



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 09:14 PM GMT

PDB ID : 2Q4Z
Title : Ensemble refinement of the protein crystal structure of an aspartoacylase from *Rattus norvegicus*
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2007-05-31
Resolution : 1.80 Å(reported)

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

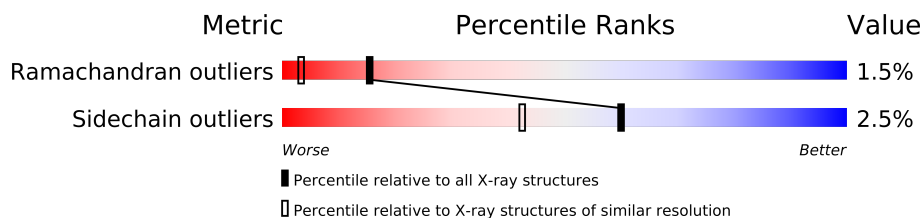
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.80 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	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	312	
1	1-B	312	
1	10-A	312	
1	10-B	312	
1	11-A	312	
1	11-B	312	
1	12-A	312	
1	12-B	312	
1	13-A	312	
1	13-B	312	
1	14-A	312	
1	14-B	312	
1	15-A	312	
1	15-B	312	
1	16-A	312	
1	16-B	312	
1	2-A	312	
1	2-B	312	
1	3-A	312	

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Mol	Chain	Length	Quality of chain
1	3-B	312	
1	4-A	312	
1	4-B	312	
1	5-A	312	
1	5-B	312	
1	6-A	312	
1	6-B	312	
1	7-A	312	
1	7-B	312	
1	8-A	312	
1	8-B	312	
1	9-A	312	
1	9-B	312	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 87056 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 Aspartoacylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	1-B	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	2-A	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	2-B	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	3-A	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	3-B	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	4-A	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	4-B	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	5-A	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	5-B	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	6-A	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	6-B	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	7-A	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	7-B	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	8-A	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	8-B	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	9-A	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	9-B	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	10-A	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	10-B	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	11-A	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	11-B	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	12-A	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	12-B	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	13-A	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	13-B	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	14-A	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	14-B	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	15-A	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	15-B	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	16-A	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	16-B	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP Q9R1T5
A	81	MSE	MET	MODIFIED RESIDUE	UNP Q9R1T5
A	121	MSE	MET	MODIFIED RESIDUE	UNP Q9R1T5
A	128	GLY	GLU	POSSIBLE ISOFORM	UNP Q9R1T5
A	131	GLY	ARG	POSSIBLE ISOFORM	UNP Q9R1T5
A	138	MSE	MET	MODIFIED RESIDUE	UNP Q9R1T5
A	146	MSE	MET	MODIFIED RESIDUE	UNP Q9R1T5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	194	MSE	MET	MODIFIED RESIDUE	UNP Q9R1T5
A	197	MSE	MET	MODIFIED RESIDUE	UNP Q9R1T5
A	225	MSE	MET	MODIFIED RESIDUE	UNP Q9R1T5
B	1	SER	-	EXPRESSION TAG	UNP Q9R1T5
B	81	MSE	MET	MODIFIED RESIDUE	UNP Q9R1T5
B	121	MSE	MET	MODIFIED RESIDUE	UNP Q9R1T5
B	128	GLY	GLU	POSSIBLE ISOFORM	UNP Q9R1T5
B	131	GLY	ARG	POSSIBLE ISOFORM	UNP Q9R1T5
B	138	MSE	MET	MODIFIED RESIDUE	UNP Q9R1T5
B	146	MSE	MET	MODIFIED RESIDUE	UNP Q9R1T5
B	194	MSE	MET	MODIFIED RESIDUE	UNP Q9R1T5
B	197	MSE	MET	MODIFIED RESIDUE	UNP Q9R1T5
B	225	MSE	MET	MODIFIED RESIDUE	UNP Q9R1T5

