



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 18, 2020 – 01:18 pm BST

PDB ID : 5EJU
Title : Ensemble refinement of the Crystal Structure of the Reversibly photoswitching chromoprotein Dathail, Ground State
Authors : Close, D.W.; Langan, P.S.; Bradbury, A.R.M.
Deposited on : 2015-11-02
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

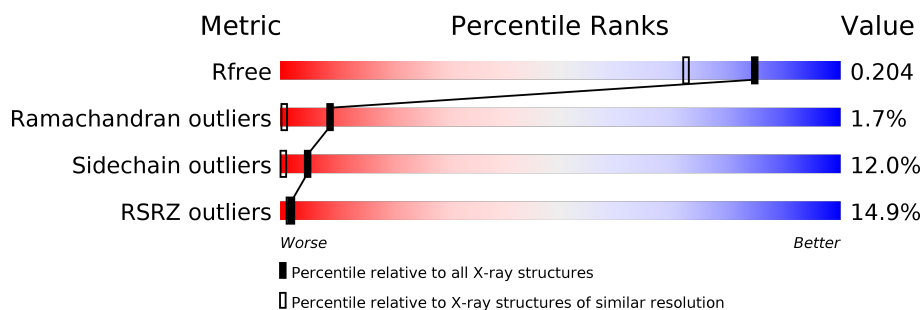
1 Overall quality at a glance ⓘ

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))
R_{free}	130704	1827 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	1-A	229	<div> <div>14%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>•</div> <div>7%</div> </div> </div>
1	10-A	229	<div> <div>14%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>7%</div> </div> </div>
1	11-A	229	<div> <div>14%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>•</div> <div>7%</div> </div> </div>
1	12-A	229	<div> <div>14%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>•</div> <div>7%</div> </div> </div>
1	13-A	229	<div> <div>14%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>•</div> <div>7%</div> </div> </div>
1	14-A	229	<div> <div>14%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>•</div> <div>7%</div> </div> </div>
1	15-A	229	<div> <div>14%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>•</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	16-A	229	
1	17-A	229	
1	18-A	229	
1	19-A	229	
1	2-A	229	
1	20-A	229	
1	21-A	229	
1	22-A	229	
1	23-A	229	
1	24-A	229	
1	25-A	229	
1	26-A	229	
1	27-A	229	
1	28-A	229	
1	29-A	229	
1	3-A	229	
1	30-A	229	
1	31-A	229	
1	32-A	229	
1	33-A	229	
1	34-A	229	
1	35-A	229	
1	36-A	229	
1	37-A	229	
1	38-A	229	

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Mol	Chain	Length	Quality of chain
1	39-A	229	
1	4-A	229	
1	40-A	229	
1	41-A	229	
1	42-A	229	
1	43-A	229	
1	44-A	229	
1	45-A	229	
1	46-A	229	
1	47-A	229	
1	5-A	229	
1	6-A	229	
1	7-A	229	
1	8-A	229	
1	9-A	229	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 167541 atoms, of which 78255 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
			3410	1118	1665	286	331	10			
1	2-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	3-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	4-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	5-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	6-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	7-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	8-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	9-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	10-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	11-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	12-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	13-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	14-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	15-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	16-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	214	Total 3410	C 1118	H 1665	N 286	O 331	S 10	0	0	0
1	18-A	214	Total 3410	C 1118	H 1665	N 286	O 331	S 10	0	0	0
1	19-A	214	Total 3410	C 1118	H 1665	N 286	O 331	S 10	0	0	0
1	20-A	214	Total 3410	C 1118	H 1665	N 286	O 331	S 10	0	0	0
1	21-A	214	Total 3410	C 1118	H 1665	N 286	O 331	S 10	0	0	0
1	22-A	214	Total 3410	C 1118	H 1665	N 286	O 331	S 10	0	0	0
1	23-A	214	Total 3410	C 1118	H 1665	N 286	O 331	S 10	0	0	0
1	24-A	214	Total 3410	C 1118	H 1665	N 286	O 331	S 10	0	0	0
1	25-A	214	Total 3410	C 1118	H 1665	N 286	O 331	S 10	0	0	0
1	26-A	214	Total 3410	C 1118	H 1665	N 286	O 331	S 10	0	0	0
1	27-A	214	Total 3410	C 1118	H 1665	N 286	O 331	S 10	0	0	0
1	28-A	214	Total 3410	C 1118	H 1665	N 286	O 331	S 10	0	0	0
1	29-A	214	Total 3410	C 1118	H 1665	N 286	O 331	S 10	0	0	0
1	30-A	214	Total 3410	C 1118	H 1665	N 286	O 331	S 10	0	0	0
1	31-A	214	Total 3410	C 1118	H 1665	N 286	O 331	S 10	0	0	0
1	32-A	214	Total 3410	C 1118	H 1665	N 286	O 331	S 10	0	0	0
1	33-A	214	Total 3410	C 1118	H 1665	N 286	O 331	S 10	0	0	0
1	34-A	214	Total 3410	C 1118	H 1665	N 286	O 331	S 10	0	0	0
1	35-A	214	Total 3410	C 1118	H 1665	N 286	O 331	S 10	0	0	0
1	36-A	214	Total 3410	C 1118	H 1665	N 286	O 331	S 10	0	0	0
1	37-A	214	Total 3410	C 1118	H 1665	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	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	39-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	40-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	41-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	42-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	43-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	44-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	45-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	46-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	47-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	165	Total	O	0	0
			165	165		
2	2-A	173	Total	O	0	0
			173	173		
2	3-A	140	Total	O	0	0
			140	140		
2	4-A	153	Total	O	0	0
			153	153		
2	5-A	167	Total	O	0	0
			167	167		
2	6-A	150	Total	O	0	0
			150	150		
2	7-A	150	Total	O	0	0
			150	150		
2	8-A	160	Total	O	0	0
			160	160		
2	9-A	160	Total	O	0	0
			160	160		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	10-A	152	Total 152	O 152	0	0
2	11-A	173	Total 173	O 173	0	0
2	12-A	160	Total 160	O 160	0	0
2	13-A	152	Total 152	O 152	0	0
2	14-A	157	Total 157	O 157	0	0
2	15-A	148	Total 148	O 148	0	0
2	16-A	152	Total 152	O 152	0	0
2	17-A	147	Total 147	O 147	0	0
2	18-A	156	Total 156	O 156	0	0
2	19-A	151	Total 151	O 151	0	0
2	20-A	147	Total 147	O 147	0	0
2	21-A	148	Total 148	O 148	0	0
2	22-A	169	Total 169	O 169	0	0
2	23-A	144	Total 144	O 144	0	0
2	24-A	138	Total 138	O 138	0	0
2	25-A	149	Total 149	O 149	0	0
2	26-A	143	Total 143	O 143	0	0
2	27-A	148	Total 148	O 148	0	0
2	28-A	165	Total 165	O 165	0	0
2	29-A	146	Total 146	O 146	0	0
2	30-A	165	Total 165	O 165	0	0

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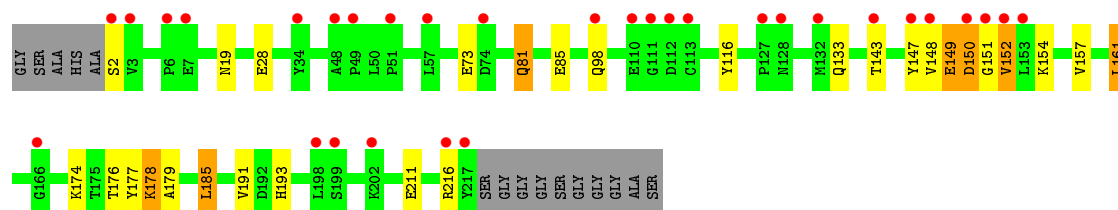
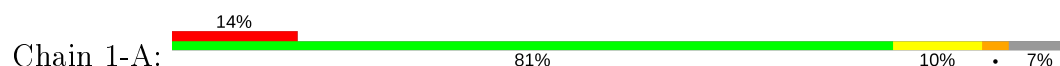
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	31-A	163	Total 163	O 163	0	0
2	32-A	163	Total 163	O 163	0	0
2	33-A	154	Total 154	O 154	0	0
2	34-A	147	Total 147	O 147	0	0
2	35-A	135	Total 135	O 135	0	0
2	36-A	160	Total 160	O 160	0	0
2	37-A	156	Total 156	O 156	0	0
2	38-A	149	Total 149	O 149	0	0
2	39-A	154	Total 154	O 154	0	0
2	40-A	164	Total 164	O 164	0	0
2	41-A	156	Total 156	O 156	0	0
2	42-A	142	Total 142	O 142	0	0
2	43-A	162	Total 162	O 162	0	0
2	44-A	159	Total 159	O 159	0	0
2	45-A	143	Total 143	O 143	0	0
2	46-A	174	Total 174	O 174	0	0
2	47-A	162	Total 162	O 162	0	0

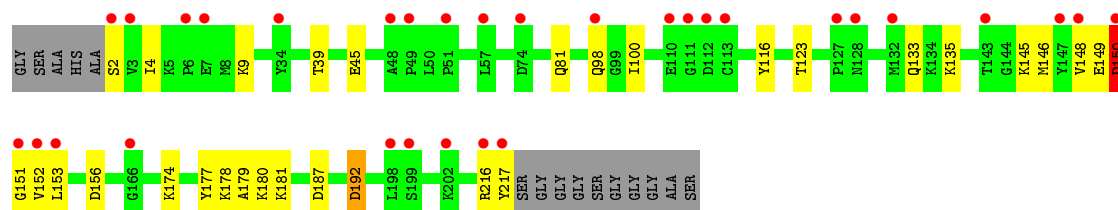
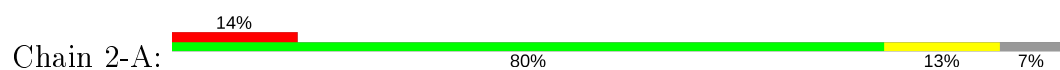
3 Residue-property plots [i](#)

