



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2016 – 02:46 PM EDT

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027457  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

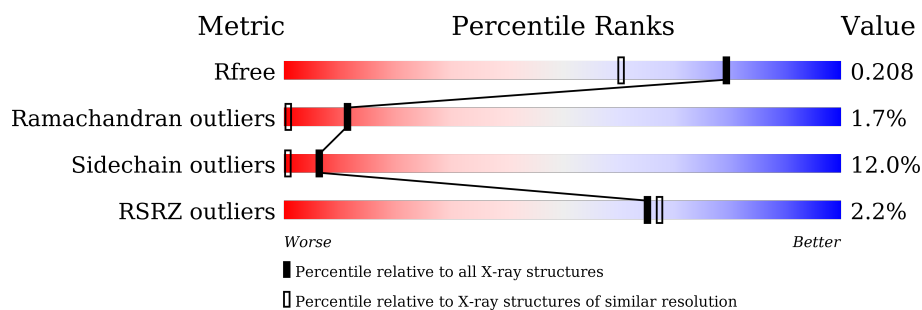
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1226 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (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.

Mol	Chain	Length	Quality of chain
1	1-A	229	<div> <div>2%</div> <div>81% 10% • 7%</div> </div>
1	10-A	229	<div> <div>2%</div> <div>79% 14% 7%</div> </div>
1	11-A	229	<div> <div>2%</div> <div>79% 11% • 7%</div> </div>
1	12-A	229	<div> <div>2%</div> <div>82% 10% • 7%</div> </div>
1	13-A	229	<div> <div>2%</div> <div>76% 15% • 7%</div> </div>
1	14-A	229	<div> <div>2%</div> <div>82% 9% • 7%</div> </div>
1	15-A	229	<div> <div>2%</div> <div>81% 11% • 7%</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	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	18-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	19-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	20-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	21-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	22-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	23-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	24-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	25-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	26-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	27-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	28-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	29-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	30-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	31-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	32-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	33-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	34-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	35-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	36-A	214	Total	C	H	N	O	S	0	0	0
			3410	1118	1665	286	331	10			
1	37-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	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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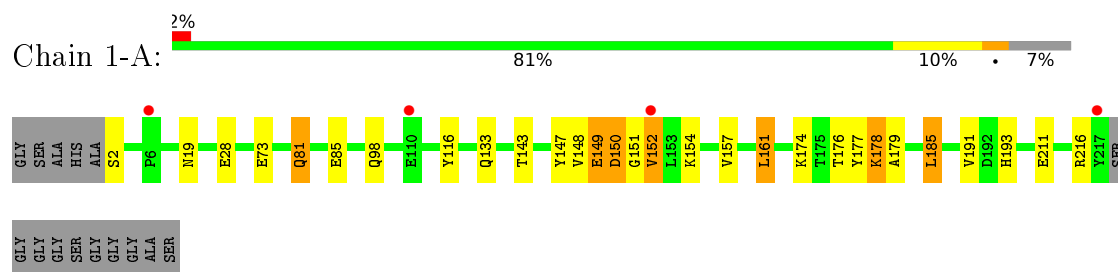
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	31-A	163	Total 163	O 163	0	0
2	32-A	163	Total 163	O 163	0	0
2	33-A	154	Total 154	O 154	0	0
2	34-A	147	Total 147	O 147	0	0
2	35-A	135	Total 135	O 135	0	0
2	36-A	160	Total 160	O 160	0	0
2	37-A	156	Total 156	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

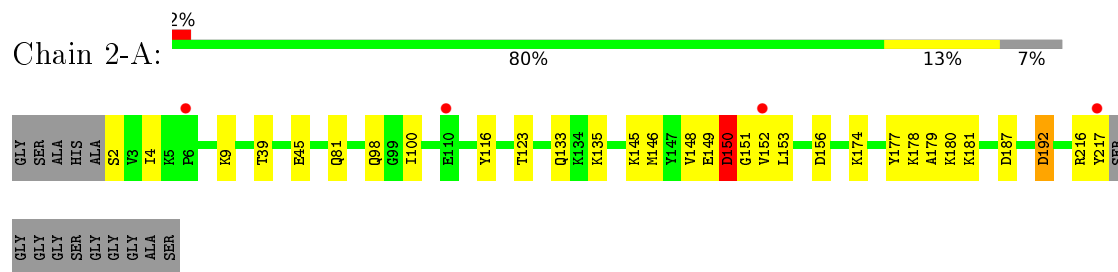
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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.

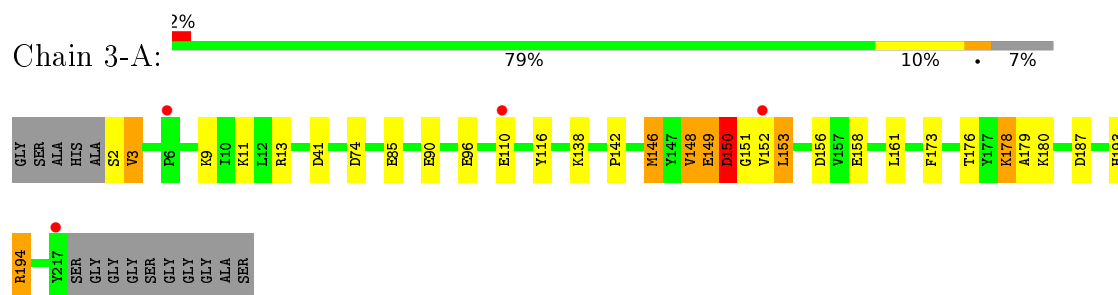
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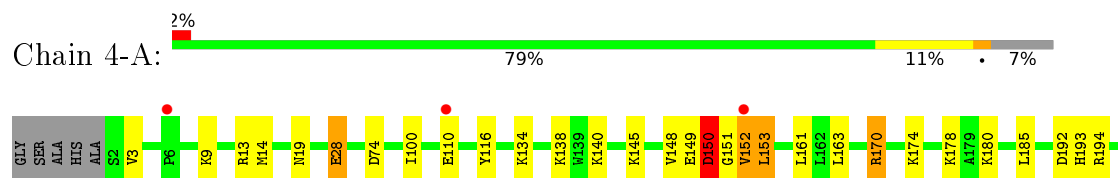
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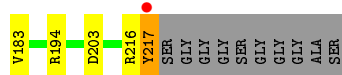
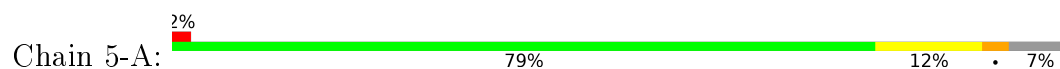


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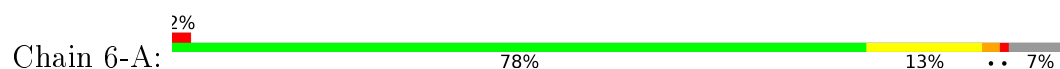




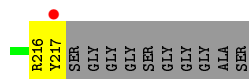
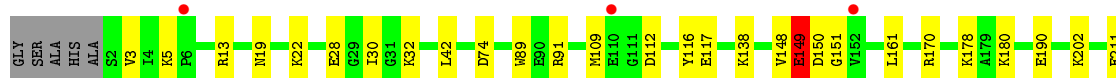
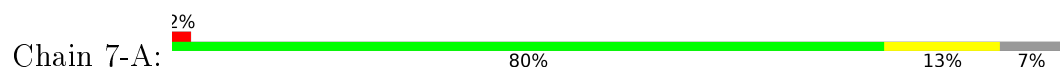
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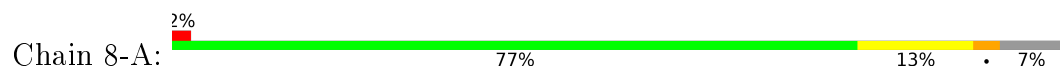
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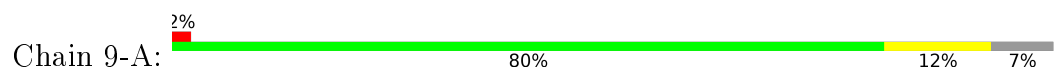
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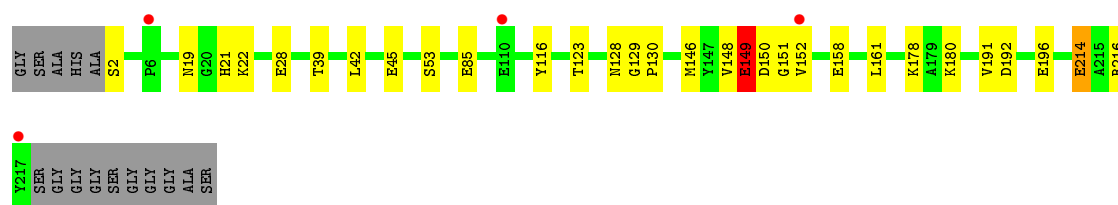


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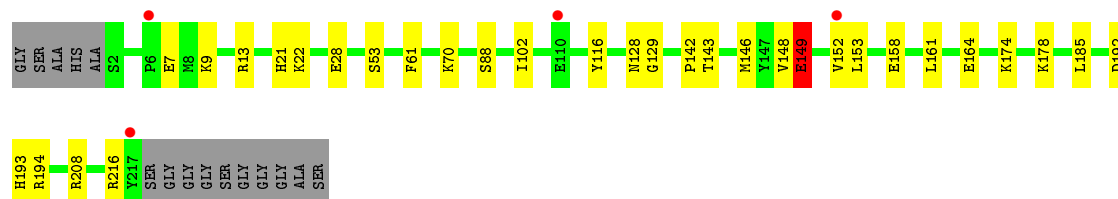
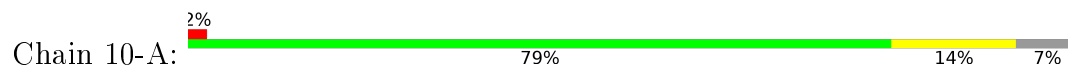


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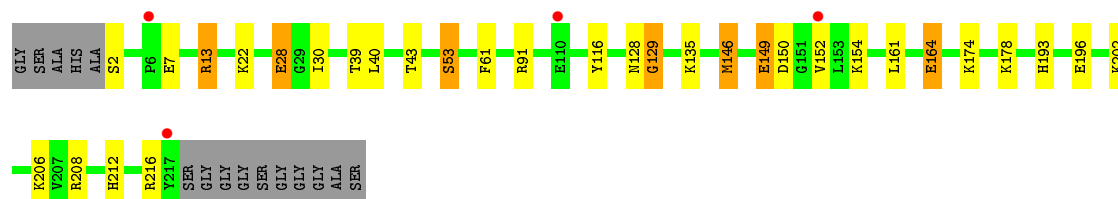
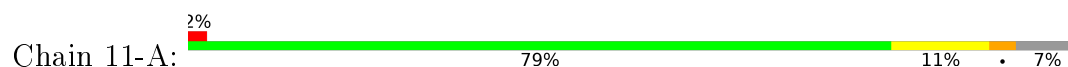




