wwPDB X-ray Structure Validation Summary Report (i)

Sep 14, 2023 – 06:16 PM EDT

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

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

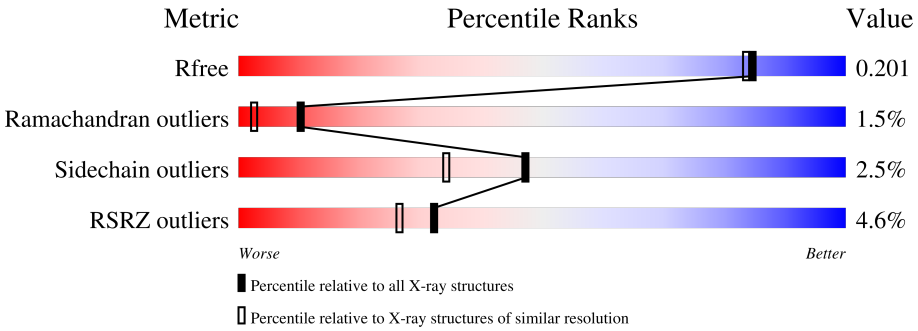
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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}	130704	5950 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 <=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	4% 95%
1	1-B	312	5% 95%
1	10-A	312	4% 96%
1	10-B	312	5% 96%
1	11-A	312	4% 96%
1	11-B	312	5% 93% 5%

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Mol	Chain	Length	Quality of chain
1	12-A	312	4% 96%
1	12-B	312	5% 96%
1	13-A	312	4% 93% 6%
1	13-B	312	5% 93% 5%
1	14-A	312	4% 92% 6%
1	14-B	312	5% 93%
1	15-A	312	4% 91% 8%
1	15-B	312	5% 96%
1	16-A	312	4% 91% 7%
1	16-B	312	5% 94%
1	2-A	312	4% 96%
1	2-B	312	5% 94%
1	3-A	312	4% 96%
1	3-B	312	5% 96%
1	4-A	312	4% 94%
1	4-B	312	5% 95%
1	5-A	312	4% 95%
1	5-B	312	5% 96%
1	6-A	312	4% 95%
1	6-B	312	5% 96%
1	7-A	312	4% 97%
1	7-B	312	5% 96%
1	8-A	312	4% 96%
1	8-B	312	5% 95%
1	9-A	312	4% 96%

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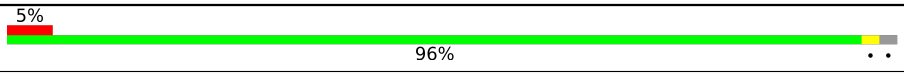
Mol	Chain	Length	Quality of chain
1	9-B	312	

2 Entry composition (i)

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 (three-letter code: 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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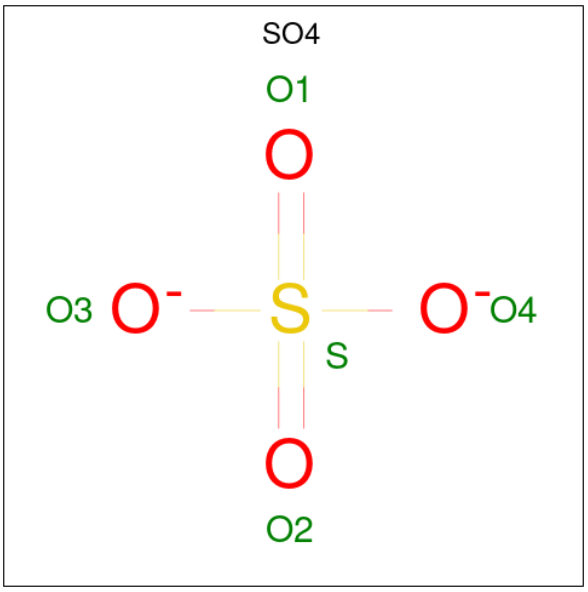
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	14-A	1	Total Zn 1 1	0	0
2	15-A	1	Total Zn 1 1	0	0
2	16-A	1	Total Zn 1 1	0	0
2	1-B	1	Total Zn 1 1	0	0
2	2-B	1	Total Zn 1 1	0	0
2	3-B	1	Total Zn 1 1	0	0
2	4-B	1	Total Zn 1 1	0	0
2	5-B	1	Total Zn 1 1	0	0
2	6-B	1	Total Zn 1 1	0	0
2	7-B	1	Total Zn 1 1	0	0
2	8-B	1	Total Zn 1 1	0	0
2	9-B	1	Total Zn 1 1	0	0
2	10-B	1	Total Zn 1 1	0	0
2	11-B	1	Total Zn 1 1	0	0
2	12-B	1	Total Zn 1 1	0	0
2	13-B	1	Total Zn 1 1	0	0
2	14-B	1	Total Zn 1 1	0	0
2	15-B	1	Total Zn 1 1	0	0
2	16-B	1	Total Zn 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

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

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1-A	288	Total O 288 288	0	0
4	2-A	284	Total O 284 284	0	0
4	3-A	282	Total O 282 282	0	0
4	4-A	284	Total O 284 284	0	0
4	5-A	283	Total O 283 283	0	0
4	6-A	292	Total O 292 292	0	0
4	7-A	291	Total O 291 291	0	0
4	8-A	293	Total O 293 293	0	0
4	9-A	292	Total O 292 292	0	0
4	10-A	280	Total O 280 280	0	0
4	11-A	294	Total O 294 294	0	0
4	12-A	285	Total O 285 285	0	0
4	13-A	291	Total O 291 291	0	0
4	14-A	289	Total O 289 289	0	0
4	15-A	285	Total O 285 285	0	0
4	16-A	284	Total O 284 284	0	0

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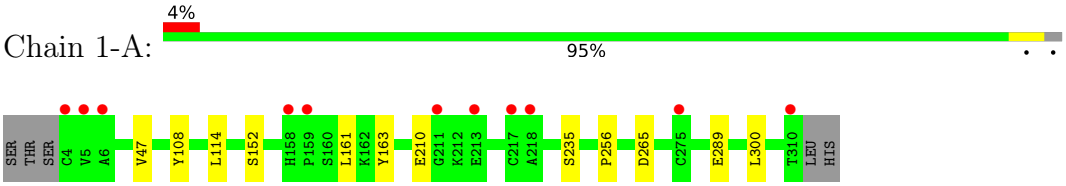
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1-B	264	Total O 264 264	0	0
4	2-B	268	Total O 268 268	0	0
4	3-B	270	Total O 270 270	0	0
4	4-B	268	Total O 268 268	0	0
4	5-B	269	Total O 269 269	0	0
4	6-B	260	Total O 260 260	0	0
4	7-B	261	Total O 261 261	0	0
4	8-B	259	Total O 259 259	0	0
4	9-B	260	Total O 260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

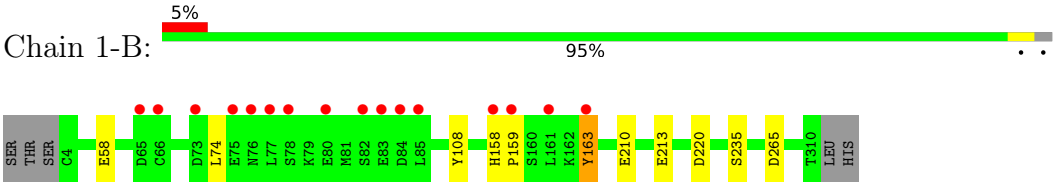
• Molecule 1: Aspartoacylase

Chain 1-A:



