



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2016 – 04:50 PM BST

PDB ID : 5EXU  
Title : Reversibly photoswitching protein Dathail, Ensemble refinement  
Authors : Close, D.W.; Langan, P.S.; Bradbury, A.R.M.  
Deposited on : 2015-11-24  
Resolution : 1.65 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : **FAILED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

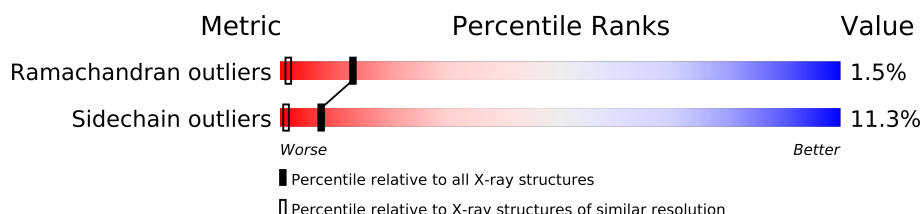
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)


























The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1-A	229	<div> <div>82%</div> <div>10% • 7%</div> </div>
1	10-A	229	<div> <div>83%</div> <div>10% • 7%</div> </div>
1	11-A	229	<div> <div>81%</div> <div>12% • 7%</div> </div>
1	12-A	229	<div> <div>81%</div> <div>11% • 7%</div> </div>
1	13-A	229	<div> <div>83%</div> <div>10% • 7%</div> </div>
1	14-A	229	<div> <div>81%</div> <div>10% • 7%</div> </div>
1	15-A	229	<div> <div>85%</div> <div>7% • 7%</div> </div>
1	16-A	229	<div> <div>83%</div> <div>10% • 7%</div> </div>
1	17-A	229	<div> <div>78%</div> <div>14% •• 7%</div> </div>


























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Mol	Chain	Length	Quality of chain
1	18-A	229	 78%14%7%
1	19-A	229	 83%9%7%
1	2-A	229	 82%11%7%
1	20-A	229	 83%10%7%
1	21-A	229	 82%11%7%
1	22-A	229	 82%10%7%
1	23-A	229	 81%11%7%
1	24-A	229	 83%10%7%
1	25-A	229	 82%9%7%
1	26-A	229	 82%9%7%
1	27-A	229	 79%13%7%
1	28-A	229	 82%10%7%
1	29-A	229	 81%11%7%
1	3-A	229	 78%13%7%
1	30-A	229	 82%10%7%
1	31-A	229	 86%6%7%
1	32-A	229	 85%8%7%
1	33-A	229	 81%11%7%
1	34-A	229	 82%10%7%
1	35-A	229	 85%9%7%
1	36-A	229	 84%10%7%
1	37-A	229	 78%14%7%
1	38-A	229	 80%12%7%
1	39-A	229	 80%12%7%
1	4-A	229	 81%10%7%

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Mol	Chain	Length	Quality of chain
1	40-A	229	 81% 11% • 7%
1	41-A	229	 81% 12% • 7%
1	42-A	229	 79% 14% • 7%
1	43-A	229	 81% 11% • 7%
1	44-A	229	 83% 9% • 7%
1	45-A	229	 83% 10% • 7%
1	46-A	229	 83% 10% • 7%
1	47-A	229	 85% 8% • 7%
1	48-A	229	 85% 9% • 7%
1	49-A	229	 84% 8% • 7%
1	5-A	229	 84% 8% • 7%
1	50-A	229	 84% 7% • 7%
1	51-A	229	 83% 9% • 7%
1	52-A	229	 82% 10% • 7%
1	53-A	229	 83% 10% • 7%
1	54-A	229	 81% 11% • 7%
1	55-A	229	 80% 13% • 7%
1	56-A	229	 81% 11% • 7%
1	57-A	229	 82% 10% • 7%
1	58-A	229	 81% 12% • 7%
1	59-A	229	 84% 9% • 7%
1	6-A	229	 84% 9% • 7%
1	60-A	229	 80% 12% • 7%
1	61-A	229	 80% 13% • 7%
1	62-A	229	 82% 10% • 7%

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Mol	Chain	Length	Quality of chain
1	63-A	229	<div><div></div><div>81%12%7%</div></div>
1	7-A	229	<div><div></div><div>82%11%7%</div></div>
1	8-A	229	<div><div></div><div>83%9%7%</div></div>
1	9-A	229	<div><div></div><div>82%11%7%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 224314 atoms, of which 105273 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 Reversibly photoswitching protein Dathail.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	214	Total	C	H	N	O	S	0	0	0
			3416	1118	1671	286	331	10			
1	2-A	214	Total	C	H	N	O	S	0	0	0
			3416	1118	1671	286	331	10			
1	3-A	214	Total	C	H	N	O	S	0	0	0
			3416	1118	1671	286	331	10			
1	4-A	214	Total	C	H	N	O	S	0	0	0
			3416	1118	1671	286	331	10			
1	5-A	214	Total	C	H	N	O	S	0	0	0
			3416	1118	1671	286	331	10			
1	6-A	214	Total	C	H	N	O	S	0	0	0
			3416	1118	1671	286	331	10			
1	7-A	214	Total	C	H	N	O	S	0	0	0
			3416	1118	1671	286	331	10			
1	8-A	214	Total	C	H	N	O	S	0	0	0
			3416	1118	1671	286	331	10			
1	9-A	214	Total	C	H	N	O	S	0	0	0
			3416	1118	1671	286	331	10			
1	10-A	214	Total	C	H	N	O	S	0	0	0
			3416	1118	1671	286	331	10			
1	11-A	214	Total	C	H	N	O	S	0	0	0
			3416	1118	1671	286	331	10			
1	12-A	214	Total	C	H	N	O	S	0	0	0
			3416	1118	1671	286	331	10			
1	13-A	214	Total	C	H	N	O	S	0	0	0
			3416	1118	1671	286	331	10			
1	14-A	214	Total	C	H	N	O	S	0	0	0
			3416	1118	1671	286	331	10			
1	15-A	214	Total	C	H	N	O	S	0	0	0
			3416	1118	1671	286	331	10			
1	16-A	214	Total	C	H	N	O	S	0	0	0
			3416	1118	1671	286	331	10			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	18-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	19-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	20-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	21-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	22-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	23-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	24-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	25-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	26-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	27-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	28-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	29-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	30-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	31-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	32-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	33-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	34-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	35-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	36-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	37-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	38-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	39-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	40-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	41-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	42-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	43-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	44-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	45-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	46-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	47-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	48-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	49-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	50-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	51-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	52-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	53-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	54-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	55-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	56-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	57-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	58-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	59-A	214	Total	C	H	N	O	S	0	0	0
			3416	1118	1671	286	331	10			
1	60-A	214	Total	C	H	N	O	S	0	0	0
			3416	1118	1671	286	331	10			
1	61-A	214	Total	C	H	N	O	S	0	0	0
			3416	1118	1671	286	331	10			
1	62-A	214	Total	C	H	N	O	S	0	0	0
			3416	1118	1671	286	331	10			
1	63-A	214	Total	C	H	N	O	S	0	0	0
			3416	1118	1671	286	331	10			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	126	Total	O	0	0
			126	126		
2	2-A	135	Total	O	0	0
			135	135		
2	3-A	140	Total	O	0	0
			140	140		
2	4-A	163	Total	O	0	0
			163	163		
2	5-A	146	Total	O	0	0
			146	146		
2	6-A	126	Total	O	0	0
			126	126		
2	7-A	124	Total	O	0	0
			124	124		
2	8-A	134	Total	O	0	0
			134	134		
2	9-A	139	Total	O	0	0
			139	139		
2	10-A	144	Total	O	0	0
			144	144		
2	11-A	140	Total	O	0	0
			140	140		
2	12-A	145	Total	O	0	0
			145	145		
2	13-A	142	Total	O	0	0
			142	142		
2	14-A	144	Total	O	0	0
			144	144		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	15-A	143	Total 143	O 143	0	0
2	16-A	144	Total 144	O 144	0	0
2	17-A	140	Total 140	O 140	0	0
2	18-A	137	Total 137	O 137	0	0
2	19-A	160	Total 160	O 160	0	0
2	20-A	161	Total 161	O 161	0	0
2	21-A	137	Total 137	O 137	0	0
2	22-A	124	Total 124	O 124	0	0
2	23-A	123	Total 123	O 123	0	0
2	24-A	148	Total 148	O 148	0	0
2	25-A	162	Total 162	O 162	0	0
2	26-A	160	Total 160	O 160	0	0
2	27-A	143	Total 143	O 143	0	0
2	28-A	140	Total 140	O 140	0	0
2	29-A	140	Total 140	O 140	0	0
2	30-A	155	Total 155	O 155	0	0
2	31-A	171	Total 171	O 171	0	0
2	32-A	143	Total 143	O 143	0	0
2	33-A	139	Total 139	O 139	0	0
2	34-A	134	Total 134	O 134	0	0
2	35-A	149	Total 149	O 149	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	36-A	149	Total 149	O 149	0	0
2	37-A	153	Total 153	O 153	0	0
2	38-A	160	Total 160	O 160	0	0
2	39-A	140	Total 140	O 140	0	0
2	40-A	139	Total 139	O 139	0	0
2	41-A	151	Total 151	O 151	0	0
2	42-A	158	Total 158	O 158	0	0
2	43-A	152	Total 152	O 152	0	0
2	44-A	140	Total 140	O 140	0	0
2	45-A	146	Total 146	O 146	0	0
2	46-A	137	Total 137	O 137	0	0
2	47-A	138	Total 138	O 138	0	0
2	48-A	140	Total 140	O 140	0	0
2	49-A	152	Total 152	O 152	0	0
2	50-A	146	Total 146	O 146	0	0
2	51-A	158	Total 158	O 158	0	0
2	52-A	136	Total 136	O 136	0	0
2	53-A	134	Total 134	O 134	0	0
2	54-A	139	Total 139	O 139	0	0
2	55-A	139	Total 139	O 139	0	0
2	56-A	138	Total 138	O 138	0	0

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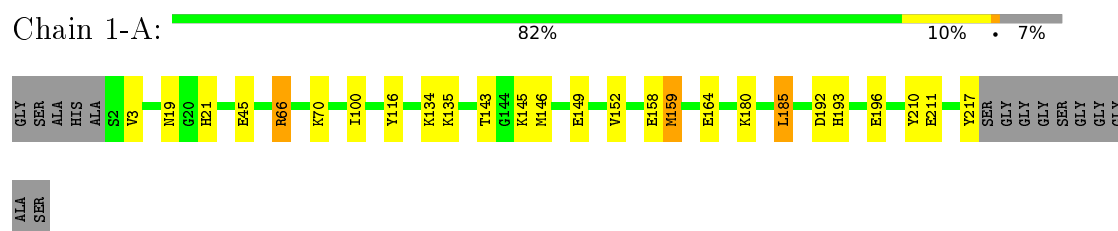
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	57-A	152	Total 152	O 152	0	0
2	58-A	150	Total 150	O 150	0	0
2	59-A	152	Total 152	O 152	0	0
2	60-A	141	Total 141	O 141	0	0
2	61-A	167	Total 167	O 167	0	0
2	62-A	155	Total 155	O 155	0	0
2	63-A	143	Total 143	O 143	0	0

### 3 Residue-property plots [i](#)

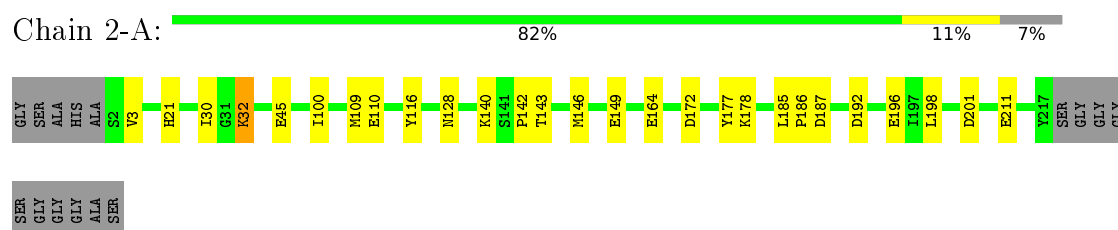
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS failed to run properly.

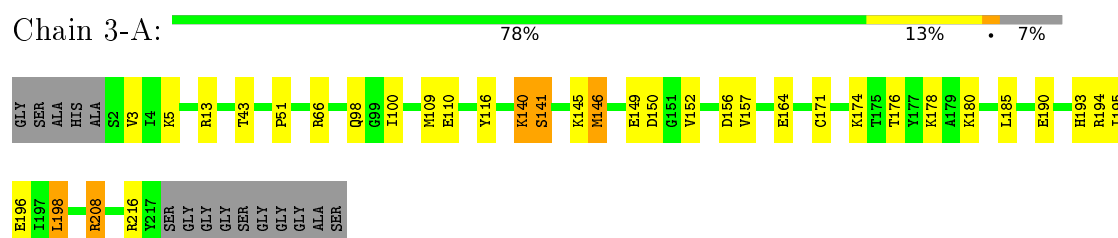
- Molecule 1: Reversibly photoswitching protein Dathail



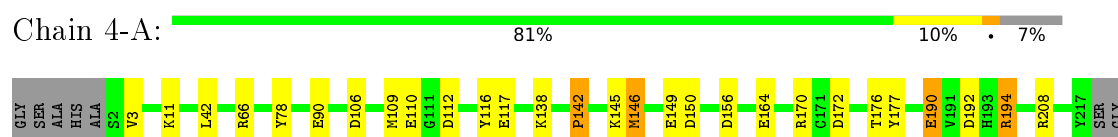
- Molecule 1: Reversibly photoswitching protein Dathail



- Molecule 1: Reversibly photoswitching protein Dathail




- Molecule 1: Reversibly photoswitching protein Dathail



GLY	SER	ALA	HIS	ALA	S2	V3	E15	E28	K32	T39	L40	D41	Q81	E90	Q98	M109	Y116	M124	K138	M139	K140	S141	P142	K145	E149	D150	D156	K174	H193	R194	L195	E196	Y217	SER	GLY	GLY	GLY	SER	GLY	GLY	ALA
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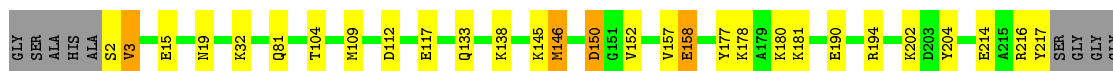
SER

- Molecule 1: Reversibly photoswitching protein Dathail

Chain 11-A:  81% 12% 7%


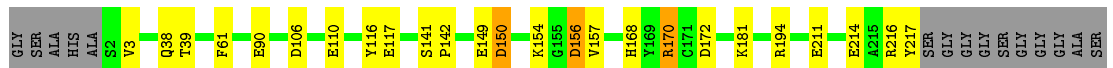
SER

- Molecule 1: Reversibly photoswitching protein Dathail


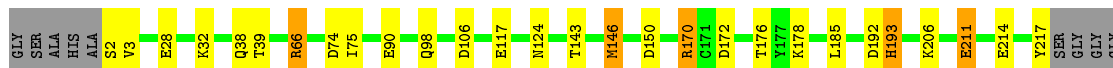
Chain 12-A:  81% 11% 7%

SER

- Molecule 1: Reversibly photoswitching protein Dathail


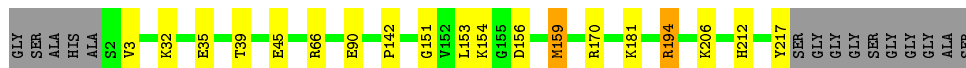
Chain 13-A:  83% 10% 7%

- Molecule 1: Reversibly photoswitching protein Dathail


Chain 14-A:  81% 10% 7%

SER

- Molecule 1: Reversibly photoswitching protein Dathail

Chain 15-A:  85% 7% 7%

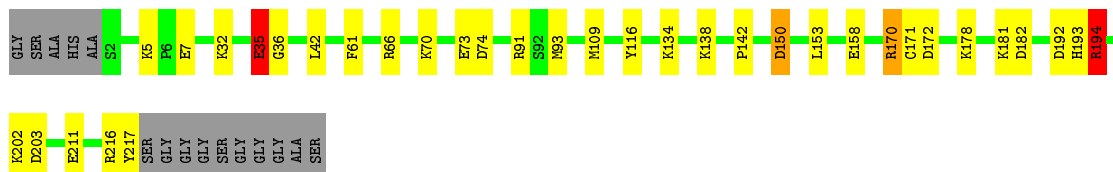
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 16-A:  83% 10% 7%




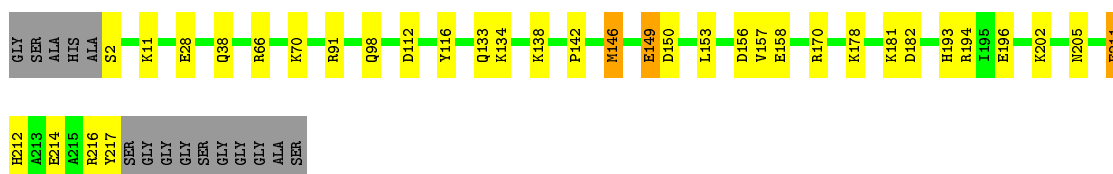
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 17-A:  78% 14% .. 7%




- Molecule 1: Reversibly photoswitching protein Dathail

Chain 18-A:  78% 14% • 7%




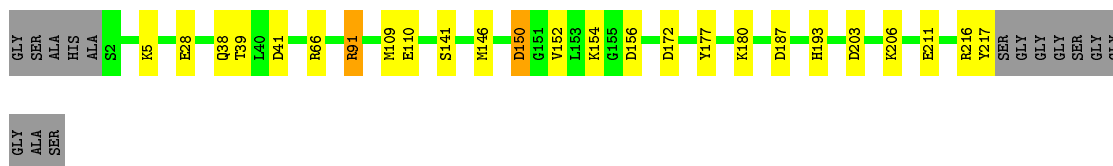
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 19-A:  83% 9% 7%




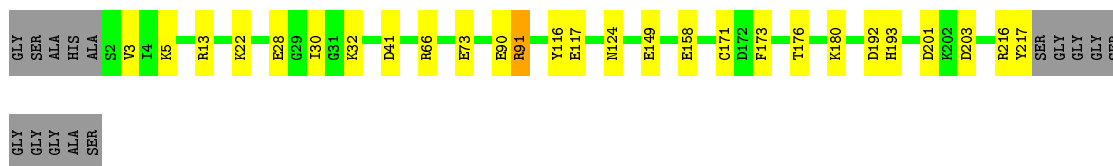
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 20-A:  83% 10% • 7%




- Molecule 1: Reversibly photoswitching protein Dathail

Chain 21-A:  82% 11% 7%




- Molecule 1: Reversibly photoswitching protein Dathail

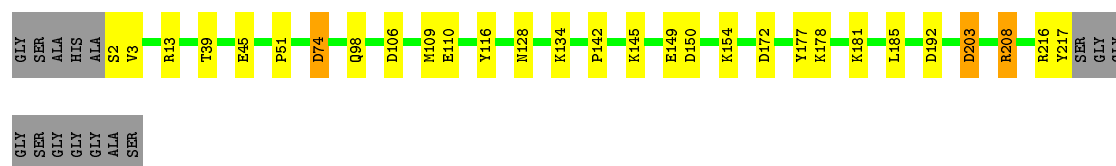


Chain 22-A: 




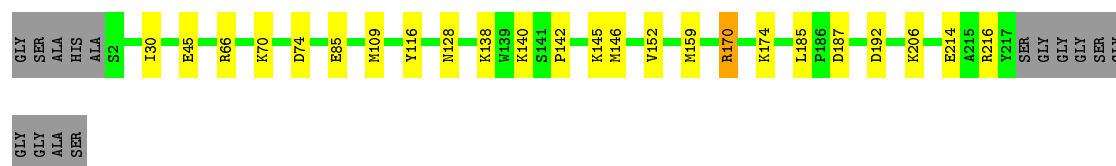
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 23-A: 




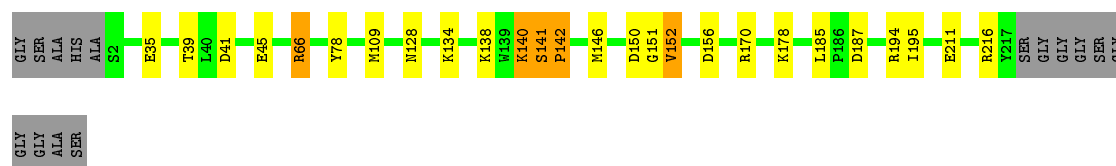
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 24-A: 




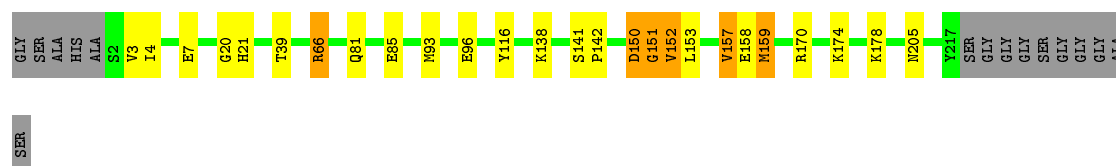
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 25-A: 




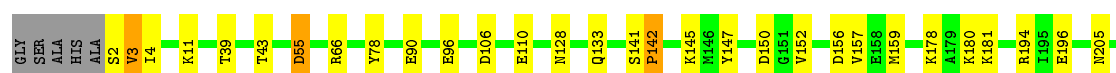
- Molecule 1: Reversibly photoswitching protein Dathail

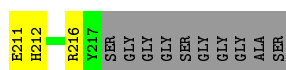
Chain 26-A: 



- Molecule 1: Reversibly photoswitching protein Dathail

Chain 27-A: 





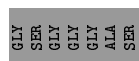
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 28-A: 82% 10% 7%



- Molecule 1: Reversibly photoswitching protein Dathail

Chain 29-A: 81% 11% 7%



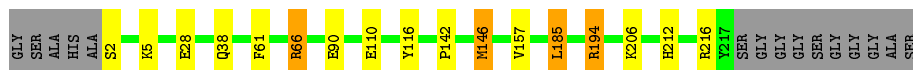
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 30-A: 82% 10% 7%



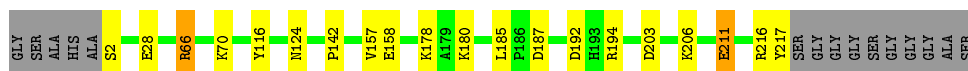
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 31-A: 86% 6% 7%



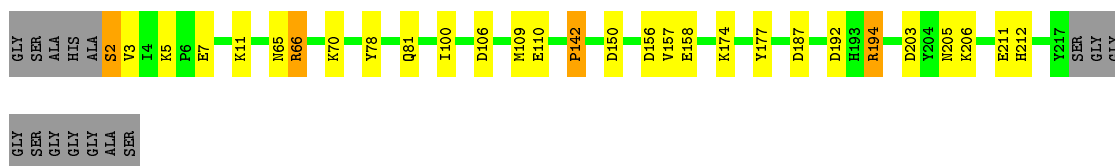
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 32-A: 85% 8% 7%



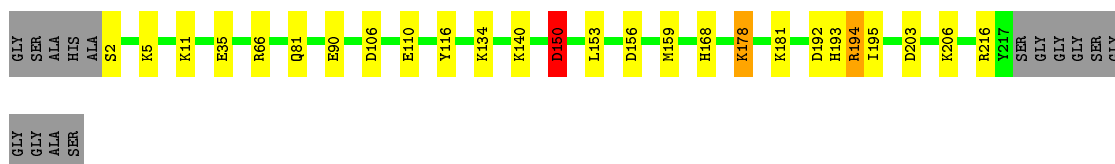
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 33-A: 81% 11% 7%



- Molecule 1: Reversibly photoswitching protein Dathail

Chain 34-A:



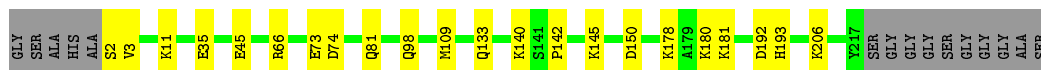
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 35-A:



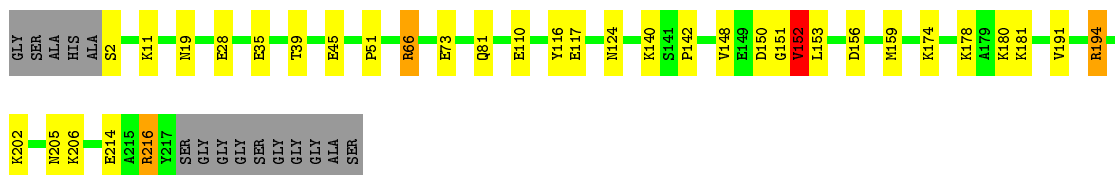
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 36-A:



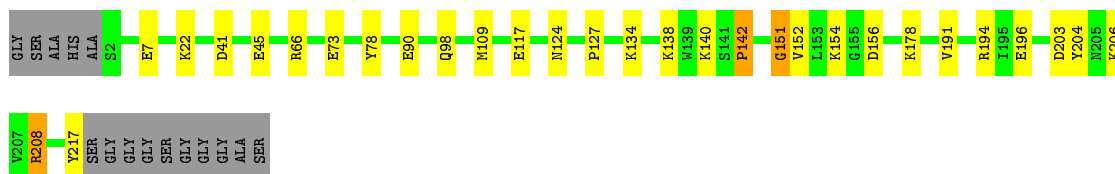
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 37-A:

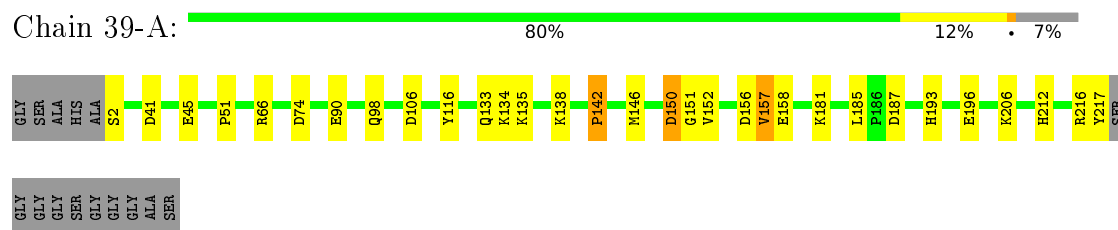


- Molecule 1: Reversibly photoswitching protein Dathail

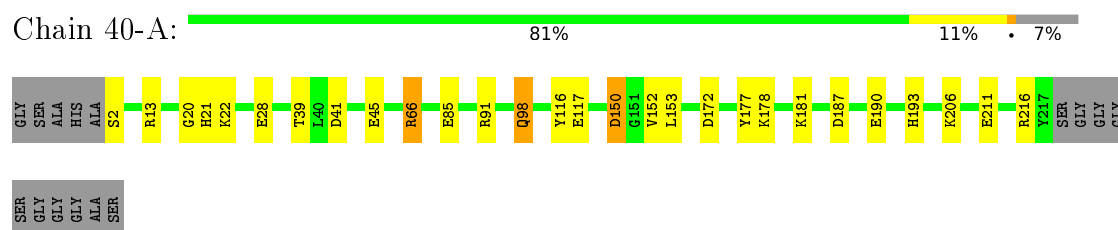
Chain 38-A:



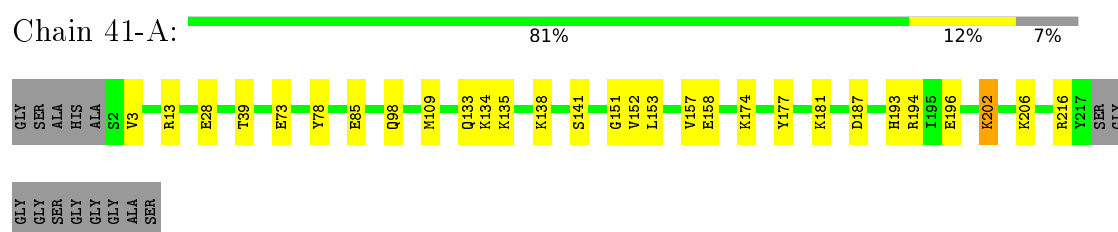
- Molecule 1: Reversibly photoswitching protein Dathail