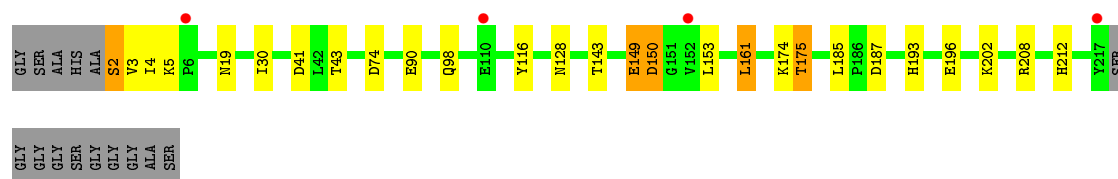
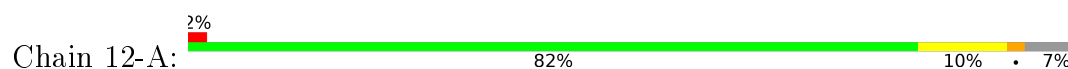
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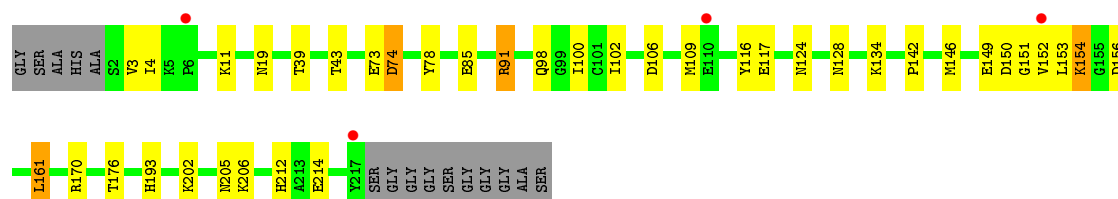
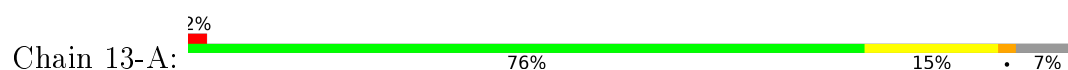
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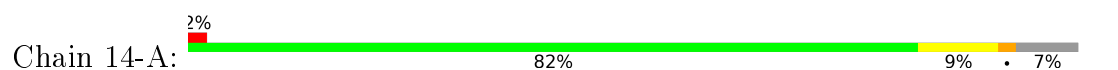
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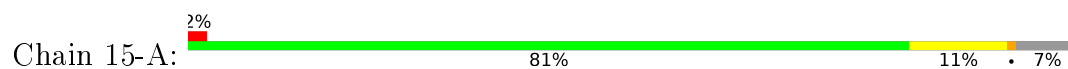
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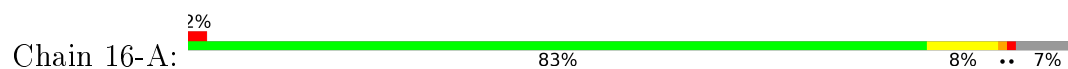
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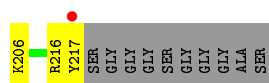
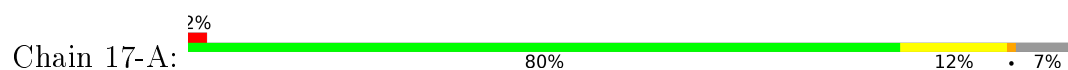
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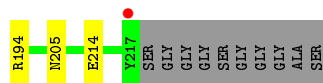
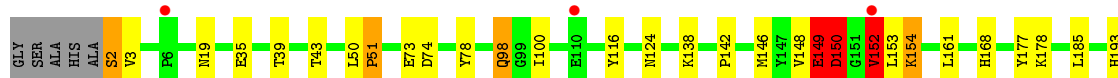
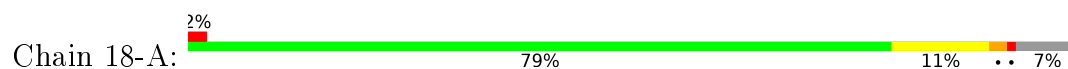
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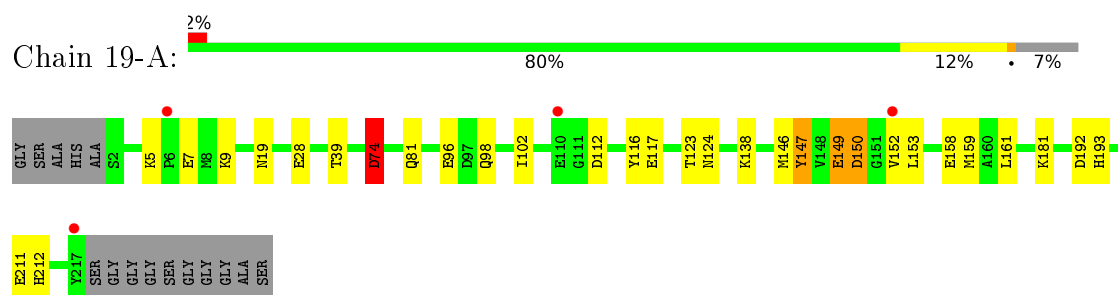
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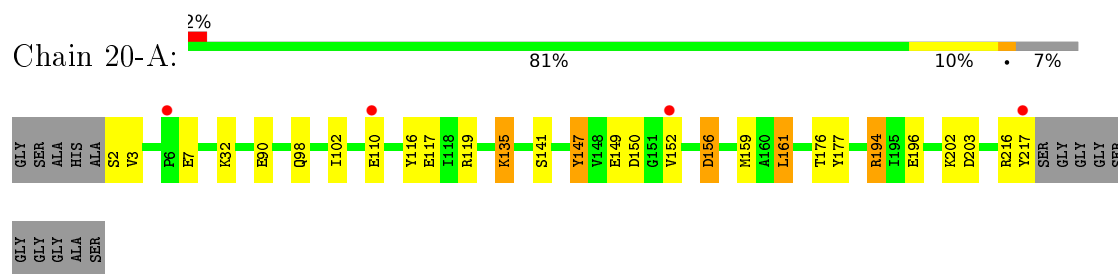
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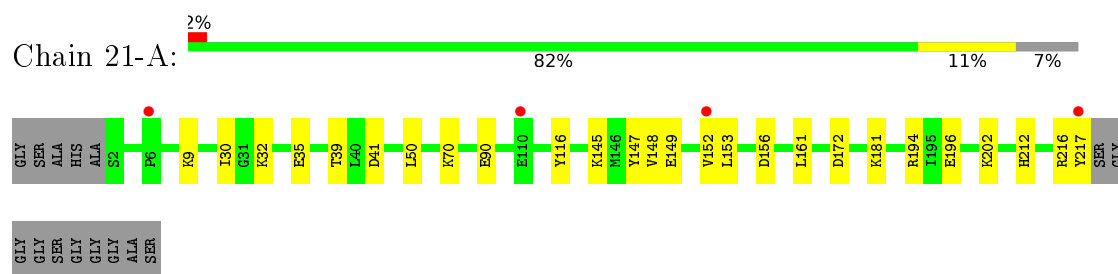
- Molecule 1: Reversibly photoswitching protein Dathail



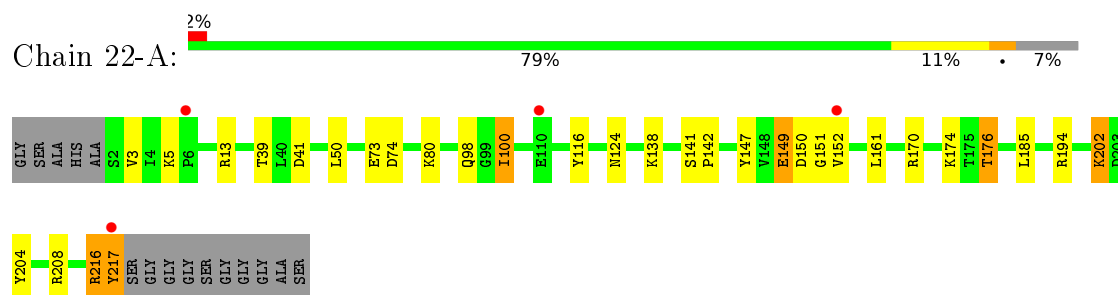
- Molecule 1: Reversibly photoswitching protein Dathail



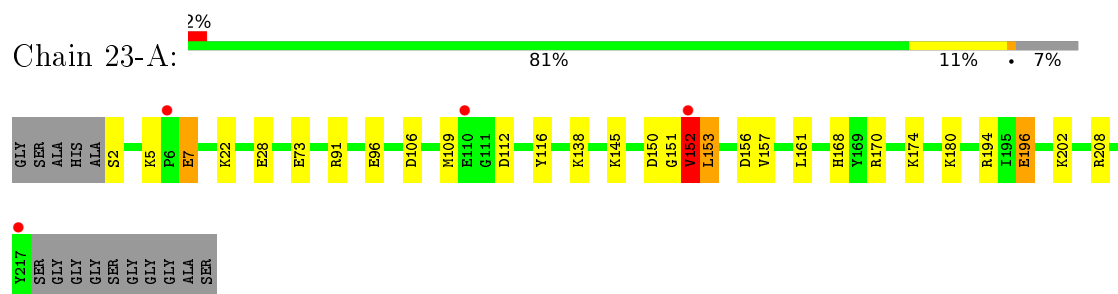
- Molecule 1: Reversibly photoswitching protein Dathail



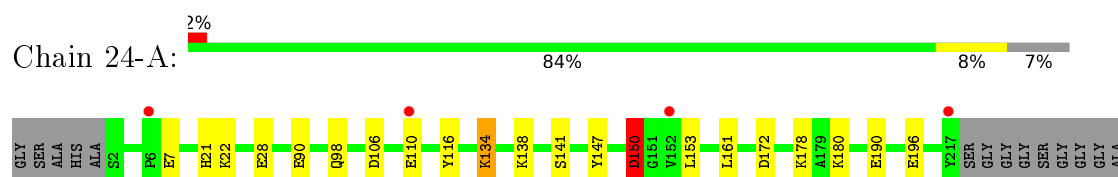
- Molecule 1: Reversibly photoswitching protein Dathail



