Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2023 – 04:41 PM EDT

PDB ID	:	2Q51
Title	:	Ensemble refinement of the protein crystal structure of an aspartoacylase from Homo sapiens
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	:	2.80 Å(reported)

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

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

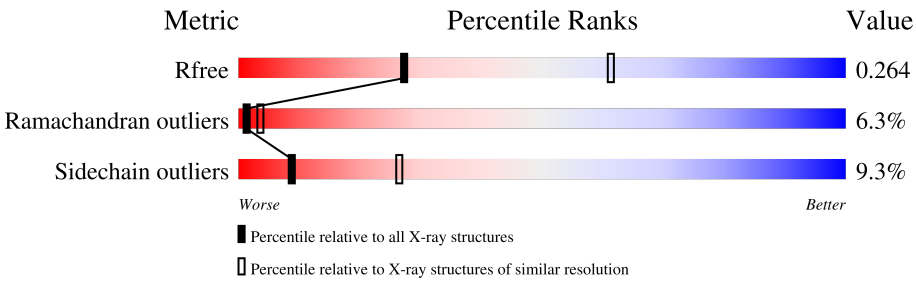
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.80 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	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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%

Mol	Chain	Length	Quality of chain
1	1-A	315	76% 19% • •
1	1-B	315	85% 10% • •
1	10-A	315	86% 9% • •
1	10-B	315	80% 16% •
1	11-A	315	85% 9% • • •
1	11-B	315	85% 8% • •
1	12-A	315	78% 17% •
1	12-B	315	84% 11% • •

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Mol	Chain	Length	Quality of chain
1	13-A	315	70% 23%
1	13-B	315	79% 15%
1	14-A	315	72% 19% 5%
1	14-B	315	79% 13%
1	15-A	315	76% 17%
1	15-B	315	74% 16%
1	16-A	315	72% 21%
1	16-B	315	75% 19%
1	2-A	315	83% 11%
1	2-B	315	87% 9%
1	3-A	315	84% 11%
1	3-B	315	87% 9%
1	4-A	315	84% 11%
1	4-B	315	85% 10%
1	5-A	315	84% 12%
1	5-B	315	83% 12%
1	6-A	315	85% 10%
1	6-B	315	85% 10%
1	7-A	315	87% 8%
1	7-B	315	82% 13%
1	8-A	315	81% 14%
1	8-B	315	83% 11%
1	9-A	315	87% 9%
1	9-B	315	84% 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 79008 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
			Total	C	N	O	S	Se			
1	1-A	302	2430	1559	411	447	7	6	0	0	0
1	2-A	302	2430	1559	411	447	7	6	0	0	0
1	3-A	302	2430	1559	411	447	7	6	0	0	0
1	4-A	302	2430	1559	411	447	7	6	0	0	0
1	5-A	302	2430	1559	411	447	7	6	0	0	0
1	6-A	302	2430	1559	411	447	7	6	0	0	0
1	7-A	302	2430	1559	411	447	7	6	0	0	0
1	8-A	302	2430	1559	411	447	7	6	0	0	0
1	9-A	302	2430	1559	411	447	7	6	0	0	0
1	10-A	302	2430	1559	411	447	7	6	0	0	0
1	11-A	302	2430	1559	411	447	7	6	0	0	0
1	12-A	302	2430	1559	411	447	7	6	0	0	0
1	13-A	302	2430	1559	411	447	7	6	0	0	0
1	14-A	302	2430	1559	411	447	7	6	0	0	0
1	15-A	302	2430	1559	411	447	7	6	0	0	0
1	16-A	302	2430	1559	411	447	7	6	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	1-B	302	2430	1559	411	447	7	6	0	0	0
1	2-B	302	2430	1559	411	447	7	6	0	0	0
1	3-B	302	2430	1559	411	447	7	6	0	0	0
1	4-B	302	2430	1559	411	447	7	6	0	0	0
1	5-B	302	2430	1559	411	447	7	6	0	0	0
1	6-B	302	2430	1559	411	447	7	6	0	0	0
1	7-B	302	2430	1559	411	447	7	6	0	0	0
1	8-B	302	2430	1559	411	447	7	6	0	0	0
1	9-B	302	2430	1559	411	447	7	6	0	0	0
1	10-B	302	2430	1559	411	447	7	6	0	0	0
1	11-B	302	2430	1559	411	447	7	6	0	0	0
1	12-B	302	2430	1559	411	447	7	6	0	0	0
1	13-B	302	2430	1559	411	447	7	6	0	0	0
1	14-B	302	2430	1559	411	447	7	6	0	0	0
1	15-B	302	2430	1559	411	447	7	6	0	0	0
1	16-B	302	2430	1559	411	447	7	6	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP P45381
A	0	ILE	-	expression tag	UNP P45381
A	1	ALA	-	expression tag	UNP P45381
A	82	MSE	MET	modified residue	UNP P45381
A	122	MSE	MET	modified residue	UNP P45381
A	139	MSE	MET	modified residue	UNP P45381
A	195	MSE	MET	modified residue	UNP P45381

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Chain	Residue	Modelled	Actual	Comment	Reference
A	198	MSE	MET	modified residue	UNP P45381
A	261	MSE	MET	modified residue	UNP P45381
B	-1	ALA	-	expression tag	UNP P45381
B	0	ILE	-	expression tag	UNP P45381
B	1	ALA	-	expression tag	UNP P45381
B	82	MSE	MET	modified residue	UNP P45381
B	122	MSE	MET	modified residue	UNP P45381
B	139	MSE	MET	modified residue	UNP P45381
B	195	MSE	MET	modified residue	UNP P45381
B	198	MSE	MET	modified residue	UNP P45381
B	261	MSE	MET	modified residue	UNP P45381

- 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
2	14-A	1	Total Zn 1 1	0	0

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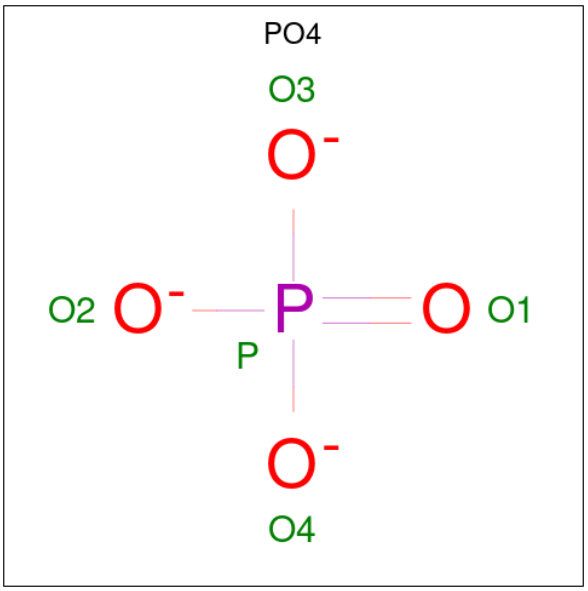
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	15-A	1	1	1	0	0
2	16-A	1	1	1	0	0
2	1-B	1	1	1	0	0
2	2-B	1	1	1	0	0
2	3-B	1	1	1	0	0
2	4-B	1	1	1	0	0
2	5-B	1	1	1	0	0
2	6-B	1	1	1	0	0
2	7-B	1	1	1	0	0
2	8-B	1	1	1	0	0
2	9-B	1	1	1	0	0
2	10-B	1	1	1	0	0
2	11-B	1	1	1	0	0
2	12-B	1	1	1	0	0
2	13-B	1	1	1	0	0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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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

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

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

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

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

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

- Molecule 4 is water.

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	11-A	14	Total O 14 14	0	0
4	12-A	14	Total O 14 14	0	0
4	13-A	14	Total O 14 14	0	0
4	14-A	14	Total O 14 14	0	0
4	15-A	13	Total O 13 13	0	0
4	16-A	13	Total O 13 13	0	0
4	1-B	23	Total O 23 23	0	0
4	2-B	22	Total O 22 22	0	0
4	3-B	23	Total O 23 23	0	0
4	4-B	23	Total O 23 23	0	0
4	5-B	22	Total O 22 22	0	0
4	6-B	22	Total O 22 22	0	0
4	7-B	22	Total O 22 22	0	0
4	8-B	22	Total O 22 22	0	0
4	9-B	22	Total O 22 22	0	0
4	10-B	22	Total O 22 22	0	0
4	11-B	22	Total O 22 22	0	0
4	12-B	22	Total O 22 22	0	0
4	13-B	22	Total O 22 22	0	0
4	14-B	22	Total O 22 22	0	0
4	15-B	23	Total O 23 23	0	0

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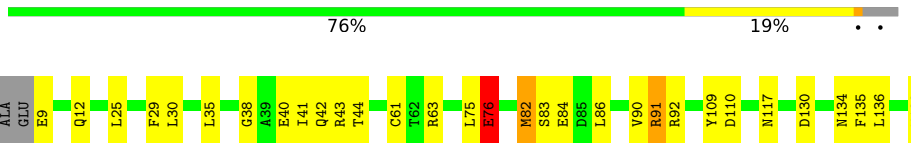
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	16-B	23	23	23	0	0

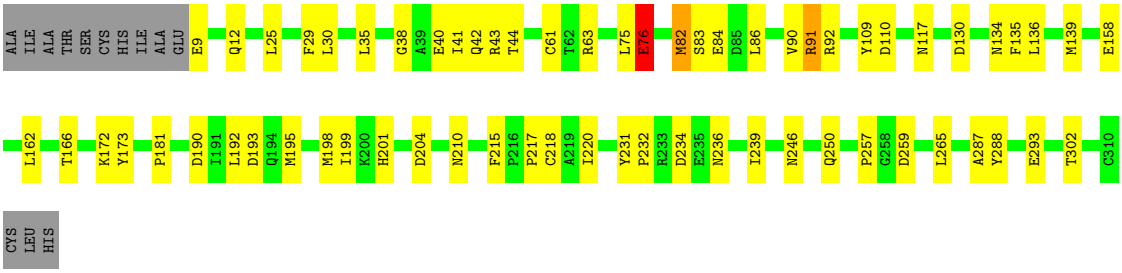
3 Residue-property plots (i)

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. 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. 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

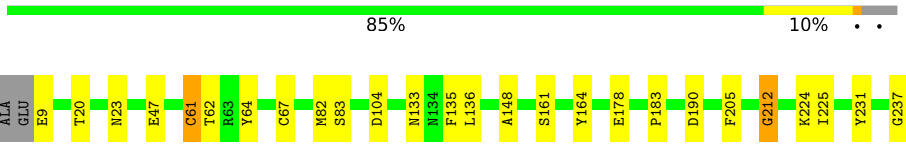
Chain 1-A:

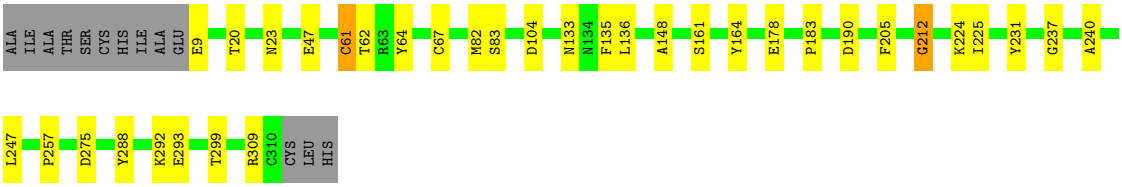




- Molecule 1: Aspartoacylase

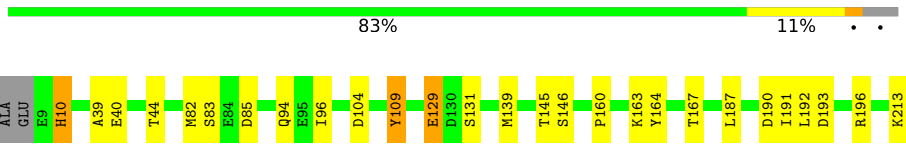
Chain 1-B:

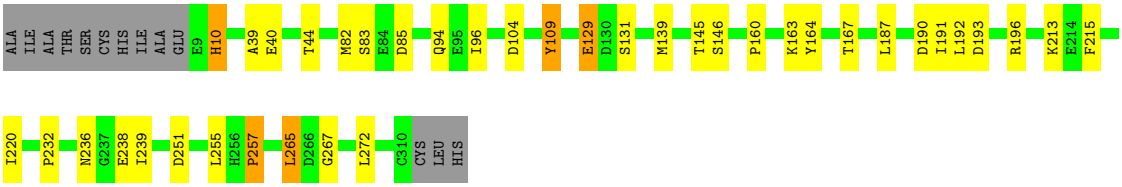




- Molecule 1: Aspartoacylase

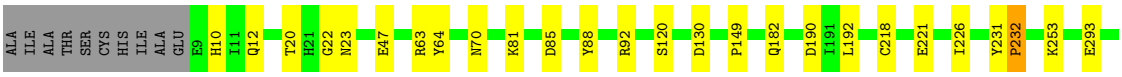
Chain 2-A:

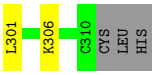




- Molecule 1: Aspartoacylase

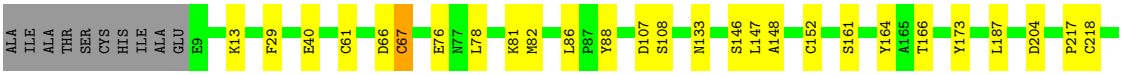
Chain 2-B:





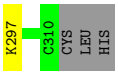
• Molecule 1: Aspartoacylase

Chain 3-A:



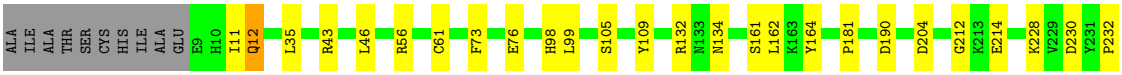
• Molecule 1: Aspartoacylase

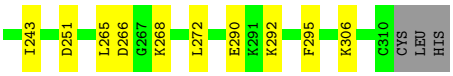
Chain 3-B:



• Molecule 1: Aspartoacylase

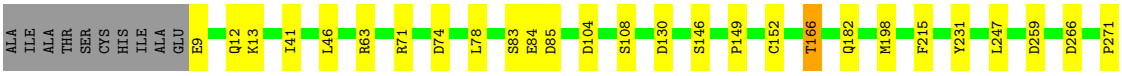
Chain 4-A:

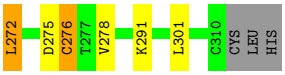




• Molecule 1: Aspartoacylase

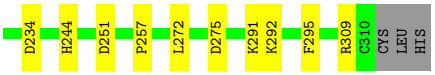
Chain 4-B:





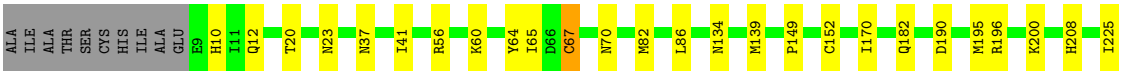
• Molecule 1: Aspartoacylase

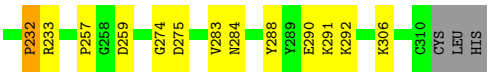
Chain 5-A:



• Molecule 1: Aspartoacylase

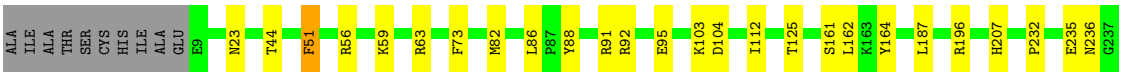
Chain 5-B:





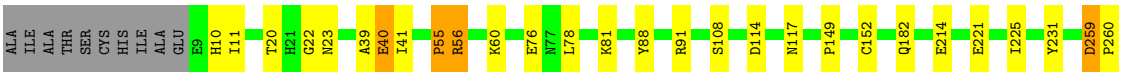
• Molecule 1: Aspartoacylase

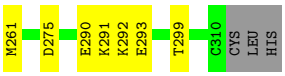
Chain 6-A:



• Molecule 1: Aspartoacylase

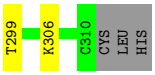
Chain 6-B:





