



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 01:52 PM UTC

PDB ID : 2Q4Z / pdb_00002q4z
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

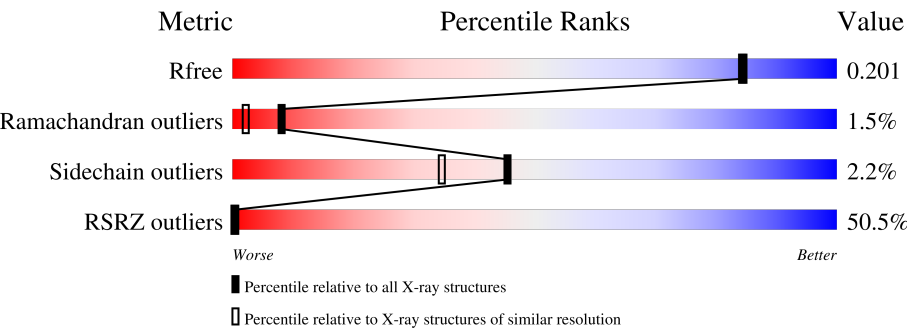
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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.



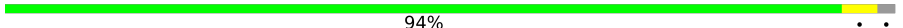
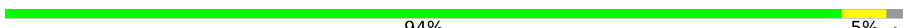
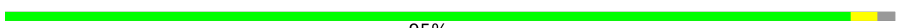
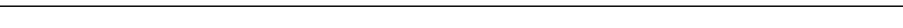
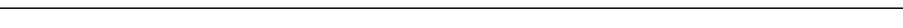
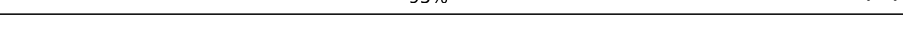
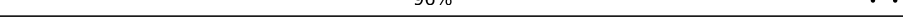
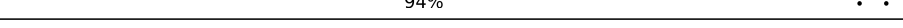
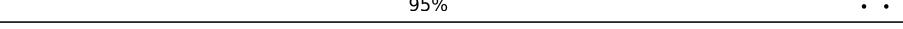
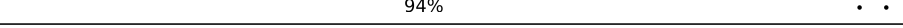
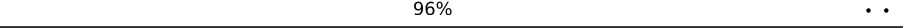
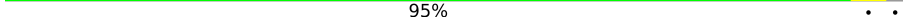
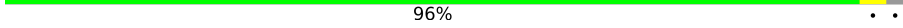
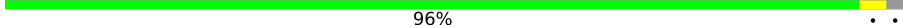
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	7662 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 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	312	45% 95%
1	1-B	312	53% 94%
1	10-A	312	96%
1	10-B	312	94%
1	11-A	312	96%
1	11-B	312	93% 5%
1	12-A	312	96%

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Mol	Chain	Length	Quality of chain
1	12-B	312	 94% . .
1	13-A	312	 94% . .
1	13-B	312	 94% 5% .
1	14-A	312	 95% . .
1	14-B	312	 93% 5% .
1	15-A	312	 94% . .
1	15-B	312	 95% . .
1	16-A	312	 94% . .
1	16-B	312	 94% . .
1	2-A	312	 96% . .
1	2-B	312	 94% . .
1	3-A	312	 96% . .
1	3-B	312	 93% 5% .
1	4-A	312	 95% . .
1	4-B	312	 95% . .
1	5-A	312	 96% . .
1	5-B	312	 94% . .
1	6-A	312	 95% . .
1	6-B	312	 94% . .
1	7-A	312	 96% . .
1	7-B	312	 95% . .
1	8-A	312	 96% . .
1	8-B	312	 93% 5% .
1	9-A	312	 96% . .
1	9-B	312	 95% . .

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	ZN	1-A	601	-	-	-	X
2	ZN	1-B	602	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 87056 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 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	2-A	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	4-A	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	6-A	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	8-A	307	Total	C	N	O	S	Se	0	0	0
			2431	1552	413	451	8	7			
1	9-A	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	11-A	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	13-A	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	15-A	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			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-B	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-B	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-B	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-B	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			
1	9-B	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-B	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-B	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-B	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	variant	UNP Q9R1T5
A	131	GLY	ARG	variant	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	variant	UNP Q9R1T5
B	131	GLY	ARG	variant	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 (CCD ID: ZN) (formula: Zn).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	14-A	1	Total 1	Zn 1	0	0
2	15-A	1	Total 1	Zn 1	0	0
2	16-A	1	Total 1	Zn 1	0	0
2	1-B	1	Total 1	Zn 1	0	0
2	2-B	1	Total 1	Zn 1	0	0
2	3-B	1	Total 1	Zn 1	0	0
2	4-B	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	7-B	1	Total 1	Zn 1	0	0
2	8-B	1	Total 1	Zn 1	0	0
2	9-B	1	Total 1	Zn 1	0	0
2	10-B	1	Total 1	Zn 1	0	0
2	11-B	1	Total 1	Zn 1	0	0
2	12-B	1	Total 1	Zn 1	0	0
2	13-B	1	Total 1	Zn 1	0	0
2	14-B	1	Total 1	Zn 1	0	0
2	15-B	1	Total 1	Zn 1	0	0
2	16-B	1	Total 1	Zn 1	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	14-B	1	Total	O	S	0	0
			5	4	1		
3	15-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	2-A	284	Total	O		0	0
			284	284			
4	3-A	282	Total	O		0	0
			282	282			
4	4-A	284	Total	O		0	0
			284	284			
4	5-A	283	Total	O		0	0
			283	283			
4	6-A	292	Total	O		0	0
			292	292			
4	7-A	291	Total	O		0	0
			291	291			
4	8-A	293	Total	O		0	0
			293	293			
4	9-A	292	Total	O		0	0
			292	292			
4	10-A	280	Total	O		0	0
			280	280			
4	11-A	294	Total	O		0	0
			294	294			
4	12-A	285	Total	O		0	0
			285	285			
4	13-A	291	Total	O		0	0
			291	291			
4	14-A	289	Total	O		0	0
			289	289			
4	15-A	285	Total	O		0	0
			285	285			
4	16-A	284	Total	O		0	0
			284	284			

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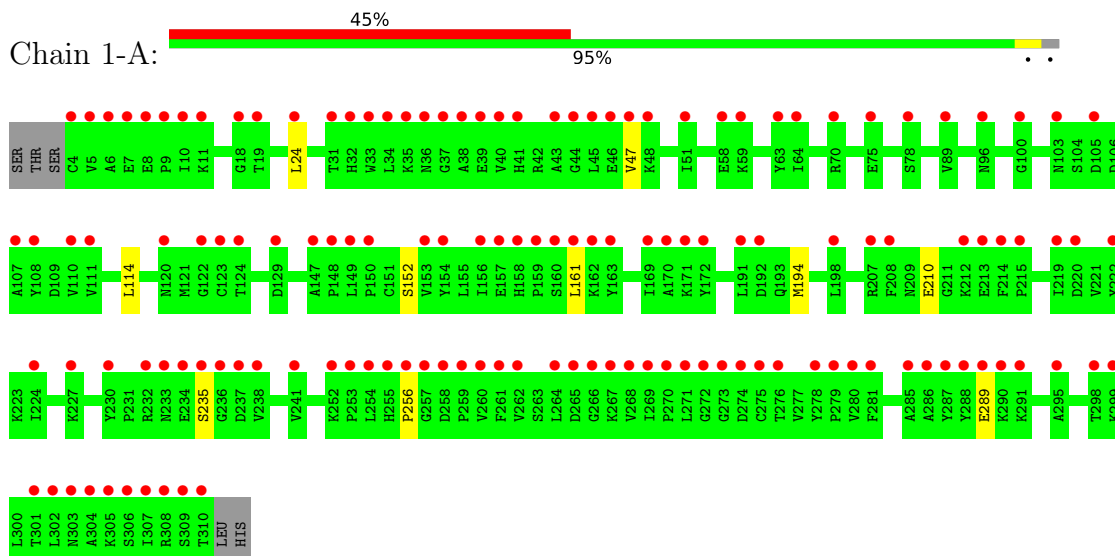
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-B	264	Total 264	O 264	0	0
4	2-B	268	Total 268	O 268	0	0
4	3-B	270	Total 270	O 270	0	0
4	4-B	268	Total 268	O 268	0	0
4	5-B	269	Total 269	O 269	0	0
4	6-B	260	Total 260	O 260	0	0
4	7-B	261	Total 261	O 261	0	0
4	8-B	259	Total 259	O 259	0	0
4	9-B	260	Total 260	O 260	0	0
4	10-B	272	Total 272	O 272	0	0
4	11-B	258	Total 258	O 258	0	0
4	12-B	267	Total 267	O 267	0	0
4	13-B	261	Total 261	O 261	0	0
4	14-B	263	Total 263	O 263	0	0
4	15-B	267	Total 267	O 267	0	0
4	16-B	268	Total 268	O 268	0	0