- Molecule 1: Reversibly photoswitching protein Dathail

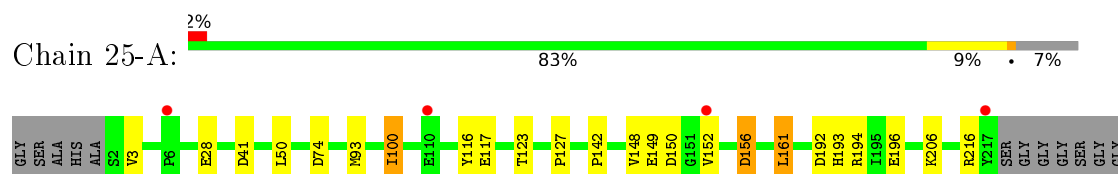


- Molecule 1: Reversibly photoswitching protein Dathail



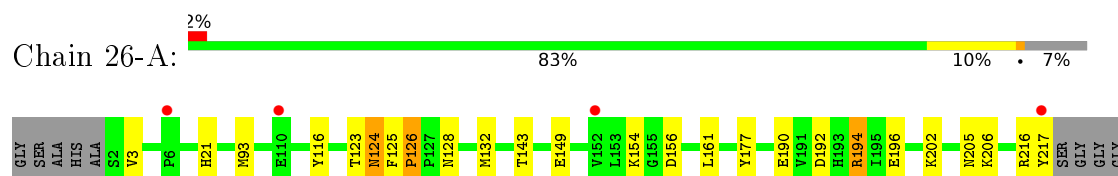
SER

- Molecule 1: Reversibly photoswitching protein Dathail



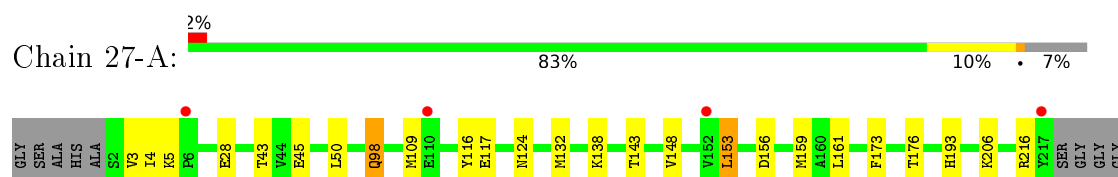
GLY  
ALA  
SER

- Molecule 1: Reversibly photoswitching protein Dathail



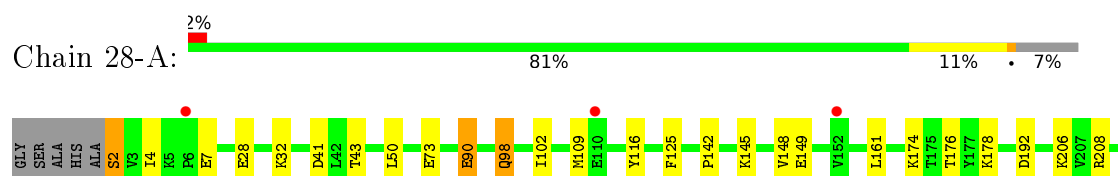
SER  
GLY  
GLY  
GLY  
ALA  
ALA  
SER

- Molecule 1: Reversibly photoswitching protein Dathail



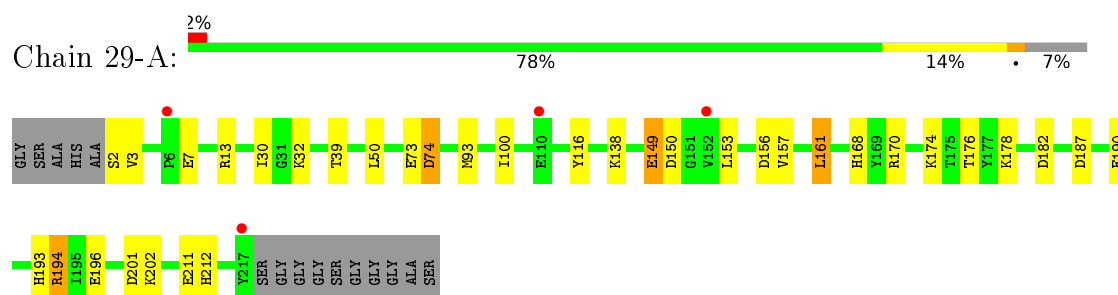
SER  
GLY  
GLY  
GLY  
ALA  
ALA  
SER

- Molecule 1: Reversibly photoswitching protein Dathail

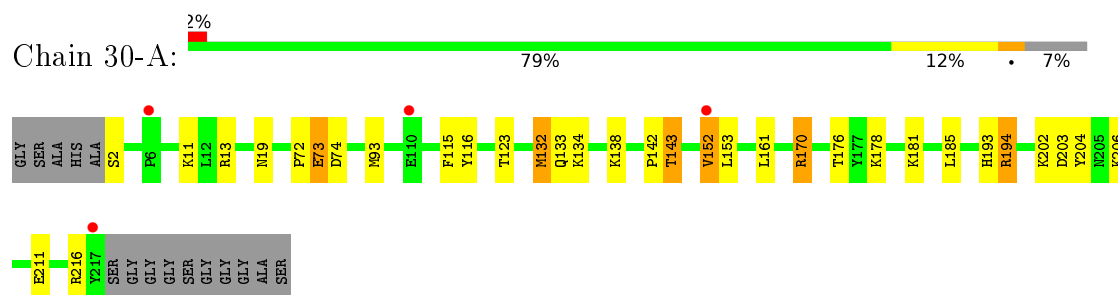


H212  
R216  
Y217  
SER  
GLY  
GLY  
GLY  
SER  
GLY  
GLY  
GLY  
ALA  
SER

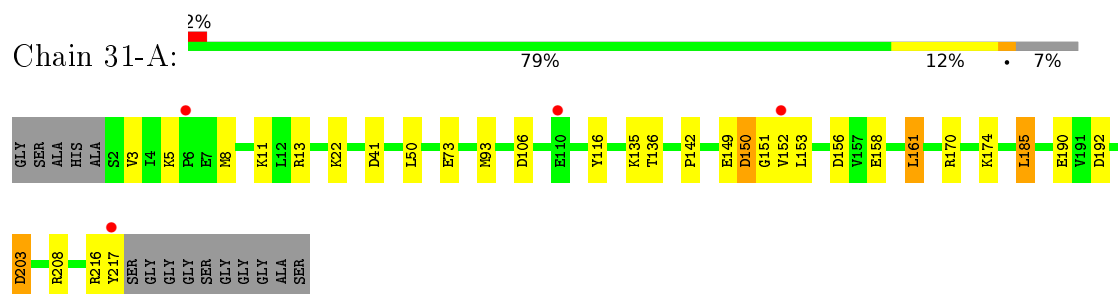
- Molecule 1: Reversibly photoswitching protein Dathail



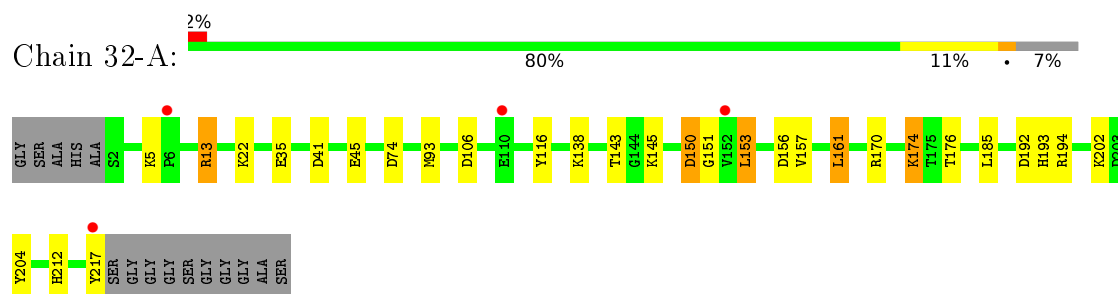
- Molecule 1: Reversibly photoswitching protein Dathail



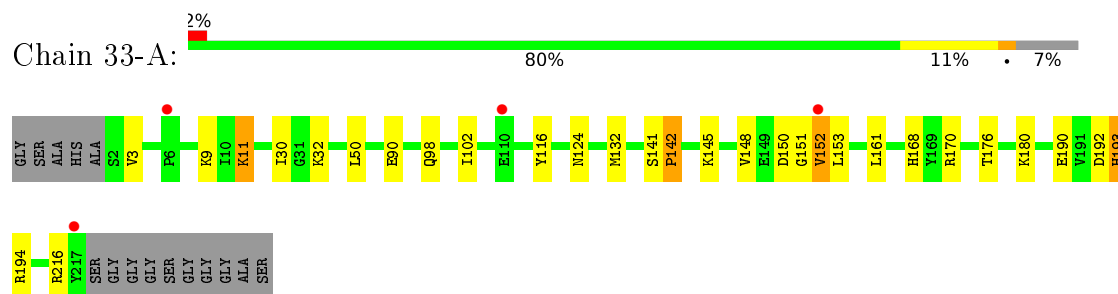
- Molecule 1: Reversibly photoswitching protein Dathail



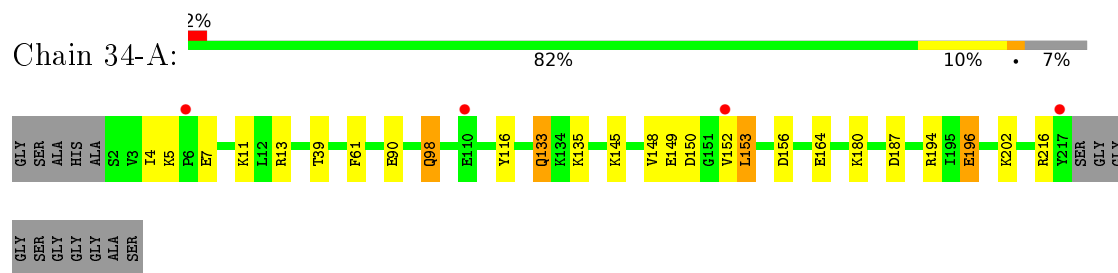
- Molecule 1: Reversibly photoswitching protein Dathail



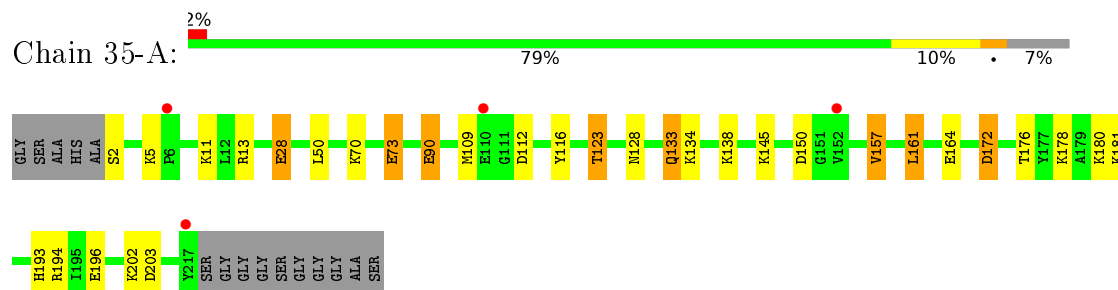
- Molecule 1: Reversibly photoswitching protein Dathail



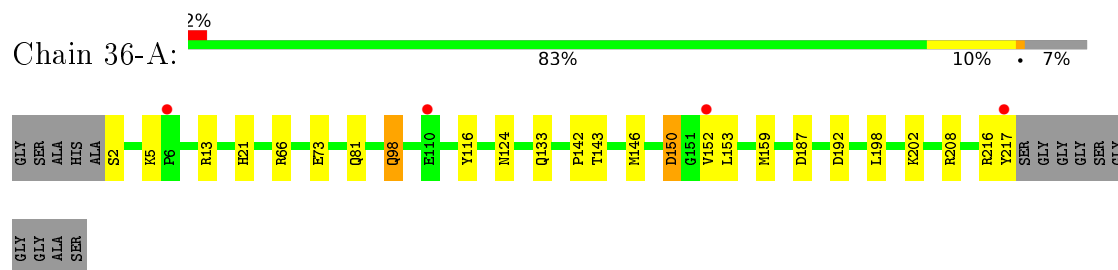
- Molecule 1: Reversibly photoswitching protein Dathail



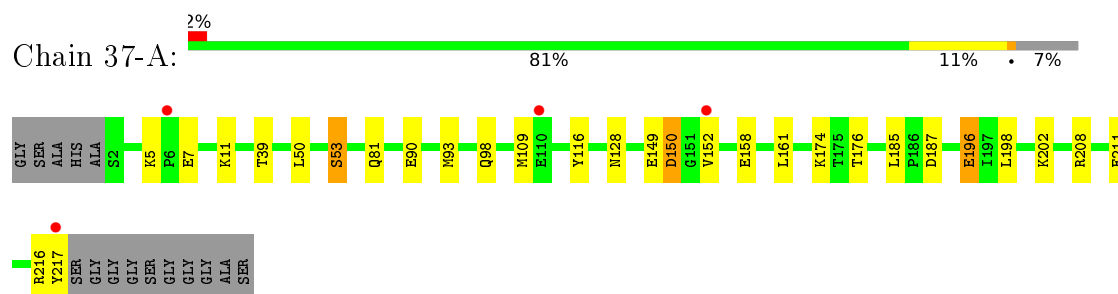
- Molecule 1: Reversibly photoswitching protein Dathail



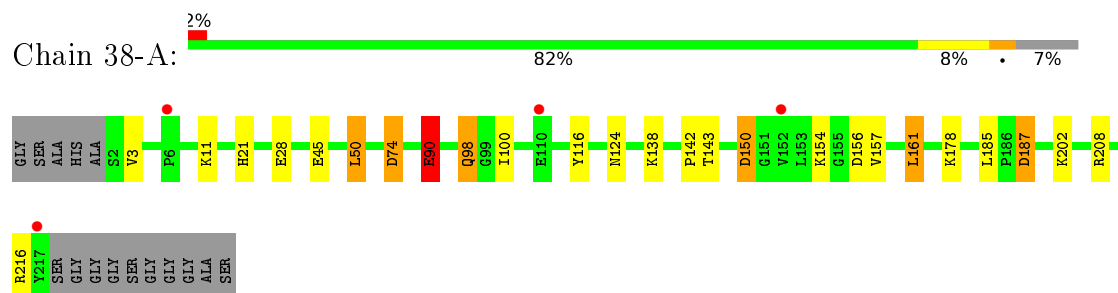
- Molecule 1: Reversibly photoswitching protein Dathail



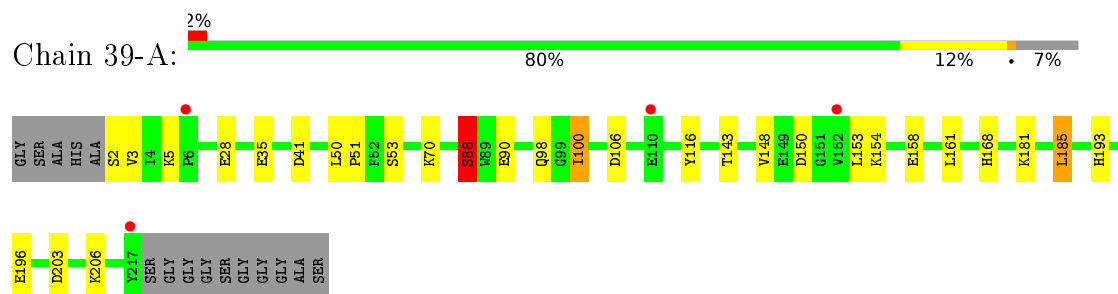
- Molecule 1: Reversibly photoswitching protein Dathail



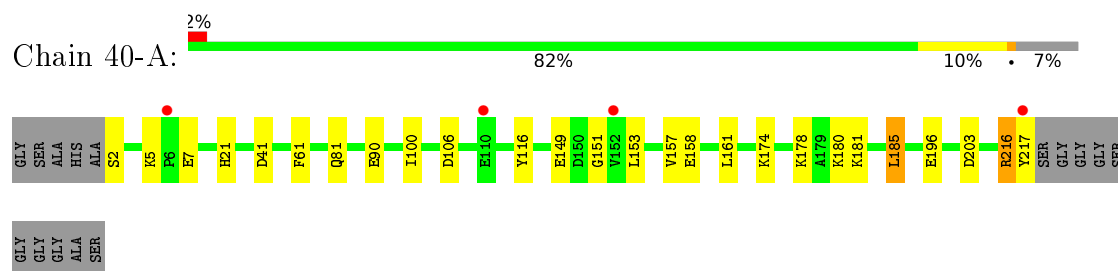
- Molecule 1: Reversibly photoswitching protein Dathail



