Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2021 – 02:44 pm BST

PDB ID	:	7AX5
Title	:	Anammox-specific acyl carrier protein from Kuenenia stuttgartiensis; ensemble refinement
Authors	:	Dietl, A.; Barends, T.
Deposited on	:	2020-11-09
Resolution	:	1.76 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 following versions of software and data (see references (1)) were used in the production of this report:

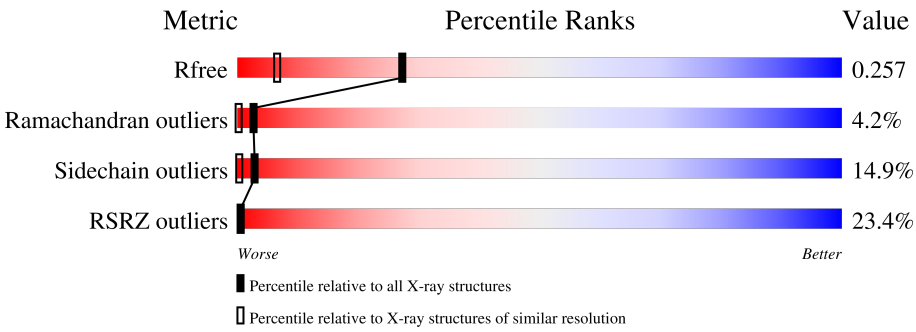
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	2340 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	94	20% 77% 17% • 5%
1	10-A	94	20% 78% 17% 5%
1	11-A	94	20% 76% 18% • 5%
1	12-A	94	20% 81% 12% • 5%
1	13-A	94	20% 78% 15% • 5%
1	14-A	94	20% 80% 12% • 5%
1	15-A	94	20% 76% 15% • 5%

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Mol	Chain	Length	Quality of chain
1	16-A	94	20% 80% 13% 5%
1	17-A	94	20% 83% 9% 5%
1	18-A	94	20% 77% 16% 5%
1	19-A	94	20% 81% 12% 5%
1	2-A	94	20% 80% 11% 5%
1	20-A	94	20% 80% 15% 5%
1	21-A	94	20% 82% 13% 5%
1	22-A	94	20% 84% 10% 5%
1	23-A	94	20% 83% 9% 5%
1	24-A	94	20% 80% 11% 5%
1	25-A	94	20% 82% 10% 5%
1	26-A	94	20% 85% 5% 5%
1	27-A	94	20% 85% 10% 5%
1	28-A	94	20% 84% 11% 5%
1	29-A	94	20% 86% 7% 5%
1	3-A	94	20% 82% 9% 5%
1	30-A	94	20% 85% 10% 5%
1	31-A	94	20% 82% 13% 5%
1	32-A	94	20% 79% 15% 5%
1	33-A	94	20% 82% 11% 5%
1	34-A	94	20% 77% 16% 5%
1	35-A	94	20% 76% 14% 5% 5%
1	36-A	94	20% 77% 16% 5%
1	37-A	94	20% 78% 13% 5%
1	38-A	94	20% 80% 13% 5%

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Mol	Chain	Length	Quality of chain
1	39-A	94	20% 80% 14% 5%
1	4-A	94	20% 81% 12% 5%
1	40-A	94	20% 86% 7% 5%
1	41-A	94	20% 73% 19% 5%
1	42-A	94	20% 74% 19% 5%
1	43-A	94	20% 81% 12% 5%
1	44-A	94	20% 80% 14% 5%
1	45-A	94	20% 78% 15% 5%
1	46-A	94	20% 74% 20% 5%
1	47-A	94	20% 79% 14% 5%
1	48-A	94	20% 79% 16% 5%
1	49-A	94	20% 76% 19% 5%
1	5-A	94	20% 72% 19% 5%
1	50-A	94	20% 77% 17% 5%
1	51-A	94	20% 74% 18% 5%
1	52-A	94	20% 72% 20% 5%
1	53-A	94	20% 77% 14% 5%
1	54-A	94	20% 68% 26% 5%
1	55-A	94	20% 77% 16% 5%
1	56-A	94	20% 81% 14% 5%
1	57-A	94	20% 82% 13% 5%
1	58-A	94	20% 80% 15% 5%
1	59-A	94	20% 80% 13% 5%
1	6-A	94	20% 81% 12% 5%
1	60-A	94	20% 79% 14% 5%

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Mol	Chain	Length	Quality of chain
1	61-A	94	20% 78% 14% 5%
1	62-A	94	20% 80% 15% 5%
1	63-A	94	20% 78% 17% 5%
1	64-A	94	20% 79% 15% 5%
1	65-A	94	20% 76% 18% 5%
1	66-A	94	20% 82% 10% 5%
1	67-A	94	20% 84% 9% 5%
1	68-A	94	20% 80% 12% 5%
1	69-A	94	20% 80% 13% 5%
1	7-A	94	20% 80% 13% 5%
1	70-A	94	20% 73% 21% 5%
1	71-A	94	20% 79% 13% 5%
1	72-A	94	20% 77% 15% 5%
1	73-A	94	20% 81% 13% 5%
1	74-A	94	20% 81% 12% 5%
1	75-A	94	20% 78% 15% 5%
1	8-A	94	20% 81% 12% 5%
1	9-A	94	20% 78% 14% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 107290 atoms, of which 53025 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 Similar to acyl carrier protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
1	1-A	89	1408	447	707	107	147	0	0	0
1	2-A	89	1408	447	707	107	147	0	0	0
1	3-A	89	1408	447	707	107	147	0	0	0
1	4-A	89	1408	447	707	107	147	0	0	0
1	5-A	89	1408	447	707	107	147	0	0	0
1	6-A	89	1408	447	707	107	147	0	0	0
1	7-A	89	1408	447	707	107	147	0	0	0
1	8-A	89	1408	447	707	107	147	0	0	0
1	9-A	89	1408	447	707	107	147	0	0	0
1	10-A	89	1408	447	707	107	147	0	0	0
1	11-A	89	1408	447	707	107	147	0	0	0
1	12-A	89	1408	447	707	107	147	0	0	0
1	13-A	89	1408	447	707	107	147	0	0	0
1	14-A	89	1408	447	707	107	147	0	0	0
1	15-A	89	1408	447	707	107	147	0	0	0
1	16-A	89	1408	447	707	107	147	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
1	17-A	89	1408	447	707	107	147	0	0	0
1	18-A	89	1408	447	707	107	147	0	0	0
1	19-A	89	1408	447	707	107	147	0	0	0
1	20-A	89	1408	447	707	107	147	0	0	0
1	21-A	89	1408	447	707	107	147	0	0	0
1	22-A	89	1408	447	707	107	147	0	0	0
1	23-A	89	1408	447	707	107	147	0	0	0
1	24-A	89	1408	447	707	107	147	0	0	0
1	25-A	89	1408	447	707	107	147	0	0	0
1	26-A	89	1408	447	707	107	147	0	0	0
1	27-A	89	1408	447	707	107	147	0	0	0
1	28-A	89	1408	447	707	107	147	0	0	0
1	29-A	89	1408	447	707	107	147	0	0	0
1	30-A	89	1408	447	707	107	147	0	0	0
1	31-A	89	1408	447	707	107	147	0	0	0
1	32-A	89	1408	447	707	107	147	0	0	0
1	33-A	89	1408	447	707	107	147	0	0	0
1	34-A	89	1408	447	707	107	147	0	0	0
1	35-A	89	1408	447	707	107	147	0	0	0
1	36-A	89	1408	447	707	107	147	0	0	0
1	37-A	89	1408	447	707	107	147	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
1	38-A	89	1408	447	707	107	147	0	0	0
1	39-A	89	1408	447	707	107	147	0	0	0
1	40-A	89	1408	447	707	107	147	0	0	0
1	41-A	89	1408	447	707	107	147	0	0	0
1	42-A	89	1408	447	707	107	147	0	0	0
1	43-A	89	1408	447	707	107	147	0	0	0
1	44-A	89	1408	447	707	107	147	0	0	0
1	45-A	89	1408	447	707	107	147	0	0	0
1	46-A	89	1408	447	707	107	147	0	0	0
1	47-A	89	1408	447	707	107	147	0	0	0
1	48-A	89	1408	447	707	107	147	0	0	0
1	49-A	89	1408	447	707	107	147	0	0	0
1	50-A	89	1408	447	707	107	147	0	0	0
1	51-A	89	1408	447	707	107	147	0	0	0
1	52-A	89	1408	447	707	107	147	0	0	0
1	53-A	89	1408	447	707	107	147	0	0	0
1	54-A	89	1408	447	707	107	147	0	0	0
1	55-A	89	1408	447	707	107	147	0	0	0
1	56-A	89	1408	447	707	107	147	0	0	0
1	57-A	89	1408	447	707	107	147	0	0	0
1	58-A	89	1408	447	707	107	147	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
1	59-A	89	1408	447	707	107	147	0	0	0
1	60-A	89	1408	447	707	107	147	0	0	0
1	61-A	89	1408	447	707	107	147	0	0	0
1	62-A	89	1408	447	707	107	147	0	0	0
1	63-A	89	1408	447	707	107	147	0	0	0
1	64-A	89	1408	447	707	107	147	0	0	0
1	65-A	89	1408	447	707	107	147	0	0	0
1	66-A	89	1408	447	707	107	147	0	0	0
1	67-A	89	1408	447	707	107	147	0	0	0
1	68-A	89	1408	447	707	107	147	0	0	0
1	69-A	89	1408	447	707	107	147	0	0	0
1	70-A	89	1408	447	707	107	147	0	0	0
1	71-A	89	1408	447	707	107	147	0	0	0
1	72-A	89	1408	447	707	107	147	0	0	0
1	73-A	89	1408	447	707	107	147	0	0	0
1	74-A	89	1408	447	707	107	147	0	0	0
1	75-A	89	1408	447	707	107	147	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q1Q2X6
A	2	ASP	-	expression tag	UNP Q1Q2X6
A	87	LEU	-	expression tag	UNP Q1Q2X6
A	88	GLU	-	expression tag	UNP Q1Q2X6
A	89	HIS	-	expression tag	UNP Q1Q2X6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	90	HIS	-	expression tag	UNP Q1Q2X6
A	91	HIS	-	expression tag	UNP Q1Q2X6
A	92	HIS	-	expression tag	UNP Q1Q2X6
A	93	HIS	-	expression tag	UNP Q1Q2X6
A	94	HIS	-	expression tag	UNP Q1Q2X6

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	1-A	7	7	7	0	0
2	2-A	7	7	7	0	0
2	3-A	7	7	7	0	0
2	4-A	7	7	7	0	0
2	5-A	7	7	7	0	0
2	6-A	7	7	7	0	0
2	7-A	7	7	7	0	0
2	8-A	7	7	7	0	0
2	9-A	7	7	7	0	0
2	10-A	7	7	7	0	0
2	11-A	7	7	7	0	0
2	12-A	7	7	7	0	0
2	13-A	7	7	7	0	0
2	14-A	7	7	7	0	0
2	15-A	7	7	7	0	0
2	16-A	7	7	7	0	0
2	17-A	7	7	7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	18-A	7	7	7	0	0
2	19-A	7	7	7	0	0
2	20-A	7	7	7	0	0
2	21-A	7	7	7	0	0
2	22-A	7	7	7	0	0
2	23-A	7	7	7	0	0
2	24-A	7	7	7	0	0
2	25-A	7	7	7	0	0
2	26-A	7	7	7	0	0
2	27-A	7	7	7	0	0
2	28-A	7	7	7	0	0
2	29-A	7	7	7	0	0
2	30-A	7	7	7	0	0
2	31-A	7	7	7	0	0
2	32-A	7	7	7	0	0
2	33-A	7	7	7	0	0
2	34-A	7	7	7	0	0
2	35-A	7	7	7	0	0
2	36-A	7	7	7	0	0
2	37-A	7	7	7	0	0
2	38-A	7	7	7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	39-A	7	7	7	0	0
2	40-A	7	7	7	0	0
2	41-A	7	7	7	0	0
2	42-A	7	7	7	0	0
2	43-A	7	7	7	0	0
2	44-A	7	7	7	0	0
2	45-A	7	7	7	0	0
2	46-A	7	7	7	0	0
2	47-A	7	7	7	0	0
2	48-A	7	7	7	0	0
2	49-A	7	7	7	0	0
2	50-A	7	7	7	0	0
2	51-A	7	7	7	0	0
2	52-A	7	7	7	0	0
2	53-A	7	7	7	0	0
2	54-A	7	7	7	0	0
2	55-A	7	7	7	0	0
2	56-A	7	7	7	0	0
2	57-A	7	7	7	0	0
2	58-A	7	7	7	0	0
2	59-A	7	7	7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	60-A	7	Total Zn 7 7	0	0
2	61-A	7	Total Zn 7 7	0	0
2	62-A	7	Total Zn 7 7	0	0
2	63-A	7	Total Zn 7 7	0	0
2	64-A	7	Total Zn 7 7	0	0
2	65-A	7	Total Zn 7 7	0	0
2	66-A	7	Total Zn 7 7	0	0
2	67-A	7	Total Zn 7 7	0	0
2	68-A	7	Total Zn 7 7	0	0
2	69-A	7	Total Zn 7 7	0	0
2	70-A	7	Total Zn 7 7	0	0
2	71-A	7	Total Zn 7 7	0	0
2	72-A	7	Total Zn 7 7	0	0
2	73-A	7	Total Zn 7 7	0	0
2	74-A	7	Total Zn 7 7	0	0
2	75-A	7	Total Zn 7 7	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	1-A	16	Total O 16 16	0	0
3	2-A	13	Total O 13 13	0	0
3	3-A	15	Total O 15 15	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	4-A	11	Total O 11 11	0	0
3	5-A	9	Total O 9 9	0	0
3	6-A	16	Total O 16 16	0	0
3	7-A	17	Total O 17 17	0	0
3	8-A	16	Total O 16 16	0	0
3	9-A	17	Total O 17 17	0	0
3	10-A	15	Total O 15 15	0	0
3	11-A	12	Total O 12 12	0	0
3	12-A	15	Total O 15 15	0	0
3	13-A	17	Total O 17 17	0	0
3	14-A	14	Total O 14 14	0	0
3	15-A	10	Total O 10 10	0	0
3	16-A	13	Total O 13 13	0	0
3	17-A	14	Total O 14 14	0	0
3	18-A	9	Total O 9 9	0	0
3	19-A	12	Total O 12 12	0	0
3	20-A	17	Total O 17 17	0	0
3	21-A	18	Total O 18 18	0	0
3	22-A	17	Total O 17 17	0	0
3	23-A	15	Total O 15 15	0	0
3	24-A	17	Total O 17 17	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	25-A	17	Total O 17 17	0	0
3	26-A	14	Total O 14 14	0	0
3	27-A	11	Total O 11 11	0	0
3	28-A	11	Total O 11 11	0	0
3	29-A	12	Total O 12 12	0	0
3	30-A	13	Total O 13 13	0	0
3	31-A	11	Total O 11 11	0	0
3	32-A	17	Total O 17 17	0	0
3	33-A	18	Total O 18 18	0	0
3	34-A	18	Total O 18 18	0	0
3	35-A	15	Total O 15 15	0	0
3	36-A	12	Total O 12 12	0	0
3	37-A	16	Total O 16 16	0	0
3	38-A	18	Total O 18 18	0	0
3	39-A	16	Total O 16 16	0	0
3	40-A	10	Total O 10 10	0	0
3	41-A	20	Total O 20 20	0	0
3	42-A	15	Total O 15 15	0	0
3	43-A	17	Total O 17 17	0	0
3	44-A	20	Total O 20 20	0	0
3	45-A	18	Total O 18 18	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	46-A	14	Total O 14 14	0	0
3	47-A	15	Total O 15 15	0	0
3	48-A	10	Total O 10 10	0	0
3	49-A	15	Total O 15 15	0	0
3	50-A	15	Total O 15 15	0	0
3	51-A	18	Total O 18 18	0	0
3	52-A	12	Total O 12 12	0	0
3	53-A	15	Total O 15 15	0	0
3	54-A	19	Total O 19 19	0	0
3	55-A	21	Total O 21 21	0	0
3	56-A	19	Total O 19 19	0	0
3	57-A	22	Total O 22 22	0	0
3	58-A	18	Total O 18 18	0	0
3	59-A	24	Total O 24 24	0	0
3	60-A	21	Total O 21 21	0	0
3	61-A	16	Total O 16 16	0	0
3	62-A	15	Total O 15 15	0	0
3	63-A	18	Total O 18 18	0	0
3	64-A	17	Total O 17 17	0	0
3	65-A	14	Total O 14 14	0	0
3	66-A	14	Total O 14 14	0	0

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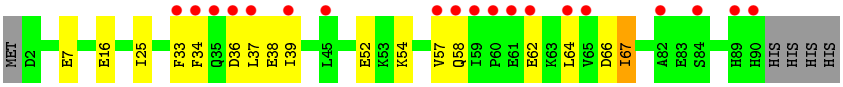
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	67-A	17	17	17	0	0
			Total	O		
3	68-A	16	16	16	0	0
			Total	O		
3	69-A	18	18	18	0	0
			Total	O		
3	70-A	20	20	20	0	0
			Total	O		
3	71-A	19	19	19	0	0
			Total	O		
3	72-A	19	19	19	0	0
			Total	O		
3	73-A	16	16	16	0	0
			Total	O		
3	74-A	14	14	14	0	0
			Total	O		
3	75-A	10	10	10	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

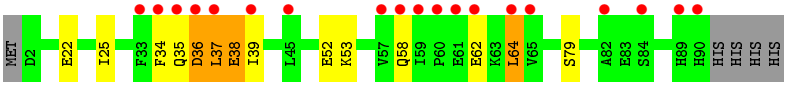
- Molecule 1: Similar to acyl carrier protein

Chain 1-A:



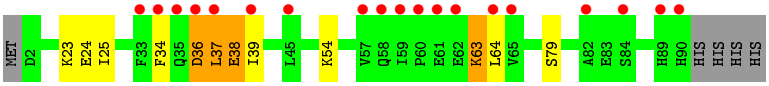
- Molecule 1: Similar to acyl carrier protein

Chain 2-A:



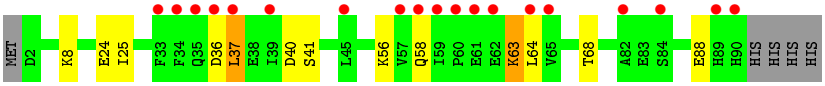
- Molecule 1: Similar to acyl carrier protein

Chain 3-A:



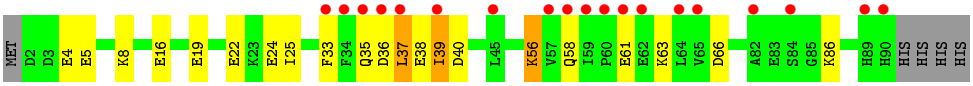
- Molecule 1: Similar to acyl carrier protein

Chain 4-A:



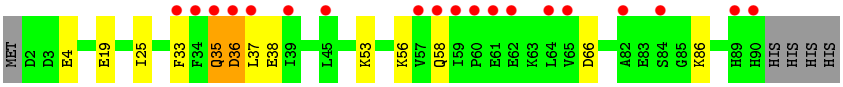
- Molecule 1: Similar to acyl carrier protein

Chain 5-A:



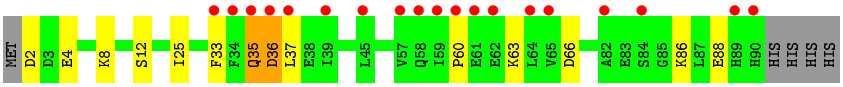
- Molecule 1: Similar to acyl carrier protein

Chain 6-A:



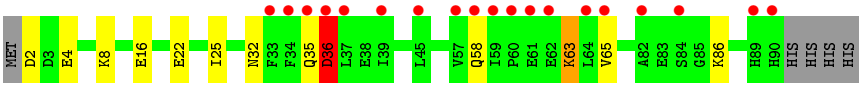
- Molecule 1: Similar to acyl carrier protein

Chain 7-A:



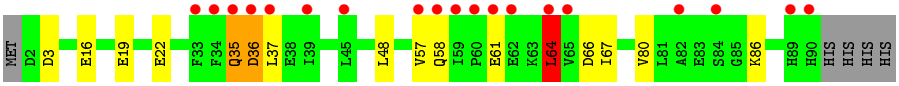
- Molecule 1: Similar to acyl carrier protein

Chain 8-A:



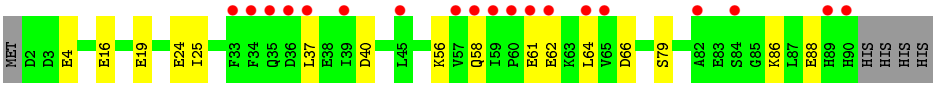
- Molecule 1: Similar to acyl carrier protein

Chain 9-A:



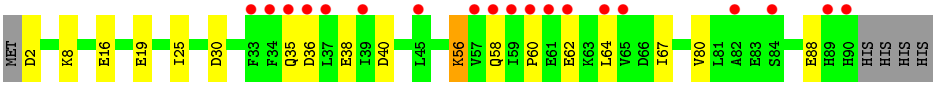
- Molecule 1: Similar to acyl carrier protein

Chain 10-A:



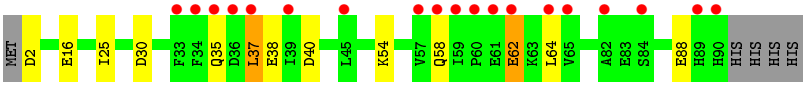
- Molecule 1: Similar to acyl carrier protein

Chain 11-A:



- Molecule 1: Similar to acyl carrier protein

Chain 12-A:

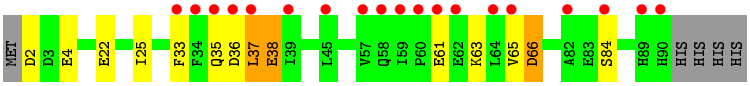


- Molecule 1: Similar to acyl carrier protein

Chain 13-A:

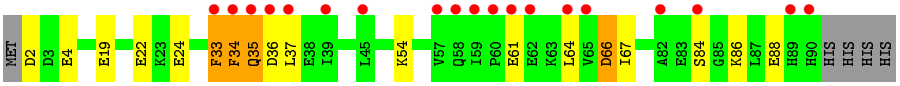
- Molecule 1: Similar to acyl carrier protein

Chain 14-A:



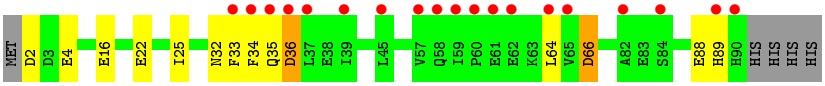
- Molecule 1: Similar to acyl carrier protein

Chain 15-A:



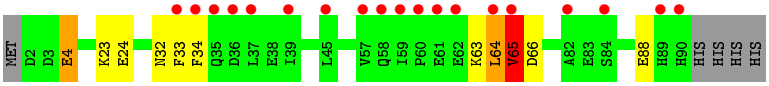
- Molecule 1: Similar to acyl carrier protein

Chain 16-A:



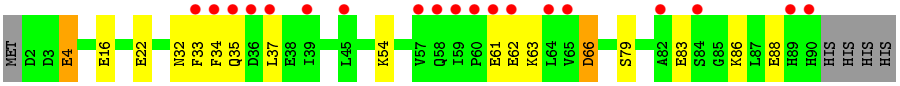
- Molecule 1: Similar to acyl carrier protein

Chain 17-A:



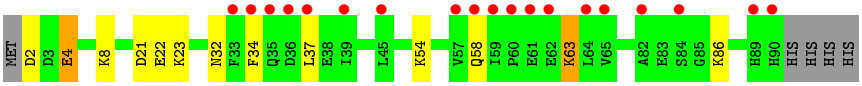
- Molecule 1: Similar to acyl carrier protein

Chain 18-A:



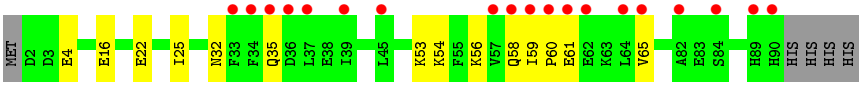
- Molecule 1: Similar to acyl carrier protein

