



# wwPDB X-ray Structure Validation Summary 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 wwPDB X-ray Structure Validation Summary 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

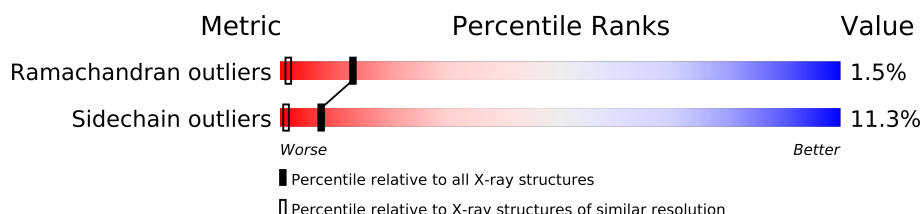
# 1 Overall quality at a glance

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	 81%12%7%
1	7-A	229	 82%11%7%
1	8-A	229	 83%9%7%
1	9-A	229	 82%11%7%

## 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 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	60-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	61-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	62-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0
1	63-A	214	Total 3416	C 1118	H 1671	N 286	O 331	S 10	0	0	0

- Molecule 2 is water.

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

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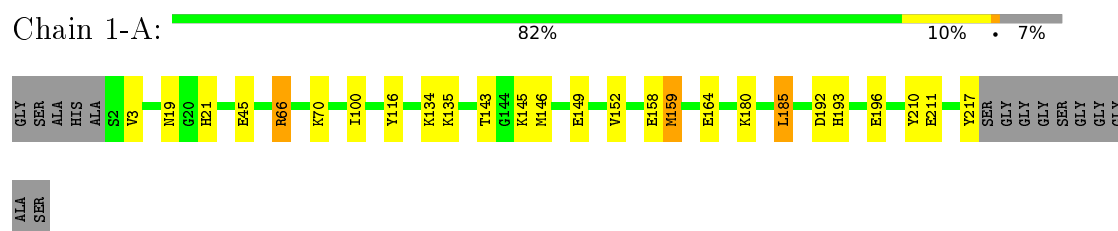
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	57-A	152	Total 152	O 152	0	0
2	58-A	150	Total 150	O 150	0	0
2	59-A	152	Total 152	O 152	0	0
2	60-A	141	Total 141	O 141	0	0
2	61-A	167	Total 167	O 167	0	0
2	62-A	155	Total 155	O 155	0	0
2	63-A	143	Total 143	O 143	0	0

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

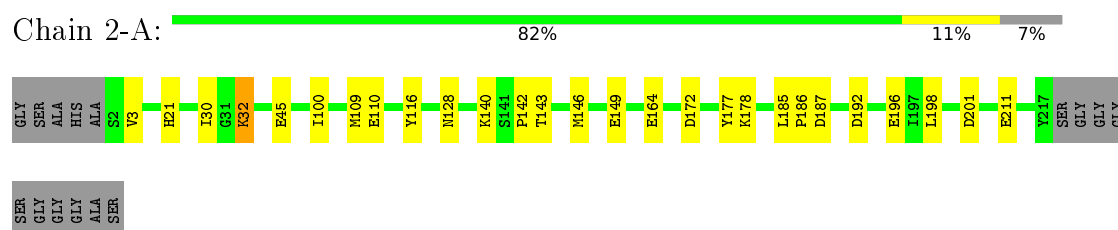
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

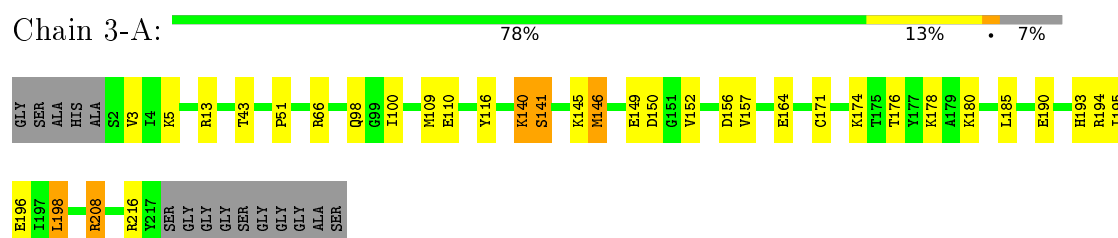
- Molecule 1: Reversibly photoswitching protein Dathail