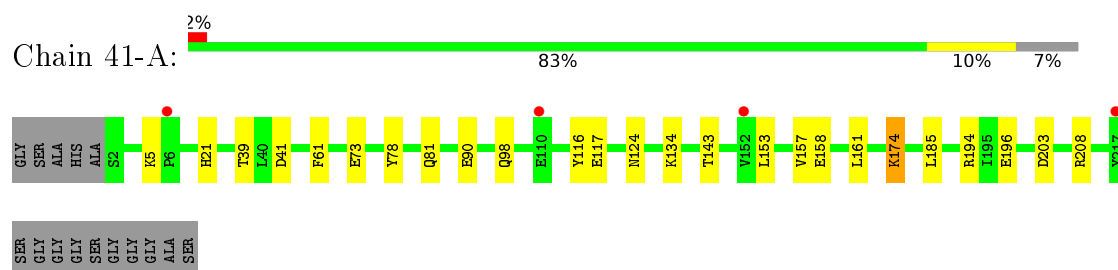
- Molecule 1: Reversibly photoswitching protein Dathail



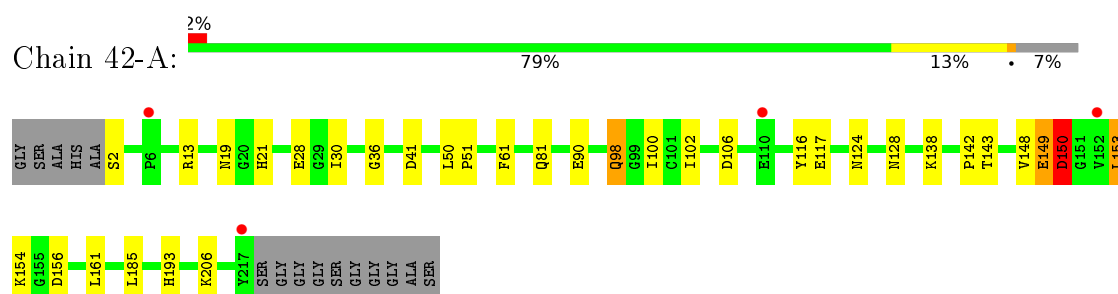
- Molecule 1: Reversibly photoswitching protein Dathail



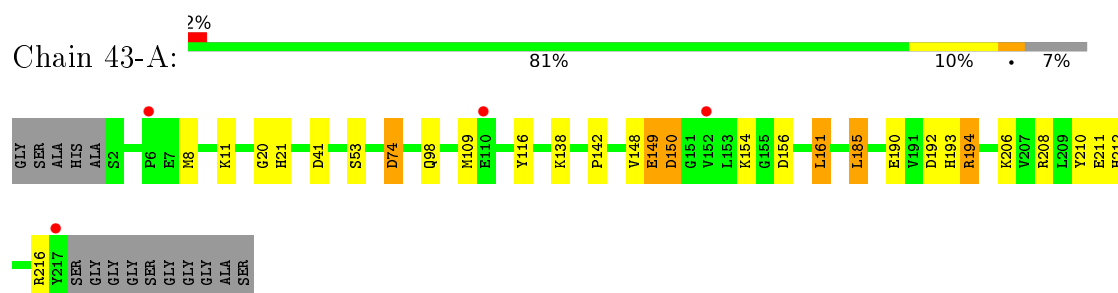
- Molecule 1: Reversibly photoswitching protein Dathail




- Molecule 1: Reversibly photoswitching protein Dathail

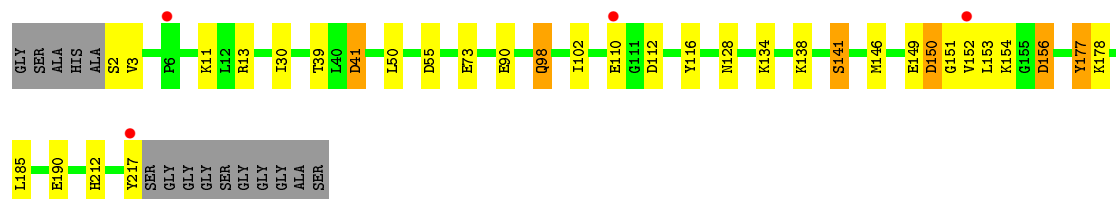


- Molecule 1: Reversibly photoswitching protein Dathail




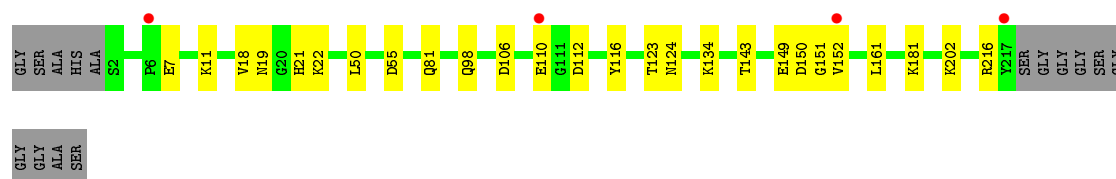
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 44-A: 




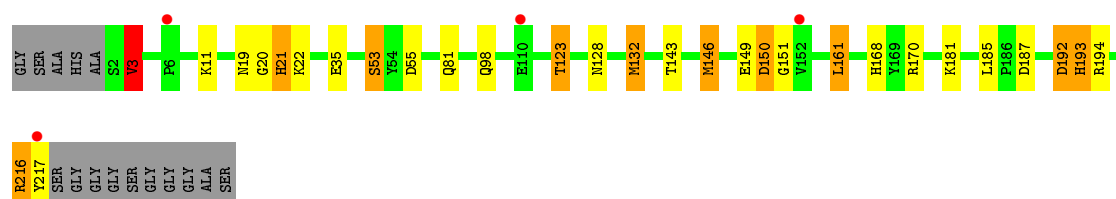
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 45-A: 




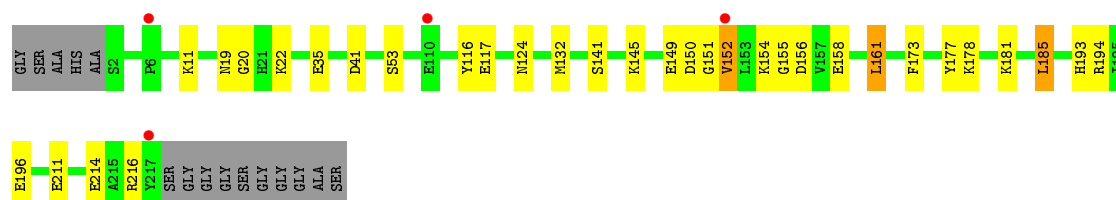
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 46-A: 



- Molecule 1: Reversibly photoswitching protein Dathail

Chain 47-A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.82 (at 1.65Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement: 1.9_1692)	Depositor
R, $R_{free}$	0.151 , 0.194 0.178 , 0.208	Depositor DCC
$R_{free}$ test set	1888 reflections (7.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.6	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<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	0.90	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

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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

All (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
1	35-A	164	GLU	CG-CD	9.21	1.65	1.51
1	35-A	133	GLN	CB-CG	9.09	1.77	1.52
1	24-A	90	GLU	CG-CD	8.63	1.65	1.51
1	32-A	157	VAL	CB-CG2	-8.36	1.35	1.52
1	15-A	176	THR	CA-CB	8.32	1.75	1.53
1	43-A	154	LYS	CG-CD	8.10	1.79	1.52
1	26-A	128	ASN	CB-CG	8.06	1.69	1.51
1	28-A	174	LYS	CD-CE	8.05	1.71	1.51
1	3-A	85	GLU	CB-CG	-8.00	1.36	1.52
1	38-A	90	GLU	CG-CD	7.93	1.63	1.51
1	33-A	90	GLU	CG-CD	7.81	1.63	1.51
1	11-A	164	GLU	CB-CG	7.76	1.66	1.52
1	33-A	161	LEU	CG-CD2	-7.66	1.23	1.51
1	29-A	196	GLU	CD-OE2	-7.62	1.17	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	40-A	161	LEU	CG-CD2	-7.55	1.24	1.51
1	44-A	177	TYR	CD2-CE2	-7.47	1.28	1.39
1	39-A	196	GLU	CB-CG	7.39	1.66	1.52
1	33-A	11	LYS	CE-NZ	-7.26	1.30	1.49
1	14-A	161	LEU	CG-CD2	-7.25	1.25	1.51
1	39-A	88	SER	CB-OG	-7.17	1.32	1.42
1	10-A	152	VAL	CB-CG2	7.14	1.67	1.52
1	23-A	161	LEU	CG-CD2	-7.10	1.25	1.51
1	30-A	161	LEU	CG-CD2	-7.05	1.25	1.51
1	13-A	154	LYS	CG-CD	7.02	1.76	1.52
1	6-A	78	TYR	CD2-CE2	6.96	1.49	1.39
1	34-A	196	GLU	CB-CG	6.90	1.65	1.52
1	26-A	132	MET	CB-CG	6.89	1.73	1.51
1	37-A	161	LEU	CG-CD2	-6.88	1.26	1.51
1	7-A	161	LEU	CG-CD2	-6.85	1.26	1.51
1	11-A	164	GLU	CG-CD	6.83	1.62	1.51
1	27-A	161	LEU	CG-CD2	-6.81	1.26	1.51
1	47-A	158	GLU	CB-CG	-6.79	1.39	1.52
1	3-A	85	GLU	CG-CD	-6.72	1.41	1.51
1	19-A	161	LEU	CG-CD2	-6.70	1.27	1.51
1	4-A	149	GLU	CB-CG	6.69	1.64	1.52
1	37-A	196	GLU	CG-CD	6.69	1.61	1.51
1	18-A	177	TYR	CD1-CE1	-6.67	1.29	1.39
1	9-A	191	VAL	CB-CG2	-6.64	1.39	1.52
1	25-A	196	GLU	CB-CG	6.61	1.64	1.52
1	17-A	73	GLU	CB-CG	6.59	1.64	1.52
1	1-A	81	GLN	CB-CG	6.57	1.70	1.52
1	2-A	135	LYS	CD-CE	6.56	1.67	1.51
1	41-A	90	GLU	CG-CD	6.48	1.61	1.51
1	22-A	161	LEU	CG-CD2	-6.47	1.27	1.51
1	34-A	133	GLN	CB-CG	6.43	1.70	1.52
1	11-A	161	LEU	CG-CD2	-6.40	1.28	1.51
1	3-A	161	LEU	CG-CD2	-6.39	1.28	1.51
1	20-A	90	GLU	CB-CG	-6.39	1.40	1.52
1	23-A	196	GLU	CG-CD	6.36	1.61	1.51
1	21-A	196	GLU	CG-CD	6.36	1.61	1.51
1	9-A	214	GLU	CB-CG	6.30	1.64	1.52
1	11-A	28	GLU	CB-CG	6.30	1.64	1.52
1	20-A	177	TYR	CD1-CE1	-6.30	1.29	1.39
1	46-A	123	THR	CA-CB	6.26	1.69	1.53
1	45-A	161	LEU	CG-CD2	-6.26	1.28	1.51
1	35-A	73	GLU	CB-CG	6.24	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	19-A	74	ASP	CB-CG	6.23	1.64	1.51
1	18-A	154	LYS	CD-CE	6.23	1.66	1.51
1	9-A	196	GLU	CB-CG	6.22	1.64	1.52
1	26-A	161	LEU	CG-CD2	-6.15	1.29	1.51
1	6-A	90	GLU	CB-CG	6.15	1.63	1.52
1	8-A	211	GLU	CB-CG	6.14	1.63	1.52
1	21-A	32	LYS	CD-CE	6.11	1.66	1.51
1	5-A	152	VAL	CB-CG2	6.11	1.65	1.52
1	11-A	28	GLU	CG-CD	6.08	1.61	1.51
1	20-A	135	LYS	CB-CG	6.07	1.69	1.52
1	44-A	156	ASP	CB-CG	6.05	1.64	1.51
1	22-A	149	GLU	CG-CD	6.03	1.60	1.51
1	22-A	176	THR	CB-CG2	-5.99	1.32	1.52
1	27-A	138	LYS	CD-CE	5.99	1.66	1.51
1	6-A	194	ARG	CG-CD	5.96	1.66	1.51
1	11-A	196	GLU	CB-CG	5.94	1.63	1.52
1	7-A	117	GLU	CG-CD	5.92	1.60	1.51
1	1-A	177	TYR	CD1-CE1	-5.92	1.30	1.39
1	38-A	157	VAL	CB-CG2	5.89	1.65	1.52
1	44-A	90	GLU	CB-CG	-5.89	1.41	1.52
1	43-A	53	SER	CB-OG	5.88	1.49	1.42
1	33-A	102	ILE	CB-CG2	-5.86	1.34	1.52
1	27-A	117	GLU	CG-CD	5.85	1.60	1.51
1	3-A	150	ASP	CB-CG	5.83	1.64	1.51
1	15-A	192	ASP	CB-CG	-5.82	1.39	1.51
1	18-A	149	GLU	CG-CD	5.78	1.60	1.51
1	29-A	161	LEU	CG-CD1	-5.78	1.30	1.51
1	4-A	152	VAL	CB-CG2	5.76	1.65	1.52
1	8-A	211	GLU	CG-CD	5.76	1.60	1.51
1	43-A	53	SER	CA-CB	5.76	1.61	1.52
1	3-A	74	ASP	CB-CG	5.74	1.63	1.51
1	28-A	102	ILE	CB-CG2	-5.70	1.35	1.52
1	9-A	149	GLU	CG-CD	5.70	1.60	1.51
1	15-A	110	GLU	CB-CG	5.69	1.62	1.52
1	9-A	158	GLU	CB-CG	-5.68	1.41	1.52
1	11-A	135	LYS	CB-CG	5.68	1.67	1.52
1	43-A	154	LYS	CD-CE	-5.67	1.37	1.51
1	27-A	138	LYS	CE-NZ	5.65	1.63	1.49
1	11-A	53	SER	CA-CB	5.64	1.61	1.52
1	2-A	192	ASP	CB-CG	-5.63	1.40	1.51
1	34-A	196	GLU	CG-CD	5.63	1.60	1.51
1	7-A	211	GLU	CB-CG	5.62	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	30-A	194	ARG	CB-CG	5.60	1.67	1.52
1	30-A	194	ARG	CG-CD	5.59	1.66	1.51
1	43-A	138	LYS	CB-CG	-5.58	1.37	1.52
1	2-A	177	TYR	CD1-CE1	-5.55	1.31	1.39
1	46-A	123	THR	CB-CG2	-5.53	1.34	1.52
1	4-A	149	GLU	N-CA	5.52	1.57	1.46
1	47-A	117	GLU	CG-CD	5.52	1.60	1.51
1	28-A	98	GLN	CB-CG	5.50	1.67	1.52
1	31-A	73	GLU	CB-CG	5.47	1.62	1.52
1	3-A	13	ARG	CG-CD	5.46	1.65	1.51
1	47-A	177	TYR	CD1-CE1	-5.46	1.31	1.39
1	1-A	149	GLU	CG-CD	5.45	1.60	1.51
1	16-A	35	GLU	CB-CG	5.42	1.62	1.52
1	5-A	78	TYR	CB-CG	5.40	1.59	1.51
1	1-A	157	VAL	CB-CG2	-5.39	1.41	1.52
1	8-A	176	THR	CB-CG2	-5.38	1.34	1.52
1	38-A	187	ASP	CB-CG	5.38	1.63	1.51
1	41-A	157	VAL	CB-CG1	-5.38	1.41	1.52
1	8-A	196	GLU	CB-CG	5.37	1.62	1.52
1	23-A	7	GLU	CG-CD	5.37	1.60	1.51
1	6-A	78	TYR	CB-CG	-5.35	1.43	1.51
1	33-A	170	ARG	CZ-NH1	5.34	1.40	1.33
1	1-A	133	GLN	CG-CD	5.29	1.63	1.51
1	28-A	90	GLU	CG-CD	5.26	1.59	1.51
1	35-A	28	GLU	CB-CG	5.25	1.62	1.52
1	18-A	149	GLU	N-CA	5.24	1.56	1.46
1	43-A	194	ARG	CB-CG	5.24	1.66	1.52
1	18-A	161	LEU	CG-CD1	-5.24	1.32	1.51
1	5-A	152	VAL	CB-CG1	5.23	1.63	1.52
1	6-A	161	LEU	CG-CD1	-5.22	1.32	1.51
1	24-A	28	GLU	CB-CG	5.22	1.62	1.52
1	35-A	196	GLU	CG-CD	5.19	1.59	1.51
1	31-A	135	LYS	CE-NZ	5.19	1.62	1.49
1	41-A	174	LYS	CE-NZ	5.19	1.62	1.49
1	4-A	152	VAL	N-CA	5.18	1.56	1.46
1	9-A	178	LYS	CE-NZ	5.17	1.61	1.49
1	1-A	81	GLN	CG-CD	5.16	1.62	1.51
1	26-A	177	TYR	CD1-CE1	-5.15	1.31	1.39
1	47-A	211	GLU	CB-CG	-5.14	1.42	1.52
1	16-A	196	GLU	CB-CG	5.13	1.61	1.52
1	37-A	187	ASP	CB-CG	5.13	1.62	1.51
1	3-A	90	GLU	CB-CG	5.13	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	32-A	174	LYS	CG-CD	-5.12	1.35	1.52
1	4-A	152	VAL	CB-CG1	5.12	1.63	1.52
1	16-A	152	VAL	CB-CG2	5.12	1.63	1.52
1	17-A	123	THR	CA-CB	5.12	1.66	1.53
1	7-A	91	ARG	CZ-NH1	5.10	1.39	1.33
1	12-A	196	GLU	CG-CD	5.10	1.59	1.51
1	29-A	196	GLU	CD-OE1	-5.10	1.20	1.25
1	12-A	90	GLU	CG-CD	5.08	1.59	1.51
1	18-A	150	ASP	CB-CG	5.07	1.62	1.51
1	10-A	146	MET	CG-SD	-5.06	1.68	1.81
1	24-A	196	GLU	CG-CD	5.05	1.59	1.51
1	22-A	13	ARG	CG-CD	5.04	1.64	1.51
1	1-A	152	VAL	CB-CG2	5.04	1.63	1.52
1	39-A	196	GLU	CG-CD	5.03	1.59	1.51

