2/13/78/90	0/4/4/4
4	EDO	7-A	401	-	-	0/1/1/1	-
3	CPS	3-A	200	-	7/7/12/15	3/13/78/90	0/4/4/4
4	EDO	9-A	403	-	-	0/1/1/1	-
4	EDO	13-A	401	-	-	1/1/1/1	-
4	EDO	8-A	402	-	-	0/1/1/1	-
4	EDO	5-A	403	-	-	1/1/1/1	-
4	EDO	12-A	402	-	-	0/1/1/1	-
4	EDO	4-A	402	-	-	0/1/1/1	-
4	EDO	8-A	401	-	-	0/1/1/1	-
4	EDO	2-A	402	-	-	0/1/1/1	-
4	EDO	9-A	404	-	-	1/1/1/1	-
3	CPS	10-A	200	-	4/4/12/15	2/13/78/90	0/4/4/4
4	EDO	13-A	402	-	-	1/1/1/1	-
4	EDO	10-A	401	-	-	1/1/1/1	-
4	EDO	8-A	403	-	-	0/1/1/1	-
4	EDO	3-A	403	-	-	0/1/1/1	-
4	EDO	9-A	401	-	-	0/1/1/1	-
4	EDO	1-A	402	-	-	0/1/1/1	-
4	EDO	1-A	404	-	-	1/1/1/1	-
4	EDO	11-A	403	-	-	0/1/1/1	-
3	CPS	13-A	200	-	5/5/12/15	4/13/78/90	0/4/4/4
3	CPS	12-A	200	-	5/5/12/15	2/13/78/90	0/4/4/4
4	EDO	15-A	402	-	-	1/1/1/1	-
4	EDO	7-A	404	-	-	1/1/1/1	-
3	CPS	4-A	200	-	4/4/12/15	4/13/78/90	0/4/4/4
3	CPS	2-A	200	-	5/5/12/15	2/13/78/90	0/4/4/4
4	EDO	13-A	403	-	-	0/1/1/1	-
4	EDO	4-A	401	-	-	0/1/1/1	-
3	CPS	8-A	200	-	5/5/12/15	5/13/78/90	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	11-A	401	-	-	0/1/1/1	-
4	EDO	15-A	403	-	-	0/1/1/1	-
4	EDO	4-A	403	-	-	1/1/1/1	-
4	EDO	15-A	404	-	-	1/1/1/1	-
4	EDO	5-A	401	-	-	1/1/1/1	-
4	EDO	1-A	401	-	-	0/1/1/1	-
4	EDO	2-A	403	-	-	1/1/1/1	-
4	EDO	3-A	402	-	-	0/1/1/1	-
4	EDO	3-A	404	-	-	1/1/1/1	-
3	CPS	11-A	200	-	5/5/12/15	4/13/78/90	0/4/4/4
4	EDO	13-A	404	-	-	1/1/1/1	-
3	CPS	5-A	200	-	4/4/12/15	3/13/78/90	0/4/4/4
3	CPS	14-A	200	-	5/5/12/15	3/13/78/90	0/4/4/4
4	EDO	3-A	401	-	-	0/1/1/1	-
4	EDO	14-A	401	-	-	1/1/1/1	-
4	EDO	16-A	402	-	-	0/1/1/1	-
4	EDO	5-A	402	-	-	0/1/1/1	-
4	EDO	14-A	402	-	-	1/1/1/1	-
4	EDO	1-A	403	-	-	1/1/1/1	-
4	EDO	4-A	404	-	-	1/1/1/1	-
4	EDO	12-A	403	-	-	1/1/1/1	-
4	EDO	2-A	404	-	-	1/1/1/1	-
4	EDO	2-A	401	-	-	1/1/1/1	-
4	EDO	16-A	401	-	-	0/1/1/1	-
3	CPS	15-A	200	-	4/4/12/15	5/13/78/90	0/4/4/4
4	EDO	6-A	404	-	-	1/1/1/1	-
4	EDO	15-A	401	-	-	0/1/1/1	-
4	EDO	16-A	403	-	-	0/1/1/1	-
3	CPS	7-A	200	-	5/5/12/15	4/13/78/90	0/4/4/4
4	EDO	6-A	402	-	-	1/1/1/1	-
4	EDO	7-A	402	-	-	0/1/1/1	-