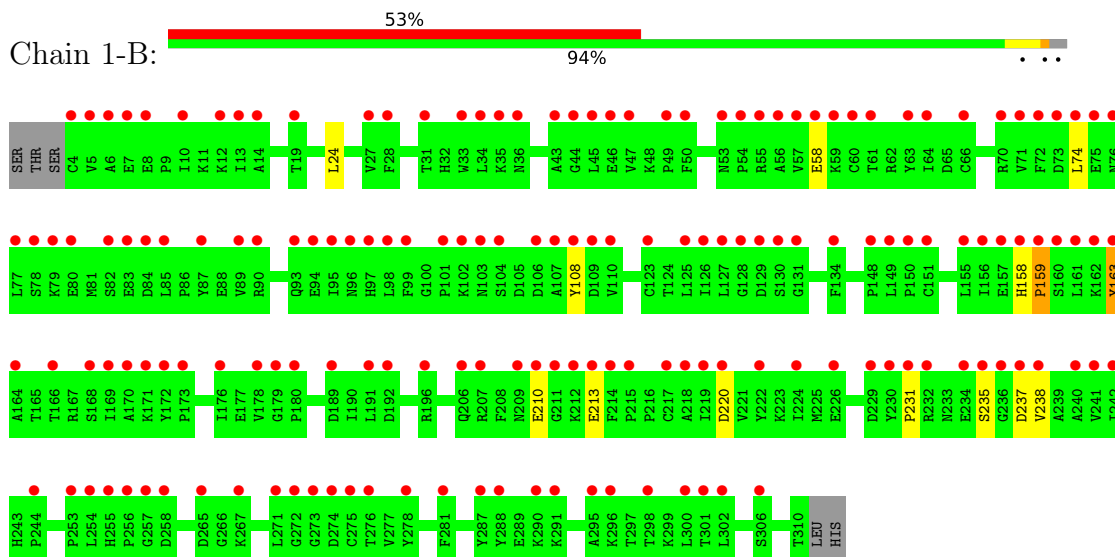
3 Residue-property plots [i](#)

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.

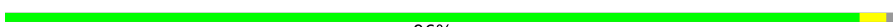
• Molecule 1: Aspartoacylase



• Molecule 1: Aspartoacylase

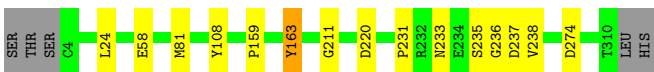


• Molecule 1: Aspartoacylase

Chain 2-A:  96% 



- Molecule 1: Aspartoacylase

Chain 2-B:  94% 



- Molecule 1: Aspartoacylase

Chain 3-A:  96% 

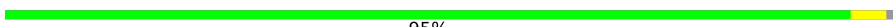


- Molecule 1: Aspartoacylase

Chain 3-B:  93% 

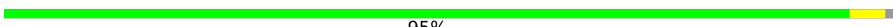


- Molecule 1: Aspartoacylase

Chain 4-A:  95% 

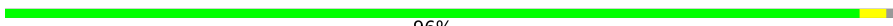


- Molecule 1: Aspartoacylase

Chain 4-B:  95% 



- Molecule 1: Aspartoacylase

Chain 5-A:  96% 

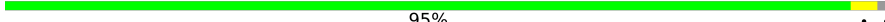


- Molecule 1: Aspartoacylase

Chain 5-B:  94% ..



- Molecule 1: Aspartoacylase

Chain 6-A:  95% ..

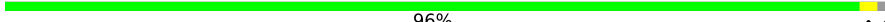


- Molecule 1: Aspartoacylase

Chain 6-B:  94% ..

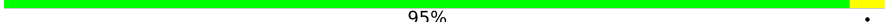


- Molecule 1: Aspartoacylase

Chain 7-A:  96% ..

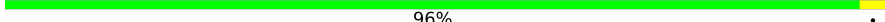


- Molecule 1: Aspartoacylase

Chain 7-B:  95% ..



- Molecule 1: Aspartoacylase

Chain 8-A:  96% ..

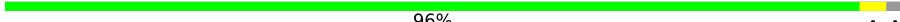


- Molecule 1: Aspartoacylase

Chain 8-B:  93% 5% ..



- Molecule 1: Aspartoacylase

Chain 9-A:  96% ..

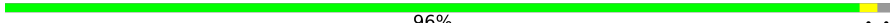


- Molecule 1: Aspartoacylase

Chain 9-B:  95% ..



- Molecule 1: Aspartoacylase

Chain 10-A:  96% ..

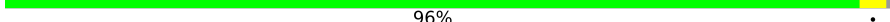


- Molecule 1: Aspartoacylase

Chain 10-B:  94% ..



- Molecule 1: Aspartoacylase

Chain 11-A:  96% ..

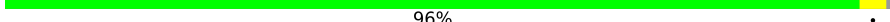


- Molecule 1: Aspartoacylase

Chain 11-B:  93% 5% .



- Molecule 1: Aspartoacylase

Chain 12-A:  96% ..

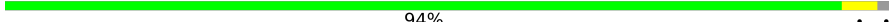


- Molecule 1: Aspartoacylase

Chain 12-B:  94% . .



- Molecule 1: Aspartoacylase

Chain 13-A:  94% . .

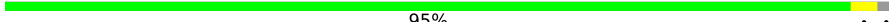


- Molecule 1: Aspartoacylase

Chain 13-B:  94% 5% .



- Molecule 1: Aspartoacylase

Chain 14-A:  95% . .

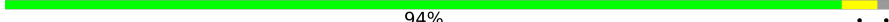


- Molecule 1: Aspartoacylase

Chain 14-B:  93% 5% .

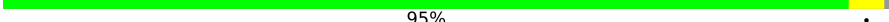


- Molecule 1: Aspartoacylase

Chain 15-A:  94% . .



- Molecule 1: Aspartoacylase

Chain 15-B:  95% . .



- Molecule 1: Aspartoacylase

Chain 16-A:  94% . .



● Molecule 1: Aspartoacylase

Chain 16-B:  94% . . .



4 Data and refinement statistics

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 40.50 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.1 (40.50-1.80) 97.2 (40.50-1.80)	Depositor EDS
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 0.151 , 0.201	Depositor DCC
R_{free} test set	2955 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.02 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
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.