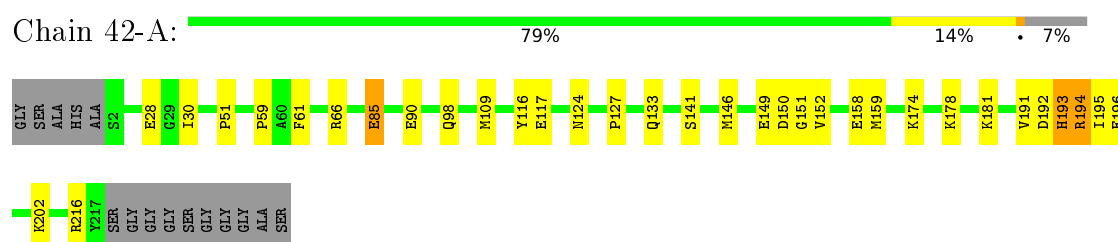
- Molecule 1: Reversibly photoswitching protein Dathail



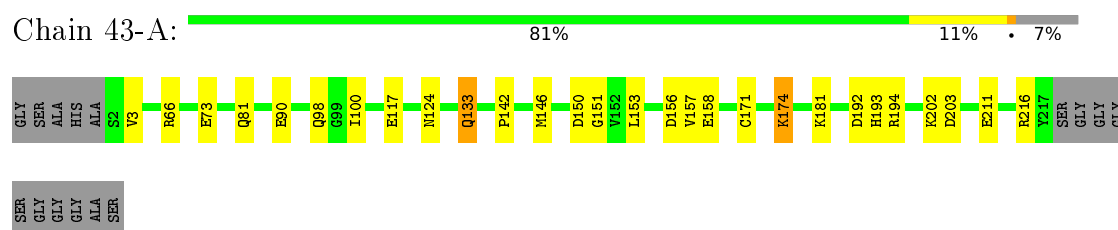
- Molecule 1: Reversibly photoswitching protein Dathail



- Molecule 1: Reversibly photoswitching protein Dathail



- Molecule 1: Reversibly photoswitching protein Dathail



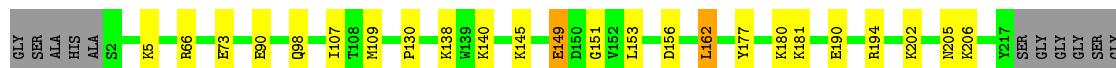
- Molecule 1: Reversibly photoswitching protein Dathail





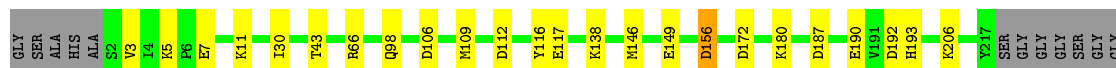
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 45-A: 83% 10% 7%



- Molecule 1: Reversibly photoswitching protein Dathail

Chain 46-A: 83% 10% 7%



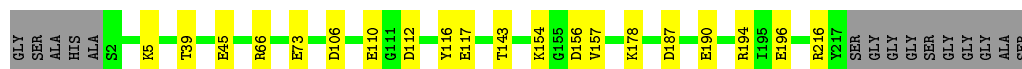
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 47-A: 85% 8% 7%



- Molecule 1: Reversibly photoswitching protein Dathail

Chain 48-A: 85% 9% 7%



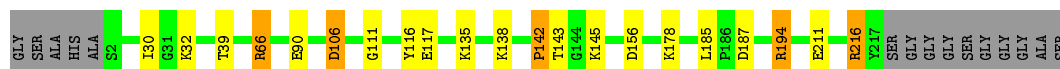
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 49-A: 84% 8% 7%




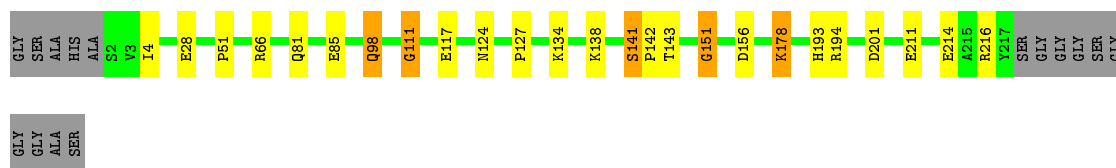
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 50-A: 84% 7% 7%




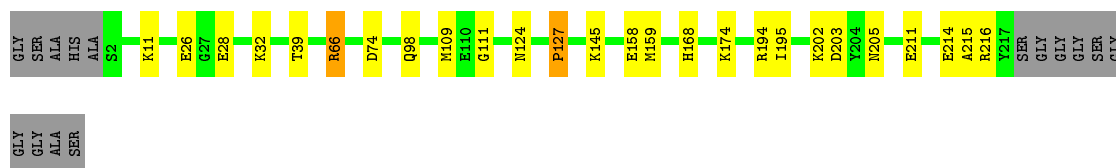
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 51-A:  83% 9% 7%




- Molecule 1: Reversibly photoswitching protein Dathail

Chain 52-A:  82% 10% 7%




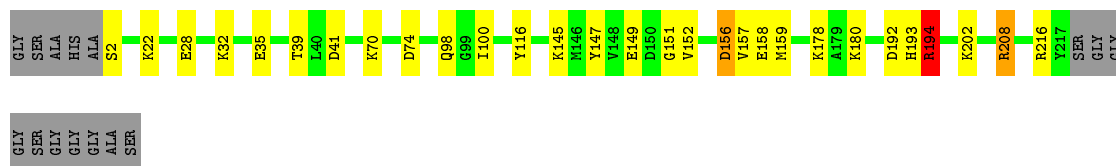
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 53-A:  83% 10% 7%




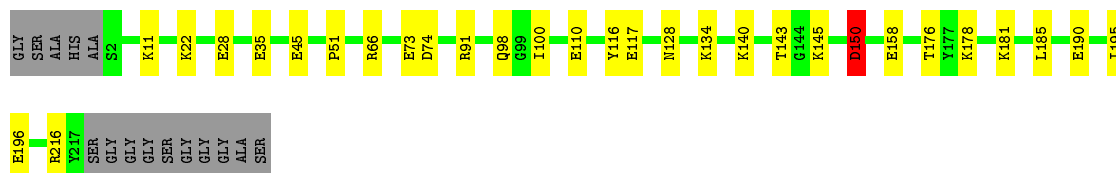
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 54-A:  81% 11% 7%




- Molecule 1: Reversibly photoswitching protein Dathail

Chain 55-A:  80% 13% 7%




- Molecule 1: Reversibly photoswitching protein Dathail

Chain 56-A:  81% 11% 7%



GLY  
SER  
GLY  
GLY  
GLY  
ALA  
ALA  
SER


- Molecule 1: Reversibly photoswitching protein Dathail

Chain 57-A:  82% 10% 7%

GLY SER GLY GLY GLY ALA HIS ALA S2 D41 E73 E90 Q98 D106 E110 G111 Y116 N124 K138 P142 T143 G144 G145 M146 D150 G151 V152 D156 R170 C171 D172 F173 K174 Y177 K178 V191 D192 H193 K206 R216 Y217 SER GLY GLY GLY SER

GLY  
GLY  
GLY  
ALA  
ALA  
SER


- Molecule 1: Reversibly photoswitching protein Dathail

Chain 58-A:  81% 12% 7%

GLY SER GLY ALA ALA S2 E7 T43 V44 E45 N65 E73 Q98 D106 M109 E110 G111 Y116 N124 K140 S141 P142 R170 T176 Y177 K180 K181 D187 Y191 D192 H193 R194 Y210 E214 A215 R216 Y217 SER GLY GLY GLY GLY


GLY  
GLY  
GLY  
ALA  
SER

- Molecule 1: Reversibly photoswitching protein Dathail

Chain 59-A:  84% 9% 7%

GLY SER GLY ALA ALA S2 N19 Q98 Y116 N124 N128 K140 S141 P142 M146 E149 D150 D156 V157 E158 R170 K178 V191 D192 H193 R208 L209 Y210 E211 R216 Y217 SER GLY GLY GLY SER GLY GLY GLY ALA SER


- Molecule 1: Reversibly photoswitching protein Dathail

Chain 60-A:  80% 12% 7%

GLY SER GLY ALA ALA S2 R66 D74 E85 M109 E110 Y116 T123 N124 K140 S141 P142 T143 D150 L153 K154 G155 G156 V157 E158 M159 G171 D172 Y177 K178 A179 K180 R194 R202 D203 Y210 E211 R216 Y217 SER GLY GLY GLY GLY

GLY  
GLY  
GLY  
ALA  
SER

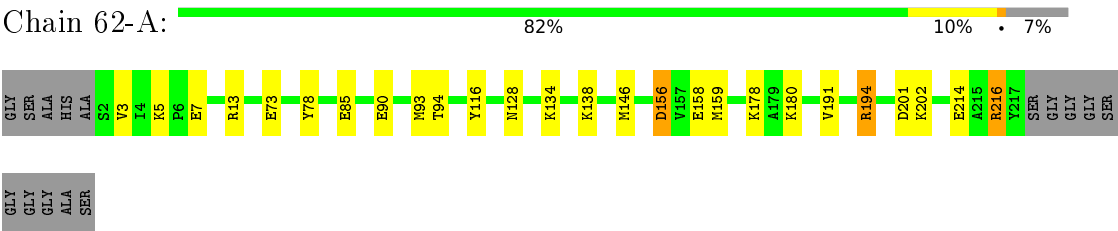
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 61-A:  80% 13% 7%

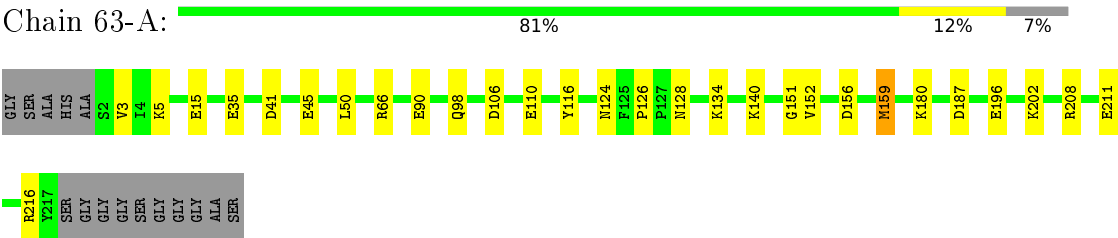
GLY SER GLY ALA ALA S2 K11 T39 P51 R66 K70 E73 E90 D97 M109 T123 K134 K138 S141 P142 T143 D150 E158 H168 F173 Y177 K178 A179 K180 V191 D192 H193 R194 I195 E196 D203 E211 R216

Y217  
SER  
GLY  
GLY  
GLY  
GLY  
GLY  
ALA  
SER

- Molecule 1: Reversibly photoswitching protein Dathail



● Molecule 1: Reversibly photoswitching protein Dathail





## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.25Å 81.18Å 39.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.18 – 1.65	Depositor
% Data completeness (in resolution range)	97.6 (32.18-1.65)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 1.65Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement: 1.10.1_2155)	Depositor
R, $R_{free}$	0.168 , 0.210	Depositor
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtriage
Anisotropy	0.569	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 29544 reflections	Xtriage
Total number of atoms	224314	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.85	3/1766 (0.2%)	0.89	5/2382 (0.2%)
1	2-A	0.84	4/1766 (0.2%)	0.86	1/2382 (0.0%)
1	3-A	0.75	3/1766 (0.2%)	0.89	6/2382 (0.3%)
1	4-A	0.84	5/1766 (0.3%)	1.00	7/2382 (0.3%)
1	5-A	0.77	2/1766 (0.1%)	0.91	5/2382 (0.2%)
1	6-A	0.81	5/1766 (0.3%)	0.91	6/2382 (0.3%)
1	7-A	0.78	3/1766 (0.2%)	0.88	1/2382 (0.0%)
1	8-A	0.81	5/1766 (0.3%)	0.89	5/2382 (0.2%)
1	9-A	0.83	2/1766 (0.1%)	0.88	1/2382 (0.0%)
1	10-A	0.77	2/1766 (0.1%)	0.88	2/2382 (0.1%)
1	11-A	0.73	0/1766	0.88	2/2382 (0.1%)
1	12-A	0.76	3/1766 (0.2%)	0.87	2/2382 (0.1%)
1	13-A	0.73	2/1766 (0.1%)	0.87	1/2382 (0.0%)
1	14-A	0.72	0/1766	0.92	7/2382 (0.3%)
1	15-A	0.70	0/1766	0.90	6/2382 (0.3%)
1	16-A	0.71	4/1766 (0.2%)	0.89	4/2382 (0.2%)
1	17-A	0.79	4/1766 (0.2%)	0.92	5/2382 (0.2%)
1	18-A	0.75	2/1766 (0.1%)	0.86	2/2382 (0.1%)
1	19-A	0.68	0/1766	0.85	1/2382 (0.0%)
1	20-A	0.79	5/1766 (0.3%)	0.88	4/2382 (0.2%)
1	21-A	0.76	1/1766 (0.1%)	0.91	5/2382 (0.2%)
1	22-A	0.74	0/1766	0.85	1/2382 (0.0%)
1	23-A	0.70	2/1766 (0.1%)	0.92	6/2382 (0.3%)
1	24-A	0.72	1/1766 (0.1%)	0.85	3/2382 (0.1%)
1	25-A	0.72	1/1766 (0.1%)	0.91	5/2382 (0.2%)
1	26-A	0.71	1/1766 (0.1%)	0.84	2/2382 (0.1%)
1	27-A	0.76	1/1766 (0.1%)	0.91	4/2382 (0.2%)
1	28-A	0.71	0/1766	0.85	2/2382 (0.1%)
1	29-A	0.73	2/1766 (0.1%)	0.90	7/2382 (0.3%)
1	30-A	0.70	2/1766 (0.1%)	0.92	3/2382 (0.1%)
1	31-A	0.78	1/1766 (0.1%)	0.93	5/2382 (0.2%)
1	32-A	0.77	3/1766 (0.2%)	0.86	1/2382 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	33-A	0.72	3/1766 (0.2%)	0.88	1/2382 (0.0%)
1	34-A	0.72	1/1766 (0.1%)	0.85	0/2382
1	35-A	0.72	2/1766 (0.1%)	0.86	2/2382 (0.1%)
1	36-A	0.70	0/1766	0.84	0/2382
1	37-A	0.77	2/1766 (0.1%)	0.90	4/2382 (0.2%)
1	38-A	0.73	2/1766 (0.1%)	0.87	3/2382 (0.1%)
1	39-A	0.74	0/1766	0.85	0/2382
1	40-A	0.72	1/1766 (0.1%)	0.94	4/2382 (0.2%)
1	41-A	0.74	2/1766 (0.1%)	0.87	0/2382
1	42-A	0.89	7/1766 (0.4%)	0.93	4/2382 (0.2%)
1	43-A	0.76	4/1766 (0.2%)	0.88	1/2382 (0.0%)
1	44-A	0.70	1/1766 (0.1%)	0.86	1/2382 (0.0%)
1	45-A	0.71	2/1766 (0.1%)	0.83	1/2382 (0.0%)
1	46-A	0.68	1/1766 (0.1%)	0.85	3/2382 (0.1%)
1	47-A	0.72	2/1766 (0.1%)	0.83	1/2382 (0.0%)
1	48-A	0.74	0/1766	0.87	2/2382 (0.1%)
1	49-A	0.67	0/1766	0.88	2/2382 (0.1%)
1	50-A	0.72	1/1766 (0.1%)	0.90	5/2382 (0.2%)
1	51-A	0.69	0/1766	0.84	1/2382 (0.0%)
1	52-A	0.74	0/1766	0.83	0/2382
1	53-A	0.72	0/1766	0.84	0/2382
1	54-A	0.71	1/1766 (0.1%)	0.88	3/2382 (0.1%)
1	55-A	0.75	1/1766 (0.1%)	0.93	4/2382 (0.2%)
1	56-A	0.72	2/1766 (0.1%)	0.86	5/2382 (0.2%)
1	57-A	0.76	3/1766 (0.2%)	0.92	4/2382 (0.2%)
1	58-A	0.73	1/1766 (0.1%)	0.85	0/2382
1	59-A	0.77	1/1766 (0.1%)	0.91	4/2382 (0.2%)
1	60-A	0.72	2/1766 (0.1%)	0.88	4/2382 (0.2%)
1	61-A	0.80	5/1766 (0.3%)	0.90	2/2382 (0.1%)
1	62-A	0.76	1/1766 (0.1%)	0.91	7/2382 (0.3%)
1	63-A	0.73	2/1766 (0.1%)	0.88	3/2382 (0.1%)
All	All	0.75	119/111258 (0.1%)	0.88	188/150066 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	1
1	2-A	0	3
1	3-A	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	4-A	0	1
1	5-A	0	1
1	7-A	0	1
1	8-A	0	2
1	10-A	0	1
1	13-A	0	3
1	14-A	0	1
1	16-A	0	1
1	17-A	0	3
1	18-A	0	1
1	19-A	0	1
1	22-A	0	1
1	23-A	0	2
1	24-A	0	1
1	25-A	0	1
1	26-A	0	3
1	27-A	0	1
1	28-A	0	1
1	30-A	0	3
1	31-A	0	1
1	32-A	0	1
1	33-A	0	1
1	34-A	0	1
1	35-A	0	1
1	36-A	0	2
1	38-A	0	2
1	39-A	0	3
1	40-A	0	2
1	41-A	0	1
1	42-A	0	2
1	43-A	0	2
1	44-A	0	4
1	45-A	0	1
1	50-A	0	2
1	51-A	0	3
1	52-A	0	3
1	53-A	0	2
1	54-A	0	1
1	55-A	0	1
1	56-A	0	2
1	57-A	0	1
1	58-A	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	59-A	0	1
All	All	0	77

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	42-A	196	GLU	CG-CD	12.80	1.71	1.51
1	2-A	164	GLU	CG-CD	12.68	1.71	1.51
1	1-A	164	GLU	CG-CD	10.39	1.67	1.51
1	2-A	32	LYS	CB-CG	-8.92	1.28	1.52
1	1-A	196	GLU	CB-CG	8.86	1.69	1.52
1	8-A	164	GLU	CB-CG	8.77	1.68	1.52
1	4-A	177	TYR	CD1-CE1	-8.27	1.26	1.39
1	9-A	117	GLU	CG-CD	8.11	1.64	1.51
1	1-A	196	GLU	CG-CD	8.07	1.64	1.51
1	4-A	90	GLU	CB-CG	8.02	1.67	1.52
1	4-A	190	GLU	CB-CG	7.98	1.67	1.52
1	4-A	164	GLU	CB-CG	7.85	1.67	1.52
1	6-A	164	GLU	CD-OE1	7.80	1.34	1.25
1	32-A	180	LYS	CD-CE	7.74	1.70	1.51
1	17-A	150	ASP	CB-CG	7.66	1.67	1.51
1	9-A	117	GLU	CB-CG	7.56	1.66	1.52
1	24-A	152	VAL	CB-CG1	7.52	1.68	1.52
1	61-A	90	GLU	CB-CG	7.48	1.66	1.52
1	16-A	117	GLU	CG-CD	7.43	1.63	1.51
1	7-A	202	LYS	CE-NZ	7.13	1.66	1.49
1	50-A	90	GLU	CB-CG	-7.11	1.38	1.52
1	8-A	117	GLU	CB-CG	7.09	1.65	1.52
1	3-A	66	ARG	CG-CD	-7.07	1.34	1.51
1	8-A	117	GLU	CG-CD	7.00	1.62	1.51
1	16-A	194	ARG	CB-CG	6.92	1.71	1.52
1	33-A	211	GLU	CG-CD	6.82	1.62	1.51
1	43-A	90	GLU	CB-CG	6.73	1.65	1.52
1	30-A	90	GLU	CG-CD	6.72	1.62	1.51
1	31-A	66	ARG	CG-CD	6.67	1.68	1.51
1	63-A	196	GLU	CG-CD	6.67	1.61	1.51
1	37-A	73	GLU	CB-CG	6.60	1.64	1.52
1	61-A	177	TYR	CD1-CE1	-6.58	1.29	1.39
1	12-A	177	TYR	CD1-CE1	-6.56	1.29	1.39
1	62-A	191	VAL	CB-CG2	-6.54	1.39	1.52
1	61-A	90	GLU	CG-CD	6.53	1.61	1.51
1	29-A	55	ASP	CB-CG	-6.52	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	55-A	196	GLU	CD-OE2	-6.51	1.18	1.25
1	20-A	211	GLU	CG-CD	6.50	1.61	1.51
1	42-A	193	HIS	CA-CB	6.46	1.68	1.53
1	18-A	211	GLU	CB-CG	6.44	1.64	1.52
1	47-A	177	TYR	CD1-CE1	-6.40	1.29	1.39
1	16-A	117	GLU	CB-CG	6.39	1.64	1.52
1	34-A	90	GLU	CG-CD	6.37	1.61	1.51
1	6-A	35	GLU	CG-CD	6.32	1.61	1.51
1	41-A	196	GLU	CB-CG	6.29	1.64	1.52
1	43-A	157	VAL	CB-CG1	-6.21	1.39	1.52
1	61-A	211	GLU	CB-CG	6.21	1.64	1.52
1	63-A	124	ASN	CB-CG	6.15	1.65	1.51
1	42-A	191	VAL	CB-CG1	-6.12	1.40	1.52
1	5-A	164	GLU	CD-OE1	6.08	1.32	1.25
1	12-A	158	GLU	CB-CG	6.06	1.63	1.52
1	40-A	177	TYR	CB-CG	-6.06	1.42	1.51
1	45-A	177	TYR	CD1-CE1	-6.05	1.30	1.39
1	42-A	149	GLU	CB-CG	6.04	1.63	1.52
1	2-A	177	TYR	CD1-CE1	-6.04	1.30	1.39
1	27-A	211	GLU	CG-CD	-5.95	1.43	1.51
1	42-A	85	GLU	CG-CD	5.91	1.60	1.51
1	59-A	191	VAL	CB-CG2	-5.88	1.40	1.52
1	29-A	159	MET	CB-CG	5.88	1.70	1.51
1	33-A	211	GLU	CB-CG	5.87	1.63	1.52
1	56-A	211	GLU	CB-CG	5.87	1.63	1.52
1	21-A	90	GLU	CB-CG	-5.84	1.41	1.52
1	56-A	90	GLU	CB-CG	-5.83	1.41	1.52
1	5-A	164	GLU	CG-CD	5.83	1.60	1.51
1	35-A	135	LYS	CD-CE	5.75	1.65	1.51
1	30-A	66	ARG	CG-CD	5.75	1.66	1.51
1	37-A	152	VAL	CB-CG1	-5.75	1.40	1.52
1	8-A	164	GLU	CG-CD	5.71	1.60	1.51
1	4-A	164	GLU	CG-CD	5.68	1.60	1.51
1	57-A	177	TYR	CD1-CE1	-5.68	1.30	1.39
1	10-A	28	GLU	CB-CG	5.67	1.62	1.52
1	13-A	117	GLU	CG-CD	5.66	1.60	1.51
1	60-A	159	MET	CB-CG	5.65	1.69	1.51
1	42-A	117	GLU	CG-CD	5.64	1.60	1.51
1	60-A	177	TYR	CD1-CE1	-5.61	1.30	1.39
1	18-A	149	GLU	CB-CG	5.57	1.62	1.52
1	43-A	90	GLU	CG-CD	5.56	1.60	1.51
1	20-A	146	MET	CG-SD	5.54	1.95	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	45-A	90	GLU	CG-CD	5.52	1.60	1.51
1	17-A	35	GLU	CG-CD	5.45	1.60	1.51
1	17-A	194	ARG	CB-CG	5.43	1.67	1.52
1	17-A	35	GLU	CB-CG	5.43	1.62	1.52
1	12-A	117	GLU	CG-CD	5.42	1.60	1.51
1	3-A	164	GLU	CB-CG	5.42	1.62	1.52
1	23-A	177	TYR	CD1-CE1	-5.42	1.31	1.39
1	20-A	177	TYR	CB-CG	-5.40	1.43	1.51
1	8-A	158	GLU	CG-CD	5.39	1.60	1.51
1	7-A	164	GLU	CB-CG	5.36	1.62	1.52
1	2-A	164	GLU	CB-CG	5.34	1.62	1.52
1	42-A	90	GLU	CG-CD	5.34	1.59	1.51
1	58-A	177	TYR	CB-CG	-5.33	1.43	1.51
1	54-A	35	GLU	CB-CG	-5.32	1.42	1.52
1	44-A	177	TYR	CD1-CE1	-5.31	1.31	1.39
1	38-A	66	ARG	CB-CG	-5.30	1.38	1.52
1	61-A	211	GLU	CG-CD	5.28	1.59	1.51
1	16-A	35	GLU	CG-CD	5.28	1.59	1.51
1	6-A	211	GLU	CB-CG	5.27	1.62	1.52
1	46-A	117	GLU	CB-CG	5.27	1.62	1.52
1	10-A	196	GLU	CG-CD	5.24	1.59	1.51
1	25-A	35	GLU	CB-CG	5.24	1.62	1.52
1	3-A	164	GLU	CG-CD	5.24	1.59	1.51
1	35-A	177	TYR	CD1-CE1	-5.22	1.31	1.39
1	57-A	90	GLU	CG-CD	5.19	1.59	1.51
1	13-A	117	GLU	CB-CG	5.17	1.61	1.52
1	20-A	91	ARG	CG-CD	-5.17	1.39	1.51
1	32-A	211	GLU	CB-CG	5.17	1.61	1.52
1	57-A	124	ASN	CB-CG	5.16	1.62	1.51
1	7-A	202	LYS	CD-CE	-5.15	1.38	1.51
1	32-A	157	VAL	CB-CG2	-5.15	1.42	1.52
1	20-A	211	GLU	CB-CG	5.14	1.61	1.52
1	41-A	177	TYR	CD1-CE1	-5.12	1.31	1.39
1	23-A	177	TYR	CB-CG	-5.11	1.44	1.51
1	38-A	117	GLU	CB-CG	-5.11	1.42	1.52
1	6-A	35	GLU	CB-CG	5.09	1.61	1.52
1	43-A	174	LYS	CD-CE	5.08	1.64	1.51
1	26-A	3	VAL	CB-CG1	5.07	1.63	1.52
1	47-A	117	GLU	CG-CD	5.01	1.59	1.51
1	33-A	177	TYR	CD1-CE1	-5.00	1.31	1.39
1	6-A	164	GLU	CG-CD	5.00	1.59	1.51