The worst 5 of 637 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-A	200	CPS	C18-C17	146.98	4.19	1.53
3	3-A	200	CPS	C12-C13	118.73	4.25	1.51
3	8-A	200	CPS	C5-C9	87.10	3.01	1.55
3	2-A	200	CPS	C3-C4	79.35	2.82	1.53
3	8-A	200	CPS	C20-C9	-76.09	0.24	1.54

The worst 5 of 745 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-A	200	CPS	C14-C13-C12	-57.61	40.34	110.62
3	3-A	200	CPS	C1-C12-C13	-54.04	38.91	110.48
3	8-A	200	CPS	C8-C9-C5	-51.48	53.61	103.54
3	13-A	200	CPS	C7-C6-C5	-48.04	56.95	103.54
3	5-A	200	CPS	C7-C6-C5	-45.36	59.55	103.54

5 of 79 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	1-A	200	CPS	C20
3	1-A	200	CPS	C18
3	1-A	200	CPS	C6
3	1-A	200	CPS	C19
3	1-A	200	CPS	C9

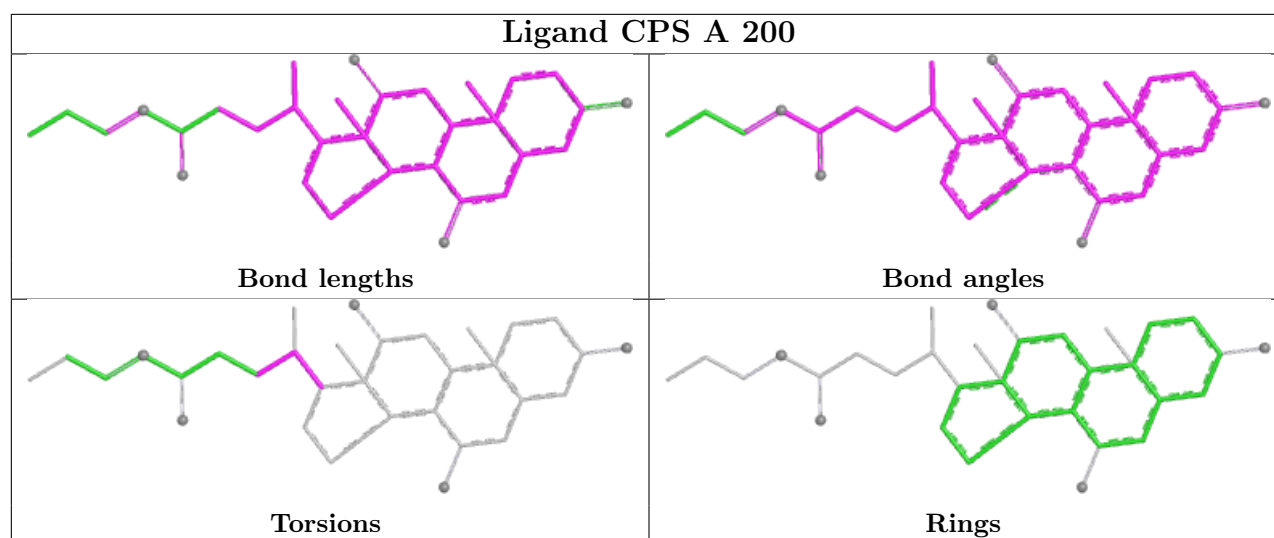
5 of 87 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	4-A	200	CPS	C22-C20-C9-C5
3	8-A	200	CPS	C22-C20-C9-C5
3	10-A	200	CPS	C22-C20-C9-C5
3	13-A	200	CPS	C22-C20-C9-C5
3	14-A	200	CPS	C21-C20-C9-C8

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	8-A	2
1	15-A	2
1	13-A	1
1	16-A	1
1	5-A	1
1	2-A	1
1	7-A	1