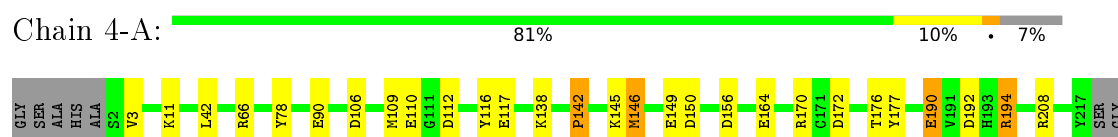
- Molecule 1: Reversibly photoswitching protein Dathail



- 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

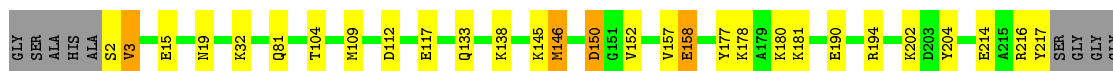
Chain 11-A:  81% 12% 7%



SER


- Molecule 1: Reversibly photoswitching protein Dathail

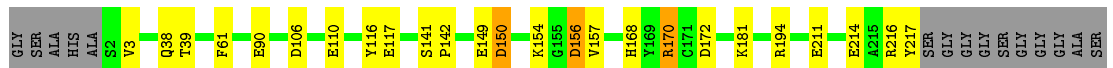
Chain 12-A:  81% 11% 7%




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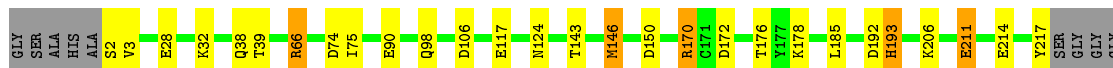
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 13-A:  83% 10% 7%




- Molecule 1: Reversibly photoswitching protein Dathail

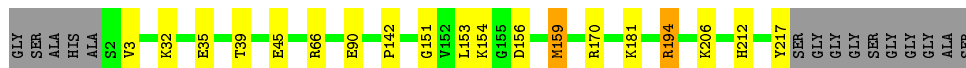
Chain 14-A:  81% 10% 7%




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- Molecule 1: Reversibly photoswitching protein Dathail

Chain 15-A:  85% 7% 7%



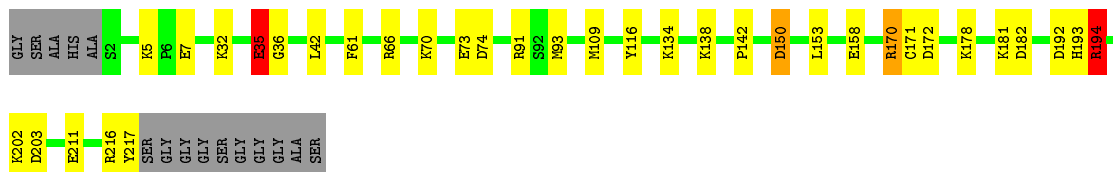
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 16-A:  83% 10% 7%



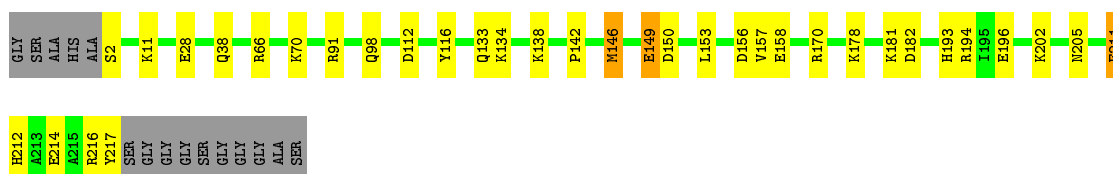
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 17-A: 78% 14% 7%