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

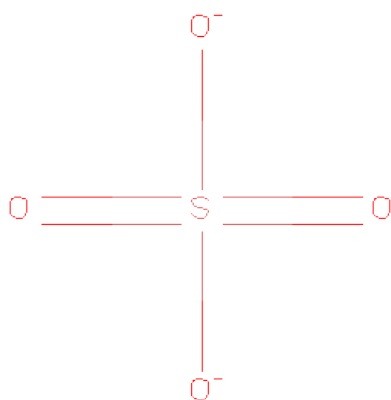
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	16-A	1	Total Zn 1 1	0	0
2	1-B	1	Total Zn 1 1	0	0
2	5-A	1	Total Zn 1 1	0	0
2	13-A	1	Total Zn 1 1	0	0
2	8-A	1	Total Zn 1 1	0	0
2	2-B	1	Total Zn 1 1	0	0
2	15-B	1	Total Zn 1 1	0	0
2	7-B	1	Total Zn 1 1	0	0
2	16-B	1	Total Zn 1 1	0	0
2	10-B	1	Total Zn 1 1	0	0
2	4-A	1	Total Zn 1 1	0	0
2	12-A	1	Total Zn 1 1	0	0
2	1-A	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	11-B	1	Total 1	Zn 1	0	0
2	8-B	1	Total 1	Zn 1	0	0
2	7-A	1	Total 1	Zn 1	0	0
2	15-A	1	Total 1	Zn 1	0	0
2	3-B	1	Total 1	Zn 1	0	0
2	12-B	1	Total 1	Zn 1	0	0
2	4-B	1	Total 1	Zn 1	0	0
2	9-B	1	Total 1	Zn 1	0	0
2	6-A	1	Total 1	Zn 1	0	0
2	14-A	1	Total 1	Zn 1	0	0
2	3-A	1	Total 1	Zn 1	0	0
2	11-A	1	Total 1	Zn 1	0	0
2	5-B	1	Total 1	Zn 1	0	0
2	6-B	1	Total 1	Zn 1	0	0
2	13-B	1	Total 1	Zn 1	0	0
2	2-A	1	Total 1	Zn 1	0	0
2	10-A	1	Total 1	Zn 1	0	0
2	9-A	1	Total 1	Zn 1	0	0
2	14-B	1	Total 1	Zn 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	3-B	1	Total	O	S	0	0
			5	4	1		
3	4-A	1	Total	O	S	0	0
			5	4	1		
3	4-A	1	Total	O	S	0	0
			5	4	1		
3	4-A	1	Total	O	S	0	0
			5	4	1		
3	4-B	1	Total	O	S	0	0
			5	4	1		
3	4-B	1	Total	O	S	0	0
			5	4	1		
3	5-A	1	Total	O	S	0	0
			5	4	1		
3	5-A	1	Total	O	S	0	0
			5	4	1		
3	5-A	1	Total	O	S	0	0
			5	4	1		
3	5-B	1	Total	O	S	0	0
			5	4	1		
3	5-B	1	Total	O	S	0	0
			5	4	1		
3	6-A	1	Total	O	S	0	0
			5	4	1		
3	6-A	1	Total	O	S	0	0
			5	4	1		
3	6-A	1	Total	O	S	0	0
			5	4	1		
3	6-B	1	Total	O	S	0	0
			5	4	1		
3	6-B	1	Total	O	S	0	0
			5	4	1		
3	7-A	1	Total	O	S	0	0
			5	4	1		
3	7-A	1	Total	O	S	0	0
			5	4	1		
3	7-A	1	Total	O	S	0	0
			5	4	1		
3	7-B	1	Total	O	S	0	0
			5	4	1		
3	7-B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	8-A	1	Total	O	S	0	0
			5	4	1		
3	8-A	1	Total	O	S	0	0
			5	4	1		
3	8-A	1	Total	O	S	0	0
			5	4	1		
3	8-B	1	Total	O	S	0	0
			5	4	1		
3	8-B	1	Total	O	S	0	0
			5	4	1		
3	9-A	1	Total	O	S	0	0
			5	4	1		
3	9-A	1	Total	O	S	0	0
			5	4	1		
3	9-A	1	Total	O	S	0	0
			5	4	1		
3	9-B	1	Total	O	S	0	0
			5	4	1		
3	9-B	1	Total	O	S	0	0
			5	4	1		
3	10-A	1	Total	O	S	0	0
			5	4	1		
3	10-A	1	Total	O	S	0	0
			5	4	1		
3	10-A	1	Total	O	S	0	0
			5	4	1		
3	10-B	1	Total	O	S	0	0
			5	4	1		
3	10-B	1	Total	O	S	0	0
			5	4	1		
3	11-A	1	Total	O	S	0	0
			5	4	1		
3	11-A	1	Total	O	S	0	0
			5	4	1		
3	11-A	1	Total	O	S	0	0
			5	4	1		
3	11-B	1	Total	O	S	0	0
			5	4	1		
3	11-B	1	Total	O	S	0	0
			5	4	1		
3	12-A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	12-A	1	Total	O	S	0	0
			5	4	1		
3	12-A	1	Total	O	S	0	0
			5	4	1		
3	12-B	1	Total	O	S	0	0
			5	4	1		
3	12-B	1	Total	O	S	0	0
			5	4	1		
3	13-A	1	Total	O	S	0	0
			5	4	1		
3	13-A	1	Total	O	S	0	0
			5	4	1		
3	13-A	1	Total	O	S	0	0
			5	4	1		
3	13-B	1	Total	O	S	0	0
			5	4	1		
3	13-B	1	Total	O	S	0	0
			5	4	1		
3	14-A	1	Total	O	S	0	0
			5	4	1		
3	14-A	1	Total	O	S	0	0
			5	4	1		
3	14-A	1	Total	O	S	0	0
			5	4	1		
3	14-B	1	Total	O	S	0	0
			5	4	1		
3	14-B	1	Total	O	S	0	0
			5	4	1		
3	15-A	1	Total	O	S	0	0
			5	4	1		
3	15-A	1	Total	O	S	0	0
			5	4	1		
3	15-A	1	Total	O	S	0	0
			5	4	1		
3	15-B	1	Total	O	S	0	0
			5	4	1		
3	15-B	1	Total	O	S	0	0
			5	4	1		
3	16-A	1	Total	O	S	0	0
			5	4	1		
3	16-A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	16-A	1	Total	O	S	0	0
			5	4	1		
3	16-B	1	Total	O	S	0	0
			5	4	1		
3	16-B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	1-A	288	Total	O		0	0
			288	288			
4	1-B	264	Total	O		0	0
			264	264			
4	2-A	284	Total	O		0	0
			284	284			
4	2-B	268	Total	O		0	0
			268	268			
4	3-A	282	Total	O		0	0
			282	282			
4	3-B	270	Total	O		0	0
			270	270			
4	4-A	284	Total	O		0	0
			284	284			
4	4-B	268	Total	O		0	0
			268	268			
4	5-A	283	Total	O		0	0
			283	283			
4	5-B	269	Total	O		0	0
			269	269			
4	6-A	292	Total	O		0	0
			292	292			
4	6-B	260	Total	O		0	0
			260	260			
4	7-A	291	Total	O		0	0
			291	291			
4	7-B	261	Total	O		0	0
			261	261			
4	8-A	293	Total	O		0	0
			293	293			
4	8-B	259	Total	O		0	0
			259	259			