The worst 5 of 9 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
13	A	65:THR	C	66:SER	N	1.67
16	A	144:PRO	C	145:MET	N	1.62
5	A	56:THR	C	57:ASN	N	1.20
8	A	147:HIS	C	148:SER	N	1.18
2	A	76:GLN	C	77:LEU	N	1.17

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	121/157 (77%)	2.42	60 (49%) 0 0	1, 1, 2, 3	121 (100%)
1	2-A	0/157	-	-	-	-
1	3-A	0/157	-	-	-	-
1	4-A	0/157	-	-	-	-
1	5-A	0/157	-	-	-	-
1	6-A	0/157	-	-	-	-
1	7-A	0/157	-	-	-	-
1	8-A	0/157	-	-	-	-
1	9-A	0/157	-	-	-	-
1	10-A	0/157	-	-	-	-
1	11-A	0/157	-	-	-	-
1	12-A	0/157	-	-	-	-
1	13-A	0/157	-	-	-	-
1	14-A	0/157	-	-	-	-
1	15-A	0/157	-	-	-	-
1	16-A	0/157	-	-	-	-
All	All	121/2512 (4%)	2.42	60 (49%) 0 0	1, 1, 2, 3	121 (100%)

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	39	LEU	8.0
1	1-A	114	THR	8.0
1	1-A	153	ILE	7.2
1	1-A	36	GLY	6.5
1	1-A	155	PRO	6.1