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	55-A	91	ARG	NE-CZ-NH1	13.52	127.06	120.30
1	31-A	66	ARG	NE-CZ-NH1	12.32	126.46	120.30
1	21-A	91	ARG	NE-CZ-NH1	11.20	125.90	120.30
1	30-A	194	ARG	NE-CZ-NH1	11.17	125.88	120.30
1	40-A	66	ARG	NE-CZ-NH1	11.06	125.83	120.30
1	40-A	66	ARG	NE-CZ-NH2	-10.70	114.95	120.30
1	55-A	91	ARG	NE-CZ-NH2	-10.35	115.12	120.30
1	4-A	146	MET	CB-CG-SD	-10.25	81.64	112.40
1	42-A	66	ARG	NE-CZ-NH2	9.22	124.91	120.30
1	11-A	66	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	59-A	170	ARG	NE-CZ-NH1	9.03	124.82	120.30
1	63-A	159	MET	CG-SD-CE	9.03	114.65	100.20
1	31-A	66	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	40-A	177	TYR	CA-CB-CG	-8.66	96.95	113.40
1	4-A	170	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	23-A	208	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	27-A	66	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	24-A	170	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	4-A	170	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	2-A	164	GLU	OE1-CD-OE2	-7.94	113.77	123.30
1	57-A	150	ASP	CB-CG-OD1	7.93	125.44	118.30
1	18-A	146	MET	CG-SD-CE	-7.87	87.60	100.20
1	27-A	55	ASP	CB-CG-OD1	-7.73	111.34	118.30
1	59-A	170	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	21-A	91	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	8-A	156	ASP	CB-CG-OD2	7.45	125.01	118.30
1	42-A	146	MET	CG-SD-CE	-7.42	88.33	100.20
1	13-A	170	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	17-A	170	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	54-A	159	MET	CG-SD-CE	7.39	112.02	100.20
1	14-A	66	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	17-A	66	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	49-A	66	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	26-A	159	MET	CG-SD-CE	7.20	111.71	100.20
1	16-A	172	ASP	CB-CG-OD1	-7.13	111.88	118.30
1	29-A	194	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	29-A	55	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	14-A	172	ASP	CB-CG-OD1	-6.99	112.01	118.30
1	56-A	141	SER	C-N-CD	-6.92	105.38	120.60
1	16-A	150	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	5-A	13	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	33-A	66	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	45-A	162	LEU	CB-CG-CD2	-6.84	99.37	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	42-A	159	MET	CG-SD-CE	-6.84	89.26	100.20
1	20-A	146	MET	CB-CG-SD	6.81	132.84	112.40
1	46-A	66	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	54-A	208	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	15-A	66	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	6-A	164	GLU	CG-CD-OE1	6.73	131.76	118.30
1	62-A	156	ASP	CB-CG-OD2	6.72	124.35	118.30
1	23-A	13	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	14-A	192	ASP	CB-CG-OD2	6.70	124.33	118.30
1	62-A	146	MET	CB-CG-SD	-6.67	92.38	112.40
1	14-A	170	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	56-A	194	ARG	NE-CZ-NH2	6.65	123.62	120.30
1	17-A	170	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	56-A	194	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	25-A	66	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	23-A	13	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	29-A	194	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	27-A	106	ASP	CB-CG-OD2	6.45	124.10	118.30
1	15-A	66	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	37-A	159	MET	CG-SD-CE	-6.37	90.00	100.20
1	46-A	66	ARG	NE-CZ-NH1	-6.35	117.12	120.30
1	14-A	170	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	4-A	194	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	12-A	146	MET	CG-SD-CE	6.32	110.31	100.20
1	6-A	93	MET	CG-SD-CE	6.30	110.28	100.20
1	3-A	208	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	21-A	173	PHE	CB-CG-CD2	-6.24	116.43	120.80
1	50-A	178	LYS	CD-CE-NZ	6.23	126.03	111.70
1	43-A	146	MET	CG-SD-CE	6.23	110.16	100.20
1	15-A	159	MET	CG-SD-CE	6.22	110.15	100.20
1	60-A	66	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	15-A	153	LEU	CB-CG-CD2	-6.21	100.44	111.00
1	23-A	208	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	1-A	164	GLU	OE1-CD-OE2	-6.16	115.91	123.30
1	60-A	153	LEU	CB-CG-CD2	-6.15	100.54	111.00
1	8-A	146	MET	CG-SD-CE	-6.15	90.36	100.20
1	28-A	194	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	62-A	194	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	6-A	140	LYS	CA-CB-CG	6.03	126.67	113.40
1	6-A	164	GLU	CG-CD-OE2	-6.02	106.25	118.30
1	3-A	208	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	23-A	106	ASP	CB-CG-OD2	-5.96	112.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	17-A	93	MET	CG-SD-CE	5.95	109.71	100.20
1	25-A	156	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	37-A	194	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	63-A	159	MET	CB-CG-SD	5.91	130.13	112.40
1	37-A	156	ASP	CB-CG-OD2	5.91	123.62	118.30
1	57-A	150	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	5-A	208	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	28-A	170	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	15-A	156	ASP	CB-CG-OD1	5.85	123.56	118.30
1	12-A	150	ASP	CB-CG-OD1	-5.84	113.04	118.30
1	24-A	170	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	15-A	156	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	29-A	55	ASP	OD1-CG-OD2	5.80	134.32	123.30
1	25-A	156	ASP	CB-CG-OD1	5.79	123.51	118.30
1	47-A	66	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	61-A	173	PHE	CB-CG-CD2	-5.77	116.76	120.80
1	42-A	194	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	11-A	8	MET	CG-SD-CE	5.74	109.38	100.20
1	24-A	159	MET	CG-SD-CE	-5.73	91.03	100.20
1	20-A	150	ASP	C-N-CA	5.72	134.31	122.30
1	56-A	211	GLU	OE1-CD-OE2	-5.71	116.44	123.30
1	9-A	178	LYS	CD-CE-NZ	5.71	124.83	111.70
1	25-A	66	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	46-A	156	ASP	CB-CG-OD2	5.70	123.43	118.30
1	4-A	172	ASP	CB-CG-OD2	5.68	123.41	118.30
1	16-A	147	TYR	CA-CB-CG	5.68	124.19	113.40
1	1-A	158	GLU	C-N-CA	-5.67	107.53	121.70
1	22-A	91	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	26-A	93	MET	CG-SD-CE	5.66	109.25	100.20
1	30-A	41	ASP	CB-CG-OD1	-5.66	113.21	118.30
1	27-A	159	MET	CG-SD-CE	-5.64	91.18	100.20
1	48-A	156	ASP	CB-CG-OD2	5.63	123.37	118.30
1	10-A	32	LYS	CD-CE-NZ	-5.63	98.75	111.70
1	20-A	91	ARG	NE-CZ-NH1	-5.63	117.49	120.30
1	44-A	133	GLN	CA-CB-CG	5.61	125.74	113.40
1	50-A	66	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	59-A	140	LYS	CA-CB-CG	5.58	125.67	113.40
1	29-A	156	ASP	CB-CG-OD1	5.57	123.31	118.30
1	23-A	203	ASP	CB-CG-OD2	5.57	123.31	118.30
1	62-A	194	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	3-A	164	GLU	OE1-CD-OE2	-5.55	116.64	123.30
1	4-A	194	ARG	NE-CZ-NH1	5.54	123.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	29-A	55	ASP	CB-CG-OD1	-5.54	113.31	118.30
1	7-A	146	MET	CG-SD-CE	-5.51	91.38	100.20
1	19-A	91	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	49-A	150	ASP	CB-CG-OD1	5.51	123.26	118.30
1	62-A	216	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	35-A	156	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	21-A	91	ARG	CD-NE-CZ	5.48	131.28	123.60
1	3-A	198	LEU	CA-CB-CG	5.47	127.89	115.30
1	57-A	156	ASP	CB-CG-OD1	5.47	123.22	118.30
1	60-A	140	LYS	CD-CE-NZ	-5.47	99.12	111.70
1	37-A	216	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	5-A	194	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	31-A	66	ARG	CD-NE-CZ	5.44	131.21	123.60
1	5-A	154	LYS	CD-CE-NZ	5.43	124.18	111.70
1	55-A	66	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	50-A	106	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	51-A	98	GLN	CA-CB-CG	5.42	125.32	113.40
1	8-A	97	ASP	CB-CG-OD1	5.41	123.17	118.30
1	56-A	66	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	40-A	91	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	5-A	13	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	48-A	194	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	21-A	173	PHE	CB-CG-CD1	5.37	124.56	120.80
1	1-A	146	MET	CG-SD-CE	-5.37	91.61	100.20
1	31-A	146	MET	CB-CG-SD	-5.36	96.33	112.40
1	59-A	208	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	31-A	185	LEU	CB-CG-CD1	5.29	119.99	111.00
1	6-A	153	LEU	CB-CG-CD2	-5.28	102.02	111.00
1	25-A	170	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	16-A	194	ARG	CB-CG-CD	5.26	125.28	111.60
1	1-A	185	LEU	CA-CB-CG	5.25	127.37	115.30
1	14-A	146	MET	CG-SD-CE	5.25	108.59	100.20
1	35-A	146	MET	CG-SD-CE	-5.25	91.81	100.20
1	18-A	66	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	29-A	54	TYR	C-N-CA	-5.22	108.64	121.70
1	1-A	66	ARG	CG-CD-NE	5.21	122.75	111.80
1	30-A	194	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	14-A	211	GLU	N-CA-CB	5.18	119.93	110.60
1	3-A	146	MET	CB-CG-SD	-5.18	96.86	112.40
1	57-A	106	ASP	CB-CG-OD1	5.18	122.96	118.30
1	10-A	194	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	6-A	216	ARG	NE-CZ-NH1	5.16	122.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-A	156	ASP	CB-CG-OD1	-5.15	113.66	118.30
1	61-A	97	ASP	CB-CG-OD1	5.14	122.93	118.30
1	63-A	208	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	62-A	216	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	38-A	194	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	50-A	135	LYS	CD-CE-NZ	5.12	123.47	111.70
1	54-A	194	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	38-A	208	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	50-A	178	LYS	CA-CB-CG	5.10	124.61	113.40
1	32-A	66	ARG	CG-CD-NE	5.09	122.49	111.80
1	17-A	66	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	62-A	201	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	60-A	194	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	38-A	208	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	8-A	90	GLU	CA-CB-CG	5.05	124.50	113.40
1	55-A	66	ARG	NE-CZ-NH2	5.03	122.81	120.30
1	3-A	146	MET	CG-SD-CE	-5.02	92.16	100.20
1	4-A	66	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	20-A	91	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (77) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	159	MET	Peptide
1	10-A	149	GLU	Peptide
1	13-A	149	GLU	Peptide
1	13-A	156	ASP	Peptide
1	13-A	61	PHE	Mainchain
1	14-A	193	HIS	Peptide
1	16-A	61	PHE	Mainchain
1	17-A	202	LYS	Peptide
1	17-A	35	GLU	Peptide
1	17-A	61	PHE	Mainchain
1	18-A	149	GLU	Peptide
1	19-A	149	GLU	Peptide
1	2-A	142	PRO	Peptide
1	2-A	186	PRO	Peptide
1	2-A	201	ASP	Peptide
1	22-A	216	ARG	Peptide
1	23-A	74	ASP	Peptide
1	23-A	98	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	24-A	74	ASP	Peptide
1	25-A	142	PRO	Peptide
1	26-A	141	SER	Peptide
1	26-A	150	ASP	Peptide
1	26-A	151	GLY	Peptide
1	27-A	3	VAL	Peptide
1	28-A	201	ASP	Peptide
1	3-A	140	LYS	Peptide
1	3-A	141	SER	Peptide
1	30-A	150	ASP	Peptide
1	30-A	151	GLY	Peptide
1	30-A	216	ARG	Peptide
1	31-A	61	PHE	Mainchain
1	32-A	142	PRO	Peptide
1	33-A	2	SER	Peptide
1	34-A	150	ASP	Peptide
1	35-A	74	ASP	Peptide
1	36-A	142	PRO	Peptide
1	36-A	74	ASP	Peptide
1	38-A	142	PRO	Peptide
1	38-A	151	GLY	Peptide
1	39-A	150	ASP	Peptide
1	39-A	151	GLY	Mainchain,Peptide
1	4-A	149	GLU	Peptide
1	40-A	150	ASP	Peptide
1	40-A	98	GLN	Peptide
1	41-A	151	GLY	Peptide
1	42-A	151	GLY	Peptide
1	42-A	61	PHE	Mainchain
1	43-A	133	GLN	Peptide
1	43-A	151	GLY	Peptide
1	44-A	127	PRO	Peptide
1	44-A	128	ASN	Peptide
1	44-A	61	PHE	Mainchain
1	44-A	74	ASP	Peptide
1	45-A	149	GLU	Peptide
1	5-A	146	MET	Peptide
1	50-A	111	GLY	Peptide
1	50-A	142	PRO	Peptide
1	51-A	111	GLY	Peptide
1	51-A	141	SER	Peptide
1	51-A	151	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	52-A	111	GLY	Peptide
1	52-A	215	ALA	Peptide
1	52-A	66	ARG	Peptide
1	53-A	142	PRO	Peptide
1	53-A	149	GLU	Peptide
1	54-A	156	ASP	Peptide
1	55-A	150	ASP	Peptide
1	56-A	111	GLY	Peptide
1	56-A	150	ASP	Peptide
1	57-A	111	GLY	Peptide
1	58-A	111	GLY	Peptide
1	58-A	142	PRO	Peptide
1	59-A	149	GLU	Peptide
1	7-A	20	GLY	Peptide
1	8-A	144	GLY	Peptide
1	8-A	145	LYS	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	1745	1671	1679	0	0
1	2-A	1745	1671	1679	0	0
1	3-A	1745	1671	1679	0	0
1	4-A	1745	1671	1679	0	0
1	5-A	1745	1671	1679	0	0
1	6-A	1745	1671	1679	0	0
1	7-A	1745	1671	1679	0	0
1	8-A	1745	1671	1679	0	0
1	9-A	1745	1671	1679	0	0
1	10-A	1745	1671	1679	0	0
1	11-A	1745	1671	1679	0	0
1	12-A	1745	1671	1679	0	0
1	13-A	1745	1671	1679	0	0
1	14-A	1745	1671	1678	0	0
1	15-A	1745	1671	1678	0	0
1	16-A	1745	1671	1679	0	0
1	17-A	1745	1671	1679	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	18-A	1745	1671	1678	0	0
1	19-A	1745	1671	1679	0	0
1	20-A	1745	1671	1678	0	0
1	21-A	1745	1671	1678	0	0
1	22-A	1745	1671	1679	0	0
1	23-A	1745	1671	1678	0	0
1	24-A	1745	1671	1679	0	0
1	25-A	1745	1671	1679	0	0
1	26-A	1745	1671	1679	0	0
1	27-A	1745	1671	1679	0	0
1	28-A	1745	1671	1679	0	0
1	29-A	1745	1671	1679	0	0
1	30-A	1745	1671	1679	0	0
1	31-A	1745	1671	1679	0	0
1	32-A	1745	1671	1679	0	0
1	33-A	1745	1671	1678	0	0
1	34-A	1745	1671	1679	0	0
1	35-A	1745	1671	1678	0	0
1	36-A	1745	1671	1679	0	0
1	37-A	1745	1671	1679	0	0
1	38-A	1745	1671	1679	0	0
1	39-A	1745	1671	1679	0	0
1	40-A	1745	1671	1679	0	0
1	41-A	1745	1671	1679	0	0
1	42-A	1745	1671	1678	0	0
1	43-A	1745	1671	1679	0	0
1	44-A	1745	1671	1679	0	0
1	45-A	1745	1671	1679	0	0
1	46-A	1745	1671	1679	0	0
1	47-A	1745	1671	1678	0	0
1	48-A	1745	1671	1679	0	0
1	49-A	1745	1671	1678	0	0
1	50-A	1745	1671	1679	0	0
1	51-A	1745	1671	1679	0	0
1	52-A	1745	1671	1677	0	0
1	53-A	1745	1671	1678	0	0
1	54-A	1745	1671	1679	0	0
1	55-A	1745	1671	1678	0	0
1	56-A	1745	1671	1678	0	0
1	57-A	1745	1671	1679	0	0
1	58-A	1745	1671	1678	0	0
1	59-A	1745	1671	1678	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	60-A	1745	1671	1679	0	0
1	61-A	1745	1671	1679	0	0
1	62-A	1745	1671	1679	0	0
1	63-A	1745	1671	1679	0	0
2	1-A	126	0	0	0	0
2	2-A	135	0	0	0	0
2	3-A	140	0	0	0	0
2	4-A	163	0	0	0	0
2	5-A	146	0	0	0	0
2	6-A	126	0	0	0	0
2	7-A	124	0	0	0	0
2	8-A	134	0	0	0	0
2	9-A	139	0	0	0	0
2	10-A	144	0	0	0	0
2	11-A	140	0	0	0	0
2	12-A	145	0	0	0	0
2	13-A	142	0	0	0	0
2	14-A	144	0	0	0	0
2	15-A	143	0	0	0	0
2	16-A	144	0	0	0	0
2	17-A	140	0	0	0	0
2	18-A	137	0	0	0	0
2	19-A	160	0	0	0	0
2	20-A	161	0	0	0	0
2	21-A	137	0	0	0	0
2	22-A	124	0	0	0	0
2	23-A	123	0	0	0	0
2	24-A	148	0	0	0	0
2	25-A	162	0	0	0	0
2	26-A	160	0	0	0	0
2	27-A	143	0	0	0	0
2	28-A	140	0	0	0	0
2	29-A	140	0	0	0	0
2	30-A	155	0	0	0	0
2	31-A	171	0	0	0	0
2	32-A	143	0	0	0	0
2	33-A	139	0	0	0	0
2	34-A	134	0	0	0	0
2	35-A	149	0	0	0	0
2	36-A	149	0	0	0	0
2	37-A	153	0	0	0	0
2	38-A	160	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	39-A	140	0	0	0	0
2	40-A	139	0	0	0	0
2	41-A	151	0	0	0	0
2	42-A	158	0	0	0	0
2	43-A	152	0	0	0	0
2	44-A	140	0	0	0	0
2	45-A	146	0	0	0	0
2	46-A	137	0	0	0	0
2	47-A	138	0	0	0	0
2	48-A	140	0	0	0	0
2	49-A	152	0	0	0	0
2	50-A	146	0	0	0	0
2	51-A	158	0	0	0	0
2	52-A	136	0	0	0	0
2	53-A	134	0	0	0	0
2	54-A	139	0	0	0	0
2	55-A	139	0	0	0	0
2	56-A	138	0	0	0	0
2	57-A	152	0	0	0	0
2	58-A	150	0	0	0	0
2	59-A	152	0	0	0	0
2	60-A	141	0	0	0	0
2	61-A	167	0	0	0	0
2	62-A	155	0	0	0	0
2	63-A	143	0	0	0	0
All	All	119041	105273	105759	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 ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	211/229 (92%)	201 (95%)	6 (3%)	4 (2%)	10	0
1	2-A	211/229 (92%)	200 (95%)	8 (4%)	3 (1%)	14	1
1	3-A	211/229 (92%)	202 (96%)	3 (1%)	6 (3%)	6	0
1	4-A	211/229 (92%)	202 (96%)	5 (2%)	4 (2%)	10	0
1	5-A	211/229 (92%)	202 (96%)	7 (3%)	2 (1%)	21	4
1	6-A	211/229 (92%)	200 (95%)	10 (5%)	1 (0%)	34	12
1	7-A	211/229 (92%)	197 (93%)	12 (6%)	2 (1%)	21	4
1	8-A	211/229 (92%)	195 (92%)	13 (6%)	3 (1%)	14	1
1	9-A	211/229 (92%)	202 (96%)	6 (3%)	3 (1%)	14	1
1	10-A	211/229 (92%)	201 (95%)	6 (3%)	4 (2%)	10	0
1	11-A	211/229 (92%)	199 (94%)	8 (4%)	4 (2%)	10	0
1	12-A	211/229 (92%)	195 (92%)	10 (5%)	6 (3%)	6	0
1	13-A	211/229 (92%)	200 (95%)	7 (3%)	4 (2%)	10	0
1	14-A	211/229 (92%)	201 (95%)	7 (3%)	3 (1%)	14	1
1	15-A	211/229 (92%)	195 (92%)	12 (6%)	4 (2%)	10	0
1	16-A	211/229 (92%)	198 (94%)	8 (4%)	5 (2%)	7	0
1	17-A	211/229 (92%)	195 (92%)	12 (6%)	4 (2%)	10	0
1	18-A	211/229 (92%)	199 (94%)	9 (4%)	3 (1%)	14	1
1	19-A	211/229 (92%)	194 (92%)	10 (5%)	7 (3%)	5	0
1	20-A	211/229 (92%)	200 (95%)	8 (4%)	3 (1%)	14	1
1	21-A	211/229 (92%)	204 (97%)	6 (3%)	1 (0%)	34	12
1	22-A	211/229 (92%)	196 (93%)	13 (6%)	2 (1%)	21	4
1	23-A	211/229 (92%)	195 (92%)	12 (6%)	4 (2%)	10	0
1	24-A	211/229 (92%)	207 (98%)	4 (2%)	0	100	100
1	25-A	211/229 (92%)	196 (93%)	10 (5%)	5 (2%)	7	0
1	26-A	211/229 (92%)	195 (92%)	8 (4%)	8 (4%)	4	0
1	27-A	211/229 (92%)	201 (95%)	4 (2%)	6 (3%)	6	0
1	28-A	211/229 (92%)	201 (95%)	4 (2%)	6 (3%)	6	0
1	29-A	211/229 (92%)	198 (94%)	9 (4%)	4 (2%)	10	0
1	30-A	211/229 (92%)	195 (92%)	13 (6%)	3 (1%)	14	1
1	31-A	211/229 (92%)	199 (94%)	10 (5%)	2 (1%)	21	4
1	32-A	211/229 (92%)	203 (96%)	7 (3%)	1 (0%)	34	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	33-A	211/229 (92%)	196 (93%)	11 (5%)	4 (2%)	10	0
1	34-A	211/229 (92%)	198 (94%)	10 (5%)	3 (1%)	14	1
1	35-A	211/229 (92%)	199 (94%)	11 (5%)	1 (0%)	34	12
1	36-A	211/229 (92%)	201 (95%)	7 (3%)	3 (1%)	14	1
1	37-A	211/229 (92%)	196 (93%)	10 (5%)	5 (2%)	7	0
1	38-A	211/229 (92%)	197 (93%)	10 (5%)	4 (2%)	10	0
1	39-A	211/229 (92%)	198 (94%)	8 (4%)	5 (2%)	7	0
1	40-A	211/229 (92%)	199 (94%)	7 (3%)	5 (2%)	7	0
1	41-A	211/229 (92%)	198 (94%)	10 (5%)	3 (1%)	14	1
1	42-A	211/229 (92%)	201 (95%)	7 (3%)	3 (1%)	14	1
1	43-A	211/229 (92%)	200 (95%)	11 (5%)	0	100	100
1	44-A	211/229 (92%)	204 (97%)	6 (3%)	1 (0%)	34	12
1	45-A	211/229 (92%)	201 (95%)	7 (3%)	3 (1%)	14	1
1	46-A	211/229 (92%)	202 (96%)	8 (4%)	1 (0%)	34	12
1	47-A	211/229 (92%)	204 (97%)	5 (2%)	2 (1%)	21	4
1	48-A	211/229 (92%)	202 (96%)	9 (4%)	0	100	100
1	49-A	211/229 (92%)	196 (93%)	12 (6%)	3 (1%)	14	1
1	50-A	211/229 (92%)	198 (94%)	11 (5%)	2 (1%)	21	4
1	51-A	211/229 (92%)	195 (92%)	9 (4%)	7 (3%)	5	0
1	52-A	211/229 (92%)	190 (90%)	17 (8%)	4 (2%)	10	0
1	53-A	211/229 (92%)	197 (93%)	10 (5%)	4 (2%)	10	0
1	54-A	211/229 (92%)	198 (94%)	8 (4%)	5 (2%)	7	0
1	55-A	211/229 (92%)	201 (95%)	7 (3%)	3 (1%)	14	1
1	56-A	211/229 (92%)	200 (95%)	8 (4%)	3 (1%)	14	1
1	57-A	211/229 (92%)	201 (95%)	7 (3%)	3 (1%)	14	1
1	58-A	211/229 (92%)	203 (96%)	7 (3%)	1 (0%)	34	12
1	59-A	211/229 (92%)	202 (96%)	8 (4%)	1 (0%)	34	12
1	60-A	211/229 (92%)	200 (95%)	8 (4%)	3 (1%)	14	1
1	61-A	211/229 (92%)	197 (93%)	12 (6%)	2 (1%)	21	4
1	62-A	211/229 (92%)	201 (95%)	10 (5%)	0	100	100
1	63-A	211/229 (92%)	199 (94%)	9 (4%)	3 (1%)	14	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	13293/14427 (92%)	12542 (94%)	547 (4%)	204 (2%)	13	1

All (204) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2-A	3	VAL
1	2-A	140	LYS
1	3-A	3	VAL
1	3-A	140	LYS
1	3-A	150	ASP
1	4-A	142	PRO
1	4-A	150	ASP
1	8-A	3	VAL
1	10-A	140	LYS
1	11-A	3	VAL
1	11-A	150	ASP
1	12-A	150	ASP
1	12-A	204	TYR
1	13-A	157	VAL
1	15-A	3	VAL
1	15-A	194	ARG
1	16-A	3	VAL
1	16-A	140	LYS
1	16-A	150	ASP
1	16-A	194	ARG
1	17-A	36	GLY
1	17-A	194	ARG
1	17-A	203	ASP
1	18-A	150	ASP
1	19-A	157	VAL
1	20-A	150	ASP
1	20-A	152	VAL
1	22-A	150	ASP
1	23-A	150	ASP
1	23-A	203	ASP
1	25-A	140	LYS
1	25-A	152	VAL
1	26-A	4	ILE
1	26-A	66	ARG
1	26-A	96	GLU
1	26-A	142	PRO
1	26-A	152	VAL

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Mol	Chain	Res	Type
1	27-A	142	PRO
1	27-A	150	ASP
1	27-A	152	VAL
1	28-A	3	VAL
1	28-A	4	ILE
1	28-A	152	VAL
1	29-A	3	VAL
1	30-A	3	VAL
1	32-A	194	ARG
1	33-A	65	ASN
1	34-A	150	ASP
1	34-A	194	ARG
1	37-A	66	ARG
1	38-A	142	PRO
1	38-A	204	TYR
1	39-A	150	ASP
1	39-A	152	VAL
1	40-A	21	HIS
1	40-A	150	ASP
1	40-A	152	VAL
1	41-A	202	LYS
1	42-A	150	ASP
1	42-A	152	VAL
1	47-A	112	ASP
1	47-A	142	PRO
1	49-A	150	ASP
1	49-A	204	TYR
1	49-A	216	ARG
1	50-A	216	ARG
1	51-A	216	ARG
1	52-A	202	LYS
1	53-A	141	SER
1	53-A	216	ARG
1	54-A	98	GLN
1	54-A	194	ARG
1	54-A	216	ARG
1	55-A	150	ASP
1	55-A	216	ARG
1	56-A	150	ASP
1	56-A	153	LEU
1	56-A	216	ARG
1	63-A	140	LYS

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Mol	Chain	Res	Type
1	1-A	192	ASP
1	2-A	187	ASP
1	4-A	112	ASP
1	5-A	3	VAL
1	7-A	127	PRO
1	9-A	3	VAL
1	12-A	3	VAL
1	12-A	19	ASN
1	12-A	157	VAL
1	13-A	3	VAL
1	13-A	150	ASP
1	18-A	157	VAL
1	19-A	150	ASP
1	22-A	203	ASP
1	23-A	51	PRO
1	25-A	142	PRO
1	25-A	151	GLY
1	27-A	4	ILE
1	29-A	203	ASP
1	30-A	151	GLY
1	30-A	152	VAL
1	33-A	194	ARG
1	33-A	203	ASP
1	34-A	178	LYS
1	36-A	3	VAL
1	38-A	152	VAL
1	39-A	142	PRO
1	40-A	20	GLY
1	41-A	152	VAL
1	45-A	98	GLN
1	45-A	140	LYS
1	51-A	151	GLY
1	52-A	216	ARG
1	53-A	150	ASP
1	54-A	157	VAL
1	57-A	216	ARG
1	60-A	110	GLU
1	60-A	150	ASP
1	61-A	142	PRO
1	63-A	98	GLN
1	1-A	19	ASN
1	3-A	98	GLN