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	9-A	292	Total 292	O 292	0	0
4	9-B	260	Total 260	O 260	0	0
4	10-A	280	Total 280	O 280	0	0
4	10-B	272	Total 272	O 272	0	0
4	11-A	294	Total 294	O 294	0	0
4	11-B	258	Total 258	O 258	0	0
4	12-A	285	Total 285	O 285	0	0
4	12-B	267	Total 267	O 267	0	0
4	13-A	291	Total 291	O 291	0	0
4	13-B	261	Total 261	O 261	0	0
4	14-A	289	Total 289	O 289	0	0
4	14-B	263	Total 263	O 263	0	0
4	15-A	285	Total 285	O 285	0	0
4	15-B	267	Total 267	O 267	0	0
4	16-A	284	Total 284	O 284	0	0
4	16-B	268	Total 268	O 268	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.

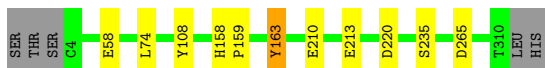
- Molecule 1: Aspartoacylase

Chain 1-A: 



- Molecule 1: Aspartoacylase

Chain 1-B: 



- Molecule 1: Aspartoacylase

Chain 2-A: 



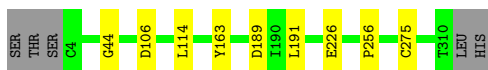
- Molecule 1: Aspartoacylase

Chain 2-B: 



- Molecule 1: Aspartoacylase

Chain 3-A: 



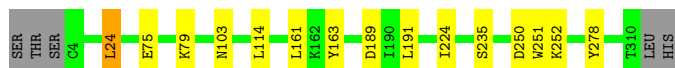
- Molecule 1: Aspartoacylase

Chain 3-B: 



- Molecule 1: Aspartoacylase

Chain 4-A: 



- Molecule 1: Aspartoacylase

Chain 4-B: 



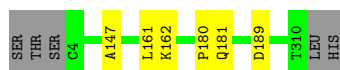
- Molecule 1: Aspartoacylase

Chain 5-A: 



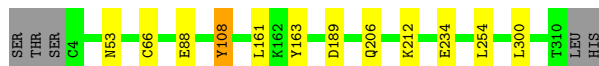
- Molecule 1: Aspartoacylase

Chain 5-B: 



- Molecule 1: Aspartoacylase

Chain 6-A: 



- Molecule 1: Aspartoacylase

Chain 6-B: 



- Molecule 1: Aspartoacylase

Chain 7-A: 



- Molecule 1: Aspartoacylase

Chain 7-B: 



- Molecule 1: Aspartoacylase

Chain 8-A: 



- Molecule 1: Aspartoacylase

Chain 8-B: 



- Molecule 1: Aspartoacylase

Chain 9-A: 



- Molecule 1: Aspartoacylase

Chain 9-B: 



- Molecule 1: Aspartoacylase

Chain 10-A: 



- Molecule 1: Aspartoacylase

Chain 10-B: 



- Molecule 1: Aspartoacylase

Chain 11-A: 



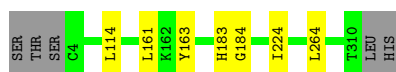
- Molecule 1: Aspartoacylase

Chain 11-B: 



- Molecule 1: Aspartoacylase

Chain 12-A: 



- Molecule 1: Aspartoacylase

Chain 12-B:



- Molecule 1: Aspartoacylase

Chain 13-A:



- Molecule 1: Aspartoacylase

Chain 13-B:



- Molecule 1: Aspartoacylase

Chain 14-A:



- Molecule 1: Aspartoacylase

Chain 14-B:



- Molecule 1: Aspartoacylase

Chain 15-A:



- Molecule 1: Aspartoacylase

Chain 15-B:



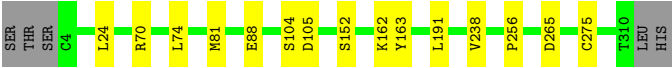
- Molecule 1: Aspartoacylase

Chain 16-A:



● Molecule 1: Aspartoacylase

Chain 16-B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.58Å 135.78Å 54.03Å 90.00° 101.49° 90.00°	Depositor
Resolution (Å)	40.50 – 1.80	Depositor
% Data completeness (in resolution range)	97.1 (40.50-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 1.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.138 , 0.191	Depositor
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.070	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 58208 reflections	Xtriage
Total number of atoms	87056	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: ZN, SO4