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: 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	0.22	0/2484	0.32	1/3360 (0.0%)
1	1-B	0.20	0/2484	0.34	2/3360 (0.1%)
1	2-A	0.22	0/2484	0.32	1/3360 (0.0%)
1	2-B	0.20	0/2484	0.34	2/3360 (0.1%)
1	3-A	0.22	0/2484	0.32	1/3360 (0.0%)
1	3-B	0.20	0/2484	0.34	2/3360 (0.1%)
1	4-A	0.22	0/2484	0.32	1/3360 (0.0%)
1	4-B	0.20	0/2484	0.34	2/3360 (0.1%)
1	5-A	0.22	0/2484	0.32	1/3360 (0.0%)
1	5-B	0.20	0/2484	0.34	2/3360 (0.1%)
1	6-A	0.22	0/2484	0.32	1/3360 (0.0%)
1	6-B	0.20	0/2484	0.34	2/3360 (0.1%)
1	7-A	0.22	0/2484	0.32	1/3360 (0.0%)
1	7-B	0.20	0/2484	0.34	2/3360 (0.1%)
1	8-A	0.22	0/2484	0.32	1/3360 (0.0%)
1	8-B	0.20	0/2484	0.34	2/3360 (0.1%)
1	9-A	0.22	0/2484	0.32	1/3360 (0.0%)
1	9-B	0.20	0/2484	0.34	2/3360 (0.1%)
1	10-A	0.22	0/2484	0.32	1/3360 (0.0%)
1	10-B	0.20	0/2484	0.34	2/3360 (0.1%)
1	11-A	0.22	0/2484	0.32	1/3360 (0.0%)
1	11-B	0.20	0/2484	0.34	2/3360 (0.1%)
1	12-A	0.22	0/2484	0.32	1/3360 (0.0%)
1	12-B	0.20	0/2484	0.34	2/3360 (0.1%)
1	13-A	0.22	0/2484	0.32	1/3360 (0.0%)
1	13-B	0.20	0/2484	0.34	2/3360 (0.1%)
1	14-A	0.22	0/2484	0.32	1/3360 (0.0%)
1	14-B	0.20	0/2484	0.34	2/3360 (0.1%)
1	15-A	0.22	0/2484	0.32	1/3360 (0.0%)
1	15-B	0.20	0/2484	0.34	2/3360 (0.1%)
1	16-A	0.22	0/2484	0.32	1/3360 (0.0%)
1	16-B	0.20	0/2484	0.34	2/3360 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.21	0/79488	0.33	48/107520 (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.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	24	LEU	N-CA-C	7.49	121.52	112.38
1	2-A	24	LEU	N-CA-C	7.49	121.52	112.38
1	3-A	24	LEU	N-CA-C	7.49	121.52	112.38
1	4-A	24	LEU	N-CA-C	7.49	121.52	112.38
1	5-A	24	LEU	N-CA-C	7.49	121.52	112.38
1	6-A	24	LEU	N-CA-C	7.49	121.52	112.38
1	7-A	24	LEU	N-CA-C	7.49	121.52	112.38
1	8-A	24	LEU	N-CA-C	7.49	121.52	112.38
1	9-A	24	LEU	N-CA-C	7.49	121.52	112.38
1	10-A	24	LEU	N-CA-C	7.49	121.52	112.38
1	11-A	24	LEU	N-CA-C	7.49	121.52	112.38
1	12-A	24	LEU	N-CA-C	7.49	121.52	112.38
1	13-A	24	LEU	N-CA-C	7.49	121.52	112.38
1	14-A	24	LEU	N-CA-C	7.49	121.52	112.38
1	15-A	24	LEU	N-CA-C	7.49	121.52	112.38
1	16-A	24	LEU	N-CA-C	7.49	121.52	112.38
1	1-B	24	LEU	N-CA-C	5.39	120.01	113.38
1	2-B	24	LEU	N-CA-C	5.39	120.01	113.38
1	3-B	24	LEU	N-CA-C	5.39	120.01	113.38
1	4-B	24	LEU	N-CA-C	5.39	120.01	113.38
1	5-B	24	LEU	N-CA-C	5.39	120.01	113.38
1	6-B	24	LEU	N-CA-C	5.39	120.01	113.38
1	7-B	24	LEU	N-CA-C	5.39	120.01	113.38
1	8-B	24	LEU	N-CA-C	5.39	120.01	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-B	24	LEU	N-CA-C	5.39	120.01	113.38
1	10-B	24	LEU	N-CA-C	5.39	120.01	113.38
1	11-B	24	LEU	N-CA-C	5.39	120.01	113.38
1	12-B	24	LEU	N-CA-C	5.39	120.01	113.38
1	13-B	24	LEU	N-CA-C	5.39	120.01	113.38
1	14-B	24	LEU	N-CA-C	5.39	120.01	113.38
1	15-B	24	LEU	N-CA-C	5.39	120.01	113.38
1	16-B	24	LEU	N-CA-C	5.39	120.01	113.38
1	1-B	231	PRO	N-CA-C	-5.10	103.11	111.21
1	2-B	231	PRO	N-CA-C	-5.10	103.11	111.21
1	3-B	231	PRO	N-CA-C	-5.10	103.11	111.21
1	4-B	231	PRO	N-CA-C	-5.10	103.11	111.21
1	5-B	231	PRO	N-CA-C	-5.10	103.11	111.21
1	6-B	231	PRO	N-CA-C	-5.10	103.11	111.21
1	7-B	231	PRO	N-CA-C	-5.10	103.11	111.21
1	8-B	231	PRO	N-CA-C	-5.10	103.11	111.21
1	9-B	231	PRO	N-CA-C	-5.10	103.11	111.21
1	10-B	231	PRO	N-CA-C	-5.10	103.11	111.21
1	11-B	231	PRO	N-CA-C	-5.10	103.11	111.21
1	12-B	231	PRO	N-CA-C	-5.10	103.11	111.21
1	13-B	231	PRO	N-CA-C	-5.10	103.11	111.21
1	14-B	231	PRO	N-CA-C	-5.10	103.11	111.21
1	15-B	231	PRO	N-CA-C	-5.10	103.11	111.21
1	16-B	231	PRO	N-CA-C	-5.10	103.11	111.21

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 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	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	0
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	0
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
2	5-B	1	0	0	0	0
2	6-A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
3	10-B	10	0	0	0	0
3	11-A	15	0	0	0	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	16-B	268	0	0	0	0
All	All	87056	0	76960	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	305/312 (98%)	275 (90%)	26 (8%)	4 (1%)	9	3
1	1-B	305/312 (98%)	270 (88%)	28 (9%)	7 (2%)	5	1
1	2-A	305/312 (98%)	278 (91%)	25 (8%)	2 (1%)	18	8
1	2-B	305/312 (98%)	274 (90%)	24 (8%)	7 (2%)	5	1
1	3-A	305/312 (98%)	277 (91%)	26 (8%)	2 (1%)	18	8
1	3-B	305/312 (98%)	273 (90%)	25 (8%)	7 (2%)	5	1
1	4-A	305/312 (98%)	277 (91%)	24 (8%)	4 (1%)	9	3
1	4-B	305/312 (98%)	273 (90%)	28 (9%)	4 (1%)	9	3
1	5-A	305/312 (98%)	277 (91%)	26 (8%)	2 (1%)	18	8
1	5-B	305/312 (98%)	272 (89%)	29 (10%)	4 (1%)	9	3
1	6-A	305/312 (98%)	277 (91%)	24 (8%)	4 (1%)	9	3
1	6-B	305/312 (98%)	274 (90%)	27 (9%)	4 (1%)	9	3
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%)	12	4
1	8-A	305/312 (98%)	265 (87%)	37 (12%)	3 (1%)	12	4
1	8-B	305/312 (98%)	275 (90%)	23 (8%)	7 (2%)	5	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	9-A	305/312 (98%)	284 (93%)	17 (6%)	4 (1%)	9	3
1	9-B	305/312 (98%)	271 (89%)	30 (10%)	4 (1%)	9	3
1	10-A	305/312 (98%)	275 (90%)	29 (10%)	1 (0%)	36	25
1	10-B	305/312 (98%)	272 (89%)	27 (9%)	6 (2%)	6	1
1	11-A	305/312 (98%)	283 (93%)	20 (7%)	2 (1%)	18	8
1	11-B	305/312 (98%)	268 (88%)	28 (9%)	9 (3%)	3	0
1	12-A	305/312 (98%)	286 (94%)	17 (6%)	2 (1%)	18	8
1	12-B	305/312 (98%)	275 (90%)	26 (8%)	4 (1%)	9	3
1	13-A	305/312 (98%)	272 (89%)	26 (8%)	7 (2%)	5	1
1	13-B	305/312 (98%)	275 (90%)	24 (8%)	6 (2%)	6	1
1	14-A	305/312 (98%)	266 (87%)	35 (12%)	4 (1%)	9	3
1	14-B	305/312 (98%)	269 (88%)	28 (9%)	8 (3%)	4	0
1	15-A	305/312 (98%)	270 (88%)	28 (9%)	7 (2%)	5	1
1	15-B	305/312 (98%)	275 (90%)	27 (9%)	3 (1%)	12	4
1	16-A	305/312 (98%)	270 (88%)	29 (10%)	6 (2%)	6	1
1	16-B	305/312 (98%)	266 (87%)	32 (10%)	7 (2%)	5	1
All	All	9760/9984 (98%)	8777 (90%)	839 (9%)	144 (2%)	8	2

All (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
1	8-B	226	GLU
1	9-A	152	SER
1	11-A	81	MSE
1	11-B	60	CYS
1	11-B	78	SER
1	11-B	168	SER
1	11-B	180	PRO
1	12-B	22	ASN
1	13-A	103	ASN
1	14-B	250	ASP

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Mol	Chain	Res	Type
1	14-B	251	TRP
1	15-A	103	ASN
1	15-A	157	GLU
1	15-B	80	GLU
1	16-B	104	SER
1	16-B	162	LYS
1	1-A	47	VAL
1	1-A	256	PRO
1	1-B	159	PRO
1	1-B	163	TYR
1	2-A	210	GLU
1	2-B	81	MSE
1	2-B	163	TYR
1	2-B	235	SER
1	3-B	99	PHE
1	3-B	167	ARG
1	4-B	168	SER
1	5-B	162	LYS
1	6-A	108	TYR
1	6-A	212	LYS
1	6-B	188	ALA
1	7-B	162	LYS
1	8-A	210	GLU
1	9-A	256	PRO
1	9-B	163	TYR
1	10-B	81	MSE
1	11-A	77	LEU
1	11-B	72	PHE
1	11-B	82	SER
1	12-B	21	GLY
1	12-B	74	LEU
1	15-A	224	ILE
1	15-A	225	MSE
1	15-B	35	LYS
1	16-B	74	LEU
1	1-B	210	GLU
1	1-B	235	SER
1	4-B	234	GLU
1	5-A	253	PRO
1	5-A	256	PRO
1	5-B	181	GLN
1	6-A	234	GLU