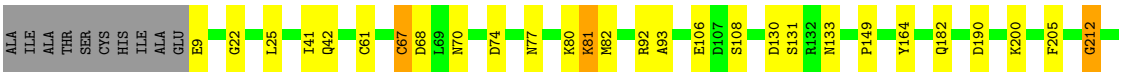
• Molecule 1: Aspartoacylase

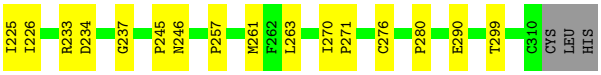
Chain 7-A:



• Molecule 1: Aspartoacylase

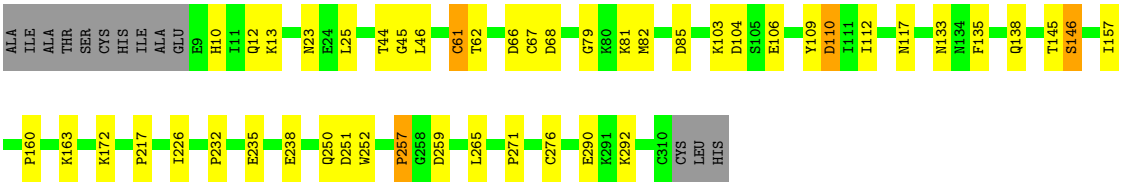
Chain 7-B:





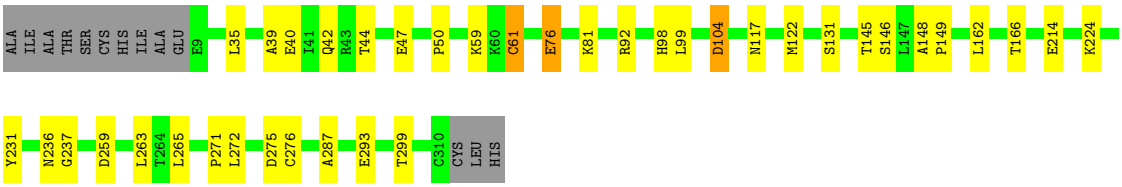
• Molecule 1: Aspartoacylase

Chain 8-A:



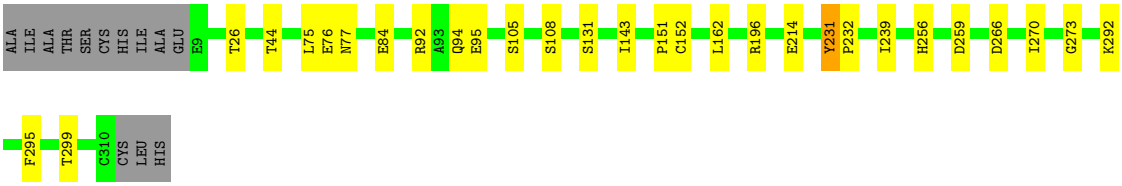
• Molecule 1: Aspartoacylase

Chain 8-B:



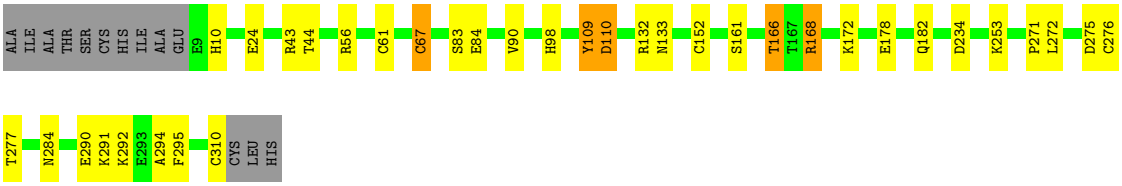
• Molecule 1: Aspartoacylase

Chain 9-A:



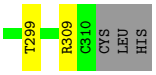
• Molecule 1: Aspartoacylase

Chain 9-B:



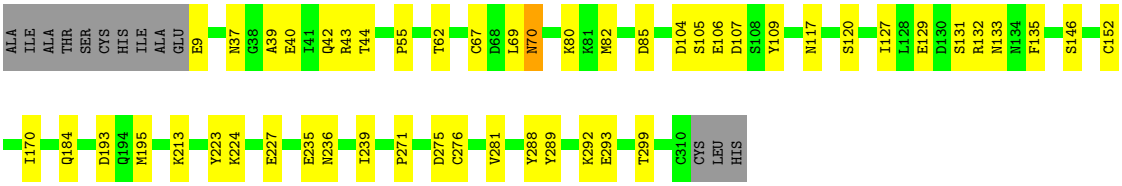
• Molecule 1: Aspartoacylase

Chain 10-A:



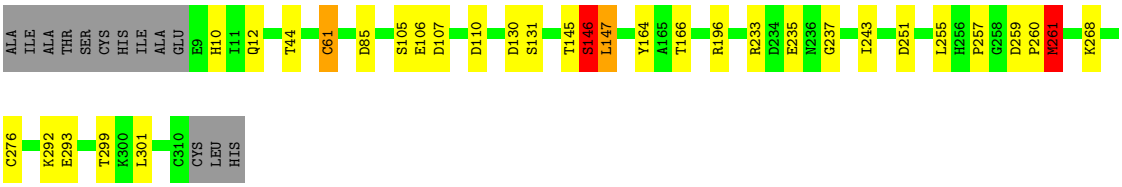
• Molecule 1: Aspartoacylase

Chain 10-B:



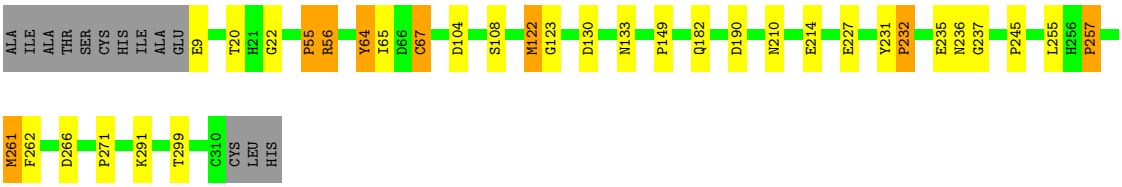
• Molecule 1: Aspartoacylase

Chain 11-A:



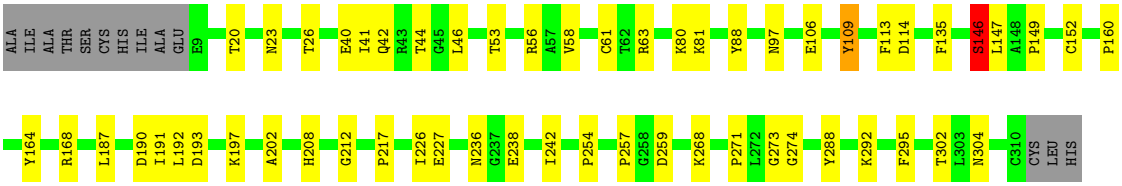
• Molecule 1: Aspartoacylase

Chain 11-B:



• Molecule 1: Aspartoacylase

Chain 12-A:

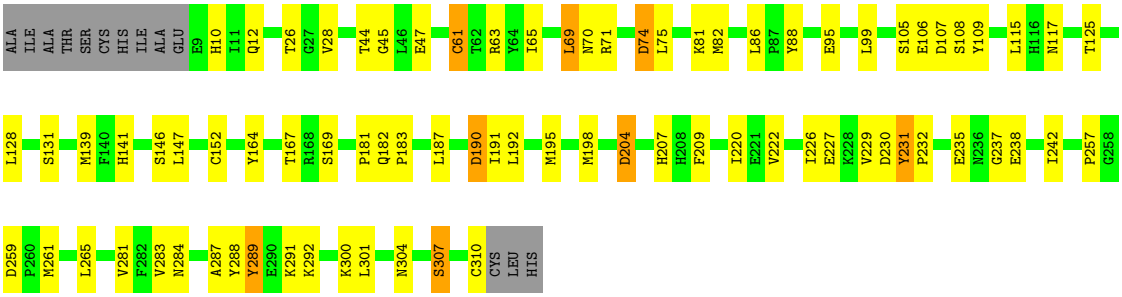


• Molecule 1: Aspartoacylase

Chain 12-B:

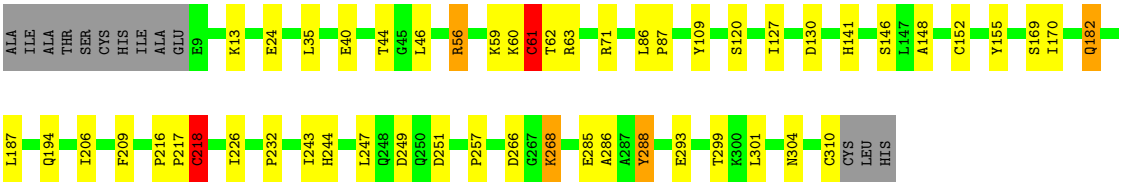
• Molecule 1: Aspartoacylase

Chain 13-A:



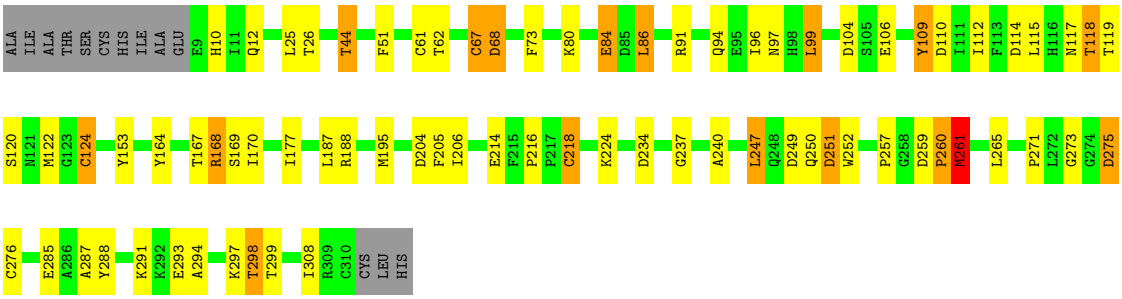
• Molecule 1: Aspartoacylase

Chain 13-B:



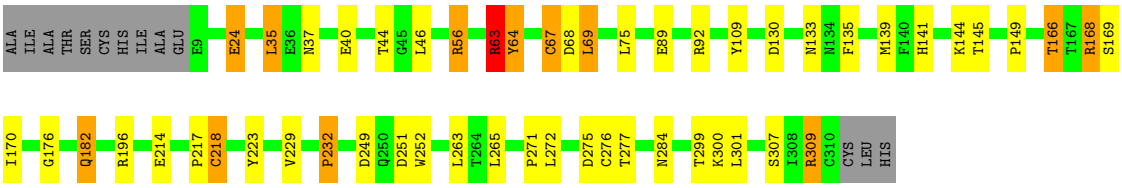
• Molecule 1: Aspartoacylase

Chain 14-A:



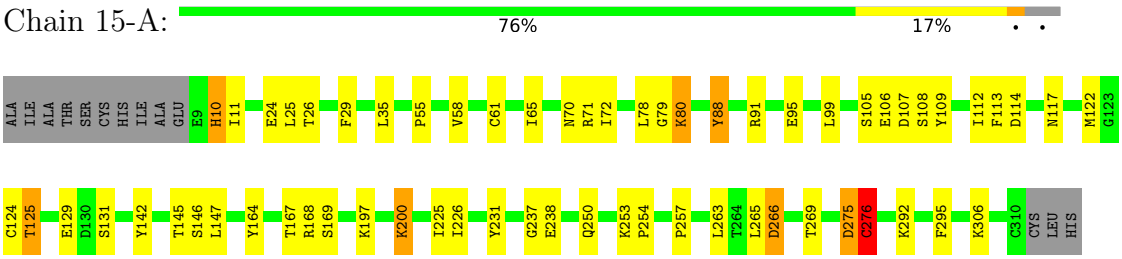
• Molecule 1: Aspartoacylase

Chain 14-B:



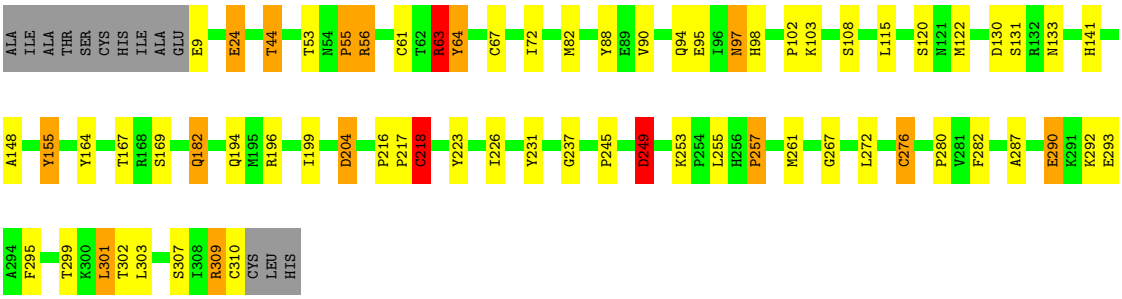
- Molecule 1: Aspartoacylase

Chain 15-A:



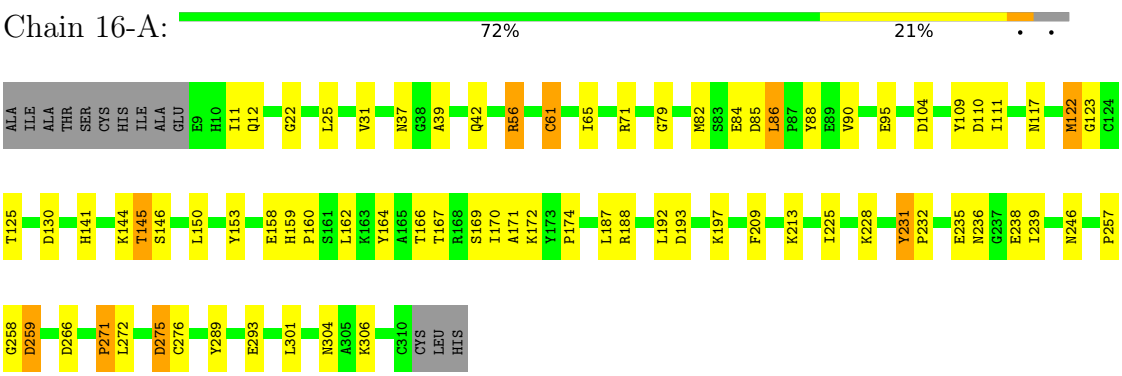
- Molecule 1: Aspartoacylase

Chain 15-B:



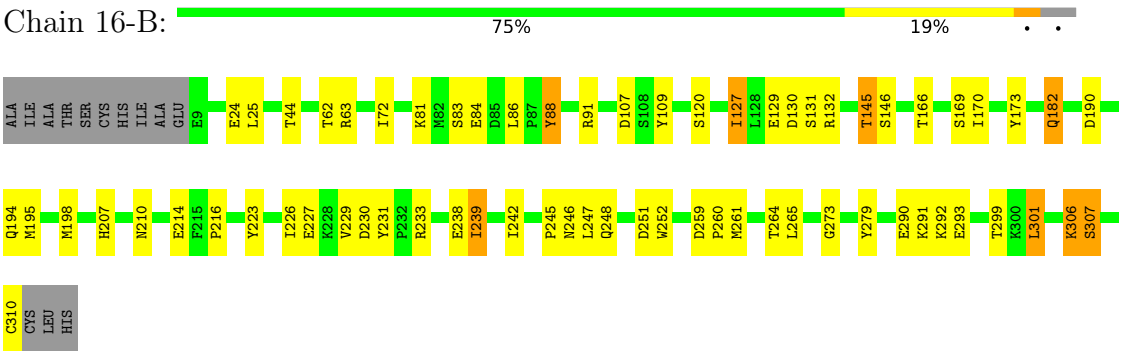
- Molecule 1: Aspartoacylase

Chain 16-A:



- Molecule 1: Aspartoacylase

Chain 16-B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	145.55Å 145.55Å 103.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.72 – 2.80 48.72 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.72-2.80) 97.8 (48.72-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.157 , 0.239 0.199 , 0.264	Depositor DCC
R_{free} test set	1374 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	53.1	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 192.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	79008	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	0.83	1/2485 (0.0%)	0.96	2/3358 (0.1%)
1	1-B	0.86	2/2485 (0.1%)	0.95	2/3358 (0.1%)
1	2-A	0.81	5/2485 (0.2%)	0.93	3/3358 (0.1%)
1	2-B	0.80	1/2485 (0.0%)	0.88	2/3358 (0.1%)
1	3-A	0.86	5/2485 (0.2%)	0.98	5/3358 (0.1%)
1	3-B	0.80	0/2485	0.89	1/3358 (0.0%)
1	4-A	0.81	2/2485 (0.1%)	0.93	2/3358 (0.1%)
1	4-B	0.80	1/2485 (0.0%)	0.88	1/3358 (0.0%)
1	5-A	0.76	2/2485 (0.1%)	0.87	1/3358 (0.0%)
1	5-B	0.85	3/2485 (0.1%)	0.95	3/3358 (0.1%)
1	6-A	0.77	1/2485 (0.0%)	0.88	1/3358 (0.0%)
1	6-B	0.82	2/2485 (0.1%)	0.90	2/3358 (0.1%)
1	7-A	0.76	1/2485 (0.0%)	0.89	3/3358 (0.1%)
1	7-B	0.81	2/2485 (0.1%)	0.91	2/3358 (0.1%)
1	8-A	0.81	1/2485 (0.0%)	0.97	9/3358 (0.3%)
1	8-B	0.82	2/2485 (0.1%)	0.94	4/3358 (0.1%)
1	9-A	0.79	1/2485 (0.0%)	0.88	1/3358 (0.0%)
1	9-B	0.80	2/2485 (0.1%)	0.95	3/3358 (0.1%)
1	10-A	0.75	1/2485 (0.0%)	0.84	0/3358
1	10-B	0.82	0/2485	0.92	1/3358 (0.0%)
1	11-A	0.79	2/2485 (0.1%)	0.91	5/3358 (0.1%)
1	11-B	0.78	1/2485 (0.0%)	0.93	2/3358 (0.1%)
1	12-A	0.83	1/2485 (0.0%)	0.97	4/3358 (0.1%)
1	12-B	0.82	3/2485 (0.1%)	0.90	1/3358 (0.0%)
1	13-A	0.96	2/2485 (0.1%)	1.08	6/3358 (0.2%)
1	13-B	0.98	2/2485 (0.1%)	1.10	5/3358 (0.1%)
1	14-A	0.96	4/2485 (0.2%)	1.15	16/3358 (0.5%)
1	14-B	0.97	3/2485 (0.1%)	1.11	12/3358 (0.4%)
1	15-A	0.94	4/2485 (0.2%)	1.12	11/3358 (0.3%)
1	15-B	0.99	3/2485 (0.1%)	1.17	13/3358 (0.4%)
1	16-A	0.98	3/2485 (0.1%)	1.09	7/3358 (0.2%)
1	16-B	0.99	1/2485 (0.0%)	1.17	12/3358 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.85	64/79520 (0.1%)	0.97	142/107456 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-B	0	2
1	2-A	0	1
1	3-A	0	2
1	4-A	0	1
1	5-A	0	1
1	6-A	0	1
1	7-A	0	2
1	7-B	0	1
1	8-B	0	1
1	9-B	0	1
1	10-A	0	1
1	10-B	0	2
1	11-A	0	1
1	11-B	0	1
1	12-A	0	1
1	13-A	0	3
1	13-B	0	2
1	14-A	0	3
1	14-B	0	1
1	15-A	0	4
1	15-B	0	4
1	16-A	0	4
1	16-B	0	3
All	All	0	43

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	13-B	61	CYS	CB-SG	10.16	1.99	1.82
1	14-B	67	CYS	CB-SG	9.39	1.98	1.82
1	12-B	276	CYS	CB-SG	8.85	1.97	1.82
1	11-A	61	CYS	CB-SG	-8.18	1.68	1.82
1	9-A	76	GLU	CB-CG	7.93	1.67	1.52
1	4-B	276	CYS	CB-SG	7.88	1.95	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	15-A	145	THR	C-O	7.42	1.37	1.23
1	5-A	61	CYS	CB-SG	-7.31	1.69	1.82
1	4-A	76	GLU	CG-CD	7.24	1.62	1.51
1	14-A	251	ASP	CB-CG	7.14	1.66	1.51
1	2-A	129	GLU	CB-CG	7.12	1.65	1.52
1	7-B	67	CYS	CB-SG	-7.03	1.70	1.82
1	3-A	76	GLU	CB-CG	7.02	1.65	1.52
1	1-B	67	CYS	CB-SG	-6.98	1.70	1.82
1	5-B	67	CYS	CB-SG	-6.66	1.71	1.82
1	15-B	218	CYS	CB-SG	-6.61	1.71	1.82
1	13-A	81	LYS	CD-CE	6.61	1.67	1.51
1	10-A	218	CYS	CB-SG	-6.43	1.71	1.82
1	2-A	129	GLU	CG-CD	6.29	1.61	1.51
1	13-B	218	CYS	CB-SG	-6.26	1.71	1.82
1	4-A	76	GLU	CB-CG	6.23	1.64	1.52
1	3-A	76	GLU	CG-CD	6.18	1.61	1.51
1	14-A	124	CYS	CB-SG	6.17	1.92	1.82
1	3-A	81	LYS	CD-CE	6.17	1.66	1.51
1	5-B	139	MSE	CG-SE	6.14	2.16	1.95
1	14-B	218	CYS	CB-SG	-6.12	1.71	1.82
1	15-A	124	CYS	CB-SG	6.11	1.92	1.82
1	9-B	276	CYS	CB-SG	6.09	1.92	1.82
1	16-B	198	MSE	CG-SE	-6.03	1.75	1.95
1	3-A	218	CYS	CB-SG	6.03	1.92	1.82
1	2-B	81	LYS	CD-CE	5.84	1.65	1.51
1	14-A	117	ASN	CB-CG	5.80	1.64	1.51
1	15-A	95	GLU	CG-CD	5.80	1.60	1.51
1	14-B	223	TYR	CD1-CE1	5.72	1.48	1.39
1	16-A	61	CYS	CB-SG	5.62	1.91	1.82
1	1-A	76	GLU	CG-CD	5.61	1.60	1.51
1	16-A	145	THR	C-O	5.59	1.33	1.23
1	11-A	146	SER	C-O	5.54	1.33	1.23
1	6-A	104	ASP	CB-CG	-5.52	1.40	1.51
1	5-A	231	TYR	CB-CG	5.49	1.59	1.51
1	15-B	290	GLU	CG-CD	5.49	1.60	1.51
1	9-B	67	CYS	CB-SG	-5.48	1.72	1.81
1	8-B	81	LYS	CD-CE	5.45	1.64	1.51
1	8-A	146	SER	C-O	5.44	1.33	1.23
1	15-A	276	CYS	CB-SG	5.36	1.91	1.82
1	7-A	81	LYS	CD-CE	5.35	1.64	1.51
1	15-B	204	ASP	CB-CG	5.32	1.62	1.51
1	11-B	67	CYS	CB-SG	5.30	1.91	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16-A	84	GLU	CG-CD	5.29	1.59	1.51
1	13-A	61	CYS	CB-SG	5.24	1.91	1.82
1	6-B	114	ASP	CB-CG	5.22	1.62	1.51
1	7-B	81	LYS	CD-CE	5.21	1.64	1.51
1	8-B	104	ASP	CB-CG	5.19	1.62	1.51
1	2-A	139	MSE	CG-SE	-5.16	1.77	1.95
1	2-A	109	TYR	CE1-CZ	5.15	1.45	1.38
1	12-B	261	MSE	CG-SE	5.14	2.12	1.95
1	6-B	40	GLU	CB-CG	5.13	1.61	1.52
1	12-B	114	ASP	CB-CG	5.12	1.62	1.51
1	1-B	82	MSE	CG-SE	5.10	2.12	1.95
1	3-A	61	CYS	CB-SG	-5.08	1.73	1.81
1	14-A	285	GLU	CG-CD	5.07	1.59	1.51
1	2-A	109	TYR	CD2-CE2	5.06	1.47	1.39
1	12-A	109	TYR	CE1-CZ	5.06	1.45	1.38
1	5-B	195	MSE	CG-SE	5.05	2.12	1.95