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	0.47	0/2484	0.65	0/3360
1	1-B	0.48	0/2484	0.65	0/3360
1	2-A	0.48	0/2484	0.64	0/3360
1	2-B	0.48	0/2484	0.65	0/3360
1	3-A	0.48	0/2484	0.64	0/3360
1	3-B	0.48	0/2484	0.66	0/3360
1	4-A	0.49	0/2484	0.66	1/3360 (0.0%)
1	4-B	0.48	0/2484	0.65	0/3360
1	5-A	0.48	0/2484	0.66	1/3360 (0.0%)
1	5-B	0.48	0/2484	0.65	0/3360
1	6-A	0.48	0/2484	0.66	1/3360 (0.0%)
1	6-B	0.48	0/2484	0.66	1/3360 (0.0%)
1	7-A	0.48	0/2484	0.64	0/3360
1	7-B	0.49	0/2484	0.63	0/3360
1	8-A	0.48	0/2484	0.64	0/3360
1	8-B	0.48	0/2484	0.65	0/3360
1	9-A	0.49	0/2484	0.64	0/3360
1	9-B	0.48	0/2484	0.64	0/3360
1	10-A	0.49	0/2484	0.66	0/3360
1	10-B	0.48	0/2484	0.66	0/3360
1	11-A	0.47	0/2484	0.66	0/3360
1	11-B	0.48	0/2484	0.64	0/3360
1	12-A	0.49	0/2484	0.65	0/3360
1	12-B	0.48	0/2484	0.64	0/3360
1	13-A	0.57	0/2484	0.74	2/3360 (0.1%)
1	13-B	0.55	0/2484	0.74	1/3360 (0.0%)
1	14-A	0.55	0/2484	0.76	3/3360 (0.1%)
1	14-B	0.57	0/2484	0.73	0/3360
1	15-A	0.54	0/2484	0.75	1/3360 (0.0%)
1	15-B	0.54	0/2484	0.73	0/3360
1	16-A	0.56	0/2484	0.77	1/3360 (0.0%)
1	16-B	0.54	0/2484	0.74	1/3360 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.50	0/79488	0.67	13/107520 (0.0%)

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	4-A	0	1
1	11-A	0	1
1	13-A	0	1
1	16-A	0	2
All	All	0	5

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	15-A	24	LEU	N-CA-C	6.39	128.25	111.00
1	14-A	24	LEU	N-CA-C	5.69	126.36	111.00
1	13-A	20	HIS	N-CA-C	-5.61	95.85	111.00
1	16-A	254	LEU	CA-CB-CG	5.34	127.59	115.30
1	4-A	24	LEU	N-CA-C	5.30	125.31	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	11-A	278	TYR	Sidechain
1	13-A	87	TYR	Sidechain
1	16-A	278	TYR	Sidechain
1	16-A	87	TYR	Sidechain
1	4-A	278	TYR	Sidechain

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	2431	0	2405	0	0
1	1-B	2431	0	2405	0	0
1	2-A	2431	0	2405	0	0
1	2-B	2431	0	2405	0	0
1	3-A	2431	0	2405	0	0
1	3-B	2431	0	2405	0	0
1	4-A	2431	0	2405	0	0
1	4-B	2431	0	2405	0	0
1	5-A	2431	0	2405	0	0
1	5-B	2431	0	2405	0	0
1	6-A	2431	0	2405	0	0
1	6-B	2431	0	2405	0	0
1	7-A	2431	0	2405	0	0
1	7-B	2431	0	2405	0	0
1	8-A	2431	0	2405	0	0
1	8-B	2431	0	2405	0	0
1	9-A	2431	0	2405	0	0
1	9-B	2431	0	2405	0	0
1	10-A	2431	0	2405	0	0
1	10-B	2431	0	2405	0	0
1	11-A	2431	0	2405	0	0
1	11-B	2431	0	2405	0	0
1	12-A	2431	0	2405	0	0
1	12-B	2431	0	2405	0	0
1	13-A	2431	0	2405	0	0
1	13-B	2431	0	2405	0	0
1	14-A	2431	0	2405	0	0
1	14-B	2431	0	2405	0	1
1	15-A	2431	0	2405	0	0
1	15-B	2431	0	2405	0	0
1	16-A	2431	0	2405	0	0
1	16-B	2431	0	2405	0	1
2	1-A	1	0	0	0	0
2	1-B	1	0	0	0	0
2	2-A	1	0	0	0	0
2	2-B	1	0	0	0	0
2	3-A	1	0	0	0	0
2	3-B	1	0	0	0	0
2	4-A	1	0	0	0	0
2	4-B	1	0	0	0	0
2	5-A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	5-B	1	0	0	0	0
2	6-A	1	0	0	0	0
2	6-B	1	0	0	0	0
2	7-A	1	0	0	0	0
2	7-B	1	0	0	0	0
2	8-A	1	0	0	0	0
2	8-B	1	0	0	0	0
2	9-A	1	0	0	0	0
2	9-B	1	0	0	0	0
2	10-A	1	0	0	0	0
2	10-B	1	0	0	0	0
2	11-A	1	0	0	0	0
2	11-B	1	0	0	0	0
2	12-A	1	0	0	0	0
2	12-B	1	0	0	0	0
2	13-A	1	0	0	0	0
2	13-B	1	0	0	0	0
2	14-A	1	0	0	0	0
2	14-B	1	0	0	0	0
2	15-A	1	0	0	0	0
2	15-B	1	0	0	0	0
2	16-A	1	0	0	0	0
2	16-B	1	0	0	0	0
3	1-A	15	0	0	0	0
3	1-B	10	0	0	0	0
3	2-A	15	0	0	0	0
3	2-B	10	0	0	0	0
3	3-A	15	0	0	0	0
3	3-B	10	0	0	0	0
3	4-A	15	0	0	0	0
3	4-B	10	0	0	0	0
3	5-A	15	0	0	0	0
3	5-B	10	0	0	0	0
3	6-A	15	0	0	0	0
3	6-B	10	0	0	0	0
3	7-A	15	0	0	0	0
3	7-B	10	0	0	0	0
3	8-A	15	0	0	0	0
3	8-B	10	0	0	0	0
3	9-A	15	0	0	0	0
3	9-B	10	0	0	0	0
3	10-A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	10-B	10	0	0	0	0
3	11-A	15	0	0	0	0
3	11-B	10	0	0	0	0
3	12-A	15	0	0	0	0
3	12-B	10	0	0	0	0
3	13-A	15	0	0	0	0
3	13-B	10	0	0	0	0
3	14-A	15	0	0	0	0
3	14-B	10	0	0	0	0
3	15-A	15	0	0	0	0
3	15-B	10	0	0	0	0
3	16-A	15	0	0	0	0
3	16-B	10	0	0	0	0
4	1-A	288	0	0	0	0
4	1-B	264	0	0	0	1
4	2-A	284	0	0	0	1
4	2-B	268	0	0	0	0
4	3-A	282	0	0	0	1
4	3-B	270	0	0	0	0
4	4-A	284	0	0	0	1
4	4-B	268	0	0	0	0
4	5-A	283	0	0	0	1
4	5-B	269	0	0	0	0
4	6-A	292	0	0	0	1
4	6-B	260	0	0	0	0
4	7-A	291	0	0	0	1
4	7-B	261	0	0	0	0
4	8-A	293	0	0	0	1
4	8-B	259	0	0	0	0
4	9-A	292	0	0	0	1
4	9-B	260	0	0	0	0
4	10-A	280	0	0	0	1
4	10-B	272	0	0	0	0
4	11-A	294	0	0	0	1
4	11-B	258	0	0	0	0
4	12-A	285	0	0	0	1
4	12-B	267	0	0	0	0
4	13-A	291	0	0	0	1
4	13-B	261	0	0	0	0
4	14-A	289	0	0	0	1
4	14-B	263	0	0	0	1
4	15-A	285	0	0	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	15-B	267	0	0	0	0
4	16-A	284	0	0	0	2
4	16-B	268	0	0	0	0
All	All	87056	0	76960	0	18