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

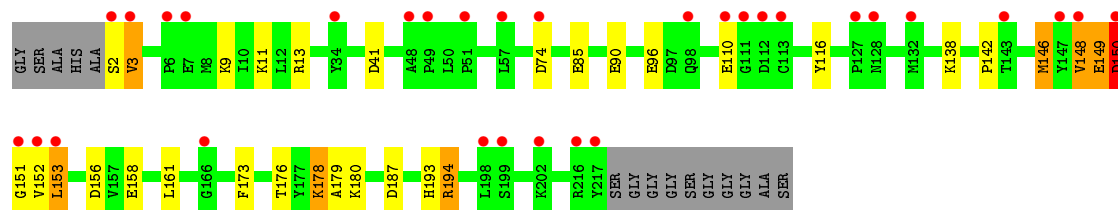
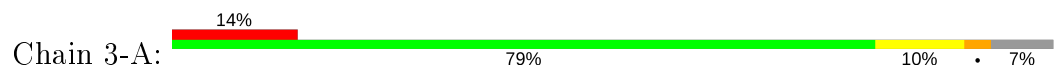
- Molecule 1: Reversibly photoswitching protein Dathail



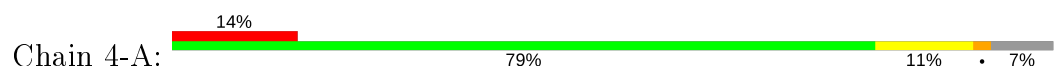
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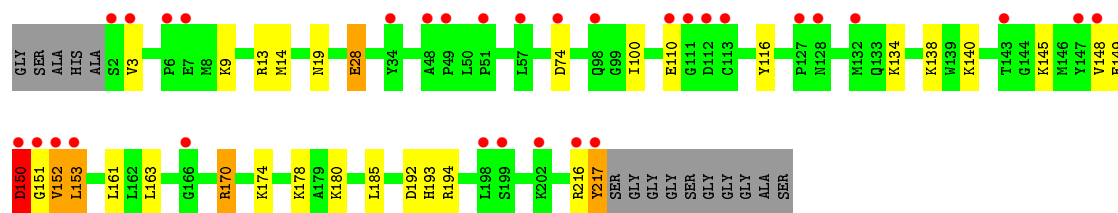


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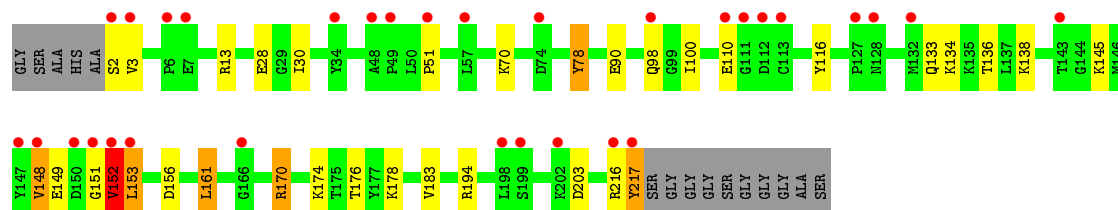
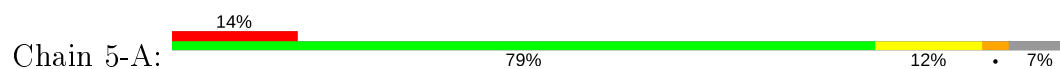


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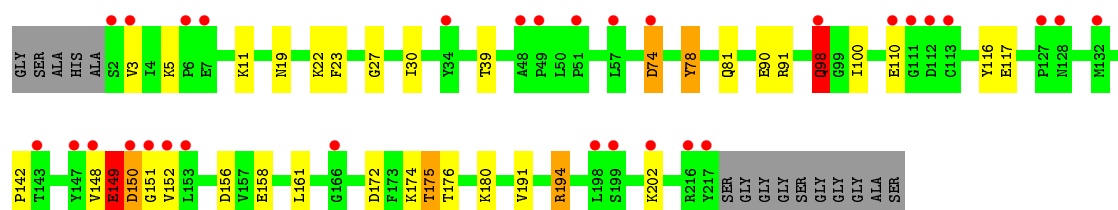
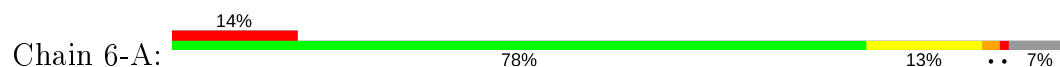




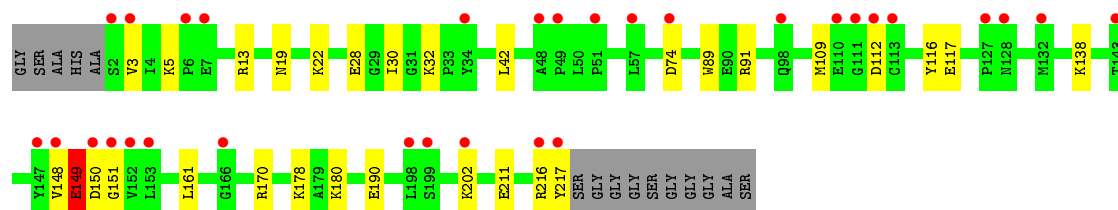
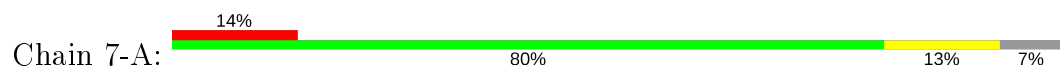
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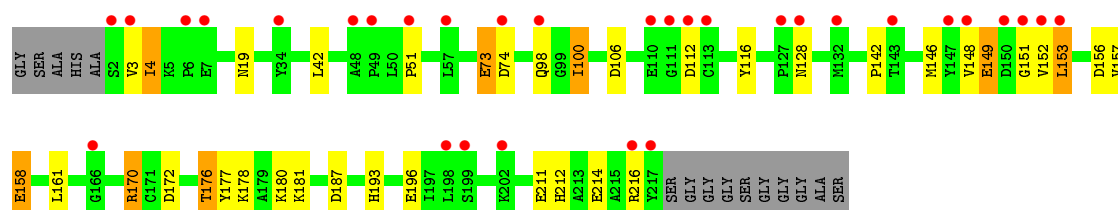
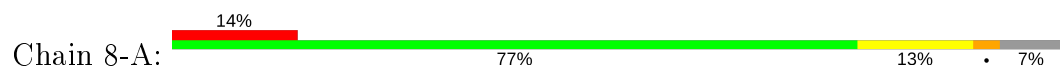
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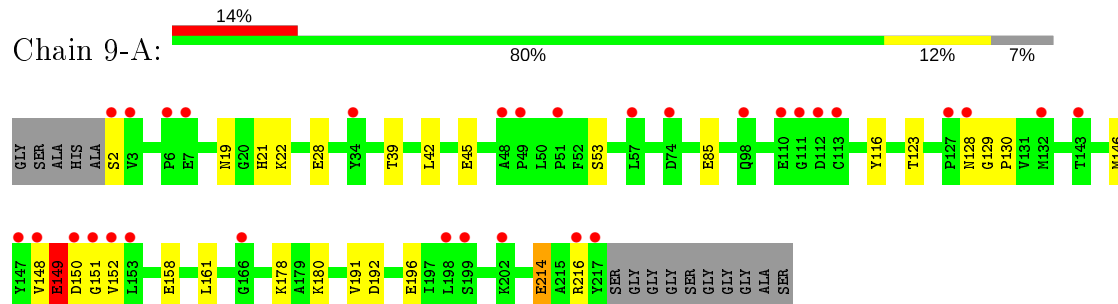
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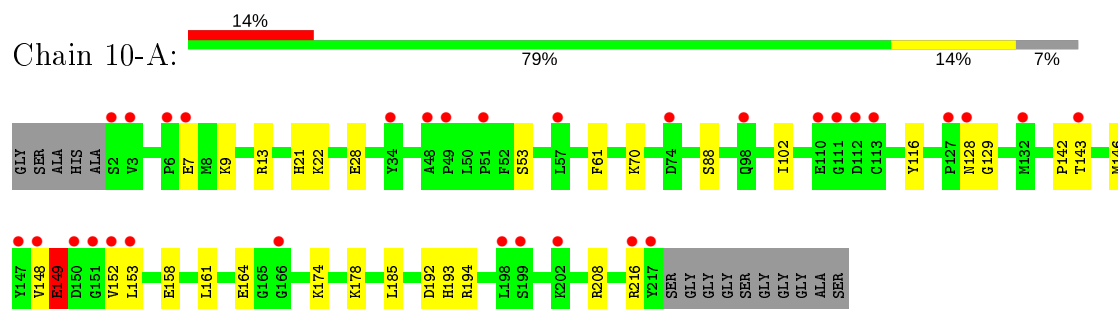
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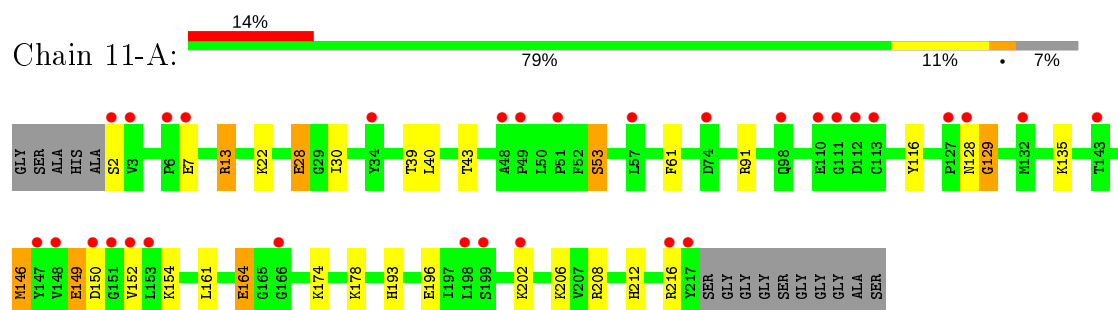
- Molecule 1: Reversibly photoswitching protein Dathail



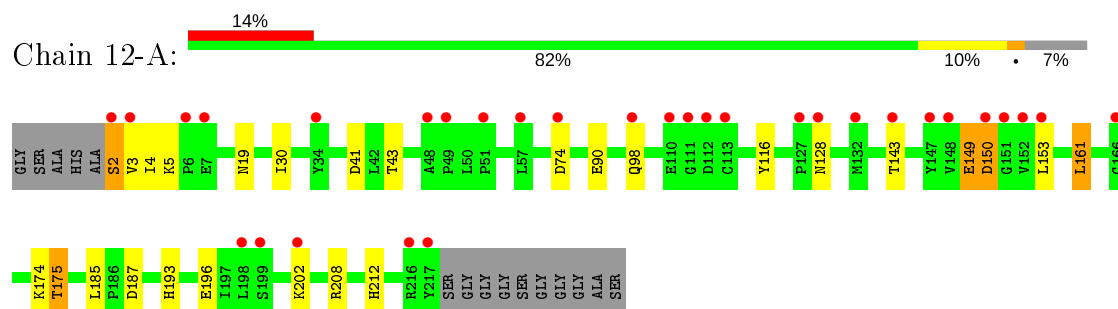
- Molecule 1: Reversibly photoswitching protein Dathail



