



Full wwPDB X-ray Structure Validation 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 full wwPDB validation 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>

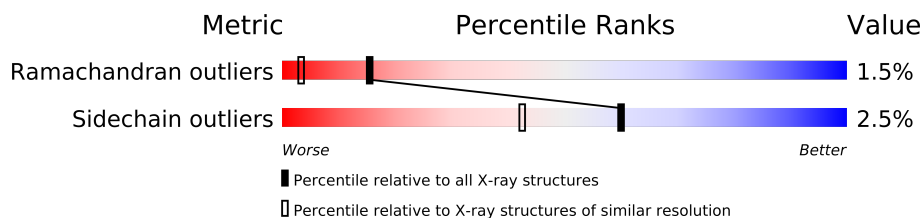
The following versions of software and data (see [references](#)) were used in the production of this report:

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	

Continued on next page...

Continued from previous page...

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			

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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).

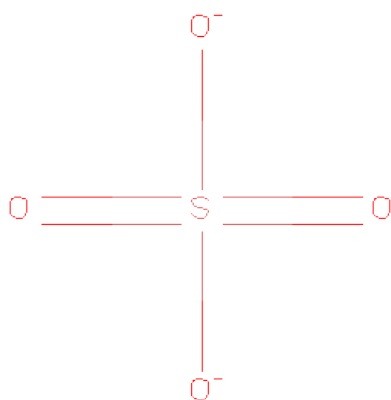
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	16-A	1	Total Zn 1 1	0	0
2	1-B	1	Total Zn 1 1	0	0
2	5-A	1	Total Zn 1 1	0	0
2	13-A	1	Total Zn 1 1	0	0
2	8-A	1	Total Zn 1 1	0	0
2	2-B	1	Total Zn 1 1	0	0
2	15-B	1	Total Zn 1 1	0	0
2	7-B	1	Total Zn 1 1	0	0
2	16-B	1	Total Zn 1 1	0	0
2	10-B	1	Total Zn 1 1	0	0
2	4-A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

Continued on next page...

Continued from previous page...

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

- 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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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			

Continued on next page...

Continued from previous page...

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 i

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: 



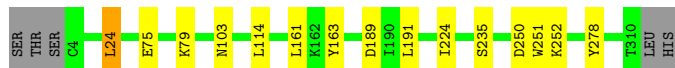
- Molecule 1: Aspartoacylase

Chain 3-B: 



- Molecule 1: Aspartoacylase

Chain 4-A: 



- Molecule 1: Aspartoacylase

Chain 4-B: 



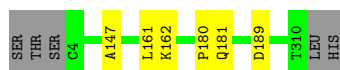
- Molecule 1: Aspartoacylase

Chain 5-A: 



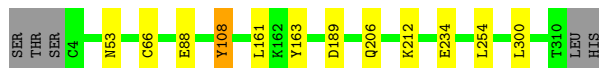
- Molecule 1: Aspartoacylase

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

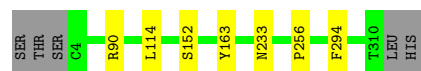
Chain 8-A:



Chain 8-B:



Chain 9-A:



Chain 9-B:



Chain 10-A:



Chain 10-B:



Chain 11-A:



Chain 11-B:



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.

All (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
1	13-B	24	LEU	N-CA-C	5.27	125.23	111.00
1	14-A	254	LEU	CA-CB-CG	5.22	127.30	115.30
1	6-B	20	HIS	N-CA-C	-5.18	97.02	111.00
1	5-A	24	LEU	N-CA-C	5.08	124.72	111.00
1	6-A	254	LEU	CA-CB-CG	5.06	126.94	115.30
1	14-A	179	GLY	N-CA-C	-5.05	100.46	113.10
1	13-A	23	GLU	N-CA-C	-5.05	97.36	111.00
1	16-B	24	LEU	N-CA-C	5.02	124.55	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
4:A:820:HOH:O	4:A:857:HOH:O[1_556]	1.89	0.31
4:A:821:HOH:O	4:A:858:HOH:O[1_556]	1.89	0.31
4:A:820:HOH:O	4:A:857:HOH:O[1_556]	1.89	0.31
4:A:816: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
4:A:819:HOH:O	4:A:853:HOH:O[1_556]	1.89	0.31
4:A:819:HOH:O	4:A:856:HOH:O[1_556]	1.89	0.31
4:A:819:HOH:O	4:A:856:HOH:O[1_556]	1.89	0.31
4:A:816:HOH:O	4:A:852:HOH:O[1_556]	1.89	0.31
4:A:818:HOH:O	4:A:854:HOH:O[1_556]	1.89	0.31
1:B:105:ASP:OD2	4:A:861:HOH:O[4_556]	1.94	0.26
4:B:786:HOH:O	4:B:900:HOH:O[1_556]	2.17	0.03
1:B:144:THR:O	4:B:738:HOH:O[2_656]	2.19	0.01