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 18 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)
4:A:818:HOH:O	4:A:853:HOH:O[1_556]	1.89	0.31
4:A:816:HOH:O	4:A:851:HOH:O[1_556]	1.89	0.31
4:A:818:HOH:O	4:A:852:HOH:O[1_556]	1.89	0.31
4:A:814:HOH:O	4:A:849:HOH:O[1_556]	1.89	0.31
4:A:819:HOH:O	4:A:856:HOH:O[1_556]	1.89	0.31

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	305/312 (98%)	275 (90%)	26 (8%)	4 (1%)	18	4
1	1-B	305/312 (98%)	270 (88%)	28 (9%)	7 (2%)	10	1
1	2-A	305/312 (98%)	278 (91%)	25 (8%)	2 (1%)	30	13
1	2-B	305/312 (98%)	274 (90%)	24 (8%)	7 (2%)	10	1
1	3-A	305/312 (98%)	277 (91%)	26 (8%)	2 (1%)	30	13
1	3-B	305/312 (98%)	273 (90%)	25 (8%)	7 (2%)	10	1
1	4-A	305/312 (98%)	277 (91%)	24 (8%)	4 (1%)	18	4
1	4-B	305/312 (98%)	273 (90%)	28 (9%)	4 (1%)	18	4
1	5-A	305/312 (98%)	277 (91%)	26 (8%)	2 (1%)	30	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5-B	305/312 (98%)	272 (89%)	29 (10%)	4 (1%)	18	4
1	6-A	305/312 (98%)	277 (91%)	24 (8%)	4 (1%)	18	4
1	6-B	305/312 (98%)	274 (90%)	27 (9%)	4 (1%)	18	4
1	7-A	305/312 (98%)	288 (94%)	17 (6%)	0	100	100
1	7-B	305/312 (98%)	275 (90%)	27 (9%)	3 (1%)	22	6
1	8-A	305/312 (98%)	265 (87%)	37 (12%)	3 (1%)	22	6
1	8-B	305/312 (98%)	275 (90%)	23 (8%)	7 (2%)	10	1
1	9-A	305/312 (98%)	284 (93%)	17 (6%)	4 (1%)	18	4
1	9-B	305/312 (98%)	271 (89%)	30 (10%)	4 (1%)	18	4
1	10-A	305/312 (98%)	275 (90%)	29 (10%)	1 (0%)	50	31
1	10-B	305/312 (98%)	272 (89%)	27 (9%)	6 (2%)	11	2
1	11-A	305/312 (98%)	283 (93%)	20 (7%)	2 (1%)	30	13
1	11-B	305/312 (98%)	268 (88%)	28 (9%)	9 (3%)	7	1
1	12-A	305/312 (98%)	286 (94%)	17 (6%)	2 (1%)	30	13
1	12-B	305/312 (98%)	275 (90%)	26 (8%)	4 (1%)	18	4
1	13-A	305/312 (98%)	272 (89%)	26 (8%)	7 (2%)	10	1
1	13-B	305/312 (98%)	275 (90%)	24 (8%)	6 (2%)	11	2
1	14-A	305/312 (98%)	266 (87%)	35 (12%)	4 (1%)	18	4
1	14-B	305/312 (98%)	269 (88%)	28 (9%)	8 (3%)	8	1
1	15-A	305/312 (98%)	270 (88%)	28 (9%)	7 (2%)	10	1
1	15-B	305/312 (98%)	275 (90%)	27 (9%)	3 (1%)	22	6
1	16-A	305/312 (98%)	270 (88%)	29 (10%)	6 (2%)	11	2
1	16-B	305/312 (98%)	266 (87%)	32 (10%)	7 (2%)	10	1
All	All	9760/9984 (98%)	8777 (90%)	839 (9%)	144 (2%)	15	3