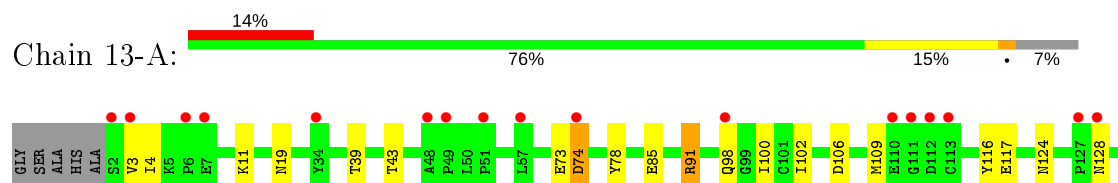
- Molecule 1: Reversibly photoswitching protein Dathail



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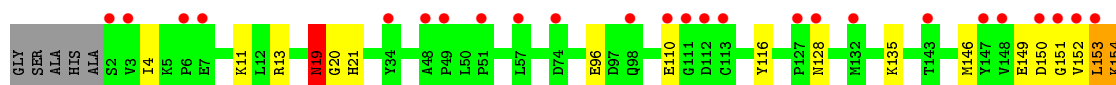
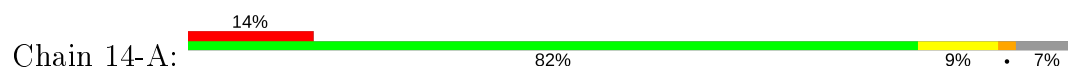


- Molecule 1: Reversibly photoswitching protein Dathail

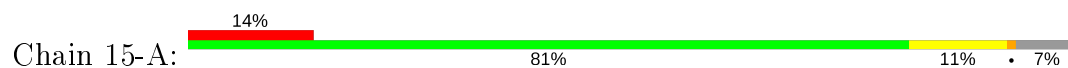




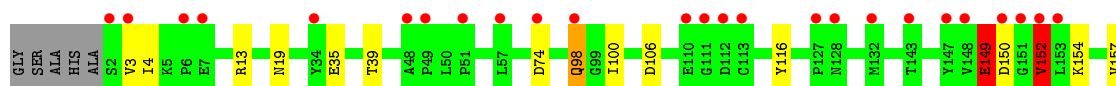
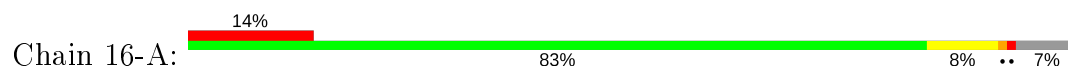
- Molecule 1: Reversibly photoswitching protein Dathail



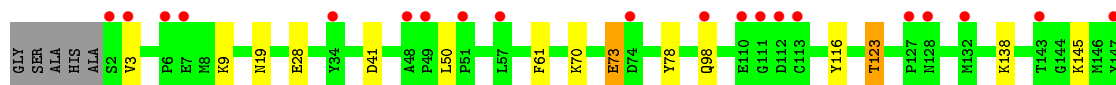
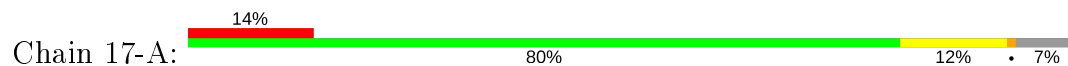
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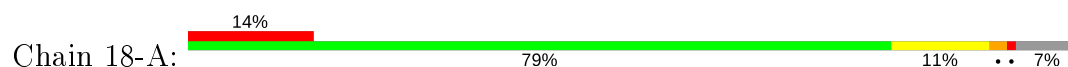
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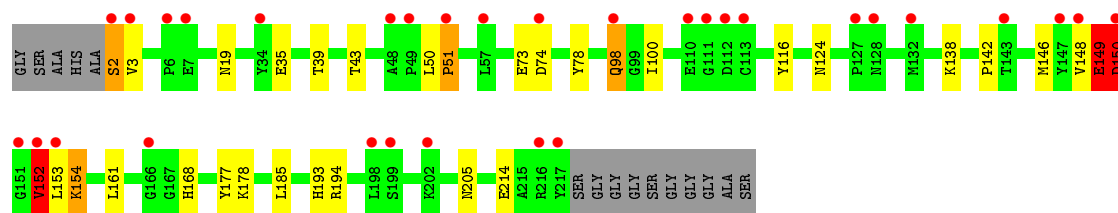


- Molecule 1: Reversibly photoswitching protein Dathail

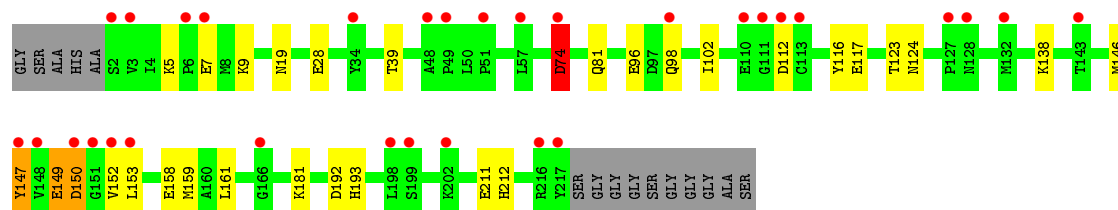
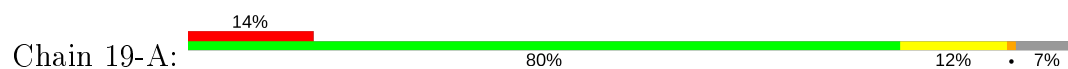


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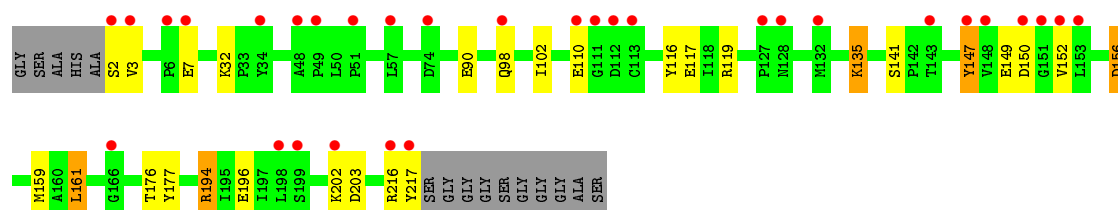
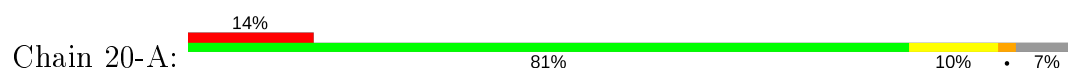




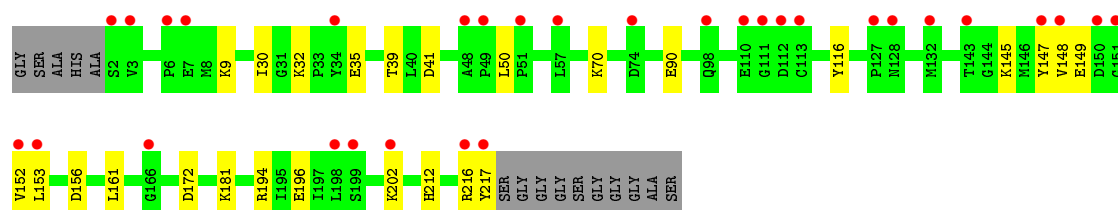
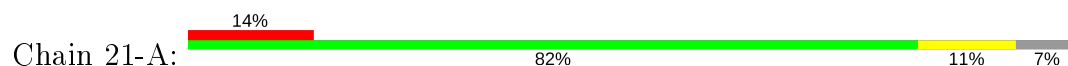
- Molecule 1: Reversibly photoswitching protein Dathail



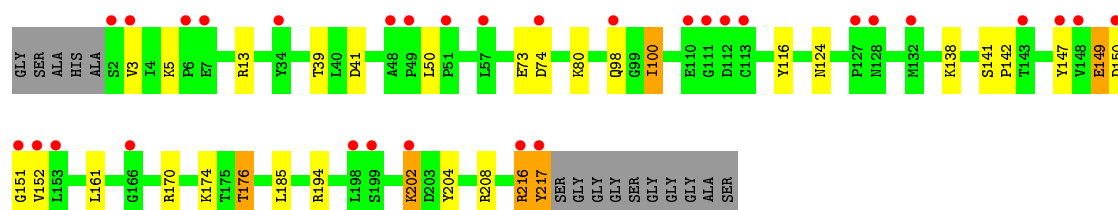
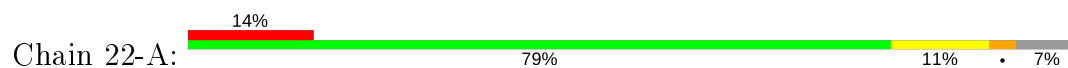
- Molecule 1: Reversibly photoswitching protein Dathail



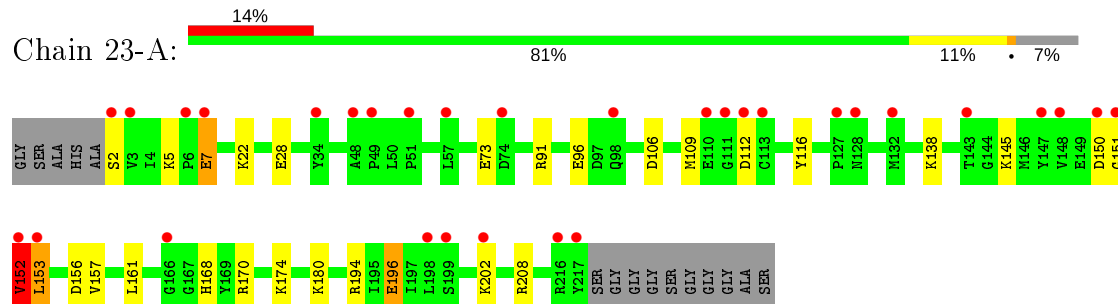
- Molecule 1: Reversibly photoswitching protein Dathail