- Molecule 1: Reversibly photoswitching protein Dathail

Chain 18-A: 78% 14% 7%



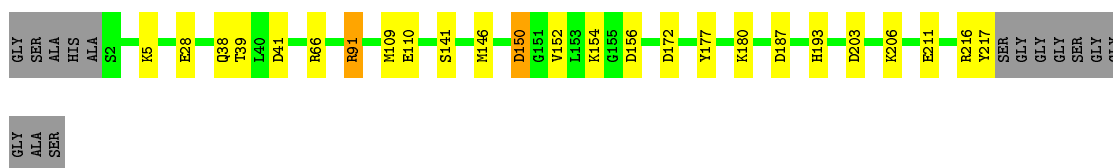
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 19-A: 83% 9% 7%



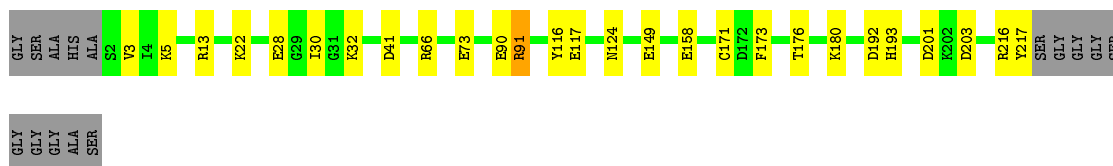
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 20-A: 83% 10% 7%



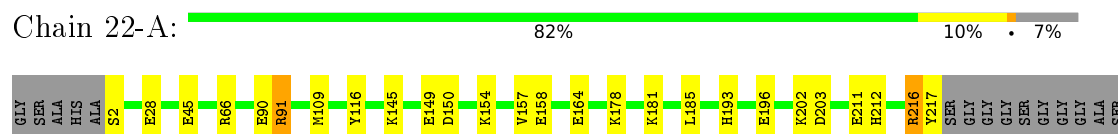
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 21-A: 82% 11% 7%

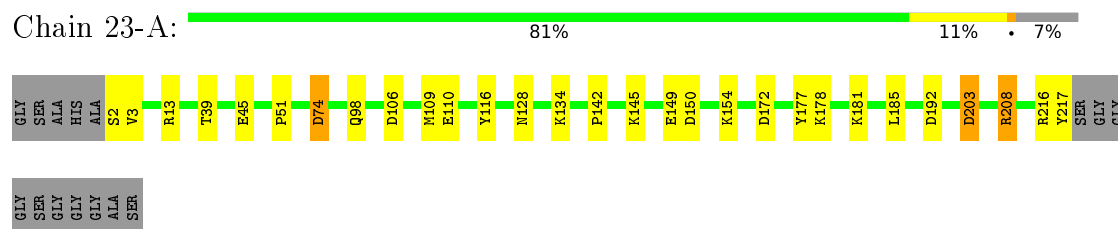


- Molecule 1: Reversibly photoswitching protein Dathail

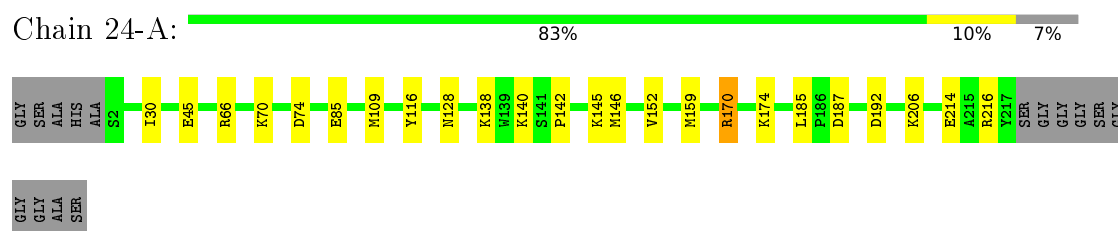




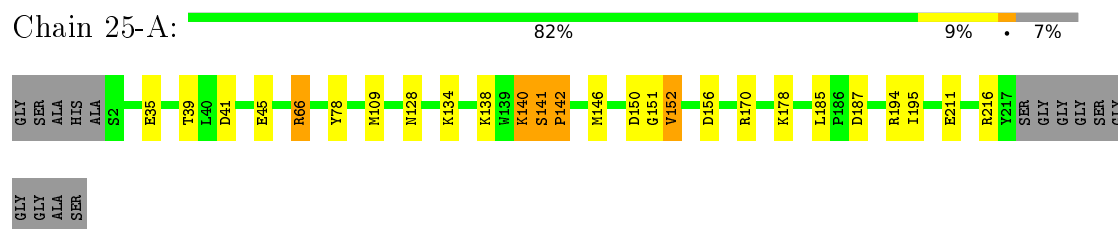
- Molecule 1: Reversibly photoswitching protein Dathail