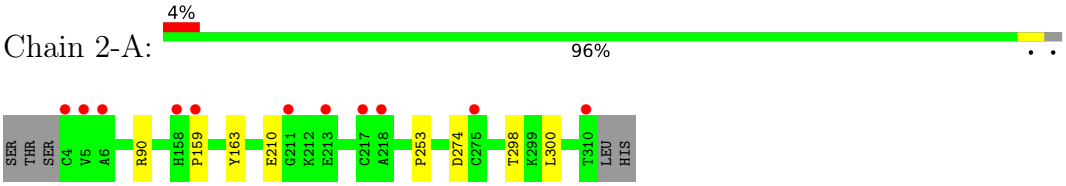
• Molecule 1: Aspartoacylase

Chain 1-B:



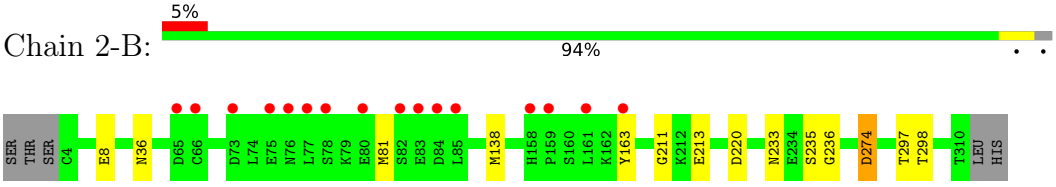
• Molecule 1: Aspartoacylase

Chain 2-A:



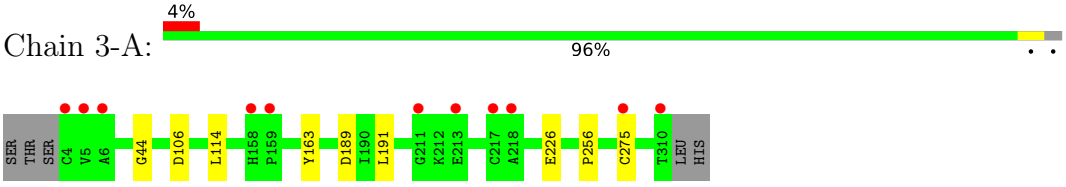
• Molecule 1: Aspartoacylase

Chain 2-B:



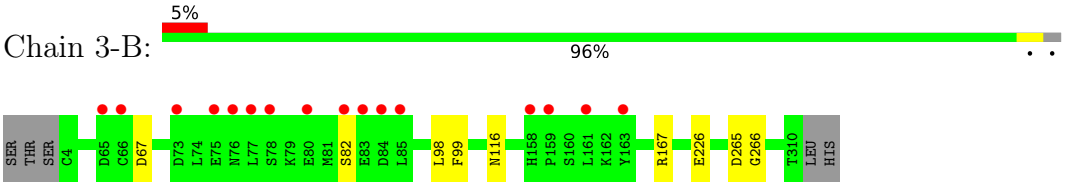
• Molecule 1: Aspartoacylase

Chain 3-A:



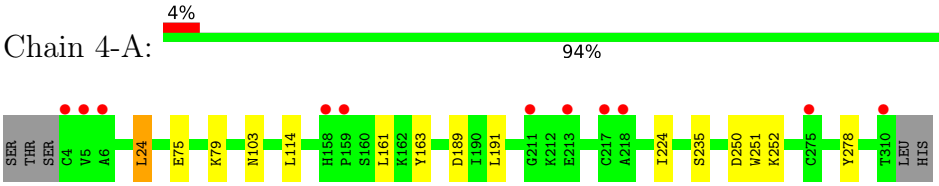
• Molecule 1: Aspartoacylase

Chain 3-B:



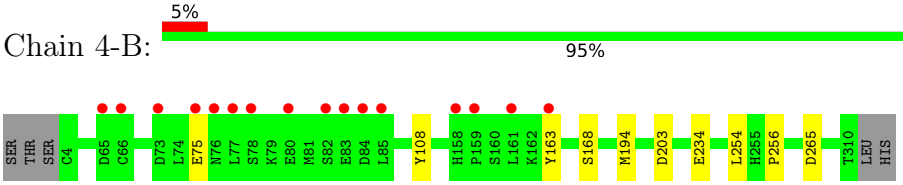
• Molecule 1: Aspartoacylase

Chain 4-A:



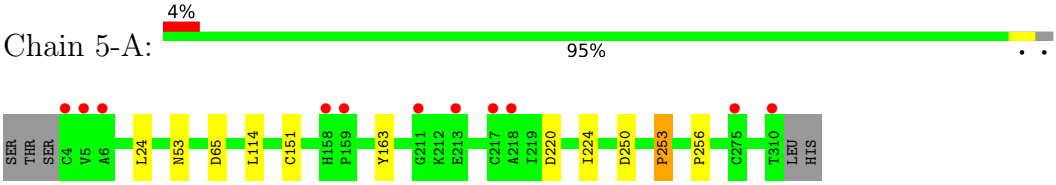
• Molecule 1: Aspartoacylase

Chain 4-B:



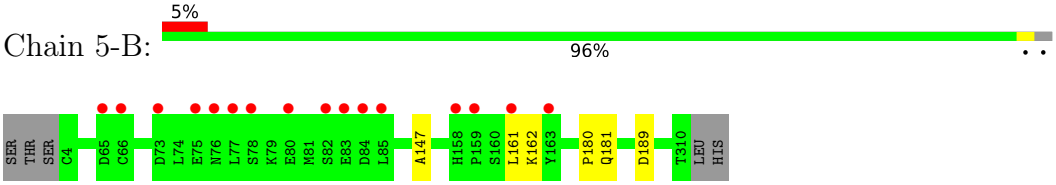
• Molecule 1: Aspartoacylase

Chain 5-A:



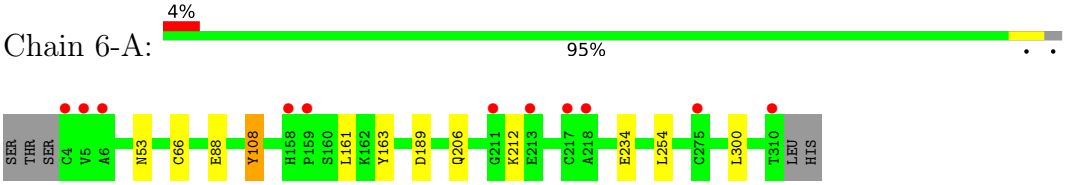
• Molecule 1: Aspartoacylase

Chain 5-B:



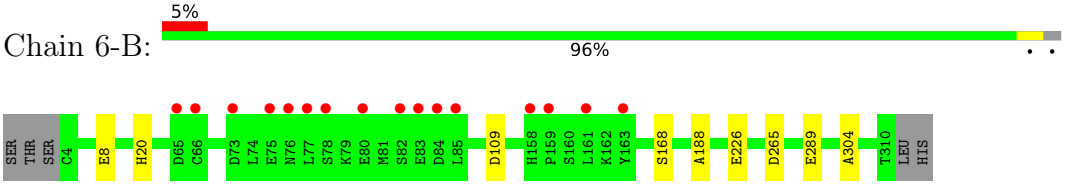
• Molecule 1: Aspartoacylase

Chain 6-A:



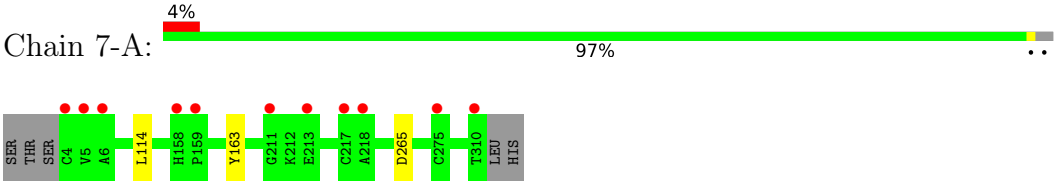
• Molecule 1: Aspartoacylase

Chain 6-B:



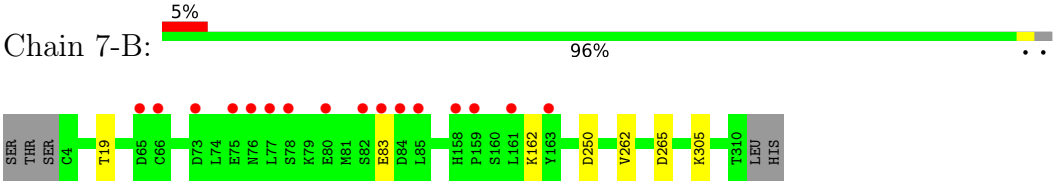
• Molecule 1: Aspartoacylase

Chain 7-A:



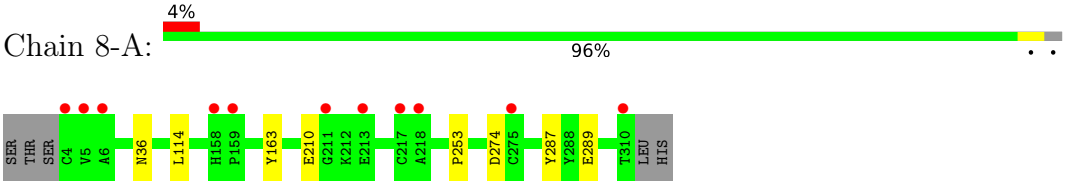
• Molecule 1: Aspartoacylase

Chain 7-B:



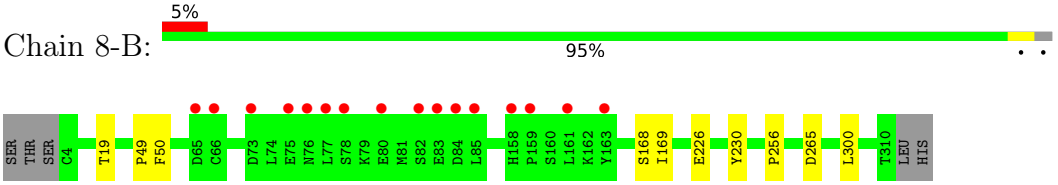
• Molecule 1: Aspartoacylase

Chain 8-A:



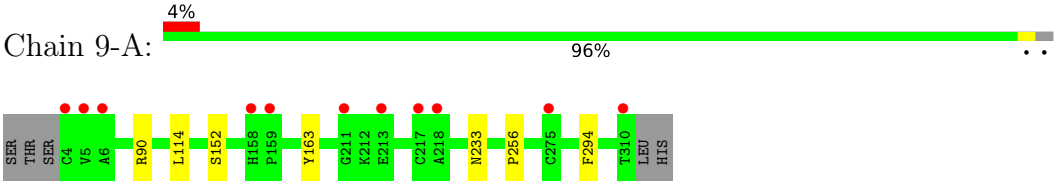
• Molecule 1: Aspartoacylase

Chain 8-B:



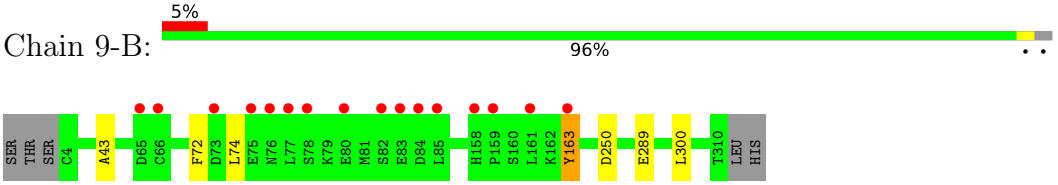
• Molecule 1: Aspartoacylase

Chain 9-A:



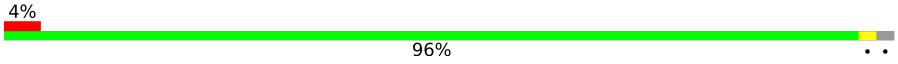
• Molecule 1: Aspartoacylase

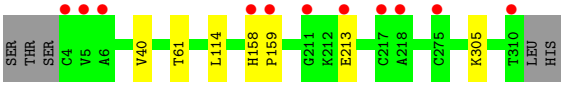
Chain 9-B:



• Molecule 1: Aspartoacylase

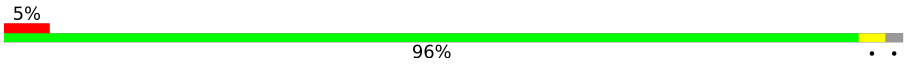
Chain 10-A:

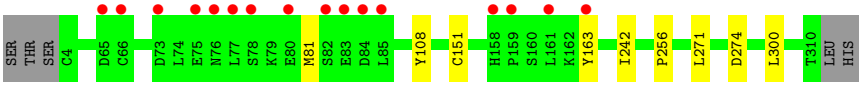




• Molecule 1: Aspartoacylase

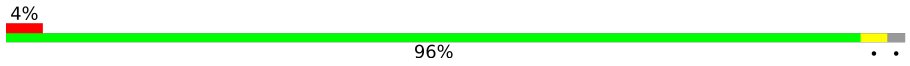
Chain 10-B:

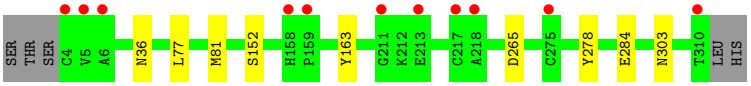




• Molecule 1: Aspartoacylase

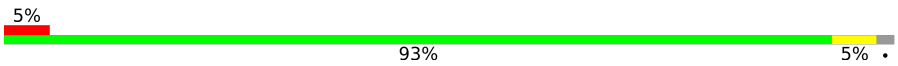
Chain 11-A:





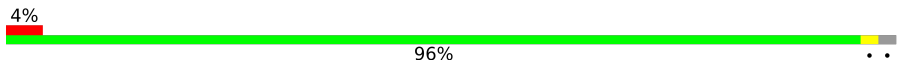
• Molecule 1: Aspartoacylase

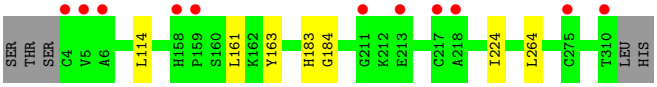
Chain 11-B:



• Molecule 1: Aspartoacylase

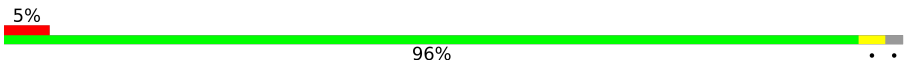
Chain 12-A:

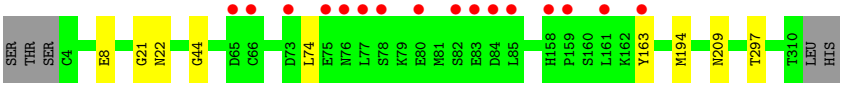




• Molecule 1: Aspartoacylase

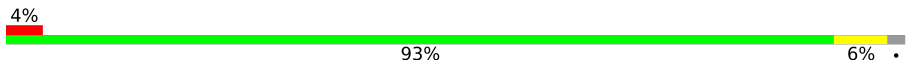
Chain 12-B:

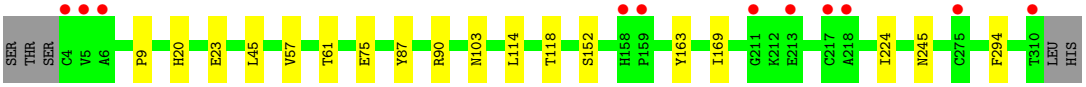




• Molecule 1: Aspartoacylase

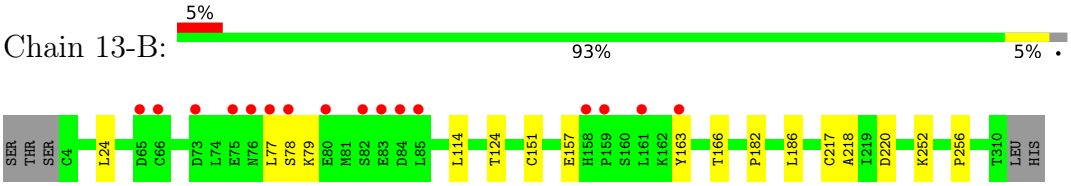
Chain 13-A:





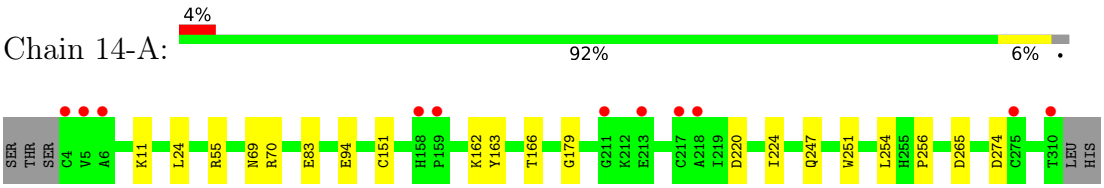
• Molecule 1: Aspartoacylase

Chain 13-B:



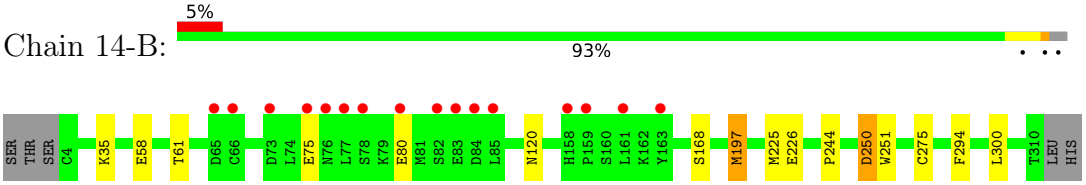
• Molecule 1: Aspartoacylase

Chain 14-A:



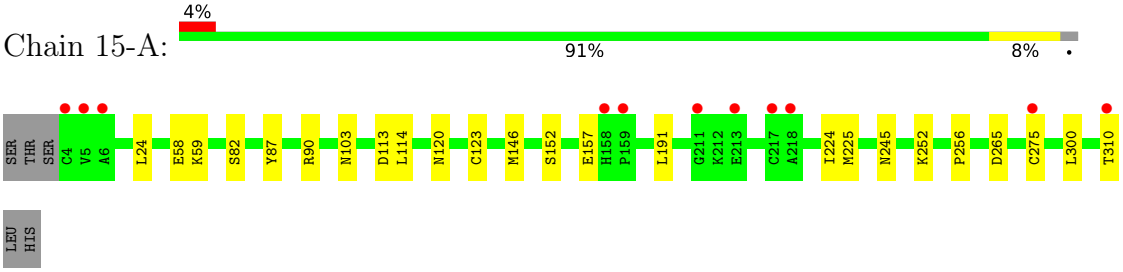
• Molecule 1: Aspartoacylase

Chain 14-B:



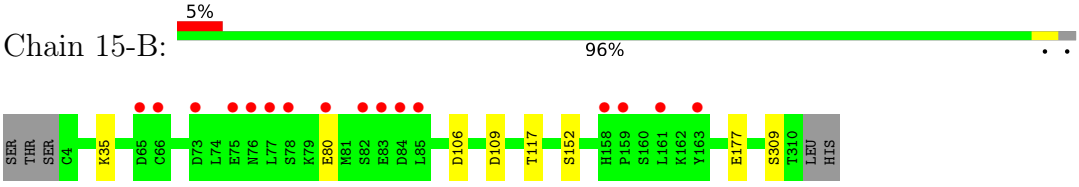
• Molecule 1: Aspartoacylase

Chain 15-A:



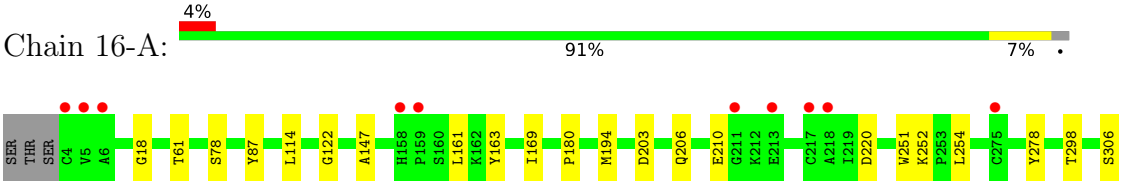
• Molecule 1: Aspartoacylase

Chain 15-B:



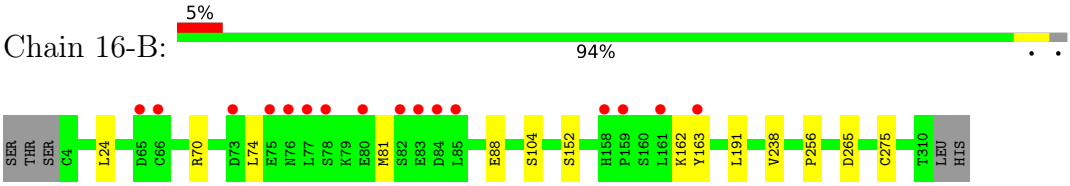
• Molecule 1: Aspartoacylase

Chain 16-A:



• Molecule 1: Aspartoacylase

Chain 16-B:


5%
94%
SER
THR
SER
C4
L24
D65
C66
R70
D73
L74
E75
N76
L77
S78
K79
E80
M81
S82
E83
D84
L85
E88
S104
S152
H158
P159
S160
L161
K162
Y163
L191
V238
P256
D265
C275
T310
LEU
HIS