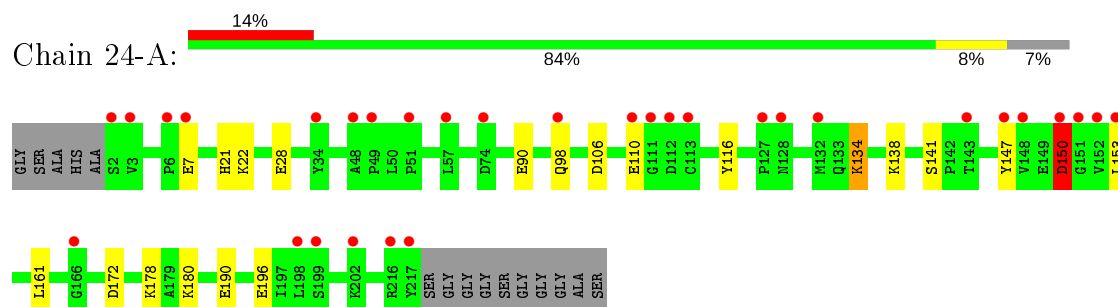
- Molecule 1: Reversibly photoswitching protein Dathail



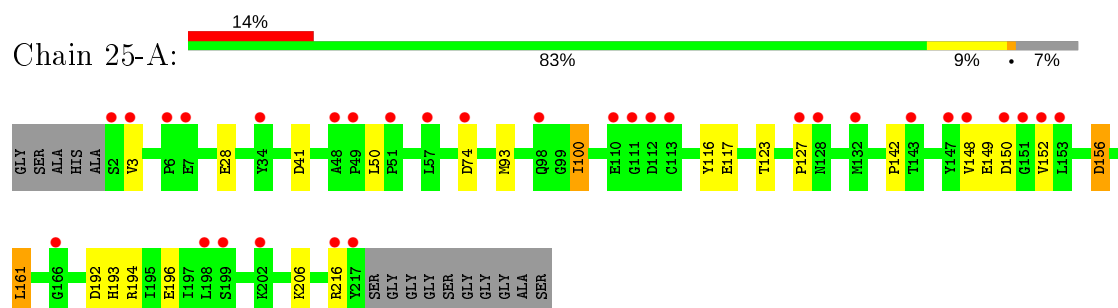
- Molecule 1: Reversibly photoswitching protein Dathail



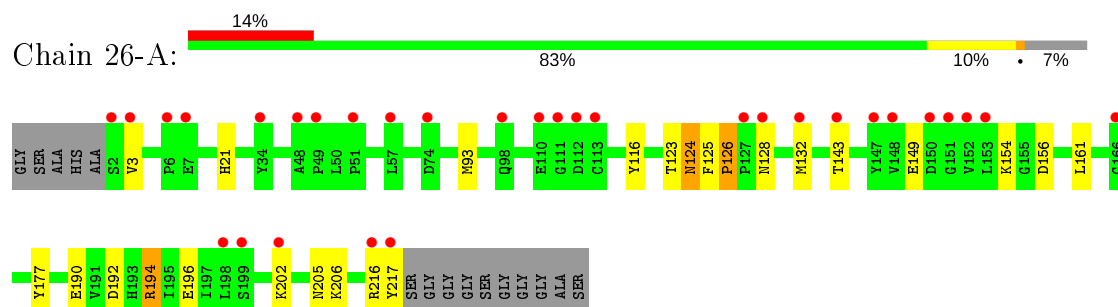
- Molecule 1: Reversibly photoswitching protein Dathail



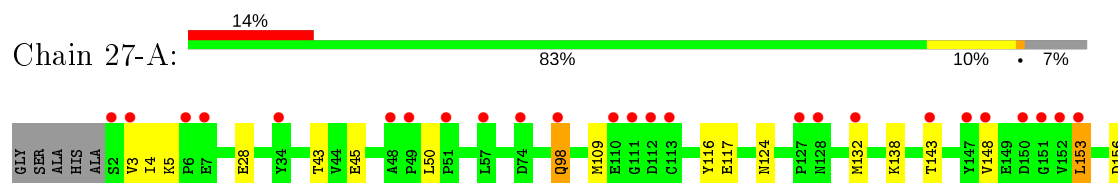
- Molecule 1: Reversibly photoswitching protein Dathail

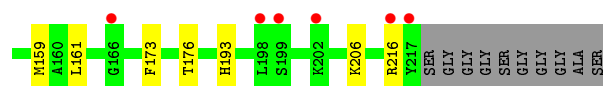


- Molecule 1: Reversibly photoswitching protein Dathail

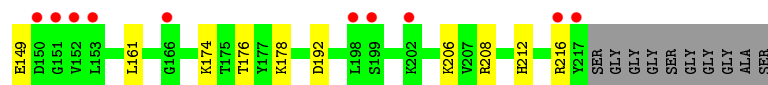
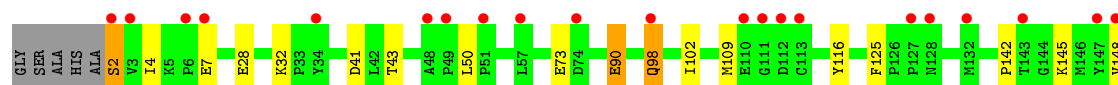
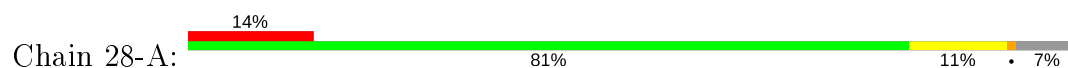


- Molecule 1: Reversibly photoswitching protein Dathail

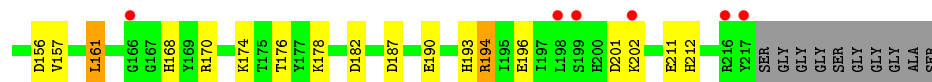
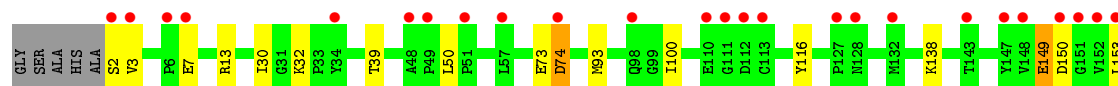
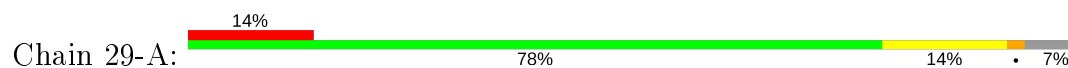




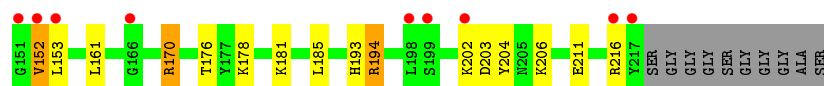
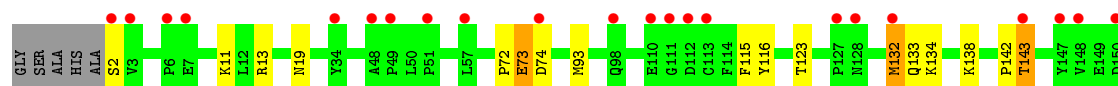
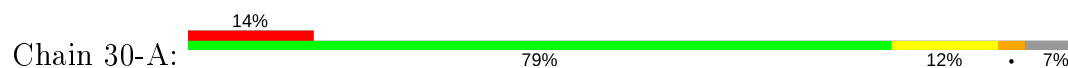
- Molecule 1: Reversibly photoswitching protein Dathail



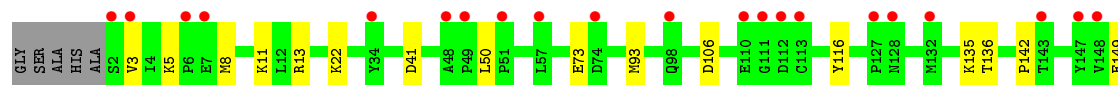
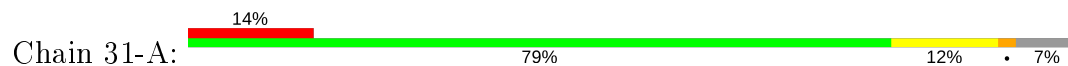
- Molecule 1: Reversibly photoswitching protein Dathail



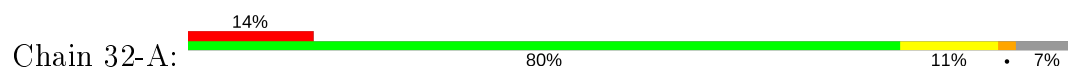
- Molecule 1: Reversibly photoswitching protein Dathail

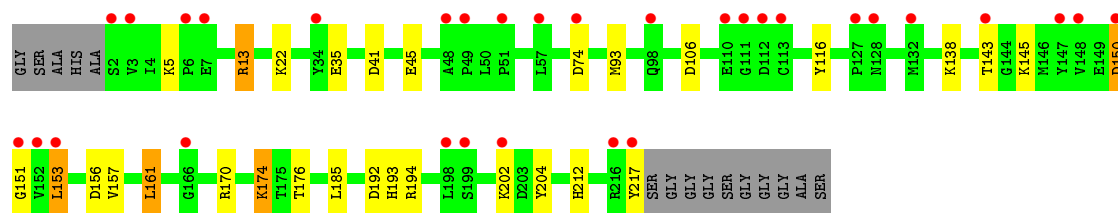


- Molecule 1: Reversibly photoswitching protein Dathail

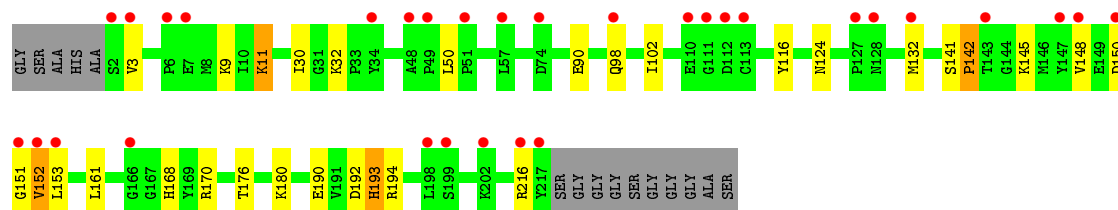
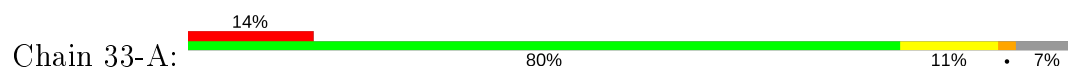