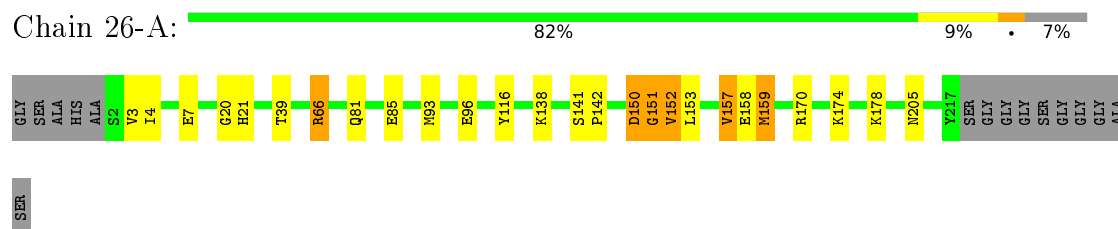
- Molecule 1: Reversibly photoswitching protein Dathail



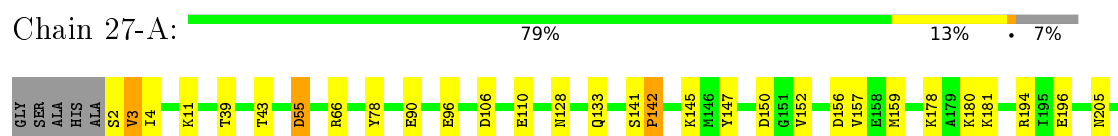
- Molecule 1: Reversibly photoswitching protein Dathail



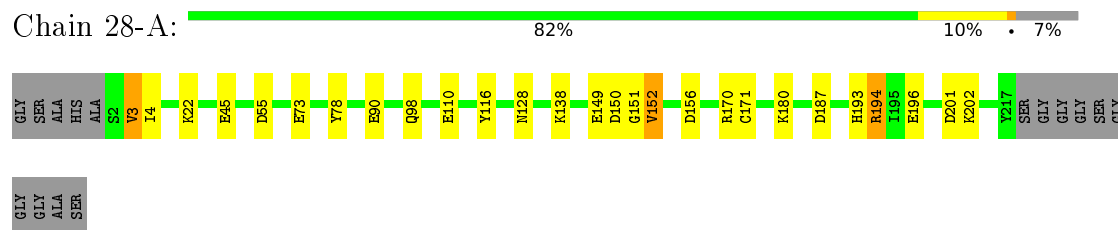
- Molecule 1: Reversibly photoswitching protein Dathail



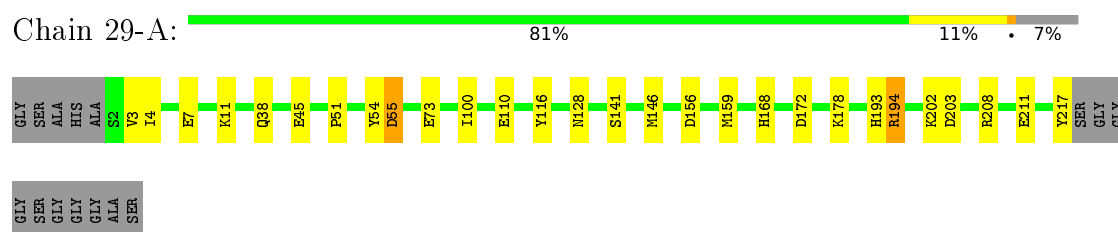
- Molecule 1: Reversibly photoswitching protein Dathail