Chain 19-A:



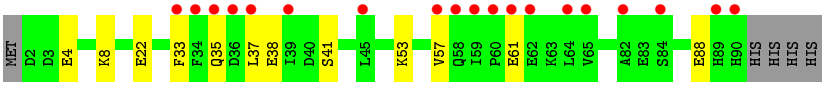
- Molecule 1: Similar to acyl carrier protein

Chain 20-A:



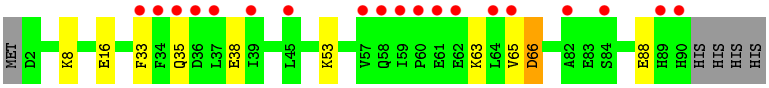
- Molecule 1: Similar to acyl carrier protein

Chain 21-A:



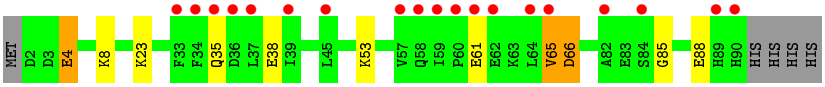
- Molecule 1: Similar to acyl carrier protein

Chain 22-A:



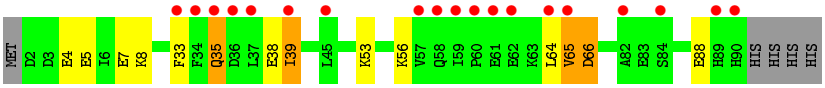
- Molecule 1: Similar to acyl carrier protein

Chain 23-A:



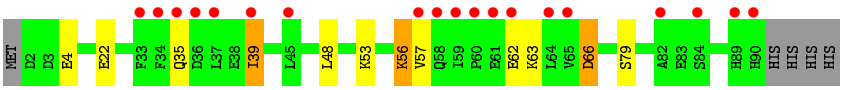
- Molecule 1: Similar to acyl carrier protein

Chain 24-A:



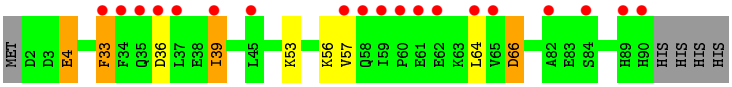
- Molecule 1: Similar to acyl carrier protein

Chain 25-A:



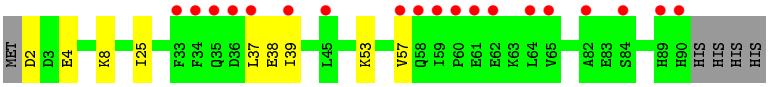
- Molecule 1: Similar to acyl carrier protein

Chain 26-A:



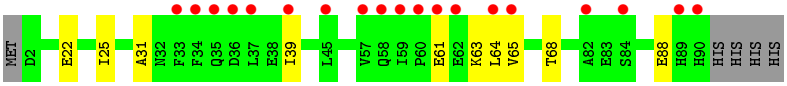
- Molecule 1: Similar to acyl carrier protein

Chain 27-A:



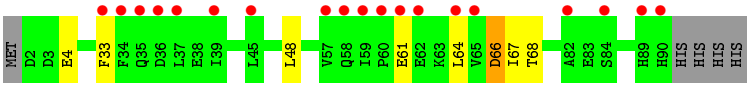
- Molecule 1: Similar to acyl carrier protein

Chain 28-A:



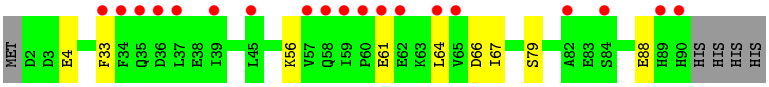
- Molecule 1: Similar to acyl carrier protein

Chain 29-A:



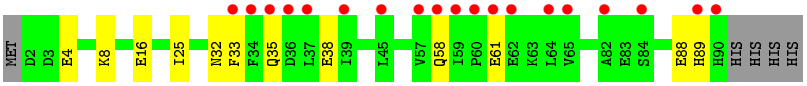
- Molecule 1: Similar to acyl carrier protein

Chain 30-A:



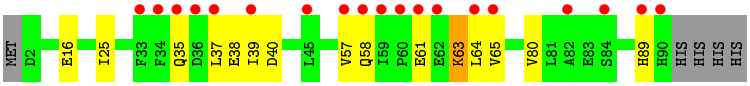
- Molecule 1: Similar to acyl carrier protein

Chain 31-A:



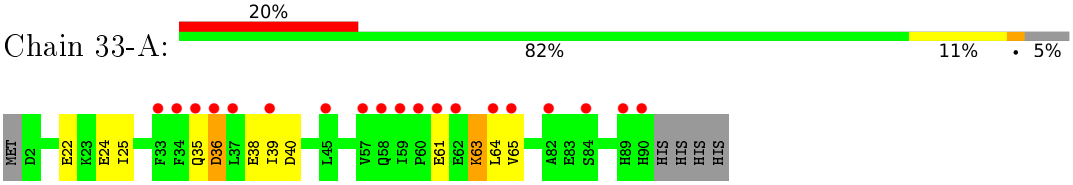
- Molecule 1: Similar to acyl carrier protein

Chain 32-A:



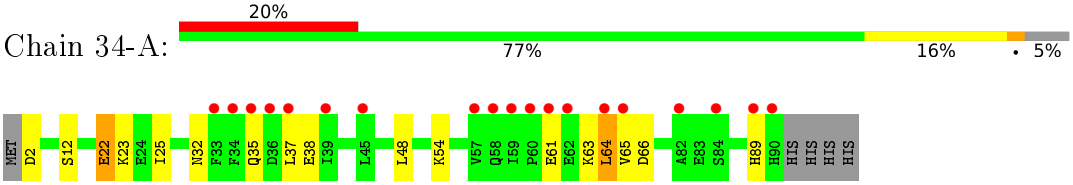
- Molecule 1: Similar to acyl carrier protein

Chain 33-A:



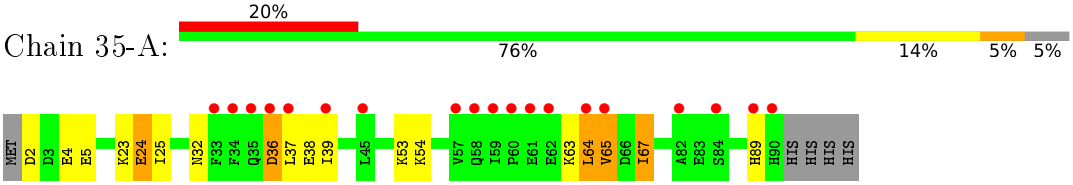
- Molecule 1: Similar to acyl carrier protein

Chain 34-A:



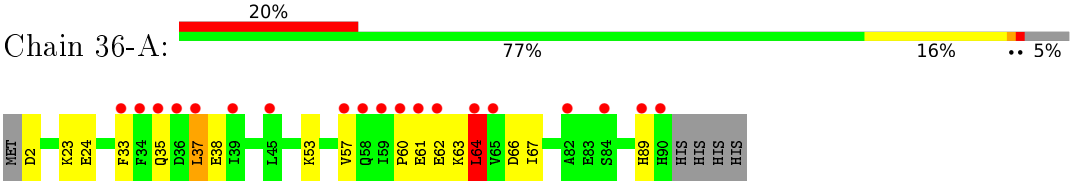
- Molecule 1: Similar to acyl carrier protein

Chain 35-A:



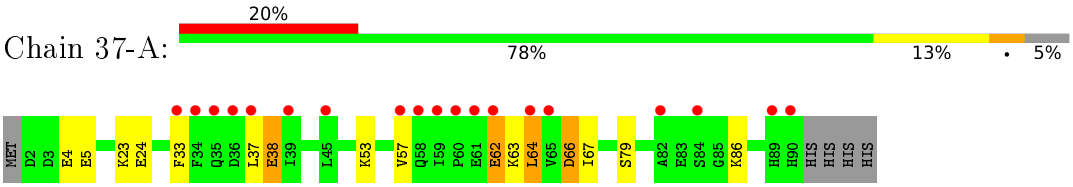
- Molecule 1: Similar to acyl carrier protein

Chain 36-A:



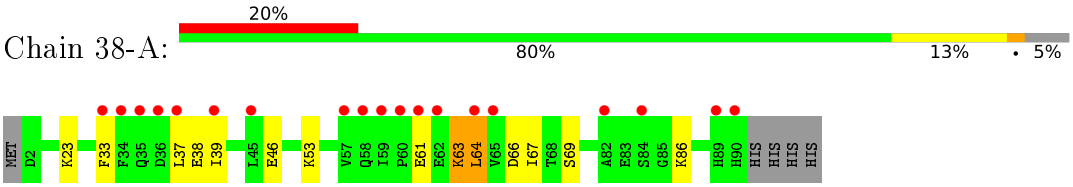
- Molecule 1: Similar to acyl carrier protein

Chain 37-A:



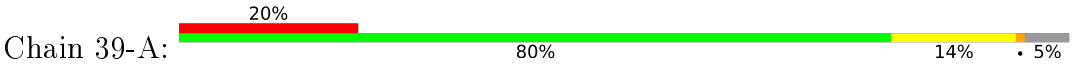
- Molecule 1: Similar to acyl carrier protein

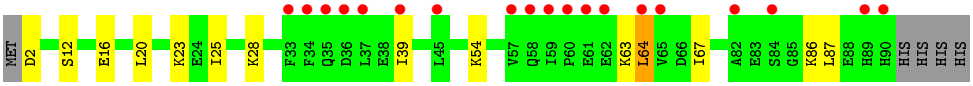
Chain 38-A:



- Molecule 1: Similar to acyl carrier protein

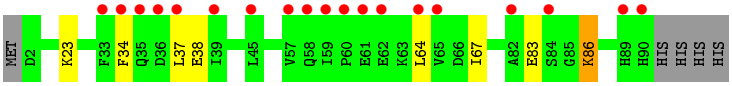
Chain 39-A:





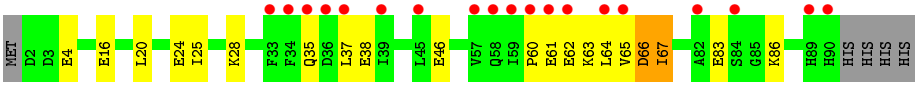
- Molecule 1: Similar to acyl carrier protein

Chain 40-A:



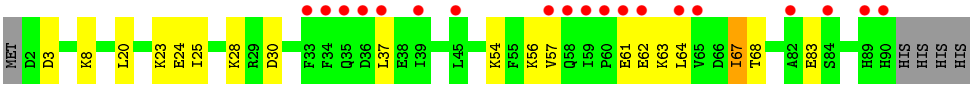
- Molecule 1: Similar to acyl carrier protein

Chain 41-A:



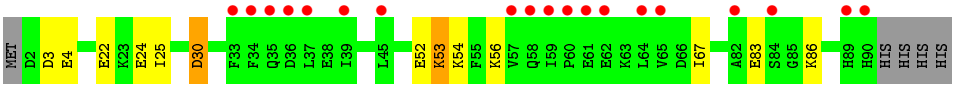
- Molecule 1: Similar to acyl carrier protein

Chain 42-A:



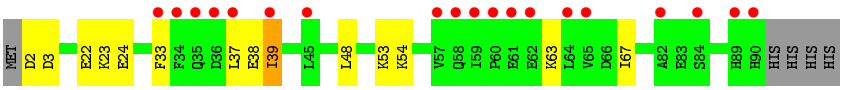
- Molecule 1: Similar to acyl carrier protein

Chain 43-A:



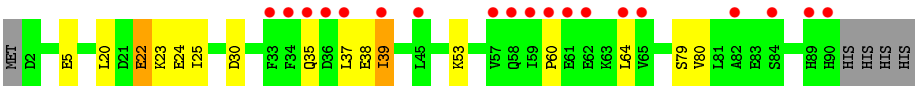
- Molecule 1: Similar to acyl carrier protein

Chain 44-A:



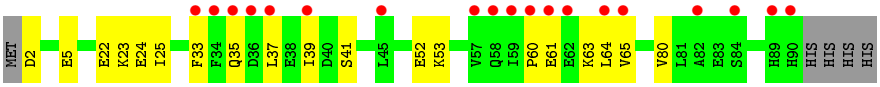
- Molecule 1: Similar to acyl carrier protein

Chain 45-A:



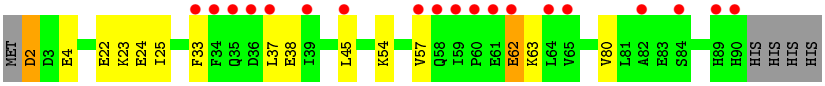
- Molecule 1: Similar to acyl carrier protein

Chain 46-A:



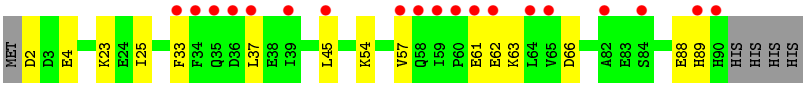
- Molecule 1: Similar to acyl carrier protein

Chain 47-A:



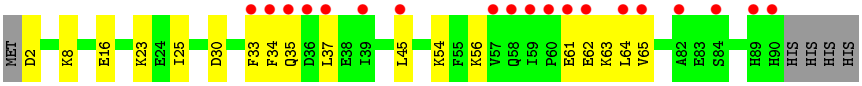
- Molecule 1: Similar to acyl carrier protein

Chain 48-A:



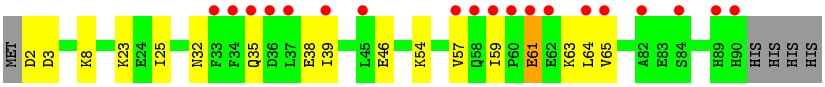
- Molecule 1: Similar to acyl carrier protein

Chain 49-A:



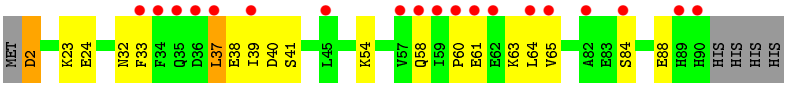
- Molecule 1: Similar to acyl carrier protein

Chain 50-A:



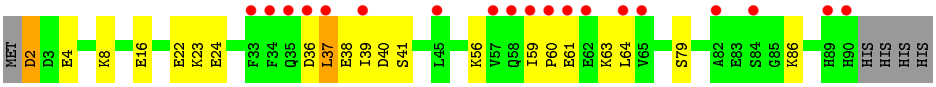
- Molecule 1: Similar to acyl carrier protein

Chain 51-A:



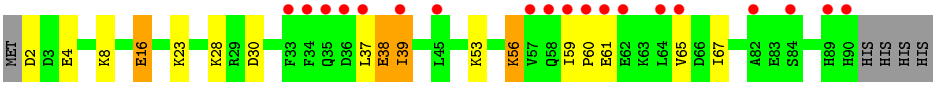
- Molecule 1: Similar to acyl carrier protein

Chain 52-A:



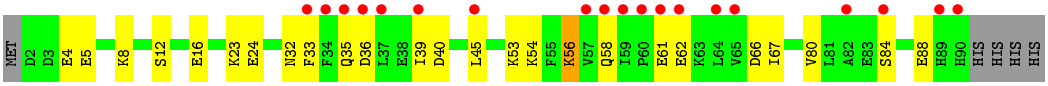
- Molecule 1: Similar to acyl carrier protein

Chain 53-A:



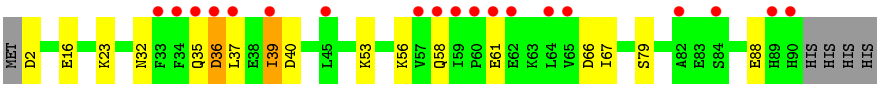
- Molecule 1: Similar to acyl carrier protein

Chain 54-A:



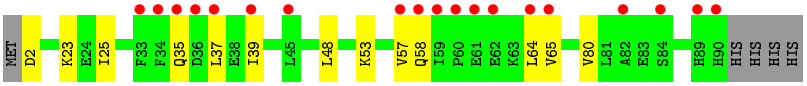
- Molecule 1: Similar to acyl carrier protein

Chain 55-A:



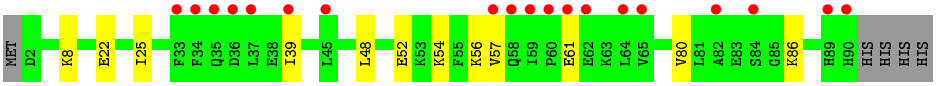
- Molecule 1: Similar to acyl carrier protein

Chain 56-A:



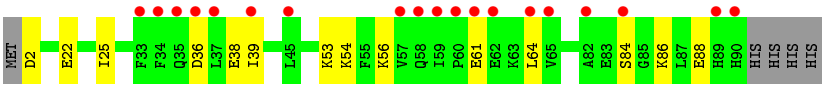
- Molecule 1: Similar to acyl carrier protein

Chain 57-A:



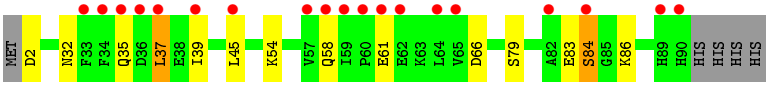
- Molecule 1: Similar to acyl carrier protein

Chain 58-A:



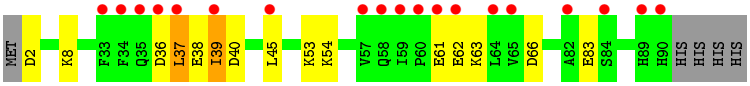
- Molecule 1: Similar to acyl carrier protein

Chain 59-A:



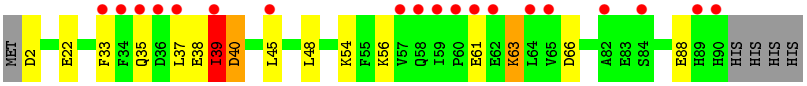
- Molecule 1: Similar to acyl carrier protein

Chain 60-A:



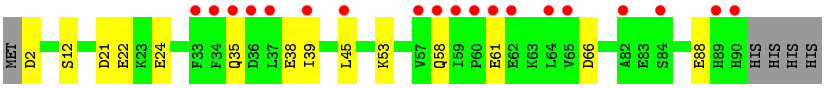
- Molecule 1: Similar to acyl carrier protein

Chain 61-A:



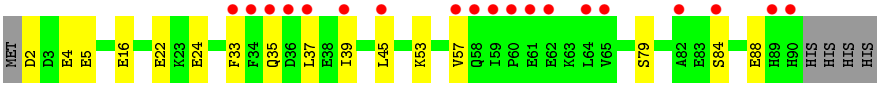
- Molecule 1: Similar to acyl carrier protein

Chain 62-A:



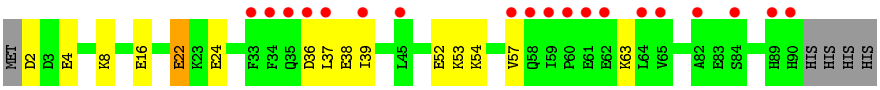
- Molecule 1: Similar to acyl carrier protein

Chain 63-A:



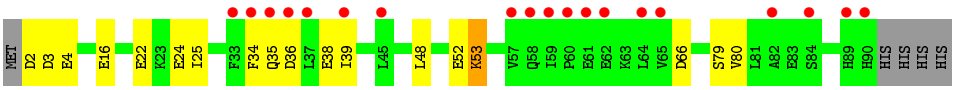
- Molecule 1: Similar to acyl carrier protein

Chain 64-A:



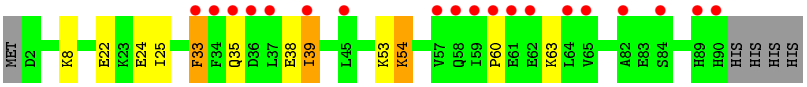
- Molecule 1: Similar to acyl carrier protein

Chain 65-A:



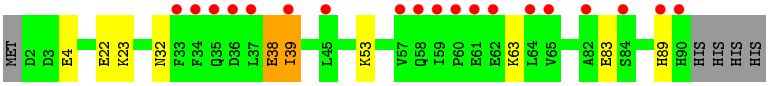
- Molecule 1: Similar to acyl carrier protein

Chain 66-A:



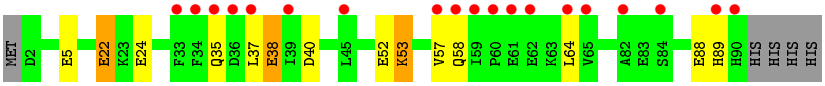
- Molecule 1: Similar to acyl carrier protein

Chain 67-A:



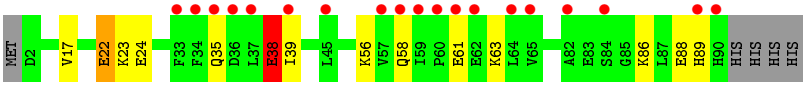
- Molecule 1: Similar to acyl carrier protein

Chain 68-A:



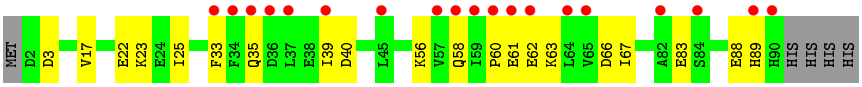
- Molecule 1: Similar to acyl carrier protein

Chain 69-A:



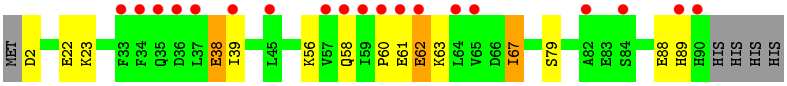
- Molecule 1: Similar to acyl carrier protein

Chain 70-A:



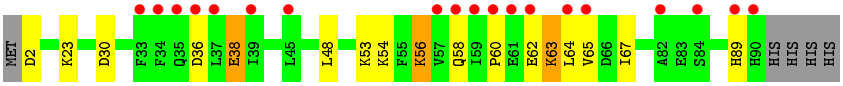
- Molecule 1: Similar to acyl carrier protein

Chain 71-A:



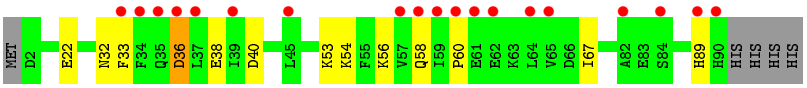
- Molecule 1: Similar to acyl carrier protein

Chain 72-A:



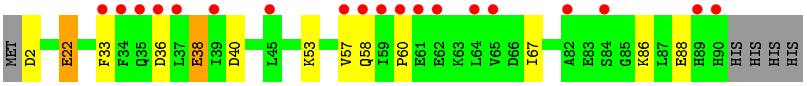
- Molecule 1: Similar to acyl carrier protein

Chain 73-A:



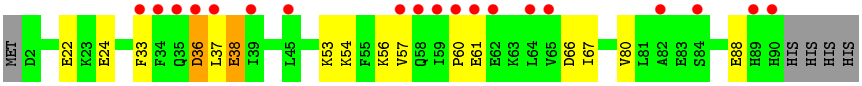
- Molecule 1: Similar to acyl carrier protein

Chain 74-A:



- Molecule 1: Similar to acyl carrier protein

Chain 75-A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α, β, γ	76.81Å 76.81Å 30.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.40 – 1.76 38.41 – 1.76	Depositor EDS
% Data completeness (in resolution range)	70.2 (38.40-1.76) 63.8 (38.41-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.48 (at 1.76Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement:1.15.2_3472)	Depositor
R, R_{free}	0.175 , 0.234 0.202 , 0.257	Depositor DCC
R_{free} test set	360 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	29.2	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 342.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.094 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	107290	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.27% 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: 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	0.55	0/707	0.69	0/953
1	2-A	0.57	0/707	0.68	1/953 (0.1%)
1	3-A	0.66	1/707 (0.1%)	0.68	0/953
1	4-A	0.67	2/707 (0.3%)	0.70	0/953
1	5-A	0.61	1/707 (0.1%)	0.69	0/953
1	6-A	0.57	0/707	0.64	0/953
1	7-A	0.62	0/707	0.65	0/953
1	8-A	0.60	0/707	0.66	0/953
1	9-A	0.58	0/707	0.68	1/953 (0.1%)
1	10-A	0.57	0/707	0.66	0/953
1	11-A	0.56	0/707	0.67	0/953
1	12-A	0.61	0/707	0.70	1/953 (0.1%)
1	13-A	0.65	1/707 (0.1%)	0.68	0/953
1	14-A	0.57	0/707	0.66	0/953
1	15-A	0.60	0/707	0.68	0/953
1	16-A	0.58	0/707	0.69	0/953
1	17-A	0.63	1/707 (0.1%)	0.74	0/953
1	18-A	0.62	1/707 (0.1%)	0.67	0/953
1	19-A	0.66	1/707 (0.1%)	0.72	1/953 (0.1%)
1	20-A	0.56	0/707	0.67	0/953
1	21-A	0.53	0/707	0.66	0/953
1	22-A	0.59	0/707	0.61	0/953
1	23-A	0.64	1/707 (0.1%)	0.65	0/953
1	24-A	0.70	2/707 (0.3%)	0.69	1/953 (0.1%)
1	25-A	0.60	0/707	0.68	0/953
1	26-A	0.61	1/707 (0.1%)	0.65	0/953
1	27-A	0.64	1/707 (0.1%)	0.65	0/953
1	28-A	0.62	0/707	0.63	0/953
1	29-A	0.61	0/707	0.69	1/953 (0.1%)
1	30-A	0.63	0/707	0.67	0/953
1	31-A	0.58	0/707	0.65	0/953
1	32-A	0.64	0/707	0.67	1/953 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	33-A	0.64	1/707 (0.1%)	0.66	0/953
1	34-A	0.70	1/707 (0.1%)	0.70	0/953
1	35-A	0.63	1/707 (0.1%)	0.65	0/953
1	36-A	0.64	0/707	0.71	1/953 (0.1%)
1	37-A	0.64	1/707 (0.1%)	0.70	0/953
1	38-A	0.55	0/707	0.69	1/953 (0.1%)
1	39-A	0.56	0/707	0.71	1/953 (0.1%)
1	40-A	0.56	0/707	0.69	0/953
1	41-A	0.55	1/707 (0.1%)	0.65	0/953
1	42-A	0.55	0/707	0.68	0/953
1	43-A	0.68	1/707 (0.1%)	0.69	0/953
1	44-A	0.65	1/707 (0.1%)	0.62	0/953
1	45-A	0.59	1/707 (0.1%)	0.69	0/953
1	46-A	0.58	0/707	0.65	0/953
1	47-A	0.61	0/707	0.67	1/953 (0.1%)
1	48-A	0.58	0/707	0.67	0/953
1	49-A	0.58	0/707	0.67	0/953
1	50-A	0.58	0/707	0.65	0/953
1	51-A	0.56	0/707	0.71	0/953
1	52-A	0.55	0/707	0.72	3/953 (0.3%)
1	53-A	0.60	0/707	0.64	0/953
1	54-A	0.68	2/707 (0.3%)	0.64	0/953
1	55-A	0.57	0/707	0.64	0/953
1	56-A	0.58	0/707	0.65	0/953
1	57-A	0.53	0/707	0.61	0/953
1	58-A	0.55	0/707	0.63	0/953
1	59-A	0.65	0/707	0.71	0/953
1	60-A	0.55	0/707	0.65	0/953
1	61-A	0.62	0/707	0.66	0/953
1	62-A	0.54	0/707	0.65	0/953
1	63-A	0.54	0/707	0.62	0/953
1	64-A	0.56	1/707 (0.1%)	0.65	0/953
1	65-A	0.62	0/707	0.68	0/953
1	66-A	0.58	0/707	0.65	0/953
1	67-A	0.56	0/707	0.65	0/953
1	68-A	0.62	2/707 (0.3%)	0.68	0/953
1	69-A	0.71	4/707 (0.6%)	0.67	0/953
1	70-A	0.63	2/707 (0.3%)	0.67	0/953
1	71-A	0.61	2/707 (0.3%)	0.67	0/953
1	72-A	0.57	0/707	0.68	0/953
1	73-A	0.57	0/707	0.66	0/953
1	74-A	0.66	1/707 (0.1%)	0.71	0/953
1	75-A	0.58	0/707	0.63	0/953

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.60	35/53025 (0.1%)	0.67	14/71475 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	1
1	2-A	0	1
1	3-A	0	1
1	4-A	0	2
1	5-A	0	2
1	6-A	0	2
1	7-A	0	2
1	8-A	0	1
1	13-A	0	1
1	14-A	0	2
1	15-A	0	2
1	17-A	0	1
1	18-A	0	1
1	23-A	0	1
1	24-A	0	1
1	28-A	0	1
1	29-A	0	1
1	30-A	0	1
1	34-A	0	1
1	48-A	0	1
1	49-A	0	1
1	51-A	0	1
1	54-A	0	1
1	56-A	0	1
1	59-A	0	1
1	60-A	0	1
1	61-A	0	1
1	69-A	0	1
1	71-A	0	1
1	72-A	0	1
All	All	0	36

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	54-A	62	GLU	CG-CD	-9.68	1.37	1.51
1	24-A	4	GLU	CB-CG	6.95	1.65	1.52
1	24-A	4	GLU	CG-CD	6.67	1.61	1.51
1	70-A	88	GLU	CB-CG	6.63	1.64	1.52
1	34-A	22	GLU	CG-CD	6.53	1.61	1.51
1	35-A	24	GLU	CB-CG	6.44	1.64	1.52
1	5-A	24	GLU	CG-CD	6.33	1.61	1.51
1	4-A	24	GLU	CG-CD	6.24	1.61	1.51
1	69-A	88	GLU	CB-CG	6.17	1.63	1.52
1	26-A	4	GLU	CG-CD	5.98	1.60	1.51
1	33-A	22	GLU	CB-CG	-5.96	1.40	1.52
1	69-A	22	GLU	CG-CD	5.96	1.60	1.51
1	45-A	22	GLU	CB-CG	5.93	1.63	1.52
1	23-A	4	GLU	CB-CG	5.88	1.63	1.52
1	27-A	4	GLU	CG-CD	5.83	1.60	1.51
1	44-A	22	GLU	CB-CG	5.82	1.63	1.52
1	18-A	4	GLU	CB-CG	5.76	1.63	1.52
1	54-A	62	GLU	CB-CG	5.68	1.62	1.52
1	19-A	4	GLU	CG-CD	5.66	1.60	1.51
1	71-A	88	GLU	CB-CG	5.51	1.62	1.52
1	3-A	24	GLU	CG-CD	5.46	1.60	1.51
1	37-A	24	GLU	CB-CG	5.34	1.62	1.52
1	71-A	88	GLU	CD-OE2	5.29	1.31	1.25
1	4-A	88	GLU	CB-CG	5.25	1.62	1.52
1	74-A	22	GLU	CB-CG	5.24	1.62	1.52
1	69-A	22	GLU	CB-CG	5.24	1.62	1.52
1	69-A	88	GLU	CD-OE2	5.22	1.31	1.25
1	70-A	88	GLU	CD-OE2	5.20	1.31	1.25
1	43-A	22	GLU	CB-CG	5.17	1.61	1.52
1	64-A	22	GLU	CG-CD	5.14	1.59	1.51
1	68-A	22	GLU	CB-CG	5.10	1.61	1.52
1	13-A	19	GLU	CG-CD	5.09	1.59	1.51
1	41-A	4	GLU	CB-CG	5.08	1.61	1.52
1	17-A	4	GLU	CB-CG	5.07	1.61	1.52
1	68-A	88	GLU	CB-CG	5.04	1.61	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	29-A	4	GLU	CA-CB-CG	7.79	130.53	113.40
1	52-A	40	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	19-A	21	ASP	CB-CG-OD1	6.33	124.00	118.30
1	24-A	4	GLU	OE1-CD-OE2	-6.24	115.82	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	9-A	64	LEU	CA-CB-CG	6.23	129.64	115.30
1	38-A	64	LEU	CA-CB-CG	6.00	129.09	115.30
1	36-A	64	LEU	CA-CB-CG	5.93	128.93	115.30
1	47-A	2	ASP	CB-CG-OD1	-5.76	113.11	118.30
1	52-A	40	ASP	CB-CG-OD1	5.63	123.37	118.30
1	12-A	40	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	39-A	64	LEU	CA-CB-CG	5.33	127.57	115.30
1	2-A	37	LEU	CA-CB-CG	5.25	127.38	115.30
1	32-A	37	LEU	CA-CB-CG	5.14	127.13	115.30
1	52-A	2	ASP	CB-CG-OD2	-5.03	113.77	118.30

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	66	ASP	Peptide
1	13-A	38	GLU	Peptide
1	14-A	33	PHE	Peptide
1	14-A	38	GLU	Peptide
1	15-A	33	PHE	Peptide
1	15-A	34	PHE	Peptide
1	17-A	65	VAL	Peptide
1	18-A	66	ASP	Peptide
1	2-A	36	ASP	Peptide
1	23-A	65	VAL	Peptide
1	24-A	65	VAL	Peptide
1	28-A	65	VAL	Peptide
1	29-A	66	ASP	Peptide
1	3-A	36	ASP	Peptide
1	30-A	66	ASP	Peptide
1	34-A	63	LYS	Peptide
1	4-A	36	ASP	Peptide
1	4-A	37	LEU	Peptide
1	48-A	61	GLU	Peptide
1	49-A	56	LYS	Peptide
1	5-A	37	LEU	Peptide
1	5-A	39	ILE	Peptide
1	51-A	2	ASP	Peptide
1	54-A	36	ASP	Peptide
1	56-A	37	LEU	Peptide
1	59-A	84	SER	Peptide
1	6-A	35	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	6-A	36	ASP	Peptide
1	60-A	66	ASP	Peptide
1	61-A	39	ILE	Peptide
1	69-A	38	GLU	Peptide
1	7-A	35	GLN	Peptide
1	7-A	36	ASP	Peptide
1	71-A	67	ILE	Peptide
1	72-A	63	LYS	Peptide
1	8-A	36	ASP	Peptide

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	701	707	711	0	0
1	2-A	701	707	711	0	0
1	3-A	701	707	711	0	0
1	4-A	701	707	711	0	0
1	5-A	701	707	711	0	0
1	6-A	701	707	711	0	0
1	7-A	701	707	711	0	0
1	8-A	701	707	711	0	0
1	9-A	701	707	711	0	0
1	10-A	701	707	711	0	0
1	11-A	701	707	711	0	0
1	12-A	701	707	711	0	0
1	13-A	701	707	711	0	0
1	14-A	701	707	711	0	0
1	15-A	701	707	711	0	0
1	16-A	701	707	711	0	0
1	17-A	701	707	711	0	0
1	18-A	701	707	711	0	0
1	19-A	701	707	711	0	0
1	20-A	701	707	711	0	0
1	21-A	701	707	711	0	0
1	22-A	701	707	711	0	0
1	23-A	701	707	711	0	0
1	24-A	701	707	711	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	25-A	701	707	711	0	0
1	26-A	701	707	711	0	0
1	27-A	701	707	711	0	0
1	28-A	701	707	711	0	0
1	29-A	701	707	711	0	0
1	30-A	701	707	711	0	0
1	31-A	701	707	711	0	0
1	32-A	701	707	711	0	0
1	33-A	701	707	711	0	0
1	34-A	701	707	711	0	0
1	35-A	701	707	711	0	0
1	36-A	701	707	711	0	0
1	37-A	701	707	711	0	0
1	38-A	701	707	711	0	0
1	39-A	701	707	711	0	0
1	40-A	701	707	711	0	0
1	41-A	701	707	711	0	0
1	42-A	701	707	710	0	0
1	43-A	701	707	711	0	0
1	44-A	701	707	711	0	0
1	45-A	701	707	711	0	0
1	46-A	701	707	711	0	0
1	47-A	701	707	711	0	0
1	48-A	701	707	710	0	0
1	49-A	701	707	711	0	0
1	50-A	701	707	711	0	0
1	51-A	701	707	711	0	0
1	52-A	701	707	711	0	0
1	53-A	701	707	710	0	0
1	54-A	701	707	711	0	0
1	55-A	701	707	711	0	0
1	56-A	701	707	711	0	0
1	57-A	701	707	711	0	0
1	58-A	701	707	711	0	0
1	59-A	701	707	711	0	0
1	60-A	701	707	711	0	0
1	61-A	701	707	711	0	0
1	62-A	701	707	711	0	0
1	63-A	701	707	711	0	0
1	64-A	701	707	711	0	0
1	65-A	701	707	711	0	0
1	66-A	701	707	711	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	67-A	701	707	711	0	0
1	68-A	701	707	711	0	0
1	69-A	701	707	711	0	0
1	70-A	701	707	711	0	0
1	71-A	701	707	711	0	0
1	72-A	701	707	711	0	0
1	73-A	701	707	711	0	0
1	74-A	701	707	711	0	0
1	75-A	701	707	711	0	0
2	1-A	7	0	0	0	0
2	2-A	7	0	0	0	0
2	3-A	7	0	0	0	0
2	4-A	7	0	0	0	0
2	5-A	7	0	0	0	0
2	6-A	7	0	0	0	0
2	7-A	7	0	0	0	0
2	8-A	7	0	0	0	0
2	9-A	7	0	0	0	0
2	10-A	7	0	0	0	0
2	11-A	7	0	0	0	0
2	12-A	7	0	0	0	0
2	13-A	7	0	0	0	0
2	14-A	7	0	0	0	0
2	15-A	7	0	0	0	0
2	16-A	7	0	0	0	0
2	17-A	7	0	0	0	0
2	18-A	7	0	0	0	0
2	19-A	7	0	0	0	0
2	20-A	7	0	0	0	0
2	21-A	7	0	0	0	0
2	22-A	7	0	0	0	0
2	23-A	7	0	0	0	0
2	24-A	7	0	0	0	0
2	25-A	7	0	0	0	0
2	26-A	7	0	0	0	0
2	27-A	7	0	0	0	0
2	28-A	7	0	0	0	0
2	29-A	7	0	0	0	0
2	30-A	7	0	0	0	0
2	31-A	7	0	0	0	0
2	32-A	7	0	0	0	0
2	33-A	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	34-A	7	0	0	0	0
2	35-A	7	0	0	0	0
2	36-A	7	0	0	0	0
2	37-A	7	0	0	0	0
2	38-A	7	0	0	0	0
2	39-A	7	0	0	0	0
2	40-A	7	0	0	0	0
2	41-A	7	0	0	0	0
2	42-A	7	0	0	0	0
2	43-A	7	0	0	0	0
2	44-A	7	0	0	0	0
2	45-A	7	0	0	0	0
2	46-A	7	0	0	0	0
2	47-A	7	0	0	0	0
2	48-A	7	0	0	0	0
2	49-A	7	0	0	0	0
2	50-A	7	0	0	0	0
2	51-A	7	0	0	0	0
2	52-A	7	0	0	0	0
2	53-A	7	0	0	0	0
2	54-A	7	0	0	0	0
2	55-A	7	0	0	0	0
2	56-A	7	0	0	0	0
2	57-A	7	0	0	0	0
2	58-A	7	0	0	0	0
2	59-A	7	0	0	0	0
2	60-A	7	0	0	0	0
2	61-A	7	0	0	0	0
2	62-A	7	0	0	0	0
2	63-A	7	0	0	0	0
2	64-A	7	0	0	0	0
2	65-A	7	0	0	0	0
2	66-A	7	0	0	0	0
2	67-A	7	0	0	0	0
2	68-A	7	0	0	0	0
2	69-A	7	0	0	0	0
2	70-A	7	0	0	0	0
2	71-A	7	0	0	0	0
2	72-A	7	0	0	0	0
2	73-A	7	0	0	0	0
2	74-A	7	0	0	0	0
2	75-A	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	1-A	16	0	0	0	0
3	2-A	13	0	0	0	0
3	3-A	15	0	0	0	0
3	4-A	11	0	0	0	0
3	5-A	9	0	0	0	0
3	6-A	16	0	0	0	0
3	7-A	17	0	0	0	0
3	8-A	16	0	0	0	0
3	9-A	17	0	0	0	0
3	10-A	15	0	0	0	0
3	11-A	12	0	0	0	0
3	12-A	15	0	0	0	0
3	13-A	17	0	0	0	0
3	14-A	14	0	0	0	0
3	15-A	10	0	0	0	0
3	16-A	13	0	0	0	0
3	17-A	14	0	0	0	0
3	18-A	9	0	0	0	0
3	19-A	12	0	0	0	0
3	20-A	17	0	0	0	0
3	21-A	18	0	0	0	0
3	22-A	17	0	0	0	0
3	23-A	15	0	0	0	0
3	24-A	17	0	0	0	0
3	25-A	17	0	0	0	0
3	26-A	14	0	0	0	0
3	27-A	11	0	0	0	0
3	28-A	11	0	0	0	0
3	29-A	12	0	0	0	0
3	30-A	13	0	0	0	0
3	31-A	11	0	0	0	0
3	32-A	17	0	0	0	0
3	33-A	18	0	0	0	0
3	34-A	18	0	0	0	0
3	35-A	15	0	0	0	0
3	36-A	12	0	0	0	0
3	37-A	16	0	0	0	0
3	38-A	18	0	0	0	0
3	39-A	16	0	0	0	0
3	40-A	10	0	0	0	0
3	41-A	20	0	0	0	0
3	42-A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	43-A	17	0	0	0	0
3	44-A	20	0	0	0	0
3	45-A	18	0	0	0	0
3	46-A	14	0	0	0	0
3	47-A	15	0	0	0	0
3	48-A	10	0	0	0	0
3	49-A	15	0	0	0	0
3	50-A	15	0	0	0	0
3	51-A	18	0	0	0	0
3	52-A	12	0	0	0	0
3	53-A	15	0	0	0	0
3	54-A	19	0	0	0	0
3	55-A	21	0	0	0	0
3	56-A	19	0	0	0	0
3	57-A	22	0	0	0	0
3	58-A	18	0	0	0	0
3	59-A	24	0	0	0	0
3	60-A	21	0	0	0	0
3	61-A	16	0	0	0	0
3	62-A	15	0	0	0	0
3	63-A	18	0	0	0	0
3	64-A	17	0	0	0	0
3	65-A	14	0	0	0	0
3	66-A	14	0	0	0	0
3	67-A	17	0	0	0	0
3	68-A	16	0	0	0	0
3	69-A	18	0	0	0	0
3	70-A	20	0	0	0	0
3	71-A	19	0	0	0	0
3	72-A	19	0	0	0	0
3	73-A	16	0	0	0	0
3	74-A	14	0	0	0	0
3	75-A	10	0	0	0	0
All	All	54265	53025	53322	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	87/94 (93%)	73 (84%)	8 (9%)	6 (7%)	1	0
1	2-A	87/94 (93%)	72 (83%)	9 (10%)	6 (7%)	1	0
1	3-A	87/94 (93%)	72 (83%)	10 (12%)	5 (6%)	1	0
1	4-A	87/94 (93%)	76 (87%)	7 (8%)	4 (5%)	2	0
1	5-A	87/94 (93%)	77 (88%)	5 (6%)	5 (6%)	1	0
1	6-A	87/94 (93%)	79 (91%)	5 (6%)	3 (3%)	3	0
1	7-A	87/94 (93%)	77 (88%)	6 (7%)	4 (5%)	2	0
1	8-A	87/94 (93%)	79 (91%)	5 (6%)	3 (3%)	3	0
1	9-A	87/94 (93%)	78 (90%)	4 (5%)	5 (6%)	1	0
1	10-A	87/94 (93%)	77 (88%)	8 (9%)	2 (2%)	6	1
1	11-A	87/94 (93%)	75 (86%)	6 (7%)	6 (7%)	1	0
1	12-A	87/94 (93%)	78 (90%)	5 (6%)	4 (5%)	2	0
1	13-A	87/94 (93%)	75 (86%)	5 (6%)	7 (8%)	1	0
1	14-A	87/94 (93%)	73 (84%)	7 (8%)	7 (8%)	1	0
1	15-A	87/94 (93%)	78 (90%)	5 (6%)	4 (5%)	2	0
1	16-A	87/94 (93%)	76 (87%)	7 (8%)	4 (5%)	2	0
1	17-A	87/94 (93%)	78 (90%)	5 (6%)	4 (5%)	2	0
1	18-A	87/94 (93%)	74 (85%)	12 (14%)	1 (1%)	14	3
1	19-A	87/94 (93%)	82 (94%)	3 (3%)	2 (2%)	6	1
1	20-A	87/94 (93%)	79 (91%)	7 (8%)	1 (1%)	14	3
1	21-A	87/94 (93%)	76 (87%)	11 (13%)	0	100	100
1	22-A	87/94 (93%)	74 (85%)	10 (12%)	3 (3%)	3	0
1	23-A	87/94 (93%)	75 (86%)	8 (9%)	4 (5%)	2	0
1	24-A	87/94 (93%)	75 (86%)	6 (7%)	6 (7%)	1	0
1	25-A	87/94 (93%)	80 (92%)	3 (3%)	4 (5%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	26-A	87/94 (93%)	76 (87%)	7 (8%)	4 (5%)	2	0
1	27-A	87/94 (93%)	78 (90%)	7 (8%)	2 (2%)	6	1
1	28-A	87/94 (93%)	78 (90%)	7 (8%)	2 (2%)	6	1
1	29-A	87/94 (93%)	77 (88%)	7 (8%)	3 (3%)	3	0
1	30-A	87/94 (93%)	73 (84%)	12 (14%)	2 (2%)	6	1
1	31-A	87/94 (93%)	77 (88%)	8 (9%)	2 (2%)	6	1
1	32-A	87/94 (93%)	74 (85%)	9 (10%)	4 (5%)	2	0
1	33-A	87/94 (93%)	75 (86%)	8 (9%)	4 (5%)	2	0
1	34-A	87/94 (93%)	76 (87%)	8 (9%)	3 (3%)	3	0
1	35-A	87/94 (93%)	74 (85%)	7 (8%)	6 (7%)	1	0
1	36-A	87/94 (93%)	73 (84%)	7 (8%)	7 (8%)	1	0
1	37-A	87/94 (93%)	76 (87%)	7 (8%)	4 (5%)	2	0
1	38-A	87/94 (93%)	78 (90%)	7 (8%)	2 (2%)	6	1
1	39-A	87/94 (93%)	76 (87%)	9 (10%)	2 (2%)	6	1
1	40-A	87/94 (93%)	76 (87%)	9 (10%)	2 (2%)	6	1
1	41-A	87/94 (93%)	76 (87%)	5 (6%)	6 (7%)	1	0
1	42-A	87/94 (93%)	75 (86%)	7 (8%)	5 (6%)	1	0
1	43-A	87/94 (93%)	72 (83%)	10 (12%)	5 (6%)	1	0
1	44-A	87/94 (93%)	77 (88%)	5 (6%)	5 (6%)	1	0
1	45-A	87/94 (93%)	73 (84%)	10 (12%)	4 (5%)	2	0
1	46-A	87/94 (93%)	76 (87%)	7 (8%)	4 (5%)	2	0
1	47-A	87/94 (93%)	74 (85%)	11 (13%)	2 (2%)	6	1
1	48-A	87/94 (93%)	77 (88%)	7 (8%)	3 (3%)	3	0
1	49-A	87/94 (93%)	78 (90%)	5 (6%)	4 (5%)	2	0
1	50-A	87/94 (93%)	77 (88%)	7 (8%)	3 (3%)	3	0
1	51-A	87/94 (93%)	78 (90%)	5 (6%)	4 (5%)	2	0
1	52-A	87/94 (93%)	73 (84%)	9 (10%)	5 (6%)	1	0
1	53-A	87/94 (93%)	75 (86%)	6 (7%)	6 (7%)	1	0
1	54-A	87/94 (93%)	77 (88%)	7 (8%)	3 (3%)	3	0
1	55-A	87/94 (93%)	76 (87%)	6 (7%)	5 (6%)	1	0
1	56-A	87/94 (93%)	79 (91%)	8 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	57-A	87/94 (93%)	80 (92%)	6 (7%)	1 (1%)	14	3
1	58-A	87/94 (93%)	81 (93%)	6 (7%)	0	100	100
1	59-A	87/94 (93%)	72 (83%)	13 (15%)	2 (2%)	6	1
1	60-A	87/94 (93%)	77 (88%)	6 (7%)	4 (5%)	2	0
1	61-A	87/94 (93%)	75 (86%)	9 (10%)	3 (3%)	3	0
1	62-A	87/94 (93%)	81 (93%)	6 (7%)	0	100	100
1	63-A	87/94 (93%)	80 (92%)	7 (8%)	0	100	100
1	64-A	87/94 (93%)	79 (91%)	6 (7%)	2 (2%)	6	1
1	65-A	87/94 (93%)	77 (88%)	6 (7%)	4 (5%)	2	0
1	66-A	87/94 (93%)	72 (83%)	8 (9%)	7 (8%)	1	0
1	67-A	87/94 (93%)	78 (90%)	4 (5%)	5 (6%)	1	0
1	68-A	87/94 (93%)	77 (88%)	6 (7%)	4 (5%)	2	0
1	69-A	87/94 (93%)	77 (88%)	5 (6%)	5 (6%)	1	0
1	70-A	87/94 (93%)	73 (84%)	10 (12%)	4 (5%)	2	0
1	71-A	87/94 (93%)	76 (87%)	6 (7%)	5 (6%)	1	0
1	72-A	87/94 (93%)	72 (83%)	7 (8%)	8 (9%)	1	0
1	73-A	87/94 (93%)	78 (90%)	5 (6%)	4 (5%)	2	0
1	74-A	87/94 (93%)	76 (87%)	8 (9%)	3 (3%)	3	0
1	75-A	87/94 (93%)	78 (90%)	6 (7%)	3 (3%)	3	0
All	All	6525/7050 (93%)	5717 (88%)	531 (8%)	277 (4%)	3	0