5 of 144 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	3-B	82	SER
1	3-B	98	LEU
1	4-A	252	LYS
1	5-B	180	PRO
1	8-B	50	PHE

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	268/266 (101%)	260 (97%)	8 (3%)	53	34
1	1-B	268/266 (101%)	263 (98%)	5 (2%)	69	56
1	2-A	268/266 (101%)	262 (98%)	6 (2%)	64	48
1	2-B	268/266 (101%)	260 (97%)	8 (3%)	53	34
1	3-A	268/266 (101%)	261 (97%)	7 (3%)	59	41
1	3-B	268/266 (101%)	266 (99%)	2 (1%)	91	88
1	4-A	268/266 (101%)	258 (96%)	10 (4%)	45	26
1	4-B	268/266 (101%)	262 (98%)	6 (2%)	64	48
1	5-A	268/266 (101%)	259 (97%)	9 (3%)	49	29
1	5-B	268/266 (101%)	266 (99%)	2 (1%)	91	88
1	6-A	268/266 (101%)	260 (97%)	8 (3%)	53	34
1	6-B	268/266 (101%)	264 (98%)	4 (2%)	76	66
1	7-A	268/266 (101%)	265 (99%)	3 (1%)	84	77
1	7-B	268/266 (101%)	264 (98%)	4 (2%)	76	66
1	8-A	268/266 (101%)	263 (98%)	5 (2%)	69	56
1	8-B	268/266 (101%)	265 (99%)	3 (1%)	84	77
1	9-A	268/266 (101%)	265 (99%)	3 (1%)	84	77
1	9-B	268/266 (101%)	264 (98%)	4 (2%)	76	66
1	10-A	268/266 (101%)	262 (98%)	6 (2%)	64	48
1	10-B	268/266 (101%)	265 (99%)	3 (1%)	84	77
1	11-A	268/266 (101%)	262 (98%)	6 (2%)	64	48
1	11-B	268/266 (101%)	260 (97%)	8 (3%)	53	34
1	12-A	268/266 (101%)	263 (98%)	5 (2%)	69	56
1	12-B	268/266 (101%)	263 (98%)	5 (2%)	69	56
1	13-A	268/266 (101%)	260 (97%)	8 (3%)	53	34
1	13-B	268/266 (101%)	258 (96%)	10 (4%)	45	26
1	14-A	268/266 (101%)	255 (95%)	13 (5%)	35	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	14-B	268/266 (101%)	258 (96%)	10 (4%)	45	26
1	15-A	268/266 (101%)	252 (94%)	16 (6%)	27	10
1	15-B	268/266 (101%)	263 (98%)	5 (2%)	69	56
1	16-A	268/266 (101%)	255 (95%)	13 (5%)	35	15
1	16-B	268/266 (101%)	262 (98%)	6 (2%)	64	48
All	All	8576/8512 (101%)	8365 (98%)	211 (2%)	60	42

5 of 211 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	9-B	289	GLU
1	11-B	274	ASP
1	16-A	161	LEU
1	10-A	61	THR
1	11-A	152	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	8-A	36	ASN
1	9-B	22	ASN
1	16-A	93	GLN
1	8-B	20	HIS
1	9-B	93	GLN