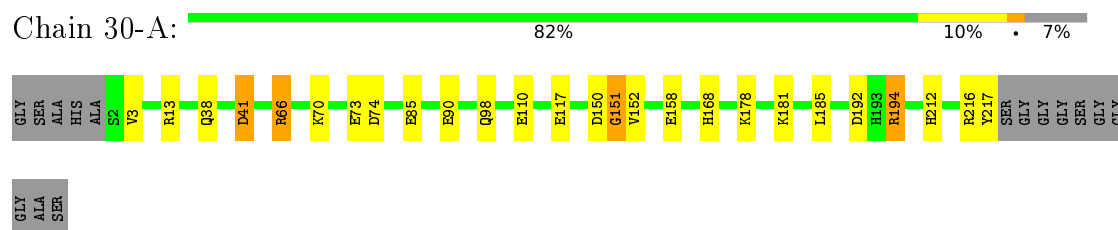
- Molecule 1: Reversibly photoswitching protein Dathail



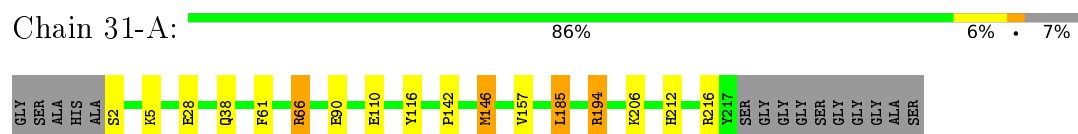
- Molecule 1: Reversibly photoswitching protein Dathail



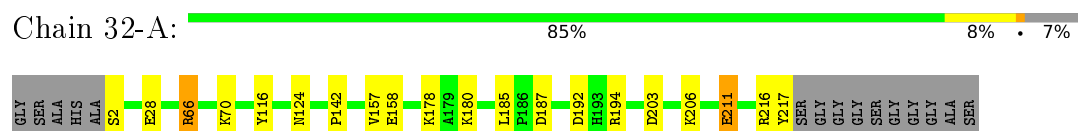
- Molecule 1: Reversibly photoswitching protein Dathail



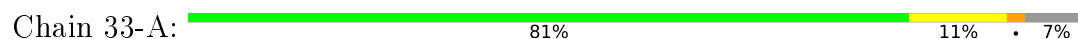
- Molecule 1: Reversibly photoswitching protein Dathail

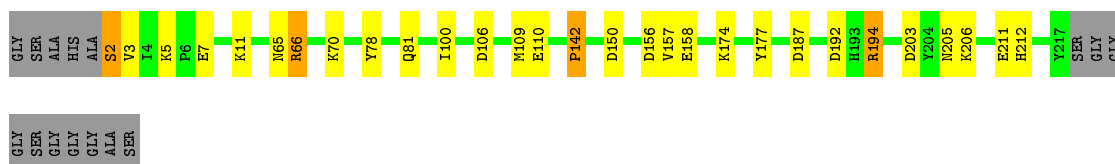


- Molecule 1: Reversibly photoswitching protein Dathail



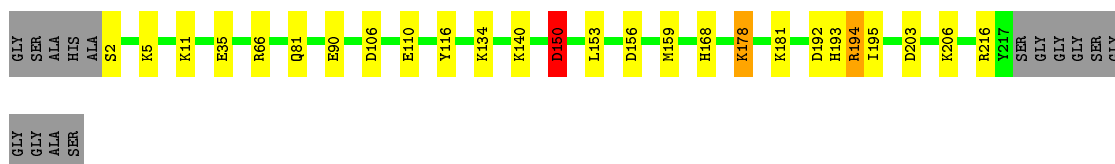
- Molecule 1: Reversibly photoswitching protein Dathail





- Molecule 1: Reversibly photoswitching protein Dathail

Chain 34-A: 82% 10% 7%



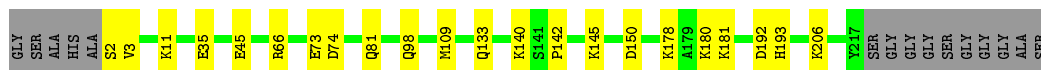
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 35-A: 85% 9% 7%