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	14-B	168	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	14-B	168	ARG	NE-CZ-NH1	9.81	125.21	120.30
1	9-B	168	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	5-B	196	ARG	NE-CZ-NH1	9.41	125.00	120.30
1	16-B	198	MSE	CB-CG-SE	-9.21	85.08	112.70
1	14-A	251	ASP	CB-CG-OD1	9.20	126.58	118.30
1	15-B	56	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	15-B	56	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	2-A	265	LEU	CA-CB-CG	8.34	134.47	115.30
1	9-B	168	ARG	NE-CZ-NH1	7.95	124.27	120.30
1	8-B	148	ALA	C-N-CD	-7.86	103.30	120.60
1	3-A	147	LEU	CA-CB-CG	7.53	132.62	115.30
1	16-A	228	LYS	N-CA-C	-7.32	91.25	111.00
1	11-B	56	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	8-A	66	ASP	CB-CG-OD1	7.27	124.84	118.30
1	14-A	114	ASP	CB-CG-OD1	7.26	124.83	118.30
1	11-B	56	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	8-A	61	CYS	CA-CB-SG	-7.17	101.10	114.00
1	14-A	204	ASP	CB-CG-OD1	7.09	124.68	118.30
1	15-A	200	LYS	CD-CE-NZ	7.03	127.86	111.70
1	4-A	228	LYS	N-CA-C	-6.95	92.23	111.00
1	16-B	182	GLN	N-CA-C	-6.88	92.44	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5-A	272	LEU	N-CA-C	6.81	129.39	111.00
1	14-A	261	MSE	CB-CG-SE	-6.74	92.47	112.70
1	13-B	148	ALA	C-N-CD	-6.73	105.80	120.60
1	13-A	190	ASP	CB-CG-OD1	6.61	124.25	118.30
1	6-B	56	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	7-A	267	GLY	N-CA-C	6.47	129.28	113.10
1	16-A	231	TYR	N-CA-C	-6.40	93.72	111.00
1	6-A	103	LYS	CD-CE-NZ	6.37	126.35	111.70
1	13-A	204	ASP	N-CA-C	-6.36	93.84	111.00
1	12-A	80	LYS	CD-CE-NZ	6.31	126.22	111.70
1	13-A	81	LYS	CD-CE-NZ	6.31	126.21	111.70
1	14-A	25	LEU	N-CA-C	6.25	127.86	111.00
1	14-A	114	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	1-B	82	MSE	CB-CG-SE	6.22	131.35	112.70
1	16-B	310	CYS	N-CA-C	-6.15	94.39	111.00
1	14-B	251	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	16-A	82	MSE	CB-CG-SE	6.13	131.09	112.70
1	11-A	261	MSE	CB-CG-SE	-6.09	94.43	112.70
1	9-A	231	TYR	N-CA-C	-6.06	94.63	111.00
1	15-A	112	ILE	CB-CA-C	-6.01	99.57	111.60
1	15-B	182	GLN	N-CA-C	-6.01	94.76	111.00
1	2-A	267	GLY	N-CA-C	5.99	128.08	113.10
1	14-A	261	MSE	N-CA-C	5.98	127.15	111.00
1	12-A	114	ASP	CB-CG-OD1	5.95	123.66	118.30
1	2-A	82	MSE	CB-CG-SE	5.92	130.46	112.70
1	15-B	95	GLU	N-CA-C	-5.91	95.04	111.00
1	11-A	146	SER	C-N-CA	5.91	136.47	121.70
1	8-B	81	LYS	CD-CE-NZ	5.88	125.24	111.70
1	15-A	145	THR	CA-C-N	-5.87	104.29	117.20
1	16-B	251	ASP	CB-CG-OD1	5.86	123.58	118.30
1	16-B	251	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	12-A	146	SER	N-CA-CB	-5.84	101.74	110.50
1	4-B	198	MSE	CB-CG-SE	-5.82	95.24	112.70
1	16-A	56	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	14-A	118	THR	N-CA-C	5.79	126.65	111.00
1	14-B	182	GLN	N-CA-C	-5.78	95.40	111.00
1	8-A	103	LYS	CD-CE-NZ	5.76	124.95	111.70
1	14-A	188	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	15-A	114	ASP	CB-CG-OD1	5.75	123.47	118.30
1	13-B	60	LYS	N-CA-C	-5.73	95.53	111.00
1	8-A	265	LEU	CA-CB-CG	5.70	128.40	115.30
1	3-A	148	ALA	N-CA-C	-5.69	95.63	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	14-A	67	CYS	CA-CB-SG	-5.68	103.77	114.00
1	2-B	81	LYS	CD-CE-NZ	5.67	124.75	111.70
1	14-B	251	ASP	CB-CG-OD1	5.65	123.38	118.30
1	3-B	152	CYS	N-CA-C	-5.63	95.79	111.00
1	14-B	68	ASP	N-CA-C	-5.61	95.85	111.00
1	15-B	90	VAL	N-CA-C	-5.60	95.89	111.00
1	15-B	249	ASP	CB-CG-OD2	5.58	123.32	118.30
1	3-A	272	LEU	N-CA-C	5.55	125.99	111.00
1	11-A	146	SER	CA-C-N	-5.55	105.00	117.20
1	12-B	261	MSE	CB-CG-SE	5.54	129.32	112.70
1	15-B	303	LEU	CA-CB-CG	5.51	127.98	115.30
1	16-B	301	LEU	CA-CB-CG	5.50	127.94	115.30
1	1-B	212	GLY	N-CA-C	5.49	126.82	113.10
1	16-B	127	ILE	CB-CA-C	-5.48	100.63	111.60
1	7-B	212	GLY	N-CA-C	5.47	126.77	113.10
1	14-B	251	ASP	N-CA-C	-5.47	96.23	111.00
1	16-B	72	ILE	N-CA-C	5.47	125.76	111.00
1	8-A	251	ASP	CB-CG-OD1	5.47	123.22	118.30
1	8-B	61	CYS	N-CA-C	5.45	125.70	111.00
1	15-A	26	THR	N-CA-CB	5.43	120.61	110.30
1	3-A	67	CYS	CA-CB-SG	-5.41	104.27	114.00
1	7-A	81	LYS	CD-CE-NZ	5.39	124.11	111.70
1	15-B	53	THR	N-CA-C	5.39	125.56	111.00
1	6-B	56	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	5-B	195	MSE	CB-CG-SE	5.38	128.83	112.70
1	13-A	69	LEU	CA-CB-CG	5.38	127.67	115.30
1	11-A	147	LEU	CB-CG-CD1	-5.38	101.86	111.00
1	3-A	81	LYS	CD-CE-NZ	5.37	124.06	111.70
1	15-B	24	GLU	N-CA-C	-5.36	96.53	111.00
1	13-B	182	GLN	N-CA-C	-5.35	96.55	111.00
1	15-A	80	LYS	N-CA-C	5.35	125.45	111.00
1	11-A	146	SER	O-C-N	5.34	131.25	122.70
1	15-A	25	LEU	N-CA-C	5.34	125.41	111.00
1	14-B	35	LEU	CB-CG-CD1	-5.33	101.94	111.00
1	4-A	46	LEU	N-CA-C	-5.33	96.61	111.00
1	7-A	190	ASP	CB-CG-OD2	5.32	123.09	118.30
1	14-A	112	ILE	CB-CA-C	-5.32	100.97	111.60
1	12-A	53	THR	N-CA-C	5.29	125.28	111.00
1	14-A	259	ASP	CB-CG-OD1	5.29	123.06	118.30
1	15-B	63	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	15-B	61	CYS	N-CA-C	-5.26	96.78	111.00
1	1-A	25	LEU	N-CA-C	5.26	125.19	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	15-B	301	LEU	CA-CB-CG	5.24	127.36	115.30
1	8-B	148	ALA	C-N-CA	5.23	143.96	122.00
1	13-B	56	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	8-A	160	PRO	N-CA-C	-5.23	98.51	112.10
1	16-A	25	LEU	N-CA-C	5.22	125.08	111.00
1	13-A	182	GLN	N-CA-C	-5.21	96.94	111.00
1	8-A	251	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	14-B	56	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	14-A	247	LEU	CA-CB-CG	5.18	127.20	115.30
1	16-B	233	ARG	N-CA-C	-5.17	97.03	111.00
1	13-B	251	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	9-B	152	CYS	N-CA-C	-5.16	97.07	111.00
1	16-A	150	LEU	CA-CB-CG	5.15	127.16	115.30
1	8-A	62	THR	N-CA-C	-5.15	97.09	111.00
1	16-A	171	ALA	N-CA-C	5.13	124.85	111.00
1	14-A	168	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	16-B	130	ASP	CB-CG-OD2	5.12	122.91	118.30
1	14-A	204	ASP	N-CA-C	-5.11	97.20	111.00
1	5-B	139	MSE	CB-CG-SE	5.09	127.97	112.70
1	14-B	24	GLU	N-CA-C	-5.09	97.25	111.00
1	14-B	176	GLY	N-CA-C	-5.09	100.38	113.10
1	2-B	22	GLY	N-CA-C	5.08	125.81	113.10
1	1-A	82	MSE	N-CA-C	5.07	124.69	111.00
1	16-B	251	ASP	N-CA-C	-5.07	97.31	111.00
1	8-A	25	LEU	N-CA-C	5.07	124.69	111.00
1	14-A	240	ALA	N-CA-C	5.06	124.67	111.00
1	13-A	74	ASP	CB-CG-OD1	5.06	122.85	118.30
1	15-A	125	THR	N-CA-C	5.04	124.61	111.00
1	15-A	72	ILE	CG1-CB-CG2	-5.04	100.32	111.40
1	14-B	63	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	16-B	25	LEU	N-CA-C	5.03	124.57	111.00
1	15-A	147	LEU	CA-CB-CG	5.02	126.84	115.30
1	15-A	78	LEU	N-CA-C	-5.01	97.48	111.00
1	15-B	267	GLY	N-CA-C	5.01	125.63	113.10
1	7-B	270	ILE	N-CA-C	-5.00	97.49	111.00
1	10-B	152	CYS	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-B	164	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	1-B	231	TYR	Sidechain
1	10-A	289	TYR	Sidechain
1	10-B	223	TYR	Sidechain
1	10-B	289	TYR	Sidechain
1	11-A	164	TYR	Sidechain
1	11-B	64	TYR	Sidechain
1	12-A	164	TYR	Sidechain
1	13-A	164	TYR	Sidechain
1	13-A	231	TYR	Sidechain
1	13-A	289	TYR	Sidechain
1	13-B	109	TYR	Sidechain
1	13-B	155	TYR	Sidechain
1	14-A	109	TYR	Sidechain
1	14-A	153	TYR	Sidechain
1	14-A	164	TYR	Sidechain
1	14-B	64	TYR	Sidechain
1	15-A	142	TYR	Sidechain
1	15-A	164	TYR	Sidechain
1	15-A	231	TYR	Sidechain
1	15-A	88	TYR	Sidechain
1	15-B	155	TYR	Sidechain
1	15-B	164	TYR	Sidechain
1	15-B	64	TYR	Sidechain
1	15-B	88	TYR	Sidechain
1	16-A	153	TYR	Sidechain
1	16-A	164	TYR	Sidechain
1	16-A	289	TYR	Sidechain
1	16-A	88	TYR	Sidechain
1	16-B	173	TYR	Sidechain
1	16-B	279	TYR	Sidechain
1	16-B	88	TYR	Sidechain
1	2-A	164	TYR	Sidechain
1	3-A	164	TYR	Sidechain
1	3-A	173	TYR	Sidechain
1	4-A	164	TYR	Sidechain
1	5-A	164	TYR	Sidechain
1	6-A	164	TYR	Sidechain
1	7-A	164	TYR	Sidechain
1	7-A	289	TYR	Sidechain
1	7-B	164	TYR	Sidechain
1	8-B	231	TYR	Sidechain
1	9-B	109	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	2430	0	2414	0	0
1	1-B	2430	0	2414	0	0
1	2-A	2430	0	2414	0	0
1	2-B	2430	0	2414	0	0
1	3-A	2430	0	2414	0	0
1	3-B	2430	0	2414	0	0
1	4-A	2430	0	2414	0	0
1	4-B	2430	0	2414	0	0
1	5-A	2430	0	2414	0	0
1	5-B	2430	0	2414	0	0
1	6-A	2430	0	2414	0	0
1	6-B	2430	0	2414	0	0
1	7-A	2430	0	2414	0	0
1	7-B	2430	0	2414	0	0
1	8-A	2430	0	2414	0	0
1	8-B	2430	0	2414	0	0
1	9-A	2430	0	2414	0	0
1	9-B	2430	0	2414	0	0
1	10-A	2430	0	2414	0	0
1	10-B	2430	0	2414	0	0
1	11-A	2430	0	2414	0	0
1	11-B	2430	0	2414	0	0
1	12-A	2430	0	2414	0	0
1	12-B	2430	0	2414	0	0
1	13-A	2430	0	2414	0	0
1	13-B	2430	0	2414	0	0
1	14-A	2430	0	2414	0	0
1	14-B	2430	0	2414	0	0
1	15-A	2430	0	2414	0	0
1	15-B	2430	0	2414	0	0
1	16-A	2430	0	2414	0	0
1	16-B	2430	0	2414	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	20	0	0	0	0
3	1-B	20	0	0	0	0
3	2-A	20	0	0	0	0
3	2-B	20	0	0	0	0
3	3-A	20	0	0	0	0
3	3-B	20	0	0	0	0
3	4-A	20	0	0	0	0
3	4-B	20	0	0	0	0
3	5-A	20	0	0	0	0
3	5-B	20	0	0	0	0
3	6-A	20	0	0	0	0
3	6-B	20	0	0	0	0
3	7-A	20	0	0	0	0
3	7-B	20	0	0	0	0
3	8-A	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	8-B	20	0	0	0	0
3	9-A	20	0	0	0	0
3	9-B	20	0	0	0	0
3	10-A	20	0	0	0	0
3	10-B	20	0	0	0	0
3	11-A	20	0	0	0	0
3	11-B	20	0	0	0	0
3	12-A	20	0	0	0	0
3	12-B	20	0	0	0	0
3	13-A	20	0	0	0	0
3	13-B	20	0	0	0	0
3	14-A	20	0	0	0	0
3	14-B	20	0	0	0	0
3	15-A	20	0	0	0	0
3	15-B	20	0	0	0	0
3	16-A	20	0	0	0	0
3	16-B	20	0	0	0	0
4	1-A	13	0	0	0	0
4	1-B	23	0	0	0	0
4	2-A	14	0	0	0	0
4	2-B	22	0	0	0	0
4	3-A	13	0	0	0	0
4	3-B	23	0	0	0	0
4	4-A	13	0	0	0	0
4	4-B	23	0	0	0	0
4	5-A	14	0	0	0	0
4	5-B	22	0	0	0	0
4	6-A	14	0	0	0	0
4	6-B	22	0	0	0	0
4	7-A	14	0	0	0	0
4	7-B	22	0	0	0	0
4	8-A	14	0	0	0	0
4	8-B	22	0	0	0	0
4	9-A	14	0	0	0	0
4	9-B	22	0	0	0	0
4	10-A	14	0	0	0	0
4	10-B	22	0	0	0	0
4	11-A	14	0	0	0	0
4	11-B	22	0	0	0	0
4	12-A	14	0	0	0	0
4	12-B	22	0	0	0	0
4	13-A	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	13-B	22	0	0	0	0
4	14-A	14	0	0	0	0
4	14-B	22	0	0	0	0
4	15-A	13	0	0	0	0
4	15-B	23	0	0	0	0
4	16-A	13	0	0	0	0
4	16-B	23	0	0	0	0
All	All	79008	0	77248	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	300/315 (95%)	209 (70%)	61 (20%)	30 (10%)	0 1
1	1-B	300/315 (95%)	243 (81%)	43 (14%)	14 (5%)	2 7
1	2-A	300/315 (95%)	248 (83%)	37 (12%)	15 (5%)	2 6
1	2-B	300/315 (95%)	264 (88%)	31 (10%)	5 (2%)	9 29
1	3-A	300/315 (95%)	239 (80%)	45 (15%)	16 (5%)	2 6
1	3-B	300/315 (95%)	249 (83%)	36 (12%)	15 (5%)	2 6
1	4-A	300/315 (95%)	237 (79%)	46 (15%)	17 (6%)	1 5
1	4-B	300/315 (95%)	242 (81%)	46 (15%)	12 (4%)	3 9
1	5-A	300/315 (95%)	252 (84%)	34 (11%)	14 (5%)	2 7
1	5-B	300/315 (95%)	239 (80%)	42 (14%)	19 (6%)	1 3
1	6-A	300/315 (95%)	240 (80%)	51 (17%)	9 (3%)	4 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	6-B	300/315 (95%)	240 (80%)	43 (14%)	17 (6%)	1	5
1	7-A	300/315 (95%)	239 (80%)	48 (16%)	13 (4%)	2	8
1	7-B	300/315 (95%)	245 (82%)	34 (11%)	21 (7%)	1	3
1	8-A	300/315 (95%)	232 (77%)	47 (16%)	21 (7%)	1	3
1	8-B	300/315 (95%)	237 (79%)	49 (16%)	14 (5%)	2	7
1	9-A	300/315 (95%)	260 (87%)	29 (10%)	11 (4%)	3	11
1	9-B	300/315 (95%)	245 (82%)	37 (12%)	18 (6%)	1	4
1	10-A	300/315 (95%)	248 (83%)	35 (12%)	17 (6%)	1	5
1	10-B	300/315 (95%)	233 (78%)	46 (15%)	21 (7%)	1	3
1	11-A	300/315 (95%)	250 (83%)	36 (12%)	14 (5%)	2	7
1	11-B	300/315 (95%)	238 (79%)	43 (14%)	19 (6%)	1	3
1	12-A	300/315 (95%)	221 (74%)	55 (18%)	24 (8%)	1	2
1	12-B	300/315 (95%)	251 (84%)	34 (11%)	15 (5%)	2	6
1	13-A	300/315 (95%)	219 (73%)	53 (18%)	28 (9%)	0	1
1	13-B	300/315 (95%)	245 (82%)	39 (13%)	16 (5%)	2	6
1	14-A	300/315 (95%)	211 (70%)	50 (17%)	39 (13%)	0	1
1	14-B	300/315 (95%)	224 (75%)	55 (18%)	21 (7%)	1	3
1	15-A	300/315 (95%)	226 (75%)	51 (17%)	23 (8%)	1	2
1	15-B	300/315 (95%)	224 (75%)	46 (15%)	30 (10%)	0	1
1	16-A	300/315 (95%)	214 (71%)	54 (18%)	32 (11%)	0	1
1	16-B	300/315 (95%)	219 (73%)	56 (19%)	25 (8%)	1	2
All	All	9600/10080 (95%)	7583 (79%)	1412 (15%)	605 (6%)	1	3

All (605) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	12	GLN
1	1-A	76	GLU
1	1-A	109	TYR
1	1-A	162	LEU
1	1-A	217	PRO
1	1-A	234	ASP
1	1-A	236	ASN
1	1-A	287	ALA
1	1-A	288	TYR

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Mol	Chain	Res	Type
1	1-B	61	CYS
1	1-B	104	ASP
1	1-B	133	ASN
1	1-B	292	LYS
1	1-B	293	GLU
1	2-A	40	GLU
1	2-A	213	LYS
1	2-A	272	LEU
1	2-B	70	ASN
1	3-A	82	MSE
1	3-A	108	SER
1	3-B	10	HIS
1	3-B	70	ASN
1	3-B	103	LYS
1	3-B	236	ASN
1	3-B	291	LYS
1	3-B	292	LYS
1	3-B	293	GLU
1	4-A	162	LEU
1	4-A	272	LEU
1	4-B	166	THR
1	4-B	272	LEU
1	5-A	70	ASN
1	5-A	234	ASP
1	5-B	37	ASN
1	5-B	64	TYR
1	5-B	275	ASP
1	6-A	63	ARG
1	6-A	88	TYR
1	6-A	162	LEU
1	6-A	235	GLU
1	6-B	39	ALA
1	6-B	40	GLU
1	6-B	56	ARG
1	6-B	60	LYS
1	6-B	260	PRO
1	6-B	261	MSE
1	6-B	292	LYS
1	6-B	293	GLU
1	7-A	39	ALA
1	7-A	40	GLU
1	7-A	238	GLU

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Mol	Chain	Res	Type
1	7-B	25	LEU
1	7-B	93	ALA
1	7-B	233	ARG
1	8-A	67	CYS
1	8-A	68	ASP
1	8-A	133	ASN
1	8-A	238	GLU
1	8-A	257	PRO
1	8-A	292	LYS
1	8-B	40	GLU
1	8-B	61	CYS
1	8-B	76	GLU
1	8-B	104	ASP
1	9-A	214	GLU
1	9-A	239	ILE
1	9-A	292	LYS
1	9-B	10	HIS
1	9-B	61	CYS
1	9-B	67	CYS
1	9-B	110	ASP
1	9-B	166	THR
1	9-B	234	ASP
1	9-B	291	LYS
1	9-B	292	LYS
1	10-A	131	SER
1	10-A	185	GLY
1	10-B	37	ASN
1	10-B	40	GLU
1	10-B	133	ASN
1	10-B	170	ILE
1	10-B	275	ASP
1	10-B	292	LYS
1	10-B	293	GLU
1	11-A	145	THR
1	11-A	261	MSE
1	11-B	56	ARG
1	11-B	108	SER
1	11-B	232	PRO
1	11-B	291	LYS
1	12-A	26	THR
1	12-A	63	ARG
1	12-A	106	GLU

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Mol	Chain	Res	Type
1	12-A	149	PRO
1	12-A	192	LEU
1	12-A	202	ALA
1	12-A	292	LYS
1	12-B	37	ASN
1	13-A	63	ARG
1	13-A	70	ASN
1	13-A	108	SER
1	13-A	131	SER
1	13-A	167	THR
1	13-A	191	ILE
1	13-A	192	LEU
1	13-A	229	VAL
1	13-A	259	ASP
1	13-A	287	ALA
1	13-A	288	TYR
1	13-B	217	PRO
1	13-B	218	CYS
1	13-B	285	GLU
1	13-B	286	ALA
1	13-B	288	TYR
1	14-A	10	HIS
1	14-A	68	ASP
1	14-A	84	GLU
1	14-A	97	ASN
1	14-A	167	THR
1	14-A	234	ASP
1	14-A	257	PRO
1	14-A	273	GLY
1	14-A	276	CYS
1	14-A	288	TYR
1	14-A	294	ALA
1	14-B	64	TYR
1	14-B	69	LEU
1	14-B	130	ASP
1	14-B	133	ASN
1	14-B	145	THR
1	14-B	166	THR
1	14-B	272	LEU
1	15-A	10	HIS
1	15-A	80	LYS
1	15-A	108	SER

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Mol	Chain	Res	Type
1	15-A	131	SER
1	15-A	167	THR
1	15-A	275	ASP
1	15-A	292	LYS
1	15-A	295	PHE
1	15-B	56	ARG
1	15-B	64	TYR
1	15-B	98	HIS
1	15-B	122	MSE
1	15-B	272	LEU
1	15-B	290	GLU
1	15-B	309	ARG
1	16-A	37	ASN
1	16-A	39	ALA
1	16-A	86	LEU
1	16-A	109	TYR
1	16-A	145	THR
1	16-A	169	SER
1	16-A	239	ILE
1	16-A	259	ASP
1	16-A	272	LEU
1	16-B	84	GLU
1	16-B	86	LEU
1	16-B	88	TYR
1	16-B	239	ILE
1	16-B	260	PRO
1	16-B	261	MSE
1	16-B	291	LYS
1	16-B	292	LYS
1	16-B	306	LYS
1	1-A	29	PHE
1	1-A	38	GLY
1	1-A	63	ARG
1	1-A	75	LEU
1	1-A	84	GLU
1	1-A	90	VAL
1	1-A	91	ARG
1	1-A	199	ILE
1	1-B	135	PHE
1	1-B	240	ALA
1	2-A	39	ALA
1	2-A	109	TYR