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 ⓘ

Of 112 ligands modelled in this entry, 32 are monoatomic - leaving 80 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	1-A	701	-	4,4,4	0.29	0	6,6,6	0.11	0
3	SO4	1-A	702	-	4,4,4	0.32	0	6,6,6	0.08	0
3	SO4	1-A	703	-	4,4,4	0.17	0	6,6,6	0.20	0
3	SO4	1-B	704	-	4,4,4	0.30	0	6,6,6	0.08	0
3	SO4	1-B	705	-	4,4,4	0.28	0	6,6,6	0.07	0
3	SO4	10-A	701	-	4,4,4	0.25	0	6,6,6	0.08	0
3	SO4	10-A	702	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	10-A	703	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	10-B	704	-	4,4,4	0.26	0	6,6,6	0.11	0
3	SO4	10-B	705	-	4,4,4	0.27	0	6,6,6	0.08	0
3	SO4	11-A	701	-	4,4,4	0.26	0	6,6,6	0.12	0
3	SO4	11-A	702	-	4,4,4	0.32	0	6,6,6	0.08	0
3	SO4	11-A	703	-	4,4,4	0.22	0	6,6,6	0.16	0
3	SO4	11-B	704	-	4,4,4	0.30	0	6,6,6	0.08	0
3	SO4	11-B	705	-	4,4,4	0.27	0	6,6,6	0.08	0
3	SO4	12-A	701	-	4,4,4	0.29	0	6,6,6	0.12	0
3	SO4	12-A	702	-	4,4,4	0.32	0	6,6,6	0.08	0
3	SO4	12-A	703	-	4,4,4	0.18	0	6,6,6	0.18	0
3	SO4	12-B	704	-	4,4,4	0.28	0	6,6,6	0.10	0
3	SO4	12-B	705	-	4,4,4	0.30	0	6,6,6	0.12	0
3	SO4	13-A	701	-	4,4,4	0.28	0	6,6,6	0.10	0
3	SO4	13-A	702	-	4,4,4	0.36	0	6,6,6	0.09	0
3	SO4	13-A	703	-	4,4,4	0.20	0	6,6,6	0.17	0
3	SO4	13-B	704	-	4,4,4	0.30	0	6,6,6	0.10	0
3	SO4	13-B	705	-	4,4,4	0.30	0	6,6,6	0.10	0
3	SO4	14-A	701	-	4,4,4	0.27	0	6,6,6	0.09	0
3	SO4	14-A	702	-	4,4,4	0.33	0	6,6,6	0.12	0
3	SO4	14-A	703	-	4,4,4	0.22	0	6,6,6	0.14	0
3	SO4	14-B	704	-	4,4,4	0.31	0	6,6,6	0.09	0
3	SO4	14-B	705	-	4,4,4	0.30	0	6,6,6	0.08	0
3	SO4	15-A	701	-	4,4,4	0.27	0	6,6,6	0.09	0
3	SO4	15-A	702	-	4,4,4	0.37	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	15-A	703	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	15-B	704	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	15-B	705	-	4,4,4	0.27	0	6,6,6	0.08	0
3	SO4	16-A	701	-	4,4,4	0.29	0	6,6,6	0.13	0
3	SO4	16-A	702	-	4,4,4	0.36	0	6,6,6	0.09	0
3	SO4	16-A	703	-	4,4,4	0.24	0	6,6,6	0.15	0
3	SO4	16-B	704	-	4,4,4	0.31	0	6,6,6	0.08	0
3	SO4	16-B	705	-	4,4,4	0.29	0	6,6,6	0.11	0
3	SO4	2-A	701	-	4,4,4	0.26	0	6,6,6	0.10	0
3	SO4	2-A	702	-	4,4,4	0.32	0	6,6,6	0.08	0
3	SO4	2-A	703	-	4,4,4	0.19	0	6,6,6	0.19	0
3	SO4	2-B	704	-	4,4,4	0.30	0	6,6,6	0.09	0
3	SO4	2-B	705	-	4,4,4	0.34	0	6,6,6	0.12	0
3	SO4	3-A	701	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	3-A	702	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	3-A	703	-	4,4,4	0.21	0	6,6,6	0.09	0
3	SO4	3-B	704	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	3-B	705	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	4-A	701	-	4,4,4	0.29	0	6,6,6	0.08	0
3	SO4	4-A	702	-	4,4,4	0.30	0	6,6,6	0.09	0
3	SO4	4-A	703	-	4,4,4	0.20	0	6,6,6	0.18	0
3	SO4	4-B	704	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	4-B	705	-	4,4,4	0.24	0	6,6,6	0.11	0
3	SO4	5-A	701	-	4,4,4	0.35	0	6,6,6	0.10	0
3	SO4	5-A	702	-	4,4,4	0.33	0	6,6,6	0.08	0
3	SO4	5-A	703	-	4,4,4	0.18	0	6,6,6	0.18	0
3	SO4	5-B	704	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	5-B	705	-	4,4,4	0.27	0	6,6,6	0.10	0
3	SO4	6-A	701	-	4,4,4	0.32	0	6,6,6	0.10	0
3	SO4	6-A	702	-	4,4,4	0.27	0	6,6,6	0.10	0
3	SO4	6-A	703	-	4,4,4	0.18	0	6,6,6	0.20	0
3	SO4	6-B	704	-	4,4,4	0.30	0	6,6,6	0.09	0
3	SO4	6-B	705	-	4,4,4	0.28	0	6,6,6	0.10	0
3	SO4	7-A	701	-	4,4,4	0.26	0	6,6,6	0.08	0
3	SO4	7-A	702	-	4,4,4	0.31	0	6,6,6	0.08	0
3	SO4	7-A	703	-	4,4,4	0.20	0	6,6,6	0.18	0
3	SO4	7-B	704	-	4,4,4	0.31	0	6,6,6	0.08	0
3	SO4	7-B	705	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	8-A	701	-	4,4,4	0.29	0	6,6,6	0.14	0