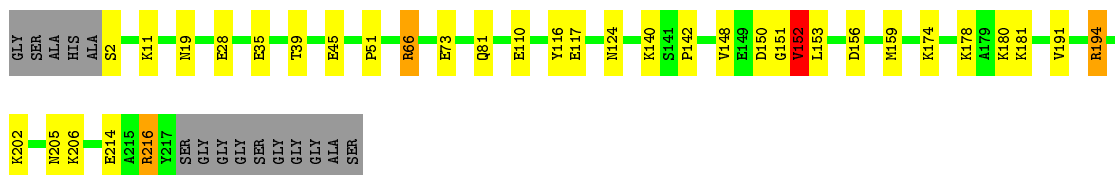
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 36-A: 84% 10% 7%



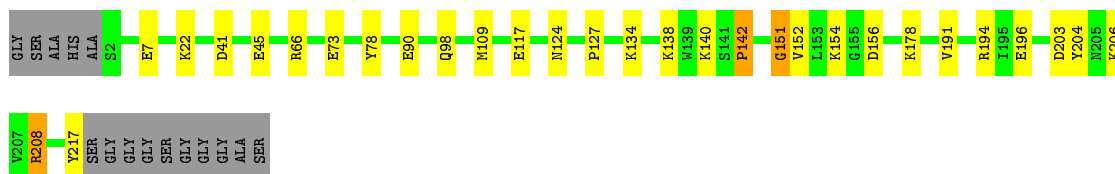
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 37-A: 78% 14% 7%

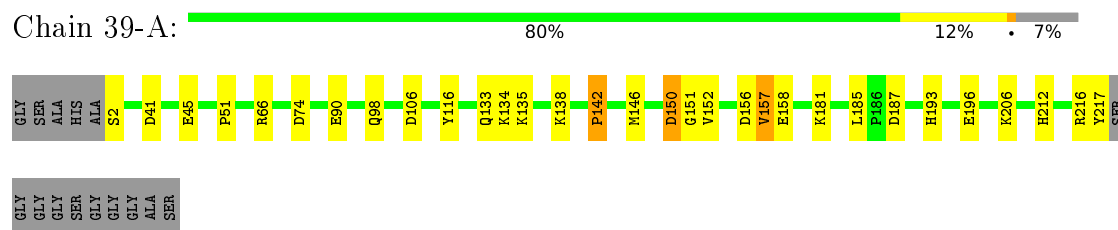


- Molecule 1: Reversibly photoswitching protein Dathail

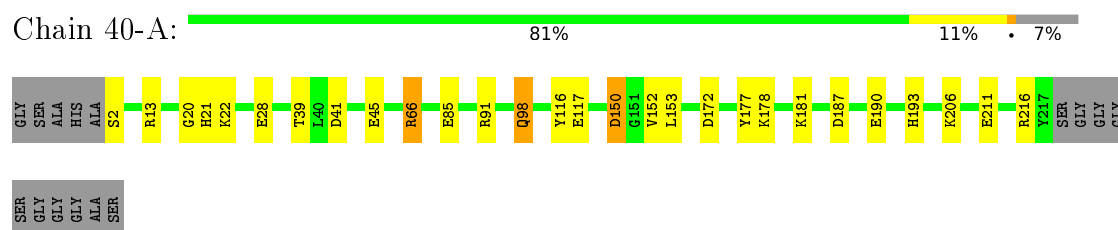
Chain 38-A: 80% 12% 7%



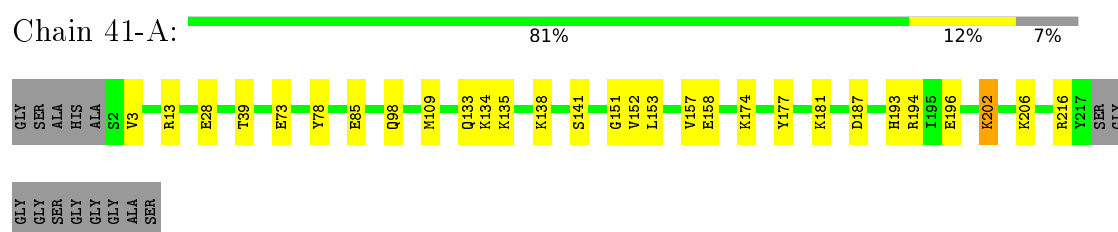
- Molecule 1: Reversibly photoswitching protein Dathail