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	8576/8512 (101%)	8365 (98%)	211 (2%)	60 42

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	108	TYR
1	1-A	114	LEU
1	1-A	152	SER
1	1-A	161	LEU
1	1-A	163	TYR
1	1-A	265	ASP
1	1-A	289	GLU
1	1-A	300	LEU
1	1-B	58	GLU
1	1-B	108	TYR
1	1-B	163	TYR
1	1-B	220	ASP
1	1-B	265	ASP
1	2-A	90	ARG
1	2-A	163	TYR
1	2-A	253	PRO
1	2-A	274	ASP
1	2-A	298	THR
1	2-A	300	LEU
1	2-B	8	GLU
1	2-B	36	ASN
1	2-B	138	MSE
1	2-B	213	GLU
1	2-B	220	ASP
1	2-B	274	ASP
1	2-B	297	THR
1	2-B	298	THR
1	3-A	106	ASP
1	3-A	114	LEU
1	3-A	163	TYR
1	3-A	189	ASP
1	3-A	191	LEU
1	3-A	226	GLU
1	3-A	275	CYS
1	3-B	116	ASN
1	3-B	265	ASP
1	4-A	24	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-A	75	GLU
1	4-A	79	LYS
1	4-A	114	LEU
1	4-A	161	LEU
1	4-A	163	TYR
1	4-A	189	ASP
1	4-A	191	LEU
1	4-A	224	ILE
1	4-A	250	ASP
1	4-B	75	GLU
1	4-B	108	TYR
1	4-B	194	MSE
1	4-B	203	ASP
1	4-B	254	LEU
1	4-B	265	ASP
1	5-A	53	ASN
1	5-A	65	ASP
1	5-A	114	LEU
1	5-A	151	CYS
1	5-A	163	TYR
1	5-A	220	ASP
1	5-A	224	ILE
1	5-A	250	ASP
1	5-A	253	PRO
1	5-B	161	LEU
1	5-B	189	ASP
1	6-A	53	ASN
1	6-A	66	CYS
1	6-A	88	GLU
1	6-A	108	TYR
1	6-A	161	LEU
1	6-A	163	TYR
1	6-A	189	ASP
1	6-A	206	GLN
1	6-B	8	GLU
1	6-B	109	ASP
1	6-B	265	ASP
1	6-B	289	GLU
1	7-A	114	LEU
1	7-A	163	TYR
1	7-A	265	ASP
1	7-B	83	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-B	250	ASP
1	7-B	265	ASP
1	7-B	305	LYS
1	8-A	36	ASN
1	8-A	114	LEU
1	8-A	163	TYR
1	8-A	274	ASP
1	8-A	289	GLU
1	8-B	256	PRO
1	8-B	265	ASP
1	8-B	300	LEU
1	9-A	90	ARG
1	9-A	114	LEU
1	9-A	163	TYR
1	9-B	163	TYR
1	9-B	250	ASP
1	9-B	289	GLU
1	9-B	300	LEU
1	10-A	40	VAL
1	10-A	61	THR
1	10-A	114	LEU
1	10-A	158	HIS
1	10-A	213	GLU
1	10-A	305	LYS
1	10-B	108	TYR
1	10-B	151	CYS
1	10-B	300	LEU
1	11-A	36	ASN
1	11-A	152	SER
1	11-A	163	TYR
1	11-A	265	ASP
1	11-A	284	GLU
1	11-A	303	ASN
1	11-B	48	LYS
1	11-B	85	LEU
1	11-B	88	GLU
1	11-B	146	MSE
1	11-B	258	ASP
1	11-B	265	ASP
1	11-B	274	ASP
1	11-B	289	GLU
1	12-A	114	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	12-A	161	LEU
1	12-A	163	TYR
1	12-A	224	ILE
1	12-A	264	LEU
1	12-B	8	GLU
1	12-B	163	TYR
1	12-B	194	MSE
1	12-B	209	ASN
1	12-B	297	THR
1	13-A	45	LEU
1	13-A	61	THR
1	13-A	75	GLU
1	13-A	90	ARG
1	13-A	114	LEU
1	13-A	152	SER