3	SO4	8-A	702	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	8-A	703	-	4,4,4	0.20	0	6,6,6	0.08	0
3	SO4	8-B	704	-	4,4,4	0.30	0	6,6,6	0.08	0
3	SO4	8-B	705	-	4,4,4	0.28	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	9-A	701	-	4,4,4	0.26	0	6,6,6	0.08	0
3	SO4	9-A	702	-	4,4,4	0.36	0	6,6,6	0.11	0
3	SO4	9-A	703	-	4,4,4	0.17	0	6,6,6	0.19	0
3	SO4	9-B	704	-	4,4,4	0.30	0	6,6,6	0.09	0
3	SO4	9-B	705	-	4,4,4	0.27	0	6,6,6	0.11	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
3	SO4	1-A	701	-	-	0/0/0/0	0/0/0/0
3	SO4	1-A	702	-	-	0/0/0/0	0/0/0/0
3	SO4	1-A	703	-	-	0/0/0/0	0/0/0/0
3	SO4	1-B	704	-	-	0/0/0/0	0/0/0/0
3	SO4	1-B	705	-	-	0/0/0/0	0/0/0/0
3	SO4	10-A	701	-	-	0/0/0/0	0/0/0/0
3	SO4	10-A	702	-	-	0/0/0/0	0/0/0/0
3	SO4	10-A	703	-	-	0/0/0/0	0/0/0/0
3	SO4	10-B	704	-	-	0/0/0/0	0/0/0/0
3	SO4	10-B	705	-	-	0/0/0/0	0/0/0/0
3	SO4	11-A	701	-	-	0/0/0/0	0/0/0/0
3	SO4	11-A	702	-	-	0/0/0/0	0/0/0/0
3	SO4	11-A	703	-	-	0/0/0/0	0/0/0/0
3	SO4	11-B	704	-	-	0/0/0/0	0/0/0/0
3	SO4	11-B	705	-	-	0/0/0/0	0/0/0/0
3	SO4	12-A	701	-	-	0/0/0/0	0/0/0/0
3	SO4	12-A	702	-	-	0/0/0/0	0/0/0/0
3	SO4	12-A	703	-	-	0/0/0/0	0/0/0/0
3	SO4	12-B	704	-	-	0/0/0/0	0/0/0/0
3	SO4	12-B	705	-	-	0/0/0/0	0/0/0/0
3	SO4	13-A	701	-	-	0/0/0/0	0/0/0/0
3	SO4	13-A	702	-	-	0/0/0/0	0/0/0/0
3	SO4	13-A	703	-	-	0/0/0/0	0/0/0/0
3	SO4	13-B	704	-	-	0/0/0/0	0/0/0/0
3	SO4	13-B	705	-	-	0/0/0/0	0/0/0/0
3	SO4	14-A	701	-	-	0/0/0/0	0/0/0/0
3	SO4	14-A	702	-	-	0/0/0/0	0/0/0/0
3	SO4	14-A	703	-	-	0/0/0/0	0/0/0/0
3	SO4	14-B	704	-	-	0/0/0/0	0/0/0/0
3	SO4	14-B	705	-	-	0/0/0/0	0/0/0/0
3	SO4	15-A	701	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	15-A	702	-	-	0/0/0/0	0/0/0/0
3	SO4	15-A	703	-	-	0/0/0/0	0/0/0/0
3	SO4	15-B	704	-	-	0/0/0/0	0/0/0/0
3	SO4	15-B	705	-	-	0/0/0/0	0/0/0/0
3	SO4	16-A	701	-	-	0/0/0/0	0/0/0/0
3	SO4	16-A	702	-	-	0/0/0/0	0/0/0/0
3	SO4	16-A	703	-	-	0/0/0/0	0/0/0/0
3	SO4	16-B	704	-	-	0/0/0/0	0/0/0/0
3	SO4	16-B	705	-	-	0/0/0/0	0/0/0/0
3	SO4	2-A	701	-	-	0/0/0/0	0/0/0/0
3	SO4	2-A	702	-	-	0/0/0/0	0/0/0/0
3	SO4	2-A	703	-	-	0/0/0/0	0/0/0/0
3	SO4	2-B	704	-	-	0/0/0/0	0/0/0/0
3	SO4	2-B	705	-	-	0/0/0/0	0/0/0/0
3	SO4	3-A	701	-	-	0/0/0/0	0/0/0/0
3	SO4	3-A	702	-	-	0/0/0/0	0/0/0/0
3	SO4	3-A	703	-	-	0/0/0/0	0/0/0/0
3	SO4	3-B	704	-	-	0/0/0/0	0/0/0/0
3	SO4	3-B	705	-	-	0/0/0/0	0/0/0/0
3	SO4	4-A	701	-	-	0/0/0/0	0/0/0/0
3	SO4	4-A	702	-	-	0/0/0/0	0/0/0/0
3	SO4	4-A	703	-	-	0/0/0/0	0/0/0/0
3	SO4	4-B	704	-	-	0/0/0/0	0/0/0/0
3	SO4	4-B	705	-	-	0/0/0/0	0/0/0/0
3	SO4	5-A	701	-	-	0/0/0/0	0/0/0/0
3	SO4	5-A	702	-	-	0/0/0/0	0/0/0/0
3	SO4	5-A	703	-	-	0/0/0/0	0/0/0/0
3	SO4	5-B	704	-	-	0/0/0/0	0/0/0/0
3	SO4	5-B	705	-	-	0/0/0/0	0/0/0/0
3	SO4	6-A	701	-	-	0/0/0/0	0/0/0/0
3	SO4	6-A	702	-	-	0/0/0/0	0/0/0/0
3	SO4	6-A	703	-	-	0/0/0/0	0/0/0/0
3	SO4	6-B	704	-	-	0/0/0/0	0/0/0/0
3	SO4	6-B	705	-	-	0/0/0/0	0/0/0/0
3	SO4	7-A	701	-	-	0/0/0/0	0/0/0/0
3	SO4	7-A	702	-	-	0/0/0/0	0/0/0/0
3	SO4	7-A	703	-	-	0/0/0/0	0/0/0/0
3	SO4	7-B	704	-	-	0/0/0/0	0/0/0/0
3	SO4	7-B	705	-	-	0/0/0/0	0/0/0/0
3	SO4	8-A	701	-	-	0/0/0/0	0/0/0/0
3	SO4	8-A	702	-	-	0/0/0/0	0/0/0/0
3	SO4	8-A	703	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	8-B	704	-	-	0/0/0/0	0/0/0/0
3	SO4	8-B	705	-	-	0/0/0/0	0/0/0/0
3	SO4	9-A	701	-	-	0/0/0/0	0/0/0/0
3	SO4	9-A	702	-	-	0/0/0/0	0/0/0/0
3	SO4	9-A	703	-	-	0/0/0/0	0/0/0/0
3	SO4	9-B	704	-	-	0/0/0/0	0/0/0/0
3	SO4	9-B	705	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

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.