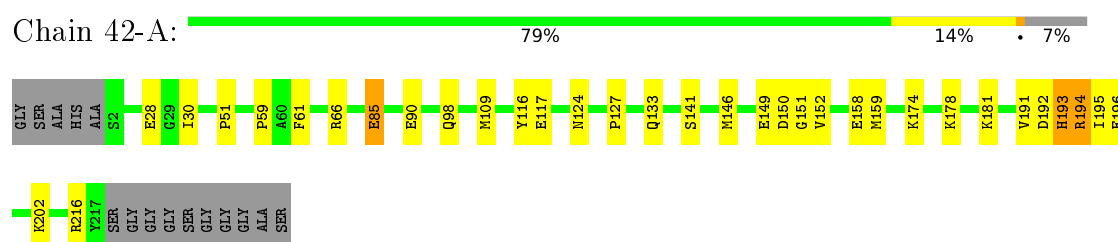
- Molecule 1: Reversibly photoswitching protein Dathail



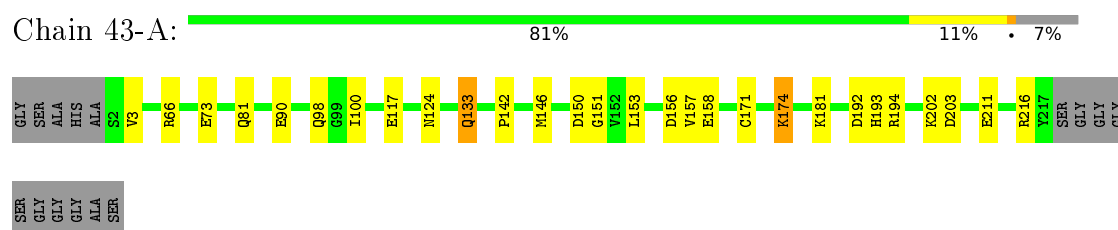
- Molecule 1: Reversibly photoswitching protein Dathail



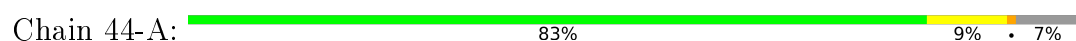
- Molecule 1: Reversibly photoswitching protein Dathail




- Molecule 1: Reversibly photoswitching protein Dathail

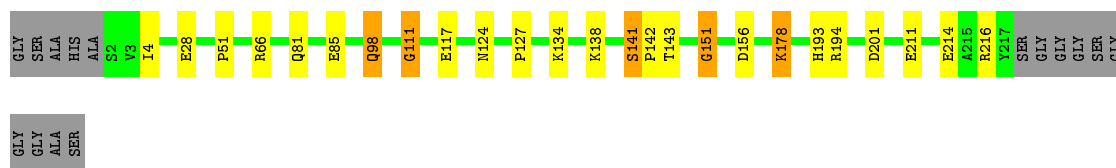


- Molecule 1: Reversibly photoswitching protein Dathail




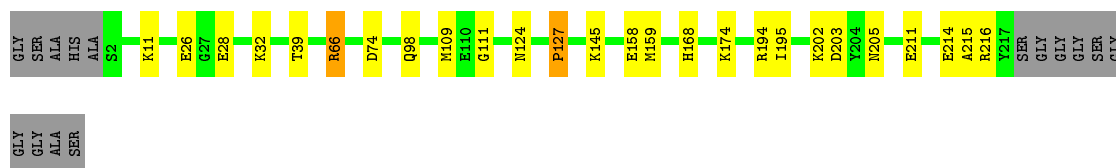


Chain 51-A:  83% 9% 7%




- Molecule 1: Reversibly photoswitching protein Dathail

Chain 52-A:  82% 10% 7%




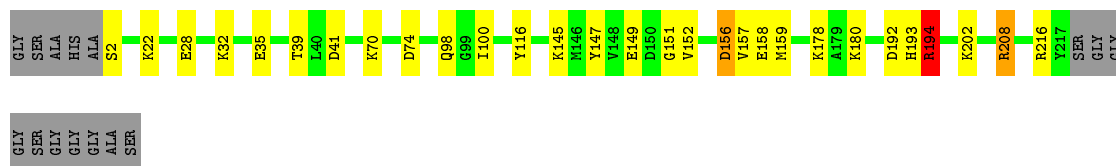
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 53-A:  83% 10% 7%