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Mol	Chain	Res	Type
1	2-A	160	PRO
1	3-A	78	LEU
1	3-A	133	ASN
1	3-A	152	CYS
1	3-A	235	GLU
1	3-A	294	ALA
1	3-B	166	THR
1	3-B	232	PRO
1	4-A	11	ILE
1	4-A	61	CYS
1	4-A	73	PHE
1	4-A	212	GLY
1	4-A	243	ILE
1	4-A	292	LYS
1	4-A	306	LYS
1	4-B	41	ILE
1	4-B	74	ASP
1	4-B	84	GLU
1	4-B	104	ASP
1	4-B	291	LYS
1	5-A	131	SER
1	5-A	210	ASN
1	5-A	291	LYS
1	5-A	292	LYS
1	5-A	295	PHE
1	5-B	60	LYS
1	5-B	233	ARG
1	5-B	257	PRO
1	5-B	274	GLY
1	5-B	288	TYR
1	5-B	292	LYS
1	5-B	306	LYS
1	6-A	292	LYS
1	6-B	11	ILE
1	6-B	22	GLY
1	6-B	76	GLU
1	6-B	291	LYS
1	7-A	134	ASN
1	7-A	234	ASP
1	7-A	271	PRO
1	7-A	293	GLU
1	7-B	22	GLY

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Mol	Chain	Res	Type
1	7-B	67	CYS
1	7-B	68	ASP
1	7-B	74	ASP
1	7-B	234	ASP
1	7-B	237	GLY
1	7-B	276	CYS
1	7-B	290	GLU
1	8-A	13	LYS
1	8-A	110	ASP
1	8-A	252	TRP
1	8-B	146	SER
1	8-B	272	LEU
1	9-A	162	LEU
1	9-A	256	HIS
1	9-A	273	GLY
1	9-B	44	THR
1	9-B	133	ASN
1	9-B	290	GLU
1	10-A	61	CYS
1	10-A	97	ASN
1	10-A	272	LEU
1	10-A	273	GLY
1	10-A	293	GLU
1	10-B	39	ALA
1	10-B	70	ASN
1	10-B	227	GLU
1	10-B	288	TYR
1	11-A	10	HIS
1	11-A	106	GLU
1	11-A	131	SER
1	11-A	147	LEU
1	11-A	292	LYS
1	11-B	64	TYR
1	11-B	123	GLY
1	11-B	210	ASN
1	11-B	257	PRO
1	11-B	261	MSE
1	12-A	58	VAL
1	12-A	109	TYR
1	12-A	135	PHE
1	12-A	146	SER
1	12-A	191	ILE

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Mol	Chain	Res	Type
1	12-A	212	GLY
1	12-A	273	GLY
1	12-B	84	GLU
1	12-B	88	TYR
1	12-B	133	ASN
1	12-B	290	GLU
1	13-A	152	CYS
1	13-A	190	ASP
1	13-A	227	GLU
1	13-A	237	GLY
1	13-A	265	LEU
1	13-A	283	VAL
1	13-A	307	SER
1	13-B	35	LEU
1	13-B	61	CYS
1	13-B	243	ILE
1	14-A	61	CYS
1	14-A	94	GLN
1	14-A	106	GLU
1	14-A	237	GLY
1	14-A	252	TRP
1	14-A	261	MSE
1	14-A	271	PRO
1	14-A	287	ALA
1	14-B	229	VAL
1	15-A	61	CYS
1	15-A	65	ILE
1	15-A	70	ASN
1	15-A	146	SER
1	15-B	63	ARG
1	15-B	97	ASN
1	15-B	108	SER
1	15-B	217	PRO
1	15-B	237	GLY
1	15-B	257	PRO
1	15-B	280	PRO
1	16-A	12	GLN
1	16-A	22	GLY
1	16-A	61	CYS
1	16-A	122	MSE
1	16-A	123	GLY
1	16-A	144	LYS

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Mol	Chain	Res	Type
1	16-A	158	GLU
1	16-A	293	GLU
1	16-A	306	LYS
1	16-B	63	ARG
1	16-B	145	THR
1	16-B	246	ASN
1	16-B	273	GLY
1	1-A	30	LEU
1	1-A	82	MSE
1	1-A	86	LEU
1	1-A	134	ASN
1	1-B	64	TYR
1	1-B	148	ALA
1	1-B	183	PRO
1	2-A	94	GLN
1	2-A	257	PRO
1	2-B	88	TYR
1	3-A	29	PHE
1	3-A	40	GLU
1	3-A	66	ASP
1	3-A	88	TYR
1	3-A	272	LEU
1	3-B	22	GLY
1	3-B	104	ASP
1	3-B	284	ASN
1	4-B	275	ASP
1	5-A	69	LEU
1	5-A	209	PHE
1	5-B	284	ASN
1	5-B	291	LYS
1	6-B	108	SER
1	6-B	259	ASP
1	7-A	292	LYS
1	7-A	306	LYS
1	7-B	77	ASN
1	7-B	80	LYS
1	8-A	46	LEU
1	8-A	61	CYS
1	8-A	104	ASP
1	8-A	145	THR
1	8-A	250	GLN
1	8-B	35	LEU

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Mol	Chain	Res	Type
1	8-B	98	HIS
1	8-B	145	THR
1	8-B	237	GLY
1	9-A	26	THR
1	9-A	295	PHE
1	9-B	98	HIS
1	9-B	284	ASN
1	9-B	295	PHE
1	10-A	73	PHE
1	10-A	109	TYR
1	10-A	184	GLN
1	10-A	292	LYS
1	10-B	107	ASP
1	10-B	146	SER
1	11-A	257	PRO
1	11-B	231	TYR
1	11-B	236	ASN
1	12-A	46	LEU
1	12-A	61	CYS
1	12-A	88	TYR
1	12-A	152	CYS
1	12-B	108	SER
1	12-B	130	ASP
1	12-B	200	LYS
1	12-B	227	GLU
1	12-B	292	LYS
1	13-A	10	HIS
1	13-A	69	LEU
1	13-A	169	SER
1	13-B	87	PRO
1	13-B	216	PRO
1	13-B	249	ASP
1	14-A	67	CYS
1	14-A	99	LEU
1	14-A	104	ASP
1	14-A	124	CYS
1	14-A	169	SER
1	14-A	205	PHE
1	14-A	218	CYS
1	14-A	249	ASP
1	14-A	250	GLN
1	14-A	275	ASP

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Mol	Chain	Res	Type
1	14-A	298	THR
1	14-A	299	THR
1	14-B	35	LEU
1	14-B	63	ARG
1	15-A	88	TYR
1	15-A	169	SER
1	15-A	254	PRO
1	15-A	263	LEU
1	15-A	265	LEU
1	15-A	276	CYS
1	15-B	103	LYS
1	15-B	133	ASN
1	15-B	218	CYS
1	15-B	249	ASP
1	16-A	146	SER
1	16-A	170	ILE
1	16-B	169	SER
1	16-B	293	GLU
1	16-B	307	SER
1	1-A	61	CYS
1	1-A	135	PHE
1	1-A	136	LEU
1	1-A	246	ASN
1	1-B	205	PHE
1	1-B	237	GLY
1	2-A	10	HIS
1	2-A	192	LEU
1	2-B	306	LYS
1	3-A	13	LYS
1	3-B	290	GLU
1	4-A	12	GLN
1	4-A	35	LEU
1	4-A	161	SER
1	4-A	181	PRO
1	4-A	295	PHE
1	4-B	63	ARG
1	4-B	108	SER
1	5-A	227	GLU
1	5-B	70	ASN
1	5-B	86	LEU
1	6-A	59	LYS
1	6-A	73	PHE

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Mol	Chain	Res	Type
1	6-A	161	SER
1	7-A	135	PHE
1	7-A	259	ASP
1	7-B	133	ASN
1	8-A	23	ASN
1	8-A	135	PHE
1	8-B	39	ALA
1	8-B	287	ALA
1	9-A	151	PRO
1	9-B	84	GLU
1	10-A	88	TYR
1	10-A	243	ILE
1	11-A	12	GLN
1	11-A	61	CYS
1	11-A	146	SER
1	11-A	243	ILE
1	11-A	293	GLU
1	11-B	122	MSE
1	12-B	103	LYS
1	12-B	266	ASP
1	13-A	88	TYR
1	13-B	63	ARG
1	13-B	169	SER
1	13-B	268	LYS
1	14-A	260	PRO
1	14-B	135	PHE
1	14-B	169	SER
1	14-B	232	PRO
1	14-B	249	ASP
1	15-A	266	ASP
1	15-B	44	THR
1	15-B	148	ALA
1	15-B	169	SER
1	15-B	231	TYR
1	15-B	276	CYS
1	16-A	104	ASP
1	16-A	174	PRO
1	16-A	236	ASN
1	16-A	275	ASP
1	16-A	301	LEU
1	16-B	146	SER
1	16-B	210	ASN

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Mol	Chain	Res	Type
1	16-B	229	VAL
1	16-B	259	ASP
1	1-A	239	ILE
1	2-A	104	ASP
1	2-A	145	THR
1	3-A	67	CYS
1	3-B	266	ASP
1	4-A	98	HIS
1	4-A	134	ASN
1	4-A	230	ASP
1	4-B	46	LEU
1	5-A	41	ILE
1	5-A	200	LYS
1	5-B	232	PRO
1	6-A	51	PHE
1	6-B	41	ILE
1	6-B	55	PRO
1	7-A	88	TYR
1	7-A	190	ASP
1	7-B	61	CYS
1	7-B	70	ASN
1	7-B	130	ASP
1	7-B	212	GLY
1	7-B	280	PRO
1	8-B	50	PRO
1	9-B	83	SER
1	9-B	294	ALA
1	10-A	217	PRO
1	10-B	69	LEU
1	10-B	106	GLU
1	10-B	131	SER
1	10-B	132	ARG
1	10-B	135	PHE
1	11-B	55	PRO
1	11-B	104	ASP
1	11-B	133	ASN
1	11-B	227	GLU
1	11-B	237	GLY
1	12-A	197	LYS
1	12-A	227	GLU
1	12-A	274	GLY
1	12-B	63	ARG

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Mol	Chain	Res	Type
1	13-A	209	PHE
1	13-B	206	ILE
1	13-B	266	ASP
1	14-A	44	THR
1	14-A	51	PHE
1	14-A	73	PHE
1	14-A	86	LEU
1	14-A	251	ASP
1	14-B	37	ASN
1	14-B	252	TRP
1	14-B	275	ASP
1	14-B	284	ASN
1	14-B	309	ARG
1	15-B	55	PRO
1	15-B	216	PRO
1	15-B	287	ALA
1	15-B	302	THR
1	16-A	11	ILE
1	16-A	65	ILE
1	16-A	162	LEU
1	16-A	266	ASP
1	16-B	131	SER
1	16-B	245	PRO
1	16-B	290	GLU
1	1-A	35	LEU
1	1-B	136	LEU
1	1-B	212	GLY
1	2-B	63	ARG
1	3-A	304	ASN
1	4-B	83	SER
1	5-A	78	LEU
1	5-B	65	ILE
1	5-B	200	LYS
1	6-B	88	TYR
1	7-B	200	LYS
1	8-A	79	GLY
1	8-A	146	SER
1	9-B	161	SER
1	10-A	62	THR
1	10-A	309	ARG
1	10-B	104	ASP
1	12-A	295	PHE

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Mol	Chain	Res	Type
1	13-A	28	VAL
1	13-A	61	CYS
1	14-B	75	LEU
1	15-A	79	GLY
1	15-B	130	ASP
1	16-A	258	GLY
1	16-B	216	PRO
1	16-B	252	TRP
1	2-A	191	ILE
1	3-A	86	LEU
1	7-B	41	ILE
1	10-B	55	PRO
1	11-A	237	GLY
1	12-A	254	PRO
1	15-A	237	GLY
1	16-A	79	GLY
1	1-A	41	ILE
1	1-A	220	ILE
1	2-A	220	ILE
1	2-A	239	ILE
1	5-A	257	PRO
1	5-B	41	ILE
1	8-A	271	PRO
1	9-A	143	ILE
1	10-B	239	ILE
1	12-A	160	PRO
1	15-A	225	ILE
1	15-B	245	PRO
1	3-B	231	TYR
1	8-A	217	PRO
1	10-A	257	PRO
1	11-B	65	ILE
1	14-A	206	ILE
1	14-B	217	PRO
1	15-A	11	ILE
1	16-A	271	PRO
1	2-B	232	PRO
1	5-B	283	VAL
1	8-A	45	GLY
1	9-A	270	ILE
1	11-B	22	GLY
1	12-B	232	PRO

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Mol	Chain	Res	Type
1	12-B	280	PRO
1	13-A	45	GLY
1	13-A	65	ILE
1	14-A	216	PRO
1	15-B	102	PRO
1	13-A	181	PRO
1	8-B	149	PRO
1	1-A	181	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1-A	267/271 (98%)	232 (87%)	35 (13%)	4 12
1	1-B	267/271 (98%)	249 (93%)	18 (7%)	16 43
1	2-A	267/271 (98%)	245 (92%)	22 (8%)	11 33
1	2-B	267/271 (98%)	245 (92%)	22 (8%)	11 33
1	3-A	267/271 (98%)	253 (95%)	14 (5%)	23 55
1	3-B	267/271 (98%)	252 (94%)	15 (6%)	21 51
1	4-A	267/271 (98%)	251 (94%)	16 (6%)	19 48
1	4-B	267/271 (98%)	245 (92%)	22 (8%)	11 33
1	5-A	267/271 (98%)	246 (92%)	21 (8%)	12 34
1	5-B	267/271 (98%)	249 (93%)	18 (7%)	16 43
1	6-A	267/271 (98%)	244 (91%)	23 (9%)	10 30
1	6-B	267/271 (98%)	248 (93%)	19 (7%)	14 39
1	7-A	267/271 (98%)	254 (95%)	13 (5%)	25 57
1	7-B	267/271 (98%)	246 (92%)	21 (8%)	12 34
1	8-A	267/271 (98%)	245 (92%)	22 (8%)	11 33
1	8-B	267/271 (98%)	244 (91%)	23 (9%)	10 30
1	9-A	267/271 (98%)	250 (94%)	17 (6%)	17 45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	9-B	267/271 (98%)	249 (93%)	18 (7%)	16	43
1	10-A	267/271 (98%)	252 (94%)	15 (6%)	21	51
1	10-B	267/271 (98%)	240 (90%)	27 (10%)	7	22
1	11-A	267/271 (98%)	247 (92%)	20 (8%)	13	37
1	11-B	267/271 (98%)	247 (92%)	20 (8%)	13	37
1	12-A	267/271 (98%)	238 (89%)	29 (11%)	6	19
1	12-B	267/271 (98%)	243 (91%)	24 (9%)	9	28
1	13-A	267/271 (98%)	217 (81%)	50 (19%)	1	5
1	13-B	267/271 (98%)	232 (87%)	35 (13%)	4	12
1	14-A	267/271 (98%)	231 (86%)	36 (14%)	4	11
1	14-B	267/271 (98%)	234 (88%)	33 (12%)	4	14
1	15-A	267/271 (98%)	236 (88%)	31 (12%)	5	17
1	15-B	267/271 (98%)	228 (85%)	39 (15%)	3	9
1	16-A	267/271 (98%)	228 (85%)	39 (15%)	3	9
1	16-B	267/271 (98%)	230 (86%)	37 (14%)	3	11
All	All	8544/8672 (98%)	7750 (91%)	794 (9%)	9	26

All (794) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	9	GLU
1	1-A	40	GLU
1	1-A	42	GLN
1	1-A	43	ARG
1	1-A	44	THR
1	1-A	76	GLU
1	1-A	83	SER
1	1-A	91	ARG
1	1-A	92	ARG
1	1-A	110	ASP
1	1-A	117	ASN
1	1-A	130	ASP
1	1-A	139	MSE
1	1-A	158	GLU
1	1-A	166	THR
1	1-A	172	LYS
1	1-A	173	TYR