4 Data and refinement statistics (i)

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 41.75 – 1.81	Depositor EDS
% Data completeness (in resolution range)	97.1 (40.50-1.80) 97.3 (41.75-1.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 1.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.138 , 0.191 0.150 , 0.201	Depositor DCC
R_{free} test set	2955 reflections (5.08%)	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)	0.33 , 69.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	1-A	0.47	0/2484	0.65	0/3360
1	1-B	0.48	0/2484	0.65	0/3360
1	2-A	0.48	0/2484	0.64	0/3360
1	2-B	0.48	0/2484	0.65	0/3360
1	3-A	0.48	0/2484	0.64	0/3360
1	3-B	0.48	0/2484	0.66	0/3360
1	4-A	0.49	0/2484	0.66	1/3360 (0.0%)
1	4-B	0.48	0/2484	0.65	0/3360
1	5-A	0.48	0/2484	0.66	1/3360 (0.0%)
1	5-B	0.48	0/2484	0.65	0/3360
1	6-A	0.48	0/2484	0.66	1/3360 (0.0%)
1	6-B	0.48	0/2484	0.66	1/3360 (0.0%)
1	7-A	0.48	0/2484	0.64	0/3360
1	7-B	0.49	0/2484	0.63	0/3360
1	8-A	0.48	0/2484	0.64	0/3360
1	8-B	0.48	0/2484	0.65	0/3360
1	9-A	0.49	0/2484	0.64	0/3360
1	9-B	0.48	0/2484	0.64	0/3360
1	10-A	0.49	0/2484	0.66	0/3360
1	10-B	0.48	0/2484	0.66	0/3360
1	11-A	0.47	0/2484	0.66	0/3360
1	11-B	0.48	0/2484	0.64	0/3360
1	12-A	0.49	0/2484	0.65	0/3360
1	12-B	0.48	0/2484	0.64	0/3360
1	13-A	0.57	0/2484	0.74	2/3360 (0.1%)
1	13-B	0.55	0/2484	0.74	1/3360 (0.0%)
1	14-A	0.55	0/2484	0.76	3/3360 (0.1%)
1	14-B	0.57	0/2484	0.73	0/3360
1	15-A	0.54	0/2484	0.75	1/3360 (0.0%)
1	15-B	0.54	0/2484	0.73	0/3360
1	16-A	0.56	0/2484	0.77	1/3360 (0.0%)
1	16-B	0.54	0/2484	0.74	1/3360 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	4-A	0	1
1	11-A	0	1
1	13-A	0	1
1	16-A	0	2
All	All	0	5

There are no bond length outliers.

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

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

There are no chirality outliers.

All (5) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

Continued on next page...

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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%)	12 3
1	1-B	305/312 (98%)	270 (88%)	28 (9%)	7 (2%)	6 1
1	2-A	305/312 (98%)	278 (91%)	25 (8%)	2 (1%)	22 10
1	2-B	305/312 (98%)	274 (90%)	24 (8%)	7 (2%)	6 1
1	3-A	305/312 (98%)	277 (91%)	26 (8%)	2 (1%)	22 10
1	3-B	305/312 (98%)	273 (90%)	25 (8%)	7 (2%)	6 1
1	4-A	305/312 (98%)	277 (91%)	24 (8%)	4 (1%)	12 3
1	4-B	305/312 (98%)	273 (90%)	28 (9%)	4 (1%)	12 3
1	5-A	305/312 (98%)	277 (91%)	26 (8%)	2 (1%)	22 10
1	5-B	305/312 (98%)	272 (89%)	29 (10%)	4 (1%)	12 3
1	6-A	305/312 (98%)	277 (91%)	24 (8%)	4 (1%)	12 3
1	6-B	305/312 (98%)	274 (90%)	27 (9%)	4 (1%)	12 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%)	15 5
1	8-A	305/312 (98%)	265 (87%)	37 (12%)	3 (1%)	15 5
1	8-B	305/312 (98%)	275 (90%)	23 (8%)	7 (2%)	6 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	9-A	305/312 (98%)	284 (93%)	17 (6%)	4 (1%)	12 3
1	9-B	305/312 (98%)	271 (89%)	30 (10%)	4 (1%)	12 3
1	10-A	305/312 (98%)	275 (90%)	29 (10%)	1 (0%)	41 27
1	10-B	305/312 (98%)	272 (89%)	27 (9%)	6 (2%)	7 1
1	11-A	305/312 (98%)	283 (93%)	20 (7%)	2 (1%)	22 10
1	11-B	305/312 (98%)	268 (88%)	28 (9%)	9 (3%)	4 0
1	12-A	305/312 (98%)	286 (94%)	17 (6%)	2 (1%)	22 10
1	12-B	305/312 (98%)	275 (90%)	26 (8%)	4 (1%)	12 3
1	13-A	305/312 (98%)	272 (89%)	26 (8%)	7 (2%)	6 1
1	13-B	305/312 (98%)	275 (90%)	24 (8%)	6 (2%)	7 1
1	14-A	305/312 (98%)	266 (87%)	35 (12%)	4 (1%)	12 3
1	14-B	305/312 (98%)	269 (88%)	28 (9%)	8 (3%)	5 1
1	15-A	305/312 (98%)	270 (88%)	28 (9%)	7 (2%)	6 1
1	15-B	305/312 (98%)	275 (90%)	27 (9%)	3 (1%)	15 5
1	16-A	305/312 (98%)	270 (88%)	29 (10%)	6 (2%)	7 1
1	16-B	305/312 (98%)	266 (87%)	32 (10%)	7 (2%)	6 1
All	All	9760/9984 (98%)	8777 (90%)	839 (9%)	144 (2%)	10 2

5 of 144 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (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%)	260 (97%)	8 (3%)	41 27
1	1-B	268/266 (101%)	263 (98%)	5 (2%)	57 46
1	2-A	268/266 (101%)	262 (98%)	6 (2%)	52 39
1	2-B	268/266 (101%)	260 (97%)	8 (3%)	41 27
1	3-A	268/266 (101%)	261 (97%)	7 (3%)	46 32
1	3-B	268/266 (101%)	266 (99%)	2 (1%)	84 81
1	4-A	268/266 (101%)	258 (96%)	10 (4%)	34 19
1	4-B	268/266 (101%)	262 (98%)	6 (2%)	52 39
1	5-A	268/266 (101%)	259 (97%)	9 (3%)	37 22
1	5-B	268/266 (101%)	266 (99%)	2 (1%)	84 81
1	6-A	268/266 (101%)	260 (97%)	8 (3%)	41 27
1	6-B	268/266 (101%)	264 (98%)	4 (2%)	65 56
1	7-A	268/266 (101%)	265 (99%)	3 (1%)	73 68
1	7-B	268/266 (101%)	264 (98%)	4 (2%)	65 56
1	8-A	268/266 (101%)	263 (98%)	5 (2%)	57 46
1	8-B	268/266 (101%)	265 (99%)	3 (1%)	73 68
1	9-A	268/266 (101%)	265 (99%)	3 (1%)	73 68
1	9-B	268/266 (101%)	264 (98%)	4 (2%)	65 56
1	10-A	268/266 (101%)	262 (98%)	6 (2%)	52 39
1	10-B	268/266 (101%)	265 (99%)	3 (1%)	73 68
1	11-A	268/266 (101%)	262 (98%)	6 (2%)	52 39
1	11-B	268/266 (101%)	260 (97%)	8 (3%)	41 27
1	12-A	268/266 (101%)	263 (98%)	5 (2%)	57 46
1	12-B	268/266 (101%)	263 (98%)	5 (2%)	57 46
1	13-A	268/266 (101%)	260 (97%)	8 (3%)	41 27
1	13-B	268/266 (101%)	258 (96%)	10 (4%)	34 19
1	14-A	268/266 (101%)	255 (95%)	13 (5%)	25 11
1	14-B	268/266 (101%)	258 (96%)	10 (4%)	34 19
1	15-A	268/266 (101%)	252 (94%)	16 (6%)	19 7
1	15-B	268/266 (101%)	263 (98%)	5 (2%)	57 46
1	16-A	268/266 (101%)	255 (95%)	13 (5%)	25 11
1	16-B	268/266 (101%)	262 (98%)	6 (2%)	52 39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	8576/8512 (101%)	8365 (98%)	211 (2%)	47 34