All (277) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	36	ASP
1	1-A	38	GLU
1	1-A	64	LEU
1	2-A	38	GLU
1	2-A	64	LEU
1	3-A	39	ILE
1	3-A	63	LYS
1	4-A	63	LYS
1	4-A	64	LEU
1	5-A	37	LEU
1	5-A	56	LYS

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Mol	Chain	Res	Type
1	6-A	36	ASP
1	7-A	36	ASP
1	8-A	36	ASP
1	9-A	35	GLN
1	9-A	36	ASP
1	9-A	67	ILE
1	10-A	40	ASP
1	11-A	38	GLU
1	11-A	40	ASP
1	12-A	35	GLN
1	12-A	37	LEU
1	12-A	38	GLU
1	13-A	35	GLN
1	13-A	36	ASP
1	14-A	35	GLN
1	14-A	36	ASP
1	14-A	37	LEU
1	14-A	66	ASP
1	15-A	35	GLN
1	15-A	66	ASP
1	15-A	67	ILE
1	16-A	36	ASP
1	17-A	64	LEU
1	18-A	63	LYS
1	22-A	65	VAL
1	23-A	38	GLU
1	25-A	62	GLU
1	25-A	66	ASP
1	26-A	66	ASP
1	27-A	38	GLU
1	29-A	66	ASP
1	29-A	67	ILE
1	30-A	64	LEU
1	31-A	89	HIS
1	32-A	38	GLU
1	32-A	63	LYS
1	32-A	89	HIS
1	33-A	63	LYS
1	35-A	36	ASP
1	35-A	38	GLU
1	35-A	67	ILE
1	35-A	89	HIS

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Mol	Chain	Res	Type
1	36-A	62	GLU
1	36-A	64	LEU
1	36-A	67	ILE
1	36-A	89	HIS
1	38-A	63	LYS
1	39-A	39	ILE
1	40-A	86	LYS
1	42-A	3	ASP
1	43-A	67	ILE
1	44-A	39	ILE
1	44-A	53	LYS
1	44-A	67	ILE
1	47-A	62	GLU
1	50-A	63	LYS
1	51-A	38	GLU
1	51-A	63	LYS
1	52-A	38	GLU
1	52-A	63	LYS
1	53-A	67	ILE
1	54-A	67	ILE
1	55-A	36	ASP
1	55-A	37	LEU
1	55-A	67	ILE
1	60-A	39	ILE
1	60-A	40	ASP
1	61-A	39	ILE
1	61-A	40	ASP
1	66-A	35	GLN
1	66-A	39	ILE
1	66-A	53	LYS
1	67-A	38	GLU
1	67-A	39	ILE
1	67-A	89	HIS
1	68-A	38	GLU
1	68-A	53	LYS
1	68-A	89	HIS
1	69-A	56	LYS
1	70-A	63	LYS
1	70-A	66	ASP
1	71-A	38	GLU
1	71-A	60	PRO
1	72-A	36	ASP

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Mol	Chain	Res	Type
1	72-A	56	LYS
1	72-A	60	PRO
1	73-A	36	ASP
1	73-A	60	PRO
1	73-A	89	HIS
1	74-A	36	ASP
1	74-A	60	PRO
1	75-A	36	ASP
1	75-A	38	GLU
1	2-A	34	PHE
1	2-A	35	GLN
1	2-A	39	ILE
1	3-A	38	GLU
1	6-A	37	LEU
1	7-A	35	GLN
1	11-A	36	ASP
1	12-A	62	GLU
1	14-A	63	LYS
1	14-A	65	VAL
1	15-A	36	ASP
1	16-A	35	GLN
1	16-A	66	ASP
1	16-A	89	HIS
1	19-A	37	LEU
1	20-A	56	LYS
1	22-A	38	GLU
1	22-A	66	ASP
1	23-A	66	ASP
1	24-A	38	GLU
1	24-A	39	ILE
1	24-A	66	ASP
1	26-A	39	ILE
1	33-A	36	ASP
1	34-A	38	GLU
1	34-A	64	LEU
1	37-A	64	LEU
1	37-A	66	ASP
1	39-A	87	LEU
1	41-A	62	GLU
1	41-A	65	VAL
1	42-A	56	LYS
1	44-A	38	GLU

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Mol	Chain	Res	Type
1	45-A	53	LYS
1	48-A	62	GLU
1	48-A	63	LYS
1	49-A	37	LEU
1	49-A	61	GLU
1	49-A	63	LYS
1	50-A	38	GLU
1	52-A	60	PRO
1	53-A	38	GLU
1	53-A	39	ILE
1	55-A	39	ILE
1	59-A	37	LEU
1	61-A	63	LYS
1	65-A	36	ASP
1	65-A	52	GLU
1	65-A	53	LYS
1	66-A	63	LYS
1	67-A	63	LYS
1	68-A	52	GLU
1	71-A	63	LYS
1	71-A	89	HIS
1	72-A	62	GLU
1	72-A	89	HIS
1	74-A	38	GLU
1	75-A	60	PRO
1	2-A	52	GLU
1	4-A	37	LEU
1	5-A	35	GLN
1	8-A	35	GLN
1	8-A	63	LYS
1	11-A	35	GLN
1	13-A	33	PHE
1	17-A	66	ASP
1	19-A	63	LYS
1	23-A	85	GLY
1	24-A	35	GLN
1	25-A	56	LYS
1	27-A	37	LEU
1	29-A	64	LEU
1	31-A	38	GLU
1	33-A	38	GLU
1	35-A	64	LEU

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Mol	Chain	Res	Type
1	36-A	38	GLU
1	37-A	62	GLU
1	42-A	62	GLU
1	42-A	68	THR
1	43-A	30	ASP
1	43-A	52	GLU
1	43-A	56	LYS
1	46-A	52	GLU
1	47-A	38	GLU
1	51-A	37	LEU
1	52-A	37	LEU
1	52-A	56	LYS
1	53-A	60	PRO
1	54-A	56	LYS
1	57-A	52	GLU
1	60-A	37	LEU
1	64-A	36	ASP
1	66-A	33	PHE
1	67-A	53	LYS
1	69-A	89	HIS
1	71-A	62	GLU
1	72-A	63	LYS
1	3-A	37	LEU
1	4-A	41	SER
1	6-A	35	GLN
1	7-A	37	LEU
1	13-A	34	PHE
1	13-A	37	LEU
1	14-A	38	GLU
1	17-A	63	LYS
1	17-A	65	VAL
1	24-A	64	LEU
1	24-A	65	VAL
1	28-A	31	ALA
1	28-A	64	LEU
1	34-A	89	HIS
1	36-A	37	LEU
1	37-A	38	GLU
1	41-A	38	GLU
1	41-A	66	ASP
1	42-A	67	ILE
1	43-A	53	LYS

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Mol	Chain	Res	Type
1	45-A	39	ILE
1	45-A	60	PRO
1	46-A	63	LYS
1	48-A	89	HIS
1	49-A	62	GLU
1	53-A	16	GLU
1	53-A	56	LYS
1	54-A	35	GLN
1	55-A	56	LYS
1	64-A	52	GLU
1	69-A	38	GLU
1	72-A	38	GLU
1	72-A	65	VAL
1	73-A	33	PHE
1	1-A	39	ILE
1	1-A	52	GLU
1	1-A	67	ILE
1	3-A	64	LEU
1	5-A	36	ASP
1	5-A	61	GLU
1	9-A	64	LEU
1	10-A	37	LEU
1	11-A	56	LYS
1	13-A	38	GLU
1	13-A	65	VAL
1	25-A	39	ILE
1	26-A	33	PHE
1	30-A	67	ILE
1	36-A	60	PRO
1	40-A	37	LEU
1	44-A	63	LYS
1	46-A	65	VAL
1	50-A	61	GLU
1	51-A	60	PRO
1	59-A	86	LYS
1	60-A	36	ASP
1	65-A	38	GLU
1	69-A	63	LYS
1	7-A	63	LYS
1	9-A	37	LEU
1	26-A	64	LEU
1	45-A	38	GLU

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Mol	Chain	Res	Type
1	46-A	60	PRO
1	66-A	54	LYS
1	70-A	89	HIS
1	35-A	65	VAL
1	66-A	60	PRO
1	69-A	39	ILE
1	70-A	60	PRO
1	23-A	65	VAL
1	32-A	65	VAL
1	41-A	60	PRO
1	41-A	67	ILE
1	11-A	60	PRO
1	33-A	65	VAL
1	38-A	39	ILE

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	79/85 (93%)	68 (86%)	11 (14%)	3	0
1	2-A	79/85 (93%)	69 (87%)	10 (13%)	4	0
1	3-A	79/85 (93%)	70 (89%)	9 (11%)	5	0
1	4-A	79/85 (93%)	72 (91%)	7 (9%)	9	1
1	5-A	79/85 (93%)	63 (80%)	16 (20%)	1	0
1	6-A	79/85 (93%)	69 (87%)	10 (13%)	4	0
1	7-A	79/85 (93%)	69 (87%)	10 (13%)	4	0
1	8-A	79/85 (93%)	67 (85%)	12 (15%)	3	0
1	9-A	79/85 (93%)	65 (82%)	14 (18%)	2	0
1	10-A	79/85 (93%)	65 (82%)	14 (18%)	2	0
1	11-A	79/85 (93%)	66 (84%)	13 (16%)	2	0
1	12-A	79/85 (93%)	69 (87%)	10 (13%)	4	0
1	13-A	79/85 (93%)	70 (89%)	9 (11%)	5	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	14-A	79/85 (93%)	71 (90%)	8 (10%)	7	1
1	15-A	79/85 (93%)	63 (80%)	16 (20%)	1	0
1	16-A	79/85 (93%)	67 (85%)	12 (15%)	3	0
1	17-A	79/85 (93%)	70 (89%)	9 (11%)	5	0
1	18-A	79/85 (93%)	63 (80%)	16 (20%)	1	0
1	19-A	79/85 (93%)	68 (86%)	11 (14%)	3	0
1	20-A	79/85 (93%)	66 (84%)	13 (16%)	2	0
1	21-A	79/85 (93%)	67 (85%)	12 (15%)	3	0
1	22-A	79/85 (93%)	71 (90%)	8 (10%)	7	1
1	23-A	79/85 (93%)	71 (90%)	8 (10%)	7	1
1	24-A	79/85 (93%)	69 (87%)	10 (13%)	4	0
1	25-A	79/85 (93%)	68 (86%)	11 (14%)	3	0
1	26-A	79/85 (93%)	71 (90%)	8 (10%)	7	1
1	27-A	79/85 (93%)	73 (92%)	6 (8%)	13	2
1	28-A	79/85 (93%)	72 (91%)	7 (9%)	9	1
1	29-A	79/85 (93%)	75 (95%)	4 (5%)	24	6
1	30-A	79/85 (93%)	73 (92%)	6 (8%)	13	2
1	31-A	79/85 (93%)	69 (87%)	10 (13%)	4	0
1	32-A	79/85 (93%)	68 (86%)	11 (14%)	3	0
1	33-A	79/85 (93%)	70 (89%)	9 (11%)	5	0
1	34-A	79/85 (93%)	65 (82%)	14 (18%)	2	0
1	35-A	79/85 (93%)	63 (80%)	16 (20%)	1	0
1	36-A	79/85 (93%)	67 (85%)	12 (15%)	3	0
1	37-A	79/85 (93%)	64 (81%)	15 (19%)	1	0
1	38-A	79/85 (93%)	66 (84%)	13 (16%)	2	0
1	39-A	79/85 (93%)	67 (85%)	12 (15%)	3	0
1	40-A	79/85 (93%)	72 (91%)	7 (9%)	9	1
1	41-A	79/85 (93%)	64 (81%)	15 (19%)	1	0
1	42-A	79/85 (93%)	64 (81%)	15 (19%)	1	0
1	43-A	79/85 (93%)	70 (89%)	9 (11%)	5	0
1	44-A	79/85 (93%)	70 (89%)	9 (11%)	5	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	45-A	79/85 (93%)	66 (84%)	13 (16%)	2	0
1	46-A	79/85 (93%)	64 (81%)	15 (19%)	1	0
1	47-A	79/85 (93%)	65 (82%)	14 (18%)	2	0
1	48-A	79/85 (93%)	68 (86%)	11 (14%)	3	0
1	49-A	79/85 (93%)	66 (84%)	13 (16%)	2	0
1	50-A	79/85 (93%)	64 (81%)	15 (19%)	1	0
1	51-A	79/85 (93%)	63 (80%)	16 (20%)	1	0
1	52-A	79/85 (93%)	63 (80%)	16 (20%)	1	0
1	53-A	79/85 (93%)	64 (81%)	15 (19%)	1	0
1	54-A	79/85 (93%)	58 (73%)	21 (27%)	0	0
1	55-A	79/85 (93%)	65 (82%)	14 (18%)	2	0
1	56-A	79/85 (93%)	67 (85%)	12 (15%)	3	0
1	57-A	79/85 (93%)	68 (86%)	11 (14%)	3	0
1	58-A	79/85 (93%)	65 (82%)	14 (18%)	2	0
1	59-A	79/85 (93%)	66 (84%)	13 (16%)	2	0
1	60-A	79/85 (93%)	67 (85%)	12 (15%)	3	0
1	61-A	79/85 (93%)	63 (80%)	16 (20%)	1	0
1	62-A	79/85 (93%)	65 (82%)	14 (18%)	2	0
1	63-A	79/85 (93%)	63 (80%)	16 (20%)	1	0
1	64-A	79/85 (93%)	66 (84%)	13 (16%)	2	0
1	65-A	79/85 (93%)	64 (81%)	15 (19%)	1	0
1	66-A	79/85 (93%)	71 (90%)	8 (10%)	7	1
1	67-A	79/85 (93%)	72 (91%)	7 (9%)	9	1
1	68-A	79/85 (93%)	68 (86%)	11 (14%)	3	0
1	69-A	79/85 (93%)	70 (89%)	9 (11%)	5	0
1	70-A	79/85 (93%)	64 (81%)	15 (19%)	1	0
1	71-A	79/85 (93%)	68 (86%)	11 (14%)	3	0
1	72-A	79/85 (93%)	68 (86%)	11 (14%)	3	0
1	73-A	79/85 (93%)	69 (87%)	10 (13%)	4	0
1	74-A	79/85 (93%)	68 (86%)	11 (14%)	3	0
1	75-A	79/85 (93%)	64 (81%)	15 (19%)	1	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5925/6375 (93%)	5041 (85%)	884 (15%)	3 0

All (884) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	7	GLU
1	1-A	16	GLU
1	1-A	25	ILE
1	1-A	33	PHE
1	1-A	34	PHE
1	1-A	37	LEU
1	1-A	54	LYS
1	1-A	57	VAL
1	1-A	58	GLN
1	1-A	62	GLU
1	1-A	67	ILE
1	2-A	22	GLU
1	2-A	25	ILE
1	2-A	36	ASP
1	2-A	37	LEU
1	2-A	38	GLU
1	2-A	53	LYS
1	2-A	58	GLN
1	2-A	62	GLU
1	2-A	64	LEU
1	2-A	79	SER
1	3-A	23	LYS
1	3-A	25	ILE
1	3-A	34	PHE
1	3-A	36	ASP
1	3-A	37	LEU
1	3-A	38	GLU
1	3-A	54	LYS
1	3-A	63	LYS
1	3-A	79	SER
1	4-A	8	LYS
1	4-A	25	ILE
1	4-A	40	ASP
1	4-A	56	LYS
1	4-A	58	GLN
1	4-A	63	LYS
1	4-A	68	THR

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Mol	Chain	Res	Type
1	5-A	4	GLU
1	5-A	5	GLU
1	5-A	8	LYS
1	5-A	16	GLU
1	5-A	19	GLU
1	5-A	22	GLU
1	5-A	25	ILE
1	5-A	33	PHE
1	5-A	38	GLU
1	5-A	39	ILE
1	5-A	40	ASP
1	5-A	56	LYS
1	5-A	58	GLN
1	5-A	63	LYS
1	5-A	66	ASP
1	5-A	86	LYS
1	6-A	4	GLU
1	6-A	19	GLU
1	6-A	25	ILE
1	6-A	33	PHE
1	6-A	38	GLU
1	6-A	53	LYS
1	6-A	56	LYS
1	6-A	58	GLN
1	6-A	66	ASP
1	6-A	86	LYS
1	7-A	2	ASP
1	7-A	4	GLU
1	7-A	8	LYS
1	7-A	12	SER
1	7-A	25	ILE
1	7-A	33	PHE
1	7-A	60	PRO
1	7-A	66	ASP
1	7-A	86	LYS
1	7-A	88	GLU
1	8-A	2	ASP
1	8-A	4	GLU
1	8-A	8	LYS
1	8-A	16	GLU
1	8-A	22	GLU
1	8-A	25	ILE

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Mol	Chain	Res	Type
1	8-A	32	ASN
1	8-A	36	ASP
1	8-A	58	GLN
1	8-A	63	LYS
1	8-A	65	VAL
1	8-A	86	LYS
1	9-A	3	ASP
1	9-A	16	GLU
1	9-A	19	GLU
1	9-A	22	GLU
1	9-A	35	GLN
1	9-A	36	ASP
1	9-A	48	LEU
1	9-A	57	VAL
1	9-A	58	GLN
1	9-A	61	GLU
1	9-A	64	LEU
1	9-A	66	ASP
1	9-A	80	VAL
1	9-A	86	LYS
1	10-A	4	GLU
1	10-A	16	GLU
1	10-A	19	GLU
1	10-A	24	GLU
1	10-A	25	ILE
1	10-A	56	LYS
1	10-A	58	GLN
1	10-A	61	GLU
1	10-A	62	GLU
1	10-A	64	LEU
1	10-A	66	ASP
1	10-A	79	SER
1	10-A	86	LYS
1	10-A	88	GLU
1	11-A	2	ASP
1	11-A	8	LYS
1	11-A	16	GLU
1	11-A	19	GLU
1	11-A	25	ILE
1	11-A	30	ASP
1	11-A	56	LYS
1	11-A	58	GLN

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Mol	Chain	Res	Type
1	11-A	62	GLU
1	11-A	64	LEU
1	11-A	67	ILE
1	11-A	80	VAL
1	11-A	88	GLU
1	12-A	2	ASP
1	12-A	16	GLU
1	12-A	25	ILE
1	12-A	30	ASP
1	12-A	37	LEU
1	12-A	54	LYS
1	12-A	58	GLN
1	12-A	62	GLU
1	12-A	64	LEU
1	12-A	88	GLU
1	13-A	2	ASP
1	13-A	4	GLU
1	13-A	8	LYS
1	13-A	22	GLU
1	13-A	25	ILE
1	13-A	34	PHE
1	13-A	54	LYS
1	13-A	58	GLN
1	13-A	61	GLU
1	14-A	2	ASP
1	14-A	4	GLU
1	14-A	22	GLU
1	14-A	25	ILE
1	14-A	37	LEU
1	14-A	61	GLU
1	14-A	66	ASP
1	14-A	84	SER
1	15-A	2	ASP
1	15-A	4	GLU
1	15-A	19	GLU
1	15-A	22	GLU
1	15-A	24	GLU
1	15-A	33	PHE
1	15-A	34	PHE
1	15-A	35	GLN
1	15-A	37	LEU
1	15-A	54	LYS

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Mol	Chain	Res	Type
1	15-A	61	GLU
1	15-A	64	LEU
1	15-A	66	ASP
1	15-A	84	SER
1	15-A	86	LYS
1	15-A	88	GLU
1	16-A	2	ASP
1	16-A	4	GLU
1	16-A	16	GLU
1	16-A	22	GLU
1	16-A	25	ILE
1	16-A	32	ASN
1	16-A	33	PHE
1	16-A	34	PHE
1	16-A	36	ASP
1	16-A	64	LEU
1	16-A	66	ASP
1	16-A	88	GLU
1	17-A	4	GLU
1	17-A	23	LYS
1	17-A	24	GLU
1	17-A	32	ASN
1	17-A	33	PHE
1	17-A	34	PHE
1	17-A	64	LEU
1	17-A	65	VAL
1	17-A	88	GLU
1	18-A	4	GLU
1	18-A	16	GLU
1	18-A	22	GLU
1	18-A	32	ASN
1	18-A	33	PHE
1	18-A	34	PHE
1	18-A	35	GLN
1	18-A	37	LEU
1	18-A	54	LYS
1	18-A	61	GLU
1	18-A	62	GLU
1	18-A	66	ASP
1	18-A	79	SER
1	18-A	83	GLU
1	18-A	86	LYS

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Mol	Chain	Res	Type
1	18-A	88	GLU
1	19-A	2	ASP
1	19-A	4	GLU
1	19-A	8	LYS
1	19-A	22	GLU
1	19-A	23	LYS
1	19-A	32	ASN
1	19-A	34	PHE
1	19-A	54	LYS
1	19-A	58	GLN
1	19-A	63	LYS
1	19-A	86	LYS
1	20-A	4	GLU
1	20-A	16	GLU
1	20-A	22	GLU
1	20-A	25	ILE
1	20-A	32	ASN
1	20-A	35	GLN
1	20-A	53	LYS
1	20-A	54	LYS
1	20-A	58	GLN
1	20-A	59	ILE
1	20-A	60	PRO
1	20-A	61	GLU
1	20-A	65	VAL
1	21-A	4	GLU
1	21-A	8	LYS
1	21-A	22	GLU
1	21-A	33	PHE
1	21-A	35	GLN
1	21-A	37	LEU
1	21-A	38	GLU
1	21-A	41	SER
1	21-A	53	LYS
1	21-A	57	VAL
1	21-A	61	GLU
1	21-A	88	GLU
1	22-A	8	LYS
1	22-A	16	GLU
1	22-A	33	PHE
1	22-A	35	GLN
1	22-A	53	LYS

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Mol	Chain	Res	Type
1	22-A	63	LYS
1	22-A	66	ASP
1	22-A	88	GLU
1	23-A	4	GLU
1	23-A	8	LYS
1	23-A	23	LYS
1	23-A	35	GLN
1	23-A	53	LYS
1	23-A	61	GLU
1	23-A	66	ASP
1	23-A	88	GLU
1	24-A	5	GLU
1	24-A	7	GLU
1	24-A	8	LYS
1	24-A	33	PHE
1	24-A	35	GLN
1	24-A	39	ILE
1	24-A	53	LYS
1	24-A	56	LYS
1	24-A	66	ASP
1	24-A	88	GLU
1	25-A	4	GLU
1	25-A	22	GLU
1	25-A	35	GLN
1	25-A	39	ILE
1	25-A	48	LEU
1	25-A	53	LYS
1	25-A	56	LYS
1	25-A	57	VAL
1	25-A	63	LYS
1	25-A	66	ASP
1	25-A	79	SER
1	26-A	4	GLU
1	26-A	33	PHE
1	26-A	36	ASP
1	26-A	39	ILE
1	26-A	53	LYS
1	26-A	56	LYS
1	26-A	57	VAL
1	26-A	66	ASP
1	27-A	2	ASP
1	27-A	8	LYS