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Mol	Chain	Res	Type
1	10-A	3	VAL
1	11-A	151	GLY
1	14-A	98	GLN
1	18-A	98	GLN
1	19-A	98	GLN
1	26-A	20	GLY
1	28-A	98	GLN
1	31-A	142	PRO
1	31-A	194	ARG
1	36-A	98	GLN
1	40-A	178	LYS
1	41-A	194	ARG
1	45-A	151	GLY
1	46-A	98	GLN
1	50-A	194	ARG
1	53-A	51	PRO
1	57-A	110	GLU
1	63-A	151	GLY
1	4-A	3	VAL
1	6-A	142	PRO
1	8-A	150	ASP
1	10-A	98	GLN
1	14-A	150	ASP
1	17-A	142	PRO
1	19-A	152	VAL
1	21-A	203	ASP
1	33-A	142	PRO
1	44-A	127	PRO
1	51-A	111	GLY
1	51-A	142	PRO
1	52-A	203	ASP
1	55-A	51	PRO
1	57-A	111	GLY
1	58-A	65	ASN
1	1-A	193	HIS
1	9-A	98	GLN
1	12-A	112	ASP
1	13-A	142	PRO
1	15-A	142	PRO
1	19-A	112	ASP
1	27-A	3	VAL
1	28-A	150	ASP

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Mol	Chain	Res	Type
1	29-A	4	ILE
1	36-A	150	ASP
1	37-A	19	ASN
1	39-A	157	VAL
1	42-A	51	PRO
1	51-A	127	PRO
1	54-A	151	GLY
1	59-A	19	ASN
1	61-A	51	PRO
1	8-A	19	ASN
1	9-A	151	GLY
1	10-A	142	PRO
1	16-A	151	GLY
1	19-A	156	ASP
1	20-A	216	ARG
1	23-A	142	PRO
1	29-A	51	PRO
1	37-A	151	GLY
1	51-A	51	PRO
1	51-A	178	LYS
1	60-A	141	SER
1	14-A	3	VAL
1	15-A	151	GLY
1	5-A	51	PRO
1	19-A	151	GLY
1	26-A	151	GLY
1	37-A	152	VAL
1	1-A	3	VAL
1	3-A	51	PRO
1	11-A	141	SER
1	26-A	157	VAL
1	27-A	141	SER
1	28-A	151	GLY
1	38-A	151	GLY
1	52-A	127	PRO
1	3-A	141	SER
1	25-A	141	SER
1	35-A	3	VAL
1	37-A	51	PRO
1	39-A	51	PRO
1	7-A	142	PRO



### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	184/189 (97%)	166 (90%)	18 (10%)	10	1
1	2-A	184/189 (97%)	165 (90%)	19 (10%)	9	1
1	3-A	184/189 (97%)	157 (85%)	27 (15%)	4	0
1	4-A	184/189 (97%)	166 (90%)	18 (10%)	10	1
1	5-A	184/189 (97%)	167 (91%)	17 (9%)	11	2
1	6-A	184/189 (97%)	168 (91%)	16 (9%)	13	2
1	7-A	184/189 (97%)	161 (88%)	23 (12%)	6	0
1	8-A	184/189 (97%)	171 (93%)	13 (7%)	18	3
1	9-A	184/189 (97%)	161 (88%)	23 (12%)	6	0
1	10-A	184/189 (97%)	168 (91%)	16 (9%)	13	2
1	11-A	184/189 (97%)	160 (87%)	24 (13%)	5	0
1	12-A	184/189 (97%)	162 (88%)	22 (12%)	6	1
1	13-A	184/189 (97%)	165 (90%)	19 (10%)	9	1
1	14-A	184/189 (97%)	161 (88%)	23 (12%)	6	0
1	15-A	184/189 (97%)	171 (93%)	13 (7%)	18	3
1	16-A	184/189 (97%)	167 (91%)	17 (9%)	11	2
1	17-A	184/189 (97%)	156 (85%)	28 (15%)	3	0
1	18-A	184/189 (97%)	154 (84%)	30 (16%)	3	0
1	19-A	184/189 (97%)	168 (91%)	16 (9%)	13	2
1	20-A	184/189 (97%)	165 (90%)	19 (10%)	9	1
1	21-A	184/189 (97%)	160 (87%)	24 (13%)	5	0
1	22-A	184/189 (97%)	160 (87%)	24 (13%)	5	0
1	23-A	184/189 (97%)	163 (89%)	21 (11%)	7	1
1	24-A	184/189 (97%)	163 (89%)	21 (11%)	7	1
1	25-A	184/189 (97%)	163 (89%)	21 (11%)	7	1
1	26-A	184/189 (97%)	166 (90%)	18 (10%)	10	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	27-A	184/189 (97%)	160 (87%)	24 (13%)	5	0
1	28-A	184/189 (97%)	163 (89%)	21 (11%)	7	1
1	29-A	184/189 (97%)	163 (89%)	21 (11%)	7	1
1	30-A	184/189 (97%)	164 (89%)	20 (11%)	8	1
1	31-A	184/189 (97%)	169 (92%)	15 (8%)	14	2
1	32-A	184/189 (97%)	168 (91%)	16 (9%)	13	2
1	33-A	184/189 (97%)	159 (86%)	25 (14%)	5	0
1	34-A	184/189 (97%)	159 (86%)	25 (14%)	5	0
1	35-A	184/189 (97%)	170 (92%)	14 (8%)	16	2
1	36-A	184/189 (97%)	167 (91%)	17 (9%)	11	2
1	37-A	184/189 (97%)	155 (84%)	29 (16%)	3	0
1	38-A	184/189 (97%)	161 (88%)	23 (12%)	6	0
1	39-A	184/189 (97%)	157 (85%)	27 (15%)	4	0
1	40-A	184/189 (97%)	163 (89%)	21 (11%)	7	1
1	41-A	184/189 (97%)	160 (87%)	24 (13%)	5	0
1	42-A	184/189 (97%)	163 (89%)	21 (11%)	7	1
1	43-A	184/189 (97%)	160 (87%)	24 (13%)	5	0
1	44-A	184/189 (97%)	166 (90%)	18 (10%)	10	1
1	45-A	184/189 (97%)	165 (90%)	19 (10%)	9	1
1	46-A	184/189 (97%)	163 (89%)	21 (11%)	7	1
1	47-A	184/189 (97%)	168 (91%)	16 (9%)	13	2
1	48-A	184/189 (97%)	166 (90%)	18 (10%)	10	1
1	49-A	184/189 (97%)	165 (90%)	19 (10%)	9	1
1	50-A	184/189 (97%)	167 (91%)	17 (9%)	11	2
1	51-A	184/189 (97%)	165 (90%)	19 (10%)	9	1
1	52-A	184/189 (97%)	163 (89%)	21 (11%)	7	1
1	53-A	184/189 (97%)	166 (90%)	18 (10%)	10	1
1	54-A	184/189 (97%)	161 (88%)	23 (12%)	6	0
1	55-A	184/189 (97%)	159 (86%)	25 (14%)	5	0
1	56-A	184/189 (97%)	163 (89%)	21 (11%)	7	1
1	57-A	184/189 (97%)	164 (89%)	20 (11%)	8	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	58-A	184/189 (97%)	160 (87%)	24 (13%)	5	0
1	59-A	184/189 (97%)	166 (90%)	18 (10%)	10	1
1	60-A	184/189 (97%)	161 (88%)	23 (12%)	6	0
1	61-A	184/189 (97%)	161 (88%)	23 (12%)	6	0
1	62-A	184/189 (97%)	161 (88%)	23 (12%)	6	0
1	63-A	184/189 (97%)	161 (88%)	23 (12%)	6	0
All	All	11592/11907 (97%)	10286 (89%)	1306 (11%)	7	1

All (1306) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	21	HIS
1	1-A	45	GLU
1	1-A	66	ARG
1	1-A	70	LYS
1	1-A	100	ILE
1	1-A	116	TYR
1	1-A	134	LYS
1	1-A	135	LYS
1	1-A	143	THR
1	1-A	145	LYS
1	1-A	149	GLU
1	1-A	152	VAL
1	1-A	159	MET
1	1-A	180	LYS
1	1-A	185	LEU
1	1-A	210	TYR
1	1-A	211	GLU
1	1-A	217	TYR
1	2-A	21	HIS
1	2-A	30	ILE
1	2-A	32	LYS
1	2-A	45	GLU
1	2-A	100	ILE
1	2-A	109	MET
1	2-A	110	GLU
1	2-A	116	TYR
1	2-A	128	ASN
1	2-A	143	THR
1	2-A	146	MET

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Mol	Chain	Res	Type
1	2-A	149	GLU
1	2-A	172	ASP
1	2-A	178	LYS
1	2-A	185	LEU
1	2-A	192	ASP
1	2-A	196	GLU
1	2-A	198	LEU
1	2-A	211	GLU
1	3-A	5	LYS
1	3-A	13	ARG
1	3-A	43	THR
1	3-A	100	ILE
1	3-A	109	MET
1	3-A	110	GLU
1	3-A	116	TYR
1	3-A	145	LYS
1	3-A	146	MET
1	3-A	149	GLU
1	3-A	152	VAL
1	3-A	156	ASP
1	3-A	157	VAL
1	3-A	171	CYS
1	3-A	174	LYS
1	3-A	176	THR
1	3-A	178	LYS
1	3-A	180	LYS
1	3-A	185	LEU
1	3-A	190	GLU
1	3-A	193	HIS
1	3-A	194	ARG
1	3-A	195	ILE
1	3-A	196	GLU
1	3-A	198	LEU
1	3-A	208	ARG
1	3-A	216	ARG
1	4-A	11	LYS
1	4-A	42	LEU
1	4-A	78	TYR
1	4-A	106	ASP
1	4-A	109	MET
1	4-A	110	GLU
1	4-A	116	TYR

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Mol	Chain	Res	Type
1	4-A	117	GLU
1	4-A	138	LYS
1	4-A	142	PRO
1	4-A	145	LYS
1	4-A	146	MET
1	4-A	156	ASP
1	4-A	176	THR
1	4-A	190	GLU
1	4-A	192	ASP
1	4-A	194	ARG
1	4-A	208	ARG
1	5-A	28	GLU
1	5-A	32	LYS
1	5-A	90	GLU
1	5-A	110	GLU
1	5-A	112	ASP
1	5-A	116	TYR
1	5-A	117	GLU
1	5-A	124	ASN
1	5-A	140	LYS
1	5-A	146	MET
1	5-A	158	GLU
1	5-A	168	HIS
1	5-A	178	LYS
1	5-A	185	LEU
1	5-A	193	HIS
1	5-A	194	ARG
1	5-A	208	ARG
1	6-A	32	LYS
1	6-A	35	GLU
1	6-A	39	THR
1	6-A	41	ASP
1	6-A	85	GLU
1	6-A	106	ASP
1	6-A	109	MET
1	6-A	116	TYR
1	6-A	117	GLU
1	6-A	138	LYS
1	6-A	187	ASP
1	6-A	193	HIS
1	6-A	194	ARG
1	6-A	202	LYS

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Mol	Chain	Res	Type
1	6-A	203	ASP
1	6-A	216	ARG
1	7-A	11	LYS
1	7-A	15	GLU
1	7-A	28	GLU
1	7-A	38	GLN
1	7-A	45	GLU
1	7-A	85	GLU
1	7-A	90	GLU
1	7-A	98	GLN
1	7-A	110	GLU
1	7-A	116	TYR
1	7-A	117	GLU
1	7-A	128	ASN
1	7-A	138	LYS
1	7-A	142	PRO
1	7-A	150	ASP
1	7-A	152	VAL
1	7-A	158	GLU
1	7-A	178	LYS
1	7-A	181	LYS
1	7-A	187	ASP
1	7-A	192	ASP
1	7-A	193	HIS
1	7-A	202	LYS
1	8-A	22	LYS
1	8-A	32	LYS
1	8-A	70	LYS
1	8-A	73	GLU
1	8-A	98	GLN
1	8-A	106	ASP
1	8-A	110	GLU
1	8-A	117	GLU
1	8-A	134	LYS
1	8-A	150	ASP
1	8-A	176	THR
1	8-A	178	LYS
1	8-A	216	ARG
1	9-A	15	GLU
1	9-A	32	LYS
1	9-A	38	GLN
1	9-A	94	THR

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Mol	Chain	Res	Type
1	9-A	106	ASP
1	9-A	110	GLU
1	9-A	112	ASP
1	9-A	116	TYR
1	9-A	117	GLU
1	9-A	128	ASN
1	9-A	135	LYS
1	9-A	141	SER
1	9-A	145	LYS
1	9-A	146	MET
1	9-A	150	ASP
1	9-A	156	ASP
1	9-A	168	HIS
1	9-A	180	LYS
1	9-A	181	LYS
1	9-A	192	ASP
1	9-A	208	ARG
1	9-A	212	HIS
1	9-A	217	TYR
1	10-A	15	GLU
1	10-A	32	LYS
1	10-A	39	THR
1	10-A	41	ASP
1	10-A	81	GLN
1	10-A	90	GLU
1	10-A	109	MET
1	10-A	116	TYR
1	10-A	124	ASN
1	10-A	138	LYS
1	10-A	145	LYS
1	10-A	150	ASP
1	10-A	156	ASP
1	10-A	174	LYS
1	10-A	193	HIS
1	10-A	217	TYR
1	11-A	2	SER
1	11-A	9	LYS
1	11-A	28	GLU
1	11-A	32	LYS
1	11-A	41	ASP
1	11-A	45	GLU
1	11-A	81	GLN

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Mol	Chain	Res	Type
1	11-A	116	TYR
1	11-A	126	PRO
1	11-A	138	LYS
1	11-A	140	LYS
1	11-A	145	LYS
1	11-A	149	GLU
1	11-A	150	ASP
1	11-A	156	ASP
1	11-A	176	THR
1	11-A	178	LYS
1	11-A	185	LEU
1	11-A	187	ASP
1	11-A	192	ASP
1	11-A	194	ARG
1	11-A	208	ARG
1	11-A	216	ARG
1	11-A	217	TYR
1	12-A	2	SER
1	12-A	3	VAL
1	12-A	15	GLU
1	12-A	32	LYS
1	12-A	81	GLN
1	12-A	104	THR
1	12-A	109	MET
1	12-A	133	GLN
1	12-A	138	LYS
1	12-A	145	LYS
1	12-A	146	MET
1	12-A	152	VAL
1	12-A	158	GLU
1	12-A	178	LYS
1	12-A	180	LYS
1	12-A	181	LYS
1	12-A	190	GLU
1	12-A	194	ARG
1	12-A	202	LYS
1	12-A	214	GLU
1	12-A	216	ARG
1	12-A	217	TYR
1	13-A	38	GLN
1	13-A	39	THR
1	13-A	90	GLU

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Mol	Chain	Res	Type
1	13-A	106	ASP
1	13-A	110	GLU
1	13-A	116	TYR
1	13-A	141	SER
1	13-A	150	ASP
1	13-A	154	LYS
1	13-A	156	ASP
1	13-A	168	HIS
1	13-A	170	ARG
1	13-A	172	ASP
1	13-A	181	LYS
1	13-A	194	ARG
1	13-A	211	GLU
1	13-A	214	GLU
1	13-A	216	ARG
1	13-A	217	TYR
1	14-A	2	SER
1	14-A	28	GLU
1	14-A	32	LYS
1	14-A	38	GLN
1	14-A	39	THR
1	14-A	66	ARG
1	14-A	74	ASP
1	14-A	75	ILE
1	14-A	90	GLU
1	14-A	106	ASP
1	14-A	117	GLU
1	14-A	124	ASN
1	14-A	143	THR
1	14-A	146	MET
1	14-A	170	ARG
1	14-A	176	THR
1	14-A	178	LYS
1	14-A	185	LEU
1	14-A	193	HIS
1	14-A	206	LYS
1	14-A	211	GLU
1	14-A	214	GLU
1	14-A	217	TYR
1	15-A	32	LYS
1	15-A	35	GLU
1	15-A	39	THR

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Mol	Chain	Res	Type
1	15-A	45	GLU
1	15-A	90	GLU
1	15-A	154	LYS
1	15-A	159	MET
1	15-A	170	ARG
1	15-A	181	LYS
1	15-A	194	ARG
1	15-A	206	LYS
1	15-A	212	HIS
1	15-A	217	TYR
1	16-A	2	SER
1	16-A	32	LYS
1	16-A	98	GLN
1	16-A	116	TYR
1	16-A	134	LYS
1	16-A	138	LYS
1	16-A	147	TYR
1	16-A	149	GLU
1	16-A	152	VAL
1	16-A	157	VAL
1	16-A	187	ASP
1	16-A	194	ARG
1	16-A	208	ARG
1	16-A	210	TYR
1	16-A	211	GLU
1	16-A	214	GLU
1	16-A	217	TYR
1	17-A	5	LYS
1	17-A	7	GLU
1	17-A	32	LYS
1	17-A	35	GLU
1	17-A	42	LEU
1	17-A	70	LYS
1	17-A	73	GLU
1	17-A	74	ASP
1	17-A	91	ARG
1	17-A	109	MET
1	17-A	116	TYR
1	17-A	134	LYS
1	17-A	138	LYS
1	17-A	150	ASP
1	17-A	153	LEU

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Mol	Chain	Res	Type
1	17-A	158	GLU
1	17-A	170	ARG
1	17-A	171	CYS
1	17-A	172	ASP
1	17-A	178	LYS
1	17-A	181	LYS
1	17-A	182	ASP
1	17-A	192	ASP
1	17-A	193	HIS
1	17-A	194	ARG
1	17-A	211	GLU
1	17-A	216	ARG
1	17-A	217	TYR
1	18-A	2	SER
1	18-A	11	LYS
1	18-A	28	GLU
1	18-A	38	GLN
1	18-A	70	LYS
1	18-A	91	ARG
1	18-A	112	ASP
1	18-A	116	TYR
1	18-A	133	GLN
1	18-A	134	LYS
1	18-A	138	LYS
1	18-A	142	PRO
1	18-A	146	MET
1	18-A	153	LEU
1	18-A	156	ASP
1	18-A	158	GLU
1	18-A	170	ARG
1	18-A	178	LYS
1	18-A	181	LYS
1	18-A	182	ASP
1	18-A	193	HIS
1	18-A	194	ARG
1	18-A	196	GLU
1	18-A	202	LYS
1	18-A	205	ASN
1	18-A	211	GLU
1	18-A	212	HIS
1	18-A	214	GLU
1	18-A	216	ARG

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Mol	Chain	Res	Type
1	18-A	217	TYR
1	19-A	2	SER
1	19-A	7	GLU
1	19-A	38	GLN
1	19-A	46	GLU
1	19-A	66	ARG
1	19-A	109	MET
1	19-A	116	TYR
1	19-A	138	LYS
1	19-A	146	MET
1	19-A	149	GLU
1	19-A	152	VAL
1	19-A	154	LYS
1	19-A	178	LYS
1	19-A	206	LYS
1	19-A	211	GLU
1	19-A	217	TYR
1	20-A	5	LYS
1	20-A	28	GLU
1	20-A	38	GLN
1	20-A	39	THR
1	20-A	41	ASP
1	20-A	66	ARG
1	20-A	91	ARG
1	20-A	109	MET
1	20-A	110	GLU
1	20-A	141	SER
1	20-A	154	LYS
1	20-A	156	ASP
1	20-A	172	ASP
1	20-A	180	LYS
1	20-A	187	ASP
1	20-A	193	HIS
1	20-A	203	ASP
1	20-A	206	LYS
1	20-A	217	TYR
1	21-A	3	VAL
1	21-A	5	LYS
1	21-A	13	ARG
1	21-A	22	LYS
1	21-A	28	GLU
1	21-A	30	ILE

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Mol	Chain	Res	Type
1	21-A	32	LYS
1	21-A	41	ASP
1	21-A	66	ARG
1	21-A	73	GLU
1	21-A	91	ARG
1	21-A	116	TYR
1	21-A	117	GLU
1	21-A	124	ASN
1	21-A	149	GLU
1	21-A	158	GLU
1	21-A	171	CYS
1	21-A	176	THR
1	21-A	180	LYS
1	21-A	192	ASP
1	21-A	193	HIS
1	21-A	201	ASP
1	21-A	216	ARG
1	21-A	217	TYR
1	22-A	2	SER
1	22-A	28	GLU
1	22-A	45	GLU
1	22-A	66	ARG
1	22-A	90	GLU
1	22-A	91	ARG
1	22-A	109	MET
1	22-A	116	TYR
1	22-A	145	LYS
1	22-A	149	GLU
1	22-A	154	LYS
1	22-A	157	VAL
1	22-A	158	GLU
1	22-A	164	GLU
1	22-A	178	LYS
1	22-A	181	LYS
1	22-A	185	LEU
1	22-A	193	HIS
1	22-A	196	GLU
1	22-A	202	LYS
1	22-A	211	GLU
1	22-A	212	HIS
1	22-A	216	ARG
1	22-A	217	TYR

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Mol	Chain	Res	Type
1	23-A	2	SER
1	23-A	3	VAL
1	23-A	39	THR
1	23-A	45	GLU
1	23-A	74	ASP
1	23-A	109	MET
1	23-A	110	GLU
1	23-A	116	TYR
1	23-A	128	ASN
1	23-A	134	LYS
1	23-A	145	LYS
1	23-A	149	GLU
1	23-A	154	LYS
1	23-A	172	ASP
1	23-A	178	LYS
1	23-A	181	LYS
1	23-A	185	LEU
1	23-A	192	ASP
1	23-A	208	ARG
1	23-A	216	ARG
1	23-A	217	TYR
1	24-A	30	ILE
1	24-A	45	GLU
1	24-A	66	ARG
1	24-A	70	LYS
1	24-A	85	GLU
1	24-A	109	MET
1	24-A	116	TYR
1	24-A	128	ASN
1	24-A	138	LYS
1	24-A	140	LYS
1	24-A	142	PRO
1	24-A	145	LYS
1	24-A	146	MET
1	24-A	170	ARG
1	24-A	174	LYS
1	24-A	185	LEU
1	24-A	187	ASP
1	24-A	192	ASP
1	24-A	206	LYS
1	24-A	214	GLU
1	24-A	216	ARG

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Mol	Chain	Res	Type
1	25-A	39	THR
1	25-A	41	ASP
1	25-A	45	GLU
1	25-A	66	ARG
1	25-A	78	TYR
1	25-A	109	MET
1	25-A	128	ASN
1	25-A	134	LYS
1	25-A	138	LYS
1	25-A	140	LYS
1	25-A	141	SER
1	25-A	146	MET
1	25-A	150	ASP
1	25-A	152	VAL
1	25-A	178	LYS
1	25-A	185	LEU
1	25-A	187	ASP
1	25-A	194	ARG
1	25-A	195	ILE
1	25-A	211	GLU
1	25-A	216	ARG
1	26-A	7	GLU
1	26-A	21	HIS
1	26-A	39	THR
1	26-A	66	ARG
1	26-A	81	GLN
1	26-A	85	GLU
1	26-A	116	TYR
1	26-A	138	LYS
1	26-A	150	ASP
1	26-A	152	VAL
1	26-A	153	LEU
1	26-A	157	VAL
1	26-A	158	GLU
1	26-A	159	MET
1	26-A	170	ARG
1	26-A	174	LYS
1	26-A	178	LYS
1	26-A	205	ASN
1	27-A	2	SER
1	27-A	11	LYS
1	27-A	39	THR

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Mol	Chain	Res	Type
1	27-A	43	THR
1	27-A	55	ASP
1	27-A	78	TYR
1	27-A	90	GLU
1	27-A	96	GLU
1	27-A	110	GLU
1	27-A	128	ASN
1	27-A	133	GLN
1	27-A	142	PRO
1	27-A	145	LYS
1	27-A	147	TYR
1	27-A	156	ASP
1	27-A	157	VAL
1	27-A	178	LYS
1	27-A	180	LYS
1	27-A	181	LYS
1	27-A	194	ARG
1	27-A	196	GLU
1	27-A	205	ASN
1	27-A	212	HIS
1	27-A	216	ARG
1	28-A	3	VAL
1	28-A	22	LYS
1	28-A	45	GLU
1	28-A	55	ASP
1	28-A	73	GLU
1	28-A	78	TYR
1	28-A	90	GLU
1	28-A	110	GLU
1	28-A	116	TYR
1	28-A	128	ASN
1	28-A	138	LYS
1	28-A	149	GLU
1	28-A	152	VAL
1	28-A	156	ASP
1	28-A	171	CYS
1	28-A	180	LYS
1	28-A	187	ASP
1	28-A	193	HIS
1	28-A	194	ARG
1	28-A	196	GLU
1	28-A	202	LYS

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Mol	Chain	Res	Type
1	29-A	7	GLU
1	29-A	11	LYS
1	29-A	38	GLN
1	29-A	45	GLU
1	29-A	55	ASP
1	29-A	73	GLU
1	29-A	100	ILE
1	29-A	110	GLU
1	29-A	116	TYR
1	29-A	128	ASN
1	29-A	141	SER
1	29-A	146	MET
1	29-A	168	HIS
1	29-A	172	ASP
1	29-A	178	LYS
1	29-A	193	HIS
1	29-A	194	ARG
1	29-A	202	LYS
1	29-A	208	ARG
1	29-A	211	GLU
1	29-A	217	TYR
1	30-A	13	ARG
1	30-A	38	GLN
1	30-A	41	ASP
1	30-A	66	ARG
1	30-A	70	LYS
1	30-A	73	GLU
1	30-A	74	ASP
1	30-A	85	GLU
1	30-A	98	GLN
1	30-A	110	GLU
1	30-A	117	GLU
1	30-A	158	GLU
1	30-A	168	HIS
1	30-A	178	LYS
1	30-A	181	LYS
1	30-A	185	LEU
1	30-A	192	ASP
1	30-A	194	ARG
1	30-A	212	HIS
1	30-A	217	TYR
1	31-A	2	SER

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Mol	Chain	Res	Type
1	31-A	5	LYS
1	31-A	28	GLU
1	31-A	38	GLN
1	31-A	66	ARG
1	31-A	90	GLU
1	31-A	110	GLU
1	31-A	116	TYR
1	31-A	146	MET
1	31-A	157	VAL
1	31-A	185	LEU
1	31-A	194	ARG
1	31-A	206	LYS
1	31-A	212	HIS
1	31-A	216	ARG
1	32-A	2	SER
1	32-A	28	GLU
1	32-A	66	ARG
1	32-A	70	LYS
1	32-A	116	TYR
1	32-A	124	ASN
1	32-A	158	GLU
1	32-A	178	LYS
1	32-A	185	LEU
1	32-A	187	ASP
1	32-A	192	ASP
1	32-A	203	ASP
1	32-A	206	LYS
1	32-A	211	GLU
1	32-A	216	ARG
1	32-A	217	TYR
1	33-A	2	SER
1	33-A	3	VAL
1	33-A	5	LYS
1	33-A	7	GLU
1	33-A	11	LYS
1	33-A	66	ARG
1	33-A	70	LYS
1	33-A	78	TYR
1	33-A	81	GLN
1	33-A	100	ILE
1	33-A	106	ASP
1	33-A	109	MET

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Mol	Chain	Res	Type
1	33-A	110	GLU
1	33-A	142	PRO
1	33-A	150	ASP
1	33-A	156	ASP
1	33-A	157	VAL
1	33-A	158	GLU
1	33-A	174	LYS
1	33-A	187	ASP
1	33-A	192	ASP
1	33-A	194	ARG
1	33-A	205	ASN
1	33-A	206	LYS
1	33-A	212	HIS
1	34-A	2	SER
1	34-A	5	LYS
1	34-A	11	LYS
1	34-A	35	GLU
1	34-A	66	ARG
1	34-A	81	GLN
1	34-A	106	ASP
1	34-A	110	GLU
1	34-A	116	TYR
1	34-A	134	LYS
1	34-A	140	LYS
1	34-A	150	ASP
1	34-A	153	LEU
1	34-A	156	ASP
1	34-A	159	MET
1	34-A	168	HIS
1	34-A	178	LYS
1	34-A	181	LYS
1	34-A	192	ASP
1	34-A	193	HIS
1	34-A	194	ARG
1	34-A	195	ILE
1	34-A	203	ASP
1	34-A	206	LYS
1	34-A	216	ARG
1	35-A	5	LYS
1	35-A	39	THR
1	35-A	66	ARG
1	35-A	81	GLN

