wwPDB X-ray Structure Validation Summary 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 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:

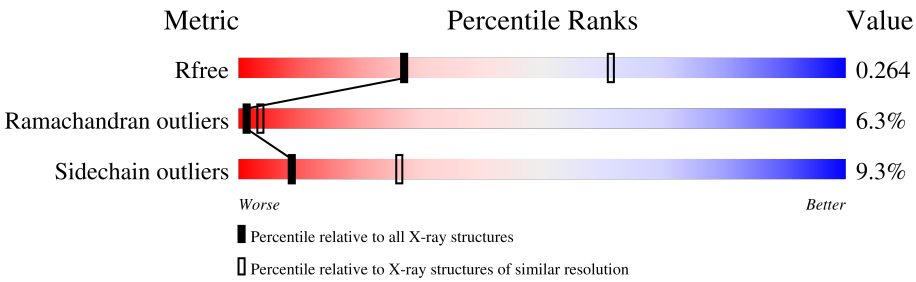
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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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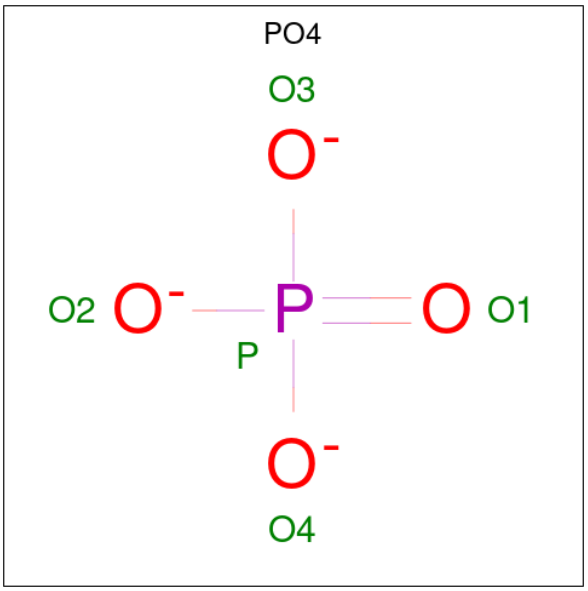
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	15-A	1	1	1	0	0
2	16-A	1	1	1	0	0
2	1-B	1	1	1	0	0
2	2-B	1	1	1	0	0
2	3-B	1	1	1	0	0
2	4-B	1	1	1	0	0
2	5-B	1	1	1	0	0
2	6-B	1	1	1	0	0
2	7-B	1	1	1	0	0
2	8-B	1	1	1	0	0
2	9-B	1	1	1	0	0
2	10-B	1	1	1	0	0
2	11-B	1	1	1	0	0
2	12-B	1	1	1	0	0
2	13-B	1	1	1	0	0
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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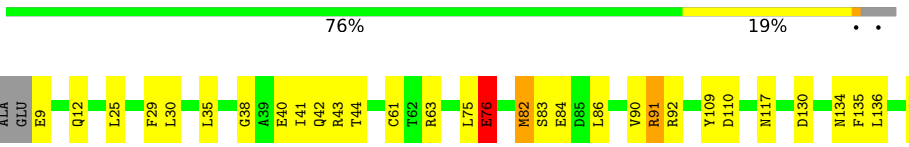
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	16-B	23	23	23	0	0

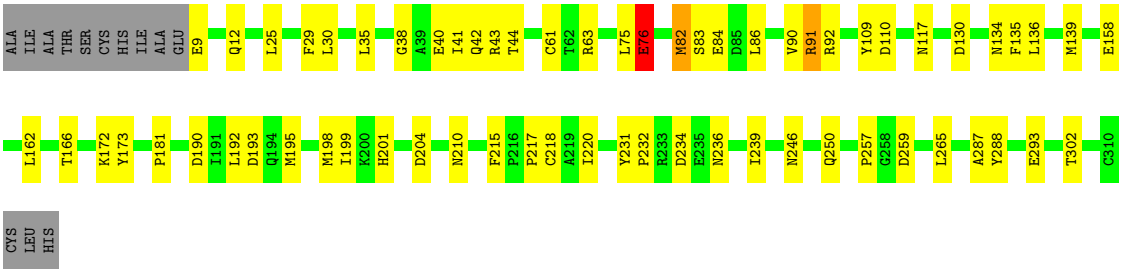
3 Residue-property plots (i)