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Mol	Chain	Res	Type
1	6-B	226	GLU
1	6-B	304	ALA
1	8-A	287	TYR
1	8-B	168	SER
1	9-A	233	ASN
1	9-A	294	PHE
1	9-B	43	ALA
1	9-B	74	LEU
1	10-A	159	PRO
1	10-B	256	PRO
1	10-B	271	LEU
1	12-A	183	HIS
1	13-A	118	THR
1	14-A	69	ASN
1	14-A	247	GLN
1	14-B	80	GLU
1	14-B	294	PHE
1	15-A	87	TYR
1	15-B	117	THR
1	16-A	206	GLN
1	16-A	210	GLU
1	16-B	163	TYR
1	16-B	238	VAL
1	1-A	210	GLU
1	1-A	235	SER
1	1-B	213	GLU
1	2-B	236	GLY
1	2-B	274	ASP
1	3-A	44	GLY
1	3-B	67	ASP
1	3-B	226	GLU
1	3-B	266	GLY
1	4-A	251	TRP
1	6-B	168	SER
1	7-B	262	VAL
1	10-B	163	TYR
1	10-B	242	ILE
1	10-B	274	ASP
1	11-B	163	TYR
1	13-A	224	ILE
1	13-A	294	PHE
1	13-B	77	LEU

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Mol	Chain	Res	Type
1	13-B	78	SER
1	13-B	79	LYS
1	14-A	166	THR
1	14-B	168	SER
1	14-B	197	MSE
1	16-A	251	TRP
1	16-B	70	ARG
1	1-B	74	LEU
1	2-B	233	ASN
1	4-A	103	ASN
1	4-B	163	TYR
1	5-B	147	ALA
1	6-A	300	LEU
1	8-B	19	THR
1	9-B	72	PHE
1	11-B	80	GLU
1	11-B	181	GLN
1	13-A	169	ILE
1	13-B	218	ALA
1	14-B	120	ASN
1	14-B	244	PRO
1	15-A	58	GLU
1	4-A	235	SER
1	4-B	256	PRO
1	7-B	19	THR
1	8-A	253	PRO
1	13-A	9	PRO
1	14-A	251	TRP
1	15-A	256	PRO
1	16-A	122	GLY
1	16-A	147	ALA
1	16-B	81	MSE
1	1-B	158	HIS
1	8-B	49	PRO
1	8-B	230	TYR
1	12-B	44	GLY
1	13-A	57	VAL
1	13-B	182	PRO
1	2-A	159	PRO
1	2-B	211	GLY
1	12-A	184	GLY
1	16-A	18	GLY

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Mol	Chain	Res	Type
1	3-A	256	PRO
1	8-B	169	ILE
1	13-B	256	PRO

5.3.2 Protein sidechains [i](#)

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%)	263 (98%)	5 (2%)	50	41
1	1-B	268/266 (101%)	261 (97%)	7 (3%)	40	28
1	2-A	268/266 (101%)	263 (98%)	5 (2%)	50	41
1	2-B	268/266 (101%)	261 (97%)	7 (3%)	40	28
1	3-A	268/266 (101%)	263 (98%)	5 (2%)	50	41
1	3-B	268/266 (101%)	261 (97%)	7 (3%)	40	28
1	4-A	268/266 (101%)	263 (98%)	5 (2%)	50	41
1	4-B	268/266 (101%)	261 (97%)	7 (3%)	40	28
1	5-A	268/266 (101%)	263 (98%)	5 (2%)	50	41
1	5-B	268/266 (101%)	261 (97%)	7 (3%)	40	28
1	6-A	268/266 (101%)	263 (98%)	5 (2%)	50	41
1	6-B	268/266 (101%)	261 (97%)	7 (3%)	40	28
1	7-A	268/266 (101%)	263 (98%)	5 (2%)	50	41
1	7-B	268/266 (101%)	261 (97%)	7 (3%)	40	28
1	8-A	268/266 (101%)	263 (98%)	5 (2%)	50	41
1	8-B	268/266 (101%)	261 (97%)	7 (3%)	40	28
1	9-A	268/266 (101%)	263 (98%)	5 (2%)	50	41
1	9-B	268/266 (101%)	261 (97%)	7 (3%)	40	28
1	10-A	268/266 (101%)	263 (98%)	5 (2%)	50	41
1	10-B	268/266 (101%)	261 (97%)	7 (3%)	40	28
1	11-A	268/266 (101%)	263 (98%)	5 (2%)	50	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	11-B	268/266 (101%)	261 (97%)	7 (3%)	40	28
1	12-A	268/266 (101%)	263 (98%)	5 (2%)	50	41
1	12-B	268/266 (101%)	261 (97%)	7 (3%)	40	28
1	13-A	268/266 (101%)	263 (98%)	5 (2%)	50	41
1	13-B	268/266 (101%)	261 (97%)	7 (3%)	40	28
1	14-A	268/266 (101%)	263 (98%)	5 (2%)	50	41
1	14-B	268/266 (101%)	261 (97%)	7 (3%)	40	28
1	15-A	268/266 (101%)	263 (98%)	5 (2%)	50	41
1	15-B	268/266 (101%)	261 (97%)	7 (3%)	40	28
1	16-A	268/266 (101%)	263 (98%)	5 (2%)	50	41
1	16-B	268/266 (101%)	261 (97%)	7 (3%)	40	28
All	All	8576/8512 (101%)	8384 (98%)	192 (2%)	45	34

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	114	LEU
1	1-A	152	SER
1	1-A	161	LEU
1	1-A	194	MSE
1	1-A	289	GLU
1	1-B	58	GLU
1	1-B	108	TYR
1	1-B	159	PRO
1	1-B	163	TYR
1	1-B	220	ASP
1	1-B	237	ASP
1	1-B	238	VAL
1	2-A	114	LEU
1	2-A	152	SER
1	2-A	161	LEU
1	2-A	194	MSE
1	2-A	289	GLU
1	2-B	58	GLU
1	2-B	108	TYR
1	2-B	159	PRO
1	2-B	163	TYR
1	2-B	220	ASP

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Mol	Chain	Res	Type
1	2-B	237	ASP
1	2-B	238	VAL
1	3-A	114	LEU
1	3-A	152	SER
1	3-A	161	LEU
1	3-A	194	MSE
1	3-A	289	GLU
1	3-B	58	GLU
1	3-B	108	TYR
1	3-B	159	PRO
1	3-B	163	TYR
1	3-B	220	ASP
1	3-B	237	ASP
1	3-B	238	VAL
1	4-A	114	LEU
1	4-A	152	SER
1	4-A	161	LEU
1	4-A	194	MSE
1	4-A	289	GLU
1	4-B	58	GLU
1	4-B	108	TYR
1	4-B	159	PRO
1	4-B	163	TYR
1	4-B	220	ASP
1	4-B	237	ASP
1	4-B	238	VAL
1	5-A	114	LEU
1	5-A	152	SER
1	5-A	161	LEU
1	5-A	194	MSE
1	5-A	289	GLU
1	5-B	58	GLU
1	5-B	108	TYR
1	5-B	159	PRO
1	5-B	163	TYR
1	5-B	220	ASP
1	5-B	237	ASP
1	5-B	238	VAL
1	6-A	114	LEU
1	6-A	152	SER
1	6-A	161	LEU
1	6-A	194	MSE

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Mol	Chain	Res	Type
1	6-A	289	GLU
1	6-B	58	GLU
1	6-B	108	TYR
1	6-B	159	PRO
1	6-B	163	TYR
1	6-B	220	ASP
1	6-B	237	ASP
1	6-B	238	VAL
1	7-A	114	LEU
1	7-A	152	SER
1	7-A	161	LEU
1	7-A	194	MSE
1	7-A	289	GLU
1	7-B	58	GLU
1	7-B	108	TYR
1	7-B	159	PRO
1	7-B	163	TYR
1	7-B	220	ASP
1	7-B	237	ASP
1	7-B	238	VAL
1	8-A	114	LEU
1	8-A	152	SER
1	8-A	161	LEU
1	8-A	194	MSE
1	8-A	289	GLU
1	8-B	58	GLU
1	8-B	108	TYR
1	8-B	159	PRO
1	8-B	163	TYR
1	8-B	220	ASP
1	8-B	237	ASP
1	8-B	238	VAL
1	9-A	114	LEU
1	9-A	152	SER
1	9-A	161	LEU
1	9-A	194	MSE
1	9-A	289	GLU
1	9-B	58	GLU
1	9-B	108	TYR
1	9-B	159	PRO
1	9-B	163	TYR
1	9-B	220	ASP