- Molecule 1: Reversibly photoswitching protein Dathail

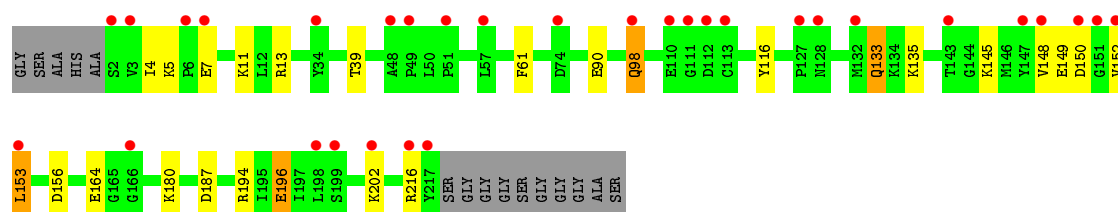
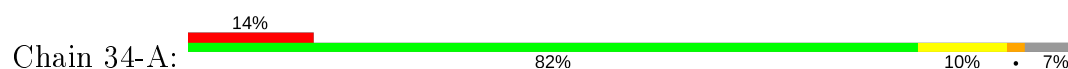




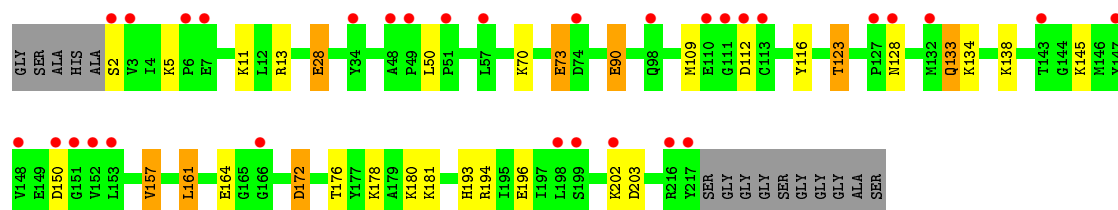
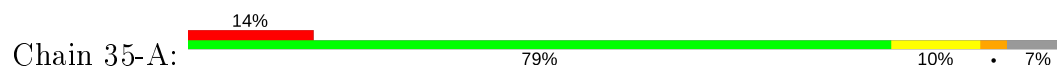
- Molecule 1: Reversibly photoswitching protein Dathail



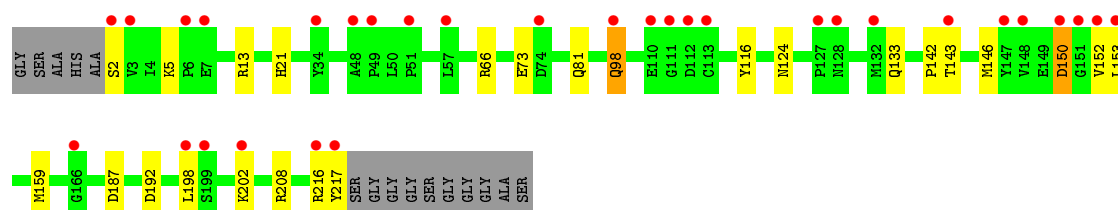
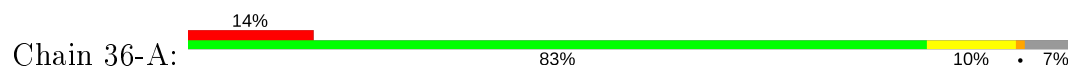
- Molecule 1: Reversibly photoswitching protein Dathail




- Molecule 1: Reversibly photoswitching protein Dathail

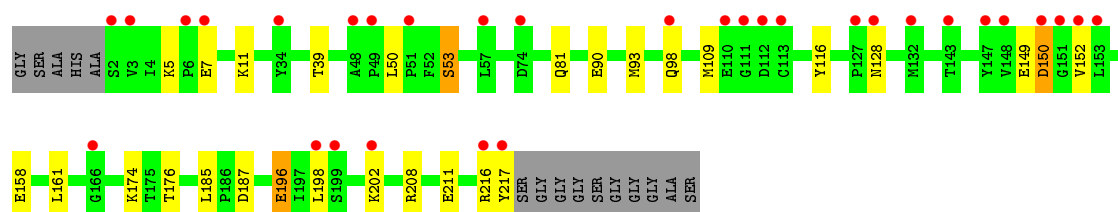


- Molecule 1: Reversibly photoswitching protein Dathail




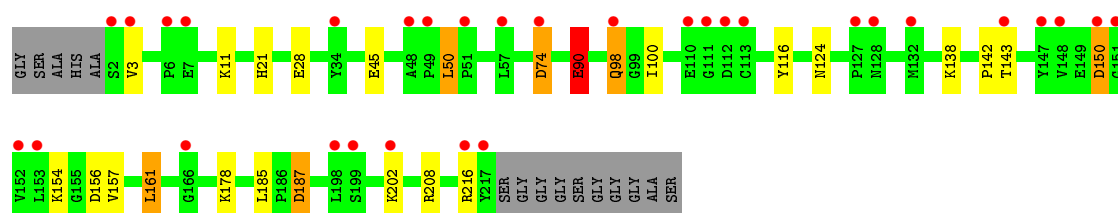
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 37-A: 




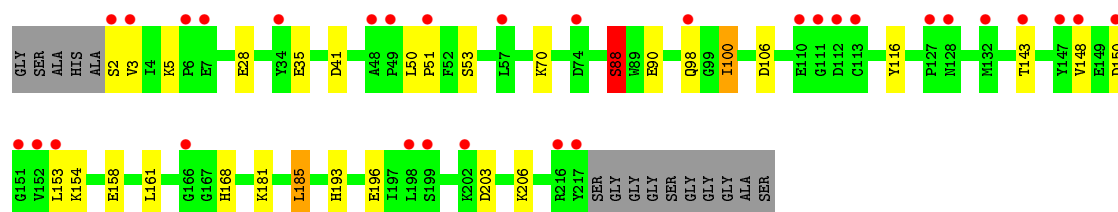
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 38-A: 




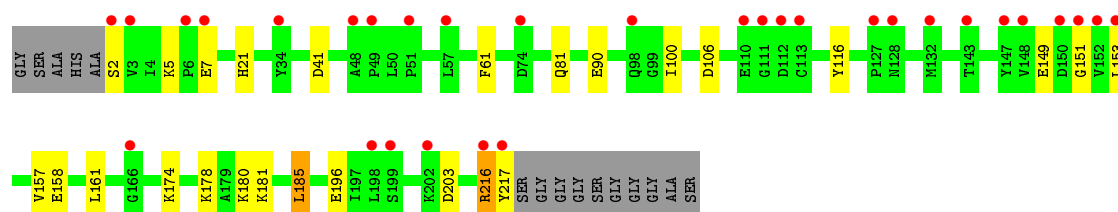
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 39-A: 




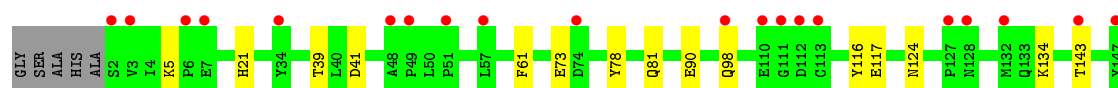
- Molecule 1: Reversibly photoswitching protein Dathail

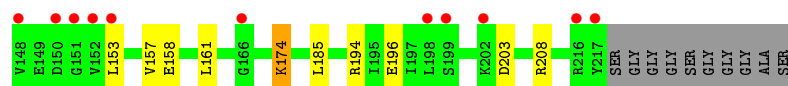
Chain 40-A: 



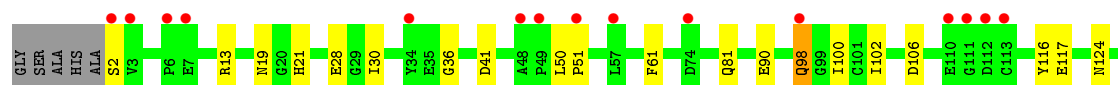
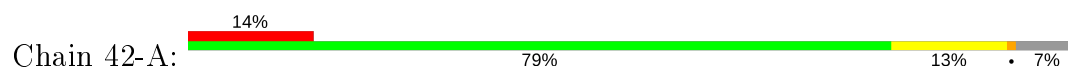
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 41-A: 

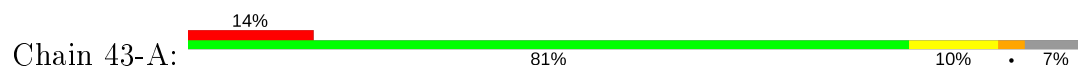




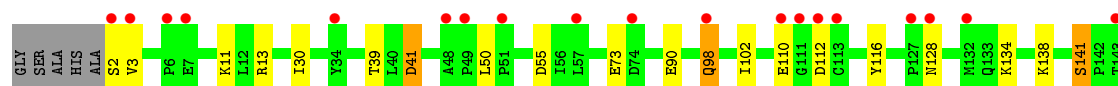
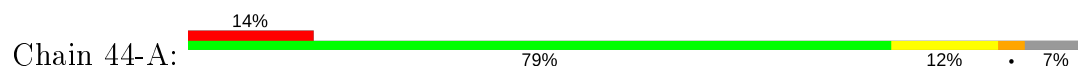
- Molecule 1: Reversibly photoswitching protein Dathail



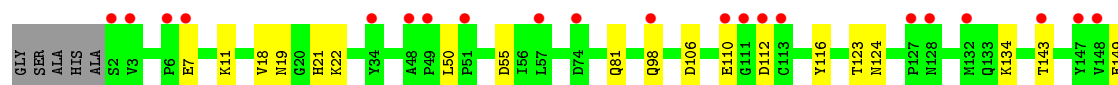
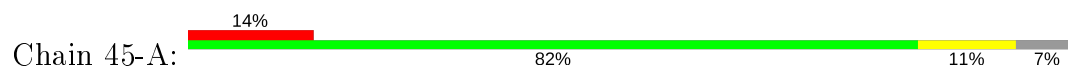
- Molecule 1: Reversibly photoswitching protein Dathail



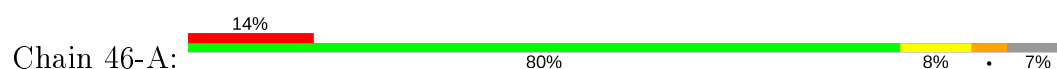
- Molecule 1: Reversibly photoswitching protein Dathail