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Mol	Chain	Res	Type
1	35-A	110	GLU
1	35-A	116	TYR
1	35-A	170	ARG
1	35-A	178	LYS
1	35-A	180	LYS
1	35-A	191	VAL
1	35-A	194	ARG
1	35-A	203	ASP
1	35-A	206	LYS
1	35-A	211	GLU
1	36-A	2	SER
1	36-A	11	LYS
1	36-A	35	GLU
1	36-A	45	GLU
1	36-A	66	ARG
1	36-A	73	GLU
1	36-A	81	GLN
1	36-A	109	MET
1	36-A	133	GLN
1	36-A	140	LYS
1	36-A	145	LYS
1	36-A	178	LYS
1	36-A	180	LYS
1	36-A	181	LYS
1	36-A	192	ASP
1	36-A	193	HIS
1	36-A	206	LYS
1	37-A	2	SER
1	37-A	11	LYS
1	37-A	28	GLU
1	37-A	35	GLU
1	37-A	39	THR
1	37-A	45	GLU
1	37-A	66	ARG
1	37-A	81	GLN
1	37-A	110	GLU
1	37-A	116	TYR
1	37-A	117	GLU
1	37-A	124	ASN
1	37-A	140	LYS
1	37-A	142	PRO
1	37-A	148	VAL

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Mol	Chain	Res	Type
1	37-A	150	ASP
1	37-A	152	VAL
1	37-A	153	LEU
1	37-A	174	LYS
1	37-A	178	LYS
1	37-A	180	LYS
1	37-A	181	LYS
1	37-A	191	VAL
1	37-A	194	ARG
1	37-A	202	LYS
1	37-A	205	ASN
1	37-A	206	LYS
1	37-A	214	GLU
1	37-A	216	ARG
1	38-A	7	GLU
1	38-A	22	LYS
1	38-A	41	ASP
1	38-A	45	GLU
1	38-A	73	GLU
1	38-A	78	TYR
1	38-A	90	GLU
1	38-A	98	GLN
1	38-A	109	MET
1	38-A	124	ASN
1	38-A	127	PRO
1	38-A	134	LYS
1	38-A	138	LYS
1	38-A	140	LYS
1	38-A	154	LYS
1	38-A	156	ASP
1	38-A	178	LYS
1	38-A	191	VAL
1	38-A	196	GLU
1	38-A	203	ASP
1	38-A	206	LYS
1	38-A	208	ARG
1	38-A	217	TYR
1	39-A	2	SER
1	39-A	41	ASP
1	39-A	45	GLU
1	39-A	66	ARG
1	39-A	74	ASP

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Mol	Chain	Res	Type
1	39-A	90	GLU
1	39-A	98	GLN
1	39-A	106	ASP
1	39-A	116	TYR
1	39-A	133	GLN
1	39-A	134	LYS
1	39-A	135	LYS
1	39-A	138	LYS
1	39-A	142	PRO
1	39-A	146	MET
1	39-A	156	ASP
1	39-A	157	VAL
1	39-A	158	GLU
1	39-A	181	LYS
1	39-A	185	LEU
1	39-A	187	ASP
1	39-A	193	HIS
1	39-A	196	GLU
1	39-A	206	LYS
1	39-A	212	HIS
1	39-A	216	ARG
1	39-A	217	TYR
1	40-A	2	SER
1	40-A	13	ARG
1	40-A	22	LYS
1	40-A	28	GLU
1	40-A	39	THR
1	40-A	41	ASP
1	40-A	45	GLU
1	40-A	66	ARG
1	40-A	85	GLU
1	40-A	98	GLN
1	40-A	116	TYR
1	40-A	117	GLU
1	40-A	153	LEU
1	40-A	172	ASP
1	40-A	181	LYS
1	40-A	187	ASP
1	40-A	190	GLU
1	40-A	193	HIS
1	40-A	206	LYS
1	40-A	211	GLU

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Mol	Chain	Res	Type
1	40-A	216	ARG
1	41-A	3	VAL
1	41-A	13	ARG
1	41-A	28	GLU
1	41-A	39	THR
1	41-A	73	GLU
1	41-A	78	TYR
1	41-A	85	GLU
1	41-A	98	GLN
1	41-A	109	MET
1	41-A	133	GLN
1	41-A	134	LYS
1	41-A	135	LYS
1	41-A	138	LYS
1	41-A	141	SER
1	41-A	153	LEU
1	41-A	157	VAL
1	41-A	158	GLU
1	41-A	174	LYS
1	41-A	181	LYS
1	41-A	187	ASP
1	41-A	193	HIS
1	41-A	202	LYS
1	41-A	206	LYS
1	41-A	216	ARG
1	42-A	28	GLU
1	42-A	30	ILE
1	42-A	59	PRO
1	42-A	85	GLU
1	42-A	98	GLN
1	42-A	109	MET
1	42-A	116	TYR
1	42-A	124	ASN
1	42-A	127	PRO
1	42-A	133	GLN
1	42-A	141	SER
1	42-A	158	GLU
1	42-A	174	LYS
1	42-A	178	LYS
1	42-A	181	LYS
1	42-A	192	ASP
1	42-A	193	HIS

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Mol	Chain	Res	Type
1	42-A	194	ARG
1	42-A	195	ILE
1	42-A	202	LYS
1	42-A	216	ARG
1	43-A	3	VAL
1	43-A	66	ARG
1	43-A	73	GLU
1	43-A	81	GLN
1	43-A	98	GLN
1	43-A	100	ILE
1	43-A	117	GLU
1	43-A	124	ASN
1	43-A	133	GLN
1	43-A	142	PRO
1	43-A	150	ASP
1	43-A	153	LEU
1	43-A	156	ASP
1	43-A	158	GLU
1	43-A	171	CYS
1	43-A	174	LYS
1	43-A	181	LYS
1	43-A	192	ASP
1	43-A	193	HIS
1	43-A	194	ARG
1	43-A	202	LYS
1	43-A	203	ASP
1	43-A	211	GLU
1	43-A	216	ARG
1	44-A	2	SER
1	44-A	11	LYS
1	44-A	39	THR
1	44-A	66	ARG
1	44-A	72	PRO
1	44-A	81	GLN
1	44-A	121	ASP
1	44-A	133	GLN
1	44-A	152	VAL
1	44-A	153	LEU
1	44-A	156	ASP
1	44-A	176	THR
1	44-A	180	LYS
1	44-A	181	LYS

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Mol	Chain	Res	Type
1	44-A	194	ARG
1	44-A	202	LYS
1	44-A	206	LYS
1	44-A	211	GLU
1	45-A	5	LYS
1	45-A	66	ARG
1	45-A	73	GLU
1	45-A	107	ILE
1	45-A	109	MET
1	45-A	130	PRO
1	45-A	138	LYS
1	45-A	145	LYS
1	45-A	149	GLU
1	45-A	153	LEU
1	45-A	156	ASP
1	45-A	162	LEU
1	45-A	180	LYS
1	45-A	181	LYS
1	45-A	190	GLU
1	45-A	194	ARG
1	45-A	202	LYS
1	45-A	205	ASN
1	45-A	206	LYS
1	46-A	3	VAL
1	46-A	5	LYS
1	46-A	7	GLU
1	46-A	11	LYS
1	46-A	30	ILE
1	46-A	43	THR
1	46-A	106	ASP
1	46-A	109	MET
1	46-A	112	ASP
1	46-A	116	TYR
1	46-A	138	LYS
1	46-A	146	MET
1	46-A	149	GLU
1	46-A	156	ASP
1	46-A	172	ASP
1	46-A	180	LYS
1	46-A	187	ASP
1	46-A	190	GLU
1	46-A	192	ASP

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Mol	Chain	Res	Type
1	46-A	193	HIS
1	46-A	206	LYS
1	47-A	2	SER
1	47-A	5	LYS
1	47-A	28	GLU
1	47-A	43	THR
1	47-A	45	GLU
1	47-A	106	ASP
1	47-A	107	ILE
1	47-A	116	TYR
1	47-A	117	GLU
1	47-A	153	LEU
1	47-A	159	MET
1	47-A	178	LYS
1	47-A	180	LYS
1	47-A	192	ASP
1	47-A	202	LYS
1	47-A	206	LYS
1	48-A	5	LYS
1	48-A	39	THR
1	48-A	45	GLU
1	48-A	66	ARG
1	48-A	73	GLU
1	48-A	106	ASP
1	48-A	110	GLU
1	48-A	112	ASP
1	48-A	116	TYR
1	48-A	117	GLU
1	48-A	143	THR
1	48-A	154	LYS
1	48-A	157	VAL
1	48-A	178	LYS
1	48-A	187	ASP
1	48-A	190	GLU
1	48-A	196	GLU
1	48-A	216	ARG
1	49-A	11	LYS
1	49-A	32	LYS
1	49-A	35	GLU
1	49-A	66	ARG
1	49-A	73	GLU
1	49-A	75	ILE

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Mol	Chain	Res	Type
1	49-A	85	GLU
1	49-A	116	TYR
1	49-A	124	ASN
1	49-A	138	LYS
1	49-A	143	THR
1	49-A	150	ASP
1	49-A	156	ASP
1	49-A	159	MET
1	49-A	168	HIS
1	49-A	180	LYS
1	49-A	181	LYS
1	49-A	193	HIS
1	49-A	212	HIS
1	50-A	30	ILE
1	50-A	32	LYS
1	50-A	39	THR
1	50-A	66	ARG
1	50-A	106	ASP
1	50-A	116	TYR
1	50-A	117	GLU
1	50-A	138	LYS
1	50-A	142	PRO
1	50-A	143	THR
1	50-A	145	LYS
1	50-A	156	ASP
1	50-A	185	LEU
1	50-A	187	ASP
1	50-A	194	ARG
1	50-A	211	GLU
1	50-A	216	ARG
1	51-A	4	ILE
1	51-A	28	GLU
1	51-A	66	ARG
1	51-A	81	GLN
1	51-A	85	GLU
1	51-A	98	GLN
1	51-A	117	GLU
1	51-A	124	ASN
1	51-A	134	LYS
1	51-A	138	LYS
1	51-A	141	SER
1	51-A	143	THR

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Mol	Chain	Res	Type
1	51-A	156	ASP
1	51-A	178	LYS
1	51-A	193	HIS
1	51-A	194	ARG
1	51-A	201	ASP
1	51-A	211	GLU
1	51-A	214	GLU
1	52-A	11	LYS
1	52-A	26	GLU
1	52-A	28	GLU
1	52-A	32	LYS
1	52-A	39	THR
1	52-A	66	ARG
1	52-A	74	ASP
1	52-A	98	GLN
1	52-A	109	MET
1	52-A	124	ASN
1	52-A	127	PRO
1	52-A	145	LYS
1	52-A	158	GLU
1	52-A	159	MET
1	52-A	168	HIS
1	52-A	174	LYS
1	52-A	194	ARG
1	52-A	195	ILE
1	52-A	205	ASN
1	52-A	211	GLU
1	52-A	214	GLU
1	53-A	2	SER
1	53-A	11	LYS
1	53-A	28	GLU
1	53-A	32	LYS
1	53-A	51	PRO
1	53-A	78	TYR
1	53-A	98	GLN
1	53-A	128	ASN
1	53-A	143	THR
1	53-A	145	LYS
1	53-A	174	LYS
1	53-A	192	ASP
1	53-A	193	HIS
1	53-A	194	ARG

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Mol	Chain	Res	Type
1	53-A	203	ASP
1	53-A	206	LYS
1	53-A	212	HIS
1	53-A	217	TYR
1	54-A	2	SER
1	54-A	22	LYS
1	54-A	28	GLU
1	54-A	32	LYS
1	54-A	39	THR
1	54-A	41	ASP
1	54-A	70	LYS
1	54-A	74	ASP
1	54-A	100	ILE
1	54-A	116	TYR
1	54-A	145	LYS
1	54-A	147	TYR
1	54-A	149	GLU
1	54-A	152	VAL
1	54-A	156	ASP
1	54-A	158	GLU
1	54-A	178	LYS
1	54-A	180	LYS
1	54-A	192	ASP
1	54-A	193	HIS
1	54-A	194	ARG
1	54-A	202	LYS
1	54-A	208	ARG
1	55-A	11	LYS
1	55-A	22	LYS
1	55-A	28	GLU
1	55-A	35	GLU
1	55-A	45	GLU
1	55-A	73	GLU
1	55-A	74	ASP
1	55-A	98	GLN
1	55-A	100	ILE
1	55-A	110	GLU
1	55-A	116	TYR
1	55-A	117	GLU
1	55-A	128	ASN
1	55-A	134	LYS
1	55-A	140	LYS

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Mol	Chain	Res	Type
1	55-A	143	THR
1	55-A	145	LYS
1	55-A	150	ASP
1	55-A	158	GLU
1	55-A	176	THR
1	55-A	178	LYS
1	55-A	181	LYS
1	55-A	185	LEU
1	55-A	190	GLU
1	55-A	195	ILE
1	56-A	2	SER
1	56-A	5	LYS
1	56-A	7	GLU
1	56-A	8	MET
1	56-A	28	GLU
1	56-A	39	THR
1	56-A	66	ARG
1	56-A	73	GLU
1	56-A	75	ILE
1	56-A	98	GLN
1	56-A	116	TYR
1	56-A	128	ASN
1	56-A	134	LYS
1	56-A	138	LYS
1	56-A	143	THR
1	56-A	145	LYS
1	56-A	152	VAL
1	56-A	156	ASP
1	56-A	178	LYS
1	56-A	194	ARG
1	56-A	217	TYR
1	57-A	41	ASP
1	57-A	73	GLU
1	57-A	98	GLN
1	57-A	110	GLU
1	57-A	116	TYR
1	57-A	138	LYS
1	57-A	142	PRO
1	57-A	143	THR
1	57-A	145	LYS
1	57-A	146	MET
1	57-A	152	VAL

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Mol	Chain	Res	Type
1	57-A	170	ARG
1	57-A	172	ASP
1	57-A	174	LYS
1	57-A	178	LYS
1	57-A	191	VAL
1	57-A	193	HIS
1	57-A	206	LYS
1	57-A	216	ARG
1	57-A	217	TYR
1	58-A	2	SER
1	58-A	7	GLU
1	58-A	43	THR
1	58-A	45	GLU
1	58-A	73	GLU
1	58-A	98	GLN
1	58-A	106	ASP
1	58-A	109	MET
1	58-A	116	TYR
1	58-A	124	ASN
1	58-A	140	LYS
1	58-A	141	SER
1	58-A	170	ARG
1	58-A	176	THR
1	58-A	180	LYS
1	58-A	181	LYS
1	58-A	187	ASP
1	58-A	191	VAL
1	58-A	192	ASP
1	58-A	194	ARG
1	58-A	210	TYR
1	58-A	214	GLU
1	58-A	216	ARG
1	58-A	217	TYR
1	59-A	2	SER
1	59-A	98	GLN
1	59-A	116	TYR
1	59-A	124	ASN
1	59-A	128	ASN
1	59-A	140	LYS
1	59-A	142	PRO
1	59-A	145	LYS
1	59-A	146	MET

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Mol	Chain	Res	Type
1	59-A	150	ASP
1	59-A	156	ASP
1	59-A	158	GLU
1	59-A	170	ARG
1	59-A	178	LYS
1	59-A	193	HIS
1	59-A	210	TYR
1	59-A	211	GLU
1	59-A	216	ARG
1	60-A	74	ASP
1	60-A	85	GLU
1	60-A	109	MET
1	60-A	116	TYR
1	60-A	123	THR
1	60-A	124	ASN
1	60-A	142	PRO
1	60-A	143	THR
1	60-A	150	ASP
1	60-A	154	LYS
1	60-A	156	ASP
1	60-A	158	GLU
1	60-A	159	MET
1	60-A	171	CYS
1	60-A	172	ASP
1	60-A	178	LYS
1	60-A	180	LYS
1	60-A	202	LYS
1	60-A	203	ASP
1	60-A	210	TYR
1	60-A	211	GLU
1	60-A	216	ARG
1	60-A	217	TYR
1	61-A	2	SER
1	61-A	11	LYS
1	61-A	39	THR
1	61-A	66	ARG
1	61-A	70	LYS
1	61-A	73	GLU
1	61-A	109	MET
1	61-A	123	THR
1	61-A	134	LYS
1	61-A	138	LYS

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Mol	Chain	Res	Type
1	61-A	141	SER
1	61-A	143	THR
1	61-A	150	ASP
1	61-A	158	GLU
1	61-A	168	HIS
1	61-A	178	LYS
1	61-A	180	LYS
1	61-A	191	VAL
1	61-A	193	HIS
1	61-A	194	ARG
1	61-A	196	GLU
1	61-A	203	ASP
1	61-A	216	ARG
1	62-A	3	VAL
1	62-A	5	LYS
1	62-A	7	GLU
1	62-A	13	ARG
1	62-A	73	GLU
1	62-A	78	TYR
1	62-A	85	GLU
1	62-A	90	GLU
1	62-A	93	MET
1	62-A	94	THR
1	62-A	116	TYR
1	62-A	128	ASN
1	62-A	134	LYS
1	62-A	138	LYS
1	62-A	156	ASP
1	62-A	158	GLU
1	62-A	159	MET
1	62-A	178	LYS
1	62-A	180	LYS
1	62-A	194	ARG
1	62-A	202	LYS
1	62-A	214	GLU
1	62-A	216	ARG
1	63-A	3	VAL
1	63-A	5	LYS
1	63-A	15	GLU
1	63-A	35	GLU
1	63-A	41	ASP
1	63-A	45	GLU

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Mol	Chain	Res	Type
1	63-A	50	LEU
1	63-A	66	ARG
1	63-A	90	GLU
1	63-A	106	ASP
1	63-A	110	GLU
1	63-A	116	TYR
1	63-A	126	PRO
1	63-A	128	ASN
1	63-A	134	LYS
1	63-A	152	VAL
1	63-A	156	ASP
1	63-A	159	MET
1	63-A	180	LYS
1	63-A	187	ASP
1	63-A	202	LYS
1	63-A	211	GLU
1	63-A	216	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (181) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	21	HIS
1	1-A	38	GLN
1	1-A	193	HIS
1	2-A	193	HIS
1	2-A	212	HIS
1	3-A	38	GLN
1	4-A	38	GLN
1	4-A	81	GLN
1	4-A	168	HIS
1	5-A	38	GLN
1	5-A	81	GLN
1	5-A	133	GLN
1	6-A	38	GLN
1	6-A	81	GLN
1	6-A	124	ASN
1	7-A	81	GLN
1	7-A	128	ASN
1	8-A	38	GLN
1	8-A	133	GLN
1	9-A	38	GLN
1	9-A	133	GLN

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Mol	Chain	Res	Type
1	9-A	168	HIS
1	9-A	205	ASN
1	9-A	212	HIS
1	10-A	38	GLN
1	10-A	81	GLN
1	10-A	133	GLN
1	10-A	205	ASN
1	11-A	81	GLN
1	11-A	205	ASN
1	11-A	212	HIS
1	12-A	133	GLN
1	12-A	205	ASN
1	12-A	212	HIS
1	13-A	81	GLN
1	13-A	124	ASN
1	13-A	133	GLN
1	13-A	205	ASN
1	14-A	38	GLN
1	14-A	124	ASN
1	14-A	133	GLN
1	14-A	205	ASN
1	15-A	193	HIS
1	15-A	205	ASN
1	16-A	133	GLN
1	16-A	205	ASN
1	17-A	38	GLN
1	17-A	193	HIS
1	17-A	205	ASN
1	18-A	38	GLN
1	18-A	98	GLN
1	19-A	38	GLN
1	19-A	81	GLN
1	19-A	128	ASN
1	19-A	133	GLN
1	19-A	205	ASN
1	20-A	38	GLN
1	20-A	193	HIS
1	20-A	205	ASN
1	21-A	38	GLN
1	21-A	133	GLN
1	21-A	193	HIS
1	21-A	205	ASN

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Mol	Chain	Res	Type
1	22-A	38	GLN
1	22-A	128	ASN
1	22-A	193	HIS
1	22-A	205	ASN
1	23-A	205	ASN
1	24-A	38	GLN
1	24-A	128	ASN
1	24-A	205	ASN
1	24-A	212	HIS
1	25-A	38	GLN
1	25-A	124	ASN
1	25-A	133	GLN
1	25-A	205	ASN
1	26-A	21	HIS
1	26-A	38	GLN
1	26-A	81	GLN
1	26-A	124	ASN
1	26-A	133	GLN
1	26-A	212	HIS
1	27-A	38	GLN
1	27-A	124	ASN
1	27-A	128	ASN
1	27-A	205	ASN
1	28-A	133	GLN
1	28-A	168	HIS
1	28-A	193	HIS
1	28-A	212	HIS
1	29-A	81	GLN
1	29-A	124	ASN
1	29-A	128	ASN
1	29-A	205	ASN
1	30-A	133	GLN
1	30-A	205	ASN
1	31-A	133	GLN
1	31-A	193	HIS
1	31-A	205	ASN
1	31-A	212	HIS
1	32-A	128	ASN
1	32-A	205	ASN
1	33-A	205	ASN
1	33-A	212	HIS
1	34-A	193	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	34-A	205	ASN
1	34-A	212	HIS
1	35-A	133	GLN
1	35-A	205	ASN
1	36-A	133	GLN
1	36-A	205	ASN
1	36-A	212	HIS
1	37-A	133	GLN
1	38-A	98	GLN
1	38-A	128	ASN
1	39-A	98	GLN
1	39-A	128	ASN
1	39-A	212	HIS
1	40-A	212	HIS
1	41-A	98	GLN
1	41-A	124	ASN
1	41-A	133	GLN
1	41-A	205	ASN
1	41-A	212	HIS
1	42-A	98	GLN
1	42-A	133	GLN
1	42-A	193	HIS
1	42-A	205	ASN
1	43-A	98	GLN
1	43-A	124	ASN
1	43-A	193	HIS
1	43-A	205	ASN
1	43-A	212	HIS
1	44-A	81	GLN
1	44-A	124	ASN
1	44-A	205	ASN
1	44-A	212	HIS
1	45-A	133	GLN
1	45-A	205	ASN
1	46-A	193	HIS
1	46-A	212	HIS
1	47-A	98	GLN
1	47-A	193	HIS
1	48-A	124	ASN
1	48-A	205	ASN
1	49-A	124	ASN
1	49-A	128	ASN

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Mol	Chain	Res	Type
1	49-A	133	GLN
1	49-A	168	HIS
1	49-A	193	HIS
1	49-A	205	ASN
1	49-A	212	HIS
1	50-A	133	GLN
1	50-A	193	HIS
1	50-A	205	ASN
1	51-A	81	GLN
1	51-A	205	ASN
1	52-A	124	ASN
1	52-A	133	GLN
1	52-A	205	ASN
1	53-A	124	ASN
1	53-A	133	GLN
1	55-A	128	ASN
1	55-A	168	HIS
1	55-A	212	HIS
1	56-A	81	GLN
1	57-A	38	GLN
1	57-A	81	GLN
1	57-A	133	GLN
1	57-A	212	HIS
1	58-A	98	GLN
1	58-A	124	ASN
1	58-A	133	GLN
1	58-A	193	HIS
1	59-A	98	GLN
1	59-A	124	ASN
1	59-A	133	GLN
1	60-A	98	GLN
1	60-A	124	ASN
1	62-A	193	HIS
1	63-A	81	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

63 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
1	CRQ	1-A	62	1	24,25,26	1.75	5 (20%)	24,34,36	1.93	6 (25%)
1	CRQ	10-A	62	1	24,25,26	1.61	5 (20%)	24,34,36	3.70	11 (45%)
1	CRQ	11-A	62	1	24,25,26	1.80	5 (20%)	24,34,36	2.21	7 (29%)
1	CRQ	12-A	62	1	24,25,26	2.31	8 (33%)	24,34,36	2.75	8 (33%)
1	CRQ	13-A	62	1	24,25,26	1.94	6 (25%)	24,34,36	3.74	7 (29%)
1	CRQ	14-A	62	1	24,25,26	1.67	4 (16%)	24,34,36	3.46	11 (45%)
1	CRQ	15-A	62	1	24,25,26	1.89	7 (29%)	24,34,36	3.34	9 (37%)
1	CRQ	16-A	62	1	24,25,26	1.81	7 (29%)	24,34,36	7.52	13 (54%)
1	CRQ	17-A	62	1	24,25,26	1.60	4 (16%)	24,34,36	4.09	10 (41%)
1	CRQ	18-A	62	1	24,25,26	1.63	5 (20%)	24,34,36	3.31	10 (41%)
1	CRQ	19-A	62	1	24,25,26	2.47	9 (37%)	24,34,36	3.17	14 (58%)
1	CRQ	2-A	62	1	24,25,26	1.71	6 (25%)	24,34,36	2.35	10 (41%)
1	CRQ	20-A	62	1	24,25,26	2.12	8 (33%)	24,34,36	4.10	10 (41%)
1	CRQ	21-A	62	1	24,25,26	2.00	7 (29%)	24,34,36	2.49	8 (33%)
1	CRQ	22-A	62	1	24,25,26	1.76	5 (20%)	24,34,36	2.75	10 (41%)
1	CRQ	23-A	62	1	24,25,26	1.93	7 (29%)	24,34,36	3.77	12 (50%)
1	CRQ	24-A	62	1	24,25,26	1.61	4 (16%)	24,34,36	2.67	6 (25%)
1	CRQ	25-A	62	1	24,25,26	1.91	6 (25%)	24,34,36	1.87	7 (29%)
1	CRQ	26-A	62	1	24,25,26	1.93	7 (29%)	24,34,36	2.16	6 (25%)
1	CRQ	27-A	62	1	24,25,26	1.74	6 (25%)	24,34,36	2.09	9 (37%)
1	CRQ	28-A	62	1	24,25,26	1.77	5 (20%)	24,34,36	1.84	9 (37%)
1	CRQ	29-A	62	1	24,25,26	1.98	4 (16%)	24,34,36	4.92	9 (37%)
1	CRQ	3-A	62	1	24,25,26	2.86	8 (33%)	24,34,36	3.26	13 (54%)
1	CRQ	30-A	62	1	24,25,26	1.87	6 (25%)	24,34,36	2.48	8 (33%)
1	CRQ	31-A	62	1	24,25,26	2.00	5 (20%)	24,34,36	3.50	10 (41%)
1	CRQ	32-A	62	1	24,25,26	1.89	7 (29%)	24,34,36	2.44	7 (29%)
1	CRQ	33-A	62	1	24,25,26	1.87	6 (25%)	24,34,36	3.47	11 (45%)
1	CRQ	34-A	62	1	24,25,26	1.63	3 (12%)	24,34,36	2.10	8 (33%)
1	CRQ	35-A	62	1	24,25,26	1.69	3 (12%)	24,34,36	2.50	7 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CRQ	36-A	62	1	24,25,26	2.15	8 (33%)	24,34,36	2.62	9 (37%)
1	CRQ	37-A	62	1	24,25,26	2.01	5 (20%)	24,34,36	3.38	10 (41%)
1	CRQ	38-A	62	1	24,25,26	1.92	7 (29%)	24,34,36	2.31	7 (29%)
1	CRQ	39-A	62	1	24,25,26	1.84	7 (29%)	24,34,36	2.07	9 (37%)
1	CRQ	4-A	62	1	24,25,26	2.06	6 (25%)	24,34,36	2.75	10 (41%)
1	CRQ	40-A	62	1	24,25,26	1.65	4 (16%)	24,34,36	2.14	5 (20%)
1	CRQ	41-A	62	1	24,25,26	1.98	5 (20%)	24,34,36	3.92	11 (45%)
1	CRQ	42-A	62	1	24,25,26	1.76	4 (16%)	24,34,36	3.46	8 (33%)
1	CRQ	43-A	62	1	24,25,26	2.37	7 (29%)	24,34,36	4.95	13 (54%)
1	CRQ	44-A	62	1	24,25,26	2.18	6 (25%)	24,34,36	4.23	14 (58%)
1	CRQ	45-A	62	1	24,25,26	1.66	6 (25%)	24,34,36	1.80	3 (12%)
1	CRQ	46-A	62	1	24,25,26	1.79	6 (25%)	24,34,36	2.05	5 (20%)
1	CRQ	47-A	62	1	24,25,26	2.21	7 (29%)	24,34,36	4.09	13 (54%)
1	CRQ	48-A	62	1	24,25,26	2.04	6 (25%)	24,34,36	1.90	6 (25%)
1	CRQ	49-A	62	1	24,25,26	1.72	5 (20%)	24,34,36	2.29	7 (29%)
1	CRQ	5-A	62	1	24,25,26	2.06	7 (29%)	24,34,36	3.98	13 (54%)
1	CRQ	50-A	62	1	24,25,26	2.00	5 (20%)	24,34,36	2.85	4 (16%)
1	CRQ	51-A	62	1	24,25,26	2.23	6 (25%)	24,34,36	3.80	10 (41%)
1	CRQ	52-A	62	1	24,25,26	1.98	4 (16%)	24,34,36	3.19	10 (41%)
1	CRQ	53-A	62	1	24,25,26	1.86	7 (29%)	24,34,36	4.01	10 (41%)
1	CRQ	54-A	62	1	24,25,26	1.61	5 (20%)	24,34,36	4.41	14 (58%)
1	CRQ	55-A	62	1	24,25,26	2.03	7 (29%)	24,34,36	3.62	10 (41%)
1	CRQ	56-A	62	1	24,25,26	1.66	5 (20%)	24,34,36	3.04	6 (25%)
1	CRQ	57-A	62	1	24,25,26	1.84	7 (29%)	24,34,36	3.30	10 (41%)
1	CRQ	58-A	62	1	24,25,26	3.06	9 (37%)	24,34,36	4.16	12 (50%)
1	CRQ	59-A	62	1	24,25,26	1.81	5 (20%)	24,34,36	3.91	13 (54%)
1	CRQ	6-A	62	1	24,25,26	1.88	4 (16%)	24,34,36	3.15	10 (41%)
1	CRQ	60-A	62	1	24,25,26	1.77	5 (20%)	24,34,36	2.17	7 (29%)
1	CRQ	61-A	62	1	24,25,26	1.71	5 (20%)	24,34,36	2.22	10 (41%)
1	CRQ	62-A	62	1	24,25,26	1.88	5 (20%)	24,34,36	2.62	7 (29%)
1	CRQ	63-A	62	1	24,25,26	2.01	4 (16%)	24,34,36	3.56	11 (45%)
1	CRQ	7-A	62	1	24,25,26	1.74	5 (20%)	24,34,36	3.88	9 (37%)
1	CRQ	8-A	62	1	24,25,26	1.87	6 (25%)	24,34,36	1.72	5 (20%)
1	CRQ	9-A	62	1	24,25,26	2.52	9 (37%)	24,34,36	2.74	11 (45%)