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Mol	Chain	Res	Type
1	9-B	237	ASP
1	9-B	238	VAL
1	10-A	114	LEU
1	10-A	152	SER
1	10-A	161	LEU
1	10-A	194	MSE
1	10-A	289	GLU
1	10-B	58	GLU
1	10-B	108	TYR
1	10-B	159	PRO
1	10-B	163	TYR
1	10-B	220	ASP
1	10-B	237	ASP
1	10-B	238	VAL
1	11-A	114	LEU
1	11-A	152	SER
1	11-A	161	LEU
1	11-A	194	MSE
1	11-A	289	GLU
1	11-B	58	GLU
1	11-B	108	TYR
1	11-B	159	PRO
1	11-B	163	TYR
1	11-B	220	ASP
1	11-B	237	ASP
1	11-B	238	VAL
1	12-A	114	LEU
1	12-A	152	SER
1	12-A	161	LEU
1	12-A	194	MSE
1	12-A	289	GLU
1	12-B	58	GLU
1	12-B	108	TYR
1	12-B	159	PRO
1	12-B	163	TYR
1	12-B	220	ASP
1	12-B	237	ASP
1	12-B	238	VAL
1	13-A	114	LEU
1	13-A	152	SER
1	13-A	161	LEU
1	13-A	194	MSE

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Mol	Chain	Res	Type
1	13-A	289	GLU
1	13-B	58	GLU
1	13-B	108	TYR
1	13-B	159	PRO
1	13-B	163	TYR
1	13-B	220	ASP
1	13-B	237	ASP
1	13-B	238	VAL
1	14-A	114	LEU
1	14-A	152	SER
1	14-A	161	LEU
1	14-A	194	MSE
1	14-A	289	GLU
1	14-B	58	GLU
1	14-B	108	TYR
1	14-B	159	PRO
1	14-B	163	TYR
1	14-B	220	ASP
1	14-B	237	ASP
1	14-B	238	VAL
1	15-A	114	LEU
1	15-A	152	SER
1	15-A	161	LEU
1	15-A	194	MSE
1	15-A	289	GLU
1	15-B	58	GLU
1	15-B	108	TYR
1	15-B	159	PRO
1	15-B	163	TYR
1	15-B	220	ASP
1	15-B	237	ASP
1	15-B	238	VAL
1	16-A	114	LEU
1	16-A	152	SER
1	16-A	161	LEU
1	16-A	194	MSE
1	16-A	289	GLU
1	16-B	58	GLU
1	16-B	108	TYR
1	16-B	159	PRO
1	16-B	163	TYR
1	16-B	220	ASP

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Mol	Chain	Res	Type
1	16-B	237	ASP
1	16-B	238	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (114) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	32	HIS
1	1-A	137	GLN
1	1-B	140	HIS
1	1-B	181	GLN
1	1-B	245	ASN
1	2-A	116	ASN
1	2-B	93	GLN
1	2-B	132	ASN
1	2-B	193	GLN
1	2-B	200	HIS
1	2-B	303	ASN
1	3-A	116	ASN
1	3-A	140	HIS
1	3-B	93	GLN
1	3-B	96	ASN
1	3-B	181	GLN
1	4-A	41	HIS
1	4-A	120	ASN
1	4-A	140	HIS
1	4-A	193	GLN
1	4-A	245	ASN
1	4-A	255	HIS
1	4-B	115	HIS
1	4-B	137	GLN
1	4-B	181	GLN
1	4-B	200	HIS
1	4-B	233	ASN
1	4-B	255	HIS
1	5-A	115	HIS
1	5-A	140	HIS
1	5-B	93	GLN
1	5-B	103	ASN
1	5-B	206	GLN
1	6-A	181	GLN
1	6-A	200	HIS
1	6-A	247	GLN

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Mol	Chain	Res	Type
1	6-A	283	ASN
1	6-B	140	HIS
1	6-B	193	GLN
1	6-B	209	ASN
1	7-A	69	ASN
1	7-A	233	ASN
1	7-B	93	GLN
1	7-B	158	HIS
1	7-B	181	GLN
1	7-B	193	GLN
1	8-A	36	ASN
1	8-A	103	ASN
1	8-B	20	HIS
1	8-B	140	HIS
1	8-B	181	GLN
1	8-B	193	GLN
1	9-A	36	ASN
1	9-A	103	ASN
1	9-A	233	ASN
1	9-A	247	GLN
1	9-A	283	ASN
1	9-B	22	ASN
1	9-B	36	ASN
1	9-B	93	GLN
1	9-B	103	ASN
1	9-B	181	GLN
1	9-B	303	ASN
1	10-A	32	HIS
1	10-A	97	HIS
1	10-A	103	ASN
1	10-A	140	HIS
1	10-A	200	HIS
1	10-A	209	ASN
1	10-A	233	ASN
1	10-A	245	ASN
1	10-A	303	ASN
1	10-B	36	ASN
1	10-B	76	ASN
1	10-B	140	HIS
1	10-B	193	GLN
1	10-B	233	ASN
1	10-B	303	ASN