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

Mol	Chain	Res	Type
1	11-B	146	MSE
1	13-B	166	THR
1	16-A	194	MSE
1	11-B	289	GLU
1	13-A	45	LEU

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

Mol	Chain	Res	Type
1	8-A	103	ASN
1	16-A	93	GLN
1	9-B	93	GLN
1	15-A	247	GLN
1	16-B	193	GLN

5.3.3 RNA (i)

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 monosaccharides 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	1-B	704	-	4,4,4	0.28	0	6,6,6	0.09	0
3	SO4	2-B	705	-	4,4,4	0.31	0	6,6,6	0.11	0
3	SO4	8-B	704	-	4,4,4	0.28	0	6,6,6	0.09	0
3	SO4	2-A	703	-	4,4,4	0.22	0	6,6,6	0.16	0
3	SO4	6-A	702	-	4,4,4	0.27	0	6,6,6	0.10	0
3	SO4	4-B	704	-	4,4,4	0.25	0	6,6,6	0.08	0
3	SO4	16-B	704	-	4,4,4	0.29	0	6,6,6	0.11	0
3	SO4	15-B	705	-	4,4,4	0.26	0	6,6,6	0.10	0
3	SO4	7-B	704	-	4,4,4	0.29	0	6,6,6	0.09	0
3	SO4	14-A	702	-	4,4,4	0.30	0	6,6,6	0.16	0
3	SO4	11-A	703	-	4,4,4	0.24	0	6,6,6	0.14	0
3	SO4	14-B	705	-	4,4,4	0.30	0	6,6,6	0.09	0
3	SO4	10-A	702	-	4,4,4	0.29	0	6,6,6	0.09	0
3	SO4	6-B	705	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	5-A	703	-	4,4,4	0.20	0	6,6,6	0.15	0
3	SO4	4-A	702	-	4,4,4	0.26	0	6,6,6	0.10	0
3	SO4	5-A	702	-	4,4,4	0.28	0	6,6,6	0.07	0
3	SO4	13-A	703	-	4,4,4	0.23	0	6,6,6	0.14	0
3	SO4	8-B	705	-	4,4,4	0.26	0	6,6,6	0.10	0
3	SO4	12-A	702	-	4,4,4	0.27	0	6,6,6	0.08	0
3	SO4	2-A	701	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	14-A	703	-	4,4,4	0.22	0	6,6,6	0.10	0
3	SO4	15-A	701	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	16-A	702	-	4,4,4	0.30	0	6,6,6	0.12	0
3	SO4	5-B	704	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	16-B	705	-	4,4,4	0.26	0	6,6,6	0.11	0
3	SO4	9-A	703	-	4,4,4	0.20	0	6,6,6	0.16	0
3	SO4	1-B	705	-	4,4,4	0.27	0	6,6,6	0.07	0
3	SO4	1-A	701	-	4,4,4	0.28	0	6,6,6	0.08	0
3	SO4	2-A	702	-	4,4,4	0.27	0	6,6,6	0.07	0
3	SO4	14-B	704	-	4,4,4	0.28	0	6,6,6	0.10	0
3	SO4	15-B	704	-	4,4,4	0.31	0	6,6,6	0.06	0
3	SO4	6-B	704	-	4,4,4	0.28	0	6,6,6	0.09	0
3	SO4	13-B	705	-	4,4,4	0.28	0	6,6,6	0.11	0
3	SO4	12-B	704	-	4,4,4	0.27	0	6,6,6	0.08	0
3	SO4	6-A	703	-	4,4,4	0.21	0	6,6,6	0.17	0
3	SO4	7-A	701	-	4,4,4	0.25	0	6,6,6	0.04	0
3	SO4	16-A	701	-	4,4,4	0.27	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	2-B	704	-	4,4,4	0.28	0	6,6,6	0.09	0
3	SO4	10-B	704	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	9-A	702	-	4,4,4	0.31	0	6,6,6	0.12	0
3	SO4	3-A	702	-	4,4,4	0.29	0	6,6,6	0.11	0
3	SO4	4-A	701	-	4,4,4	0.27	0	6,6,6	0.07	0
3	SO4	10-A	703	-	4,4,4	0.25	0	6,6,6	0.07	0
3	SO4	4-A	703	-	4,4,4	0.23	0	6,6,6	0.15	0
3	SO4	5-A	701	-	4,4,4	0.33	0	6,6,6	0.06	0
3	SO4	9-A	701	-	4,4,4	0.27	0	6,6,6	0.07	0
3	SO4	3-B	705	-	4,4,4	0.27	0	6,6,6	0.07	0
3	SO4	11-A	701	-	4,4,4	0.26	0	6,6,6	0.10	0
3	SO4	3-A	703	-	4,4,4	0.22	0	6,6,6	0.07	0
3	SO4	1-A	703	-	4,4,4	0.21	0	6,6,6	0.17	0
3	SO4	8-A	703	-	4,4,4	0.22	0	6,6,6	0.09	0
3	SO4	8-A	702	-	4,4,4	0.30	0	6,6,6	0.10	0
3	SO4	10-B	705	-	4,4,4	0.27	0	6,6,6	0.10	0
3	SO4	11-B	704	-	4,4,4	0.28	0	6,6,6	0.11	0
3	SO4	3-A	701	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	7-A	702	-	4,4,4	0.27	0	6,6,6	0.08	0
3	SO4	13-B	704	-	4,4,4	0.30	0	6,6,6	0.07	0
3	SO4	4-B	705	-	4,4,4	0.25	0	6,6,6	0.07	0
3	SO4	9-B	704	-	4,4,4	0.28	0	6,6,6	0.09	0
3	SO4	8-A	701	-	4,4,4	0.28	0	6,6,6	0.11	0