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	1-A	302	5/5	0.56	0.26	85,85,85,85	5
2	SO4	2-A	300	5/5	-	-	17,17,19,21	5
2	SO4	3-A	300	5/5	-	-	17,18,20,21	5
2	SO4	4-A	300	5/5	-	-	17,17,19,20	5
2	SO4	5-A	300	5/5	-	-	17,17,19,20	5
2	SO4	6-A	300	5/5	-	-	17,17,19,21	5
2	SO4	7-A	300	5/5	-	-	17,17,19,20	5
2	SO4	8-A	300	5/5	-	-	18,19,21,21	5
2	SO4	9-A	300	5/5	-	-	17,17,19,20	5
2	SO4	10-A	300	5/5	-	-	17,17,19,20	5
2	SO4	11-A	300	5/5	-	-	16,19,21,21	5
2	SO4	12-A	300	5/5	-	-	17,17,19,21	5
2	SO4	13-A	300	5/5	-	-	17,18,20,20	5
2	SO4	14-A	300	5/5	-	-	16,17,19,21	5
2	SO4	15-A	300	5/5	-	-	17,18,20,21	5
2	SO4	16-A	300	5/5	-	-	16,17,19,21	5
2	SO4	1-A	300	5/5	0.64	0.27	19,19,21,21	5
2	SO4	2-A	301	5/5	-	-	28,30,32,33	5
2	SO4	3-A	301	5/5	-	-	27,29,33,33	5
2	SO4	4-A	301	5/5	-	-	27,29,33,33	5
2	SO4	5-A	301	5/5	-	-	27,29,33,33	5
2	SO4	6-A	301	5/5	-	-	27,29,33,33	5
2	SO4	7-A	301	5/5	-	-	29,29,32,33	5
2	SO4	8-A	301	5/5	-	-	28,29,31,33	5
2	SO4	9-A	301	5/5	-	-	28,29,32,33	5
2	SO4	10-A	301	5/5	-	-	30,31,32,32	5
2	SO4	11-A	301	5/5	-	-	27,29,33,33	5
2	SO4	12-A	301	5/5	-	-	27,29,32,33	5
2	SO4	13-A	301	5/5	-	-	30,31,32,32	5
2	SO4	14-A	301	5/5	-	-	29,30,31,32	5
2	SO4	15-A	301	5/5	-	-	27,29,32,33	5
2	SO4	16-A	301	5/5	-	-	27,28,33,33	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CPS	1-A	200	32/42	0.67	0.25	8,14,47,55	32
2	SO4	2-A	302	5/5	-	-	85,85,85,85	5
2	SO4	3-A	302	5/5	-	-	85,85,85,85	5
2	SO4	4-A	302	5/5	-	-	85,85,85,85	5
2	SO4	5-A	302	5/5	-	-	85,85,85,85	5
2	SO4	6-A	302	5/5	-	-	85,85,85,85	5
2	SO4	7-A	302	5/5	-	-	85,85,85,85	5
2	SO4	8-A	302	5/5	-	-	85,85,85,85	5
2	SO4	9-A	302	5/5	-	-	85,85,85,85	5
2	SO4	10-A	302	5/5	-	-	85,85,85,85	5
2	SO4	11-A	302	5/5	-	-	85,85,85,85	5
2	SO4	12-A	302	5/5	-	-	85,85,85,85	5
2	SO4	13-A	302	5/5	-	-	85,85,85,85	5
2	SO4	14-A	302	5/5	-	-	85,85,85,85	5
2	SO4	15-A	302	5/5	-	-	85,85,85,85	5
2	SO4	16-A	302	5/5	-	-	85,85,85,85	5
4	EDO	1-A	404	4/4	0.67	0.26	28,31,34,35	4
3	CPS	2-A	200	32/42	-	-	8,14,47,55	32
3	CPS	3-A	200	32/42	-	-	7,14,47,55	32
3	CPS	4-A	200	32/42	-	-	8,15,47,55	32
3	CPS	5-A	200	32/42	-	-	9,15,47,55	32
3	CPS	6-A	200	32/42	-	-	3,14,47,55	32
3	CPS	7-A	200	32/42	-	-	8,14,47,55	32
3	CPS	8-A	200	32/42	-	-	5,14,47,55	32
3	CPS	9-A	200	32/42	-	-	8,15,47,55	32
3	CPS	10-A	200	32/42	-	-	9,14,47,55	32
3	CPS	11-A	200	32/42	-	-	1,14,47,55	32
3	CPS	12-A	200	32/42	-	-	7,14,47,55	32
3	CPS	13-A	200	32/42	-	-	1,13,46,55	32
3	CPS	14-A	200	32/42	-	-	1,13,46,55	32
3	CPS	15-A	200	32/42	-	-	1,13,46,55	32
3	CPS	16-A	200	32/42	-	-	1,13,47,55	32
4	EDO	1-A	403	4/4	0.76	0.19	27,32,32,35	4
4	EDO	2-A	401	4/4	-	-	16,17,18,20	4
4	EDO	3-A	401	4/4	-	-	16,17,18,20	4
4	EDO	4-A	401	4/4	-	-	16,17,18,20	4
4	EDO	5-A	401	4/4	-	-	16,17,18,20	4
4	EDO	6-A	401	4/4	-	-	16,17,18,20	4
4	EDO	7-A	401	4/4	-	-	16,17,18,20	4
4	EDO	8-A	401	4/4	-	-	16,17,19,20	4
4	EDO	9-A	401	4/4	-	-	16,17,18,20	4
4	EDO	10-A	401	4/4	-	-	16,17,18,20	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	11-A	401	4/4	-	-	16,17,18,20	4
4	EDO	12-A	401	4/4	-	-	16,17,19,20	4
4	EDO	13-A	401	4/4	-	-	16,17,18,20	4
4	EDO	14-A	401	4/4	-	-	16,17,18,21	4
4	EDO	15-A	401	4/4	-	-	15,17,19,20	4
4	EDO	16-A	401	4/4	-	-	15,17,18,20	4
4	EDO	1-A	401	4/4	0.85	0.16	16,17,18,20	4
4	EDO	2-A	402	4/4	-	-	18,22,22,26	4
4	EDO	3-A	402	4/4	-	-	18,22,22,26	4
4	EDO	4-A	402	4/4	-	-	18,22,22,26	4
4	EDO	5-A	402	4/4	-	-	18,22,22,26	4
4	EDO	6-A	402	4/4	-	-	18,22,22,26	4
4	EDO	7-A	402	4/4	-	-	18,22,22,26	4
4	EDO	8-A	402	4/4	-	-	18,22,22,26	4
4	EDO	9-A	402	4/4	-	-	18,22,22,26	4
4	EDO	10-A	402	4/4	-	-	18,22,22,26	4
4	EDO	11-A	402	4/4	-	-	18,22,22,26	4
4	EDO	12-A	402	4/4	-	-	18,22,22,26	4
4	EDO	13-A	402	4/4	-	-	18,22,22,25	4
4	EDO	14-A	402	4/4	-	-	18,22,22,26	4
4	EDO	15-A	402	4/4	-	-	18,22,22,26	4
4	EDO	16-A	402	4/4	-	-	18,22,22,26	4
4	EDO	1-A	402	4/4	0.88	0.16	18,22,22,26	4
4	EDO	2-A	403	4/4	-	-	27,32,32,35	4
4	EDO	3-A	403	4/4	-	-	27,32,33,35	4
4	EDO	4-A	403	4/4	-	-	28,32,32,35	4
4	EDO	5-A	403	4/4	-	-	28,32,32,35	4
4	EDO	6-A	403	4/4	-	-	27,32,33,35	4
4	EDO	7-A	403	4/4	-	-	28,32,32,35	4
4	EDO	8-A	403	4/4	-	-	27,32,33,35	4
4	EDO	9-A	403	4/4	-	-	28,32,32,35	4
4	EDO	10-A	403	4/4	-	-	28,32,32,35	4
4	EDO	11-A	403	4/4	-	-	28,32,33,35	4
4	EDO	12-A	403	4/4	-	-	28,32,32,35	4
4	EDO	13-A	403	4/4	-	-	27,32,33,34	4
4	EDO	14-A	403	4/4	-	-	28,32,33,35	4
4	EDO	15-A	403	4/4	-	-	27,33,33,34	4
4	EDO	16-A	403	4/4	-	-	27,31,33,35	4
2	SO4	1-A	301	5/5	0.92	0.23	27,29,33,33	5
4	EDO	2-A	404	4/4	-	-	28,31,34,35	4
4	EDO	3-A	404	4/4	-	-	28,31,34,35	4
4	EDO	4-A	404	4/4	-	-	28,31,34,35	4