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Mol	Chain	Res	Type
1	27-A	25	ILE
1	27-A	39	ILE
1	27-A	53	LYS
1	27-A	57	VAL
1	28-A	22	GLU
1	28-A	25	ILE
1	28-A	39	ILE
1	28-A	61	GLU
1	28-A	63	LYS
1	28-A	68	THR
1	28-A	88	GLU
1	29-A	33	PHE
1	29-A	48	LEU
1	29-A	61	GLU
1	29-A	68	THR
1	30-A	4	GLU
1	30-A	33	PHE
1	30-A	56	LYS
1	30-A	61	GLU
1	30-A	79	SER
1	30-A	88	GLU
1	31-A	4	GLU
1	31-A	8	LYS
1	31-A	16	GLU
1	31-A	25	ILE
1	31-A	32	ASN
1	31-A	33	PHE
1	31-A	35	GLN
1	31-A	58	GLN
1	31-A	61	GLU
1	31-A	88	GLU
1	32-A	16	GLU
1	32-A	25	ILE
1	32-A	35	GLN
1	32-A	39	ILE
1	32-A	40	ASP
1	32-A	57	VAL
1	32-A	58	GLN
1	32-A	61	GLU
1	32-A	63	LYS
1	32-A	64	LEU
1	32-A	80	VAL

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Mol	Chain	Res	Type
1	33-A	24	GLU
1	33-A	25	ILE
1	33-A	35	GLN
1	33-A	36	ASP
1	33-A	39	ILE
1	33-A	40	ASP
1	33-A	61	GLU
1	33-A	63	LYS
1	33-A	64	LEU
1	34-A	2	ASP
1	34-A	12	SER
1	34-A	22	GLU
1	34-A	23	LYS
1	34-A	25	ILE
1	34-A	32	ASN
1	34-A	35	GLN
1	34-A	37	LEU
1	34-A	48	LEU
1	34-A	54	LYS
1	34-A	61	GLU
1	34-A	64	LEU
1	34-A	65	VAL
1	34-A	66	ASP
1	35-A	2	ASP
1	35-A	4	GLU
1	35-A	5	GLU
1	35-A	23	LYS
1	35-A	24	GLU
1	35-A	25	ILE
1	35-A	32	ASN
1	35-A	36	ASP
1	35-A	37	LEU
1	35-A	39	ILE
1	35-A	53	LYS
1	35-A	54	LYS
1	35-A	63	LYS
1	35-A	64	LEU
1	35-A	65	VAL
1	35-A	67	ILE
1	36-A	2	ASP
1	36-A	23	LYS
1	36-A	24	GLU

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Mol	Chain	Res	Type
1	36-A	33	PHE
1	36-A	35	GLN
1	36-A	37	LEU
1	36-A	53	LYS
1	36-A	57	VAL
1	36-A	61	GLU
1	36-A	63	LYS
1	36-A	64	LEU
1	36-A	66	ASP
1	37-A	4	GLU
1	37-A	5	GLU
1	37-A	23	LYS
1	37-A	33	PHE
1	37-A	37	LEU
1	37-A	38	GLU
1	37-A	53	LYS
1	37-A	57	VAL
1	37-A	62	GLU
1	37-A	63	LYS
1	37-A	64	LEU
1	37-A	66	ASP
1	37-A	67	ILE
1	37-A	79	SER
1	37-A	86	LYS
1	38-A	23	LYS
1	38-A	33	PHE
1	38-A	37	LEU
1	38-A	38	GLU
1	38-A	46	GLU
1	38-A	53	LYS
1	38-A	61	GLU
1	38-A	63	LYS
1	38-A	64	LEU
1	38-A	66	ASP
1	38-A	67	ILE
1	38-A	69	SER
1	38-A	86	LYS
1	39-A	2	ASP
1	39-A	12	SER
1	39-A	16	GLU
1	39-A	20	LEU
1	39-A	23	LYS

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Mol	Chain	Res	Type
1	39-A	25	ILE
1	39-A	28	LYS
1	39-A	54	LYS
1	39-A	63	LYS
1	39-A	64	LEU
1	39-A	67	ILE
1	39-A	86	LYS
1	40-A	23	LYS
1	40-A	34	PHE
1	40-A	38	GLU
1	40-A	64	LEU
1	40-A	67	ILE
1	40-A	83	GLU
1	40-A	86	LYS
1	41-A	16	GLU
1	41-A	20	LEU
1	41-A	24	GLU
1	41-A	25	ILE
1	41-A	28	LYS
1	41-A	35	GLN
1	41-A	37	LEU
1	41-A	46	GLU
1	41-A	61	GLU
1	41-A	63	LYS
1	41-A	64	LEU
1	41-A	66	ASP
1	41-A	67	ILE
1	41-A	83	GLU
1	41-A	86	LYS
1	42-A	8	LYS
1	42-A	20	LEU
1	42-A	23	LYS
1	42-A	24	GLU
1	42-A	25	ILE
1	42-A	28	LYS
1	42-A	30	ASP
1	42-A	37	LEU
1	42-A	54	LYS
1	42-A	57	VAL
1	42-A	61	GLU
1	42-A	63	LYS
1	42-A	64	LEU

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Mol	Chain	Res	Type
1	42-A	67	ILE
1	42-A	83	GLU
1	43-A	3	ASP
1	43-A	4	GLU
1	43-A	24	GLU
1	43-A	25	ILE
1	43-A	30	ASP
1	43-A	53	LYS
1	43-A	54	LYS
1	43-A	83	GLU
1	43-A	86	LYS
1	44-A	2	ASP
1	44-A	3	ASP
1	44-A	23	LYS
1	44-A	24	GLU
1	44-A	33	PHE
1	44-A	37	LEU
1	44-A	39	ILE
1	44-A	48	LEU
1	44-A	54	LYS
1	45-A	5	GLU
1	45-A	20	LEU
1	45-A	22	GLU
1	45-A	23	LYS
1	45-A	24	GLU
1	45-A	25	ILE
1	45-A	30	ASP
1	45-A	35	GLN
1	45-A	37	LEU
1	45-A	39	ILE
1	45-A	64	LEU
1	45-A	79	SER
1	45-A	80	VAL
1	46-A	2	ASP
1	46-A	5	GLU
1	46-A	22	GLU
1	46-A	23	LYS
1	46-A	24	GLU
1	46-A	25	ILE
1	46-A	33	PHE
1	46-A	35	GLN
1	46-A	37	LEU

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Mol	Chain	Res	Type
1	46-A	39	ILE
1	46-A	41	SER
1	46-A	53	LYS
1	46-A	61	GLU
1	46-A	64	LEU
1	46-A	80	VAL
1	47-A	2	ASP
1	47-A	4	GLU
1	47-A	22	GLU
1	47-A	23	LYS
1	47-A	24	GLU
1	47-A	25	ILE
1	47-A	33	PHE
1	47-A	37	LEU
1	47-A	45	LEU
1	47-A	54	LYS
1	47-A	57	VAL
1	47-A	62	GLU
1	47-A	63	LYS
1	47-A	80	VAL
1	48-A	2	ASP
1	48-A	4	GLU
1	48-A	23	LYS
1	48-A	25	ILE
1	48-A	33	PHE
1	48-A	37	LEU
1	48-A	45	LEU
1	48-A	54	LYS
1	48-A	57	VAL
1	48-A	66	ASP
1	48-A	88	GLU
1	49-A	2	ASP
1	49-A	8	LYS
1	49-A	16	GLU
1	49-A	23	LYS
1	49-A	25	ILE
1	49-A	30	ASP
1	49-A	33	PHE
1	49-A	34	PHE
1	49-A	35	GLN
1	49-A	45	LEU
1	49-A	54	LYS

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Mol	Chain	Res	Type
1	49-A	64	LEU
1	49-A	65	VAL
1	50-A	2	ASP
1	50-A	3	ASP
1	50-A	8	LYS
1	50-A	23	LYS
1	50-A	25	ILE
1	50-A	32	ASN
1	50-A	35	GLN
1	50-A	39	ILE
1	50-A	46	GLU
1	50-A	54	LYS
1	50-A	57	VAL
1	50-A	59	ILE
1	50-A	61	GLU
1	50-A	64	LEU
1	50-A	65	VAL
1	51-A	2	ASP
1	51-A	23	LYS
1	51-A	24	GLU
1	51-A	32	ASN
1	51-A	33	PHE
1	51-A	37	LEU
1	51-A	39	ILE
1	51-A	40	ASP
1	51-A	41	SER
1	51-A	54	LYS
1	51-A	58	GLN
1	51-A	61	GLU
1	51-A	64	LEU
1	51-A	65	VAL
1	51-A	84	SER
1	51-A	88	GLU
1	52-A	2	ASP
1	52-A	4	GLU
1	52-A	8	LYS
1	52-A	16	GLU
1	52-A	22	GLU
1	52-A	23	LYS
1	52-A	24	GLU
1	52-A	36	ASP
1	52-A	37	LEU

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Mol	Chain	Res	Type
1	52-A	39	ILE
1	52-A	41	SER
1	52-A	59	ILE
1	52-A	61	GLU
1	52-A	64	LEU
1	52-A	79	SER
1	52-A	86	LYS
1	53-A	2	ASP
1	53-A	4	GLU
1	53-A	8	LYS
1	53-A	16	GLU
1	53-A	23	LYS
1	53-A	28	LYS
1	53-A	30	ASP
1	53-A	37	LEU
1	53-A	38	GLU
1	53-A	39	ILE
1	53-A	53	LYS
1	53-A	56	LYS
1	53-A	59	ILE
1	53-A	61	GLU
1	53-A	65	VAL
1	54-A	4	GLU
1	54-A	5	GLU
1	54-A	8	LYS
1	54-A	12	SER
1	54-A	16	GLU
1	54-A	23	LYS
1	54-A	24	GLU
1	54-A	32	ASN
1	54-A	33	PHE
1	54-A	39	ILE
1	54-A	40	ASP
1	54-A	45	LEU
1	54-A	53	LYS
1	54-A	54	LYS
1	54-A	56	LYS
1	54-A	58	GLN
1	54-A	61	GLU
1	54-A	66	ASP
1	54-A	80	VAL
1	54-A	84	SER

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Mol	Chain	Res	Type
1	54-A	88	GLU
1	55-A	2	ASP
1	55-A	16	GLU
1	55-A	23	LYS
1	55-A	32	ASN
1	55-A	35	GLN
1	55-A	36	ASP
1	55-A	39	ILE
1	55-A	40	ASP
1	55-A	53	LYS
1	55-A	58	GLN
1	55-A	61	GLU
1	55-A	66	ASP
1	55-A	79	SER
1	55-A	88	GLU
1	56-A	2	ASP
1	56-A	23	LYS
1	56-A	25	ILE
1	56-A	35	GLN
1	56-A	39	ILE
1	56-A	48	LEU
1	56-A	53	LYS
1	56-A	57	VAL
1	56-A	58	GLN
1	56-A	64	LEU
1	56-A	65	VAL
1	56-A	80	VAL
1	57-A	8	LYS
1	57-A	22	GLU
1	57-A	25	ILE
1	57-A	39	ILE
1	57-A	48	LEU
1	57-A	54	LYS
1	57-A	56	LYS
1	57-A	57	VAL
1	57-A	61	GLU
1	57-A	80	VAL
1	57-A	86	LYS
1	58-A	2	ASP
1	58-A	22	GLU
1	58-A	25	ILE
1	58-A	36	ASP

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Mol	Chain	Res	Type
1	58-A	38	GLU
1	58-A	39	ILE
1	58-A	53	LYS
1	58-A	54	LYS
1	58-A	56	LYS
1	58-A	61	GLU
1	58-A	64	LEU
1	58-A	84	SER
1	58-A	86	LYS
1	58-A	88	GLU
1	59-A	2	ASP
1	59-A	32	ASN
1	59-A	35	GLN
1	59-A	37	LEU
1	59-A	39	ILE
1	59-A	45	LEU
1	59-A	54	LYS
1	59-A	58	GLN
1	59-A	61	GLU
1	59-A	66	ASP
1	59-A	79	SER
1	59-A	83	GLU
1	59-A	84	SER
1	60-A	2	ASP
1	60-A	8	LYS
1	60-A	37	LEU
1	60-A	38	GLU
1	60-A	39	ILE
1	60-A	45	LEU
1	60-A	53	LYS
1	60-A	54	LYS
1	60-A	61	GLU
1	60-A	62	GLU
1	60-A	63	LYS
1	60-A	83	GLU
1	61-A	2	ASP
1	61-A	22	GLU
1	61-A	33	PHE
1	61-A	35	GLN
1	61-A	37	LEU
1	61-A	38	GLU
1	61-A	39	ILE

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Mol	Chain	Res	Type
1	61-A	40	ASP
1	61-A	45	LEU
1	61-A	48	LEU
1	61-A	54	LYS
1	61-A	56	LYS
1	61-A	61	GLU
1	61-A	63	LYS
1	61-A	66	ASP
1	61-A	88	GLU
1	62-A	2	ASP
1	62-A	12	SER
1	62-A	21	ASP
1	62-A	22	GLU
1	62-A	24	GLU
1	62-A	35	GLN
1	62-A	38	GLU
1	62-A	39	ILE
1	62-A	45	LEU
1	62-A	53	LYS
1	62-A	58	GLN
1	62-A	61	GLU
1	62-A	66	ASP
1	62-A	88	GLU
1	63-A	2	ASP
1	63-A	4	GLU
1	63-A	5	GLU
1	63-A	16	GLU
1	63-A	22	GLU
1	63-A	24	GLU
1	63-A	33	PHE
1	63-A	35	GLN
1	63-A	37	LEU
1	63-A	39	ILE
1	63-A	45	LEU
1	63-A	53	LYS
1	63-A	57	VAL
1	63-A	79	SER
1	63-A	84	SER
1	63-A	88	GLU
1	64-A	2	ASP
1	64-A	4	GLU
1	64-A	8	LYS

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Mol	Chain	Res	Type
1	64-A	16	GLU
1	64-A	22	GLU
1	64-A	24	GLU
1	64-A	37	LEU
1	64-A	38	GLU
1	64-A	39	ILE
1	64-A	53	LYS
1	64-A	54	LYS
1	64-A	57	VAL
1	64-A	63	LYS
1	65-A	2	ASP
1	65-A	3	ASP
1	65-A	4	GLU
1	65-A	16	GLU
1	65-A	22	GLU
1	65-A	24	GLU
1	65-A	25	ILE
1	65-A	34	PHE
1	65-A	35	GLN
1	65-A	39	ILE
1	65-A	48	LEU
1	65-A	53	LYS
1	65-A	66	ASP
1	65-A	79	SER
1	65-A	80	VAL
1	66-A	8	LYS
1	66-A	22	GLU
1	66-A	24	GLU
1	66-A	25	ILE
1	66-A	33	PHE
1	66-A	38	GLU
1	66-A	39	ILE
1	66-A	54	LYS
1	67-A	4	GLU
1	67-A	22	GLU
1	67-A	23	LYS
1	67-A	32	ASN
1	67-A	38	GLU
1	67-A	39	ILE
1	67-A	83	GLU
1	68-A	5	GLU
1	68-A	22	GLU

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Mol	Chain	Res	Type
1	68-A	24	GLU
1	68-A	35	GLN
1	68-A	37	LEU
1	68-A	38	GLU
1	68-A	40	ASP
1	68-A	53	LYS
1	68-A	57	VAL
1	68-A	58	GLN
1	68-A	64	LEU
1	69-A	17	VAL
1	69-A	22	GLU
1	69-A	23	LYS
1	69-A	24	GLU
1	69-A	35	GLN
1	69-A	38	GLU
1	69-A	58	GLN
1	69-A	61	GLU
1	69-A	86	LYS
1	70-A	3	ASP
1	70-A	17	VAL
1	70-A	22	GLU
1	70-A	23	LYS
1	70-A	25	ILE
1	70-A	33	PHE
1	70-A	35	GLN
1	70-A	39	ILE
1	70-A	40	ASP
1	70-A	56	LYS
1	70-A	58	GLN
1	70-A	61	GLU
1	70-A	62	GLU
1	70-A	67	ILE
1	70-A	83	GLU
1	71-A	2	ASP
1	71-A	22	GLU
1	71-A	23	LYS
1	71-A	38	GLU
1	71-A	39	ILE
1	71-A	56	LYS
1	71-A	58	GLN
1	71-A	61	GLU
1	71-A	62	GLU

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Mol	Chain	Res	Type
1	71-A	67	ILE
1	71-A	79	SER
1	72-A	2	ASP
1	72-A	23	LYS
1	72-A	30	ASP
1	72-A	38	GLU
1	72-A	48	LEU
1	72-A	53	LYS
1	72-A	54	LYS
1	72-A	56	LYS
1	72-A	58	GLN
1	72-A	64	LEU
1	72-A	67	ILE
1	73-A	22	GLU
1	73-A	32	ASN
1	73-A	36	ASP
1	73-A	38	GLU
1	73-A	40	ASP
1	73-A	53	LYS
1	73-A	54	LYS
1	73-A	56	LYS
1	73-A	58	GLN
1	73-A	67	ILE
1	74-A	2	ASP
1	74-A	22	GLU
1	74-A	33	PHE
1	74-A	38	GLU
1	74-A	40	ASP
1	74-A	53	LYS
1	74-A	57	VAL
1	74-A	58	GLN
1	74-A	67	ILE
1	74-A	86	LYS
1	74-A	88	GLU
1	75-A	22	GLU
1	75-A	24	GLU
1	75-A	33	PHE
1	75-A	36	ASP
1	75-A	37	LEU
1	75-A	38	GLU
1	75-A	53	LYS
1	75-A	54	LYS

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Mol	Chain	Res	Type
1	75-A	56	LYS
1	75-A	57	VAL
1	75-A	61	GLU
1	75-A	66	ASP
1	75-A	67	ILE
1	75-A	80	VAL
1	75-A	88	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 525 ligands modelled in this entry, 525 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	1-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	2-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	3-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	4-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	5-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	6-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	7-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	8-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	9-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	10-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	11-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	12-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	13-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	14-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	15-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	16-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	17-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	18-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	19-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	20-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	21-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	22-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	23-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	24-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	25-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	26-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	27-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	28-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	29-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	30-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	31-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	32-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	33-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	34-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	35-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	36-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	37-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	38-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	39-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	40-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	41-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	42-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	43-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	44-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	45-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	46-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	47-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	48-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	49-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	50-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	51-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	52-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	53-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	54-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	55-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	56-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	57-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	58-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	59-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	60-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	61-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	62-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	63-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	64-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	65-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	66-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	67-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	68-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	69-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	70-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	71-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	72-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	73-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	74-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
1	75-A	89/94 (94%)	1.27	19 (21%)	0	1	35, 45, 57, 64	89 (100%)
All	All	6675/7050 (94%)	1.27	1425 (21%)	0	1	35, 45, 57, 64	6675 (100%)

All (1425) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	37	LEU	8.3
1	2-A	37	LEU	8.3
1	3-A	37	LEU	8.3
1	4-A	37	LEU	8.3
1	5-A	37	LEU	8.3
1	6-A	37	LEU	8.3
1	7-A	37	LEU	8.3
1	8-A	37	LEU	8.3
1	9-A	37	LEU	8.3
1	10-A	37	LEU	8.3

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Mol	Chain	Res	Type	RSRZ
1	11-A	37	LEU	8.3
1	12-A	37	LEU	8.3
1	13-A	37	LEU	8.3
1	14-A	37	LEU	8.3
1	15-A	37	LEU	8.3
1	16-A	37	LEU	8.3
1	17-A	37	LEU	8.3
1	18-A	37	LEU	8.3
1	19-A	37	LEU	8.3
1	20-A	37	LEU	8.3
1	21-A	37	LEU	8.3
1	22-A	37	LEU	8.3
1	23-A	37	LEU	8.3
1	24-A	37	LEU	8.3
1	25-A	37	LEU	8.3
1	26-A	37	LEU	8.3
1	27-A	37	LEU	8.3
1	28-A	37	LEU	8.3
1	29-A	37	LEU	8.3
1	30-A	37	LEU	8.3
1	31-A	37	LEU	8.3
1	32-A	37	LEU	8.3
1	33-A	37	LEU	8.3
1	34-A	37	LEU	8.3
1	35-A	37	LEU	8.3
1	36-A	37	LEU	8.3
1	37-A	37	LEU	8.3
1	38-A	37	LEU	8.3
1	39-A	37	LEU	8.3
1	40-A	37	LEU	8.3
1	41-A	37	LEU	8.3
1	42-A	37	LEU	8.3
1	43-A	37	LEU	8.3
1	44-A	37	LEU	8.3
1	45-A	37	LEU	8.3
1	46-A	37	LEU	8.3
1	47-A	37	LEU	8.3
1	48-A	37	LEU	8.3
1	49-A	37	LEU	8.3
1	50-A	37	LEU	8.3
1	51-A	37	LEU	8.3
1	52-A	37	LEU	8.3

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Mol	Chain	Res	Type	RSRZ
1	53-A	37	LEU	8.3
1	54-A	37	LEU	8.3
1	55-A	37	LEU	8.3
1	56-A	37	LEU	8.3
1	57-A	37	LEU	8.3
1	58-A	37	LEU	8.3
1	59-A	37	LEU	8.3
1	60-A	37	LEU	8.3
1	61-A	37	LEU	8.3
1	62-A	37	LEU	8.3
1	63-A	37	LEU	8.3
1	64-A	37	LEU	8.3
1	65-A	37	LEU	8.3
1	66-A	37	LEU	8.3
1	67-A	37	LEU	8.3
1	68-A	37	LEU	8.3
1	69-A	37	LEU	8.3
1	70-A	37	LEU	8.3
1	71-A	37	LEU	8.3
1	72-A	37	LEU	8.3
1	73-A	37	LEU	8.3
1	74-A	37	LEU	8.3
1	75-A	37	LEU	8.3
1	1-A	60	PRO	6.2
1	2-A	60	PRO	6.2
1	3-A	60	PRO	6.2
1	4-A	60	PRO	6.2
1	5-A	60	PRO	6.2
1	6-A	60	PRO	6.2
1	7-A	60	PRO	6.2
1	8-A	60	PRO	6.2
1	9-A	60	PRO	6.2
1	10-A	60	PRO	6.2
1	11-A	60	PRO	6.2
1	12-A	60	PRO	6.2
1	13-A	60	PRO	6.2
1	14-A	60	PRO	6.2
1	15-A	60	PRO	6.2
1	16-A	60	PRO	6.2
1	17-A	60	PRO	6.2
1	18-A	60	PRO	6.2
1	19-A	60	PRO	6.2

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Mol	Chain	Res	Type	RSRZ
1	20-A	60	PRO	6.2
1	21-A	60	PRO	6.2
1	22-A	60	PRO	6.2
1	23-A	60	PRO	6.2
1	24-A	60	PRO	6.2
1	25-A	60	PRO	6.2
1	26-A	60	PRO	6.2
1	27-A	60	PRO	6.2
1	28-A	60	PRO	6.2
1	29-A	60	PRO	6.2
1	30-A	60	PRO	6.2
1	31-A	60	PRO	6.2
1	32-A	60	PRO	6.2
1	33-A	60	PRO	6.2
1	34-A	60	PRO	6.2
1	35-A	60	PRO	6.2
1	36-A	60	PRO	6.2
1	37-A	60	PRO	6.2
1	38-A	60	PRO	6.2
1	39-A	60	PRO	6.2
1	40-A	60	PRO	6.2
1	41-A	60	PRO	6.2
1	42-A	60	PRO	6.2
1	43-A	60	PRO	6.2
1	44-A	60	PRO	6.2
1	45-A	60	PRO	6.2
1	46-A	60	PRO	6.2
1	47-A	60	PRO	6.2
1	48-A	60	PRO	6.2
1	49-A	60	PRO	6.2
1	50-A	60	PRO	6.2
1	51-A	60	PRO	6.2
1	52-A	60	PRO	6.2
1	53-A	60	PRO	6.2
1	54-A	60	PRO	6.2
1	55-A	60	PRO	6.2
1	56-A	60	PRO	6.2
1	57-A	60	PRO	6.2
1	58-A	60	PRO	6.2
1	59-A	60	PRO	6.2
1	60-A	60	PRO	6.2
1	61-A	60	PRO	6.2