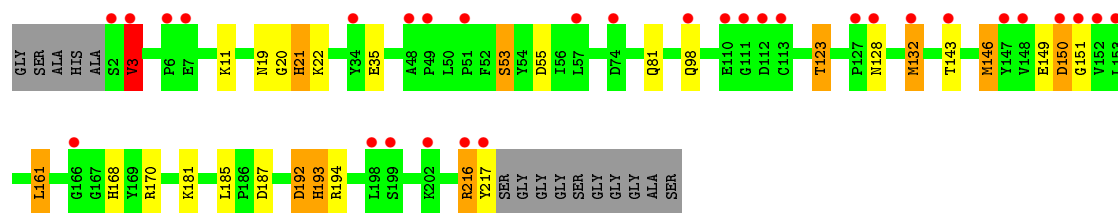


- Molecule 1: Reversibly photoswitching protein Dathail

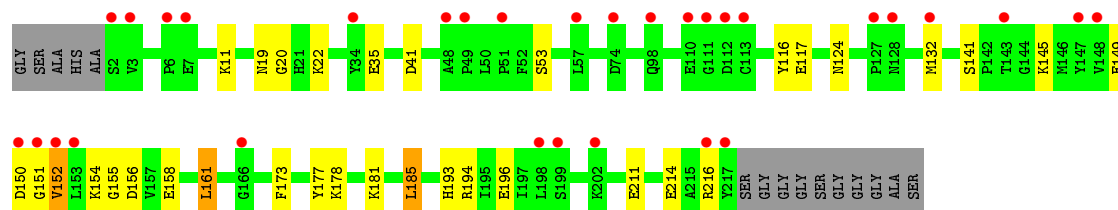
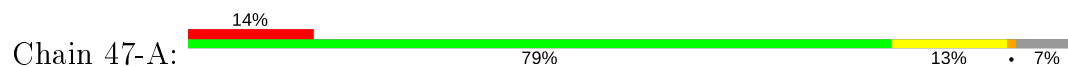


- Molecule 1: Reversibly photoswitching protein Dathail





- Molecule 1: Reversibly photoswitching protein Dathail



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	75.97Å 81.09Å 39.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.27 – 1.65 32.14 – 1.65	Depositor EDS
% Data completeness (in resolution range)	97.4 (28.27-1.65) 95.6 (32.14-1.65)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.47 (at 1.65Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.151 , 0.194 0.169 , 0.204	Depositor DCC
R_{free} test set	1888 reflections (6.43%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 357.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	167541	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.90	7/1766 (0.4%)	0.99	6/2382 (0.3%)
1	2-A	0.91	3/1766 (0.2%)	1.01	3/2382 (0.1%)
1	3-A	0.99	7/1766 (0.4%)	1.06	9/2382 (0.4%)
1	4-A	0.91	5/1766 (0.3%)	1.03	6/2382 (0.3%)
1	5-A	0.88	3/1766 (0.2%)	1.05	11/2382 (0.5%)
1	6-A	0.91	5/1766 (0.3%)	1.04	6/2382 (0.3%)
1	7-A	0.89	4/1766 (0.2%)	1.02	7/2382 (0.3%)
1	8-A	1.00	6/1766 (0.3%)	1.09	10/2382 (0.4%)
1	9-A	0.90	6/1766 (0.3%)	0.96	1/2382 (0.0%)
1	10-A	0.85	2/1766 (0.1%)	0.99	6/2382 (0.3%)
1	11-A	0.98	8/1766 (0.5%)	1.11	12/2382 (0.5%)
1	12-A	0.84	2/1766 (0.1%)	0.98	3/2382 (0.1%)
1	13-A	0.88	1/1766 (0.1%)	1.08	8/2382 (0.3%)
1	14-A	0.89	1/1766 (0.1%)	1.07	9/2382 (0.4%)
1	15-A	0.89	3/1766 (0.2%)	1.00	2/2382 (0.1%)
1	16-A	0.83	3/1766 (0.2%)	0.97	3/2382 (0.1%)
1	17-A	0.88	2/1766 (0.1%)	1.00	3/2382 (0.1%)
1	18-A	0.91	6/1766 (0.3%)	1.02	5/2382 (0.2%)
1	19-A	0.88	2/1766 (0.1%)	1.00	9/2382 (0.4%)
1	20-A	0.89	3/1766 (0.2%)	1.04	7/2382 (0.3%)
1	21-A	0.90	3/1766 (0.2%)	1.06	4/2382 (0.2%)
1	22-A	0.84	4/1766 (0.2%)	0.97	5/2382 (0.2%)
1	23-A	0.90	3/1766 (0.2%)	1.02	8/2382 (0.3%)
1	24-A	0.89	3/1766 (0.2%)	0.96	4/2382 (0.2%)
1	25-A	0.87	1/1766 (0.1%)	1.00	4/2382 (0.2%)
1	26-A	0.91	4/1766 (0.2%)	1.00	8/2382 (0.3%)
1	27-A	0.85	4/1766 (0.2%)	1.01	7/2382 (0.3%)
1	28-A	0.90	4/1766 (0.2%)	0.97	3/2382 (0.1%)
1	29-A	0.88	3/1766 (0.2%)	1.02	7/2382 (0.3%)
1	30-A	0.87	3/1766 (0.2%)	1.05	4/2382 (0.2%)
1	31-A	0.85	2/1766 (0.1%)	0.99	6/2382 (0.3%)
1	32-A	0.87	2/1766 (0.1%)	1.06	11/2382 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	33-A	0.97	5/1766 (0.3%)	1.03	7/2382 (0.3%)
1	34-A	0.83	3/1766 (0.2%)	0.97	3/2382 (0.1%)
1	35-A	0.91	6/1766 (0.3%)	1.03	7/2382 (0.3%)
1	36-A	0.86	0/1766	1.01	5/2382 (0.2%)
1	37-A	0.89	3/1766 (0.2%)	0.96	2/2382 (0.1%)
1	38-A	0.88	3/1766 (0.2%)	0.96	4/2382 (0.2%)
1	39-A	0.85	3/1766 (0.2%)	0.99	5/2382 (0.2%)
1	40-A	0.82	1/1766 (0.1%)	0.97	4/2382 (0.2%)
1	41-A	0.87	4/1766 (0.2%)	0.99	7/2382 (0.3%)
1	42-A	0.75	0/1766	0.95	2/2382 (0.1%)
1	43-A	0.90	6/1766 (0.3%)	1.09	13/2382 (0.5%)
1	44-A	0.89	3/1766 (0.2%)	0.99	5/2382 (0.2%)
1	45-A	0.88	1/1766 (0.1%)	1.01	3/2382 (0.1%)
1	46-A	0.83	2/1766 (0.1%)	1.00	7/2382 (0.3%)
1	47-A	0.89	4/1766 (0.2%)	1.00	6/2382 (0.3%)
All	All	0.89	159/83002 (0.2%)	1.01	277/111954 (0.2%)

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	2-A	0	4
1	3-A	0	6
1	4-A	0	2
1	5-A	0	1
1	6-A	0	4
1	7-A	0	2
1	8-A	0	2
1	9-A	0	3
1	10-A	0	4
1	11-A	0	2
1	12-A	0	4
1	14-A	0	5
1	15-A	0	1
1	17-A	0	3
1	18-A	0	5
1	19-A	0	1
1	22-A	0	1
1	23-A	0	2
1	25-A	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	26-A	0	1
1	28-A	0	1
1	30-A	0	1
1	31-A	0	2
1	32-A	0	1
1	34-A	0	1
1	36-A	0	1
1	37-A	0	1
1	38-A	0	2
1	39-A	0	1
1	40-A	0	2
1	41-A	0	1
1	42-A	0	5
1	43-A	0	2
1	44-A	0	1
1	45-A	0	4
1	46-A	0	4
1	47-A	0	1
All	All	0	86

The worst 5 of 159 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-A	152	VAL	CB-CG2	-10.82	1.30	1.52
1	8-A	73	GLU	CB-CG	-10.15	1.32	1.52
1	41-A	41	ASP	CB-CG	9.69	1.72	1.51
1	35-A	164	GLU	CB-CG	9.36	1.70	1.52
1	21-A	196	GLU	CB-CG	9.32	1.69	1.52

The worst 5 of 277 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	17-A	170	ARG	NE-CZ-NH1	14.47	127.53	120.30
1	13-A	91	ARG	NE-CZ-NH1	13.14	126.87	120.30
1	11-A	91	ARG	NE-CZ-NH1	12.58	126.59	120.30
1	46-A	55	ASP	CB-CG-OD1	-12.49	107.06	118.30
1	3-A	146	MET	CB-CG-SD	-11.64	77.48	112.40

There are no chirality outliers.