3	SO4	10-A	701	-	4,4,4	0.23	0	6,6,6	0.06	0
3	SO4	12-A	701	-	4,4,4	0.28	0	6,6,6	0.10	0
3	SO4	12-B	705	-	4,4,4	0.28	0	6,6,6	0.11	0
3	SO4	7-B	705	-	4,4,4	0.24	0	6,6,6	0.10	0
3	SO4	16-A	703	-	4,4,4	0.25	0	6,6,6	0.13	0
3	SO4	9-B	705	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	6-A	701	-	4,4,4	0.28	0	6,6,6	0.09	0
3	SO4	11-A	702	-	4,4,4	0.28	0	6,6,6	0.08	0
3	SO4	11-B	705	-	4,4,4	0.26	0	6,6,6	0.10	0
3	SO4	1-A	702	-	4,4,4	0.27	0	6,6,6	0.08	0
3	SO4	14-A	701	-	4,4,4	0.24	0	6,6,6	0.11	0
3	SO4	13-A	702	-	4,4,4	0.30	0	6,6,6	0.12	0
3	SO4	15-A	703	-	4,4,4	0.26	0	6,6,6	0.09	0
3	SO4	15-A	702	-	4,4,4	0.34	0	6,6,6	0.11	0
3	SO4	3-B	704	-	4,4,4	0.27	0	6,6,6	0.07	0
3	SO4	12-A	703	-	4,4,4	0.20	0	6,6,6	0.15	0
3	SO4	5-B	705	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	7-A	703	-	4,4,4	0.22	0	6,6,6	0.15	0
3	SO4	13-A	701	-	4,4,4	0.25	0	6,6,6	0.11	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, 95^{th} 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%)	-0.04	11 (3%)	41	36	5, 14, 34, 60	300 (100%)
1	1-B	300/312 (96%)	-0.03	16 (5%)	26	21	8, 15, 33, 55	300 (100%)
1	2-A	300/312 (96%)	-0.04	11 (3%)	41	36	5, 14, 34, 60	300 (100%)
1	2-B	300/312 (96%)	-0.03	16 (5%)	26	21	8, 15, 33, 55	300 (100%)
1	3-A	300/312 (96%)	-0.04	11 (3%)	41	36	5, 14, 34, 60	300 (100%)
1	3-B	300/312 (96%)	-0.03	16 (5%)	26	21	8, 15, 33, 55	300 (100%)
1	4-A	300/312 (96%)	-0.04	11 (3%)	41	36	5, 14, 34, 60	300 (100%)
1	4-B	300/312 (96%)	-0.03	16 (5%)	26	21	8, 15, 33, 55	300 (100%)
1	5-A	300/312 (96%)	-0.04	11 (3%)	41	36	5, 14, 34, 60	300 (100%)
1	5-B	300/312 (96%)	-0.03	16 (5%)	26	21	8, 15, 33, 55	300 (100%)
1	6-A	300/312 (96%)	-0.04	11 (3%)	41	36	5, 14, 34, 60	300 (100%)
1	6-B	300/312 (96%)	-0.03	16 (5%)	26	21	8, 15, 33, 55	300 (100%)
1	7-A	300/312 (96%)	-0.04	11 (3%)	41	36	5, 14, 34, 60	300 (100%)
1	7-B	300/312 (96%)	-0.03	16 (5%)	26	21	8, 15, 33, 55	300 (100%)
1	8-A	300/312 (96%)	-0.04	11 (3%)	41	36	5, 14, 34, 60	300 (100%)
1	8-B	300/312 (96%)	-0.03	16 (5%)	26	21	8, 15, 33, 55	300 (100%)
1	9-A	300/312 (96%)	-0.04	11 (3%)	41	36	5, 14, 34, 60	300 (100%)
1	9-B	300/312 (96%)	-0.03	16 (5%)	26	21	8, 15, 33, 55	300 (100%)
1	10-A	300/312 (96%)	-0.04	11 (3%)	41	36	5, 14, 34, 60	300 (100%)
1	10-B	300/312 (96%)	-0.03	16 (5%)	26	21	8, 15, 33, 55	300 (100%)
1	11-A	300/312 (96%)	-0.04	11 (3%)	41	36	5, 14, 34, 60	300 (100%)
1	11-B	300/312 (96%)	-0.03	16 (5%)	26	21	8, 15, 33, 55	300 (100%)
1	12-A	300/312 (96%)	-0.04	11 (3%)	41	36	5, 14, 34, 60	300 (100%)
1	12-B	300/312 (96%)	-0.03	16 (5%)	26	21	8, 15, 33, 55	300 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	13-A	300/312 (96%)	-0.04	11 (3%)	41	36	5, 14, 34, 60	300 (100%)
1	13-B	300/312 (96%)	-0.03	16 (5%)	26	21	8, 15, 33, 55	300 (100%)
1	14-A	300/312 (96%)	-0.04	11 (3%)	41	36	5, 14, 34, 60	300 (100%)
1	14-B	300/312 (96%)	-0.03	16 (5%)	26	21	8, 15, 33, 55	300 (100%)
1	15-A	300/312 (96%)	-0.04	11 (3%)	41	36	5, 14, 34, 60	300 (100%)
1	15-B	300/312 (96%)	-0.03	16 (5%)	26	21	8, 15, 33, 55	300 (100%)
1	16-A	300/312 (96%)	-0.04	11 (3%)	41	36	5, 14, 34, 60	300 (100%)
1	16-B	300/312 (96%)	-0.03	16 (5%)	26	21	8, 15, 33, 55	300 (100%)
All	All	9600/9984 (96%)	-0.03	432 (4%)	32	27	5, 15, 33, 60	9600 (100%)