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Mol	Chain	Res	Type
1	1-A	190	ASP
1	1-A	192	LEU
1	1-A	193	ASP
1	1-A	195	MSE
1	1-A	198	MSE
1	1-A	201	HIS
1	1-A	204	ASP
1	1-A	210	ASN
1	1-A	215	PHE
1	1-A	218	CYS
1	1-A	231	TYR
1	1-A	232	PRO
1	1-A	250	GLN
1	1-A	257	PRO
1	1-A	259	ASP
1	1-A	265	LEU
1	1-A	293	GLU
1	1-A	302	THR
1	1-B	9	GLU
1	1-B	20	THR
1	1-B	23	ASN
1	1-B	47	GLU
1	1-B	61	CYS
1	1-B	62	THR
1	1-B	83	SER
1	1-B	161	SER
1	1-B	178	GLU
1	1-B	190	ASP
1	1-B	224	LYS
1	1-B	225	ILE
1	1-B	247	LEU
1	1-B	257	PRO
1	1-B	275	ASP
1	1-B	288	TYR
1	1-B	299	THR
1	1-B	309	ARG
1	2-A	10	HIS
1	2-A	44	THR
1	2-A	83	SER
1	2-A	85	ASP
1	2-A	96	ILE
1	2-A	129	GLU

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Mol	Chain	Res	Type
1	2-A	131	SER
1	2-A	146	SER
1	2-A	163	LYS
1	2-A	167	THR
1	2-A	187	LEU
1	2-A	190	ASP
1	2-A	193	ASP
1	2-A	196	ARG
1	2-A	215	PHE
1	2-A	232	PRO
1	2-A	236	ASN
1	2-A	238	GLU
1	2-A	251	ASP
1	2-A	255	LEU
1	2-A	257	PRO
1	2-A	265	LEU
1	2-B	10	HIS
1	2-B	12	GLN
1	2-B	20	THR
1	2-B	23	ASN
1	2-B	47	GLU
1	2-B	64	TYR
1	2-B	85	ASP
1	2-B	92	ARG
1	2-B	120	SER
1	2-B	130	ASP
1	2-B	149	PRO
1	2-B	182	GLN
1	2-B	190	ASP
1	2-B	192	LEU
1	2-B	218	CYS
1	2-B	221	GLU
1	2-B	226	ILE
1	2-B	231	TYR
1	2-B	232	PRO
1	2-B	253	LYS
1	2-B	293	GLU
1	2-B	301	LEU
1	3-A	107	ASP
1	3-A	146	SER
1	3-A	161	SER
1	3-A	166	THR

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Mol	Chain	Res	Type
1	3-A	187	LEU
1	3-A	204	ASP
1	3-A	217	PRO
1	3-A	224	LYS
1	3-A	226	ILE
1	3-A	229	VAL
1	3-A	231	TYR
1	3-A	232	PRO
1	3-A	238	GLU
1	3-A	301	LEU
1	3-B	9	GLU
1	3-B	47	GLU
1	3-B	64	TYR
1	3-B	67	CYS
1	3-B	82	MSE
1	3-B	138	GLN
1	3-B	182	GLN
1	3-B	224	LYS
1	3-B	227	GLU
1	3-B	232	PRO
1	3-B	247	LEU
1	3-B	257	PRO
1	3-B	266	ASP
1	3-B	275	ASP
1	3-B	297	LYS
1	4-A	12	GLN
1	4-A	43	ARG
1	4-A	56	ARG
1	4-A	99	LEU
1	4-A	105	SER
1	4-A	109	TYR
1	4-A	132	ARG
1	4-A	190	ASP
1	4-A	204	ASP
1	4-A	214	GLU
1	4-A	232	PRO
1	4-A	251	ASP
1	4-A	265	LEU
1	4-A	266	ASP
1	4-A	268	LYS
1	4-A	290	GLU
1	4-B	9	GLU

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Mol	Chain	Res	Type
1	4-B	12	GLN
1	4-B	13	LYS
1	4-B	71	ARG
1	4-B	78	LEU
1	4-B	85	ASP
1	4-B	130	ASP
1	4-B	146	SER
1	4-B	149	PRO
1	4-B	152	CYS
1	4-B	166	THR
1	4-B	182	GLN
1	4-B	215	PHE
1	4-B	231	TYR
1	4-B	247	LEU
1	4-B	259	ASP
1	4-B	266	ASP
1	4-B	271	PRO
1	4-B	272	LEU
1	4-B	276	CYS
1	4-B	278	VAL
1	4-B	301	LEU
1	5-A	9	GLU
1	5-A	42	GLN
1	5-A	44	THR
1	5-A	47	GLU
1	5-A	105	SER
1	5-A	109	TYR
1	5-A	117	ASN
1	5-A	130	ASP
1	5-A	146	SER
1	5-A	166	THR
1	5-A	170	ILE
1	5-A	213	LYS
1	5-A	214	GLU
1	5-A	217	PRO
1	5-A	221	GLU
1	5-A	225	ILE
1	5-A	231	TYR
1	5-A	244	HIS
1	5-A	251	ASP
1	5-A	275	ASP
1	5-A	309	ARG

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Mol	Chain	Res	Type
1	5-B	10	HIS
1	5-B	12	GLN
1	5-B	20	THR
1	5-B	23	ASN
1	5-B	56	ARG
1	5-B	67	CYS
1	5-B	82	MSE
1	5-B	134	ASN
1	5-B	149	PRO
1	5-B	152	CYS
1	5-B	170	ILE
1	5-B	182	GLN
1	5-B	190	ASP
1	5-B	208	HIS
1	5-B	225	ILE
1	5-B	232	PRO
1	5-B	259	ASP
1	5-B	290	GLU
1	6-A	23	ASN
1	6-A	44	THR
1	6-A	51	PHE
1	6-A	56	ARG
1	6-A	82	MSE
1	6-A	86	LEU
1	6-A	91	ARG
1	6-A	92	ARG
1	6-A	95	GLU
1	6-A	112	ILE
1	6-A	125	THR
1	6-A	187	LEU
1	6-A	196	ARG
1	6-A	207	HIS
1	6-A	232	PRO
1	6-A	236	ASN
1	6-A	238	GLU
1	6-A	244	HIS
1	6-A	251	ASP
1	6-A	257	PRO
1	6-A	268	LYS
1	6-A	279	TYR
1	6-A	301	LEU
1	6-B	10	HIS

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Mol	Chain	Res	Type
1	6-B	20	THR
1	6-B	23	ASN
1	6-B	55	PRO
1	6-B	78	LEU
1	6-B	81	LYS
1	6-B	91	ARG
1	6-B	117	ASN
1	6-B	149	PRO
1	6-B	152	CYS
1	6-B	182	GLN
1	6-B	214	GLU
1	6-B	221	GLU
1	6-B	225	ILE
1	6-B	231	TYR
1	6-B	259	ASP
1	6-B	275	ASP
1	6-B	290	GLU
1	6-B	299	THR
1	7-A	12	GLN
1	7-A	44	THR
1	7-A	105	SER
1	7-A	107	ASP
1	7-A	108	SER
1	7-A	166	THR
1	7-A	190	ASP
1	7-A	196	ARG
1	7-A	220	ILE
1	7-A	225	ILE
1	7-A	259	ASP
1	7-A	275	ASP
1	7-A	299	THR
1	7-B	9	GLU
1	7-B	42	GLN
1	7-B	81	LYS
1	7-B	82	MSE
1	7-B	92	ARG
1	7-B	106	GLU
1	7-B	108	SER
1	7-B	131	SER
1	7-B	149	PRO
1	7-B	182	GLN
1	7-B	190	ASP

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Mol	Chain	Res	Type
1	7-B	205	PHE
1	7-B	225	ILE
1	7-B	226	ILE
1	7-B	245	PRO
1	7-B	246	ASN
1	7-B	257	PRO
1	7-B	261	MSE
1	7-B	263	LEU
1	7-B	271	PRO
1	7-B	299	THR
1	8-A	10	HIS
1	8-A	12	GLN
1	8-A	44	THR
1	8-A	81	LYS
1	8-A	82	MSE
1	8-A	85	ASP
1	8-A	106	GLU
1	8-A	109	TYR
1	8-A	110	ASP
1	8-A	112	ILE
1	8-A	117	ASN
1	8-A	138	GLN
1	8-A	157	ILE
1	8-A	163	LYS
1	8-A	172	LYS
1	8-A	226	ILE
1	8-A	232	PRO
1	8-A	235	GLU
1	8-A	257	PRO
1	8-A	259	ASP
1	8-A	276	CYS
1	8-A	290	GLU
1	8-B	42	GLN
1	8-B	44	THR
1	8-B	47	GLU
1	8-B	59	LYS
1	8-B	76	GLU
1	8-B	92	ARG
1	8-B	99	LEU
1	8-B	117	ASN
1	8-B	122	MSE
1	8-B	131	SER

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Mol	Chain	Res	Type
1	8-B	162	LEU
1	8-B	166	THR
1	8-B	214	GLU
1	8-B	224	LYS
1	8-B	236	ASN
1	8-B	259	ASP
1	8-B	263	LEU
1	8-B	265	LEU
1	8-B	271	PRO
1	8-B	275	ASP
1	8-B	276	CYS
1	8-B	293	GLU
1	8-B	299	THR
1	9-A	44	THR
1	9-A	75	LEU
1	9-A	77	ASN
1	9-A	84	GLU
1	9-A	92	ARG
1	9-A	94	GLN
1	9-A	95	GLU
1	9-A	105	SER
1	9-A	108	SER
1	9-A	131	SER
1	9-A	152	CYS
1	9-A	196	ARG
1	9-A	231	TYR
1	9-A	232	PRO
1	9-A	259	ASP
1	9-A	266	ASP
1	9-A	299	THR
1	9-B	24	GLU
1	9-B	43	ARG
1	9-B	56	ARG
1	9-B	90	VAL
1	9-B	109	TYR
1	9-B	110	ASP
1	9-B	132	ARG
1	9-B	166	THR
1	9-B	168	ARG
1	9-B	172	LYS
1	9-B	178	GLU
1	9-B	182	GLN

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Mol	Chain	Res	Type
1	9-B	253	LYS
1	9-B	271	PRO
1	9-B	272	LEU
1	9-B	275	ASP
1	9-B	277	THR
1	9-B	310	CYS
1	10-A	9	GLU
1	10-A	12	GLN
1	10-A	25	LEU
1	10-A	63	ARG
1	10-A	71	ARG
1	10-A	166	THR
1	10-A	217	PRO
1	10-A	218	CYS
1	10-A	232	PRO
1	10-A	257	PRO
1	10-A	261	MSE
1	10-A	268	LYS
1	10-A	271	PRO
1	10-A	279	TYR
1	10-A	299	THR
1	10-B	9	GLU
1	10-B	42	GLN
1	10-B	43	ARG
1	10-B	44	THR
1	10-B	62	THR
1	10-B	67	CYS
1	10-B	70	ASN
1	10-B	80	LYS
1	10-B	82	MSE
1	10-B	85	ASP
1	10-B	105	SER
1	10-B	109	TYR
1	10-B	117	ASN
1	10-B	120	SER
1	10-B	127	ILE
1	10-B	129	GLU
1	10-B	184	GLN
1	10-B	193	ASP
1	10-B	195	MSE
1	10-B	213	LYS
1	10-B	224	LYS

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Mol	Chain	Res	Type
1	10-B	235	GLU
1	10-B	236	ASN
1	10-B	271	PRO
1	10-B	276	CYS
1	10-B	281	VAL
1	10-B	299	THR
1	11-A	44	THR
1	11-A	85	ASP
1	11-A	105	SER
1	11-A	107	ASP
1	11-A	110	ASP
1	11-A	130	ASP
1	11-A	146	SER
1	11-A	166	THR
1	11-A	196	ARG
1	11-A	233	ARG
1	11-A	235	GLU
1	11-A	251	ASP
1	11-A	255	LEU
1	11-A	259	ASP
1	11-A	260	PRO
1	11-A	261	MSE
1	11-A	268	LYS
1	11-A	276	CYS
1	11-A	299	THR
1	11-A	301	LEU
1	11-B	9	GLU
1	11-B	20	THR
1	11-B	55	PRO
1	11-B	67	CYS
1	11-B	122	MSE
1	11-B	130	ASP
1	11-B	149	PRO
1	11-B	182	GLN
1	11-B	190	ASP
1	11-B	214	GLU
1	11-B	232	PRO
1	11-B	235	GLU
1	11-B	245	PRO
1	11-B	255	LEU
1	11-B	257	PRO
1	11-B	261	MSE

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Mol	Chain	Res	Type
1	11-B	262	PHE
1	11-B	266	ASP
1	11-B	271	PRO
1	11-B	299	THR
1	12-A	20	THR
1	12-A	23	ASN
1	12-A	40	GLU
1	12-A	41	ILE
1	12-A	42	GLN
1	12-A	44	THR
1	12-A	56	ARG
1	12-A	81	LYS
1	12-A	97	ASN
1	12-A	113	PHE
1	12-A	146	SER
1	12-A	147	LEU
1	12-A	168	ARG
1	12-A	187	LEU
1	12-A	190	ASP
1	12-A	193	ASP
1	12-A	208	HIS
1	12-A	217	PRO
1	12-A	226	ILE
1	12-A	236	ASN
1	12-A	238	GLU
1	12-A	242	ILE
1	12-A	257	PRO
1	12-A	259	ASP
1	12-A	268	LYS
1	12-A	271	PRO
1	12-A	288	TYR
1	12-A	302	THR
1	12-A	304	ASN
1	12-B	9	GLU
1	12-B	46	LEU
1	12-B	47	GLU
1	12-B	62	THR
1	12-B	64	TYR
1	12-B	67	CYS
1	12-B	108	SER
1	12-B	117	ASN
1	12-B	118	THR

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Mol	Chain	Res	Type
1	12-B	146	SER
1	12-B	149	PRO
1	12-B	161	SER
1	12-B	170	ILE
1	12-B	182	GLN
1	12-B	214	GLU
1	12-B	232	PRO
1	12-B	235	GLU
1	12-B	242	ILE
1	12-B	257	PRO
1	12-B	259	ASP
1	12-B	266	ASP
1	12-B	268	LYS
1	12-B	276	CYS
1	12-B	277	THR
1	13-A	12	GLN
1	13-A	26	THR
1	13-A	44	THR
1	13-A	47	GLU
1	13-A	71	ARG
1	13-A	74	ASP
1	13-A	75	LEU
1	13-A	82	MSE
1	13-A	86	LEU
1	13-A	95	GLU
1	13-A	99	LEU
1	13-A	105	SER
1	13-A	106	GLU
1	13-A	107	ASP
1	13-A	109	TYR
1	13-A	115	LEU
1	13-A	117	ASN
1	13-A	125	THR
1	13-A	128	LEU
1	13-A	139	MSE
1	13-A	141	HIS
1	13-A	146	SER
1	13-A	147	LEU
1	13-A	183	PRO
1	13-A	187	LEU
1	13-A	195	MSE
1	13-A	198	MSE

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Mol	Chain	Res	Type
1	13-A	204	ASP
1	13-A	207	HIS
1	13-A	220	ILE
1	13-A	222	VAL
1	13-A	226	ILE
1	13-A	230	ASP
1	13-A	231	TYR
1	13-A	232	PRO
1	13-A	235	GLU
1	13-A	238	GLU
1	13-A	242	ILE
1	13-A	257	PRO
1	13-A	261	MSE
1	13-A	281	VAL
1	13-A	284	ASN
1	13-A	289	TYR
1	13-A	291	LYS
1	13-A	292	LYS
1	13-A	300	LYS
1	13-A	301	LEU
1	13-A	304	ASN
1	13-A	307	SER
1	13-A	310	CYS
1	13-B	13	LYS
1	13-B	24	GLU
1	13-B	40	GLU
1	13-B	44	THR
1	13-B	46	LEU
1	13-B	56	ARG
1	13-B	59	LYS
1	13-B	61	CYS
1	13-B	62	THR
1	13-B	71	ARG
1	13-B	86	LEU
1	13-B	120	SER
1	13-B	127	ILE
1	13-B	130	ASP
1	13-B	141	HIS
1	13-B	146	SER
1	13-B	152	CYS
1	13-B	170	ILE
1	13-B	182	GLN