5 of 86 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2-A	149	GLU	Peptide
1	2-A	150	ASP	Peptide
1	2-A	179	ALA	Peptide
1	2-A	2	SER	Peptide
1	3-A	2	SER	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	1665	1678	0	0
1	2-A	1745	1665	1679	0	0
1	3-A	1745	1665	1679	0	0
1	4-A	1745	1665	1679	0	0
1	5-A	1745	1665	1679	0	0
1	6-A	1745	1665	1679	0	0
1	7-A	1745	1665	1679	0	0
1	8-A	1745	1665	1677	0	0
1	9-A	1745	1665	1679	0	0
1	10-A	1745	1665	1678	0	0
1	11-A	1745	1665	1679	0	0
1	12-A	1745	1665	1679	0	0
1	13-A	1745	1665	1679	0	0
1	14-A	1745	1665	1679	0	0
1	15-A	1745	1665	1679	0	0
1	16-A	1745	1665	1679	0	0
1	17-A	1745	1665	1678	0	0
1	18-A	1745	1665	1679	0	0
1	19-A	1745	1665	1678	0	0
1	20-A	1745	1665	1679	0	0
1	21-A	1745	1665	1679	0	0
1	22-A	1745	1665	1678	0	0
1	23-A	1745	1665	1679	0	0
1	24-A	1745	1665	1679	0	0
1	25-A	1745	1665	1679	0	0
1	26-A	1745	1665	1679	0	0
1	27-A	1745	1665	1679	0	0
1	28-A	1745	1665	1679	0	0
1	29-A	1745	1665	1679	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	30-A	1745	1665	1679	0	0
1	31-A	1745	1665	1679	0	0
1	32-A	1745	1665	1679	0	0
1	33-A	1745	1665	1679	0	0
1	34-A	1745	1665	1678	0	0
1	35-A	1745	1665	1678	0	0
1	36-A	1745	1665	1679	0	0
1	37-A	1745	1665	1679	0	0
1	38-A	1745	1665	1679	0	0
1	39-A	1745	1665	1679	0	0
1	40-A	1745	1665	1679	0	0
1	41-A	1745	1665	1679	0	0
1	42-A	1745	1665	1679	0	0
1	43-A	1745	1665	1679	0	0
1	44-A	1745	1665	1679	0	0
1	45-A	1745	1665	1679	0	0
1	46-A	1745	1665	1679	0	0
1	47-A	1745	1665	1678	0	0
2	1-A	165	0	0	0	0
2	2-A	173	0	0	0	0
2	3-A	140	0	0	0	0
2	4-A	153	0	0	0	0
2	5-A	167	0	0	0	0
2	6-A	150	0	0	0	0
2	7-A	150	0	0	0	0
2	8-A	160	0	0	0	0
2	9-A	160	0	0	0	0
2	10-A	152	0	0	0	0
2	11-A	173	0	0	0	0
2	12-A	160	0	0	0	0
2	13-A	152	0	0	0	0
2	14-A	157	0	0	0	0
2	15-A	148	0	0	0	0
2	16-A	152	0	0	0	0
2	17-A	147	0	0	0	0
2	18-A	156	0	0	0	0
2	19-A	151	0	0	0	0
2	20-A	147	0	0	0	0
2	21-A	148	0	0	0	0
2	22-A	169	0	0	0	0
2	23-A	144	0	0	0	0
2	24-A	138	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	25-A	149	0	0	0	0
2	26-A	143	0	0	0	0
2	27-A	148	0	0	0	0
2	28-A	165	0	0	0	0
2	29-A	146	0	0	0	0
2	30-A	165	0	0	0	0
2	31-A	163	0	0	0	0
2	32-A	163	0	0	0	0
2	33-A	154	0	0	0	0
2	34-A	147	0	0	0	0
2	35-A	135	0	0	0	0
2	36-A	160	0	0	0	0
2	37-A	156	0	0	0	0
2	38-A	149	0	0	0	0
2	39-A	154	0	0	0	0
2	40-A	164	0	0	0	0
2	41-A	156	0	0	0	0
2	42-A	142	0	0	0	0
2	43-A	162	0	0	0	0
2	44-A	159	0	0	0	0
2	45-A	143	0	0	0	0
2	46-A	174	0	0	0	0
2	47-A	162	0	0	0	0
All	All	89286	78255	78903	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	211/229 (92%)	196 (93%)	9 (4%)	6 (3%)	5	0
1	2-A	211/229 (92%)	195 (92%)	13 (6%)	3 (1%)	11	1
1	3-A	211/229 (92%)	194 (92%)	11 (5%)	6 (3%)	5	0
1	4-A	211/229 (92%)	200 (95%)	7 (3%)	4 (2%)	8	0
1	5-A	211/229 (92%)	200 (95%)	5 (2%)	6 (3%)	5	0
1	6-A	211/229 (92%)	196 (93%)	6 (3%)	9 (4%)	2	0
1	7-A	211/229 (92%)	199 (94%)	8 (4%)	4 (2%)	8	0
1	8-A	211/229 (92%)	201 (95%)	3 (1%)	7 (3%)	4	0
1	9-A	211/229 (92%)	200 (95%)	7 (3%)	4 (2%)	8	0
1	10-A	211/229 (92%)	202 (96%)	7 (3%)	2 (1%)	17	4
1	11-A	211/229 (92%)	199 (94%)	9 (4%)	3 (1%)	11	1
1	12-A	211/229 (92%)	198 (94%)	11 (5%)	2 (1%)	17	4
1	13-A	211/229 (92%)	197 (93%)	10 (5%)	4 (2%)	8	0
1	14-A	211/229 (92%)	199 (94%)	9 (4%)	3 (1%)	11	1
1	15-A	211/229 (92%)	200 (95%)	8 (4%)	3 (1%)	11	1
1	16-A	211/229 (92%)	199 (94%)	8 (4%)	4 (2%)	8	0
1	17-A	211/229 (92%)	197 (93%)	10 (5%)	4 (2%)	8	0
1	18-A	211/229 (92%)	200 (95%)	6 (3%)	5 (2%)	6	0
1	19-A	211/229 (92%)	199 (94%)	7 (3%)	5 (2%)	6	0
1	20-A	211/229 (92%)	201 (95%)	7 (3%)	3 (1%)	11	1
1	21-A	211/229 (92%)	199 (94%)	11 (5%)	1 (0%)	29	11
1	22-A	211/229 (92%)	196 (93%)	8 (4%)	7 (3%)	4	0
1	23-A	211/229 (92%)	202 (96%)	8 (4%)	1 (0%)	29	11
1	24-A	211/229 (92%)	201 (95%)	7 (3%)	3 (1%)	11	1
1	25-A	211/229 (92%)	200 (95%)	9 (4%)	2 (1%)	17	4
1	26-A	211/229 (92%)	196 (93%)	13 (6%)	2 (1%)	17	4
1	27-A	211/229 (92%)	202 (96%)	7 (3%)	2 (1%)	17	4
1	28-A	211/229 (92%)	204 (97%)	5 (2%)	2 (1%)	17	4
1	29-A	211/229 (92%)	201 (95%)	9 (4%)	1 (0%)	29	11
1	30-A	211/229 (92%)	191 (90%)	13 (6%)	7 (3%)	4	0
1	31-A	211/229 (92%)	200 (95%)	7 (3%)	4 (2%)	8	0
1	32-A	211/229 (92%)	202 (96%)	8 (4%)	1 (0%)	29	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	33-A	211/229 (92%)	194 (92%)	13 (6%)	4 (2%)	8	0
1	34-A	211/229 (92%)	198 (94%)	10 (5%)	3 (1%)	11	1
1	35-A	211/229 (92%)	202 (96%)	8 (4%)	1 (0%)	29	11
1	36-A	211/229 (92%)	197 (93%)	11 (5%)	3 (1%)	11	1
1	37-A	211/229 (92%)	200 (95%)	10 (5%)	1 (0%)	29	11
1	38-A	211/229 (92%)	199 (94%)	9 (4%)	3 (1%)	11	1
1	39-A	211/229 (92%)	199 (94%)	9 (4%)	3 (1%)	11	1
1	40-A	211/229 (92%)	206 (98%)	4 (2%)	1 (0%)	29	11
1	41-A	211/229 (92%)	204 (97%)	6 (3%)	1 (0%)	29	11
1	42-A	211/229 (92%)	192 (91%)	14 (7%)	5 (2%)	6	0
1	43-A	211/229 (92%)	200 (95%)	10 (5%)	1 (0%)	29	11
1	44-A	211/229 (92%)	200 (95%)	7 (3%)	4 (2%)	8	0
1	45-A	211/229 (92%)	199 (94%)	6 (3%)	6 (3%)	5	0
1	46-A	211/229 (92%)	193 (92%)	11 (5%)	7 (3%)	4	0
1	47-A	211/229 (92%)	197 (93%)	10 (5%)	4 (2%)	8	0
All	All	9917/10763 (92%)	9346 (94%)	404 (4%)	167 (2%)	9	1

5 of 167 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	98	GLN
1	1-A	149	GLU
1	1-A	151	GLY
1	1-A	152	VAL
1	1-A	179	ALA

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%)	164 (89%)	20 (11%)	6	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2-A	184/189 (97%)	162 (88%)	22 (12%)	5	0
1	3-A	184/189 (97%)	163 (89%)	21 (11%)	5	1
1	4-A	184/189 (97%)	158 (86%)	26 (14%)	3	0
1	5-A	184/189 (97%)	157 (85%)	27 (15%)	3	0
1	6-A	184/189 (97%)	161 (88%)	23 (12%)	4	0
1	7-A	184/189 (97%)	166 (90%)	18 (10%)	8	1
1	8-A	184/189 (97%)	160 (87%)	24 (13%)	4	0
1	9-A	184/189 (97%)	163 (89%)	21 (11%)	5	1
1	10-A	184/189 (97%)	161 (88%)	23 (12%)	4	0
1	11-A	184/189 (97%)	163 (89%)	21 (11%)	5	1
1	12-A	184/189 (97%)	163 (89%)	21 (11%)	5	1
1	13-A	184/189 (97%)	152 (83%)	32 (17%)	2	0
1	14-A	184/189 (97%)	168 (91%)	16 (9%)	10	1
1	15-A	184/189 (97%)	161 (88%)	23 (12%)	4	0
1	16-A	184/189 (97%)	165 (90%)	19 (10%)	7	1
1	17-A	184/189 (97%)	162 (88%)	22 (12%)	5	0
1	18-A	184/189 (97%)	157 (85%)	27 (15%)	3	0
1	19-A	184/189 (97%)	162 (88%)	22 (12%)	5	0
1	20-A	184/189 (97%)	163 (89%)	21 (11%)	5	1
1	21-A	184/189 (97%)	163 (89%)	21 (11%)	5	1
1	22-A	184/189 (97%)	162 (88%)	22 (12%)	5	0
1	23-A	184/189 (97%)	162 (88%)	22 (12%)	5	0
1	24-A	184/189 (97%)	168 (91%)	16 (9%)	10	1
1	25-A	184/189 (97%)	166 (90%)	18 (10%)	8	1
1	26-A	184/189 (97%)	169 (92%)	15 (8%)	11	2
1	27-A	184/189 (97%)	166 (90%)	18 (10%)	8	1
1	28-A	184/189 (97%)	161 (88%)	23 (12%)	4	0
1	29-A	184/189 (97%)	153 (83%)	31 (17%)	2	0
1	30-A	184/189 (97%)	159 (86%)	25 (14%)	3	0
1	31-A	184/189 (97%)	161 (88%)	23 (12%)	4	0
1	32-A	184/189 (97%)	161 (88%)	23 (12%)	4	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	33-A	184/189 (97%)	163 (89%)	21 (11%)	5	1
1	34-A	184/189 (97%)	163 (89%)	21 (11%)	5	1
1	35-A	184/189 (97%)	155 (84%)	29 (16%)	2	0
1	36-A	184/189 (97%)	165 (90%)	19 (10%)	7	1
1	37-A	184/189 (97%)	159 (86%)	25 (14%)	3	0
1	38-A	184/189 (97%)	161 (88%)	23 (12%)	4	0
1	39-A	184/189 (97%)	159 (86%)	25 (14%)	3	0
1	40-A	184/189 (97%)	164 (89%)	20 (11%)	6	1
1	41-A	184/189 (97%)	167 (91%)	17 (9%)	9	1
1	42-A	184/189 (97%)	157 (85%)	27 (15%)	3	0
1	43-A	184/189 (97%)	164 (89%)	20 (11%)	6	1
1	44-A	184/189 (97%)	157 (85%)	27 (15%)	3	0
1	45-A	184/189 (97%)	172 (94%)	12 (6%)	17	3
1	46-A	184/189 (97%)	161 (88%)	23 (12%)	4	0
1	47-A	184/189 (97%)	163 (89%)	21 (11%)	5	1
All	All	8648/8883 (97%)	7612 (88%)	1036 (12%)	5	0