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Mol	Chain	Res	Type
1	11-A	116	ASN
1	11-B	69	ASN
1	11-B	193	GLN
1	12-A	116	ASN
1	12-A	137	GLN
1	12-A	181	GLN
1	12-A	206	GLN
1	12-A	233	ASN
1	12-A	303	ASN
1	12-B	193	GLN
1	13-A	76	ASN
1	13-A	193	GLN
1	13-A	206	GLN
1	13-B	93	GLN
1	13-B	181	GLN
1	13-B	200	HIS
1	14-A	41	HIS
1	14-A	116	ASN
1	14-A	183	HIS
1	14-A	193	GLN
1	14-A	247	GLN
1	14-B	140	HIS
1	14-B	193	GLN
1	15-A	115	HIS
1	15-A	120	ASN
1	15-A	193	GLN
1	15-A	247	GLN
1	16-A	93	GLN
1	16-A	193	GLN
1	16-B	32	HIS
1	16-B	76	ASN
1	16-B	93	GLN
1	16-B	97	HIS
1	16-B	132	ASN
1	16-B	193	GLN
1	16-B	303	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	11-B	704	-	4,4,4	0.38	0	6,6,6	0.12	0
3	SO4	16-A	701	-	4,4,4	0.38	0	6,6,6	0.15	0
3	SO4	16-A	702	-	4,4,4	0.40	0	6,6,6	0.09	0
3	SO4	6-A	701	-	4,4,4	0.39	0	6,6,6	0.12	0
3	SO4	15-A	703	-	4,4,4	0.37	0	6,6,6	0.09	0
3	SO4	1-B	704	-	4,4,4	0.39	0	6,6,6	0.10	0
3	SO4	5-A	703	-	4,4,4	0.32	0	6,6,6	0.18	0
3	SO4	13-A	701	-	4,4,4	0.36	0	6,6,6	0.13	0
3	SO4	10-B	704	-	4,4,4	0.36	0	6,6,6	0.10	0
3	SO4	3-A	702	-	4,4,4	0.40	0	6,6,6	0.09	0
3	SO4	16-A	703	-	4,4,4	0.36	0	6,6,6	0.15	0
3	SO4	12-A	702	-	4,4,4	0.38	0	6,6,6	0.08	0
3	SO4	6-A	703	-	4,4,4	0.33	0	6,6,6	0.19	0
3	SO4	8-A	703	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	1-B	705	-	4,4,4	0.38	0	6,6,6	0.06	0
3	SO4	9-A	701	-	4,4,4	0.38	0	6,6,6	0.08	0
3	SO4	12-A	701	-	4,4,4	0.39	0	6,6,6	0.13	0
3	SO4	14-B	704	-	4,4,4	0.39	0	6,6,6	0.11	0
3	SO4	4-B	705	-	4,4,4	0.36	0	6,6,6	0.11	0
3	SO4	16-B	704	-	4,4,4	0.40	0	6,6,6	0.11	0
3	SO4	6-B	704	-	4,4,4	0.39	0	6,6,6	0.11	0
3	SO4	16-B	705	-	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	3-B	704	-	4,4,4	0.37	0	6,6,6	0.10	0
3	SO4	10-A	702	-	4,4,4	0.40	0	6,6,6	0.08	0
3	SO4	4-B	704	-	4,4,4	0.36	0	6,6,6	0.06	0
3	SO4	2-A	703	-	4,4,4	0.33	0	6,6,6	0.19	0
3	SO4	7-A	701	-	4,4,4	0.36	0	6,6,6	0.08	0
3	SO4	2-B	705	-	4,4,4	0.42	0	6,6,6	0.14	0
3	SO4	11-A	703	-	4,4,4	0.35	0	6,6,6	0.17	0
3	SO4	10-A	701	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	13-A	703	-	4,4,4	0.34	0	6,6,6	0.17	0
3	SO4	11-A	701	-	4,4,4	0.37	0	6,6,6	0.13	0
3	SO4	14-B	705	-	4,4,4	0.40	0	6,6,6	0.07	0
3	SO4	11-A	702	-	4,4,4	0.38	0	6,6,6	0.08	0
3	SO4	14-A	702	-	4,4,4	0.40	0	6,6,6	0.12	0
3	SO4	3-B	705	-	4,4,4	0.38	0	6,6,6	0.09	0
3	SO4	12-B	704	-	4,4,4	0.38	0	6,6,6	0.10	0
3	SO4	7-A	702	-	4,4,4	0.38	0	6,6,6	0.08	0
3	SO4	10-B	705	-	4,4,4	0.38	0	6,6,6	0.10	0
3	SO4	13-B	705	-	4,4,4	0.38	0	6,6,6	0.12	0
3	SO4	9-A	703	-	4,4,4	0.31	0	6,6,6	0.18	0
3	SO4	3-A	701	-	4,4,4	0.34	0	6,6,6	0.10	0
3	SO4	1-A	703	-	4,4,4	0.32	0	6,6,6	0.19	0
3	SO4	5-B	704	-	4,4,4	0.36	0	6,6,6	0.08	0
3	SO4	9-A	702	-	4,4,4	0.41	0	6,6,6	0.14	0
3	SO4	10-A	703	-	4,4,4	0.36	0	6,6,6	0.09	0
3	SO4	15-A	702	-	4,4,4	0.44	0	6,6,6	0.06	0
3	SO4	2-A	701	-	4,4,4	0.34	0	6,6,6	0.11	0
3	SO4	13-B	704	-	4,4,4	0.40	0	6,6,6	0.09	0
3	SO4	13-A	702	-	4,4,4	0.41	0	6,6,6	0.10	0
3	SO4	8-B	705	-	4,4,4	0.37	0	6,6,6	0.09	0
3	SO4	8-A	702	-	4,4,4	0.40	0	6,6,6	0.09	0
3	SO4	15-A	701	-	4,4,4	0.34	0	6,6,6	0.10	0
3	SO4	12-B	705	-	4,4,4	0.39	0	6,6,6	0.12	0
3	SO4	12-A	703	-	4,4,4	0.31	0	6,6,6	0.18	0
3	SO4	5-A	702	-	4,4,4	0.38	0	6,6,6	0.08	0
3	SO4	14-A	701	-	4,4,4	0.35	0	6,6,6	0.13	0
3	SO4	1-A	702	-	4,4,4	0.38	0	6,6,6	0.08	0
3	SO4	9-B	704	-	4,4,4	0.39	0	6,6,6	0.11	0
3	SO4	8-A	701	-	4,4,4	0.39	0	6,6,6	0.14	0
3	SO4	2-A	702	-	4,4,4	0.38	0	6,6,6	0.08	0
3	SO4	11-B	705	-	4,4,4	0.37	0	6,6,6	0.09	0
3	SO4	3-A	703	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	7-A	703	-	4,4,4	0.33	0	6,6,6	0.18	0
3	SO4	7-B	704	-	4,4,4	0.39	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	14-A	703	-	4,4,4	0.33	0	6,6,6	0.14	0
3	SO4	15-B	704	-	4,4,4	0.42	0	6,6,6	0.09	0
3	SO4	9-B	705	-	4,4,4	0.36	0	6,6,6	0.10	0
3	SO4	4-A	703	-	4,4,4	0.34	0	6,6,6	0.18	0
3	SO4	1-A	701	-	4,4,4	0.39	0	6,6,6	0.12	0
3	SO4	4-A	701	-	4,4,4	0.38	0	6,6,6	0.10	0
3	SO4	4-A	702	-	4,4,4	0.37	0	6,6,6	0.06	0
3	SO4	15-B	705	-	4,4,4	0.37	0	6,6,6	0.10	0
3	SO4	8-B	704	-	4,4,4	0.39	0	6,6,6	0.10	0
3	SO4	2-B	704	-	4,4,4	0.39	0	6,6,6	0.10	0
3	SO4	7-B	705	-	4,4,4	0.35	0	6,6,6	0.10	0
3	SO4	6-B	705	-	4,4,4	0.36	0	6,6,6	0.10	0
3	SO4	5-A	701	-	4,4,4	0.44	0	6,6,6	0.10	0
3	SO4	6-A	702	-	4,4,4	0.38	0	6,6,6	0.12	0
3	SO4	5-B	705	-	4,4,4	0.36	0	6,6,6	0.10	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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	300/312 (96%)	2.21	139 (46%) 0 0	0, 1, 2, 4	300 (100%)
1	1-B	300/312 (96%)	2.35	164 (54%) 0 0	0, 1, 2, 3	300 (100%)
1	2-A	0/312	-	-	-	-
1	2-B	0/312	-	-	-	-
1	3-A	0/312	-	-	-	-
1	3-B	0/312	-	-	-	-
1	4-A	0/312	-	-	-	-
1	4-B	0/312	-	-	-	-
1	5-A	0/312	-	-	-	-
1	5-B	0/312	-	-	-	-
1	6-A	0/312	-	-	-	-
1	6-B	0/312	-	-	-	-
1	7-A	0/312	-	-	-	-
1	7-B	0/312	-	-	-	-
1	8-A	0/312	-	-	-	-
1	8-B	0/312	-	-	-	-
1	9-A	0/312	-	-	-	-
1	9-B	0/312	-	-	-	-
1	10-A	0/312	-	-	-	-
1	10-B	0/312	-	-	-	-
1	11-A	0/312	-	-	-	-
1	11-B	0/312	-	-	-	-
1	12-A	0/312	-	-	-	-
1	12-B	0/312	-	-	-	-
1	13-A	0/312	-	-	-	-
1	13-B	0/312	-	-	-	-
1	14-A	0/312	-	-	-	-
1	14-B	0/312	-	-	-	-
1	15-A	0/312	-	-	-	-
1	15-B	0/312	-	-	-	-
1	16-A	0/312	-	-	-	-
1	16-B	0/312	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	600/9984 (6%)	2.28	303 (50%) 0 0	0, 1, 2, 4	600 (100%)