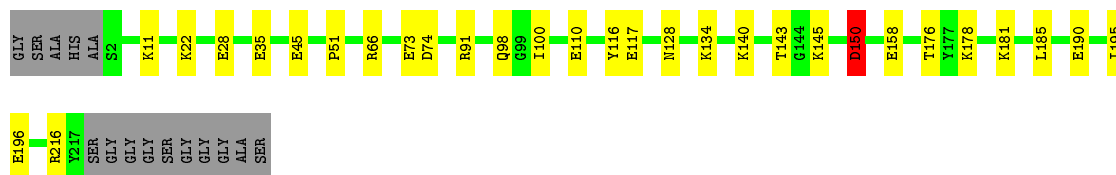
- Molecule 1: Reversibly photoswitching protein Dathail

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 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 S143 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

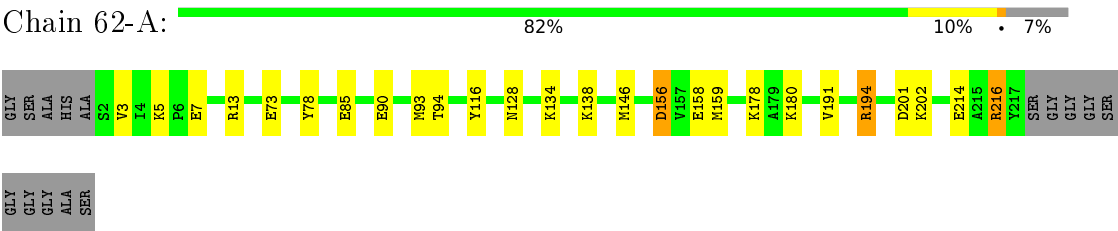
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 61-A:  80% 13% 7%

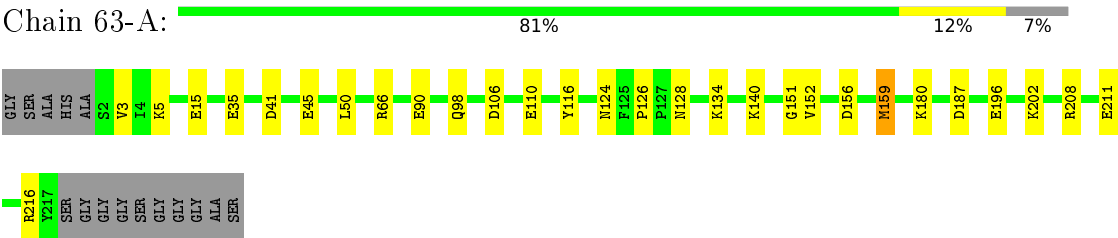
GLY SER GLY ALA ALA S2 K11 T39 P51 R66 K70 E73 E90 D97 M109 T123 K134 K138 S141 P142 T143 D150 E158 H168 F173 Y177 K178 A179 K180 V191 D192 H193 R194 I195 E196 D203 E211 R216

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

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 77 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	159	MET	Peptide
1	2-A	142	PRO	Peptide
1	2-A	186	PRO	Peptide
1	2-A	201	ASP	Peptide
1	3-A	140	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

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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

5 of 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

### 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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

5 of 1306 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	29-A	193	HIS
1	37-A	35	GLU
1	59-A	158	GLU
1	30-A	168	HIS
1	33-A	157	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 181 such sidechains are listed below:

Mol	Chain	Res	Type
1	26-A	212	HIS
1	32-A	205	ASN
1	57-A	81	GLN
1	27-A	128	ASN
1	29-A	124	ASN

### 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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 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

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

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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