All (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
1	21-A	194	ARG	NE-CZ-NH2	-11.34	114.63	120.30
1	7-A	91	ARG	NE-CZ-NH2	-11.06	114.77	120.30
1	14-A	153	LEU	CB-CG-CD1	-10.69	92.83	111.00
1	11-A	91	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	21-A	194	ARG	NE-CZ-NH1	10.49	125.55	120.30
1	33-A	170	ARG	NE-CZ-NH2	-10.14	115.23	120.30
1	29-A	93	MET	CG-SD-CE	9.71	115.73	100.20
1	35-A	157	VAL	CB-CA-C	-9.66	93.04	111.40
1	32-A	93	MET	CG-SD-CE	9.62	115.58	100.20
1	20-A	194	ARG	NE-CZ-NH1	9.45	125.02	120.30
1	43-A	53	SER	CB-CA-C	-9.33	92.38	110.10
1	32-A	170	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	8-A	172	ASP	CB-CG-OD1	-8.79	110.39	118.30
1	17-A	151	GLY	N-CA-C	-8.71	91.33	113.10
1	11-A	53	SER	N-CA-CB	8.59	123.39	110.50
1	32-A	156	ASP	CB-CG-OD1	-8.59	110.57	118.30
1	33-A	170	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	14-A	208	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	12-A	150	ASP	CB-CG-OD1	8.41	125.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5-A	217	TYR	CB-CG-CD1	8.41	126.04	121.00
1	30-A	152	VAL	CB-CA-C	-8.28	95.66	111.40
1	43-A	53	SER	N-CA-CB	8.24	122.86	110.50
1	4-A	149	GLU	N-CA-C	8.23	133.21	111.00
1	39-A	185	LEU	CA-CB-CG	8.21	134.18	115.30
1	7-A	138	LYS	CD-CE-NZ	8.18	130.52	111.70
1	36-A	208	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	12-A	175	THR	CB-CA-C	-8.03	89.92	111.60
1	8-A	152	VAL	CB-CA-C	-8.01	96.17	111.40
1	18-A	194	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	8-A	170	ARG	NE-CZ-NH2	-7.81	116.40	120.30
1	43-A	150	ASP	CB-CG-OD2	7.79	125.31	118.30
1	11-A	152	VAL	N-CA-C	-7.78	90.01	111.00
1	24-A	134	LYS	CD-CE-NZ	7.76	129.55	111.70
1	45-A	106	ASP	CB-CG-OD1	7.74	125.26	118.30
1	43-A	208	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	42-A	153	LEU	CB-CG-CD1	-7.64	98.02	111.00
1	2-A	174	LYS	CD-CE-NZ	7.62	129.23	111.70
1	33-A	102	ILE	CB-CA-C	7.61	126.83	111.60
1	5-A	217	TYR	CB-CG-CD2	-7.57	116.46	121.00
1	8-A	161	LEU	CA-CB-CG	7.54	132.65	115.30
1	25-A	93	MET	CG-SD-CE	7.45	112.12	100.20
1	7-A	91	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	19-A	159	MET	CG-SD-CE	7.36	111.98	100.20
1	22-A	151	GLY	N-CA-C	-7.33	94.77	113.10
1	43-A	185	LEU	CA-CB-CG	7.31	132.11	115.30
1	29-A	196	GLU	OE1-CD-OE2	-7.29	114.55	123.30
1	27-A	159	MET	CG-SD-CE	-7.29	88.53	100.20
1	15-A	176	THR	CB-CA-C	7.28	131.26	111.60
1	10-A	152	VAL	CB-CA-C	7.28	125.22	111.40
1	40-A	185	LEU	CA-CB-CG	7.27	132.03	115.30
1	47-A	185	LEU	CB-CG-CD1	7.26	123.34	111.00
1	32-A	170	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	16-A	161	LEU	CB-CG-CD1	-7.17	98.82	111.00
1	11-A	13	ARG	NE-CZ-NH1	-7.13	116.73	120.30
1	14-A	170	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	1-A	154	LYS	CD-CE-NZ	7.08	127.99	111.70
1	43-A	216	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	5-A	170	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	3-A	194	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	30-A	170	ARG	NE-CZ-NH2	6.97	123.79	120.30
1	24-A	196	GLU	OE1-CD-OE2	-6.94	114.97	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-A	14	MET	CG-SD-CE	6.93	111.28	100.20
1	26-A	93	MET	CG-SD-CE	6.92	111.28	100.20
1	24-A	150	ASP	CB-CG-OD2	6.89	124.50	118.30
1	10-A	194	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	31-A	170	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	11-A	13	ARG	NE-CZ-NH2	6.81	123.71	120.30
1	35-A	172	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	33-A	132	MET	CG-SD-CE	6.77	111.03	100.20
1	3-A	150	ASP	N-CA-C	-6.73	92.84	111.00
1	7-A	151	GLY	N-CA-C	6.72	129.91	113.10
1	35-A	123	THR	CB-CA-C	-6.72	93.46	111.60
1	33-A	193	HIS	CB-CA-C	-6.71	96.98	110.40
1	10-A	208	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	14-A	13	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	47-A	41	ASP	CB-CG-OD1	6.63	124.27	118.30
1	5-A	217	TYR	CA-CB-CG	6.63	125.99	113.40
1	43-A	208	ARG	NE-CZ-NH2	-6.63	116.99	120.30
1	14-A	154	LYS	N-CA-CB	6.61	122.49	110.60
1	39-A	185	LEU	CB-CG-CD2	6.58	122.19	111.00
1	44-A	152	VAL	N-CA-C	-6.52	93.39	111.00
1	6-A	175	THR	CB-CA-C	-6.48	94.11	111.60
1	47-A	152	VAL	N-CA-C	-6.47	93.53	111.00
1	44-A	138	LYS	CD-CE-NZ	6.46	126.57	111.70
1	8-A	158	GLU	CB-CA-C	-6.46	97.47	110.40
1	13-A	161	LEU	CB-CG-CD1	6.46	121.97	111.00
1	37-A	93	MET	CG-SD-CE	6.44	110.50	100.20
1	2-A	151	GLY	N-CA-C	-6.41	97.07	113.10
1	23-A	170	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	32-A	106	ASP	CB-CG-OD2	6.41	124.06	118.30
1	3-A	161	LEU	CB-CG-CD2	-6.40	100.11	111.00
1	28-A	102	ILE	CB-CA-C	6.38	124.37	111.60
1	37-A	53	SER	N-CA-CB	6.34	120.00	110.50
1	29-A	190	GLU	CB-CA-C	-6.32	97.75	110.40
1	9-A	191	VAL	CB-CA-C	-6.31	99.42	111.40
1	45-A	55	ASP	CB-CG-OD1	-6.27	112.66	118.30
1	1-A	185	LEU	CB-CG-CD2	-6.26	100.36	111.00
1	46-A	53	SER	N-CA-CB	-6.26	101.12	110.50
1	46-A	21	HIS	CB-CA-C	6.24	122.87	110.40
1	23-A	91	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	26-A	156	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	13-A	91	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	31-A	161	LEU	CA-CB-CG	6.15	129.44	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	14-A	170	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	8-A	100	ILE	CB-CA-C	-6.12	99.37	111.60
1	20-A	156	ASP	CB-CG-OD1	-6.12	112.79	118.30
1	19-A	147	TYR	CA-CB-CG	6.10	125.00	113.40
1	27-A	161	LEU	CB-CG-CD2	-6.10	100.63	111.00
1	44-A	102	ILE	CB-CA-C	-6.09	99.43	111.60
1	41-A	41	ASP	CB-CG-OD1	6.07	123.76	118.30
1	28-A	208	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	8-A	170	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	11-A	91	ARG	CD-NE-CZ	6.05	132.07	123.60
1	3-A	150	ASP	CB-CG-OD1	6.05	123.74	118.30
1	5-A	170	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	34-A	90	GLU	OE1-CD-OE2	-6.03	116.06	123.30
1	10-A	192	ASP	CB-CG-OD1	-6.03	112.88	118.30
1	32-A	13	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	14-A	20	GLY	N-CA-C	-6.02	98.06	113.10
1	32-A	106	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	43-A	156	ASP	CB-CA-C	5.98	122.37	110.40
1	20-A	147	TYR	CA-CB-CG	5.96	124.72	113.40
1	25-A	156	ASP	N-CA-CB	5.96	121.32	110.60
1	13-A	146	MET	CG-SD-CE	-5.96	90.67	100.20
1	15-A	161	LEU	CB-CG-CD2	-5.94	100.90	111.00
1	29-A	194	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	41-A	161	LEU	CB-CG-CD2	-5.91	100.95	111.00
1	46-A	3	VAL	N-CA-C	5.91	126.96	111.00
1	3-A	150	ASP	CB-CA-C	5.91	122.22	110.40
1	26-A	194	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	29-A	74	ASP	N-CA-CB	-5.89	100.00	110.60
1	36-A	159	MET	CG-SD-CE	-5.89	90.78	100.20
1	42-A	150	ASP	N-CA-C	-5.89	95.11	111.00
1	13-A	91	ARG	CB-CA-C	-5.88	98.63	110.40