All (303) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	272	GLY	10.2
1	1-A	286	ALA	8.7
1	1-B	164	ALA	8.7
1	1-B	162	LYS	8.1
1	1-A	268	VAL	7.8
1	1-B	163	TYR	7.3
1	1-B	149	LEU	7.1
1	1-A	273	GLY	6.8
1	1-B	159	PRO	6.7
1	1-A	254	LEU	6.5
1	1-A	36	ASN	6.5
1	1-A	7	GLU	6.4
1	1-A	5	VAL	6.4
1	1-A	6	ALA	6.1
1	1-A	301	THR	5.9
1	1-B	4	CYS	5.9
1	1-A	289	GLU	5.8
1	1-A	4	CYS	5.8
1	1-B	103	ASN	5.7
1	1-B	160	SER	5.7
1	1-B	161	LEU	5.6
1	1-B	151	CYS	5.4
1	1-A	260	VAL	5.3
1	1-B	44	GLY	5.3
1	1-A	285	ALA	5.1
1	1-A	40	VAL	5.1
1	1-A	45	LEU	5.0
1	1-B	158	HIS	5.0
1	1-B	241	VAL	5.0
1	1-B	59	LYS	4.9
1	1-B	5	VAL	4.9
1	1-A	156	ILE	4.9
1	1-B	128	GLY	4.8
1	1-A	10	ILE	4.8
1	1-A	279	PRO	4.8
1	1-A	38	ALA	4.8
1	1-B	169	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	1-B	104	SER	4.8
1	1-B	90	ARG	4.7
1	1-A	257	GLY	4.7
1	1-B	73	ASP	4.7
1	1-A	287	TYR	4.7
1	1-A	256	PRO	4.7
1	1-B	272	GLY	4.7
1	1-A	274	ASP	4.7
1	1-B	75	GLU	4.7
1	1-A	170	ALA	4.7
1	1-A	149	LEU	4.6
1	1-A	44	GLY	4.6
1	1-A	163	TYR	4.6
1	1-A	275	CYS	4.6
1	1-A	46	GLU	4.5
1	1-B	178	VAL	4.5
1	1-B	211	GLY	4.5
1	1-A	11	LYS	4.5
1	1-B	238	VAL	4.4
1	1-B	78	SER	4.4
1	1-A	33	TRP	4.4
1	1-B	222	TYR	4.4
1	1-B	84	ASP	4.4
1	1-A	37	GLY	4.3
1	1-A	34	LEU	4.3
1	1-B	234	GLU	4.3
1	1-B	74	LEU	4.2
1	1-A	255	HIS	4.2
1	1-A	161	LEU	4.2
1	1-A	100	GLY	4.2
1	1-B	82	SER	4.2
1	1-B	79	LYS	4.2
1	1-B	217	CYS	4.1
1	1-B	212	LYS	4.1
1	1-B	8	GLU	4.1
1	1-A	298	THR	4.1
1	1-A	290	LYS	4.1
1	1-B	58	GLU	4.1
1	1-B	107	ALA	4.1
1	1-B	66	CYS	4.1
1	1-A	122	GLY	4.0
1	1-A	158	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
1	1-B	265	ASP	4.0
1	1-A	159	PRO	4.0
1	1-A	237	ASP	3.9
1	1-A	107	ALA	3.9
1	1-B	98	LEU	3.9
1	1-A	234	GLU	3.9
1	1-B	172	TYR	3.9
1	1-B	240	ALA	3.9
1	1-B	106	ASP	3.8
1	1-B	126	ILE	3.8
1	1-B	83	GLU	3.8
1	1-A	308	ARG	3.8
1	1-B	123	CYS	3.7
1	1-B	95	ILE	3.7
1	1-A	280	VAL	3.7
1	1-A	258	ASP	3.7
1	1-A	252	LYS	3.7
1	1-A	70	ARG	3.7
1	1-B	85	LEU	3.6
1	1-A	35	LYS	3.6
1	1-A	150	PRO	3.6
1	1-B	218	ALA	3.6
1	1-B	76	ASN	3.6
1	1-B	46	GLU	3.6
1	1-A	160	SER	3.6
1	1-B	131	GLY	3.5
1	1-A	103	ASN	3.5
1	1-A	220	ASP	3.5
1	1-A	172	TYR	3.5
1	1-B	54	PRO	3.5
1	1-B	36	ASN	3.4
1	1-B	34	LEU	3.4
1	1-B	274	ASP	3.4
1	1-A	9	PRO	3.4
1	1-B	148	PRO	3.4
1	1-B	179	GLY	3.4
1	1-B	242	ILE	3.3
1	1-B	96	ASN	3.3
1	1-A	299	LYS	3.3
1	1-A	261	PHE	3.3
1	1-B	214	PHE	3.2
1	1-B	27	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	1-B	57	VAL	3.2
1	1-B	50	PHE	3.2
1	1-B	55	ARG	3.2
1	1-B	77	LEU	3.1
1	1-A	219	ILE	3.1
1	1-A	269	ILE	3.1
1	1-B	278	TYR	3.1
1	1-A	47	VAL	3.1
1	1-B	45	LEU	3.1
1	1-A	8	GLU	3.1
1	1-B	80	GLU	3.1
1	1-B	157	GLU	3.1
1	1-A	270	PRO	3.1
1	1-B	64	ILE	3.1
1	1-B	210	GLU	3.1
1	1-A	288	TYR	3.1
1	1-A	271	LEU	3.0
1	1-B	302	LEU	3.0
1	1-A	310	THR	3.0
1	1-B	275	CYS	3.0
1	1-B	12	LYS	3.0
1	1-A	233	ASN	3.0
1	1-B	288	TYR	3.0
1	1-A	259	PRO	3.0
1	1-B	150	PRO	3.0
1	1-B	244	PRO	3.0
1	1-A	41	HIS	3.0
1	1-A	281	PHE	3.0
1	1-B	60	CYS	3.0
1	1-A	224	ILE	3.0
1	1-B	300	LEU	2.9
1	1-B	192	ASP	2.9
1	1-B	298	THR	2.9
1	1-A	230	TYR	2.9
1	1-B	281	PHE	2.9
1	1-B	43	ALA	2.9
1	1-B	156	ILE	2.9
1	1-B	166	THR	2.9
1	1-A	32	HIS	2.9
1	1-B	99	PHE	2.9
1	1-A	48	LYS	2.9
1	1-A	235	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	1-B	213	GLU	2.9
1	1-B	256	PRO	2.8
1	1-B	33	TRP	2.8
1	1-A	31	THR	2.8
1	1-A	58	GLU	2.8
1	1-A	208	PHE	2.8
1	1-B	130	SER	2.8
1	1-B	236	GLY	2.8
1	1-A	59	LYS	2.8
1	1-A	238	VAL	2.8
1	1-A	64	ILE	2.8
1	1-A	253	PRO	2.8
1	1-A	192	ASP	2.8
1	1-A	278	TYR	2.7
1	1-A	147	ALA	2.7
1	1-B	196	ARG	2.7
1	1-A	157	GLU	2.7
1	1-A	302	LEU	2.7
1	1-B	173	PRO	2.7
1	1-B	63	TYR	2.7
1	1-B	72	PHE	2.7
1	1-A	266	GLY	2.7
1	1-A	276	THR	2.7
1	1-B	127	LEU	2.7
1	1-A	305	LYS	2.7
1	1-A	129	ASP	2.6
1	1-B	28	PHE	2.6
1	1-B	291	LYS	2.6
1	1-B	53	ASN	2.6
1	1-B	224	ILE	2.6
1	1-B	94	GLU	2.6
1	1-B	31	THR	2.6
1	1-B	301	THR	2.6
1	1-B	235	SER	2.6
1	1-B	101	PRO	2.6
1	1-A	105	ASP	2.6
1	1-A	43	ALA	2.6
1	1-A	291	LYS	2.6
1	1-B	230	TYR	2.6
1	1-A	51	ILE	2.6
1	1-B	220	ASP	2.6
1	1-B	171	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	1-B	215	PRO	2.5
1	1-B	206	GLN	2.5
1	1-B	254	LEU	2.5
1	1-B	102	LYS	2.5
1	1-B	176	ILE	2.5
1	1-B	56	ALA	2.5
1	1-A	110	VAL	2.5
1	1-B	71	VAL	2.5
1	1-B	287	TYR	2.5
1	1-A	171	LYS	2.5
1	1-B	271	LEU	2.5
1	1-B	237	ASP	2.5
1	1-B	168	SER	2.5
1	1-B	14	ALA	2.5
1	1-A	111	VAL	2.5
1	1-A	227	LYS	2.5
1	1-A	207	ARG	2.4
1	1-A	303	ASN	2.4
1	1-A	212	LYS	2.4
1	1-B	267	LYS	2.4
1	1-B	47	VAL	2.4
1	1-B	89	VAL	2.4
1	1-A	162	LYS	2.4
1	1-A	267	LYS	2.4
1	1-B	10	ILE	2.4
1	1-B	231	PRO	2.4
1	1-A	236	GLY	2.4
1	1-A	78	SER	2.4
1	1-A	123	CYS	2.4
1	1-A	264	LEU	2.4
1	1-B	125	LEU	2.4
1	1-B	226	GLU	2.4
1	1-A	120	ASN	2.4
1	1-B	255	HIS	2.3
1	1-B	70	ARG	2.3
1	1-B	155	LEU	2.3
1	1-B	61	THR	2.3
1	1-B	13	ILE	2.3
1	1-B	253	PRO	2.3
1	1-B	273	GLY	2.3
1	1-B	189	ASP	2.3
1	1-B	290	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	1-A	148	PRO	2.3
1	1-B	258	ASP	2.3
1	1-A	232	ARG	2.2
1	1-A	215	PRO	2.2
1	1-A	304	ALA	2.2
1	1-B	7	GLU	2.2
1	1-B	229	ASP	2.2
1	1-B	110	VAL	2.2
1	1-A	19	THR	2.2
1	1-A	124	THR	2.2
1	1-B	276	THR	2.2
1	1-A	24	LEU	2.2
1	1-A	198	LEU	2.2
1	1-B	49	PRO	2.2
1	1-B	257	GLY	2.2
1	1-B	109	ASP	2.2
1	1-A	75	GLU	2.2
1	1-B	191	LEU	2.2
1	1-A	265	ASP	2.2
1	1-A	306	SER	2.2
1	1-A	309	SER	2.2
1	1-B	306	SER	2.2
1	1-B	87	TYR	2.2
1	1-A	169	ILE	2.2
1	1-B	219	ILE	2.2
1	1-B	296	LYS	2.2
1	1-B	232	ARG	2.2
1	1-A	153	VAL	2.2
1	1-A	262	VAL	2.2
1	1-A	295	ALA	2.2
1	1-B	170	ALA	2.2
1	1-A	108	TYR	2.1
1	1-A	39	GLU	2.1
1	1-A	154	TYR	2.1
1	1-A	213	GLU	2.1
1	1-B	97	HIS	2.1
1	1-A	191	LEU	2.1
1	1-B	209	ASN	2.1
1	1-B	6	ALA	2.1
1	1-B	93	GLN	2.1
1	1-A	63	TYR	2.1
1	1-B	129	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	1-A	241	VAL	2.1
1	1-A	214	PHE	2.0
1	1-B	108	TYR	2.0
1	1-B	19	THR	2.0
1	1-A	18	GLY	2.0
1	1-B	207	ARG	2.0
1	1-B	295	ALA	2.0
1	1-B	35	LYS	2.0
1	1-A	307	ILE	2.0
1	1-B	134	PHE	2.0
1	1-A	96	ASN	2.0
1	1-A	222	TYR	2.0
1	1-B	180	PRO	2.0
1	1-A	89	VAL	2.0