In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CRQ	1-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	10-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	11-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	12-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	13-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	14-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	15-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	16-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	17-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	18-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	19-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	2-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	20-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	21-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	22-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	23-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	24-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	25-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	26-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	27-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	28-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	29-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	3-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	30-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	31-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	32-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	33-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	34-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	35-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	36-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	37-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	38-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	39-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	4-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	40-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	41-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	42-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	43-A	62	1	-	0/10/32/33	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CRQ	44-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	45-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	46-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	47-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	48-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	49-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	5-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	50-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	51-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	52-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	53-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	54-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	55-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	56-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	57-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	58-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	59-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	6-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	60-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	61-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	62-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	63-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	7-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	8-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	9-A	62	1	-	0/10/32/33	0/2/2/2

All (367) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	51-A	62	CRQ	CA2-C2	-6.38	1.41	1.48
1	29-A	62	CRQ	CA2-C2	-6.33	1.41	1.48
1	44-A	62	CRQ	CA2-C2	-6.31	1.41	1.48
1	4-A	62	CRQ	CA2-C2	-6.21	1.41	1.48
1	37-A	62	CRQ	CA2-C2	-6.18	1.41	1.48
1	47-A	62	CRQ	CA2-C2	-6.08	1.42	1.48
1	63-A	62	CRQ	CA2-C2	-5.67	1.42	1.48
1	43-A	62	CRQ	CA2-C2	-5.35	1.42	1.48
1	41-A	62	CRQ	CA2-C2	-5.23	1.42	1.48
1	31-A	62	CRQ	CA2-C2	-5.14	1.43	1.48
1	61-A	62	CRQ	CA2-C2	-4.64	1.43	1.48
1	6-A	62	CRQ	CA2-C2	-4.61	1.43	1.48
1	21-A	62	CRQ	CA2-C2	-4.46	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	15-A	62	CRQ	CA2-C2	-4.39	1.43	1.48
1	57-A	62	CRQ	CA2-C2	-4.27	1.44	1.48
1	55-A	62	CRQ	CA2-C2	-4.25	1.44	1.48
1	32-A	62	CRQ	CA2-C2	-4.12	1.44	1.48
1	23-A	62	CRQ	CA2-C2	-4.06	1.44	1.48
1	1-A	62	CRQ	CA2-C2	-4.04	1.44	1.48
1	28-A	62	CRQ	CA2-C2	-3.90	1.44	1.48
1	47-A	62	CRQ	CA3-N3	-3.79	1.39	1.47
1	23-A	62	CRQ	CA3-N3	-3.75	1.39	1.47
1	5-A	62	CRQ	CA2-C2	-3.74	1.44	1.48
1	46-A	62	CRQ	CA3-N3	-3.66	1.39	1.47
1	16-A	62	CRQ	CA3-N3	-3.64	1.39	1.47
1	20-A	62	CRQ	CA3-N3	-3.55	1.39	1.47
1	30-A	62	CRQ	CA2-C2	-3.51	1.44	1.48
1	59-A	62	CRQ	CB2-CA2	-3.48	1.31	1.35
1	41-A	62	CRQ	CA3-N3	-3.46	1.39	1.47
1	19-A	62	CRQ	CA2-C2	-3.45	1.44	1.48
1	47-A	62	CRQ	CB2-CA2	-3.45	1.32	1.35
1	44-A	62	CRQ	CB2-CA2	-3.39	1.32	1.35
1	3-A	62	CRQ	CA3-N3	-3.39	1.40	1.47
1	49-A	62	CRQ	CA2-C2	-3.38	1.44	1.48
1	43-A	62	CRQ	CA3-N3	-3.37	1.40	1.47
1	57-A	62	CRQ	CB2-CA2	-3.33	1.32	1.35
1	21-A	62	CRQ	CA3-N3	-3.32	1.40	1.47
1	18-A	62	CRQ	CA3-N3	-3.26	1.40	1.47
1	54-A	62	CRQ	CA3-N3	-3.23	1.40	1.47
1	45-A	62	CRQ	CA2-C2	-3.17	1.45	1.48
1	37-A	62	CRQ	CA3-N3	-3.16	1.40	1.47
1	40-A	62	CRQ	CA2-C2	-3.15	1.45	1.48
1	42-A	62	CRQ	CA2-C2	-3.09	1.45	1.48
1	15-A	62	CRQ	CA3-N3	-3.04	1.40	1.47
1	2-A	62	CRQ	CA3-N3	-3.03	1.40	1.47
1	4-A	62	CRQ	CA3-N3	-3.01	1.40	1.47
1	14-A	62	CRQ	CA3-N3	-3.00	1.40	1.47
1	57-A	62	CRQ	CA3-N3	-2.98	1.40	1.47
1	45-A	62	CRQ	CA3-N3	-2.97	1.41	1.47
1	7-A	62	CRQ	CA3-N3	-2.97	1.41	1.47
1	10-A	62	CRQ	CA3-N3	-2.95	1.41	1.47
1	56-A	62	CRQ	CA3-N3	-2.91	1.41	1.47
1	11-A	62	CRQ	CA2-C2	-2.91	1.45	1.48
1	24-A	62	CRQ	CA3-N3	-2.90	1.41	1.47
1	53-A	62	CRQ	C1-N2	-2.86	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	59-A	62	CRQ	CA3-N3	-2.85	1.41	1.47
1	17-A	62	CRQ	CA3-N3	-2.85	1.41	1.47
1	49-A	62	CRQ	CA3-N3	-2.85	1.41	1.47
1	58-A	62	CRQ	CA3-N3	-2.81	1.41	1.47
1	12-A	62	CRQ	CA2-C2	-2.81	1.45	1.48
1	59-A	62	CRQ	C1-N2	-2.79	1.27	1.33
1	22-A	62	CRQ	CA3-N3	-2.77	1.41	1.47
1	14-A	62	CRQ	C1-N2	-2.77	1.27	1.33
1	16-A	62	CRQ	C1-N2	-2.76	1.27	1.33
1	2-A	62	CRQ	CA2-C2	-2.76	1.45	1.48
1	1-A	62	CRQ	CA3-N3	-2.72	1.41	1.47
1	23-A	62	CRQ	C1-N2	-2.71	1.27	1.33
1	11-A	62	CRQ	CA3-N3	-2.69	1.41	1.47
1	7-A	62	CRQ	CA2-C2	-2.68	1.45	1.48
1	31-A	62	CRQ	CA3-N3	-2.68	1.41	1.47
1	29-A	62	CRQ	CA3-N3	-2.67	1.41	1.47
1	48-A	62	CRQ	CA3-N3	-2.64	1.41	1.47
1	53-A	62	CRQ	CA3-N3	-2.63	1.41	1.47
1	30-A	62	CRQ	CA3-N3	-2.62	1.41	1.47
1	39-A	62	CRQ	CA2-C2	-2.59	1.45	1.48
1	25-A	62	CRQ	CA3-N3	-2.59	1.41	1.47
1	60-A	62	CRQ	CA3-N3	-2.57	1.41	1.47
1	33-A	62	CRQ	CA2-C2	-2.57	1.45	1.48
1	40-A	62	CRQ	CA3-N3	-2.56	1.41	1.47
1	28-A	62	CRQ	CA3-N3	-2.53	1.41	1.47
1	5-A	62	CRQ	CA3-N3	-2.51	1.41	1.47
1	13-A	62	CRQ	CA3-N3	-2.50	1.42	1.47
1	53-A	62	CRQ	CA2-C2	-2.47	1.45	1.48
1	39-A	62	CRQ	CA3-N3	-2.46	1.42	1.47
1	10-A	62	CRQ	CA2-C2	-2.44	1.45	1.48
1	61-A	62	CRQ	CA3-N3	-2.44	1.42	1.47
1	25-A	62	CRQ	CA2-C2	-2.43	1.45	1.48
1	51-A	62	CRQ	CA3-N3	-2.40	1.42	1.47
1	13-A	62	CRQ	CA2-C2	-2.39	1.45	1.48
1	57-A	62	CRQ	C1-N2	-2.35	1.28	1.33
1	4-A	62	CRQ	CB2-CA2	-2.34	1.33	1.35
1	34-A	62	CRQ	CA3-N3	-2.34	1.42	1.47
1	60-A	62	CRQ	CA2-C2	-2.33	1.46	1.48
1	12-A	62	CRQ	CA3-N3	-2.31	1.42	1.47
1	35-A	62	CRQ	CA3-N3	-2.30	1.42	1.47
1	10-A	62	CRQ	C1-N2	-2.29	1.28	1.33
1	32-A	62	CRQ	CA3-N3	-2.26	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	9-A	62	CRQ	CA2-C2	-2.25	1.46	1.48
1	27-A	62	CRQ	CA3-N3	-2.24	1.42	1.47
1	6-A	62	CRQ	CA3-N3	-2.22	1.42	1.47
1	36-A	62	CRQ	CA3-N3	-2.19	1.42	1.47
1	26-A	62	CRQ	CA3-N3	-2.19	1.42	1.47
1	47-A	62	CRQ	CD1-CG2	-2.19	1.35	1.39
1	8-A	62	CRQ	CA3-N3	-2.18	1.42	1.47
1	44-A	62	CRQ	CA3-N3	-2.16	1.42	1.47
1	55-A	62	CRQ	CA3-N3	-2.16	1.42	1.47
1	17-A	62	CRQ	C1-N2	-2.15	1.29	1.33
1	38-A	62	CRQ	CA3-N3	-2.15	1.42	1.47
1	18-A	62	CRQ	C1-N2	-2.15	1.29	1.33
1	42-A	62	CRQ	CA3-N3	-2.14	1.42	1.47
1	16-A	62	CRQ	CD1-CG2	-2.09	1.35	1.39
1	53-A	62	CRQ	CB2-CA2	-2.02	1.33	1.35
1	8-A	62	CRQ	CA2-N2	2.01	1.42	1.38
1	22-A	62	CRQ	O2-C2	2.01	1.27	1.23
1	39-A	62	CRQ	CA1-N	2.01	1.34	1.27
1	27-A	62	CRQ	O2-C2	2.01	1.27	1.23
1	28-A	62	CRQ	CA1-N	2.02	1.34	1.27
1	53-A	62	CRQ	O2-C2	2.02	1.27	1.23
1	3-A	62	CRQ	OH-CZ	2.02	1.41	1.37
1	45-A	62	CRQ	CA1-N	2.03	1.34	1.27
1	56-A	62	CRQ	C2-N3	2.03	1.44	1.39
1	19-A	62	CRQ	CA1-N	2.04	1.34	1.27
1	63-A	62	CRQ	CA1-N	2.05	1.34	1.27
1	16-A	62	CRQ	CE2-CZ	2.05	1.43	1.38
1	5-A	62	CRQ	C2-N3	2.06	1.44	1.39
1	7-A	62	CRQ	CA1-N	2.06	1.34	1.27
1	58-A	62	CRQ	CE1-CD1	2.07	1.42	1.38
1	9-A	62	CRQ	CA1-N	2.07	1.34	1.27
1	32-A	62	CRQ	O2-C2	2.07	1.27	1.23
1	8-A	62	CRQ	CA1-N	2.08	1.34	1.27
1	41-A	62	CRQ	CA2-N2	2.09	1.43	1.38
1	57-A	62	CRQ	O2-C2	2.09	1.27	1.23
1	32-A	62	CRQ	CA1-N	2.10	1.34	1.27
1	24-A	62	CRQ	CB2-CA2	2.11	1.37	1.35
1	2-A	62	CRQ	CA1-N	2.11	1.34	1.27
1	49-A	62	CRQ	CA1-N	2.13	1.34	1.27
1	32-A	62	CRQ	CB2-CA2	2.13	1.37	1.35
1	4-A	62	CRQ	CE1-CZ	2.14	1.43	1.38
1	37-A	62	CRQ	CA1-N	2.14	1.34	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	36-A	62	CRQ	CA1-N	2.18	1.34	1.27
1	1-A	62	CRQ	CB2-CA2	2.18	1.37	1.35
1	26-A	62	CRQ	CA1-N	2.19	1.34	1.27
1	62-A	62	CRQ	CA1-N	2.19	1.34	1.27
1	50-A	62	CRQ	CA1-N	2.20	1.34	1.27
1	27-A	62	CRQ	CA1-N	2.20	1.34	1.27
1	9-A	62	CRQ	O2-C2	2.21	1.27	1.23
1	54-A	62	CRQ	CA1-N	2.21	1.34	1.27
1	22-A	62	CRQ	CA1-N	2.21	1.34	1.27
1	44-A	62	CRQ	CE2-CZ	2.21	1.43	1.38
1	38-A	62	CRQ	CA1-N	2.22	1.34	1.27
1	5-A	62	CRQ	CA1-N	2.22	1.34	1.27
1	3-A	62	CRQ	CA2-N2	2.23	1.43	1.38
1	36-A	62	CRQ	O2-C2	2.24	1.27	1.23
1	61-A	62	CRQ	CA1-N	2.24	1.34	1.27
1	51-A	62	CRQ	CA1-N	2.24	1.34	1.27
1	39-A	62	CRQ	CB2-CA2	2.24	1.37	1.35
1	26-A	62	CRQ	CG2-CB2	2.26	1.51	1.46
1	12-A	62	CRQ	CD2-CG2	2.26	1.43	1.39
1	23-A	62	CRQ	C2-N3	2.26	1.45	1.39
1	47-A	62	CRQ	CA1-N	2.27	1.34	1.27
1	30-A	62	CRQ	CB2-CA2	2.27	1.37	1.35
1	20-A	62	CRQ	CB2-CA2	2.28	1.37	1.35
1	48-A	62	CRQ	CA1-N	2.29	1.35	1.27
1	12-A	62	CRQ	CA2-N2	2.29	1.43	1.38
1	30-A	62	CRQ	CA1-N	2.29	1.35	1.27
1	9-A	62	CRQ	C2-N3	2.32	1.45	1.39
1	21-A	62	CRQ	CA2-N2	2.32	1.43	1.38
1	13-A	62	CRQ	O2-C2	2.35	1.28	1.23
1	55-A	62	CRQ	C2-N3	2.36	1.45	1.39
1	59-A	62	CRQ	CD3-NE1	2.36	1.40	1.32
1	57-A	62	CRQ	CD3-NE1	2.36	1.40	1.32
1	62-A	62	CRQ	O2-C2	2.36	1.28	1.23
1	20-A	62	CRQ	O2-C2	2.38	1.28	1.23
1	3-A	62	CRQ	CA1-N	2.40	1.35	1.27
1	27-A	62	CRQ	CB2-CA2	2.41	1.37	1.35
1	23-A	62	CRQ	CA1-N	2.42	1.35	1.27
1	15-A	62	CRQ	CA2-N2	2.42	1.43	1.38
1	38-A	62	CRQ	CG2-CB2	2.44	1.51	1.46
1	19-A	62	CRQ	OH-CZ	2.44	1.42	1.37
1	26-A	62	CRQ	O2-C2	2.45	1.28	1.23
1	43-A	62	CRQ	CA1-N	2.45	1.35	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	54-A	62	CRQ	O2-C2	2.45	1.28	1.23
1	21-A	62	CRQ	CG2-CB2	2.46	1.51	1.46
1	1-A	62	CRQ	CD3-NE1	2.47	1.40	1.32
1	19-A	62	CRQ	CE2-CZ	2.50	1.43	1.38
1	48-A	62	CRQ	CG2-CB2	2.51	1.51	1.46
1	18-A	62	CRQ	CD3-NE1	2.51	1.41	1.32
1	7-A	62	CRQ	CD3-NE1	2.52	1.41	1.32
1	4-A	62	CRQ	CD3-NE1	2.52	1.41	1.32
1	33-A	62	CRQ	CA1-N	2.53	1.35	1.27
1	55-A	62	CRQ	CD3-NE1	2.53	1.41	1.32
1	5-A	62	CRQ	CD3-NE1	2.53	1.41	1.32
1	61-A	62	CRQ	CD3-NE1	2.54	1.41	1.32
1	46-A	62	CRQ	CA1-N	2.55	1.35	1.27
1	10-A	62	CRQ	CD3-NE1	2.56	1.41	1.32
1	60-A	62	CRQ	CG2-CB2	2.56	1.51	1.46
1	56-A	62	CRQ	CD3-NE1	2.56	1.41	1.32
1	37-A	62	CRQ	CD3-NE1	2.57	1.41	1.32
1	16-A	62	CRQ	CD3-NE1	2.57	1.41	1.32
1	46-A	62	CRQ	CG2-CB2	2.59	1.51	1.46
1	58-A	62	CRQ	CA1-N	2.59	1.35	1.27
1	31-A	62	CRQ	CD3-NE1	2.61	1.41	1.32
1	40-A	62	CRQ	CD3-NE1	2.62	1.41	1.32
1	24-A	62	CRQ	CD3-NE1	2.65	1.41	1.32
1	43-A	62	CRQ	CA2-N2	2.66	1.44	1.38
1	49-A	62	CRQ	CD3-NE1	2.67	1.41	1.32
1	21-A	62	CRQ	CA1-N	2.67	1.36	1.27
1	2-A	62	CRQ	CD3-NE1	2.68	1.41	1.32
1	6-A	62	CRQ	CD3-NE1	2.69	1.41	1.32
1	53-A	62	CRQ	CD3-NE1	2.71	1.41	1.32
1	20-A	62	CRQ	CB1-CA1	2.73	1.60	1.50
1	52-A	62	CRQ	O2-C2	2.74	1.28	1.23
1	15-A	62	CRQ	CA1-N	2.74	1.36	1.27
1	62-A	62	CRQ	CD3-NE1	2.74	1.41	1.32
1	9-A	62	CRQ	CD3-NE1	2.76	1.41	1.32
1	2-A	62	CRQ	CB2-CA2	2.76	1.37	1.35
1	23-A	62	CRQ	CD3-NE1	2.77	1.41	1.32
1	36-A	62	CRQ	OH-CZ	2.77	1.43	1.37
1	55-A	62	CRQ	CA1-N	2.77	1.36	1.27
1	3-A	62	CRQ	CD3-NE1	2.78	1.41	1.32
1	50-A	62	CRQ	CG2-CB2	2.78	1.52	1.46
1	9-A	62	CRQ	OH-CZ	2.81	1.43	1.37
1	20-A	62	CRQ	CA2-N2	2.82	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	48-A	62	CRQ	CD3-NE1	2.83	1.42	1.32
1	50-A	62	CRQ	CD3-NE1	2.83	1.42	1.32
1	27-A	62	CRQ	CD3-NE1	2.83	1.42	1.32
1	45-A	62	CRQ	CD3-NE1	2.84	1.42	1.32
1	33-A	62	CRQ	C2-N3	2.84	1.46	1.39
1	51-A	62	CRQ	CD3-NE1	2.85	1.42	1.32
1	63-A	62	CRQ	CD3-NE1	2.85	1.42	1.32
1	32-A	62	CRQ	CD3-NE1	2.86	1.42	1.32
1	60-A	62	CRQ	CD3-NE1	2.86	1.42	1.32
1	30-A	62	CRQ	CD3-NE1	2.87	1.42	1.32
1	39-A	62	CRQ	CD3-NE1	2.87	1.42	1.32
1	11-A	62	CRQ	CD3-NE1	2.87	1.42	1.32
1	46-A	62	CRQ	CD3-NE1	2.88	1.42	1.32
1	44-A	62	CRQ	CD3-NE1	2.88	1.42	1.32
1	15-A	62	CRQ	CD3-NE1	2.88	1.42	1.32
1	25-A	62	CRQ	CD3-NE1	2.90	1.42	1.32
1	25-A	62	CRQ	CG2-CB2	2.91	1.52	1.46
1	29-A	62	CRQ	CD3-NE1	2.92	1.42	1.32
1	36-A	62	CRQ	CD3-NE1	2.93	1.42	1.32
1	21-A	62	CRQ	CD3-NE1	2.93	1.42	1.32
1	45-A	62	CRQ	CB2-CA2	2.93	1.37	1.35
1	58-A	62	CRQ	OH-CZ	2.94	1.44	1.37
1	22-A	62	CRQ	CD3-NE1	2.94	1.42	1.32
1	28-A	62	CRQ	CD3-NE1	2.94	1.42	1.32
1	34-A	62	CRQ	CD3-NE1	2.95	1.42	1.32
1	38-A	62	CRQ	OH-CZ	2.95	1.44	1.37
1	54-A	62	CRQ	CD3-NE1	2.96	1.42	1.32
1	13-A	62	CRQ	CD3-NE1	2.97	1.42	1.32
1	19-A	62	CRQ	CA2-N2	2.99	1.45	1.38
1	19-A	62	CRQ	CD3-NE1	3.00	1.42	1.32
1	47-A	62	CRQ	CD3-NE1	3.00	1.42	1.32
1	33-A	62	CRQ	CD3-NE1	3.00	1.42	1.32
1	58-A	62	CRQ	C1-N3	3.01	1.44	1.38
1	43-A	62	CRQ	CD3-NE1	3.01	1.42	1.32
1	52-A	62	CRQ	CD3-NE1	3.02	1.42	1.32
1	26-A	62	CRQ	CD3-NE1	3.02	1.42	1.32
1	14-A	62	CRQ	CD3-NE1	3.02	1.42	1.32
1	38-A	62	CRQ	CD3-NE1	3.04	1.42	1.32
1	42-A	62	CRQ	CD3-NE1	3.06	1.42	1.32
1	17-A	62	CRQ	CD3-NE1	3.07	1.42	1.32
1	8-A	62	CRQ	CD3-NE1	3.08	1.42	1.32
1	12-A	62	CRQ	CD3-NE1	3.09	1.42	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	35-A	62	CRQ	CD3-NE1	3.11	1.43	1.32
1	16-A	62	CRQ	CA2-C2	3.11	1.51	1.48
1	56-A	62	CRQ	CB2-CA2	3.18	1.38	1.35
1	58-A	62	CRQ	CD3-NE1	3.28	1.43	1.32
1	41-A	62	CRQ	CD3-NE1	3.33	1.43	1.32
1	8-A	62	CRQ	CB2-CA2	3.34	1.38	1.35
1	9-A	62	CRQ	CG2-CB2	3.44	1.53	1.46
1	39-A	62	CRQ	OH-CZ	3.44	1.45	1.37
1	15-A	62	CRQ	C1-N3	3.45	1.45	1.38
1	15-A	62	CRQ	CB2-CA2	3.46	1.38	1.35
1	36-A	62	CRQ	CG2-CB2	3.47	1.53	1.46
1	18-A	62	CRQ	CB2-CA2	3.48	1.38	1.35
1	3-A	62	CRQ	C1-N3	3.62	1.46	1.38
1	46-A	62	CRQ	C1-N3	3.63	1.46	1.38
1	20-A	62	CRQ	C2-N3	3.67	1.48	1.39
1	38-A	62	CRQ	CB2-CA2	3.68	1.38	1.35
1	25-A	62	CRQ	CB2-CA2	3.70	1.38	1.35
1	58-A	62	CRQ	CA2-N2	3.75	1.46	1.38
1	11-A	62	CRQ	CB2-CA2	3.78	1.38	1.35
1	33-A	62	CRQ	CB2-CA2	3.85	1.38	1.35
1	20-A	62	CRQ	CD3-NE1	3.91	1.45	1.32
1	18-A	62	CRQ	C1-N3	3.91	1.46	1.38
1	3-A	62	CRQ	CG2-CB2	3.92	1.54	1.46
1	62-A	62	CRQ	CB2-CA2	3.94	1.38	1.35
1	16-A	62	CRQ	C1-N3	4.11	1.47	1.38
1	45-A	62	CRQ	C1-N3	4.16	1.47	1.38
1	19-A	62	CRQ	C1-N3	4.17	1.47	1.38
1	51-A	62	CRQ	CB2-CA2	4.18	1.38	1.35
1	12-A	62	CRQ	CG2-CB2	4.23	1.55	1.46
1	57-A	62	CRQ	C1-N3	4.24	1.47	1.38
1	54-A	62	CRQ	C1-N3	4.32	1.47	1.38
1	31-A	62	CRQ	C1-N3	4.33	1.47	1.38
1	43-A	62	CRQ	C1-N3	4.34	1.47	1.38
1	13-A	62	CRQ	C1-N3	4.44	1.47	1.38
1	46-A	62	CRQ	CB2-CA2	4.47	1.39	1.35
1	56-A	62	CRQ	C1-N3	4.52	1.47	1.38
1	55-A	62	CRQ	CB2-CA2	4.53	1.39	1.35
1	36-A	62	CRQ	C1-N3	4.54	1.47	1.38
1	55-A	62	CRQ	C1-N3	4.59	1.48	1.38
1	61-A	62	CRQ	C1-N3	4.61	1.48	1.38
1	23-A	62	CRQ	C1-N3	4.63	1.48	1.38
1	52-A	62	CRQ	C1-N3	4.65	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	14-A	62	CRQ	C1-N3	4.67	1.48	1.38
1	19-A	62	CRQ	CG2-CB2	4.67	1.56	1.46
1	24-A	62	CRQ	C1-N3	4.71	1.48	1.38
1	20-A	62	CRQ	C1-N3	4.72	1.48	1.38
1	11-A	62	CRQ	C1-N3	4.72	1.48	1.38
1	10-A	62	CRQ	C1-N3	4.73	1.48	1.38
1	2-A	62	CRQ	C1-N3	4.76	1.48	1.38
1	62-A	62	CRQ	C1-N3	4.76	1.48	1.38
1	26-A	62	CRQ	C1-N3	4.80	1.48	1.38
1	1-A	62	CRQ	C1-N3	4.81	1.48	1.38
1	31-A	62	CRQ	CB2-CA2	4.82	1.39	1.35
1	41-A	62	CRQ	C1-N3	4.84	1.48	1.38
1	37-A	62	CRQ	C1-N3	4.86	1.48	1.38
1	39-A	62	CRQ	C1-N3	4.86	1.48	1.38
1	44-A	62	CRQ	C1-N3	5.00	1.48	1.38
1	33-A	62	CRQ	C1-N3	5.01	1.48	1.38
1	21-A	62	CRQ	C1-N3	5.02	1.48	1.38
1	17-A	62	CRQ	C1-N3	5.03	1.48	1.38
1	29-A	62	CRQ	C1-N3	5.03	1.48	1.38
1	12-A	62	CRQ	C1-N3	5.04	1.48	1.38
1	50-A	62	CRQ	C1-N3	5.05	1.48	1.38
1	47-A	62	CRQ	C1-N3	5.06	1.49	1.38
1	26-A	62	CRQ	CB2-CA2	5.08	1.39	1.35
1	40-A	62	CRQ	C1-N3	5.11	1.49	1.38
1	30-A	62	CRQ	C1-N3	5.14	1.49	1.38
1	60-A	62	CRQ	C1-N3	5.15	1.49	1.38
1	4-A	62	CRQ	C1-N3	5.17	1.49	1.38
1	38-A	62	CRQ	C1-N3	5.18	1.49	1.38
1	34-A	62	CRQ	C1-N3	5.20	1.49	1.38
1	27-A	62	CRQ	C1-N3	5.20	1.49	1.38
1	59-A	62	CRQ	C1-N3	5.20	1.49	1.38
1	48-A	62	CRQ	C1-N3	5.22	1.49	1.38
1	53-A	62	CRQ	C1-N3	5.23	1.49	1.38
1	28-A	62	CRQ	C1-N3	5.29	1.49	1.38
1	49-A	62	CRQ	C1-N3	5.29	1.49	1.38
1	5-A	62	CRQ	CB2-CA2	5.31	1.40	1.35
1	9-A	62	CRQ	C1-N3	5.35	1.49	1.38
1	5-A	62	CRQ	C1-N3	5.36	1.49	1.38
1	7-A	62	CRQ	C1-N3	5.36	1.49	1.38
1	51-A	62	CRQ	C1-N3	5.36	1.49	1.38
1	25-A	62	CRQ	C1-N3	5.37	1.49	1.38
1	48-A	62	CRQ	CB2-CA2	5.50	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	36-A	62	CRQ	CB2-CA2	5.56	1.40	1.35
1	52-A	62	CRQ	CB2-CA2	5.61	1.40	1.35
1	35-A	62	CRQ	C1-N3	5.63	1.50	1.38
1	32-A	62	CRQ	C1-N3	5.63	1.50	1.38
1	8-A	62	CRQ	C1-N3	5.63	1.50	1.38
1	6-A	62	CRQ	C1-N3	5.64	1.50	1.38
1	22-A	62	CRQ	C1-N3	5.68	1.50	1.38
1	42-A	62	CRQ	C1-N3	5.71	1.50	1.38
1	58-A	62	CRQ	CG2-CB2	5.71	1.58	1.46
1	50-A	62	CRQ	CB2-CA2	5.80	1.40	1.35
1	13-A	62	CRQ	CB2-CA2	5.94	1.40	1.35
1	63-A	62	CRQ	C1-N3	6.02	1.50	1.38
1	12-A	62	CRQ	CB2-CA2	6.09	1.40	1.35
1	43-A	62	CRQ	CB2-CA2	6.66	1.41	1.35
1	19-A	62	CRQ	CB2-CA2	6.88	1.41	1.35
1	9-A	62	CRQ	CB2-CA2	7.94	1.42	1.35
1	58-A	62	CRQ	CB2-CA2	10.38	1.44	1.35
1	3-A	62	CRQ	CB2-CA2	10.98	1.45	1.35