1	26-A	124	ASN	CA-C-N	-5.88	104.27	117.20
1	33-A	152	VAL	N-CA-C	-5.86	95.19	111.00
1	47-A	149	GLU	CB-CA-C	5.85	122.11	110.40
1	23-A	138	LYS	CD-CE-NZ	5.85	125.15	111.70
1	4-A	170	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	17-A	170	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	20-A	194	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	23-A	153	LEU	CB-CG-CD2	-5.80	101.13	111.00
1	13-A	74	ASP	CB-CG-OD1	5.79	123.51	118.30
1	16-A	149	GLU	N-CA-C	5.78	126.61	111.00
1	43-A	149	GLU	N-CA-C	-5.78	95.40	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	46-A	132	MET	CG-SD-CE	-5.77	90.97	100.20
1	35-A	90	GLU	CB-CA-C	5.75	121.91	110.40
1	29-A	149	GLU	N-CA-C	-5.74	95.50	111.00
1	5-A	161	LEU	CB-CG-CD1	5.73	120.75	111.00
1	41-A	208	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	22-A	100	ILE	CB-CA-C	-5.73	100.15	111.60
1	5-A	153	LEU	CB-CG-CD2	5.72	120.73	111.00
1	20-A	119	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	33-A	192	ASP	CB-CG-OD1	5.72	123.45	118.30
1	12-A	161	LEU	CB-CG-CD1	5.71	120.71	111.00
1	23-A	170	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	38-A	50	LEU	CB-CG-CD1	5.71	120.71	111.00
1	4-A	151	GLY	N-CA-C	-5.69	98.87	113.10
1	34-A	153	LEU	CB-CG-CD2	5.67	120.65	111.00
1	11-A	146	MET	CA-CB-CG	5.66	122.92	113.30
1	5-A	194	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	47-A	161	LEU	CB-CG-CD1	5.62	120.55	111.00
1	19-A	102	ILE	CB-CA-C	-5.60	100.39	111.60
1	5-A	156	ASP	CB-CG-OD1	5.60	123.34	118.30
1	19-A	193	HIS	CB-CA-C	-5.60	99.20	110.40
1	41-A	208	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	23-A	208	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	21-A	196	GLU	CA-CB-CG	5.59	125.70	113.40
1	11-A	154	LYS	CD-CE-NZ	5.54	124.44	111.70
1	32-A	150	ASP	CB-CG-OD1	5.54	123.28	118.30
1	26-A	125	PHE	N-CA-C	-5.53	96.06	111.00
1	30-A	143	THR	N-CA-C	-5.51	96.12	111.00
1	43-A	161	LEU	CB-CG-CD1	5.50	120.36	111.00
1	8-A	106	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	7-A	161	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	11-A	164	GLU	OE1-CD-OE2	-5.49	116.72	123.30
1	18-A	161	LEU	CB-CG-CD1	-5.48	101.68	111.00
1	18-A	150	ASP	CB-CA-C	5.47	121.34	110.40
1	25-A	100	ILE	CG1-CB-CG2	-5.45	99.42	111.40
1	45-A	98	GLN	CA-CB-CG	5.45	125.38	113.40
1	27-A	153	LEU	CA-CB-CG	5.44	127.82	115.30
1	40-A	157	VAL	CB-CA-C	-5.44	101.06	111.40
1	6-A	156	ASP	CB-CG-OD1	5.43	123.19	118.30
1	41-A	158	GLU	CA-CB-CG	5.42	125.33	113.40
1	20-A	159	MET	CG-SD-CE	-5.42	91.53	100.20
1	13-A	78	TYR	OH-CZ-CE2	-5.42	105.48	120.10
1	27-A	153	LEU	CB-CA-C	5.42	120.49	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	31-A	185	LEU	CA-CB-CG	5.41	127.75	115.30
1	8-A	153	LEU	CB-CG-CD2	-5.41	101.80	111.00
1	26-A	3	VAL	CB-CA-C	-5.38	101.18	111.40
1	10-A	208	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	27-A	138	LYS	CD-CE-NZ	5.38	124.07	111.70
1	19-A	161	LEU	CB-CG-CD2	-5.37	101.87	111.00
1	6-A	161	LEU	CB-CG-CD1	-5.37	101.88	111.00
1	7-A	13	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	44-A	41	ASP	CB-CG-OD1	5.36	123.12	118.30
1	28-A	174	LYS	CD-CE-NZ	5.36	124.02	111.70
1	32-A	161	LEU	CA-CB-CG	5.36	127.62	115.30
1	43-A	216	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	38-A	161	LEU	CA-CB-CG	5.35	127.61	115.30
1	3-A	173	PHE	CB-CG-CD2	-5.33	117.07	120.80
1	32-A	161	LEU	CB-CG-CD1	5.33	120.05	111.00
1	40-A	41	ASP	CB-CG-OD1	5.32	123.09	118.30
1	25-A	161	LEU	CB-CG-CD1	5.30	120.01	111.00
1	41-A	41	ASP	N-CA-CB	5.29	120.12	110.60
1	39-A	100	ILE	CB-CA-C	-5.29	101.02	111.60
1	11-A	129	GLY	N-CA-C	5.29	126.32	113.10
1	46-A	161	LEU	CA-CB-CG	5.28	127.45	115.30
1	4-A	217	TYR	CA-CB-CG	5.28	123.43	113.40
1	26-A	156	ASP	CB-CG-OD1	5.27	123.04	118.30
1	1-A	157	VAL	CB-CA-C	-5.27	101.39	111.40
1	38-A	90	GLU	CB-CA-C	5.26	120.92	110.40
1	39-A	53	SER	CB-CA-C	-5.26	100.11	110.10
1	21-A	156	ASP	CB-CG-OD1	5.25	123.03	118.30
1	27-A	98	GLN	CB-CA-C	-5.25	99.89	110.40
1	46-A	146	MET	CB-CG-SD	5.25	128.16	112.40
1	1-A	161	LEU	CA-CB-CG	5.23	127.34	115.30
1	14-A	154	LYS	CB-CG-CD	5.23	125.20	111.60
1	41-A	90	GLU	CB-CA-C	-5.23	99.94	110.40
1	38-A	208	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	40-A	106	ASP	CB-CA-C	5.23	120.85	110.40
1	16-A	217	TYR	CA-CB-CG	5.21	123.31	113.40
1	35-A	133	GLN	CA-CB-CG	5.21	124.87	113.40
1	6-A	150	ASP	CB-CG-OD2	5.21	122.99	118.30
1	22-A	13	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	4-A	153	LEU	CB-CG-CD1	5.20	119.84	111.00
1	35-A	161	LEU	CA-CB-CG	5.19	127.24	115.30
1	27-A	173	PHE	CB-CG-CD2	-5.19	117.17	120.80
1	10-A	194	ARG	NE-CZ-NH1	5.19	122.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	24-A	90	GLU	OE1-CD-OE2	-5.19	117.08	123.30
1	19-A	146	MET	CB-CG-SD	-5.18	96.84	112.40
1	23-A	161	LEU	CB-CG-CD2	-5.18	102.20	111.00
1	31-A	152	VAL	CA-CB-CG2	5.18	118.66	110.90
1	1-A	178	LYS	N-CA-C	5.16	124.93	111.00
1	47-A	173	PHE	CB-CA-C	-5.16	100.08	110.40
1	3-A	74	ASP	CB-CG-OD2	5.16	122.94	118.30
1	34-A	194	ARG	CG-CD-NE	5.15	122.62	111.80
1	39-A	88	SER	CB-CA-C	-5.15	100.31	110.10
1	43-A	210	TYR	CA-CB-CG	5.15	123.18	113.40
1	26-A	125	PHE	N-CA-CB	-5.14	101.34	110.60
1	36-A	208	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	6-A	74	ASP	CB-CG-OD1	-5.14	113.67	118.30
1	14-A	146	MET	CG-SD-CE	5.14	108.42	100.20
1	18-A	194	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	30-A	132	MET	CB-CG-SD	5.14	127.81	112.40
1	7-A	170	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	32-A	153	LEU	CA-CB-CG	5.13	127.11	115.30
1	43-A	161	LEU	CA-CB-CG	5.13	127.11	115.30
1	19-A	153	LEU	CB-CG-CD1	-5.13	102.28	111.00
1	22-A	217	TYR	N-CA-CB	5.13	119.84	110.60
1	5-A	161	LEU	CA-CB-CG	5.13	127.09	115.30
1	1-A	81	GLN	CB-CG-CD	5.12	124.91	111.60
1	13-A	106	ASP	CB-CG-OD1	5.12	122.91	118.30
1	29-A	194	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	31-A	161	LEU	CB-CG-CD1	5.11	119.69	111.00
1	11-A	193	HIS	CB-CA-C	-5.10	100.19	110.40
1	36-A	66	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	31-A	93	MET	CG-SD-CE	-5.09	92.06	100.20
1	20-A	161	LEU	CA-CB-CG	5.08	126.98	115.30
1	23-A	152	VAL	N-CA-C	5.07	124.68	111.00
1	35-A	157	VAL	CG1-CB-CG2	5.07	119.00	110.90
1	6-A	149	GLU	N-CA-C	5.06	124.67	111.00
1	22-A	80	LYS	CD-CE-NZ	-5.06	100.06	111.70
1	2-A	135	LYS	CD-CE-NZ	5.06	123.34	111.70
1	36-A	146	MET	CG-SD-CE	-5.06	92.10	100.20
1	3-A	194	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	18-A	149	GLU	N-CA-C	5.05	124.62	111.00
1	19-A	153	LEU	N-CA-C	5.04	124.62	111.00
1	44-A	146	MET	CG-SD-CE	5.04	108.26	100.20
1	5-A	194	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	19-A	153	LEU	CB-CA-C	-5.03	100.64	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-A	146	MET	CB-CG-SD	5.01	127.44	112.40