5 of 1036 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	21-A	216	ARG
1	27-A	206	LYS
1	44-A	30	ILE
1	22-A	150	ASP
1	24-A	172	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 142 such sidechains are listed below:

Mol	Chain	Res	Type
1	20-A	19	ASN
1	26-A	205	ASN
1	45-A	193	HIS
1	20-A	81	GLN
1	22-A	193	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

47 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	29-A	62	1	24,25,26	2.02	5 (20%)	27,34,36	2.16	11 (40%)
1	CRQ	16-A	62	1	24,25,26	1.98	7 (29%)	27,34,36	1.58	3 (11%)
1	CRQ	25-A	62	1	24,25,26	2.04	7 (29%)	27,34,36	1.68	6 (22%)
1	CRQ	31-A	62	1	24,25,26	1.95	6 (25%)	27,34,36	1.37	4 (14%)
1	CRQ	30-A	62	1	24,25,26	1.93	7 (29%)	27,34,36	1.54	6 (22%)
1	CRQ	35-A	62	1	24,25,26	2.10	6 (25%)	27,34,36	2.26	10 (37%)
1	CRQ	24-A	62	1	24,25,26	1.81	6 (25%)	27,34,36	1.41	5 (18%)
1	CRQ	3-A	62	1	24,25,26	1.95	7 (29%)	27,34,36	1.69	5 (18%)
1	CRQ	2-A	62	1	24,25,26	2.09	8 (33%)	27,34,36	1.35	4 (14%)
1	CRQ	7-A	62	1	24,25,26	2.32	8 (33%)	27,34,36	1.58	4 (14%)
1	CRQ	18-A	62	1	24,25,26	2.17	6 (25%)	27,34,36	1.55	5 (18%)
1	CRQ	4-A	62	1	24,25,26	2.21	6 (25%)	27,34,36	1.80	7 (25%)
1	CRQ	13-A	62	1	24,25,26	2.16	7 (29%)	27,34,36	1.48	3 (11%)
1	CRQ	27-A	62	1	24,25,26	1.96	7 (29%)	27,34,36	1.29	3 (11%)
1	CRQ	22-A	62	1	24,25,26	2.04	6 (25%)	27,34,36	1.61	8 (29%)
1	CRQ	21-A	62	1	24,25,26	2.10	7 (29%)	27,34,36	1.58	4 (14%)
1	CRQ	41-A	62	1	24,25,26	2.12	7 (29%)	27,34,36	1.51	6 (22%)
1	CRQ	47-A	62	1	24,25,26	2.04	6 (25%)	27,34,36	1.83	7 (25%)
1	CRQ	20-A	62	1	24,25,26	1.81	6 (25%)	27,34,36	1.24	3 (11%)
1	CRQ	36-A	62	1	24,25,26	2.04	8 (33%)	27,34,36	1.73	4 (14%)
1	CRQ	6-A	62	1	24,25,26	2.06	6 (25%)	27,34,36	2.09	9 (33%)
1	CRQ	33-A	62	1	24,25,26	1.88	5 (20%)	27,34,36	1.98	10 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CRQ	37-A	62	1	24,25,26	2.13	7 (29%)	27,34,36	1.56	6 (22%)
1	CRQ	1-A	62	1	24,25,26	1.94	5 (20%)	27,34,36	2.07	10 (37%)
1	CRQ	39-A	62	1	24,25,26	2.07	7 (29%)	27,34,36	1.36	4 (14%)
1	CRQ	23-A	62	1	24,25,26	2.00	7 (29%)	27,34,36	1.53	3 (11%)
1	CRQ	10-A	62	1	24,25,26	1.98	6 (25%)	27,34,36	1.48	5 (18%)
1	CRQ	44-A	62	1	24,25,26	1.84	6 (25%)	27,34,36	1.43	4 (14%)
1	CRQ	45-A	62	1	24,25,26	2.10	7 (29%)	27,34,36	1.49	3 (11%)
1	CRQ	40-A	62	1	24,25,26	1.92	7 (29%)	27,34,36	1.54	7 (25%)
1	CRQ	11-A	62	1	24,25,26	2.03	7 (29%)	27,34,36	1.65	5 (18%)
1	CRQ	28-A	62	1	24,25,26	2.02	6 (25%)	27,34,36	1.58	5 (18%)
1	CRQ	8-A	62	1	24,25,26	1.91	6 (25%)	27,34,36	1.51	5 (18%)
1	CRQ	26-A	62	1	24,25,26	1.74	6 (25%)	27,34,36	1.70	6 (22%)
1	CRQ	38-A	62	1	24,25,26	1.92	6 (25%)	27,34,36	1.94	6 (22%)
1	CRQ	5-A	62	1	24,25,26	1.97	6 (25%)	27,34,36	1.62	5 (18%)
1	CRQ	17-A	62	1	24,25,26	1.80	6 (25%)	27,34,36	1.54	4 (14%)
1	CRQ	12-A	62	1	24,25,26	2.13	6 (25%)	27,34,36	1.91	8 (29%)
1	CRQ	9-A	62	1	24,25,26	1.80	5 (20%)	27,34,36	1.93	7 (25%)
1	CRQ	19-A	62	1	24,25,26	2.11	5 (20%)	27,34,36	2.44	9 (33%)
1	CRQ	14-A	62	1	24,25,26	2.10	6 (25%)	27,34,36	1.87	7 (25%)
1	CRQ	34-A	62	1	24,25,26	1.98	6 (25%)	27,34,36	1.38	4 (14%)
1	CRQ	32-A	62	1	24,25,26	2.24	6 (25%)	27,34,36	2.45	10 (37%)
1	CRQ	15-A	62	1	24,25,26	2.11	6 (25%)	27,34,36	2.03	11 (40%)
1	CRQ	43-A	62	1	24,25,26	2.06	8 (33%)	27,34,36	1.58	4 (14%)
1	CRQ	46-A	62	1	24,25,26	2.22	6 (25%)	27,34,36	1.54	4 (14%)
1	CRQ	42-A	62	1	24,25,26	2.06	7 (29%)	27,34,36	1.70	4 (14%)

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	29-A	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	16-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	25-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	31-A	62	1	-	2/10/32/33	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CRQ	30-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	35-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	24-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	3-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	2-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	7-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	18-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	4-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	13-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	27-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	22-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	21-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	41-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	47-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	20-A	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	36-A	62	1	-	5/10/32/33	0/2/2/2
1	CRQ	6-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	33-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	37-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	1-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	39-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	23-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	10-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	44-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	45-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	40-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	11-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	28-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	8-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	26-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	38-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	5-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	17-A	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	12-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	9-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	19-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	14-A	62	1	-	2/10/32/33	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CRQ	34-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	32-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	15-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	43-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	46-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	42-A	62	1	-	0/10/32/33	0/2/2/2

The worst 5 of 300 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-A	62	CRQ	CB2-CA2	6.28	1.40	1.35
1	19-A	62	CRQ	C1-N3	6.14	1.48	1.38
1	32-A	62	CRQ	CA2-C2	-6.00	1.42	1.48
1	37-A	62	CRQ	C1-N3	5.94	1.48	1.38
1	1-A	62	CRQ	C1-N3	5.84	1.48	1.38

The worst 5 of 273 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	32-A	62	CRQ	CA2-C2-N3	8.19	107.24	103.37
1	19-A	62	CRQ	O2-C2-CA2	-8.00	126.47	130.96
1	35-A	62	CRQ	CG2-CB2-CA2	-6.16	122.40	129.94
1	1-A	62	CRQ	O2-C2-CA2	-5.65	127.79	130.96
1	42-A	62	CRQ	CA2-C2-N3	5.52	105.98	103.37

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	29-A	62	CRQ	C-CA3-N3-C1
1	29-A	62	CRQ	C-CA3-N3-C2
1	25-A	62	CRQ	C-CA3-N3-C2
1	31-A	62	CRQ	C-CA3-N3-C1
1	31-A	62	CRQ	C-CA3-N3-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

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	1-A	1
1	5-A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
5	A	62:CRQ	C	65:ASN	N	1.20
1	A	62:CRQ	C	65:ASN	N	1.18

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	2-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	3-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	4-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	5-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	6-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	7-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	8-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	9-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	10-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	11-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	12-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	13-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	14-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	15-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	16-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	17-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	18-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	19-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	20-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	21-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	22-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	23-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	24-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	25-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	26-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	27-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	28-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	29-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	30-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	31-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	32-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	33-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	34-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	35-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	36-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	37-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	38-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	39-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	40-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	41-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	42-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	43-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	44-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	45-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	46-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
1	47-A	213/229 (93%)	0.91	31 (14%) 2 2	22, 29, 37, 41	213 (100%)
All	All	10011/10763 (93%)	0.91	1457 (14%) 2 2	22, 29, 37, 41	10011 (100%)

The worst 5 of 1457 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	217	TYR	11.3
1	2-A	217	TYR	11.3
1	3-A	217	TYR	11.3
1	4-A	217	TYR	11.3
1	5-A	217	TYR	11.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CRQ	29-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	16-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	25-A	62	24/25	0.94	0.16	22,23,24,25	24
1	CRQ	31-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	30-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	35-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	24-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	3-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	2-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	7-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	18-A	62	24/25	0.94	0.16	22,23,24,25	24
1	CRQ	4-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	23-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	13-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	27-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	22-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	21-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	41-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	47-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	20-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	36-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	6-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	33-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	37-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	1-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	39-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	19-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	10-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	44-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	45-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	40-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	11-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	28-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	8-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	26-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	38-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	5-A	62	24/25	0.94	0.16	22,22,24,25	24

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	CRQ	17-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	12-A	62	24/25	0.94	0.16	22,23,24,25	24
1	CRQ	9-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	14-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	34-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	32-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	15-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	43-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	46-A	62	24/25	0.94	0.16	22,22,24,25	24
1	CRQ	42-A	62	24/25	0.94	0.16	22,23,24,25	24

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.