All (578) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	29-A	62	CRQ	CG2-CB2-CA2	-16.99	108.77	130.27
1	54-A	62	CRQ	CG2-CB2-CA2	-16.63	109.23	130.27
1	17-A	62	CRQ	CG2-CB2-CA2	-16.57	109.30	130.27
1	7-A	62	CRQ	CG2-CB2-CA2	-16.11	109.88	130.27
1	13-A	62	CRQ	CG2-CB2-CA2	-14.55	111.86	130.27
1	41-A	62	CRQ	CG2-CB2-CA2	-14.47	111.96	130.27
1	63-A	62	CRQ	O2-C2-CA2	-13.64	123.13	130.97
1	16-A	62	CRQ	CB2-CA2-N2	-13.01	105.65	128.71
1	10-A	62	CRQ	CG2-CB2-CA2	-12.74	114.15	130.27
1	37-A	62	CRQ	CG2-CB2-CA2	-12.52	114.43	130.27
1	29-A	62	CRQ	O2-C2-CA2	-12.49	123.79	130.97
1	16-A	62	CRQ	CA2-C2-N3	-12.29	97.28	103.37
1	44-A	62	CRQ	O2-C2-CA2	-12.22	123.95	130.97
1	43-A	62	CRQ	O2-C2-CA2	-12.20	123.96	130.97
1	20-A	62	CRQ	N3-C1-N2	-12.06	100.24	113.16
1	59-A	62	CRQ	CG2-CB2-CA2	-12.05	115.03	130.27
1	42-A	62	CRQ	CG2-CB2-CA2	-11.81	115.33	130.27
1	51-A	62	CRQ	O2-C2-CA2	-11.66	124.27	130.97
1	43-A	62	CRQ	CB2-CA2-C2	-11.49	106.08	122.24
1	31-A	62	CRQ	O2-C2-CA2	-11.47	124.38	130.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	57-A	62	CRQ	CG2-CB2-CA2	-11.43	115.80	130.27
1	33-A	62	CRQ	O2-C2-CA2	-11.38	124.43	130.97
1	6-A	62	CRQ	CG2-CB2-CA2	-11.13	116.18	130.27
1	55-A	62	CRQ	CG2-CB2-CA2	-11.05	116.28	130.27
1	53-A	62	CRQ	CG2-CB2-CA2	-10.13	117.45	130.27
1	58-A	62	CRQ	N3-C1-N2	-9.90	102.55	113.16
1	51-A	62	CRQ	CB2-CA2-C2	-9.88	108.34	122.24
1	58-A	62	CRQ	CG2-CB2-CA2	-9.62	118.10	130.27
1	53-A	62	CRQ	CB2-CA2-N2	-9.53	111.82	128.71
1	18-A	62	CRQ	CG2-CB2-CA2	-9.32	118.47	130.27
1	14-A	62	CRQ	CB2-CA2-N2	-8.99	112.77	128.71
1	15-A	62	CRQ	N3-C1-N2	-8.88	103.65	113.16
1	20-A	62	CRQ	CA2-C2-N3	-8.77	99.03	103.37
1	35-A	62	CRQ	CG2-CB2-CA2	-8.62	119.36	130.27
1	47-A	62	CRQ	CG2-CB2-CA2	-8.52	119.49	130.27
1	56-A	62	CRQ	CG2-CB2-CA2	-8.34	119.72	130.27
1	49-A	62	CRQ	CG2-CB2-CA2	-7.95	120.21	130.27
1	44-A	62	CRQ	CE2-CD2-CG2	-7.93	111.51	121.29
1	55-A	62	CRQ	N3-C1-N2	-7.93	104.67	113.16
1	30-A	62	CRQ	O2-C2-CA2	-7.80	126.48	130.97
1	47-A	62	CRQ	O2-C2-CA2	-7.75	126.52	130.97
1	16-A	62	CRQ	CG2-CB2-CA2	-7.69	120.54	130.27
1	32-A	62	CRQ	CG2-CB2-CA2	-7.50	120.78	130.27
1	23-A	62	CRQ	CG2-CB2-CA2	-7.44	120.85	130.27
1	58-A	62	CRQ	C2-CA2-N2	-7.43	103.37	109.03
1	20-A	62	CRQ	CB1-CA1-N	-7.05	110.88	124.73
1	4-A	62	CRQ	O2-C2-CA2	-7.02	126.93	130.97
1	23-A	62	CRQ	N3-C1-N2	-6.99	105.67	113.16
1	47-A	62	CRQ	CA2-C2-N3	-6.95	99.93	103.37
1	41-A	62	CRQ	N3-C1-N2	-6.94	105.72	113.16
1	24-A	62	CRQ	CB2-CA2-N2	-6.86	116.56	128.71
1	42-A	62	CRQ	CB2-CA2-N2	-6.83	116.61	128.71
1	19-A	62	CRQ	O2-C2-CA2	-6.82	127.05	130.97
1	19-A	62	CRQ	N3-C1-N2	-6.78	105.90	113.16
1	3-A	62	CRQ	N3-C1-N2	-6.76	105.92	113.16
1	56-A	62	CRQ	CB2-CA2-N2	-6.67	116.90	128.71
1	55-A	62	CRQ	O2-C2-CA2	-6.59	127.18	130.97
1	5-A	62	CRQ	N3-C1-N2	-6.59	106.10	113.16
1	18-A	62	CRQ	CB2-CA2-N2	-6.58	117.05	128.71
1	23-A	62	CRQ	CB2-CA2-N2	-6.32	117.52	128.71
1	31-A	62	CRQ	CB2-CA2-C2	-6.31	113.36	122.24
1	1-A	62	CRQ	O2-C2-CA2	-6.23	127.39	130.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	12-A	62	CRQ	N3-C1-N2	-6.19	106.53	113.16
1	12-A	62	CRQ	CB1-CA1-N	-6.18	112.59	124.73
1	29-A	62	CRQ	CE2-CD2-CG2	-6.16	113.70	121.29
1	62-A	62	CRQ	CB2-CA2-N2	-6.07	117.95	128.71
1	45-A	62	CRQ	CG2-CB2-CA2	-6.01	122.67	130.27
1	22-A	62	CRQ	CB2-CA2-N2	-5.97	118.12	128.71
1	13-A	62	CRQ	N3-C1-N2	-5.97	106.77	113.16
1	14-A	62	CRQ	CG2-CB2-CA2	-5.90	122.80	130.27
1	59-A	62	CRQ	CB2-CA2-N2	-5.90	118.26	128.71
1	9-A	62	CRQ	N3-C1-N2	-5.89	106.85	113.16
1	16-A	62	CRQ	N3-C1-N2	-5.87	106.88	113.16
1	52-A	62	CRQ	CB2-CA2-N2	-5.81	118.41	128.71
1	54-A	62	CRQ	CB2-CA2-N2	-5.79	118.44	128.71
1	23-A	62	CRQ	CA2-C2-N3	-5.75	100.52	103.37
1	44-A	62	CRQ	CD1-CG2-CB2	-5.74	101.66	121.24
1	40-A	62	CRQ	O2-C2-CA2	-5.74	127.67	130.97
1	16-A	62	CRQ	CE2-CD2-CG2	-5.73	114.22	121.29
1	37-A	62	CRQ	O2-C2-CA2	-5.69	127.70	130.97
1	23-A	62	CRQ	O2-C2-CA2	-5.61	127.74	130.97
1	58-A	62	CRQ	CE2-CZ-CE1	-5.53	112.19	119.78
1	15-A	62	CRQ	CE2-CD2-CG2	-5.47	114.55	121.29
1	22-A	62	CRQ	CG2-CB2-CA2	-5.39	123.45	130.27
1	5-A	62	CRQ	CA3-N3-C2	-5.30	113.22	124.21
1	20-A	62	CRQ	CB2-CA2-N2	-5.27	119.36	128.71
1	9-A	62	CRQ	O2-C2-CA2	-5.27	127.94	130.97
1	10-A	62	CRQ	CB2-CA2-N2	-5.23	119.44	128.71
1	2-A	62	CRQ	CG2-CB2-CA2	-5.20	123.69	130.27
1	5-A	62	CRQ	CB2-CA2-N2	-5.17	119.56	128.71
1	10-A	62	CRQ	CE2-CD2-CG2	-5.17	114.92	121.29
1	33-A	62	CRQ	CB1-CA1-N	-5.13	114.66	124.73
1	62-A	62	CRQ	CG2-CB2-CA2	-5.08	123.84	130.27
1	26-A	62	CRQ	CB2-CA2-N2	-5.07	119.72	128.71
1	23-A	62	CRQ	CB1-CA1-N	-5.05	114.81	124.73
1	9-A	62	CRQ	CB1-CA1-N	-5.02	114.87	124.73
1	17-A	62	CRQ	CB2-CA2-N2	-5.00	119.86	128.71
1	50-A	62	CRQ	O2-C2-CA2	-4.99	128.10	130.97
1	41-A	62	CRQ	CE2-CD2-CG2	-4.96	115.17	121.29
1	38-A	62	CRQ	O2-C2-CA2	-4.96	128.12	130.97
1	3-A	62	CRQ	C2-CA2-N2	-4.95	105.26	109.03
1	15-A	62	CRQ	CD1-CE1-CZ	-4.90	114.24	119.86
1	52-A	62	CRQ	CE1-CD1-CG2	-4.82	115.34	121.29
1	34-A	62	CRQ	CB2-CA2-N2	-4.81	120.18	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	59-A	62	CRQ	CE2-CD2-CG2	-4.80	115.37	121.29
1	47-A	62	CRQ	CE1-CD1-CG2	-4.70	115.50	121.29
1	7-A	62	CRQ	CB2-CA2-N2	-4.65	120.47	128.71
1	52-A	62	CRQ	N3-C1-N2	-4.64	108.19	113.16
1	58-A	62	CRQ	CB1-CA1-N	-4.63	115.64	124.73
1	19-A	62	CRQ	CE2-CZ-CE1	-4.60	113.45	119.78
1	5-A	62	CRQ	CB1-CA1-N	-4.57	115.75	124.73
1	61-A	62	CRQ	O2-C2-CA2	-4.55	128.35	130.97
1	58-A	62	CRQ	CD2-CG2-CD1	-4.54	110.82	117.62
1	32-A	62	CRQ	O2-C2-CA2	-4.54	128.36	130.97
1	2-A	62	CRQ	CB2-CA2-N2	-4.54	120.67	128.71
1	39-A	62	CRQ	CE2-CZ-CE1	-4.50	113.60	119.78
1	11-A	62	CRQ	CG2-CB2-CA2	-4.50	124.57	130.27
1	47-A	62	CRQ	CB2-CA2-C2	-4.48	115.94	122.24
1	24-A	62	CRQ	CG2-CB2-CA2	-4.45	124.64	130.27
1	46-A	62	CRQ	CB2-CA2-N2	-4.42	120.87	128.71
1	36-A	62	CRQ	CB2-CA2-N2	-4.40	120.91	128.71
1	6-A	62	CRQ	CE1-CD1-CG2	-4.38	115.89	121.29
1	55-A	62	CRQ	CB1-CA1-N	-4.32	116.24	124.73
1	4-A	62	CRQ	CE1-CD1-CG2	-4.30	115.98	121.29
1	22-A	62	CRQ	N3-C1-N2	-4.30	108.55	113.16
1	44-A	62	CRQ	CD1-CE1-CZ	-4.29	114.94	119.86
1	44-A	62	CRQ	CB2-CA2-C2	-4.27	116.24	122.24
1	57-A	62	CRQ	CA2-C2-N3	-4.26	101.26	103.37
1	28-A	62	CRQ	O2-C2-CA2	-4.24	128.53	130.97
1	3-A	62	CRQ	CB2-CA2-N2	-4.24	121.20	128.71
1	30-A	62	CRQ	CB1-CA1-N	-4.17	116.54	124.73
1	27-A	62	CRQ	CB2-CA2-N2	-4.16	121.34	128.71
1	15-A	62	CRQ	CG2-CB2-CA2	-4.14	125.03	130.27
1	47-A	62	CRQ	C-CA3-N3	-4.10	104.51	112.97
1	41-A	62	CRQ	C-CA3-N3	-4.07	104.56	112.97
1	54-A	62	CRQ	CE1-CD1-CG2	-4.03	116.32	121.29
1	19-A	62	CRQ	CD2-CG2-CD1	-4.03	111.59	117.62
1	6-A	62	CRQ	O2-C2-CA2	-4.02	128.66	130.97
1	59-A	62	CRQ	C-CA3-N3	-4.00	104.71	112.97
1	31-A	62	CRQ	N3-C1-N2	-3.99	108.89	113.16
1	15-A	62	CRQ	CB1-CA1-N	-3.98	116.91	124.73
1	32-A	62	CRQ	N3-C1-N2	-3.98	108.90	113.16
1	16-A	62	CRQ	OE1-CD3-NE1	-3.97	111.27	122.52
1	45-A	62	CRQ	N3-C1-N2	-3.96	108.92	113.16
1	53-A	62	CRQ	CA2-C2-N3	-3.96	101.41	103.37
1	21-A	62	CRQ	CB1-CA1-N	-3.96	116.96	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	53-A	62	CRQ	CB1-CA1-N	-3.93	117.01	124.73
1	35-A	62	CRQ	N3-C1-N2	-3.93	108.96	113.16
1	3-A	62	CRQ	CB1-CA1-N	-3.84	117.19	124.73
1	46-A	62	CRQ	N3-C1-N2	-3.78	109.11	113.16
1	57-A	62	CRQ	CE2-CD2-CG2	-3.78	116.63	121.29
1	16-A	62	CRQ	CD1-CG2-CB2	-3.74	108.49	121.24
1	38-A	62	CRQ	CB1-CA1-N	-3.74	117.39	124.73
1	57-A	62	CRQ	CD1-CE1-CZ	-3.72	115.60	119.86
1	47-A	62	CRQ	N3-C1-N2	-3.69	109.21	113.16
1	14-A	62	CRQ	CA2-C2-N3	-3.66	101.56	103.37
1	48-A	62	CRQ	N3-C1-N2	-3.65	109.25	113.16
1	49-A	62	CRQ	N3-C1-N2	-3.65	109.25	113.16
1	14-A	62	CRQ	N3-C1-N2	-3.62	109.29	113.16
1	49-A	62	CRQ	C-CA3-N3	-3.61	105.52	112.97
1	55-A	62	CRQ	CE1-CD1-CG2	-3.60	116.85	121.29
1	18-A	62	CRQ	CE2-CD2-CG2	-3.60	116.85	121.29
1	11-A	62	CRQ	N3-C1-N2	-3.59	109.31	113.16
1	32-A	62	CRQ	CB2-CA2-N2	-3.57	122.38	128.71
1	63-A	62	CRQ	CG2-CB2-CA2	-3.56	125.77	130.27
1	34-A	62	CRQ	CE2-CD2-CG2	-3.55	116.91	121.29
1	1-A	62	CRQ	CB2-CA2-N2	-3.51	122.49	128.71
1	43-A	62	CRQ	N3-C1-N2	-3.51	109.40	113.16
1	23-A	62	CRQ	CE1-CD1-CG2	-3.49	116.98	121.29
1	32-A	62	CRQ	CB1-CA1-N	-3.45	117.95	124.73
1	60-A	62	CRQ	CD2-CG2-CB2	-3.44	109.51	121.24
1	20-A	62	CRQ	CE2-CD2-CG2	-3.42	117.07	121.29
1	59-A	62	CRQ	N3-C1-N2	-3.42	109.50	113.16
1	25-A	62	CRQ	N3-C1-N2	-3.40	109.52	113.16
1	15-A	62	CRQ	C2-CA2-N2	-3.38	106.46	109.03
1	54-A	62	CRQ	CE2-CD2-CG2	-3.38	117.13	121.29
1	51-A	62	CRQ	N3-C1-N2	-3.34	109.58	113.16
1	31-A	62	CRQ	CE1-CD1-CG2	-3.34	117.17	121.29
1	8-A	62	CRQ	N3-C1-N2	-3.34	109.58	113.16
1	31-A	62	CRQ	CG2-CB2-CA2	-3.33	126.06	130.27
1	62-A	62	CRQ	N3-C1-N2	-3.30	109.62	113.16
1	52-A	62	CRQ	CD2-CE2-CZ	-3.28	116.10	119.86
1	29-A	62	CRQ	CB1-CA1-N	-3.28	118.29	124.73
1	38-A	62	CRQ	CB2-CA2-N2	-3.28	122.91	128.71
1	41-A	62	CRQ	CD1-CE1-CZ	-3.28	116.10	119.86
1	53-A	62	CRQ	CE1-CD1-CG2	-3.26	117.27	121.29
1	16-A	62	CRQ	O2-C2-N3	-3.26	117.62	124.70
1	11-A	62	CRQ	CB2-CA2-N2	-3.25	122.95	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	40-A	62	CRQ	CB1-CA1-N	-3.23	118.39	124.73
1	17-A	62	CRQ	CE1-CD1-CG2	-3.23	117.31	121.29
1	63-A	62	CRQ	N3-C1-N2	-3.21	109.72	113.16
1	25-A	62	CRQ	O2-C2-CA2	-3.19	129.13	130.97
1	22-A	62	CRQ	CB1-CA1-N	-3.17	118.50	124.73
1	39-A	62	CRQ	O2-C2-CA2	-3.17	129.15	130.97
1	12-A	62	CRQ	CB2-CA2-N2	-3.17	123.09	128.71
1	6-A	62	CRQ	N3-C1-N2	-3.17	109.77	113.16
1	26-A	62	CRQ	N3-C1-N2	-3.16	109.77	113.16
1	24-A	62	CRQ	N3-C1-N2	-3.16	109.77	113.16
1	22-A	62	CRQ	CD1-CE1-CZ	-3.15	116.24	119.86
1	54-A	62	CRQ	N3-C1-N2	-3.14	109.80	113.16
1	43-A	62	CRQ	CB1-CA1-N	-3.10	118.64	124.73
1	20-A	62	CRQ	OE1-CD3-NE1	-3.10	113.72	122.52
1	47-A	62	CRQ	CD2-CE2-CZ	-3.09	116.31	119.86
1	5-A	62	CRQ	O2-C2-CA2	-3.07	129.20	130.97
1	21-A	62	CRQ	CD2-CE2-CZ	-3.07	116.34	119.86
1	42-A	62	CRQ	N3-C1-N2	-3.06	109.89	113.16
1	27-A	62	CRQ	N3-C1-N2	-3.03	109.91	113.16
1	55-A	62	CRQ	CA2-C2-N3	-2.99	101.89	103.37
1	59-A	62	CRQ	CA2-C2-N3	-2.98	101.89	103.37
1	34-A	62	CRQ	CB1-CA1-N	-2.98	118.87	124.73
1	35-A	62	CRQ	CB2-CA2-N2	-2.98	123.43	128.71
1	48-A	62	CRQ	CB1-CA1-N	-2.97	118.90	124.73
1	14-A	62	CRQ	CB1-CA1-N	-2.96	118.91	124.73
1	17-A	62	CRQ	N3-C1-N2	-2.93	110.02	113.16
1	61-A	62	CRQ	CE1-CD1-CG2	-2.93	117.67	121.29
1	8-A	62	CRQ	CB2-CA2-N2	-2.93	123.52	128.71
1	9-A	62	CRQ	CB2-CA2-N2	-2.93	123.52	128.71
1	21-A	62	CRQ	CB2-CA2-C2	-2.92	118.13	122.24
1	4-A	62	CRQ	CB1-CA1-N	-2.90	119.03	124.73
1	18-A	62	CRQ	N3-C1-N2	-2.88	110.07	113.16
1	63-A	62	CRQ	CE2-CD2-CG2	-2.86	117.76	121.29
1	60-A	62	CRQ	N3-C1-N2	-2.86	110.10	113.16
1	9-A	62	CRQ	CE2-CZ-CE1	-2.85	115.86	119.78
1	55-A	62	CRQ	CD2-CE2-CZ	-2.85	116.59	119.86
1	2-A	62	CRQ	CE2-CD2-CG2	-2.85	117.77	121.29
1	36-A	62	CRQ	N3-C1-N2	-2.85	110.11	113.16
1	52-A	62	CRQ	CB1-CA1-N	-2.83	119.17	124.73
1	10-A	62	CRQ	CB1-CA1-N	-2.82	119.18	124.73
1	7-A	62	CRQ	CB1-CA1-N	-2.82	119.19	124.73
1	33-A	62	CRQ	CE1-CD1-CG2	-2.81	117.82	121.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	56-A	62	CRQ	N3-C1-N2	-2.81	110.15	113.16
1	49-A	62	CRQ	CB1-CA1-N	-2.80	119.23	124.73
1	56-A	62	CRQ	CD2-CE2-CZ	-2.78	116.67	119.86
1	61-A	62	CRQ	CB2-CA2-C2	-2.75	118.37	122.24
1	5-A	62	CRQ	C2-CA2-N2	-2.73	106.95	109.03
1	30-A	62	CRQ	N3-C1-N2	-2.73	110.23	113.16
1	4-A	62	CRQ	CB2-CA2-N2	-2.72	123.89	128.71
1	41-A	62	CRQ	O2-C2-CA2	-2.71	129.41	130.97
1	26-A	62	CRQ	CB1-CA1-N	-2.70	119.43	124.73
1	29-A	62	CRQ	N3-C1-N2	-2.69	110.28	113.16
1	28-A	62	CRQ	N3-C1-N2	-2.69	110.28	113.16
1	19-A	62	CRQ	CB1-CA1-N	-2.68	119.47	124.73
1	34-A	62	CRQ	N3-C1-N2	-2.64	110.33	113.16
1	37-A	62	CRQ	CB2-CA2-C2	-2.63	118.54	122.24
1	3-A	62	CRQ	CE2-CZ-CE1	-2.63	116.16	119.78
1	22-A	62	CRQ	CE2-CD2-CG2	-2.62	118.06	121.29
1	21-A	62	CRQ	N3-C1-N2	-2.60	110.38	113.16
1	30-A	62	CRQ	OH-CZ-CE2	-2.58	112.75	120.04
1	42-A	62	CRQ	CB1-CA1-N	-2.58	119.66	124.73
1	44-A	62	CRQ	OH-CZ-CE1	-2.57	112.79	120.04
1	21-A	62	CRQ	O2-C2-CA2	-2.56	129.50	130.97
1	2-A	62	CRQ	N3-C1-N2	-2.55	110.42	113.16
1	54-A	62	CRQ	CD2-CG2-CB2	-2.55	112.53	121.24
1	60-A	62	CRQ	CE1-CD1-CG2	-2.54	118.16	121.29
1	57-A	62	CRQ	N3-C1-N2	-2.54	110.44	113.16
1	10-A	62	CRQ	N3-C1-N2	-2.53	110.45	113.16
1	28-A	62	CRQ	CE1-CD1-CG2	-2.49	118.22	121.29
1	2-A	62	CRQ	CB1-CA1-N	-2.49	119.84	124.73
1	54-A	62	CRQ	CB1-CA1-N	-2.48	119.86	124.73
1	41-A	62	CRQ	CA2-C2-N3	-2.48	102.14	103.37
1	40-A	62	CRQ	CG2-CB2-CA2	-2.48	127.14	130.27
1	28-A	62	CRQ	CD2-CG2-CB2	-2.46	112.85	121.24
1	27-A	62	CRQ	CE2-CZ-CE1	-2.46	116.40	119.78
1	13-A	62	CRQ	C2-CA2-N2	-2.45	107.17	109.03
1	17-A	62	CRQ	CB1-CA1-N	-2.45	119.93	124.73
1	37-A	62	CRQ	OH-CZ-CE2	-2.45	113.14	120.04
1	37-A	62	CRQ	N3-C1-N2	-2.44	110.54	113.16
1	4-A	62	CRQ	N3-C1-N2	-2.44	110.55	113.16
1	14-A	62	CRQ	CE1-CD1-CG2	-2.43	118.29	121.29
1	51-A	62	CRQ	CB1-CA1-N	-2.43	119.96	124.73
1	40-A	62	CRQ	CD2-CG2-CB2	-2.42	113.00	121.24
1	13-A	62	CRQ	CE2-CD2-CG2	-2.40	118.33	121.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	19-A	62	CRQ	C2-CA2-N2	-2.40	107.21	109.03
1	43-A	62	CRQ	CE1-CD1-CG2	-2.39	118.34	121.29
1	9-A	62	CRQ	C2-CA2-N2	-2.38	107.22	109.03
1	2-A	62	CRQ	O2-C2-CA2	-2.38	129.60	130.97
1	34-A	62	CRQ	CG2-CB2-CA2	-2.37	127.27	130.27
1	63-A	62	CRQ	CB1-CA1-N	-2.37	120.08	124.73
1	8-A	62	CRQ	CG2-CB2-CA2	-2.37	127.27	130.27
1	57-A	62	CRQ	C-CA3-N3	-2.36	108.09	112.97
1	49-A	62	CRQ	CE1-CD1-CG2	-2.35	118.39	121.29
1	17-A	62	CRQ	CE2-CD2-CG2	-2.34	118.40	121.29
1	63-A	62	CRQ	CB2-CA2-C2	-2.33	118.96	122.24
1	37-A	62	CRQ	CB1-CA1-N	-2.33	120.15	124.73
1	7-A	62	CRQ	CE2-CD2-CG2	-2.33	118.42	121.29
1	61-A	62	CRQ	CD2-CG2-CB2	-2.33	113.30	121.24
1	47-A	62	CRQ	CB1-CA1-N	-2.32	120.17	124.73
1	18-A	62	CRQ	CB1-CA1-N	-2.30	120.21	124.73
1	5-A	62	CRQ	CE1-CD1-CG2	-2.29	118.46	121.29
1	33-A	62	CRQ	N3-C1-N2	-2.29	110.71	113.16
1	61-A	62	CRQ	N3-C1-N2	-2.28	110.72	113.16
1	38-A	62	CRQ	CE2-CZ-CE1	-2.27	116.66	119.78
1	5-A	62	CRQ	CE2-CD2-CG2	-2.26	118.50	121.29
1	25-A	62	CRQ	CB1-CA1-N	-2.25	120.31	124.73