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Mol	Chain	Res	Type	RSRZ
1	62-A	60	PRO	6.2
1	63-A	60	PRO	6.2
1	64-A	60	PRO	6.2
1	65-A	60	PRO	6.2
1	66-A	60	PRO	6.2
1	67-A	60	PRO	6.2
1	68-A	60	PRO	6.2
1	69-A	60	PRO	6.2
1	70-A	60	PRO	6.2
1	71-A	60	PRO	6.2
1	72-A	60	PRO	6.2
1	73-A	60	PRO	6.2
1	74-A	60	PRO	6.2
1	75-A	60	PRO	6.2
1	1-A	39	ILE	5.8
1	2-A	39	ILE	5.8
1	3-A	39	ILE	5.8
1	4-A	39	ILE	5.8
1	5-A	39	ILE	5.8
1	6-A	39	ILE	5.8
1	7-A	39	ILE	5.8
1	8-A	39	ILE	5.8
1	9-A	39	ILE	5.8
1	10-A	39	ILE	5.8
1	11-A	39	ILE	5.8
1	12-A	39	ILE	5.8
1	13-A	39	ILE	5.8
1	14-A	39	ILE	5.8
1	15-A	39	ILE	5.8
1	16-A	39	ILE	5.8
1	17-A	39	ILE	5.8
1	18-A	39	ILE	5.8
1	19-A	39	ILE	5.8
1	20-A	39	ILE	5.8
1	21-A	39	ILE	5.8
1	22-A	39	ILE	5.8
1	23-A	39	ILE	5.8
1	24-A	39	ILE	5.8
1	25-A	39	ILE	5.8
1	26-A	39	ILE	5.8
1	27-A	39	ILE	5.8
1	28-A	39	ILE	5.8

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Mol	Chain	Res	Type	RSRZ
1	29-A	39	ILE	5.8
1	30-A	39	ILE	5.8
1	31-A	39	ILE	5.8
1	32-A	39	ILE	5.8
1	33-A	39	ILE	5.8
1	34-A	39	ILE	5.8
1	35-A	39	ILE	5.8
1	36-A	39	ILE	5.8
1	37-A	39	ILE	5.8
1	38-A	39	ILE	5.8
1	39-A	39	ILE	5.8
1	40-A	39	ILE	5.8
1	41-A	39	ILE	5.8
1	42-A	39	ILE	5.8
1	43-A	39	ILE	5.8
1	44-A	39	ILE	5.8
1	45-A	39	ILE	5.8
1	46-A	39	ILE	5.8
1	47-A	39	ILE	5.8
1	48-A	39	ILE	5.8
1	49-A	39	ILE	5.8
1	50-A	39	ILE	5.8
1	51-A	39	ILE	5.8
1	52-A	39	ILE	5.8
1	53-A	39	ILE	5.8
1	54-A	39	ILE	5.8
1	55-A	39	ILE	5.8
1	56-A	39	ILE	5.8
1	57-A	39	ILE	5.8
1	58-A	39	ILE	5.8
1	59-A	39	ILE	5.8
1	60-A	39	ILE	5.8
1	61-A	39	ILE	5.8
1	62-A	39	ILE	5.8
1	63-A	39	ILE	5.8
1	64-A	39	ILE	5.8
1	65-A	39	ILE	5.8
1	66-A	39	ILE	5.8
1	67-A	39	ILE	5.8
1	68-A	39	ILE	5.8
1	69-A	39	ILE	5.8
1	70-A	39	ILE	5.8

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Mol	Chain	Res	Type	RSRZ
1	71-A	39	ILE	5.8
1	72-A	39	ILE	5.8
1	73-A	39	ILE	5.8
1	74-A	39	ILE	5.8
1	75-A	39	ILE	5.8
1	1-A	57	VAL	5.2
1	2-A	57	VAL	5.2
1	3-A	57	VAL	5.2
1	4-A	57	VAL	5.2
1	5-A	57	VAL	5.2
1	6-A	57	VAL	5.2
1	7-A	57	VAL	5.2
1	8-A	57	VAL	5.2
1	9-A	57	VAL	5.2
1	10-A	57	VAL	5.2
1	11-A	57	VAL	5.2
1	12-A	57	VAL	5.2
1	13-A	57	VAL	5.2
1	14-A	57	VAL	5.2
1	15-A	57	VAL	5.2
1	16-A	57	VAL	5.2
1	17-A	57	VAL	5.2
1	18-A	57	VAL	5.2
1	19-A	57	VAL	5.2
1	20-A	57	VAL	5.2
1	21-A	57	VAL	5.2
1	22-A	57	VAL	5.2
1	23-A	57	VAL	5.2
1	24-A	57	VAL	5.2
1	25-A	57	VAL	5.2
1	26-A	57	VAL	5.2
1	27-A	57	VAL	5.2
1	28-A	57	VAL	5.2
1	29-A	57	VAL	5.2
1	30-A	57	VAL	5.2
1	31-A	57	VAL	5.2
1	32-A	57	VAL	5.2
1	33-A	57	VAL	5.2
1	34-A	57	VAL	5.2
1	35-A	57	VAL	5.2
1	36-A	57	VAL	5.2
1	37-A	57	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	38-A	57	VAL	5.2
1	39-A	57	VAL	5.2
1	40-A	57	VAL	5.2
1	41-A	57	VAL	5.2
1	42-A	57	VAL	5.2
1	43-A	57	VAL	5.2
1	44-A	57	VAL	5.2
1	45-A	57	VAL	5.2
1	46-A	57	VAL	5.2
1	47-A	57	VAL	5.2
1	48-A	57	VAL	5.2
1	49-A	57	VAL	5.2
1	50-A	57	VAL	5.2
1	51-A	57	VAL	5.2
1	52-A	57	VAL	5.2
1	53-A	57	VAL	5.2
1	54-A	57	VAL	5.2
1	55-A	57	VAL	5.2
1	56-A	57	VAL	5.2
1	57-A	57	VAL	5.2
1	58-A	57	VAL	5.2
1	59-A	57	VAL	5.2
1	60-A	57	VAL	5.2
1	61-A	57	VAL	5.2
1	62-A	57	VAL	5.2
1	63-A	57	VAL	5.2
1	64-A	57	VAL	5.2
1	65-A	57	VAL	5.2
1	66-A	57	VAL	5.2
1	67-A	57	VAL	5.2
1	68-A	57	VAL	5.2
1	69-A	57	VAL	5.2
1	70-A	57	VAL	5.2
1	71-A	57	VAL	5.2
1	72-A	57	VAL	5.2
1	73-A	57	VAL	5.2
1	74-A	57	VAL	5.2
1	75-A	57	VAL	5.2
1	1-A	90	HIS	5.0
1	2-A	90	HIS	5.0
1	3-A	90	HIS	5.0
1	4-A	90	HIS	5.0

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Mol	Chain	Res	Type	RSRZ
1	5-A	90	HIS	5.0
1	6-A	90	HIS	5.0
1	7-A	90	HIS	5.0
1	8-A	90	HIS	5.0
1	9-A	90	HIS	5.0
1	10-A	90	HIS	5.0
1	11-A	90	HIS	5.0
1	12-A	90	HIS	5.0
1	13-A	90	HIS	5.0
1	14-A	90	HIS	5.0
1	15-A	90	HIS	5.0
1	16-A	90	HIS	5.0
1	17-A	90	HIS	5.0
1	18-A	90	HIS	5.0
1	19-A	90	HIS	5.0
1	20-A	90	HIS	5.0
1	21-A	90	HIS	5.0
1	22-A	90	HIS	5.0
1	23-A	90	HIS	5.0
1	24-A	90	HIS	5.0
1	25-A	90	HIS	5.0
1	26-A	90	HIS	5.0
1	27-A	90	HIS	5.0
1	28-A	90	HIS	5.0
1	29-A	90	HIS	5.0
1	30-A	90	HIS	5.0
1	31-A	90	HIS	5.0
1	32-A	90	HIS	5.0
1	33-A	90	HIS	5.0
1	34-A	90	HIS	5.0
1	35-A	90	HIS	5.0
1	36-A	90	HIS	5.0
1	37-A	90	HIS	5.0
1	38-A	90	HIS	5.0
1	39-A	90	HIS	5.0
1	40-A	90	HIS	5.0
1	41-A	90	HIS	5.0
1	42-A	90	HIS	5.0
1	43-A	90	HIS	5.0
1	44-A	90	HIS	5.0
1	45-A	90	HIS	5.0
1	46-A	90	HIS	5.0