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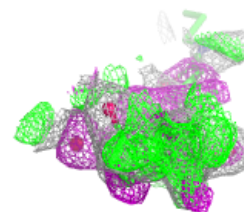
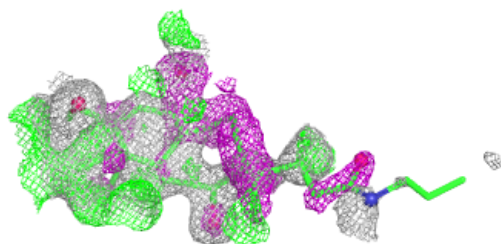
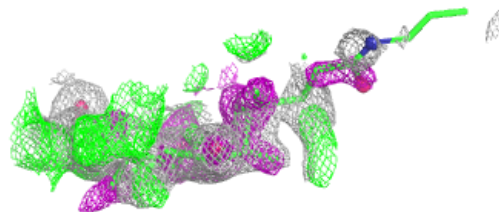
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	5-A	404	4/4	-	-	27,31,34,35	4
4	EDO	6-A	404	4/4	-	-	27,31,34,35	4
4	EDO	7-A	404	4/4	-	-	27,31,34,35	4
4	EDO	8-A	404	4/4	-	-	28,31,34,35	4
4	EDO	9-A	404	4/4	-	-	27,31,34,35	4
4	EDO	10-A	404	4/4	-	-	27,31,34,35	4
4	EDO	11-A	404	4/4	-	-	27,31,34,35	4
4	EDO	12-A	404	4/4	-	-	28,31,34,35	4
4	EDO	13-A	404	4/4	-	-	27,31,34,35	4
4	EDO	14-A	404	4/4	-	-	27,31,33,35	4
4	EDO	15-A	404	4/4	-	-	27,31,33,35	4
4	EDO	16-A	404	4/4	-	-	27,31,34,35	4

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

Electron density around CPS A 200:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.