1	59-A	62	CRQ	CE1-CD1-CG2	-2.24	118.52	121.29
1	44-A	62	CRQ	N3-C1-N2	-2.24	110.76	113.16
1	59-A	62	CRQ	CD1-CE1-CZ	-2.22	117.32	119.86
1	20-A	62	CRQ	CD1-CE1-CZ	-2.22	117.32	119.86
1	36-A	62	CRQ	CE2-CZ-CE1	-2.21	116.74	119.78
1	35-A	62	CRQ	CB1-CA1-N	-2.20	120.41	124.73
1	63-A	62	CRQ	CE1-CD1-CG2	-2.19	118.59	121.29
1	4-A	62	CRQ	OH-CZ-CE2	-2.18	113.88	120.04
1	46-A	62	CRQ	CB1-CA1-N	-2.18	120.45	124.73
1	27-A	62	CRQ	CB1-CA1-N	-2.18	120.45	124.73
1	10-A	62	CRQ	CE1-CD1-CG2	-2.17	118.62	121.29
1	4-A	62	CRQ	CE2-CD2-CG2	-2.16	118.62	121.29
1	53-A	62	CRQ	CD2-CE2-CZ	-2.16	117.39	119.86
1	37-A	62	CRQ	CE1-CD1-CG2	-2.15	118.64	121.29
1	16-A	62	CRQ	OH-CZ-CE1	-2.14	114.01	120.04
1	39-A	62	CRQ	CB1-CA1-N	-2.13	120.54	124.73
1	42-A	62	CRQ	CE2-CD2-CG2	-2.13	118.67	121.29
1	35-A	62	CRQ	OH-CZ-CE1	-2.12	114.05	120.04
1	36-A	62	CRQ	CB1-CA1-N	-2.12	120.57	124.73
1	11-A	62	CRQ	OH-CZ-CE2	-2.12	114.06	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	14-A	62	CRQ	OE1-CD3-NE1	-2.12	116.52	122.52
1	27-A	62	CRQ	CD2-CG2-CB2	-2.11	114.03	121.24
1	7-A	62	CRQ	CE1-CD1-CG2	-2.11	118.69	121.29
1	41-A	62	CRQ	CB1-CA1-N	-2.09	120.63	124.73
1	22-A	62	CRQ	CA2-C2-N3	-2.09	102.33	103.37
1	6-A	62	CRQ	CD2-CG2-CB2	-2.08	114.15	121.24
1	33-A	62	CRQ	CD2-CE2-CZ	-2.07	117.49	119.86
1	56-A	62	CRQ	CE1-CD1-CG2	-2.05	118.76	121.29
1	18-A	62	CRQ	CD1-CG2-CB2	-2.05	114.24	121.24
1	28-A	62	CRQ	CB1-CA1-N	-2.05	120.70	124.73
1	43-A	62	CRQ	CD2-CE2-CZ	-2.05	117.51	119.86
1	7-A	62	CRQ	O2-C2-CA2	-2.03	129.80	130.97
1	33-A	62	CRQ	CD1-CE1-CZ	-2.03	117.53	119.86
1	39-A	62	CRQ	CB2-CA2-N2	-2.02	125.13	128.71
1	48-A	62	CRQ	CE2-CZ-CE1	-2.02	117.00	119.78
1	61-A	62	CRQ	CA2-C2-N3	-2.00	102.38	103.37
1	12-A	62	CRQ	CD1-CG2-CB2	-2.00	114.41	121.24
1	28-A	62	CRQ	CD2-CG2-CD1	2.03	120.66	117.62
1	54-A	62	CRQ	CA3-N3-C2	2.05	128.46	124.21
1	19-A	62	CRQ	CG1-CD3-NE1	2.05	123.47	116.54
1	61-A	62	CRQ	C-CA3-N3	2.06	117.22	112.97
1	47-A	62	CRQ	CE2-CZ-CE1	2.06	122.61	119.78
1	61-A	62	CRQ	O2-C2-N3	2.06	129.19	124.70
1	17-A	62	CRQ	C2-CA2-N2	2.07	110.61	109.03
1	28-A	62	CRQ	CG2-CB2-CA2	2.07	132.89	130.27
1	24-A	62	CRQ	C-CA3-N3	2.07	117.25	112.97
1	55-A	62	CRQ	CD1-CE1-CZ	2.08	122.25	119.86
1	49-A	62	CRQ	CD2-CG2-CD1	2.09	120.75	117.62
1	18-A	62	CRQ	CA3-N3-C2	2.10	128.55	124.21
1	19-A	62	CRQ	CE2-CD2-CG2	2.11	123.89	121.29
1	25-A	62	CRQ	CE2-CD2-CG2	2.11	123.89	121.29
1	53-A	62	CRQ	C-CA3-N3	2.13	117.36	112.97
1	27-A	62	CRQ	O2-C2-CA2	2.13	132.19	130.97
1	52-A	62	CRQ	CD1-CE1-CZ	2.15	122.33	119.86
1	22-A	62	CRQ	CD2-CG2-CD1	2.15	120.84	117.62
1	25-A	62	CRQ	CD1-CG2-CB2	2.15	128.58	121.24
1	9-A	62	CRQ	CE1-CD1-CG2	2.15	123.94	121.29
1	41-A	62	CRQ	C2-CA2-N2	2.16	110.68	109.03
1	9-A	62	CRQ	OH-CZ-CE2	2.17	126.18	120.04
1	6-A	62	CRQ	OH-CZ-CE1	2.20	126.25	120.04
1	57-A	62	CRQ	O2-C2-CA2	2.21	132.23	130.97
1	14-A	62	CRQ	CD2-CG2-CD1	2.21	120.94	117.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	63-A	62	CRQ	C2-CA2-N2	2.22	110.72	109.03
1	30-A	62	CRQ	CD2-CG2-CD1	2.23	120.96	117.62
1	55-A	62	CRQ	CE2-CD2-CG2	2.23	124.04	121.29
1	6-A	62	CRQ	CE2-CD2-CG2	2.24	124.05	121.29
1	1-A	62	CRQ	CA2-C2-N3	2.26	104.48	103.37
1	28-A	62	CRQ	C-CA3-N3	2.26	117.64	112.97
1	27-A	62	CRQ	CD1-CG2-CB2	2.27	128.96	121.24
1	30-A	62	CRQ	OH-CZ-CE1	2.27	126.45	120.04
1	51-A	62	CRQ	CD2-CG2-CD1	2.27	121.03	117.62
1	54-A	62	CRQ	C2-CA2-N2	2.29	110.78	109.03
1	62-A	62	CRQ	CD2-CE2-CZ	2.30	122.50	119.86
1	12-A	62	CRQ	CD2-CG2-CB2	2.30	129.08	121.24
1	21-A	62	CRQ	CB2-CA2-N2	2.31	132.80	128.71
1	26-A	62	CRQ	CA3-N3-C2	2.31	128.99	124.21
1	3-A	62	CRQ	CE1-CD1-CG2	2.31	124.14	121.29
1	12-A	62	CRQ	CA2-C2-N3	2.31	104.51	103.37
1	45-A	62	CRQ	CD2-CE2-CZ	2.32	122.52	119.86
1	43-A	62	CRQ	CD2-CG2-CD1	2.33	121.12	117.62
1	48-A	62	CRQ	CB2-CA2-C2	2.33	125.53	122.24
1	33-A	62	CRQ	C-CA3-N3	2.34	117.81	112.97
1	54-A	62	CRQ	CE2-CZ-CE1	2.35	123.01	119.78
1	51-A	62	CRQ	CG2-CB2-CA2	2.36	133.26	130.27
1	39-A	62	CRQ	CG2-CB2-CA2	2.37	133.26	130.27
1	54-A	62	CRQ	O2-C2-CA2	2.37	132.33	130.97
1	10-A	62	CRQ	C-CA3-N3	2.38	117.88	112.97
1	43-A	62	CRQ	O2-C2-N3	2.39	129.89	124.70
1	49-A	62	CRQ	CA2-C2-N3	2.39	104.55	103.37
1	3-A	62	CRQ	CA2-C2-N3	2.39	104.55	103.37
1	62-A	62	CRQ	O2-C2-CA2	2.40	132.34	130.97
1	11-A	62	CRQ	OH-CZ-CE1	2.40	126.83	120.04
1	2-A	62	CRQ	C-CA3-N3	2.42	117.98	112.97
1	14-A	62	CRQ	O2-C2-CA2	2.43	132.36	130.97
1	9-A	62	CRQ	CD2-CE2-CZ	2.43	122.66	119.86
1	36-A	62	CRQ	CA2-C2-N3	2.46	104.58	103.37
1	1-A	62	CRQ	CG2-CB2-CA2	2.46	133.38	130.27
1	50-A	62	CRQ	CA3-N3-C2	2.47	129.32	124.21
1	60-A	62	CRQ	C2-CA2-N2	2.49	110.93	109.03
1	2-A	62	CRQ	CD2-CE2-CZ	2.54	122.77	119.86
1	24-A	62	CRQ	CD2-CE2-CZ	2.56	122.81	119.86
1	6-A	62	CRQ	C2-CA2-N2	2.59	111.00	109.03
1	41-A	62	CRQ	CD2-CE2-CZ	2.59	122.84	119.86
1	58-A	62	CRQ	CD1-CE1-CZ	2.60	122.84	119.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	60-A	62	CRQ	C-CA3-N3	2.63	118.40	112.97
1	2-A	62	CRQ	CA3-N3-C2	2.63	129.66	124.21
1	22-A	62	CRQ	C2-CA2-N2	2.64	111.04	109.03
1	34-A	62	CRQ	CD2-CG2-CD1	2.64	121.58	117.62
1	37-A	62	CRQ	OH-CZ-CE1	2.64	127.50	120.04
1	51-A	62	CRQ	O2-C2-N3	2.66	130.48	124.70
1	4-A	62	CRQ	O2-C2-N3	2.66	130.49	124.70
1	19-A	62	CRQ	CD2-CG2-CB2	2.68	130.36	121.24
1	25-A	62	CRQ	C-CA3-N3	2.70	118.55	112.97
1	1-A	62	CRQ	CB2-CA2-C2	2.71	126.05	122.24
1	33-A	62	CRQ	CA3-N3-C2	2.72	129.84	124.21
1	48-A	62	CRQ	CA2-C2-N3	2.72	104.71	103.37
1	63-A	62	CRQ	O2-C2-N3	2.73	130.65	124.70
1	23-A	62	CRQ	CD2-CG2-CD1	2.74	121.72	117.62
1	20-A	62	CRQ	O2-C2-N3	2.76	130.70	124.70
1	39-A	62	CRQ	CD1-CE1-CZ	2.78	123.05	119.86
1	32-A	62	CRQ	C2-CA2-N2	2.78	111.15	109.03
1	59-A	62	CRQ	C2-CA2-N2	2.78	111.15	109.03
1	32-A	62	CRQ	CB2-CA2-C2	2.79	126.16	122.24
1	20-A	62	CRQ	CD2-CG2-CD1	2.80	121.83	117.62
1	3-A	62	CRQ	CG2-CB2-CA2	2.81	133.82	130.27
1	35-A	62	CRQ	O2-C2-CA2	2.81	132.58	130.97
1	58-A	62	CRQ	CE2-CD2-CG2	2.83	124.78	121.29
1	43-A	62	CRQ	CA3-N3-C2	2.85	130.12	124.21
1	7-A	62	CRQ	CD2-CG2-CD1	2.86	121.91	117.62
1	13-A	62	CRQ	CB2-CA2-C2	2.86	126.26	122.24
1	55-A	62	CRQ	O2-C2-N3	2.86	130.92	124.70
1	10-A	62	CRQ	C2-CA2-N2	2.87	111.22	109.03
1	44-A	62	CRQ	CE2-CZ-CE1	2.87	123.72	119.78
1	52-A	62	CRQ	CD2-CG2-CD1	2.90	121.97	117.62
1	37-A	62	CRQ	CD2-CG2-CD1	2.91	121.98	117.62
1	46-A	62	CRQ	CA3-N3-C2	2.92	130.26	124.21
1	31-A	62	CRQ	CD1-CE1-CZ	2.92	123.21	119.86
1	23-A	62	CRQ	C2-CA2-N2	2.93	111.27	109.03
1	35-A	62	CRQ	CB2-CA2-C2	2.93	126.37	122.24
1	14-A	62	CRQ	C2-CA2-N2	2.94	111.27	109.03
1	43-A	62	CRQ	C-CA3-N3	2.96	119.08	112.97
1	1-A	62	CRQ	C2-CA2-N2	3.00	111.32	109.03
1	54-A	62	CRQ	C-CA3-N3	3.00	119.17	112.97
1	58-A	62	CRQ	CE1-CD1-CG2	3.01	125.00	121.29
1	34-A	62	CRQ	C2-CA2-N2	3.04	111.35	109.03
1	19-A	62	CRQ	OH-CZ-CE2	3.05	128.65	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	42-A	62	CRQ	CD2-CG2-CD1	3.05	122.19	117.62
1	16-A	62	CRQ	C2-CA2-N2	3.07	111.37	109.03
1	39-A	62	CRQ	OH-CZ-CE2	3.07	128.71	120.04
1	19-A	62	CRQ	CD1-CE1-CZ	3.08	123.40	119.86
1	31-A	62	CRQ	C2-CA2-N2	3.09	111.39	109.03
1	61-A	62	CRQ	CD2-CG2-CD1	3.12	122.30	117.62
1	18-A	62	CRQ	C-CA3-N3	3.14	119.46	112.97
1	44-A	62	CRQ	CG2-CB2-CA2	3.14	134.24	130.27
1	60-A	62	CRQ	CD1-CG2-CB2	3.17	132.03	121.24
1	28-A	62	CRQ	C2-CA2-N2	3.17	111.45	109.03
1	19-A	62	CRQ	CA2-C2-N3	3.18	104.94	103.37
1	6-A	62	CRQ	CA2-C2-N3	3.18	104.94	103.37
1	31-A	62	CRQ	O2-C2-N3	3.19	131.63	124.70
1	18-A	62	CRQ	CD2-CG2-CD1	3.20	122.42	117.62
1	23-A	62	CRQ	O2-C2-N3	3.20	131.67	124.70
1	30-A	62	CRQ	CA2-C2-N3	3.21	104.95	103.37
1	41-A	62	CRQ	CD2-CG2-CD1	3.24	122.49	117.62
1	8-A	62	CRQ	CA2-C2-N3	3.28	104.99	103.37
1	3-A	62	CRQ	O2-C2-CA2	3.29	132.85	130.97
1	42-A	62	CRQ	C2-CA2-N2	3.31	111.56	109.03
1	7-A	62	CRQ	CB2-CA2-C2	3.31	126.90	122.24
1	62-A	62	CRQ	C-CA3-N3	3.32	119.83	112.97
1	59-A	62	CRQ	CE2-CZ-CE1	3.34	124.37	119.78
1	5-A	62	CRQ	CD2-CG2-CD1	3.39	122.70	117.62
1	3-A	62	CRQ	CD2-CE2-CZ	3.39	123.75	119.86
1	30-A	62	CRQ	CG2-CB2-CA2	3.39	134.56	130.27
1	38-A	62	CRQ	CD2-CE2-CZ	3.40	123.76	119.86
1	44-A	62	CRQ	CD2-CG2-CB2	3.47	133.08	121.24
1	36-A	62	CRQ	C-CA3-N3	3.48	120.17	112.97
1	52-A	62	CRQ	C-CA3-N3	3.51	120.22	112.97
1	29-A	62	CRQ	O2-C2-N3	3.52	132.35	124.70
1	11-A	62	CRQ	CB2-CA2-C2	3.52	127.19	122.24
1	44-A	62	CRQ	O2-C2-N3	3.56	132.44	124.70
1	26-A	62	CRQ	C-CA3-N3	3.57	120.34	112.97
1	57-A	62	CRQ	CD2-CE2-CZ	3.59	123.98	119.86
1	57-A	62	CRQ	CE1-CD1-CG2	3.65	125.79	121.29
1	8-A	62	CRQ	CB2-CA2-C2	3.68	127.41	122.24
1	31-A	62	CRQ	CB2-CA2-N2	3.68	135.24	128.71
1	39-A	62	CRQ	C2-CA2-N2	3.69	111.84	109.03
1	33-A	62	CRQ	CD2-CG2-CD1	3.73	123.21	117.62
1	63-A	62	CRQ	CD2-CG2-CD1	3.74	123.23	117.62
1	58-A	62	CRQ	CA2-C2-N3	3.76	105.23	103.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	53-A	62	CRQ	CD2-CG2-CD1	3.76	123.27	117.62
1	51-A	62	CRQ	CA2-C2-N3	3.77	105.23	103.37
1	33-A	62	CRQ	CE2-CZ-CE1	3.78	124.98	119.78
1	17-A	62	CRQ	O2-C2-CA2	3.79	133.14	130.97
1	29-A	62	CRQ	CD2-CG2-CD1	3.87	123.43	117.62
1	9-A	62	CRQ	CA2-C2-N3	3.90	105.30	103.37
1	58-A	62	CRQ	CD2-CE2-CZ	3.92	124.36	119.86
1	25-A	62	CRQ	CA2-C2-N3	3.93	105.31	103.37
1	38-A	62	CRQ	CB2-CA2-C2	3.96	127.81	122.24
1	51-A	62	CRQ	C2-CA2-N2	3.96	112.05	109.03
1	19-A	62	CRQ	CE1-CD1-CG2	3.98	126.19	121.29
1	3-A	62	CRQ	C-CA3-N3	3.99	121.22	112.97
1	29-A	62	CRQ	CD2-CE2-CZ	4.00	124.46	119.86
1	3-A	62	CRQ	CA3-N3-C2	4.05	132.60	124.21
1	47-A	62	CRQ	O2-C2-N3	4.06	133.52	124.70
1	39-A	62	CRQ	CD2-CE2-CZ	4.06	124.52	119.86
1	23-A	62	CRQ	CA3-N3-C2	4.21	132.92	124.21
1	34-A	62	CRQ	CB2-CA2-C2	4.23	128.19	122.24
1	17-A	62	CRQ	CD2-CG2-CD1	4.23	123.97	117.62
1	13-A	62	CRQ	CA2-C2-N3	4.24	105.46	103.37
1	15-A	62	CRQ	CB2-CA2-C2	4.33	128.34	122.24
1	58-A	62	CRQ	O2-C2-CA2	4.38	133.48	130.97
1	6-A	62	CRQ	CD1-CE1-CZ	4.38	124.89	119.86
1	16-A	62	CRQ	CD2-CG2-CD1	4.39	124.20	117.62
1	10-A	62	CRQ	O2-C2-CA2	4.41	133.50	130.97
1	4-A	62	CRQ	CD2-CG2-CD1	4.42	124.24	117.62
1	19-A	62	CRQ	C-CA3-N3	4.44	122.14	112.97
1	7-A	62	CRQ	C2-CA2-N2	4.44	112.42	109.03
1	27-A	62	CRQ	CD2-CE2-CZ	4.47	124.99	119.86
1	12-A	62	CRQ	CB2-CA2-C2	4.48	128.55	122.24
1	27-A	62	CRQ	CB2-CA2-C2	4.50	128.57	122.24
1	59-A	62	CRQ	O2-C2-CA2	4.58	133.60	130.97
1	15-A	62	CRQ	CE1-CD1-CG2	4.71	127.09	121.29
1	36-A	62	CRQ	CG2-CB2-CA2	4.72	136.24	130.27
1	2-A	62	CRQ	CB2-CA2-C2	4.78	128.96	122.24
1	10-A	62	CRQ	CD2-CG2-CD1	4.83	124.86	117.62
1	40-A	62	CRQ	C2-CA2-N2	4.90	112.76	109.03
1	5-A	62	CRQ	CA2-C2-N3	4.97	105.83	103.37
1	44-A	62	CRQ	CD2-CG2-CD1	4.97	125.08	117.62
1	9-A	62	CRQ	CB2-CA2-C2	4.98	129.24	122.24
1	10-A	62	CRQ	CB2-CA2-C2	4.98	129.25	122.24
1	29-A	62	CRQ	C2-CA2-N2	4.99	112.84	109.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	47-A	62	CRQ	CD2-CG2-CD1	5.03	125.17	117.62
1	11-A	62	CRQ	C-CA3-N3	5.08	123.46	112.97
1	44-A	62	CRQ	C-CA3-N3	5.08	123.46	112.97
1	17-A	62	CRQ	CB2-CA2-C2	5.08	129.38	122.24
1	31-A	62	CRQ	C-CA3-N3	5.08	123.47	112.97
1	54-A	62	CRQ	CD2-CG2-CD1	5.25	125.49	117.62
1	43-A	62	CRQ	CA2-C2-N3	5.31	105.99	103.37
1	37-A	62	CRQ	C2-CA2-N2	5.31	113.08	109.03
1	48-A	62	CRQ	C-CA3-N3	5.38	124.08	112.97
1	46-A	62	CRQ	CB2-CA2-C2	5.43	129.88	122.24
1	59-A	62	CRQ	CD2-CG2-CD1	5.48	125.84	117.62
1	38-A	62	CRQ	CA2-C2-N3	5.53	106.10	103.37
1	36-A	62	CRQ	O2-C2-CA2	5.53	134.14	130.97
1	53-A	62	CRQ	C2-CA2-N2	5.66	113.34	109.03
1	21-A	62	CRQ	CA3-N3-C2	5.67	135.95	124.21
1	15-A	62	CRQ	CD2-CE2-CZ	5.68	126.38	119.86
1	57-A	62	CRQ	C2-CA2-N2	5.75	113.41	109.03
1	63-A	62	CRQ	CA2-C2-N3	5.76	106.22	103.37
1	50-A	62	CRQ	CG2-CB2-CA2	5.85	137.67	130.27
1	61-A	62	CRQ	C2-CA2-N2	5.86	113.50	109.03
1	44-A	62	CRQ	C2-CA2-N2	5.87	113.51	109.03
1	13-A	62	CRQ	C-CA3-N3	5.88	125.11	112.97
1	59-A	62	CRQ	CB2-CA2-C2	5.94	130.59	122.24
1	51-A	62	CRQ	CB2-CA2-N2	5.97	139.30	128.71
1	54-A	62	CRQ	CB2-CA2-C2	6.06	130.77	122.24
1	22-A	62	CRQ	CB2-CA2-C2	6.07	130.77	122.24
1	36-A	62	CRQ	CB2-CA2-C2	6.14	130.88	122.24
1	26-A	62	CRQ	CB2-CA2-C2	6.18	130.93	122.24
1	52-A	62	CRQ	O2-C2-CA2	6.28	134.57	130.97
1	23-A	62	CRQ	CB2-CA2-C2	6.38	131.21	122.24
1	5-A	62	CRQ	CG2-CB2-CA2	6.46	138.44	130.27
1	12-A	62	CRQ	CG2-CB2-CA2	6.56	138.57	130.27
1	4-A	62	CRQ	C2-CA2-N2	6.57	114.04	109.03
1	21-A	62	CRQ	CA2-C2-N3	6.58	106.63	103.37
1	42-A	62	CRQ	CB2-CA2-C2	6.78	131.77	122.24
1	60-A	62	CRQ	CG2-CB2-CA2	6.78	138.85	130.27
1	20-A	62	CRQ	CB2-CA2-C2	6.84	131.86	122.24
1	33-A	62	CRQ	CA2-C2-N3	7.13	106.90	103.37
1	62-A	62	CRQ	CB2-CA2-C2	7.32	132.53	122.24
1	24-A	62	CRQ	CB2-CA2-C2	7.56	132.88	122.24
1	18-A	62	CRQ	CB2-CA2-C2	7.72	133.10	122.24
1	52-A	62	CRQ	CB2-CA2-C2	7.92	133.38	122.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5-A	62	CRQ	CB2-CA2-C2	8.00	133.49	122.24
1	3-A	62	CRQ	CB2-CA2-C2	8.02	133.52	122.24
1	56-A	62	CRQ	CB2-CA2-C2	8.03	133.53	122.24
1	43-A	62	CRQ	CB2-CA2-N2	8.47	143.72	128.71
1	47-A	62	CRQ	C2-CA2-N2	8.93	115.84	109.03
1	53-A	62	CRQ	CB2-CA2-C2	8.94	134.82	122.24
1	5-A	62	CRQ	C-CA3-N3	9.10	131.77	112.97
1	14-A	62	CRQ	CB2-CA2-C2	9.71	135.90	122.24
1	50-A	62	CRQ	CA2-C2-N3	10.51	108.57	103.37
1	43-A	62	CRQ	CG2-CB2-CA2	11.77	145.16	130.27
1	16-A	62	CRQ	CB2-CA2-C2	14.60	142.78	122.24
1	16-A	62	CRQ	O2-C2-CA2	24.53	145.05	130.97

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	39-A	62	CRQ	CG2-CB2-CA2-C2
1	62-A	62	CRQ	CG2-CB2-CA2-N2
1	26-A	62	CRQ	CG2-CB2-CA2-C2
1	26-A	62	CRQ	CG2-CB2-CA2-N2
1	62-A	62	CRQ	CG2-CB2-CA2-C2
1	16-A	62	CRQ	CG2-CB2-CA2-N2
1	24-A	62	CRQ	CG2-CB2-CA2-N2
1	42-A	62	CRQ	CG2-CB2-CA2-N2
1	4-A	62	CRQ	CG2-CB2-CA2-C2
1	16-A	62	CRQ	CG2-CB2-CA2-C2
1	24-A	62	CRQ	CG2-CB2-CA2-C2
1	42-A	62	CRQ	CG2-CB2-CA2-C2
1	21-A	62	CRQ	C-CA3-N3-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	52-A	1
1	15-A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
52	A	62:CRQ	C	65:ASN	N	1.19
15	A	62:CRQ	C	65:ASN	N	1.18

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS failed to run properly - this section will therefore be empty.