The worst 5 of 432 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	78	SER	8.7
1	2-B	78	SER	8.7
1	3-B	78	SER	8.7
1	4-B	78	SER	8.7
1	5-B	78	SER	8.7

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 monosaccharides 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-A	702	5/5	0.95	0.11	42,44,44,45	5
3	SO4	2-A	702	5/5	0.95	0.11	42,44,44,45	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	3-A	702	5/5	0.95	0.11	43,44,44,46	5
3	SO4	4-A	702	5/5	0.95	0.11	43,44,45,45	5
3	SO4	5-A	702	5/5	0.95	0.11	42,44,44,45	5
3	SO4	6-A	702	5/5	0.95	0.11	44,44,45,45	5
3	SO4	7-A	702	5/5	0.95	0.11	42,44,44,45	5
3	SO4	8-A	702	5/5	0.95	0.11	43,44,44,46	5
3	SO4	9-A	702	5/5	0.95	0.11	43,43,45,45	5
3	SO4	10-A	702	5/5	0.95	0.11	43,44,44,46	5
3	SO4	11-A	702	5/5	0.95	0.11	42,44,44,45	5
3	SO4	12-A	702	5/5	0.95	0.11	42,44,44,45	5
3	SO4	13-A	702	5/5	0.95	0.11	42,43,43,45	5
3	SO4	14-A	702	5/5	0.95	0.11	42,43,44,44	5
3	SO4	15-A	702	5/5	0.95	0.11	42,43,45,45	5
3	SO4	16-A	702	5/5	0.95	0.11	42,43,44,45	5
3	SO4	1-B	704	5/5	0.95	0.14	50,51,51,53	5
3	SO4	2-B	704	5/5	0.95	0.14	50,51,51,53	5
3	SO4	3-B	704	5/5	0.95	0.14	52,52,53,53	5
3	SO4	4-B	704	5/5	0.95	0.14	50,51,52,52	5
3	SO4	5-B	704	5/5	0.95	0.14	50,51,52,52	5
3	SO4	6-B	704	5/5	0.95	0.14	50,51,52,53	5
3	SO4	7-B	704	5/5	0.95	0.14	50,51,52,53	5
3	SO4	8-B	704	5/5	0.95	0.14	50,51,51,53	5
3	SO4	9-B	704	5/5	0.95	0.14	51,51,52,53	5
3	SO4	10-B	704	5/5	0.95	0.14	50,51,52,52	5
3	SO4	11-B	704	5/5	0.95	0.14	51,51,52,53	5
3	SO4	12-B	704	5/5	0.95	0.14	50,51,51,52	5
3	SO4	13-B	704	5/5	0.95	0.14	49,50,51,52	5
3	SO4	14-B	704	5/5	0.95	0.14	50,50,51,53	5
3	SO4	15-B	704	5/5	0.95	0.14	51,52,52,53	5
3	SO4	16-B	704	5/5	0.95	0.14	50,51,52,53	5
2	ZN	1-B	602	1/1	0.97	0.50	14,14,14,14	1
2	ZN	2-B	602	1/1	0.97	0.50	21,21,21,21	1
2	ZN	3-B	602	1/1	0.97	0.50	15,15,15,15	1
2	ZN	4-B	602	1/1	0.97	0.50	21,21,21,21	1
2	ZN	5-B	602	1/1	0.97	0.50	23,23,23,23	1
2	ZN	6-B	602	1/1	0.97	0.50	19,19,19,19	1
2	ZN	7-B	602	1/1	0.97	0.50	19,19,19,19	1
2	ZN	8-B	602	1/1	0.97	0.50	7,7,7,7	1
2	ZN	9-B	602	1/1	0.97	0.50	16,16,16,16	1
2	ZN	10-B	602	1/1	0.97	0.50	16,16,16,16	1
2	ZN	11-B	602	1/1	0.97	0.50	11,11,11,11	1
2	ZN	12-B	602	1/1	0.97	0.50	0,0,0,0	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	13-B	602	1/1	0.97	0.50	28,28,28,28	1
2	ZN	14-B	602	1/1	0.97	0.50	12,12,12,12	1
2	ZN	15-B	602	1/1	0.97	0.50	27,27,27,27	1
2	ZN	16-B	602	1/1	0.97	0.50	29,29,29,29	1
3	SO4	1-A	703	5/5	0.98	0.08	47,48,49,49	5
3	SO4	2-A	703	5/5	0.98	0.08	47,48,49,49	5
3	SO4	3-A	703	5/5	0.98	0.08	46,47,48,49	5
3	SO4	4-A	703	5/5	0.98	0.08	47,48,49,49	5
3	SO4	5-A	703	5/5	0.98	0.08	46,48,49,49	5
3	SO4	6-A	703	5/5	0.98	0.08	47,48,49,49	5
3	SO4	7-A	703	5/5	0.98	0.08	47,48,49,49	5
3	SO4	8-A	703	5/5	0.98	0.08	46,47,47,48	5
3	SO4	9-A	703	5/5	0.98	0.08	47,48,49,49	5
3	SO4	10-A	703	5/5	0.98	0.08	46,48,49,49	5
3	SO4	11-A	703	5/5	0.98	0.08	48,48,49,50	5
3	SO4	12-A	703	5/5	0.98	0.08	47,48,49,49	5
3	SO4	13-A	703	5/5	0.98	0.08	47,48,49,50	5
3	SO4	14-A	703	5/5	0.98	0.08	48,48,49,49	5
3	SO4	15-A	703	5/5	0.98	0.08	46,48,48,48	5
3	SO4	16-A	703	5/5	0.98	0.08	48,48,49,50	5
3	SO4	1-A	701	5/5	0.98	0.18	38,39,39,40	5
3	SO4	2-A	701	5/5	0.98	0.18	37,37,38,38	5
3	SO4	3-A	701	5/5	0.98	0.18	37,37,38,39	5
3	SO4	4-A	701	5/5	0.98	0.18	38,39,40,40	5
3	SO4	5-A	701	5/5	0.98	0.18	39,39,40,41	5
3	SO4	6-A	701	5/5	0.98	0.18	38,39,39,40	5
3	SO4	7-A	701	5/5	0.98	0.18	38,39,39,41	5
3	SO4	8-A	701	5/5	0.98	0.18	37,38,39,39	5
3	SO4	9-A	701	5/5	0.98	0.18	37,37,39,39	5
3	SO4	10-A	701	5/5	0.98	0.18	37,38,38,39	5
3	SO4	11-A	701	5/5	0.98	0.18	37,38,39,39	5
3	SO4	12-A	701	5/5	0.98	0.18	37,38,39,39	5
3	SO4	13-A	701	5/5	0.98	0.18	37,38,39,39	5
3	SO4	14-A	701	5/5	0.98	0.18	38,38,40,41	5
3	SO4	15-A	701	5/5	0.98	0.18	36,37,38,38	5
3	SO4	16-A	701	5/5	0.98	0.18	36,38,38,38	5
3	SO4	1-B	705	5/5	0.98	0.08	48,48,49,49	5
3	SO4	2-B	705	5/5	0.98	0.08	46,47,48,48	5
3	SO4	3-B	705	5/5	0.98	0.08	48,49,49,49	5
3	SO4	4-B	705	5/5	0.98	0.08	47,48,49,49	5
3	SO4	5-B	705	5/5	0.98	0.08	45,46,47,48	5
3	SO4	6-B	705	5/5	0.98	0.08	45,46,47,47	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	7-B	705	5/5	0.98	0.08	46,47,49,49	5
3	SO4	8-B	705	5/5	0.98	0.08	45,46,47,47	5
3	SO4	9-B	705	5/5	0.98	0.08	45,46,47,47	5
3	SO4	10-B	705	5/5	0.98	0.08	45,46,47,48	5
3	SO4	11-B	705	5/5	0.98	0.08	45,46,47,47	5
3	SO4	12-B	705	5/5	0.98	0.08	46,47,47,47	5
3	SO4	13-B	705	5/5	0.98	0.08	46,47,47,48	5
3	SO4	14-B	705	5/5	0.98	0.08	49,49,50,51	5
3	SO4	15-B	705	5/5	0.98	0.08	44,45,47,47	5
3	SO4	16-B	705	5/5	0.98	0.08	44,45,47,47	5
2	ZN	1-A	601	1/1	0.99	0.04	24,24,24,24	1
2	ZN	2-A	601	1/1	0.99	0.04	13,13,13,13	1
2	ZN	3-A	601	1/1	0.99	0.04	15,15,15,15	1
2	ZN	4-A	601	1/1	0.99	0.04	4,4,4,4	1
2	ZN	5-A	601	1/1	0.99	0.04	16,16,16,16	1
2	ZN	6-A	601	1/1	0.99	0.04	6,6,6,6	1
2	ZN	7-A	601	1/1	0.99	0.04	18,18,18,18	1
2	ZN	8-A	601	1/1	0.99	0.04	11,11,11,11	1
2	ZN	9-A	601	1/1	0.99	0.04	0,0,0,0	1
2	ZN	10-A	601	1/1	0.99	0.04	25,25,25,25	1
2	ZN	11-A	601	1/1	0.99	0.04	17,17,17,17	1
2	ZN	12-A	601	1/1	0.99	0.04	12,12,12,12	1
2	ZN	13-A	601	1/1	0.99	0.04	23,23,23,23	1
2	ZN	14-A	601	1/1	0.99	0.04	17,17,17,17	1
2	ZN	15-A	601	1/1	0.99	0.04	23,23,23,23	1
2	ZN	16-A	601	1/1	0.99	0.04	15,15,15,15	1

6.5 Other polymers (i)

There are no such residues in this entry.