There are no chirality outliers.

All (86) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	10-A	129	GLY	Peptide
1	10-A	148	VAL	Peptide
1	10-A	149	GLU	Peptide
1	10-A	61	PHE	Mainchain
1	11-A	149	GLU	Peptide
1	11-A	61	PHE	Mainchain
1	12-A	128	ASN	Peptide
1	12-A	149	GLU	Peptide
1	12-A	2	SER	Peptide
1	12-A	74	ASP	Peptide
1	14-A	149	GLU	Peptide
1	14-A	150	ASP	Peptide
1	14-A	151	GLY	Peptide
1	14-A	19	ASN	Peptide
1	14-A	21	HIS	Peptide
1	15-A	216	ARG	Peptide
1	17-A	148	VAL	Peptide
1	17-A	216	ARG	Peptide
1	17-A	61	PHE	Mainchain
1	18-A	148	VAL	Peptide
1	18-A	150	ASP	Peptide
1	18-A	152	VAL	Peptide
1	18-A	2	SER	Peptide
1	18-A	98	GLN	Peptide
1	19-A	149	GLU	Peptide
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	22-A	216	ARG	Peptide
1	23-A	150	ASP	Peptide
1	23-A	151	GLY	Peptide
1	25-A	149	GLU	Peptide
1	25-A	152	VAL	Peptide
1	26-A	123	THR	Peptide
1	28-A	2	SER	Peptide

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Mol	Chain	Res	Type	Group
1	3-A	148	VAL	Peptide
1	3-A	150	ASP	Peptide
1	3-A	151	GLY	Peptide
1	3-A	178	LYS	Peptide
1	3-A	2	SER	Peptide
1	3-A	3	VAL	Peptide
1	30-A	73	GLU	Peptide
1	31-A	150	ASP	Peptide
1	31-A	216	ARG	Peptide
1	32-A	151	GLY	Peptide
1	34-A	61	PHE	Mainchain
1	36-A	150	ASP	Peptide
1	37-A	149	GLU	Peptide
1	38-A	74	ASP	Peptide
1	38-A	90	GLU	Peptide
1	39-A	88	SER	Peptide
1	4-A	148	VAL	Peptide
1	4-A	150	ASP	Peptide
1	40-A	216	ARG	Peptide
1	40-A	61	PHE	Mainchain
1	41-A	61	PHE	Mainchain
1	42-A	149	GLU	Peptide
1	42-A	150	ASP	Peptide
1	42-A	21	HIS	Peptide
1	42-A	61	PHE	Mainchain
1	42-A	98	GLN	Peptide
1	43-A	20	GLY	Peptide
1	43-A	74	ASP	Peptide
1	44-A	149	GLU	Peptide
1	45-A	123	THR	Peptide
1	45-A	149	GLU	Peptide
1	45-A	152	VAL	Peptide
1	45-A	18	VAL	Peptide
1	46-A	149	GLU	Peptide
1	46-A	192	ASP	Peptide
1	46-A	20	GLY	Peptide
1	46-A	216	ARG	Peptide
1	47-A	155	GLY	Peptide
1	5-A	148	VAL	Peptide
1	6-A	148	VAL	Peptide
1	6-A	149	GLU	Peptide
1	6-A	27	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	6-A	98	GLN	Peptide
1	7-A	148	VAL	Peptide
1	7-A	149	GLU	Peptide
1	8-A	148	VAL	Peptide
1	8-A	149	GLU	Peptide
1	9-A	148	VAL	Peptide
1	9-A	149	GLU	Peptide
1	9-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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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%)	6	0
1	2-A	211/229 (92%)	195 (92%)	13 (6%)	3 (1%)	14	1
1	3-A	211/229 (92%)	194 (92%)	11 (5%)	6 (3%)	6	0
1	4-A	211/229 (92%)	200 (95%)	7 (3%)	4 (2%)	10	0
1	5-A	211/229 (92%)	200 (95%)	5 (2%)	6 (3%)	6	0
1	6-A	211/229 (92%)	196 (93%)	6 (3%)	9 (4%)	3	0
1	7-A	211/229 (92%)	199 (94%)	8 (4%)	4 (2%)	10	0
1	8-A	211/229 (92%)	201 (95%)	3 (1%)	7 (3%)	5	0
1	9-A	211/229 (92%)	200 (95%)	7 (3%)	4 (2%)	10	0
1	10-A	211/229 (92%)	202 (96%)	7 (3%)	2 (1%)	21	4
1	11-A	211/229 (92%)	199 (94%)	9 (4%)	3 (1%)	14	1
1	12-A	211/229 (92%)	198 (94%)	11 (5%)	2 (1%)	21	4
1	13-A	211/229 (92%)	197 (93%)	10 (5%)	4 (2%)	10	0
1	14-A	211/229 (92%)	199 (94%)	9 (4%)	3 (1%)	14	1
1	15-A	211/229 (92%)	200 (95%)	8 (4%)	3 (1%)	14	1
1	16-A	211/229 (92%)	199 (94%)	8 (4%)	4 (2%)	10	0
1	17-A	211/229 (92%)	197 (93%)	10 (5%)	4 (2%)	10	0
1	18-A	211/229 (92%)	200 (95%)	6 (3%)	5 (2%)	7	0
1	19-A	211/229 (92%)	199 (94%)	7 (3%)	5 (2%)	7	0
1	20-A	211/229 (92%)	201 (95%)	7 (3%)	3 (1%)	14	1
1	21-A	211/229 (92%)	199 (94%)	11 (5%)	1 (0%)	34	12
1	22-A	211/229 (92%)	196 (93%)	8 (4%)	7 (3%)	5	0
1	23-A	211/229 (92%)	202 (96%)	8 (4%)	1 (0%)	34	12
1	24-A	211/229 (92%)	201 (95%)	7 (3%)	3 (1%)	14	1
1	25-A	211/229 (92%)	200 (95%)	9 (4%)	2 (1%)	21	4
1	26-A	211/229 (92%)	196 (93%)	13 (6%)	2 (1%)	21	4
1	27-A	211/229 (92%)	202 (96%)	7 (3%)	2 (1%)	21	4
1	28-A	211/229 (92%)	204 (97%)	5 (2%)	2 (1%)	21	4
1	29-A	211/229 (92%)	201 (95%)	9 (4%)	1 (0%)	34	12
1	30-A	211/229 (92%)	191 (90%)	13 (6%)	7 (3%)	5	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	31-A	211/229 (92%)	200 (95%)	7 (3%)	4 (2%)	10	0
1	32-A	211/229 (92%)	202 (96%)	8 (4%)	1 (0%)	34	12
1	33-A	211/229 (92%)	194 (92%)	13 (6%)	4 (2%)	10	0
1	34-A	211/229 (92%)	198 (94%)	10 (5%)	3 (1%)	14	1
1	35-A	211/229 (92%)	202 (96%)	8 (4%)	1 (0%)	34	12
1	36-A	211/229 (92%)	197 (93%)	11 (5%)	3 (1%)	14	1
1	37-A	211/229 (92%)	200 (95%)	10 (5%)	1 (0%)	34	12
1	38-A	211/229 (92%)	199 (94%)	9 (4%)	3 (1%)	14	1
1	39-A	211/229 (92%)	199 (94%)	9 (4%)	3 (1%)	14	1
1	40-A	211/229 (92%)	206 (98%)	4 (2%)	1 (0%)	34	12
1	41-A	211/229 (92%)	204 (97%)	6 (3%)	1 (0%)	34	12
1	42-A	211/229 (92%)	192 (91%)	14 (7%)	5 (2%)	7	0
1	43-A	211/229 (92%)	200 (95%)	10 (5%)	1 (0%)	34	12
1	44-A	211/229 (92%)	200 (95%)	7 (3%)	4 (2%)	10	0
1	45-A	211/229 (92%)	199 (94%)	6 (3%)	6 (3%)	6	0
1	46-A	211/229 (92%)	193 (92%)	11 (5%)	7 (3%)	5	0
1	47-A	211/229 (92%)	197 (93%)	10 (5%)	4 (2%)	10	0
All	All	9917/10763 (92%)	9346 (94%)	404 (4%)	167 (2%)	11	1

All (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
1	2-A	150	ASP
1	2-A	152	VAL
1	3-A	3	VAL
1	3-A	179	ALA
1	4-A	3	VAL
1	4-A	150	ASP
1	5-A	3	VAL
1	5-A	98	GLN
1	5-A	152	VAL

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Mol	Chain	Res	Type
1	6-A	98	GLN
1	6-A	149	GLU
1	6-A	150	ASP
1	6-A	152	VAL
1	7-A	149	GLU
1	7-A	150	ASP
1	8-A	149	GLU
1	9-A	149	GLU
1	10-A	149	GLU
1	11-A	128	ASN
1	11-A	129	GLY
1	11-A	149	GLU
1	12-A	150	ASP
1	13-A	98	GLN
1	13-A	149	GLU
1	13-A	152	VAL
1	14-A	19	ASN
1	14-A	152	VAL
1	15-A	151	GLY
1	17-A	149	GLU
1	17-A	152	VAL
1	18-A	98	GLN
1	18-A	149	GLU
1	19-A	150	ASP
1	20-A	150	ASP
1	20-A	152	VAL
1	21-A	152	VAL
1	22-A	142	PRO
1	22-A	152	VAL
1	23-A	152	VAL
1	24-A	150	ASP
1	25-A	142	PRO
1	25-A	150	ASP
1	26-A	124	ASN
1	27-A	4	ILE
1	27-A	5	LYS
1	30-A	19	ASN
1	30-A	72	PRO
1	31-A	203	ASP
1	32-A	204	TYR
1	34-A	5	LYS
1	35-A	203	ASP

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Mol	Chain	Res	Type
1	38-A	150	ASP
1	42-A	19	ASN
1	43-A	21	HIS
1	44-A	150	ASP
1	45-A	19	ASN
1	45-A	21	HIS
1	45-A	22	LYS
1	45-A	150	ASP
1	45-A	151	GLY
1	46-A	3	VAL
1	46-A	21	HIS
1	46-A	151	GLY
1	47-A	22	LYS
1	3-A	149	GLU
1	5-A	28	GLU
1	6-A	3	VAL
1	6-A	151	GLY
1	7-A	3	VAL
1	7-A	202	LYS
1	8-A	151	GLY
1	9-A	150	ASP
1	13-A	151	GLY
1	15-A	152	VAL
1	16-A	3	VAL
1	16-A	149	GLU
1	16-A	152	VAL
1	18-A	152	VAL
1	19-A	74	ASP
1	19-A	98	GLN
1	22-A	204	TYR
1	28-A	98	GLN
1	30-A	73	GLU
1	30-A	74	ASP
1	30-A	133	GLN
1	31-A	150	ASP
1	31-A	151	GLY
1	33-A	150	ASP
1	34-A	98	GLN
1	36-A	98	GLN
1	37-A	150	ASP
1	39-A	150	ASP
1	41-A	98	GLN

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Mol	Chain	Res	Type
1	42-A	36	GLY
1	44-A	151	GLY
1	45-A	124	ASN
1	1-A	150	ASP
1	3-A	150	ASP
1	4-A	28	GLU
1	5-A	51	PRO
1	5-A	151	GLY
1	6-A	22	LYS
1	8-A	4	ILE
1	8-A	19	ASN
1	14-A	187	ASP
1	15-A	111	GLY
1	17-A	150	ASP
1	22-A	124	ASN
1	22-A	149	GLU
1	28-A	142	PRO
1	29-A	74	ASP
1	30-A	204	TYR
1	34-A	4	ILE
1	38-A	98	GLN
1	38-A	124	ASN
1	2-A	98	GLN
1	3-A	153	LEU
1	6-A	23	PHE
1	8-A	3	VAL
1	16-A	98	GLN
1	18-A	142	PRO
1	19-A	19	ASN
1	19-A	152	VAL
1	22-A	98	GLN
1	24-A	98	GLN
1	33-A	98	GLN
1	36-A	142	PRO
1	36-A	150	ASP
1	39-A	181	LYS
1	40-A	151	GLY
1	42-A	51	PRO
1	46-A	98	GLN
1	47-A	20	GLY
1	3-A	142	PRO
1	8-A	51	PRO

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Mol	Chain	Res	Type
1	12-A	98	GLN
1	33-A	142	PRO
1	33-A	151	GLY
1	42-A	98	GLN
1	46-A	22	LYS
1	46-A	193	HIS
1	47-A	193	HIS
1	4-A	152	VAL
1	9-A	129	GLY
1	17-A	3	VAL
1	20-A	141	SER
1	22-A	202	LYS
1	42-A	142	PRO
1	44-A	98	GLN
1	46-A	150	ASP
1	26-A	126	PRO
1	47-A	151	GLY
1	9-A	151	GLY
1	18-A	51	PRO
1	30-A	142	PRO
1	31-A	142	PRO
1	39-A	51	PRO
1	6-A	142	PRO
1	8-A	142	PRO
1	10-A	142	PRO
1	24-A	141	SER
1	44-A	141	SER