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Mol	Chain	Res	Type	RSRZ
1	47-A	90	HIS	5.0
1	48-A	90	HIS	5.0
1	49-A	90	HIS	5.0
1	50-A	90	HIS	5.0
1	51-A	90	HIS	5.0
1	52-A	90	HIS	5.0
1	53-A	90	HIS	5.0
1	54-A	90	HIS	5.0
1	55-A	90	HIS	5.0
1	56-A	90	HIS	5.0
1	57-A	90	HIS	5.0
1	58-A	90	HIS	5.0
1	59-A	90	HIS	5.0
1	60-A	90	HIS	5.0
1	61-A	90	HIS	5.0
1	62-A	90	HIS	5.0
1	63-A	90	HIS	5.0
1	64-A	90	HIS	5.0
1	65-A	90	HIS	5.0
1	66-A	90	HIS	5.0
1	67-A	90	HIS	5.0
1	68-A	90	HIS	5.0
1	69-A	90	HIS	5.0
1	70-A	90	HIS	5.0
1	71-A	90	HIS	5.0
1	72-A	90	HIS	5.0
1	73-A	90	HIS	5.0
1	74-A	90	HIS	5.0
1	75-A	90	HIS	5.0
1	1-A	45	LEU	4.7
1	2-A	45	LEU	4.7
1	3-A	45	LEU	4.7
1	4-A	45	LEU	4.7
1	5-A	45	LEU	4.7
1	6-A	45	LEU	4.7
1	7-A	45	LEU	4.7
1	8-A	45	LEU	4.7
1	9-A	45	LEU	4.7
1	10-A	45	LEU	4.7
1	11-A	45	LEU	4.7
1	12-A	45	LEU	4.7
1	13-A	45	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	14-A	45	LEU	4.7
1	15-A	45	LEU	4.7
1	16-A	45	LEU	4.7
1	17-A	45	LEU	4.7
1	18-A	45	LEU	4.7
1	19-A	45	LEU	4.7
1	20-A	45	LEU	4.7
1	21-A	45	LEU	4.7
1	22-A	45	LEU	4.7
1	23-A	45	LEU	4.7
1	24-A	45	LEU	4.7
1	25-A	45	LEU	4.7
1	26-A	45	LEU	4.7
1	27-A	45	LEU	4.7
1	28-A	45	LEU	4.7
1	29-A	45	LEU	4.7
1	30-A	45	LEU	4.7
1	31-A	45	LEU	4.7
1	32-A	45	LEU	4.7
1	33-A	45	LEU	4.7
1	34-A	45	LEU	4.7
1	35-A	45	LEU	4.7
1	36-A	45	LEU	4.7
1	37-A	45	LEU	4.7
1	38-A	45	LEU	4.7
1	39-A	45	LEU	4.7
1	40-A	45	LEU	4.7
1	41-A	45	LEU	4.7
1	42-A	45	LEU	4.7
1	43-A	45	LEU	4.7
1	44-A	45	LEU	4.7
1	45-A	45	LEU	4.7
1	46-A	45	LEU	4.7
1	47-A	45	LEU	4.7
1	48-A	45	LEU	4.7
1	49-A	45	LEU	4.7
1	50-A	45	LEU	4.7
1	51-A	45	LEU	4.7
1	52-A	45	LEU	4.7
1	53-A	45	LEU	4.7
1	54-A	45	LEU	4.7
1	55-A	45	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	56-A	45	LEU	4.7
1	57-A	45	LEU	4.7
1	58-A	45	LEU	4.7
1	59-A	45	LEU	4.7
1	60-A	45	LEU	4.7
1	61-A	45	LEU	4.7
1	62-A	45	LEU	4.7
1	63-A	45	LEU	4.7
1	64-A	45	LEU	4.7
1	65-A	45	LEU	4.7
1	66-A	45	LEU	4.7
1	67-A	45	LEU	4.7
1	68-A	45	LEU	4.7
1	69-A	45	LEU	4.7
1	70-A	45	LEU	4.7
1	71-A	45	LEU	4.7
1	72-A	45	LEU	4.7
1	73-A	45	LEU	4.7
1	74-A	45	LEU	4.7
1	75-A	45	LEU	4.7
1	1-A	34	PHE	4.6
1	2-A	34	PHE	4.6
1	3-A	34	PHE	4.6
1	4-A	34	PHE	4.6
1	5-A	34	PHE	4.6
1	6-A	34	PHE	4.6
1	7-A	34	PHE	4.6
1	8-A	34	PHE	4.6
1	9-A	34	PHE	4.6
1	10-A	34	PHE	4.6
1	11-A	34	PHE	4.6
1	12-A	34	PHE	4.6
1	13-A	34	PHE	4.6
1	14-A	34	PHE	4.6
1	15-A	34	PHE	4.6
1	16-A	34	PHE	4.6
1	17-A	34	PHE	4.6
1	18-A	34	PHE	4.6
1	19-A	34	PHE	4.6
1	20-A	34	PHE	4.6
1	21-A	34	PHE	4.6
1	22-A	34	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	23-A	34	PHE	4.6
1	24-A	34	PHE	4.6
1	25-A	34	PHE	4.6
1	26-A	34	PHE	4.6
1	27-A	34	PHE	4.6
1	28-A	34	PHE	4.6
1	29-A	34	PHE	4.6
1	30-A	34	PHE	4.6
1	31-A	34	PHE	4.6
1	32-A	34	PHE	4.6
1	33-A	34	PHE	4.6
1	34-A	34	PHE	4.6
1	35-A	34	PHE	4.6
1	36-A	34	PHE	4.6
1	37-A	34	PHE	4.6
1	38-A	34	PHE	4.6
1	39-A	34	PHE	4.6
1	40-A	34	PHE	4.6
1	41-A	34	PHE	4.6
1	42-A	34	PHE	4.6
1	43-A	34	PHE	4.6
1	44-A	34	PHE	4.6
1	45-A	34	PHE	4.6
1	46-A	34	PHE	4.6
1	47-A	34	PHE	4.6
1	48-A	34	PHE	4.6
1	49-A	34	PHE	4.6
1	50-A	34	PHE	4.6
1	51-A	34	PHE	4.6
1	52-A	34	PHE	4.6
1	53-A	34	PHE	4.6
1	54-A	34	PHE	4.6
1	55-A	34	PHE	4.6
1	56-A	34	PHE	4.6
1	57-A	34	PHE	4.6
1	58-A	34	PHE	4.6
1	59-A	34	PHE	4.6
1	60-A	34	PHE	4.6
1	61-A	34	PHE	4.6
1	62-A	34	PHE	4.6
1	63-A	34	PHE	4.6
1	64-A	34	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	65-A	34	PHE	4.6
1	66-A	34	PHE	4.6
1	67-A	34	PHE	4.6
1	68-A	34	PHE	4.6
1	69-A	34	PHE	4.6
1	70-A	34	PHE	4.6
1	71-A	34	PHE	4.6
1	72-A	34	PHE	4.6
1	73-A	34	PHE	4.6
1	74-A	34	PHE	4.6
1	75-A	34	PHE	4.6
1	1-A	64	LEU	3.7
1	2-A	64	LEU	3.7
1	3-A	64	LEU	3.7
1	4-A	64	LEU	3.7
1	5-A	64	LEU	3.7
1	6-A	64	LEU	3.7
1	7-A	64	LEU	3.7
1	8-A	64	LEU	3.7
1	9-A	64	LEU	3.7
1	10-A	64	LEU	3.7
1	11-A	64	LEU	3.7
1	12-A	64	LEU	3.7
1	13-A	64	LEU	3.7
1	14-A	64	LEU	3.7
1	15-A	64	LEU	3.7
1	16-A	64	LEU	3.7
1	17-A	64	LEU	3.7
1	18-A	64	LEU	3.7
1	19-A	64	LEU	3.7
1	20-A	64	LEU	3.7
1	21-A	64	LEU	3.7
1	22-A	64	LEU	3.7
1	23-A	64	LEU	3.7
1	24-A	64	LEU	3.7
1	25-A	64	LEU	3.7
1	26-A	64	LEU	3.7
1	27-A	64	LEU	3.7
1	28-A	64	LEU	3.7
1	29-A	64	LEU	3.7
1	30-A	64	LEU	3.7
1	31-A	64	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	32-A	64	LEU	3.7
1	33-A	64	LEU	3.7
1	34-A	64	LEU	3.7
1	35-A	64	LEU	3.7
1	36-A	64	LEU	3.7
1	37-A	64	LEU	3.7
1	38-A	64	LEU	3.7
1	39-A	64	LEU	3.7
1	40-A	64	LEU	3.7
1	41-A	64	LEU	3.7
1	42-A	64	LEU	3.7
1	43-A	64	LEU	3.7
1	44-A	64	LEU	3.7
1	45-A	64	LEU	3.7
1	46-A	64	LEU	3.7
1	47-A	64	LEU	3.7
1	48-A	64	LEU	3.7
1	49-A	64	LEU	3.7
1	50-A	64	LEU	3.7
1	51-A	64	LEU	3.7
1	52-A	64	LEU	3.7
1	53-A	64	LEU	3.7
1	54-A	64	LEU	3.7
1	55-A	64	LEU	3.7
1	56-A	64	LEU	3.7
1	57-A	64	LEU	3.7
1	58-A	64	LEU	3.7
1	59-A	64	LEU	3.7
1	60-A	64	LEU	3.7
1	61-A	64	LEU	3.7
1	62-A	64	LEU	3.7
1	63-A	64	LEU	3.7
1	64-A	64	LEU	3.7
1	65-A	64	LEU	3.7
1	66-A	64	LEU	3.7
1	67-A	64	LEU	3.7
1	68-A	64	LEU	3.7
1	69-A	64	LEU	3.7
1	70-A	64	LEU	3.7
1	71-A	64	LEU	3.7
1	72-A	64	LEU	3.7
1	73-A	64	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	74-A	64	LEU	3.7
1	75-A	64	LEU	3.7
1	1-A	59	ILE	3.5
1	1-A	62	GLU	3.5
1	2-A	59	ILE	3.5
1	2-A	62	GLU	3.5
1	3-A	59	ILE	3.5
1	3-A	62	GLU	3.5
1	4-A	59	ILE	3.5
1	4-A	62	GLU	3.5
1	5-A	59	ILE	3.5
1	5-A	62	GLU	3.5
1	6-A	59	ILE	3.5
1	6-A	62	GLU	3.5
1	7-A	59	ILE	3.5
1	7-A	62	GLU	3.5
1	8-A	59	ILE	3.5
1	8-A	62	GLU	3.5
1	9-A	59	ILE	3.5
1	9-A	62	GLU	3.5
1	10-A	59	ILE	3.5
1	10-A	62	GLU	3.5
1	11-A	59	ILE	3.5
1	11-A	62	GLU	3.5
1	12-A	59	ILE	3.5
1	12-A	62	GLU	3.5
1	13-A	59	ILE	3.5
1	13-A	62	GLU	3.5
1	14-A	59	ILE	3.5
1	14-A	62	GLU	3.5
1	15-A	59	ILE	3.5
1	15-A	62	GLU	3.5
1	16-A	59	ILE	3.5
1	16-A	62	GLU	3.5
1	17-A	59	ILE	3.5
1	17-A	62	GLU	3.5
1	18-A	59	ILE	3.5
1	18-A	62	GLU	3.5
1	19-A	59	ILE	3.5
1	19-A	62	GLU	3.5
1	20-A	59	ILE	3.5
1	20-A	62	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	21-A	59	ILE	3.5
1	21-A	62	GLU	3.5
1	22-A	59	ILE	3.5
1	22-A	62	GLU	3.5
1	23-A	59	ILE	3.5
1	23-A	62	GLU	3.5
1	24-A	59	ILE	3.5
1	24-A	62	GLU	3.5
1	25-A	59	ILE	3.5
1	25-A	62	GLU	3.5
1	26-A	59	ILE	3.5
1	26-A	62	GLU	3.5
1	27-A	59	ILE	3.5
1	27-A	62	GLU	3.5
1	28-A	59	ILE	3.5
1	28-A	62	GLU	3.5
1	29-A	59	ILE	3.5
1	29-A	62	GLU	3.5
1	30-A	59	ILE	3.5
1	30-A	62	GLU	3.5
1	31-A	59	ILE	3.5
1	31-A	62	GLU	3.5
1	32-A	59	ILE	3.5
1	32-A	62	GLU	3.5
1	33-A	59	ILE	3.5
1	33-A	62	GLU	3.5
1	34-A	59	ILE	3.5
1	34-A	62	GLU	3.5
1	35-A	59	ILE	3.5
1	35-A	62	GLU	3.5
1	36-A	59	ILE	3.5
1	36-A	62	GLU	3.5
1	37-A	59	ILE	3.5
1	37-A	62	GLU	3.5
1	38-A	59	ILE	3.5
1	38-A	62	GLU	3.5
1	39-A	59	ILE	3.5
1	39-A	62	GLU	3.5
1	40-A	59	ILE	3.5
1	40-A	62	GLU	3.5
1	41-A	59	ILE	3.5
1	41-A	62	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	42-A	59	ILE	3.5
1	42-A	62	GLU	3.5
1	43-A	59	ILE	3.5
1	43-A	62	GLU	3.5
1	44-A	59	ILE	3.5
1	44-A	62	GLU	3.5
1	45-A	59	ILE	3.5
1	45-A	62	GLU	3.5
1	46-A	59	ILE	3.5
1	46-A	62	GLU	3.5
1	47-A	59	ILE	3.5
1	47-A	62	GLU	3.5
1	48-A	59	ILE	3.5
1	48-A	62	GLU	3.5
1	49-A	59	ILE	3.5
1	49-A	62	GLU	3.5
1	50-A	59	ILE	3.5
1	50-A	62	GLU	3.5
1	51-A	59	ILE	3.5
1	51-A	62	GLU	3.5
1	52-A	59	ILE	3.5
1	52-A	62	GLU	3.5
1	53-A	59	ILE	3.5
1	53-A	62	GLU	3.5
1	54-A	59	ILE	3.5
1	54-A	62	GLU	3.5
1	55-A	59	ILE	3.5
1	55-A	62	GLU	3.5
1	56-A	59	ILE	3.5
1	56-A	62	GLU	3.5
1	57-A	59	ILE	3.5
1	57-A	62	GLU	3.5
1	58-A	59	ILE	3.5
1	58-A	62	GLU	3.5
1	59-A	59	ILE	3.5
1	59-A	62	GLU	3.5
1	60-A	59	ILE	3.5
1	60-A	62	GLU	3.5
1	61-A	59	ILE	3.5
1	61-A	62	GLU	3.5
1	62-A	59	ILE	3.5
1	62-A	62	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	63-A	59	ILE	3.5
1	63-A	62	GLU	3.5
1	64-A	59	ILE	3.5
1	64-A	62	GLU	3.5
1	65-A	59	ILE	3.5
1	65-A	62	GLU	3.5
1	66-A	59	ILE	3.5
1	66-A	62	GLU	3.5
1	67-A	59	ILE	3.5
1	67-A	62	GLU	3.5
1	68-A	59	ILE	3.5
1	68-A	62	GLU	3.5
1	69-A	59	ILE	3.5
1	69-A	62	GLU	3.5
1	70-A	59	ILE	3.5
1	70-A	62	GLU	3.5
1	71-A	59	ILE	3.5
1	71-A	62	GLU	3.5
1	72-A	59	ILE	3.5
1	72-A	62	GLU	3.5
1	73-A	59	ILE	3.5
1	73-A	62	GLU	3.5
1	74-A	59	ILE	3.5
1	74-A	62	GLU	3.5
1	75-A	59	ILE	3.5
1	75-A	62	GLU	3.5
1	1-A	61	GLU	3.2
1	2-A	61	GLU	3.2
1	3-A	61	GLU	3.2
1	4-A	61	GLU	3.2
1	5-A	61	GLU	3.2
1	6-A	61	GLU	3.2
1	7-A	61	GLU	3.2
1	8-A	61	GLU	3.2
1	9-A	61	GLU	3.2
1	10-A	61	GLU	3.2
1	11-A	61	GLU	3.2
1	12-A	61	GLU	3.2
1	13-A	61	GLU	3.2
1	14-A	61	GLU	3.2
1	15-A	61	GLU	3.2
1	16-A	61	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	17-A	61	GLU	3.2
1	18-A	61	GLU	3.2
1	19-A	61	GLU	3.2
1	20-A	61	GLU	3.2
1	21-A	61	GLU	3.2
1	22-A	61	GLU	3.2
1	23-A	61	GLU	3.2
1	24-A	61	GLU	3.2
1	25-A	61	GLU	3.2
1	26-A	61	GLU	3.2
1	27-A	61	GLU	3.2
1	28-A	61	GLU	3.2
1	29-A	61	GLU	3.2
1	30-A	61	GLU	3.2
1	31-A	61	GLU	3.2
1	32-A	61	GLU	3.2
1	33-A	61	GLU	3.2
1	34-A	61	GLU	3.2
1	35-A	61	GLU	3.2
1	36-A	61	GLU	3.2
1	37-A	61	GLU	3.2
1	38-A	61	GLU	3.2
1	39-A	61	GLU	3.2
1	40-A	61	GLU	3.2
1	41-A	61	GLU	3.2
1	42-A	61	GLU	3.2
1	43-A	61	GLU	3.2
1	44-A	61	GLU	3.2
1	45-A	61	GLU	3.2
1	46-A	61	GLU	3.2
1	47-A	61	GLU	3.2
1	48-A	61	GLU	3.2
1	49-A	61	GLU	3.2
1	50-A	61	GLU	3.2
1	51-A	61	GLU	3.2
1	52-A	61	GLU	3.2
1	53-A	61	GLU	3.2
1	54-A	61	GLU	3.2
1	55-A	61	GLU	3.2
1	56-A	61	GLU	3.2
1	57-A	61	GLU	3.2
1	58-A	61	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	59-A	61	GLU	3.2
1	60-A	61	GLU	3.2
1	61-A	61	GLU	3.2
1	62-A	61	GLU	3.2
1	63-A	61	GLU	3.2
1	64-A	61	GLU	3.2
1	65-A	61	GLU	3.2
1	66-A	61	GLU	3.2
1	67-A	61	GLU	3.2
1	68-A	61	GLU	3.2
1	69-A	61	GLU	3.2
1	70-A	61	GLU	3.2
1	71-A	61	GLU	3.2
1	72-A	61	GLU	3.2
1	73-A	61	GLU	3.2
1	74-A	61	GLU	3.2
1	75-A	61	GLU	3.2
1	1-A	36	ASP	3.1
1	2-A	36	ASP	3.1
1	3-A	36	ASP	3.1
1	4-A	36	ASP	3.1
1	5-A	36	ASP	3.1
1	6-A	36	ASP	3.1
1	7-A	36	ASP	3.1
1	8-A	36	ASP	3.1
1	9-A	36	ASP	3.1
1	10-A	36	ASP	3.1
1	11-A	36	ASP	3.1
1	12-A	36	ASP	3.1
1	13-A	36	ASP	3.1
1	14-A	36	ASP	3.1
1	15-A	36	ASP	3.1
1	16-A	36	ASP	3.1
1	17-A	36	ASP	3.1
1	18-A	36	ASP	3.1
1	19-A	36	ASP	3.1
1	20-A	36	ASP	3.1
1	21-A	36	ASP	3.1
1	22-A	36	ASP	3.1
1	23-A	36	ASP	3.1
1	24-A	36	ASP	3.1
1	25-A	36	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	26-A	36	ASP	3.1
1	27-A	36	ASP	3.1
1	28-A	36	ASP	3.1
1	29-A	36	ASP	3.1
1	30-A	36	ASP	3.1
1	31-A	36	ASP	3.1
1	32-A	36	ASP	3.1
1	33-A	36	ASP	3.1
1	34-A	36	ASP	3.1
1	35-A	36	ASP	3.1
1	36-A	36	ASP	3.1
1	37-A	36	ASP	3.1
1	38-A	36	ASP	3.1
1	39-A	36	ASP	3.1
1	40-A	36	ASP	3.1
1	41-A	36	ASP	3.1
1	42-A	36	ASP	3.1
1	43-A	36	ASP	3.1
1	44-A	36	ASP	3.1
1	45-A	36	ASP	3.1
1	46-A	36	ASP	3.1
1	47-A	36	ASP	3.1
1	48-A	36	ASP	3.1
1	49-A	36	ASP	3.1
1	50-A	36	ASP	3.1
1	51-A	36	ASP	3.1
1	52-A	36	ASP	3.1
1	53-A	36	ASP	3.1
1	54-A	36	ASP	3.1
1	55-A	36	ASP	3.1
1	56-A	36	ASP	3.1
1	57-A	36	ASP	3.1
1	58-A	36	ASP	3.1
1	59-A	36	ASP	3.1
1	60-A	36	ASP	3.1
1	61-A	36	ASP	3.1
1	62-A	36	ASP	3.1
1	63-A	36	ASP	3.1
1	64-A	36	ASP	3.1
1	65-A	36	ASP	3.1
1	66-A	36	ASP	3.1
1	67-A	36	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	68-A	36	ASP	3.1
1	69-A	36	ASP	3.1
1	70-A	36	ASP	3.1
1	71-A	36	ASP	3.1
1	72-A	36	ASP	3.1
1	73-A	36	ASP	3.1
1	74-A	36	ASP	3.1
1	75-A	36	ASP	3.1
1	1-A	65	VAL	2.6
1	2-A	65	VAL	2.6
1	3-A	65	VAL	2.6
1	4-A	65	VAL	2.6
1	5-A	65	VAL	2.6
1	6-A	65	VAL	2.6
1	7-A	65	VAL	2.6
1	8-A	65	VAL	2.6
1	9-A	65	VAL	2.6
1	10-A	65	VAL	2.6
1	11-A	65	VAL	2.6
1	12-A	65	VAL	2.6
1	13-A	65	VAL	2.6
1	14-A	65	VAL	2.6
1	15-A	65	VAL	2.6
1	16-A	65	VAL	2.6
1	17-A	65	VAL	2.6
1	18-A	65	VAL	2.6
1	19-A	65	VAL	2.6
1	20-A	65	VAL	2.6
1	21-A	65	VAL	2.6
1	22-A	65	VAL	2.6
1	23-A	65	VAL	2.6
1	24-A	65	VAL	2.6
1	25-A	65	VAL	2.6
1	26-A	65	VAL	2.6
1	27-A	65	VAL	2.6
1	28-A	65	VAL	2.6
1	29-A	65	VAL	2.6
1	30-A	65	VAL	2.6
1	31-A	65	VAL	2.6
1	32-A	65	VAL	2.6
1	33-A	65	VAL	2.6
1	34-A	65	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	35-A	65	VAL	2.6
1	36-A	65	VAL	2.6
1	37-A	65	VAL	2.6
1	38-A	65	VAL	2.6
1	39-A	65	VAL	2.6
1	40-A	65	VAL	2.6
1	41-A	65	VAL	2.6
1	42-A	65	VAL	2.6
1	43-A	65	VAL	2.6
1	44-A	65	VAL	2.6
1	45-A	65	VAL	2.6
1	46-A	65	VAL	2.6
1	47-A	65	VAL	2.6
1	48-A	65	VAL	2.6
1	49-A	65	VAL	2.6
1	50-A	65	VAL	2.6
1	51-A	65	VAL	2.6
1	52-A	65	VAL	2.6
1	53-A	65	VAL	2.6
1	54-A	65	VAL	2.6
1	55-A	65	VAL	2.6
1	56-A	65	VAL	2.6
1	57-A	65	VAL	2.6
1	58-A	65	VAL	2.6
1	59-A	65	VAL	2.6
1	60-A	65	VAL	2.6
1	61-A	65	VAL	2.6
1	62-A	65	VAL	2.6
1	63-A	65	VAL	2.6
1	64-A	65	VAL	2.6
1	65-A	65	VAL	2.6
1	66-A	65	VAL	2.6
1	67-A	65	VAL	2.6
1	68-A	65	VAL	2.6
1	69-A	65	VAL	2.6
1	70-A	65	VAL	2.6
1	71-A	65	VAL	2.6
1	72-A	65	VAL	2.6
1	73-A	65	VAL	2.6
1	74-A	65	VAL	2.6
1	75-A	65	VAL	2.6
1	1-A	33	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	2-A	33	PHE	2.6
1	3-A	33	PHE	2.6
1	4-A	33	PHE	2.6
1	5-A	33	PHE	2.6
1	6-A	33	PHE	2.6
1	7-A	33	PHE	2.6
1	8-A	33	PHE	2.6
1	9-A	33	PHE	2.6
1	10-A	33	PHE	2.6
1	11-A	33	PHE	2.6
1	12-A	33	PHE	2.6
1	13-A	33	PHE	2.6
1	14-A	33	PHE	2.6
1	15-A	33	PHE	2.6
1	16-A	33	PHE	2.6
1	17-A	33	PHE	2.6
1	18-A	33	PHE	2.6
1	19-A	33	PHE	2.6
1	20-A	33	PHE	2.6
1	21-A	33	PHE	2.6
1	22-A	33	PHE	2.6
1	23-A	33	PHE	2.6
1	24-A	33	PHE	2.6
1	25-A	33	PHE	2.6
1	26-A	33	PHE	2.6
1	27-A	33	PHE	2.6
1	28-A	33	PHE	2.6
1	29-A	33	PHE	2.6
1	30-A	33	PHE	2.6
1	31-A	33	PHE	2.6
1	32-A	33	PHE	2.6
1	33-A	33	PHE	2.6
1	34-A	33	PHE	2.6
1	35-A	33	PHE	2.6
1	36-A	33	PHE	2.6
1	37-A	33	PHE	2.6
1	38-A	33	PHE	2.6
1	39-A	33	PHE	2.6
1	40-A	33	PHE	2.6
1	41-A	33	PHE	2.6
1	42-A	33	PHE	2.6
1	43-A	33	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	44-A	33	PHE	2.6
1	45-A	33	PHE	2.6
1	46-A	33	PHE	2.6
1	47-A	33	PHE	2.6
1	48-A	33	PHE	2.6
1	49-A	33	PHE	2.6
1	50-A	33	PHE	2.6
1	51-A	33	PHE	2.6
1	52-A	33	PHE	2.6
1	53-A	33	PHE	2.6
1	54-A	33	PHE	2.6
1	55-A	33	PHE	2.6
1	56-A	33	PHE	2.6
1	57-A	33	PHE	2.6
1	58-A	33	PHE	2.6
1	59-A	33	PHE	2.6
1	60-A	33	PHE	2.6
1	61-A	33	PHE	2.6
1	62-A	33	PHE	2.6
1	63-A	33	PHE	2.6
1	64-A	33	PHE	2.6
1	65-A	33	PHE	2.6
1	66-A	33	PHE	2.6
1	67-A	33	PHE	2.6
1	68-A	33	PHE	2.6
1	69-A	33	PHE	2.6
1	70-A	33	PHE	2.6
1	71-A	33	PHE	2.6
1	72-A	33	PHE	2.6
1	73-A	33	PHE	2.6
1	74-A	33	PHE	2.6
1	75-A	33	PHE	2.6
1	1-A	35	GLN	2.3
1	2-A	35	GLN	2.3
1	3-A	35	GLN	2.3
1	4-A	35	GLN	2.3
1	5-A	35	GLN	2.3
1	6-A	35	GLN	2.3
1	7-A	35	GLN	2.3
1	8-A	35	GLN	2.3
1	9-A	35	GLN	2.3
1	10-A	35	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	11-A	35	GLN	2.3
1	12-A	35	GLN	2.3
1	13-A	35	GLN	2.3
1	14-A	35	GLN	2.3
1	15-A	35	GLN	2.3
1	16-A	35	GLN	2.3
1	17-A	35	GLN	2.3
1	18-A	35	GLN	2.3
1	19-A	35	GLN	2.3
1	20-A	35	GLN	2.3
1	21-A	35	GLN	2.3
1	22-A	35	GLN	2.3
1	23-A	35	GLN	2.3
1	24-A	35	GLN	2.3
1	25-A	35	GLN	2.3
1	26-A	35	GLN	2.3
1	27-A	35	GLN	2.3
1	28-A	35	GLN	2.3
1	29-A	35	GLN	2.3
1	30-A	35	GLN	2.3
1	31-A	35	GLN	2.3
1	32-A	35	GLN	2.3
1	33-A	35	GLN	2.3
1	34-A	35	GLN	2.3
1	35-A	35	GLN	2.3
1	36-A	35	GLN	2.3
1	37-A	35	GLN	2.3
1	38-A	35	GLN	2.3
1	39-A	35	GLN	2.3
1	40-A	35	GLN	2.3
1	41-A	35	GLN	2.3
1	42-A	35	GLN	2.3
1	43-A	35	GLN	2.3
1	44-A	35	GLN	2.3
1	45-A	35	GLN	2.3
1	46-A	35	GLN	2.3
1	47-A	35	GLN	2.3
1	48-A	35	GLN	2.3
1	49-A	35	GLN	2.3
1	50-A	35	GLN	2.3
1	51-A	35	GLN	2.3
1	52-A	35	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	53-A	35	GLN	2.3
1	54-A	35	GLN	2.3
1	55-A	35	GLN	2.3
1	56-A	35	GLN	2.3
1	57-A	35	GLN	2.3
1	58-A	35	GLN	2.3
1	59-A	35	GLN	2.3
1	60-A	35	GLN	2.3
1	61-A	35	GLN	2.3
1	62-A	35	GLN	2.3
1	63-A	35	GLN	2.3
1	64-A	35	GLN	2.3
1	65-A	35	GLN	2.3
1	66-A	35	GLN	2.3
1	67-A	35	GLN	2.3
1	68-A	35	GLN	2.3
1	69-A	35	GLN	2.3
1	70-A	35	GLN	2.3
1	71-A	35	GLN	2.3
1	72-A	35	GLN	2.3
1	73-A	35	GLN	2.3
1	74-A	35	GLN	2.3
1	75-A	35	GLN	2.3
1	1-A	84	SER	2.3
1	2-A	84	SER	2.3
1	3-A	84	SER	2.3
1	4-A	84	SER	2.3
1	5-A	84	SER	2.3
1	6-A	84	SER	2.3
1	7-A	84	SER	2.3
1	8-A	84	SER	2.3
1	9-A	84	SER	2.3
1	10-A	84	SER	2.3
1	11-A	84	SER	2.3
1	12-A	84	SER	2.3
1	13-A	84	SER	2.3
1	14-A	84	SER	2.3
1	15-A	84	SER	2.3
1	16-A	84	SER	2.3
1	17-A	84	SER	2.3
1	18-A	84	SER	2.3
1	19-A	84	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	20-A	84	SER	2.3
1	21-A	84	SER	2.3
1	22-A	84	SER	2.3
1	23-A	84	SER	2.3
1	24-A	84	SER	2.3
1	25-A	84	SER	2.3
1	26-A	84	SER	2.3
1	27-A	84	SER	2.3
1	28-A	84	SER	2.3
1	29-A	84	SER	2.3
1	30-A	84	SER	2.3
1	31-A	84	SER	2.3
1	32-A	84	SER	2.3
1	33-A	84	SER	2.3
1	34-A	84	SER	2.3
1	35-A	84	SER	2.3
1	36-A	84	SER	2.3
1	37-A	84	SER	2.3
1	38-A	84	SER	2.3
1	39-A	84	SER	2.3
1	40-A	84	SER	2.3
1	41-A	84	SER	2.3
1	42-A	84	SER	2.3
1	43-A	84	SER	2.3
1	44-A	84	SER	2.3
1	45-A	84	SER	2.3
1	46-A	84	SER	2.3
1	47-A	84	SER	2.3
1	48-A	84	SER	2.3
1	49-A	84	SER	2.3
1	50-A	84	SER	2.3
1	51-A	84	SER	2.3
1	52-A	84	SER	2.3
1	53-A	84	SER	2.3
1	54-A	84	SER	2.3
1	55-A	84	SER	2.3
1	56-A	84	SER	2.3
1	57-A	84	SER	2.3
1	58-A	84	SER	2.3
1	59-A	84	SER	2.3
1	60-A	84	SER	2.3
1	61-A	84	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	62-A	84	SER	2.3
1	63-A	84	SER	2.3
1	64-A	84	SER	2.3
1	65-A	84	SER	2.3
1	66-A	84	SER	2.3
1	67-A	84	SER	2.3
1	68-A	84	SER	2.3
1	69-A	84	SER	2.3
1	70-A	84	SER	2.3
1	71-A	84	SER	2.3
1	72-A	84	SER	2.3
1	73-A	84	SER	2.3
1	74-A	84	SER	2.3
1	75-A	84	SER	2.3
1	1-A	82	ALA	2.3
1	2-A	82	ALA	2.3
1	3-A	82	ALA	2.3
1	4-A	82	ALA	2.3
1	5-A	82	ALA	2.3
1	6-A	82	ALA	2.3
1	7-A	82	ALA	2.3
1	8-A	82	ALA	2.3
1	9-A	82	ALA	2.3
1	10-A	82	ALA	2.3
1	11-A	82	ALA	2.3
1	12-A	82	ALA	2.3
1	13-A	82	ALA	2.3
1	14-A	82	ALA	2.3
1	15-A	82	ALA	2.3
1	16-A	82	ALA	2.3
1	17-A	82	ALA	2.3
1	18-A	82	ALA	2.3
1	19-A	82	ALA	2.3
1	20-A	82	ALA	2.3
1	21-A	82	ALA	2.3
1	22-A	82	ALA	2.3
1	23-A	82	ALA	2.3
1	24-A	82	ALA	2.3
1	25-A	82	ALA	2.3
1	26-A	82	ALA	2.3
1	27-A	82	ALA	2.3
1	28-A	82	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	29-A	82	ALA	2.3
1	30-A	82	ALA	2.3
1	31-A	82	ALA	2.3
1	32-A	82	ALA	2.3
1	33-A	82	ALA	2.3
1	34-A	82	ALA	2.3
1	35-A	82	ALA	2.3
1	36-A	82	ALA	2.3
1	37-A	82	ALA	2.3
1	38-A	82	ALA	2.3
1	39-A	82	ALA	2.3
1	40-A	82	ALA	2.3
1	41-A	82	ALA	2.3
1	42-A	82	ALA	2.3
1	43-A	82	ALA	2.3
1	44-A	82	ALA	2.3
1	45-A	82	ALA	2.3
1	46-A	82	ALA	2.3
1	47-A	82	ALA	2.3
1	48-A	82	ALA	2.3
1	49-A	82	ALA	2.3
1	50-A	82	ALA	2.3
1	51-A	82	ALA	2.3
1	52-A	82	ALA	2.3
1	53-A	82	ALA	2.3
1	54-A	82	ALA	2.3
1	55-A	82	ALA	2.3
1	56-A	82	ALA	2.3
1	57-A	82	ALA	2.3
1	58-A	82	ALA	2.3
1	59-A	82	ALA	2.3
1	60-A	82	ALA	2.3
1	61-A	82	ALA	2.3
1	62-A	82	ALA	2.3
1	63-A	82	ALA	2.3
1	64-A	82	ALA	2.3
1	65-A	82	ALA	2.3
1	66-A	82	ALA	2.3
1	67-A	82	ALA	2.3
1	68-A	82	ALA	2.3
1	69-A	82	ALA	2.3
1	70-A	82	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	71-A	82	ALA	2.3
1	72-A	82	ALA	2.3
1	73-A	82	ALA	2.3
1	74-A	82	ALA	2.3
1	75-A	82	ALA	2.3
1	1-A	89	HIS	2.2
1	2-A	89	HIS	2.2
1	3-A	89	HIS	2.2
1	4-A	89	HIS	2.2
1	5-A	89	HIS	2.2
1	6-A	89	HIS	2.2
1	7-A	89	HIS	2.2
1	8-A	89	HIS	2.2
1	9-A	89	HIS	2.2
1	10-A	89	HIS	2.2
1	11-A	89	HIS	2.2
1	12-A	89	HIS	2.2
1	13-A	89	HIS	2.2
1	14-A	89	HIS	2.2
1	15-A	89	HIS	2.2
1	16-A	89	HIS	2.2
1	17-A	89	HIS	2.2
1	18-A	89	HIS	2.2
1	19-A	89	HIS	2.2
1	20-A	89	HIS	2.2
1	21-A	89	HIS	2.2
1	22-A	89	HIS	2.2
1	23-A	89	HIS	2.2
1	24-A	89	HIS	2.2
1	25-A	89	HIS	2.2
1	26-A	89	HIS	2.2
1	27-A	89	HIS	2.2
1	28-A	89	HIS	2.2
1	29-A	89	HIS	2.2
1	30-A	89	HIS	2.2
1	31-A	89	HIS	2.2
1	32-A	89	HIS	2.2
1	33-A	89	HIS	2.2
1	34-A	89	HIS	2.2
1	35-A	89	HIS	2.2
1	36-A	89	HIS	2.2
1	37-A	89	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	38-A	89	HIS	2.2
1	39-A	89	HIS	2.2
1	40-A	89	HIS	2.2
1	41-A	89	HIS	2.2
1	42-A	89	HIS	2.2
1	43-A	89	HIS	2.2
1	44-A	89	HIS	2.2
1	45-A	89	HIS	2.2
1	46-A	89	HIS	2.2
1	47-A	89	HIS	2.2
1	48-A	89	HIS	2.2
1	49-A	89	HIS	2.2
1	50-A	89	HIS	2.2
1	51-A	89	HIS	2.2
1	52-A	89	HIS	2.2
1	53-A	89	HIS	2.2
1	54-A	89	HIS	2.2
1	55-A	89	HIS	2.2
1	56-A	89	HIS	2.2
1	57-A	89	HIS	2.2
1	58-A	89	HIS	2.2
1	59-A	89	HIS	2.2
1	60-A	89	HIS	2.2
1	61-A	89	HIS	2.2
1	62-A	89	HIS	2.2
1	63-A	89	HIS	2.2
1	64-A	89	HIS	2.2
1	65-A	89	HIS	2.2
1	66-A	89	HIS	2.2
1	67-A	89	HIS	2.2
1	68-A	89	HIS	2.2
1	69-A	89	HIS	2.2
1	70-A	89	HIS	2.2
1	71-A	89	HIS	2.2
1	72-A	89	HIS	2.2
1	73-A	89	HIS	2.2
1	74-A	89	HIS	2.2
1	75-A	89	HIS	2.2
1	1-A	58	GLN	2.2
1	2-A	58	GLN	2.2
1	3-A	58	GLN	2.2
1	4-A	58	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	5-A	58	GLN	2.2
1	6-A	58	GLN	2.2
1	7-A	58	GLN	2.2
1	8-A	58	GLN	2.2
1	9-A	58	GLN	2.2
1	10-A	58	GLN	2.2
1	11-A	58	GLN	2.2
1	12-A	58	GLN	2.2
1	13-A	58	GLN	2.2
1	14-A	58	GLN	2.2
1	15-A	58	GLN	2.2
1	16-A	58	GLN	2.2
1	17-A	58	GLN	2.2
1	18-A	58	GLN	2.2
1	19-A	58	GLN	2.2
1	20-A	58	GLN	2.2
1	21-A	58	GLN	2.2
1	22-A	58	GLN	2.2
1	23-A	58	GLN	2.2
1	24-A	58	GLN	2.2
1	25-A	58	GLN	2.2
1	26-A	58	GLN	2.2
1	27-A	58	GLN	2.2
1	28-A	58	GLN	2.2
1	29-A	58	GLN	2.2
1	30-A	58	GLN	2.2
1	31-A	58	GLN	2.2
1	32-A	58	GLN	2.2
1	33-A	58	GLN	2.2
1	34-A	58	GLN	2.2
1	35-A	58	GLN	2.2
1	36-A	58	GLN	2.2
1	37-A	58	GLN	2.2
1	38-A	58	GLN	2.2
1	39-A	58	GLN	2.2
1	40-A	58	GLN	2.2
1	41-A	58	GLN	2.2
1	42-A	58	GLN	2.2
1	43-A	58	GLN	2.2
1	44-A	58	GLN	2.2
1	45-A	58	GLN	2.2
1	46-A	58	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	47-A	58	GLN	2.2
1	48-A	58	GLN	2.2
1	49-A	58	GLN	2.2
1	50-A	58	GLN	2.2
1	51-A	58	GLN	2.2
1	52-A	58	GLN	2.2
1	53-A	58	GLN	2.2
1	54-A	58	GLN	2.2
1	55-A	58	GLN	2.2
1	56-A	58	GLN	2.2
1	57-A	58	GLN	2.2
1	58-A	58	GLN	2.2
1	59-A	58	GLN	2.2
1	60-A	58	GLN	2.2
1	61-A	58	GLN	2.2
1	62-A	58	GLN	2.2
1	63-A	58	GLN	2.2
1	64-A	58	GLN	2.2
1	65-A	58	GLN	2.2
1	66-A	58	GLN	2.2
1	67-A	58	GLN	2.2
1	68-A	58	GLN	2.2
1	69-A	58	GLN	2.2
1	70-A	58	GLN	2.2
1	71-A	58	GLN	2.2
1	72-A	58	GLN	2.2
1	73-A	58	GLN	2.2
1	74-A	58	GLN	2.2
1	75-A	58	GLN	2.2