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Mol	Chain	Res	Type
1	13-B	187	LEU
1	13-B	194	GLN
1	13-B	209	PHE
1	13-B	218	CYS
1	13-B	226	ILE
1	13-B	232	PRO
1	13-B	244	HIS
1	13-B	247	LEU
1	13-B	257	PRO
1	13-B	268	LYS
1	13-B	288	TYR
1	13-B	293	GLU
1	13-B	299	THR
1	13-B	301	LEU
1	13-B	304	ASN
1	13-B	310	CYS
1	14-A	12	GLN
1	14-A	26	THR
1	14-A	44	THR
1	14-A	62	THR
1	14-A	68	ASP
1	14-A	80	LYS
1	14-A	84	GLU
1	14-A	86	LEU
1	14-A	91	ARG
1	14-A	96	ILE
1	14-A	99	LEU
1	14-A	109	TYR
1	14-A	110	ASP
1	14-A	115	LEU
1	14-A	118	THR
1	14-A	119	THR
1	14-A	120	SER
1	14-A	122	MSE
1	14-A	168	ARG
1	14-A	170	ILE
1	14-A	177	ILE
1	14-A	187	LEU
1	14-A	195	MSE
1	14-A	214	GLU
1	14-A	218	CYS
1	14-A	224	LYS

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Mol	Chain	Res	Type
1	14-A	247	LEU
1	14-A	260	PRO
1	14-A	261	MSE
1	14-A	265	LEU
1	14-A	275	ASP
1	14-A	291	LYS
1	14-A	293	GLU
1	14-A	297	LYS
1	14-A	298	THR
1	14-A	308	ILE
1	14-B	24	GLU
1	14-B	40	GLU
1	14-B	44	THR
1	14-B	46	LEU
1	14-B	56	ARG
1	14-B	63	ARG
1	14-B	67	CYS
1	14-B	69	LEU
1	14-B	89	GLU
1	14-B	92	ARG
1	14-B	109	TYR
1	14-B	139	MSE
1	14-B	141	HIS
1	14-B	144	LYS
1	14-B	149	PRO
1	14-B	166	THR
1	14-B	168	ARG
1	14-B	170	ILE
1	14-B	182	GLN
1	14-B	196	ARG
1	14-B	214	GLU
1	14-B	218	CYS
1	14-B	232	PRO
1	14-B	263	LEU
1	14-B	265	LEU
1	14-B	271	PRO
1	14-B	276	CYS
1	14-B	277	THR
1	14-B	299	THR
1	14-B	300	LYS
1	14-B	301	LEU
1	14-B	307	SER

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Mol	Chain	Res	Type
1	14-B	309	ARG
1	15-A	10	HIS
1	15-A	24	GLU
1	15-A	29	PHE
1	15-A	35	LEU
1	15-A	55	PRO
1	15-A	58	VAL
1	15-A	71	ARG
1	15-A	91	ARG
1	15-A	99	LEU
1	15-A	105	SER
1	15-A	106	GLU
1	15-A	107	ASP
1	15-A	109	TYR
1	15-A	113	PHE
1	15-A	117	ASN
1	15-A	122	MSE
1	15-A	125	THR
1	15-A	129	GLU
1	15-A	168	ARG
1	15-A	197	LYS
1	15-A	200	LYS
1	15-A	226	ILE
1	15-A	238	GLU
1	15-A	250	GLN
1	15-A	253	LYS
1	15-A	257	PRO
1	15-A	266	ASP
1	15-A	269	THR
1	15-A	275	ASP
1	15-A	276	CYS
1	15-A	306	LYS
1	15-B	9	GLU
1	15-B	24	GLU
1	15-B	44	THR
1	15-B	55	PRO
1	15-B	63	ARG
1	15-B	67	CYS
1	15-B	72	ILE
1	15-B	82	MSE
1	15-B	94	GLN
1	15-B	97	ASN

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Mol	Chain	Res	Type
1	15-B	115	LEU
1	15-B	120	SER
1	15-B	131	SER
1	15-B	141	HIS
1	15-B	155	TYR
1	15-B	167	THR
1	15-B	182	GLN
1	15-B	194	GLN
1	15-B	196	ARG
1	15-B	199	ILE
1	15-B	204	ASP
1	15-B	218	CYS
1	15-B	223	TYR
1	15-B	226	ILE
1	15-B	249	ASP
1	15-B	253	LYS
1	15-B	255	LEU
1	15-B	257	PRO
1	15-B	261	MSE
1	15-B	276	CYS
1	15-B	282	PHE
1	15-B	292	LYS
1	15-B	293	GLU
1	15-B	295	PHE
1	15-B	299	THR
1	15-B	301	LEU
1	15-B	307	SER
1	15-B	309	ARG
1	15-B	310	CYS
1	16-A	31	VAL
1	16-A	42	GLN
1	16-A	56	ARG
1	16-A	71	ARG
1	16-A	85	ASP
1	16-A	86	LEU
1	16-A	90	VAL
1	16-A	95	GLU
1	16-A	110	ASP
1	16-A	111	ILE
1	16-A	117	ASN
1	16-A	122	MSE
1	16-A	125	THR

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Mol	Chain	Res	Type
1	16-A	130	ASP
1	16-A	141	HIS
1	16-A	159	HIS
1	16-A	160	PRO
1	16-A	166	THR
1	16-A	167	THR
1	16-A	172	LYS
1	16-A	187	LEU
1	16-A	188	ARG
1	16-A	192	LEU
1	16-A	193	ASP
1	16-A	197	LYS
1	16-A	209	PHE
1	16-A	213	LYS
1	16-A	225	ILE
1	16-A	231	TYR
1	16-A	232	PRO
1	16-A	235	GLU
1	16-A	238	GLU
1	16-A	246	ASN
1	16-A	257	PRO
1	16-A	259	ASP
1	16-A	271	PRO
1	16-A	275	ASP
1	16-A	276	CYS
1	16-A	304	ASN
1	16-B	24	GLU
1	16-B	44	THR
1	16-B	62	THR
1	16-B	81	LYS
1	16-B	83	SER
1	16-B	91	ARG
1	16-B	107	ASP
1	16-B	109	TYR
1	16-B	120	SER
1	16-B	127	ILE
1	16-B	129	GLU
1	16-B	132	ARG
1	16-B	145	THR
1	16-B	166	THR
1	16-B	170	ILE
1	16-B	182	GLN

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Mol	Chain	Res	Type
1	16-B	190	ASP
1	16-B	194	GLN
1	16-B	195	MSE
1	16-B	207	HIS
1	16-B	214	GLU
1	16-B	223	TYR
1	16-B	226	ILE
1	16-B	227	GLU
1	16-B	230	ASP
1	16-B	231	TYR
1	16-B	238	GLU
1	16-B	239	ILE
1	16-B	242	ILE
1	16-B	247	LEU
1	16-B	248	GLN
1	16-B	264	THR
1	16-B	265	LEU
1	16-B	299	THR
1	16-B	301	LEU
1	16-B	306	LYS
1	16-B	307	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (245) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	10	HIS
1	1-A	42	GLN
1	1-A	77	ASN
1	1-A	97	ASN
1	1-A	98	HIS
1	1-A	117	ASN
1	1-A	194	GLN
1	1-A	210	ASN
1	1-A	246	ASN
1	1-A	250	GLN
1	1-B	10	HIS
1	1-B	12	GLN
1	1-B	23	ASN
1	1-B	33	HIS
1	1-B	42	GLN
1	1-B	98	HIS
1	1-B	117	ASN

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Mol	Chain	Res	Type
1	1-B	141	HIS
1	1-B	182	GLN
1	1-B	184	GLN
1	1-B	194	GLN
1	1-B	208	HIS
1	2-A	33	HIS
1	2-A	77	ASN
1	2-A	133	ASN
1	2-A	201	HIS
1	2-A	246	ASN
1	2-B	23	ASN
1	2-B	184	GLN
1	2-B	208	HIS
1	3-A	10	HIS
1	3-A	21	HIS
1	3-A	94	GLN
1	3-A	98	HIS
1	3-A	134	ASN
1	3-A	248	GLN
1	3-B	10	HIS
1	3-B	12	GLN
1	3-B	77	ASN
1	3-B	97	ASN
1	3-B	98	HIS
1	3-B	117	ASN
1	3-B	138	GLN
1	3-B	159	HIS
1	3-B	182	GLN
1	3-B	194	GLN
1	3-B	201	HIS
1	3-B	208	HIS
1	4-A	12	GLN
1	4-A	77	ASN
1	4-A	94	GLN
1	4-A	208	HIS
1	4-B	12	GLN
1	4-B	42	GLN
1	4-B	94	GLN
1	4-B	117	ASN
1	4-B	201	HIS
1	4-B	244	HIS
1	5-A	10	HIS

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Mol	Chain	Res	Type
1	5-A	21	HIS
1	5-A	94	GLN
1	5-A	117	ASN
1	5-A	138	GLN
1	5-A	141	HIS
1	5-A	182	GLN
1	5-A	194	GLN
1	5-A	246	ASN
1	5-A	248	GLN
1	5-A	284	ASN
1	5-B	12	GLN
1	5-B	42	GLN
1	5-B	94	GLN
1	5-B	117	ASN
1	5-B	133	ASN
1	5-B	194	GLN
1	5-B	207	HIS
1	5-B	208	HIS
1	6-A	10	HIS
1	6-A	12	GLN
1	6-A	23	ASN
1	6-A	98	HIS
1	6-A	141	HIS
1	6-A	210	ASN
1	6-B	12	GLN
1	6-B	33	HIS
1	6-B	42	GLN
1	6-B	77	ASN
1	6-B	117	ASN
1	6-B	138	GLN
1	6-B	182	GLN
1	6-B	194	GLN
1	6-B	208	HIS
1	6-B	246	ASN
1	7-A	12	GLN
1	7-A	117	ASN
1	7-A	133	ASN
1	7-A	248	GLN
1	7-A	250	GLN
1	7-A	284	ASN
1	7-B	42	GLN
1	7-B	246	ASN

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Mol	Chain	Res	Type
1	7-B	248	GLN
1	8-A	12	GLN
1	8-A	21	HIS
1	8-A	33	HIS
1	8-A	77	ASN
1	8-A	94	GLN
1	8-A	97	ASN
1	8-A	98	HIS
1	8-A	159	HIS
1	8-A	201	HIS
1	8-A	207	HIS
1	8-A	248	GLN
1	8-A	284	ASN
1	8-B	12	GLN
1	8-B	33	HIS
1	8-B	42	GLN
1	8-B	98	HIS
1	8-B	141	HIS
1	8-B	159	HIS
1	8-B	194	GLN
1	8-B	246	ASN
1	9-A	10	HIS
1	9-A	23	ASN
1	9-A	94	GLN
1	9-A	194	GLN
1	9-A	207	HIS
1	9-A	208	HIS
1	9-A	236	ASN
1	9-A	250	GLN
1	9-A	256	HIS
1	9-B	42	GLN
1	9-B	94	GLN
1	9-B	117	ASN
1	9-B	133	ASN
1	9-B	141	HIS
1	9-B	201	HIS
1	9-B	246	ASN
1	9-B	248	GLN
1	10-A	12	GLN
1	10-A	21	HIS
1	10-A	77	ASN
1	10-A	194	GLN

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Mol	Chain	Res	Type
1	10-A	248	GLN
1	10-A	284	ASN
1	10-B	33	HIS
1	10-B	134	ASN
1	10-B	138	GLN
1	10-B	194	GLN
1	10-B	201	HIS
1	10-B	236	ASN
1	10-B	246	ASN
1	10-B	248	GLN
1	11-A	194	GLN
1	11-A	207	HIS
1	11-A	236	ASN
1	11-A	248	GLN
1	11-A	284	ASN
1	11-B	10	HIS
1	11-B	12	GLN
1	11-B	121	ASN
1	11-B	133	ASN
1	11-B	246	ASN
1	12-A	23	ASN
1	12-A	33	HIS
1	12-A	42	GLN
1	12-A	94	GLN
1	12-A	134	ASN
1	12-A	248	GLN
1	12-A	284	ASN
1	12-A	304	ASN
1	12-B	37	ASN
1	12-B	138	GLN
1	12-B	246	ASN
1	13-A	10	HIS
1	13-A	12	GLN
1	13-A	21	HIS
1	13-A	42	GLN
1	13-A	77	ASN
1	13-A	94	GLN
1	13-A	121	ASN
1	13-A	138	GLN
1	13-A	141	HIS
1	13-A	182	GLN
1	13-A	184	GLN

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Mol	Chain	Res	Type
1	13-A	246	ASN
1	13-A	250	GLN
1	13-A	304	ASN
1	13-B	12	GLN
1	13-B	117	ASN
1	13-B	121	ASN
1	13-B	138	GLN
1	13-B	141	HIS
1	13-B	248	GLN
1	14-A	12	GLN
1	14-A	77	ASN
1	14-A	117	ASN
1	14-A	184	GLN
1	14-A	208	HIS
1	14-A	210	ASN
1	14-A	236	ASN
1	14-A	248	GLN
1	14-A	256	HIS
1	14-B	12	GLN
1	14-B	33	HIS
1	14-B	117	ASN
1	14-B	121	ASN
1	14-B	138	GLN
1	14-B	141	HIS
1	14-B	182	GLN
1	14-B	194	GLN
1	14-B	246	ASN
1	15-A	10	HIS
1	15-A	12	GLN
1	15-A	33	HIS
1	15-A	94	GLN
1	15-A	117	ASN
1	15-A	194	GLN
1	15-A	246	ASN
1	15-A	248	GLN
1	15-A	250	GLN
1	15-A	284	ASN
1	15-B	77	ASN
1	15-B	97	ASN
1	15-B	98	HIS
1	15-B	117	ASN
1	15-B	141	HIS

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Mol	Chain	Res	Type
1	15-B	184	GLN
1	15-B	194	GLN
1	15-B	201	HIS
1	15-B	210	ASN
1	15-B	246	ASN
1	15-B	250	GLN
1	16-A	33	HIS
1	16-A	77	ASN
1	16-A	184	GLN
1	16-A	201	HIS
1	16-A	207	HIS
1	16-A	246	ASN
1	16-A	304	ASN
1	16-B	12	GLN
1	16-B	42	GLN
1	16-B	133	ASN
1	16-B	208	HIS
1	16-B	256	HIS