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

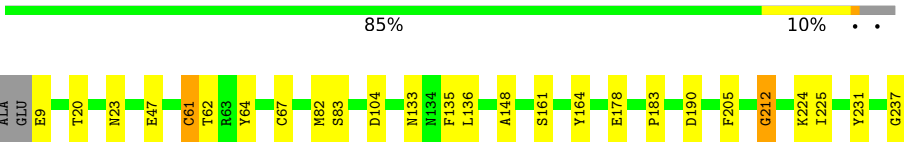
Chain 1-A:

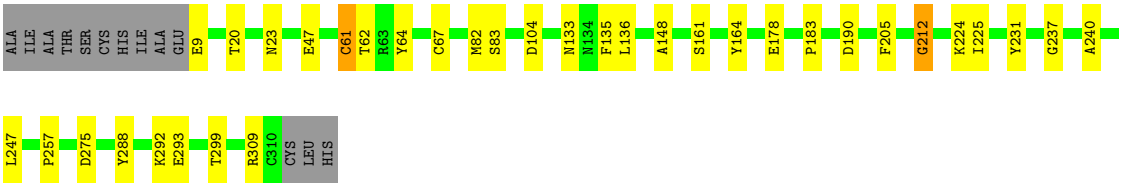




- Molecule 1: Aspartoacylase

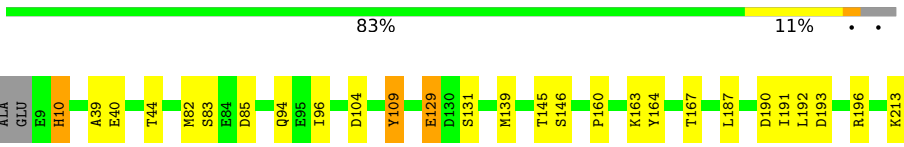
Chain 1-B:

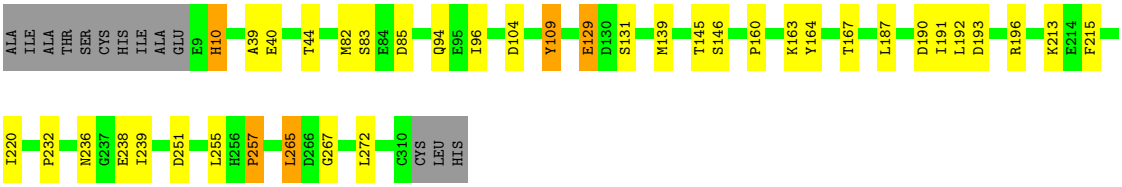




- Molecule 1: Aspartoacylase

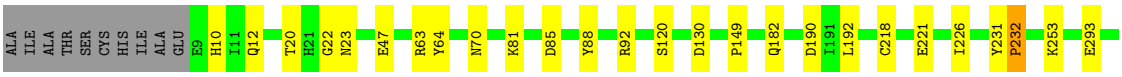
Chain 2-A:

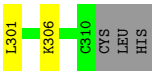




- Molecule 1: Aspartoacylase

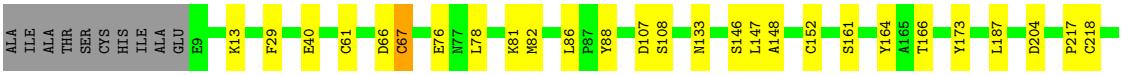
Chain 2-B:

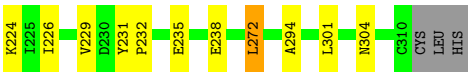




• Molecule 1: Aspartoacylase

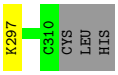
Chain 3-A:





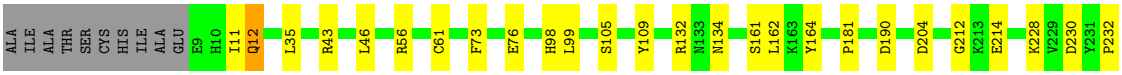
• Molecule 1: Aspartoacylase

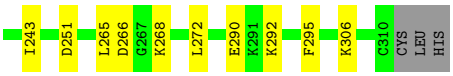
Chain 3-B:



• Molecule 1: Aspartoacylase

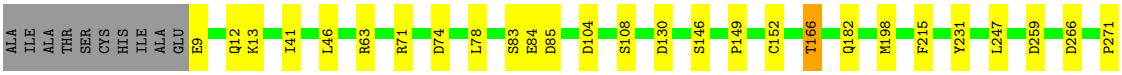
Chain 4-A:

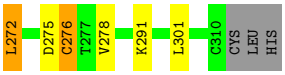




• Molecule 1: Aspartoacylase

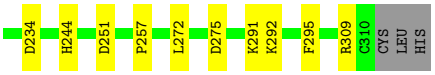
Chain 4-B:





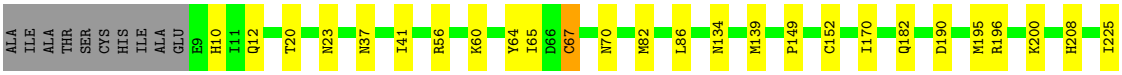
• Molecule 1: Aspartoacylase

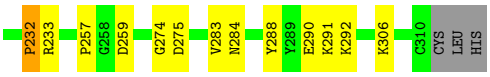
Chain 5-A:



- Molecule 1: Aspartoacylase

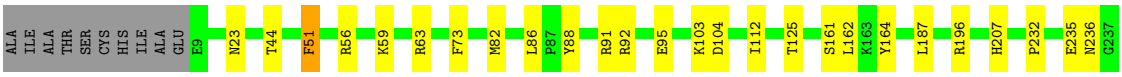
Chain 5-B:





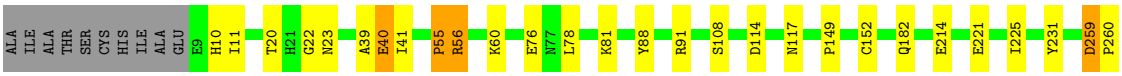
- Molecule 1: Aspartoacylase

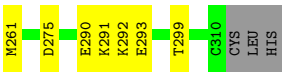
Chain 6-A:



- Molecule 1: Aspartoacylase

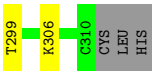
Chain 6-B:





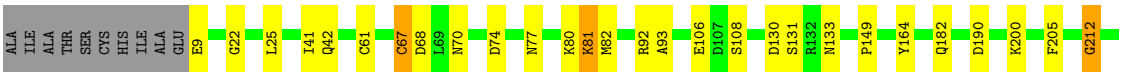
- Molecule 1: Aspartoacylase

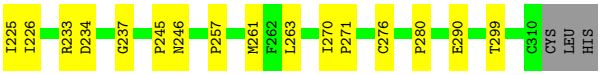
Chain 7-A:



- Molecule 1: Aspartoacylase

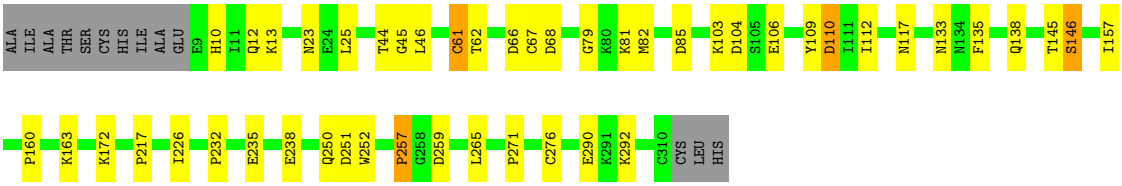
Chain 7-B:





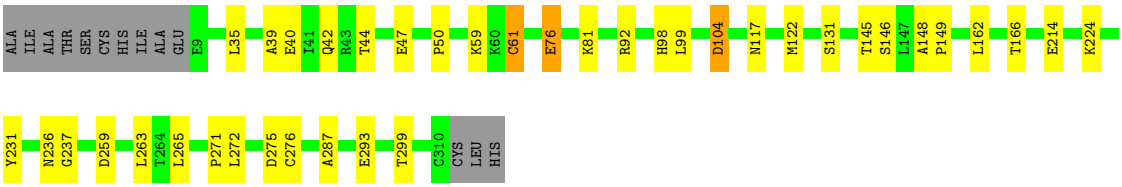
• Molecule 1: Aspartoacylase

Chain 8-A:



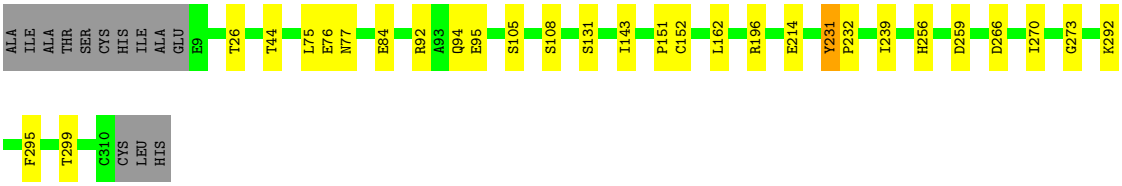
• Molecule 1: Aspartoacylase

Chain 8-B:



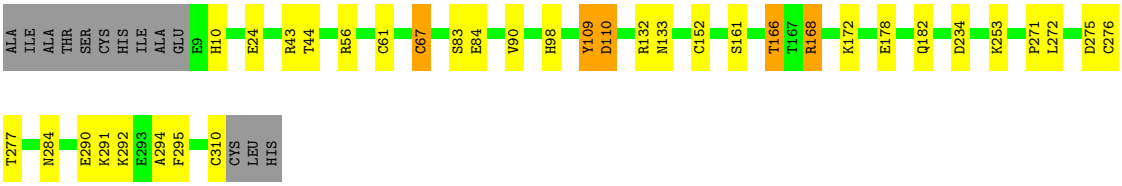
• Molecule 1: Aspartoacylase

Chain 9-A:



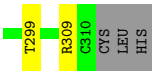
• Molecule 1: Aspartoacylase

Chain 9-B:



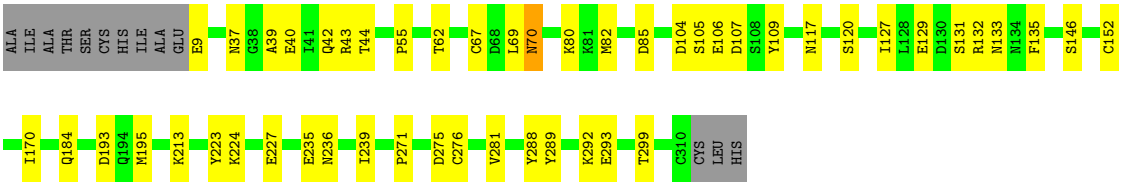
• Molecule 1: Aspartoacylase

Chain 10-A:



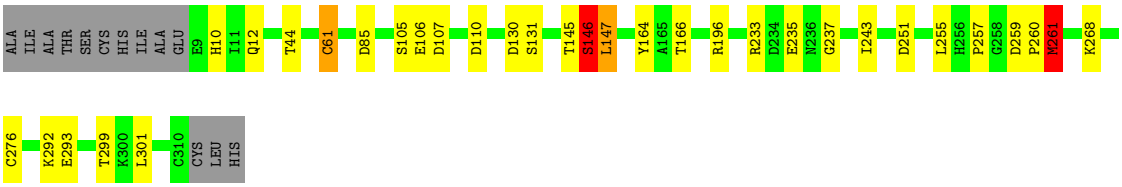
• Molecule 1: Aspartoacylase

Chain 10-B:



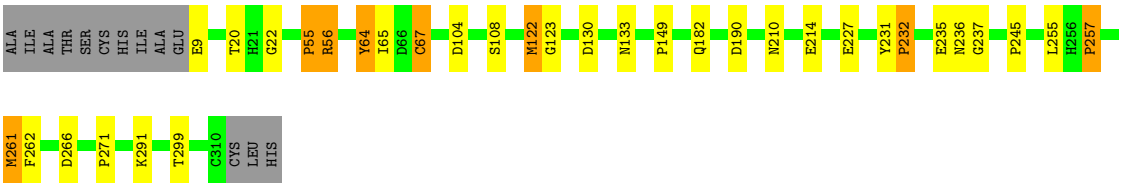
• Molecule 1: Aspartoacylase

Chain 11-A:



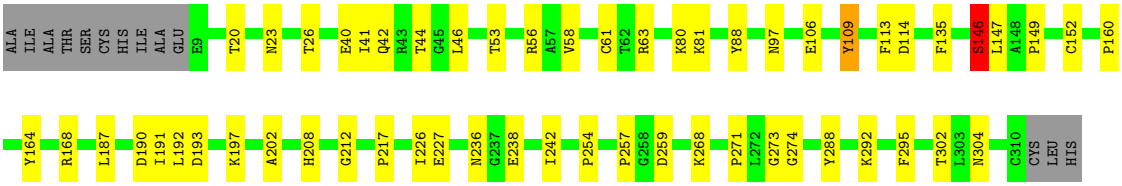
• Molecule 1: Aspartoacylase

Chain 11-B:



• Molecule 1: Aspartoacylase

Chain 12-A:

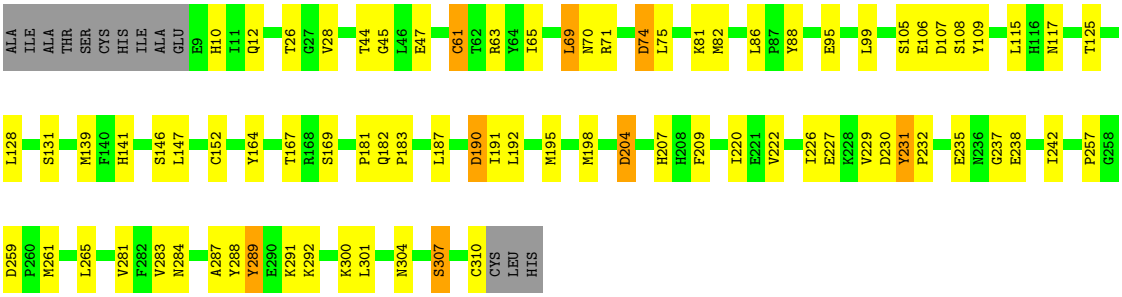


• Molecule 1: Aspartoacylase

Chain 12-B:

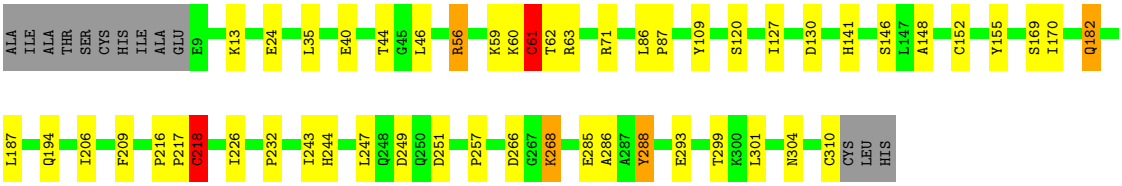
• Molecule 1: Aspartoacylase

Chain 13-A:



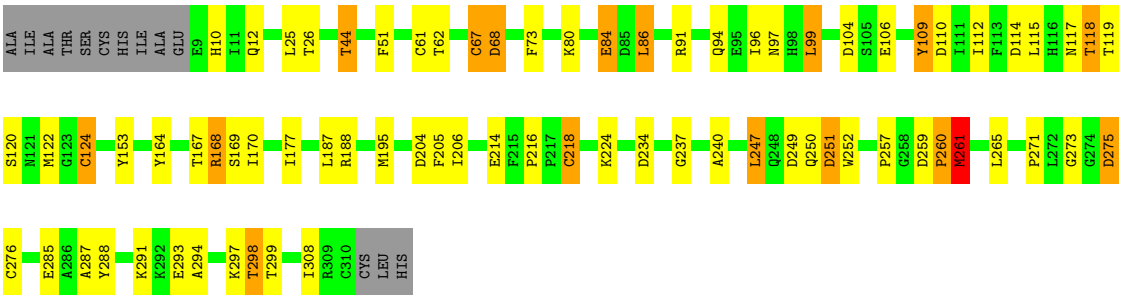
• Molecule 1: Aspartoacylase

Chain 13-B:



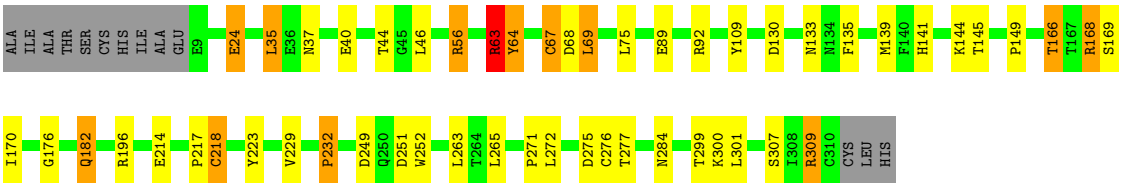
• Molecule 1: Aspartoacylase

Chain 14-A:



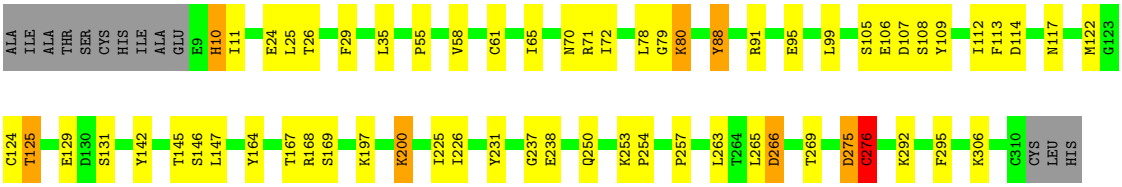
• Molecule 1: Aspartoacylase

Chain 14-B:



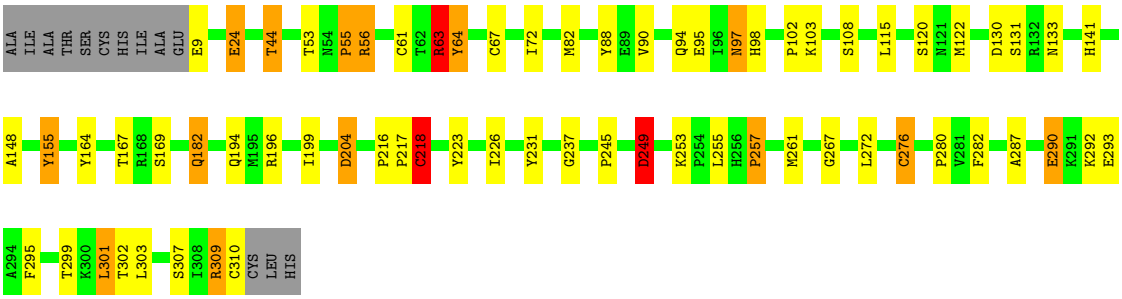
- Molecule 1: Aspartoacylase

Chain 15-A:



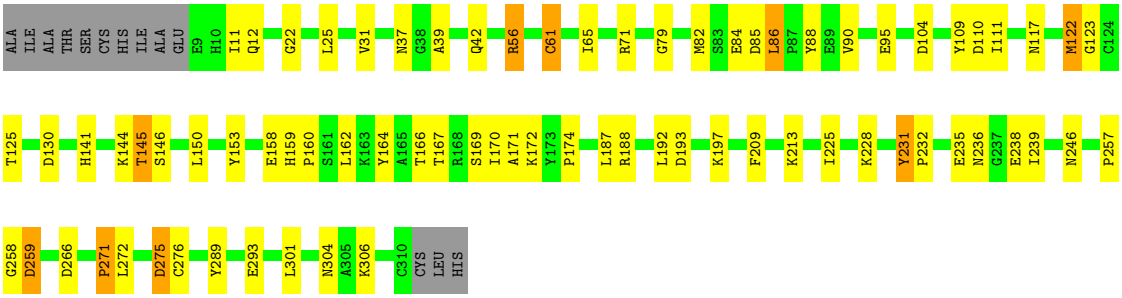
- Molecule 1: Aspartoacylase

Chain 15-B:



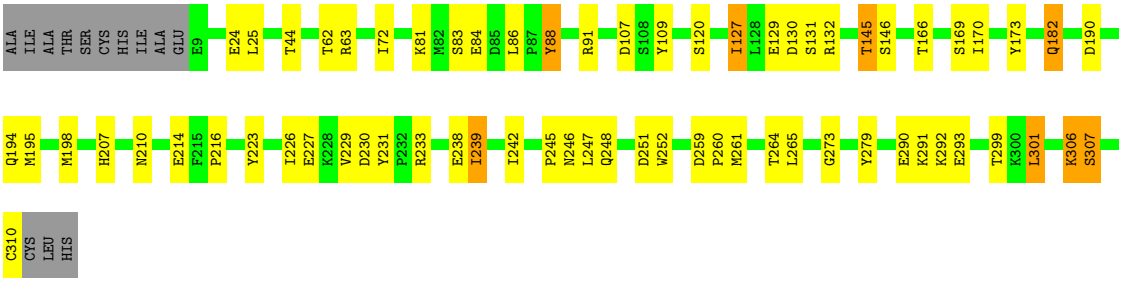
- Molecule 1: Aspartoacylase

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

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-B	164	TYR	Sidechain
1	1-B	231	TYR	Sidechain
1	2-A	164	TYR	Sidechain
1	3-A	164	TYR	Sidechain
1	3-A	173	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

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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

5 of 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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

5 of 794 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	12-A	257	PRO
1	13-B	288	TYR
1	12-B	108	SER
1	12-A	242	ILE
1	13-A	198	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 245 such sidechains are listed below:

Mol	Chain	Res	Type
1	8-B	33	HIS

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Mol	Chain	Res	Type
1	15-A	284	ASN
1	10-A	248	GLN
1	15-A	248	GLN
1	16-A	201	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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
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

The worst 5 of 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

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.