1	13-A	163	TYR
1	13-A	245	ASN
1	13-B	114	LEU
1	13-B	124	THR
1	13-B	151	CYS
1	13-B	157	GLU
1	13-B	163	TYR
1	13-B	166	THR
1	13-B	186	LEU
1	13-B	217	CYS
1	13-B	220	ASP
1	13-B	252	LYS
1	14-A	11	LYS
1	14-A	55	ARG
1	14-A	70	ARG
1	14-A	83	GLU
1	14-A	94	GLU
1	14-A	151	CYS
1	14-A	162	LYS
1	14-A	163	TYR
1	14-A	220	ASP
1	14-A	224	ILE
1	14-A	256	PRO
1	14-A	265	ASP
1	14-A	274	ASP
1	14-B	35	LYS
1	14-B	58	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	14-B	61	THR
1	14-B	75	GLU
1	14-B	197	MSE
1	14-B	225	MSE
1	14-B	226	GLU
1	14-B	250	ASP
1	14-B	275	CYS
1	14-B	300	LEU
1	15-A	59	LYS
1	15-A	82	SER
1	15-A	90	ARG
1	15-A	113	ASP
1	15-A	114	LEU
1	15-A	120	ASN
1	15-A	123	CYS
1	15-A	146	MSE
1	15-A	152	SER
1	15-A	191	LEU
1	15-A	245	ASN
1	15-A	252	LYS
1	15-A	265	ASP
1	15-A	275	CYS
1	15-A	300	LEU
1	15-A	310	THR
1	15-B	106	ASP
1	15-B	109	ASP
1	15-B	152	SER
1	15-B	177	GLU
1	15-B	309	SER
1	16-A	61	THR
1	16-A	78	SER
1	16-A	114	LEU
1	16-A	161	LEU
1	16-A	163	TYR
1	16-A	169	ILE
1	16-A	180	PRO
1	16-A	194	MSE
1	16-A	203	ASP
1	16-A	220	ASP
1	16-A	252	LYS
1	16-A	298	THR
1	16-A	306	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	16-B	88	GLU
1	16-B	152	SER
1	16-B	191	LEU
1	16-B	256	PRO
1	16-B	265	ASP
1	16-B	275	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	32	HIS
1	1-A	36	ASN
1	1-A	137	GLN
1	1-A	233	ASN
1	2-B	93	GLN
1	2-B	200	HIS
1	3-A	116	ASN
1	3-B	96	ASN
1	3-B	181	GLN
1	4-A	36	ASN
1	4-A	41	HIS
1	4-A	120	ASN
1	4-A	140	HIS
1	4-A	193	GLN
1	4-B	103	ASN
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-B	93	GLN
1	5-B	103	ASN
1	5-B	206	GLN
1	6-A	200	HIS
1	6-B	140	HIS
1	6-B	209	ASN
1	7-B	103	ASN
1	8-A	36	ASN
1	8-A	103	ASN
1	8-A	209	ASN
1	8-B	20	HIS
1	9-A	36	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-A	233	ASN
1	9-B	22	ASN
1	9-B	36	ASN
1	9-B	93	GLN
1	9-B	103	ASN
1	10-A	32	HIS
1	10-A	36	ASN
1	10-A	209	ASN
1	10-A	245	ASN
1	10-B	233	ASN
1	11-A	93	GLN
1	12-A	116	ASN
1	12-A	137	GLN
1	12-A	233	ASN
1	13-B	181	GLN
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	15-A	120	ASN
1	15-A	193	GLN
1	15-A	247	GLN
1	16-A	93	GLN
1	16-B	32	HIS
1	16-B	93	GLN
1	16-B	97	HIS
1	16-B	193	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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.