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 160 ligands modelled in this entry, 32 are monoatomic - leaving 128 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	PO4	2-B	316	-	4,4,4	1.64	0	6,6,6	0.46	0
3	PO4	6-A	315	-	4,4,4	1.60	0	6,6,6	0.42	0
3	PO4	5-A	318	-	4,4,4	1.47	0	6,6,6	0.44	0
3	PO4	4-A	315	-	4,4,4	1.54	0	6,6,6	0.43	0
3	PO4	5-A	317	-	4,4,4	1.18	0	6,6,6	0.46	0
3	PO4	1-B	316	-	4,4,4	1.55	0	6,6,6	0.45	0
3	PO4	1-A	317	-	4,4,4	1.16	0	6,6,6	0.45	0
3	PO4	6-B	315	-	4,4,4	1.68	1 (25%)	6,6,6	0.43	0
3	PO4	14-B	315	-	4,4,4	1.60	1 (25%)	6,6,6	0.51	0
3	PO4	9-A	315	-	4,4,4	1.62	0	6,6,6	0.43	0
3	PO4	7-B	316	-	4,4,4	1.45	1 (25%)	6,6,6	0.44	0
3	PO4	10-A	316	-	4,4,4	1.71	1 (25%)	6,6,6	0.45	0
3	PO4	7-B	315	-	4,4,4	1.85	2 (50%)	6,6,6	0.43	0
3	PO4	4-A	316	-	4,4,4	1.49	0	6,6,6	0.43	0
3	PO4	11-A	316	-	4,4,4	1.58	0	6,6,6	0.44	0
3	PO4	12-A	318	-	4,4,4	1.97	2 (50%)	6,6,6	0.44	0
3	PO4	11-A	315	-	4,4,4	1.57	0	6,6,6	0.40	0
3	PO4	10-B	317	-	4,4,4	1.65	1 (25%)	6,6,6	0.41	0
3	PO4	9-A	317	-	4,4,4	1.35	0	6,6,6	0.41	0
3	PO4	10-B	315	-	4,4,4	1.78	1 (25%)	6,6,6	0.46	0
3	PO4	6-B	317	-	4,4,4	1.69	1 (25%)	6,6,6	0.45	0
3	PO4	15-B	315	-	4,4,4	1.60	0	6,6,6	0.45	0
3	PO4	16-A	317	-	4,4,4	1.11	0	6,6,6	0.45	0
3	PO4	14-A	318	-	4,4,4	1.34	0	6,6,6	0.47	0
3	PO4	3-B	317	-	4,4,4	1.95	3 (75%)	6,6,6	0.38	0
3	PO4	9-B	317	-	4,4,4	1.69	1 (25%)	6,6,6	0.40	0
3	PO4	1-A	315	-	4,4,4	3.63	3 (75%)	6,6,6	0.88	0
3	PO4	1-B	315	-	4,4,4	1.75	2 (50%)	6,6,6	0.34	0
3	PO4	6-B	316	-	4,4,4	1.70	2 (50%)	6,6,6	0.47	0
3	PO4	4-B	318	-	4,4,4	1.52	0	6,6,6	0.40	0
3	PO4	8-B	318	-	4,4,4	3.03	3 (75%)	6,6,6	0.55	0
3	PO4	3-B	318	-	4,4,4	1.59	0	6,6,6	0.43	0
3	PO4	6-A	318	-	4,4,4	1.51	0	6,6,6	0.43	0
3	PO4	4-A	318	-	4,4,4	1.49	0	6,6,6	0.42	0
3	PO4	8-A	318	-	4,4,4	1.65	0	6,6,6	0.42	0
3	PO4	2-A	318	-	4,4,4	1.48	0	6,6,6	0.44	0
3	PO4	4-B	317	-	4,4,4	1.73	1 (25%)	6,6,6	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PO4	8-B	317	-	4,4,4	1.94	3 (75%)	6,6,6	0.46	0
3	PO4	1-B	317	-	4,4,4	1.84	2 (50%)	6,6,6	0.40	0
3	PO4	10-A	315	-	4,4,4	1.34	0	6,6,6	0.42	0
3	PO4	15-A	316	-	4,4,4	1.53	1 (25%)	6,6,6	0.47	0
3	PO4	2-A	317	-	4,4,4	1.66	1 (25%)	6,6,6	0.44	0
3	PO4	7-A	316	-	4,4,4	1.77	2 (50%)	6,6,6	0.46	0
3	PO4	13-B	316	-	4,4,4	1.57	0	6,6,6	0.47	0
3	PO4	4-A	317	-	4,4,4	1.30	0	6,6,6	0.44	0
3	PO4	8-A	317	-	4,4,4	1.69	1 (25%)	6,6,6	0.38	0
3	PO4	5-B	315	-	4,4,4	1.80	1 (25%)	6,6,6	0.42	0
3	PO4	7-A	315	-	4,4,4	1.64	0	6,6,6	0.46	0
3	PO4	12-B	317	-	4,4,4	1.99	3 (75%)	6,6,6	0.39	0
3	PO4	3-A	317	-	4,4,4	1.33	0	6,6,6	0.47	0
3	PO4	14-B	317	-	4,4,4	1.77	2 (50%)	6,6,6	0.44	0
3	PO4	7-B	317	-	4,4,4	1.54	1 (25%)	6,6,6	0.40	0
3	PO4	13-B	318	-	4,4,4	1.43	0	6,6,6	0.38	0
3	PO4	10-B	318	-	4,4,4	1.36	0	6,6,6	0.43	0
3	PO4	3-A	318	-	4,4,4	1.45	0	6,6,6	0.45	0
3	PO4	9-A	318	-	4,4,4	1.68	0	6,6,6	0.43	0
3	PO4	11-B	316	-	4,4,4	1.29	0	6,6,6	0.48	0
3	PO4	16-B	316	-	4,4,4	1.63	1 (25%)	6,6,6	0.42	0
3	PO4	7-A	317	-	4,4,4	1.46	0	6,6,6	0.46	0
3	PO4	16-B	315	-	4,4,4	1.53	0	6,6,6	0.43	0
3	PO4	10-A	317	-	4,4,4	1.60	0	6,6,6	0.45	0
3	PO4	12-B	316	-	4,4,4	1.69	1 (25%)	6,6,6	0.44	0
3	PO4	15-A	315	-	4,4,4	1.64	0	6,6,6	0.44	0
3	PO4	8-A	316	-	4,4,4	1.15	0	6,6,6	0.54	0
3	PO4	11-B	315	-	4,4,4	1.68	1 (25%)	6,6,6	0.45	0
3	PO4	1-B	318	-	4,4,4	1.49	0	6,6,6	0.41	0
3	PO4	16-A	316	-	4,4,4	1.71	2 (50%)	6,6,6	0.47	0
3	PO4	3-B	316	-	4,4,4	1.25	0	6,6,6	0.49	0
3	PO4	16-A	315	-	4,4,4	1.61	0	6,6,6	0.48	0
3	PO4	13-A	316	-	4,4,4	1.81	2 (50%)	6,6,6	0.44	0
3	PO4	12-A	315	-	4,4,4	1.65	0	6,6,6	0.47	0
3	PO4	3-B	315	-	4,4,4	1.67	0	6,6,6	0.45	0
3	PO4	13-A	315	-	4,4,4	1.49	1 (25%)	6,6,6	0.46	0
3	PO4	15-A	318	-	4,4,4	1.54	1 (25%)	6,6,6	0.50	0
3	PO4	8-A	315	-	4,4,4	1.39	0	6,6,6	0.43	0
3	PO4	5-B	316	-	4,4,4	1.42	0	6,6,6	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PO4	6-B	318	-	4,4,4	1.54	0	6,6,6	0.41	0
3	PO4	14-B	318	-	4,4,4	1.51	1 (25%)	6,6,6	0.41	0
3	PO4	10-B	316	-	4,4,4	2.43	3 (75%)	6,6,6	0.33	0
3	PO4	12-A	316	-	4,4,4	1.61	1 (25%)	6,6,6	0.47	0
3	PO4	7-B	318	-	4,4,4	1.54	1 (25%)	6,6,6	0.49	0
3	PO4	2-B	317	-	4,4,4	1.44	1 (25%)	6,6,6	0.42	0
3	PO4	6-A	317	-	4,4,4	1.26	0	6,6,6	0.47	0
3	PO4	2-B	315	-	4,4,4	1.70	1 (25%)	6,6,6	0.45	0
3	PO4	7-A	318	-	4,4,4	1.66	0	6,6,6	0.41	0
3	PO4	2-A	316	-	4,4,4	1.79	2 (50%)	6,6,6	0.43	0
3	PO4	15-B	318	-	4,4,4	1.42	0	6,6,6	0.37	0
3	PO4	2-A	315	-	4,4,4	1.55	2 (50%)	6,6,6	0.47	0
3	PO4	15-A	317	-	4,4,4	1.12	0	6,6,6	0.45	0
3	PO4	6-A	316	-	4,4,4	1.80	1 (25%)	6,6,6	0.45	0
3	PO4	16-A	318	-	4,4,4	1.47	0	6,6,6	0.45	0
3	PO4	11-B	317	-	4,4,4	1.36	0	6,6,6	0.40	0
3	PO4	9-B	315	-	4,4,4	1.72	1 (25%)	6,6,6	0.37	0
3	PO4	5-A	316	-	4,4,4	1.82	2 (50%)	6,6,6	0.43	0
3	PO4	12-B	318	-	4,4,4	1.56	0	6,6,6	0.40	0
3	PO4	13-B	315	-	4,4,4	1.67	0	6,6,6	0.37	0
3	PO4	1-A	318	-	4,4,4	1.45	0	6,6,6	0.44	0
3	PO4	13-B	317	-	4,4,4	1.62	1 (25%)	6,6,6	0.46	0
3	PO4	11-B	318	-	4,4,4	1.55	0	6,6,6	0.40	0
3	PO4	15-B	317	-	4,4,4	1.62	1 (25%)	6,6,6	0.44	0
3	PO4	9-B	316	-	4,4,4	1.42	0	6,6,6	0.41	0
3	PO4	16-B	318	-	4,4,4	1.63	2 (50%)	6,6,6	0.47	0
3	PO4	5-A	315	-	4,4,4	1.64	1 (25%)	6,6,6	0.34	0
3	PO4	13-A	317	-	4,4,4	1.15	0	6,6,6	0.46	0
3	PO4	3-A	316	-	4,4,4	2.06	2 (50%)	6,6,6	0.42	0
3	PO4	2-B	318	-	4,4,4	1.63	1 (25%)	6,6,6	0.48	0
3	PO4	12-B	315	-	4,4,4	1.60	0	6,6,6	0.39	0
3	PO4	14-A	317	-	4,4,4	1.20	0	6,6,6	0.47	0
3	PO4	3-A	315	-	4,4,4	1.43	0	6,6,6	0.36	0
3	PO4	9-B	318	-	4,4,4	1.52	0	6,6,6	0.40	0
3	PO4	10-A	318	-	4,4,4	1.62	0	6,6,6	0.42	0
3	PO4	5-B	317	-	4,4,4	1.52	1 (25%)	6,6,6	0.40	0
3	PO4	13-A	318	-	4,4,4	1.64	1 (25%)	6,6,6	0.46	0
3	PO4	15-B	316	-	4,4,4	1.54	0	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PO4	1-A	316	-	4,4,4	1.75	1 (25%)	6,6,6	0.44	0
3	PO4	11-A	318	-	4,4,4	1.48	0	6,6,6	0.42	0
3	PO4	12-A	317	-	4,4,4	1.22	0	6,6,6	0.47	0
3	PO4	14-A	315	-	4,4,4	1.48	1 (25%)	6,6,6	0.46	0
3	PO4	4-B	316	-	4,4,4	1.59	0	6,6,6	0.45	0
3	PO4	8-B	316	-	4,4,4	1.64	1 (25%)	6,6,6	0.43	0
3	PO4	5-B	318	-	4,4,4	1.56	0	6,6,6	0.40	0
3	PO4	11-A	317	-	4,4,4	1.36	0	6,6,6	0.45	0
3	PO4	4-B	315	-	4,4,4	1.60	0	6,6,6	0.39	0
3	PO4	8-B	315	-	4,4,4	1.58	0	6,6,6	0.40	0
3	PO4	14-A	316	-	4,4,4	1.60	0	6,6,6	0.45	0
3	PO4	9-A	316	-	4,4,4	1.30	0	6,6,6	0.52	0
3	PO4	16-B	317	-	4,4,4	1.64	0	6,6,6	0.40	0
3	PO4	14-B	316	-	4,4,4	1.64	2 (50%)	6,6,6	0.42	0

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-A	315	PO4	P-O3	-6.06	1.36	1.54
3	8-B	318	PO4	P-O2	-3.92	1.42	1.54
3	10-B	316	PO4	P-O4	-3.70	1.43	1.54
3	8-B	318	PO4	P-O4	-3.38	1.44	1.54
3	1-A	315	PO4	P-O4	-3.18	1.45	1.54
3	8-B	318	PO4	P-O3	-2.70	1.46	1.54
3	3-A	316	PO4	P-O3	-2.64	1.46	1.54
3	3-A	316	PO4	P-O4	-2.60	1.46	1.54
3	7-B	315	PO4	P-O2	-2.42	1.47	1.54
3	14-B	317	PO4	P-O4	-2.40	1.47	1.54
3	5-A	316	PO4	P-O4	-2.39	1.47	1.54
3	6-A	316	PO4	P-O4	-2.37	1.47	1.54
3	12-A	318	PO4	P-O4	-2.35	1.47	1.54
3	5-B	315	PO4	P-O2	-2.35	1.47	1.54
3	10-B	316	PO4	P-O3	-2.33	1.47	1.54
3	8-B	317	PO4	P-O3	-2.32	1.47	1.54
3	13-A	316	PO4	P-O4	-2.30	1.47	1.54
3	2-A	316	PO4	P-O4	-2.29	1.47	1.54
3	16-B	318	PO4	P-O3	-2.29	1.47	1.54
3	2-B	318	PO4	P-O2	-2.28	1.47	1.54
3	4-B	317	PO4	P-O2	-2.28	1.47	1.54
3	1-B	317	PO4	P-O4	-2.28	1.47	1.54
3	1-B	315	PO4	P-O3	-2.27	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	12-A	318	PO4	P-O2	-2.27	1.47	1.54
3	3-B	317	PO4	P-O3	-2.26	1.47	1.54
3	12-B	317	PO4	P-O4	-2.25	1.47	1.54
3	10-A	316	PO4	P-O2	-2.24	1.47	1.54
3	12-B	317	PO4	P-O2	-2.23	1.47	1.54
3	6-B	317	PO4	P-O2	-2.23	1.47	1.54
3	9-B	315	PO4	P-O2	-2.23	1.47	1.54
3	12-B	317	PO4	P-O3	-2.22	1.47	1.54
3	1-A	316	PO4	P-O4	-2.21	1.47	1.54
3	1-B	317	PO4	P-O3	-2.21	1.47	1.54
3	16-B	316	PO4	P-O4	-2.21	1.48	1.54
3	12-B	316	PO4	P-O4	-2.21	1.48	1.54
3	7-A	316	PO4	P-O4	-2.20	1.48	1.54
3	14-B	315	PO4	P-O3	-2.18	1.48	1.54
3	9-B	317	PO4	P-O2	-2.16	1.48	1.54
3	15-A	318	PO4	P-O3	-2.16	1.48	1.54
3	10-B	315	PO4	P-O2	-2.15	1.48	1.54
3	7-B	317	PO4	P-O4	-2.14	1.48	1.54
3	10-B	316	PO4	P-O2	-2.13	1.48	1.54
3	5-B	317	PO4	P-O4	-2.13	1.48	1.54
3	3-B	317	PO4	P-O2	-2.13	1.48	1.54
3	8-B	316	PO4	P-O4	-2.12	1.48	1.54
3	3-B	317	PO4	P-O4	-2.12	1.48	1.54
3	1-A	315	PO4	P-O2	-2.12	1.48	1.54
3	7-B	318	PO4	P-O2	-2.11	1.48	1.54
3	13-A	316	PO4	P-O3	-2.10	1.48	1.54
3	14-B	316	PO4	P-O3	-2.10	1.48	1.54
3	15-B	317	PO4	P-O3	-2.09	1.48	1.54
3	6-B	315	PO4	P-O3	-2.09	1.48	1.54
3	10-B	317	PO4	P-O3	-2.08	1.48	1.54
3	7-B	316	PO4	P-O2	-2.08	1.48	1.54
3	13-B	317	PO4	P-O3	-2.07	1.48	1.54
3	8-B	317	PO4	P-O4	-2.07	1.48	1.54
3	14-B	318	PO4	P-O3	-2.07	1.48	1.54
3	8-A	317	PO4	P-O4	-2.07	1.48	1.54
3	15-A	316	PO4	P-O3	-2.06	1.48	1.54
3	2-A	317	PO4	P-O2	-2.05	1.48	1.54
3	2-B	315	PO4	P-O3	-2.05	1.48	1.54
3	6-B	316	PO4	P-O4	-2.05	1.48	1.54
3	11-B	315	PO4	P-O2	-2.05	1.48	1.54
3	16-A	316	PO4	P-O3	-2.05	1.48	1.54
3	5-A	316	PO4	P-O3	-2.05	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	8-B	317	PO4	P-O2	-2.04	1.48	1.54
3	2-A	315	PO4	P-O2	-2.04	1.48	1.54
3	1-B	315	PO4	P-O4	-2.04	1.48	1.54
3	13-A	318	PO4	P-O2	-2.04	1.48	1.54
3	14-B	316	PO4	P-O4	-2.04	1.48	1.54
3	13-A	315	PO4	P-O2	-2.03	1.48	1.54
3	16-A	316	PO4	P-O4	-2.03	1.48	1.54
3	2-B	317	PO4	P-O4	-2.02	1.48	1.54
3	7-B	315	PO4	P-O3	-2.02	1.48	1.54
3	2-A	316	PO4	P-O3	-2.02	1.48	1.54
3	2-A	315	PO4	P-O3	-2.02	1.48	1.54
3	14-A	315	PO4	P-O2	-2.02	1.48	1.54
3	5-A	315	PO4	P-O4	-2.01	1.48	1.54
3	6-B	316	PO4	P-O2	-2.01	1.48	1.54
3	16-B	318	PO4	P-O2	-2.01	1.48	1.54
3	14-B	317	PO4	P-O3	-2.00	1.48	1.54
3	7-A	316	PO4	P-O3	-2.00	1.48	1.54
3	12-A	316	PO4	P-O2	-2.00	1.48	1.54

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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.