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	1-A	104	1/1	0.66	0.28	45,45,45,45	1
2	ZN	2-A	104	1/1	0.66	0.28	46,46,46,46	1
2	ZN	3-A	104	1/1	0.66	0.28	45,45,45,45	1
2	ZN	4-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	5-A	104	1/1	0.66	0.28	44,44,44,44	1
2	ZN	6-A	104	1/1	0.66	0.28	45,45,45,45	1
2	ZN	7-A	104	1/1	0.66	0.28	44,44,44,44	1
2	ZN	8-A	104	1/1	0.66	0.28	41,41,41,41	1
2	ZN	9-A	104	1/1	0.66	0.28	42,42,42,42	1
2	ZN	10-A	104	1/1	0.66	0.28	42,42,42,42	1
2	ZN	11-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	12-A	104	1/1	0.66	0.28	42,42,42,42	1
2	ZN	13-A	104	1/1	0.66	0.28	40,40,40,40	1
2	ZN	14-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	15-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	16-A	104	1/1	0.66	0.28	45,45,45,45	1
2	ZN	17-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	18-A	104	1/1	0.66	0.28	44,44,44,44	1
2	ZN	19-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	20-A	104	1/1	0.66	0.28	42,42,42,42	1
2	ZN	21-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	22-A	104	1/1	0.66	0.28	44,44,44,44	1
2	ZN	23-A	104	1/1	0.66	0.28	44,44,44,44	1
2	ZN	24-A	104	1/1	0.66	0.28	44,44,44,44	1
2	ZN	25-A	104	1/1	0.66	0.28	42,42,42,42	1
2	ZN	26-A	104	1/1	0.66	0.28	44,44,44,44	1
2	ZN	27-A	104	1/1	0.66	0.28	44,44,44,44	1
2	ZN	28-A	104	1/1	0.66	0.28	41,41,41,41	1
2	ZN	29-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	30-A	104	1/1	0.66	0.28	41,41,41,41	1
2	ZN	31-A	104	1/1	0.66	0.28	41,41,41,41	1
2	ZN	32-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	33-A	104	1/1	0.66	0.28	42,42,42,42	1
2	ZN	34-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	35-A	104	1/1	0.66	0.28	42,42,42,42	1
2	ZN	36-A	104	1/1	0.66	0.28	42,42,42,42	1
2	ZN	37-A	104	1/1	0.66	0.28	43,43,43,43	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	38-A	104	1/1	0.66	0.28	42,42,42,42	1
2	ZN	39-A	104	1/1	0.66	0.28	42,42,42,42	1
2	ZN	40-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	41-A	104	1/1	0.66	0.28	44,44,44,44	1
2	ZN	42-A	104	1/1	0.66	0.28	42,42,42,42	1
2	ZN	43-A	104	1/1	0.66	0.28	42,42,42,42	1
2	ZN	44-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	45-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	46-A	104	1/1	0.66	0.28	42,42,42,42	1
2	ZN	47-A	104	1/1	0.66	0.28	45,45,45,45	1
2	ZN	48-A	104	1/1	0.66	0.28	45,45,45,45	1
2	ZN	49-A	104	1/1	0.66	0.28	45,45,45,45	1
2	ZN	50-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	51-A	104	1/1	0.66	0.28	41,41,41,41	1
2	ZN	52-A	104	1/1	0.66	0.28	42,42,42,42	1
2	ZN	53-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	54-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	55-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	56-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	57-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	58-A	104	1/1	0.66	0.28	45,45,45,45	1
2	ZN	59-A	104	1/1	0.66	0.28	45,45,45,45	1
2	ZN	60-A	104	1/1	0.66	0.28	44,44,44,44	1
2	ZN	61-A	104	1/1	0.66	0.28	42,42,42,42	1
2	ZN	62-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	63-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	64-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	65-A	104	1/1	0.66	0.28	42,42,42,42	1
2	ZN	66-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	67-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	68-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	69-A	104	1/1	0.66	0.28	42,42,42,42	1
2	ZN	70-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	71-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	72-A	104	1/1	0.66	0.28	44,44,44,44	1
2	ZN	73-A	104	1/1	0.66	0.28	42,42,42,42	1
2	ZN	74-A	104	1/1	0.66	0.28	43,43,43,43	1
2	ZN	75-A	104	1/1	0.66	0.28	41,41,41,41	1
2	ZN	1-A	107	1/1	0.83	0.08	59,59,59,59	1
2	ZN	2-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	3-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	4-A	107	1/1	0.83	0.08	59,59,59,59	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	5-A	107	1/1	0.83	0.08	61,61,61,61	1
2	ZN	6-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	7-A	107	1/1	0.83	0.08	56,56,56,56	1
2	ZN	8-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	9-A	107	1/1	0.83	0.08	59,59,59,59	1
2	ZN	10-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	11-A	107	1/1	0.83	0.08	59,59,59,59	1
2	ZN	12-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	13-A	107	1/1	0.83	0.08	56,56,56,56	1
2	ZN	14-A	107	1/1	0.83	0.08	53,53,53,53	1
2	ZN	15-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	16-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	17-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	18-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	19-A	107	1/1	0.83	0.08	54,54,54,54	1
2	ZN	20-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	21-A	107	1/1	0.83	0.08	56,56,56,56	1
2	ZN	22-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	23-A	107	1/1	0.83	0.08	59,59,59,59	1
2	ZN	24-A	107	1/1	0.83	0.08	59,59,59,59	1
2	ZN	25-A	107	1/1	0.83	0.08	61,61,61,61	1
2	ZN	26-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	27-A	107	1/1	0.83	0.08	58,58,58,58	1
2	ZN	28-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	29-A	107	1/1	0.83	0.08	62,62,62,62	1
2	ZN	30-A	107	1/1	0.83	0.08	56,56,56,56	1
2	ZN	31-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	32-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	33-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	34-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	35-A	107	1/1	0.83	0.08	55,55,55,55	1
2	ZN	36-A	107	1/1	0.83	0.08	54,54,54,54	1
2	ZN	37-A	107	1/1	0.83	0.08	52,52,52,52	1
2	ZN	38-A	107	1/1	0.83	0.08	56,56,56,56	1
2	ZN	39-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	40-A	107	1/1	0.83	0.08	59,59,59,59	1
2	ZN	41-A	107	1/1	0.83	0.08	61,61,61,61	1
2	ZN	42-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	43-A	107	1/1	0.83	0.08	59,59,59,59	1
2	ZN	44-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	45-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	46-A	107	1/1	0.83	0.08	58,58,58,58	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	47-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	48-A	107	1/1	0.83	0.08	59,59,59,59	1
2	ZN	49-A	107	1/1	0.83	0.08	56,56,56,56	1
2	ZN	50-A	107	1/1	0.83	0.08	56,56,56,56	1
2	ZN	51-A	107	1/1	0.83	0.08	58,58,58,58	1
2	ZN	52-A	107	1/1	0.83	0.08	58,58,58,58	1
2	ZN	53-A	107	1/1	0.83	0.08	58,58,58,58	1
2	ZN	54-A	107	1/1	0.83	0.08	58,58,58,58	1
2	ZN	55-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	56-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	57-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	58-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	59-A	107	1/1	0.83	0.08	61,61,61,61	1
2	ZN	60-A	107	1/1	0.83	0.08	60,60,60,60	1
2	ZN	61-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	62-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	63-A	107	1/1	0.83	0.08	55,55,55,55	1
2	ZN	64-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	65-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	66-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	67-A	107	1/1	0.83	0.08	56,56,56,56	1
2	ZN	68-A	107	1/1	0.83	0.08	53,53,53,53	1
2	ZN	69-A	107	1/1	0.83	0.08	59,59,59,59	1
2	ZN	70-A	107	1/1	0.83	0.08	56,56,56,56	1
2	ZN	71-A	107	1/1	0.83	0.08	59,59,59,59	1
2	ZN	72-A	107	1/1	0.83	0.08	60,60,60,60	1
2	ZN	73-A	107	1/1	0.83	0.08	62,62,62,62	1
2	ZN	74-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	75-A	107	1/1	0.83	0.08	57,57,57,57	1
2	ZN	1-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	2-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	3-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	4-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	5-A	102	1/1	0.91	0.15	41,41,41,41	1
2	ZN	6-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	7-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	8-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	9-A	102	1/1	0.91	0.15	41,41,41,41	1
2	ZN	10-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	11-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	12-A	102	1/1	0.91	0.15	38,38,38,38	1
2	ZN	13-A	102	1/1	0.91	0.15	39,39,39,39	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	14-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	15-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	16-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	17-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	18-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	19-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	20-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	21-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	22-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	23-A	102	1/1	0.91	0.15	38,38,38,38	1
2	ZN	24-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	25-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	26-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	27-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	28-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	29-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	30-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	31-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	32-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	33-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	34-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	35-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	36-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	37-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	38-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	39-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	40-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	41-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	42-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	43-A	102	1/1	0.91	0.15	41,41,41,41	1
2	ZN	44-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	45-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	46-A	102	1/1	0.91	0.15	41,41,41,41	1
2	ZN	47-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	48-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	49-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	50-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	51-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	52-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	53-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	54-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	55-A	102	1/1	0.91	0.15	39,39,39,39	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	56-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	57-A	102	1/1	0.91	0.15	41,41,41,41	1
2	ZN	58-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	59-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	60-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	61-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	62-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	63-A	102	1/1	0.91	0.15	37,37,37,37	1
2	ZN	64-A	102	1/1	0.91	0.15	38,38,38,38	1
2	ZN	65-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	66-A	102	1/1	0.91	0.15	38,38,38,38	1
2	ZN	67-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	68-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	69-A	102	1/1	0.91	0.15	41,41,41,41	1
2	ZN	70-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	71-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	72-A	102	1/1	0.91	0.15	41,41,41,41	1
2	ZN	73-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	74-A	102	1/1	0.91	0.15	39,39,39,39	1
2	ZN	75-A	102	1/1	0.91	0.15	40,40,40,40	1
2	ZN	1-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	2-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	3-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	4-A	106	1/1	0.93	0.29	36,36,36,36	1
2	ZN	5-A	106	1/1	0.93	0.29	36,36,36,36	1
2	ZN	6-A	106	1/1	0.93	0.29	36,36,36,36	1
2	ZN	7-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	8-A	106	1/1	0.93	0.29	36,36,36,36	1
2	ZN	9-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	10-A	106	1/1	0.93	0.29	36,36,36,36	1
2	ZN	11-A	106	1/1	0.93	0.29	36,36,36,36	1
2	ZN	12-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	13-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	14-A	106	1/1	0.93	0.29	36,36,36,36	1
2	ZN	15-A	106	1/1	0.93	0.29	36,36,36,36	1
2	ZN	16-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	17-A	106	1/1	0.93	0.29	36,36,36,36	1
2	ZN	18-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	19-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	20-A	106	1/1	0.93	0.29	36,36,36,36	1
2	ZN	21-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	22-A	106	1/1	0.93	0.29	35,35,35,35	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	23-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	24-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	25-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	26-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	27-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	28-A	106	1/1	0.93	0.29	36,36,36,36	1
2	ZN	29-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	30-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	31-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	32-A	106	1/1	0.93	0.29	36,36,36,36	1
2	ZN	33-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	34-A	106	1/1	0.93	0.29	36,36,36,36	1
2	ZN	35-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	36-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	37-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	38-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	39-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	40-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	41-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	42-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	43-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	44-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	45-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	46-A	106	1/1	0.93	0.29	36,36,36,36	1
2	ZN	47-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	48-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	49-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	50-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	51-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	52-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	53-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	54-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	55-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	56-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	57-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	58-A	106	1/1	0.93	0.29	36,36,36,36	1
2	ZN	59-A	106	1/1	0.93	0.29	36,36,36,36	1
2	ZN	60-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	61-A	106	1/1	0.93	0.29	36,36,36,36	1
2	ZN	62-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	63-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	64-A	106	1/1	0.93	0.29	35,35,35,35	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	65-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	66-A	106	1/1	0.93	0.29	36,36,36,36	1
2	ZN	67-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	68-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	69-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	70-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	71-A	106	1/1	0.93	0.29	36,36,36,36	1
2	ZN	72-A	106	1/1	0.93	0.29	36,36,36,36	1
2	ZN	73-A	106	1/1	0.93	0.29	36,36,36,36	1
2	ZN	74-A	106	1/1	0.93	0.29	36,36,36,36	1
2	ZN	75-A	106	1/1	0.93	0.29	35,35,35,35	1
2	ZN	1-A	105	1/1	0.97	0.11	43,43,43,43	1
2	ZN	2-A	105	1/1	0.97	0.11	41,41,41,41	1
2	ZN	3-A	105	1/1	0.97	0.11	41,41,41,41	1
2	ZN	4-A	105	1/1	0.97	0.11	44,44,44,44	1
2	ZN	5-A	105	1/1	0.97	0.11	46,46,46,46	1
2	ZN	6-A	105	1/1	0.97	0.11	44,44,44,44	1
2	ZN	7-A	105	1/1	0.97	0.11	43,43,43,43	1
2	ZN	8-A	105	1/1	0.97	0.11	42,42,42,42	1
2	ZN	9-A	105	1/1	0.97	0.11	42,42,42,42	1
2	ZN	10-A	105	1/1	0.97	0.11	42,42,42,42	1
2	ZN	11-A	105	1/1	0.97	0.11	45,45,45,45	1
2	ZN	12-A	105	1/1	0.97	0.11	43,43,43,43	1
2	ZN	13-A	105	1/1	0.97	0.11	46,46,46,46	1
2	ZN	14-A	105	1/1	0.97	0.11	46,46,46,46	1
2	ZN	15-A	105	1/1	0.97	0.11	42,42,42,42	1
2	ZN	16-A	105	1/1	0.97	0.11	43,43,43,43	1
2	ZN	17-A	105	1/1	0.97	0.11	43,43,43,43	1
2	ZN	18-A	105	1/1	0.97	0.11	44,44,44,44	1
2	ZN	19-A	105	1/1	0.97	0.11	41,41,41,41	1
2	ZN	20-A	105	1/1	0.97	0.11	41,41,41,41	1
2	ZN	21-A	105	1/1	0.97	0.11	43,43,43,43	1
2	ZN	22-A	105	1/1	0.97	0.11	41,41,41,41	1
2	ZN	23-A	105	1/1	0.97	0.11	43,43,43,43	1
2	ZN	24-A	105	1/1	0.97	0.11	43,43,43,43	1
2	ZN	25-A	105	1/1	0.97	0.11	45,45,45,45	1
2	ZN	26-A	105	1/1	0.97	0.11	44,44,44,44	1
2	ZN	27-A	105	1/1	0.97	0.11	44,44,44,44	1
2	ZN	28-A	105	1/1	0.97	0.11	43,43,43,43	1
2	ZN	29-A	105	1/1	0.97	0.11	46,46,46,46	1
2	ZN	30-A	105	1/1	0.97	0.11	43,43,43,43	1
2	ZN	31-A	105	1/1	0.97	0.11	44,44,44,44	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	32-A	105	1/1	0.97	0.11	43,43,43,43	1
2	ZN	33-A	105	1/1	0.97	0.11	46,46,46,46	1
2	ZN	34-A	105	1/1	0.97	0.11	43,43,43,43	1
2	ZN	35-A	105	1/1	0.97	0.11	41,41,41,41	1
2	ZN	36-A	105	1/1	0.97	0.11	42,42,42,42	1
2	ZN	37-A	105	1/1	0.97	0.11	44,44,44,44	1
2	ZN	38-A	105	1/1	0.97	0.11	41,41,41,41	1
2	ZN	39-A	105	1/1	0.97	0.11	42,42,42,42	1
2	ZN	40-A	105	1/1	0.97	0.11	46,46,46,46	1
2	ZN	41-A	105	1/1	0.97	0.11	47,47,47,47	1
2	ZN	42-A	105	1/1	0.97	0.11	45,45,45,45	1
2	ZN	43-A	105	1/1	0.97	0.11	42,42,42,42	1
2	ZN	44-A	105	1/1	0.97	0.11	42,42,42,42	1
2	ZN	45-A	105	1/1	0.97	0.11	44,44,44,44	1
2	ZN	46-A	105	1/1	0.97	0.11	42,42,42,42	1
2	ZN	47-A	105	1/1	0.97	0.11	43,43,43,43	1
2	ZN	48-A	105	1/1	0.97	0.11	43,43,43,43	1
2	ZN	49-A	105	1/1	0.97	0.11	41,41,41,41	1
2	ZN	50-A	105	1/1	0.97	0.11	45,45,45,45	1
2	ZN	51-A	105	1/1	0.97	0.11	47,47,47,47	1
2	ZN	52-A	105	1/1	0.97	0.11	44,44,44,44	1
2	ZN	53-A	105	1/1	0.97	0.11	42,42,42,42	1
2	ZN	54-A	105	1/1	0.97	0.11	42,42,42,42	1
2	ZN	55-A	105	1/1	0.97	0.11	44,44,44,44	1
2	ZN	56-A	105	1/1	0.97	0.11	42,42,42,42	1
2	ZN	57-A	105	1/1	0.97	0.11	43,43,43,43	1
2	ZN	58-A	105	1/1	0.97	0.11	44,44,44,44	1
2	ZN	59-A	105	1/1	0.97	0.11	44,44,44,44	1
2	ZN	60-A	105	1/1	0.97	0.11	44,44,44,44	1
2	ZN	61-A	105	1/1	0.97	0.11	46,46,46,46	1
2	ZN	62-A	105	1/1	0.97	0.11	43,43,43,43	1
2	ZN	63-A	105	1/1	0.97	0.11	42,42,42,42	1
2	ZN	64-A	105	1/1	0.97	0.11	43,43,43,43	1
2	ZN	65-A	105	1/1	0.97	0.11	42,42,42,42	1
2	ZN	66-A	105	1/1	0.97	0.11	43,43,43,43	1
2	ZN	67-A	105	1/1	0.97	0.11	42,42,42,42	1
2	ZN	68-A	105	1/1	0.97	0.11	41,41,41,41	1
2	ZN	69-A	105	1/1	0.97	0.11	44,44,44,44	1
2	ZN	70-A	105	1/1	0.97	0.11	42,42,42,42	1
2	ZN	71-A	105	1/1	0.97	0.11	45,45,45,45	1
2	ZN	72-A	105	1/1	0.97	0.11	45,45,45,45	1
2	ZN	73-A	105	1/1	0.97	0.11	43,43,43,43	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	74-A	105	1/1	0.97	0.11	42,42,42,42	1
2	ZN	75-A	105	1/1	0.97	0.11	42,42,42,42	1
2	ZN	1-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	2-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	3-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	4-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	5-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	6-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	7-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	8-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	9-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	10-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	11-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	12-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	13-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	14-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	15-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	16-A	101	1/1	0.98	0.04	56,56,56,56	1
2	ZN	17-A	101	1/1	0.98	0.04	57,57,57,57	1
2	ZN	18-A	101	1/1	0.98	0.04	56,56,56,56	1
2	ZN	19-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	20-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	21-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	22-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	23-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	24-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	25-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	26-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	27-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	28-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	29-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	30-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	31-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	32-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	33-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	34-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	35-A	101	1/1	0.98	0.04	51,51,51,51	1
2	ZN	36-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	37-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	38-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	39-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	40-A	101	1/1	0.98	0.04	53,53,53,53	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	41-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	42-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	43-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	44-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	45-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	46-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	47-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	48-A	101	1/1	0.98	0.04	51,51,51,51	1
2	ZN	49-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	50-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	51-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	52-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	53-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	54-A	101	1/1	0.98	0.04	55,55,55,55	1
2	ZN	55-A	101	1/1	0.98	0.04	57,57,57,57	1
2	ZN	56-A	101	1/1	0.98	0.04	56,56,56,56	1
2	ZN	57-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	58-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	59-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	60-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	61-A	101	1/1	0.98	0.04	51,51,51,51	1
2	ZN	62-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	63-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	64-A	101	1/1	0.98	0.04	51,51,51,51	1
2	ZN	65-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	66-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	67-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	68-A	101	1/1	0.98	0.04	55,55,55,55	1
2	ZN	69-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	70-A	101	1/1	0.98	0.04	50,50,50,50	1
2	ZN	71-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	72-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	73-A	101	1/1	0.98	0.04	53,53,53,53	1
2	ZN	74-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	75-A	101	1/1	0.98	0.04	52,52,52,52	1
2	ZN	1-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	2-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	3-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	4-A	103	1/1	0.98	0.11	40,40,40,40	1
2	ZN	5-A	103	1/1	0.98	0.11	41,41,41,41	1
2	ZN	6-A	103	1/1	0.98	0.11	40,40,40,40	1
2	ZN	7-A	103	1/1	0.98	0.11	42,42,42,42	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	8-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	9-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	10-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	11-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	12-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	13-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	14-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	15-A	103	1/1	0.98	0.11	40,40,40,40	1
2	ZN	16-A	103	1/1	0.98	0.11	41,41,41,41	1
2	ZN	17-A	103	1/1	0.98	0.11	44,44,44,44	1
2	ZN	18-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	19-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	20-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	21-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	22-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	23-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	24-A	103	1/1	0.98	0.11	46,46,46,46	1
2	ZN	25-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	26-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	27-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	28-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	29-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	30-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	31-A	103	1/1	0.98	0.11	41,41,41,41	1
2	ZN	32-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	33-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	34-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	35-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	36-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	37-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	38-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	39-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	40-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	41-A	103	1/1	0.98	0.11	44,44,44,44	1
2	ZN	42-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	43-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	44-A	103	1/1	0.98	0.11	45,45,45,45	1
2	ZN	45-A	103	1/1	0.98	0.11	44,44,44,44	1
2	ZN	46-A	103	1/1	0.98	0.11	45,45,45,45	1
2	ZN	47-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	48-A	103	1/1	0.98	0.11	40,40,40,40	1
2	ZN	49-A	103	1/1	0.98	0.11	41,41,41,41	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	50-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	51-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	52-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	53-A	103	1/1	0.98	0.11	41,41,41,41	1
2	ZN	54-A	103	1/1	0.98	0.11	44,44,44,44	1
2	ZN	55-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	56-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	57-A	103	1/1	0.98	0.11	44,44,44,44	1
2	ZN	58-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	59-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	60-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	61-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	62-A	103	1/1	0.98	0.11	44,44,44,44	1
2	ZN	63-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	64-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	65-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	66-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	67-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	68-A	103	1/1	0.98	0.11	40,40,40,40	1
2	ZN	69-A	103	1/1	0.98	0.11	41,41,41,41	1
2	ZN	70-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	71-A	103	1/1	0.98	0.11	40,40,40,40	1
2	ZN	72-A	103	1/1	0.98	0.11	42,42,42,42	1
2	ZN	73-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	74-A	103	1/1	0.98	0.11	43,43,43,43	1
2	ZN	75-A	103	1/1	0.98	0.11	43,43,43,43	1

6.5 Other polymers (i)

There are no such residues in this entry.