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	1-B	705	5/5	0.53	0.21	48,48,49,49	5
2	ZN	2-A	601	1/1	-	-	13,13,13,13	1
2	ZN	3-A	601	1/1	-	-	15,15,15,15	1
2	ZN	4-A	601	1/1	-	-	4,4,4,4	1
2	ZN	5-A	601	1/1	-	-	16,16,16,16	1
2	ZN	6-A	601	1/1	-	-	6,6,6,6	1
2	ZN	7-A	601	1/1	-	-	18,18,18,18	1
2	ZN	8-A	601	1/1	-	-	11,11,11,11	1
2	ZN	9-A	601	1/1	-	-	0,0,0,0	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	10-A	601	1/1	-	-	25,25,25,25	1
2	ZN	11-A	601	1/1	-	-	17,17,17,17	1
2	ZN	12-A	601	1/1	-	-	12,12,12,12	1
2	ZN	13-A	601	1/1	-	-	23,23,23,23	1
2	ZN	14-A	601	1/1	-	-	17,17,17,17	1
2	ZN	15-A	601	1/1	-	-	23,23,23,23	1
2	ZN	16-A	601	1/1	-	-	15,15,15,15	1
2	ZN	1-A	601	1/1	0.70	0.49	24,24,24,24	1
2	ZN	2-B	602	1/1	-	-	21,21,21,21	1
2	ZN	3-B	602	1/1	-	-	15,15,15,15	1
2	ZN	4-B	602	1/1	-	-	21,21,21,21	1
2	ZN	5-B	602	1/1	-	-	23,23,23,23	1
2	ZN	6-B	602	1/1	-	-	19,19,19,19	1
2	ZN	7-B	602	1/1	-	-	19,19,19,19	1
2	ZN	8-B	602	1/1	-	-	7,7,7,7	1
2	ZN	9-B	602	1/1	-	-	16,16,16,16	1
2	ZN	10-B	602	1/1	-	-	16,16,16,16	1
2	ZN	11-B	602	1/1	-	-	11,11,11,11	1
2	ZN	12-B	602	1/1	-	-	0,0,0,0	1
2	ZN	13-B	602	1/1	-	-	28,28,28,28	1
2	ZN	14-B	602	1/1	-	-	12,12,12,12	1
2	ZN	15-B	602	1/1	-	-	27,27,27,27	1
2	ZN	16-B	602	1/1	-	-	29,29,29,29	1
2	ZN	1-B	602	1/1	0.72	0.46	14,14,14,14	1
3	SO4	2-A	701	5/5	-	-	37,37,38,38	5
3	SO4	3-A	701	5/5	-	-	37,37,38,39	5
3	SO4	4-A	701	5/5	-	-	38,39,40,40	5
3	SO4	5-A	701	5/5	-	-	39,39,40,41	5
3	SO4	6-A	701	5/5	-	-	38,39,39,40	5
3	SO4	7-A	701	5/5	-	-	38,39,39,41	5
3	SO4	8-A	701	5/5	-	-	37,38,39,39	5
3	SO4	9-A	701	5/5	-	-	37,37,39,39	5
3	SO4	10-A	701	5/5	-	-	37,38,38,39	5
3	SO4	11-A	701	5/5	-	-	37,38,39,39	5
3	SO4	12-A	701	5/5	-	-	37,38,39,39	5
3	SO4	13-A	701	5/5	-	-	37,38,39,39	5
3	SO4	14-A	701	5/5	-	-	38,38,40,41	5
3	SO4	15-A	701	5/5	-	-	36,37,38,38	5
3	SO4	16-A	701	5/5	-	-	36,38,38,38	5
3	SO4	1-B	704	5/5	0.73	0.19	50,51,51,53	5
3	SO4	2-A	702	5/5	-	-	42,44,44,45	5
3	SO4	3-A	702	5/5	-	-	43,44,44,46	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	4-A	702	5/5	-	-	43,44,45,45	5
3	SO4	5-A	702	5/5	-	-	42,44,44,45	5
3	SO4	6-A	702	5/5	-	-	44,44,45,45	5
3	SO4	7-A	702	5/5	-	-	42,44,44,45	5
3	SO4	8-A	702	5/5	-	-	43,44,44,46	5
3	SO4	9-A	702	5/5	-	-	43,43,45,45	5
3	SO4	10-A	702	5/5	-	-	43,44,44,46	5
3	SO4	11-A	702	5/5	-	-	42,44,44,45	5
3	SO4	12-A	702	5/5	-	-	42,44,44,45	5
3	SO4	13-A	702	5/5	-	-	42,43,43,45	5
3	SO4	14-A	702	5/5	-	-	42,43,44,44	5
3	SO4	15-A	702	5/5	-	-	42,43,45,45	5
3	SO4	16-A	702	5/5	-	-	42,43,44,45	5
3	SO4	1-A	701	5/5	0.80	0.22	38,39,39,40	5
3	SO4	2-A	703	5/5	-	-	47,48,49,49	5
3	SO4	3-A	703	5/5	-	-	46,47,48,49	5
3	SO4	4-A	703	5/5	-	-	47,48,49,49	5
3	SO4	5-A	703	5/5	-	-	46,48,49,49	5
3	SO4	6-A	703	5/5	-	-	47,48,49,49	5
3	SO4	7-A	703	5/5	-	-	47,48,49,49	5
3	SO4	8-A	703	5/5	-	-	46,47,47,48	5
3	SO4	9-A	703	5/5	-	-	47,48,49,49	5
3	SO4	10-A	703	5/5	-	-	46,48,49,49	5
3	SO4	11-A	703	5/5	-	-	48,48,49,50	5
3	SO4	12-A	703	5/5	-	-	47,48,49,49	5
3	SO4	13-A	703	5/5	-	-	47,48,49,50	5
3	SO4	14-A	703	5/5	-	-	48,48,49,49	5
3	SO4	15-A	703	5/5	-	-	46,48,48,48	5
3	SO4	16-A	703	5/5	-	-	48,48,49,50	5
3	SO4	1-A	702	5/5	0.85	0.15	42,44,44,45	5
3	SO4	2-B	704	5/5	-	-	50,51,51,53	5
3	SO4	3-B	704	5/5	-	-	52,52,53,53	5
3	SO4	4-B	704	5/5	-	-	50,51,52,52	5
3	SO4	5-B	704	5/5	-	-	50,51,52,52	5
3	SO4	6-B	704	5/5	-	-	50,51,52,53	5
3	SO4	7-B	704	5/5	-	-	50,51,52,53	5
3	SO4	8-B	704	5/5	-	-	50,51,51,53	5
3	SO4	9-B	704	5/5	-	-	51,51,52,53	5
3	SO4	10-B	704	5/5	-	-	50,51,52,52	5
3	SO4	11-B	704	5/5	-	-	51,51,52,53	5
3	SO4	12-B	704	5/5	-	-	50,51,51,52	5
3	SO4	13-B	704	5/5	-	-	49,50,51,52	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	14-B	704	5/5	-	-	50,50,51,53	5
3	SO4	15-B	704	5/5	-	-	51,52,52,53	5
3	SO4	16-B	704	5/5	-	-	50,51,52,53	5
3	SO4	1-A	703	5/5	0.90	0.14	47,48,49,49	5
3	SO4	2-B	705	5/5	-	-	46,47,48,48	5
3	SO4	3-B	705	5/5	-	-	48,49,49,49	5
3	SO4	4-B	705	5/5	-	-	47,48,49,49	5
3	SO4	5-B	705	5/5	-	-	45,46,47,48	5
3	SO4	6-B	705	5/5	-	-	45,46,47,47	5
3	SO4	7-B	705	5/5	-	-	46,47,49,49	5
3	SO4	8-B	705	5/5	-	-	45,46,47,47	5
3	SO4	9-B	705	5/5	-	-	45,46,47,47	5
3	SO4	10-B	705	5/5	-	-	45,46,47,48	5
3	SO4	11-B	705	5/5	-	-	45,46,47,47	5
3	SO4	12-B	705	5/5	-	-	46,47,47,47	5
3	SO4	13-B	705	5/5	-	-	46,47,47,48	5
3	SO4	14-B	705	5/5	-	-	49,49,50,51	5
3	SO4	15-B	705	5/5	-	-	44,45,47,47	5
3	SO4	16-B	705	5/5	-	-	44,45,47,47	5

6.5 Other polymers [i](#)

There are no such residues in this entry.