### 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%)	8	1
1	2-A	184/189 (97%)	162 (88%)	22 (12%)	6	1
1	3-A	184/189 (97%)	163 (89%)	21 (11%)	7	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4-A	184/189 (97%)	158 (86%)	26 (14%)	4	0
1	5-A	184/189 (97%)	157 (85%)	27 (15%)	4	0
1	6-A	184/189 (97%)	161 (88%)	23 (12%)	6	0
1	7-A	184/189 (97%)	166 (90%)	18 (10%)	10	1
1	8-A	184/189 (97%)	160 (87%)	24 (13%)	5	0
1	9-A	184/189 (97%)	163 (89%)	21 (11%)	7	1
1	10-A	184/189 (97%)	161 (88%)	23 (12%)	6	0
1	11-A	184/189 (97%)	163 (89%)	21 (11%)	7	1
1	12-A	184/189 (97%)	163 (89%)	21 (11%)	7	1
1	13-A	184/189 (97%)	152 (83%)	32 (17%)	2	0
1	14-A	184/189 (97%)	168 (91%)	16 (9%)	13	2
1	15-A	184/189 (97%)	161 (88%)	23 (12%)	6	0
1	16-A	184/189 (97%)	165 (90%)	19 (10%)	9	1
1	17-A	184/189 (97%)	162 (88%)	22 (12%)	6	1
1	18-A	184/189 (97%)	157 (85%)	27 (15%)	4	0
1	19-A	184/189 (97%)	162 (88%)	22 (12%)	6	1
1	20-A	184/189 (97%)	163 (89%)	21 (11%)	7	1
1	21-A	184/189 (97%)	163 (89%)	21 (11%)	7	1
1	22-A	184/189 (97%)	162 (88%)	22 (12%)	6	1
1	23-A	184/189 (97%)	162 (88%)	22 (12%)	6	1
1	24-A	184/189 (97%)	168 (91%)	16 (9%)	13	2
1	25-A	184/189 (97%)	166 (90%)	18 (10%)	10	1
1	26-A	184/189 (97%)	169 (92%)	15 (8%)	14	2
1	27-A	184/189 (97%)	166 (90%)	18 (10%)	10	1
1	28-A	184/189 (97%)	161 (88%)	23 (12%)	6	0
1	29-A	184/189 (97%)	153 (83%)	31 (17%)	2	0
1	30-A	184/189 (97%)	159 (86%)	25 (14%)	5	0
1	31-A	184/189 (97%)	161 (88%)	23 (12%)	6	0
1	32-A	184/189 (97%)	161 (88%)	23 (12%)	6	0
1	33-A	184/189 (97%)	163 (89%)	21 (11%)	7	1
1	34-A	184/189 (97%)	163 (89%)	21 (11%)	7	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	35-A	184/189 (97%)	155 (84%)	29 (16%)	3	0
1	36-A	184/189 (97%)	165 (90%)	19 (10%)	9	1
1	37-A	184/189 (97%)	159 (86%)	25 (14%)	5	0
1	38-A	184/189 (97%)	161 (88%)	23 (12%)	6	0
1	39-A	184/189 (97%)	159 (86%)	25 (14%)	5	0
1	40-A	184/189 (97%)	164 (89%)	20 (11%)	8	1
1	41-A	184/189 (97%)	167 (91%)	17 (9%)	11	2
1	42-A	184/189 (97%)	157 (85%)	27 (15%)	4	0
1	43-A	184/189 (97%)	164 (89%)	20 (11%)	8	1
1	44-A	184/189 (97%)	157 (85%)	27 (15%)	4	0
1	45-A	184/189 (97%)	172 (94%)	12 (6%)	21	4
1	46-A	184/189 (97%)	161 (88%)	23 (12%)	6	0
1	47-A	184/189 (97%)	163 (89%)	21 (11%)	7	1
All	All	8648/8883 (97%)	7612 (88%)	1036 (12%)	6	1

All (1036) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	2	SER
1	1-A	19	ASN
1	1-A	28	GLU
1	1-A	73	GLU
1	1-A	81	GLN
1	1-A	85	GLU
1	1-A	116	TYR
1	1-A	143	THR
1	1-A	147	TYR
1	1-A	148	VAL
1	1-A	150	ASP
1	1-A	161	LEU
1	1-A	174	LYS
1	1-A	176	THR
1	1-A	178	LYS
1	1-A	185	LEU
1	1-A	191	VAL
1	1-A	193	HIS
1	1-A	211	GLU

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Mol	Chain	Res	Type
1	1-A	216	ARG
1	2-A	4	ILE
1	2-A	9	LYS
1	2-A	39	THR
1	2-A	45	GLU
1	2-A	81	GLN
1	2-A	100	ILE
1	2-A	116	TYR
1	2-A	123	THR
1	2-A	133	GLN
1	2-A	145	LYS
1	2-A	146	MET
1	2-A	148	VAL
1	2-A	150	ASP
1	2-A	153	LEU
1	2-A	156	ASP
1	2-A	178	LYS
1	2-A	180	LYS
1	2-A	181	LYS
1	2-A	187	ASP
1	2-A	192	ASP
1	2-A	216	ARG
1	2-A	217	TYR
1	3-A	9	LYS
1	3-A	11	LYS
1	3-A	41	ASP
1	3-A	96	GLU
1	3-A	110	GLU
1	3-A	116	TYR
1	3-A	138	LYS
1	3-A	146	MET
1	3-A	148	VAL
1	3-A	149	GLU
1	3-A	150	ASP
1	3-A	152	VAL
1	3-A	153	LEU
1	3-A	156	ASP
1	3-A	158	GLU
1	3-A	176	THR
1	3-A	178	LYS
1	3-A	180	LYS
1	3-A	187	ASP

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Mol	Chain	Res	Type
1	3-A	193	HIS
1	3-A	194	ARG
1	4-A	9	LYS
1	4-A	13	ARG
1	4-A	19	ASN
1	4-A	28	GLU
1	4-A	74	ASP
1	4-A	100	ILE
1	4-A	110	GLU
1	4-A	116	TYR
1	4-A	134	LYS
1	4-A	138	LYS
1	4-A	140	LYS
1	4-A	145	LYS
1	4-A	150	ASP
1	4-A	153	LEU
1	4-A	161	LEU
1	4-A	163	LEU
1	4-A	170	ARG
1	4-A	174	LYS
1	4-A	178	LYS
1	4-A	180	LYS
1	4-A	185	LEU
1	4-A	192	ASP
1	4-A	193	HIS
1	4-A	194	ARG
1	4-A	216	ARG
1	4-A	217	TYR
1	5-A	2	SER
1	5-A	13	ARG
1	5-A	30	ILE
1	5-A	70	LYS
1	5-A	78	TYR
1	5-A	90	GLU
1	5-A	100	ILE
1	5-A	110	GLU
1	5-A	116	TYR
1	5-A	133	GLN
1	5-A	134	LYS
1	5-A	136	THR
1	5-A	138	LYS
1	5-A	145	LYS

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Mol	Chain	Res	Type
1	5-A	148	VAL
1	5-A	149	GLU
1	5-A	152	VAL
1	5-A	153	LEU
1	5-A	161	LEU
1	5-A	170	ARG
1	5-A	174	LYS
1	5-A	176	THR
1	5-A	178	LYS
1	5-A	183	VAL
1	5-A	203	ASP
1	5-A	216	ARG
1	5-A	217	TYR
1	6-A	5	LYS
1	6-A	11	LYS
1	6-A	19	ASN
1	6-A	30	ILE
1	6-A	39	THR
1	6-A	74	ASP
1	6-A	78	TYR
1	6-A	81	GLN
1	6-A	91	ARG
1	6-A	98	GLN
1	6-A	100	ILE
1	6-A	110	GLU
1	6-A	116	TYR
1	6-A	117	GLU
1	6-A	158	GLU
1	6-A	172	ASP
1	6-A	174	LYS
1	6-A	175	THR
1	6-A	176	THR
1	6-A	180	LYS
1	6-A	191	VAL
1	6-A	194	ARG
1	6-A	202	LYS
1	7-A	5	LYS
1	7-A	19	ASN
1	7-A	22	LYS
1	7-A	28	GLU
1	7-A	30	ILE
1	7-A	32	LYS

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Mol	Chain	Res	Type
1	7-A	42	LEU
1	7-A	74	ASP
1	7-A	89	TRP
1	7-A	109	MET
1	7-A	112	ASP
1	7-A	116	TYR
1	7-A	149	GLU
1	7-A	178	LYS
1	7-A	180	LYS
1	7-A	190	GLU
1	7-A	216	ARG
1	7-A	217	TYR
1	8-A	4	ILE
1	8-A	42	LEU
1	8-A	73	GLU
1	8-A	74	ASP
1	8-A	98	GLN
1	8-A	100	ILE
1	8-A	112	ASP
1	8-A	116	TYR
1	8-A	128	ASN
1	8-A	153	LEU
1	8-A	156	ASP
1	8-A	157	VAL
1	8-A	158	GLU
1	8-A	170	ARG
1	8-A	176	THR
1	8-A	177	TYR
1	8-A	178	LYS
1	8-A	180	LYS
1	8-A	181	LYS
1	8-A	187	ASP
1	8-A	193	HIS
1	8-A	212	HIS
1	8-A	214	GLU
1	8-A	216	ARG
1	9-A	19	ASN
1	9-A	21	HIS
1	9-A	22	LYS
1	9-A	28	GLU
1	9-A	39	THR
1	9-A	42	LEU

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Mol	Chain	Res	Type
1	9-A	45	GLU
1	9-A	53	SER
1	9-A	85	GLU
1	9-A	116	TYR
1	9-A	123	THR
1	9-A	128	ASN
1	9-A	130	PRO
1	9-A	146	MET
1	9-A	149	GLU
1	9-A	152	VAL
1	9-A	161	LEU
1	9-A	180	LYS
1	9-A	192	ASP
1	9-A	214	GLU
1	9-A	216	ARG
1	10-A	7	GLU
1	10-A	9	LYS
1	10-A	13	ARG
1	10-A	21	HIS
1	10-A	22	LYS
1	10-A	28	GLU
1	10-A	53	SER
1	10-A	70	LYS
1	10-A	88	SER
1	10-A	102	ILE
1	10-A	116	TYR
1	10-A	128	ASN
1	10-A	143	THR
1	10-A	149	GLU
1	10-A	153	LEU
1	10-A	158	GLU
1	10-A	161	LEU
1	10-A	164	GLU
1	10-A	174	LYS
1	10-A	178	LYS
1	10-A	185	LEU
1	10-A	193	HIS
1	10-A	216	ARG
1	11-A	2	SER
1	11-A	7	GLU
1	11-A	13	ARG
1	11-A	22	LYS

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Mol	Chain	Res	Type
1	11-A	28	GLU
1	11-A	30	ILE
1	11-A	39	THR
1	11-A	40	LEU
1	11-A	43	THR
1	11-A	53	SER
1	11-A	116	TYR
1	11-A	146	MET
1	11-A	150	ASP
1	11-A	164	GLU
1	11-A	174	LYS
1	11-A	178	LYS
1	11-A	202	LYS
1	11-A	206	LYS
1	11-A	208	ARG
1	11-A	212	HIS
1	11-A	216	ARG
1	12-A	2	SER
1	12-A	3	VAL
1	12-A	4	ILE
1	12-A	5	LYS
1	12-A	19	ASN
1	12-A	30	ILE
1	12-A	41	ASP
1	12-A	43	THR
1	12-A	116	TYR
1	12-A	143	THR
1	12-A	149	GLU
1	12-A	153	LEU
1	12-A	161	LEU
1	12-A	174	LYS
1	12-A	175	THR
1	12-A	185	LEU
1	12-A	187	ASP
1	12-A	193	HIS
1	12-A	202	LYS
1	12-A	208	ARG
1	12-A	212	HIS
1	13-A	3	VAL
1	13-A	4	ILE
1	13-A	11	LYS
1	13-A	19	ASN

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Mol	Chain	Res	Type
1	13-A	39	THR
1	13-A	43	THR
1	13-A	73	GLU
1	13-A	74	ASP
1	13-A	85	GLU
1	13-A	91	ARG
1	13-A	100	ILE
1	13-A	102	ILE
1	13-A	109	MET
1	13-A	116	TYR
1	13-A	117	GLU
1	13-A	124	ASN
1	13-A	128	ASN
1	13-A	134	LYS
1	13-A	142	PRO
1	13-A	150	ASP
1	13-A	153	LEU
1	13-A	154	LYS
1	13-A	156	ASP
1	13-A	161	LEU
1	13-A	170	ARG
1	13-A	176	THR
1	13-A	193	HIS
1	13-A	202	LYS
1	13-A	205	ASN
1	13-A	206	LYS
1	13-A	212	HIS
1	13-A	214	GLU
1	14-A	4	ILE
1	14-A	11	LYS
1	14-A	19	ASN
1	14-A	96	GLU
1	14-A	110	GLU
1	14-A	116	TYR
1	14-A	128	ASN
1	14-A	135	LYS
1	14-A	153	LEU
1	14-A	154	LYS
1	14-A	174	LYS
1	14-A	187	ASP
1	14-A	193	HIS
1	14-A	198	LEU

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Mol	Chain	Res	Type
1	14-A	208	ARG
1	14-A	216	ARG
1	15-A	2	SER
1	15-A	3	VAL
1	15-A	4	ILE
1	15-A	11	LYS
1	15-A	39	THR
1	15-A	90	GLU
1	15-A	110	GLU
1	15-A	116	TYR
1	15-A	128	ASN
1	15-A	134	LYS
1	15-A	138	LYS
1	15-A	143	THR
1	15-A	147	TYR
1	15-A	153	LEU
1	15-A	154	LYS
1	15-A	158	GLU
1	15-A	176	THR
1	15-A	178	LYS
1	15-A	181	LYS
1	15-A	193	HIS
1	15-A	198	LEU
1	15-A	216	ARG
1	15-A	217	TYR
1	16-A	4	ILE
1	16-A	13	ARG
1	16-A	19	ASN
1	16-A	39	THR
1	16-A	74	ASP
1	16-A	98	GLN
1	16-A	100	ILE
1	16-A	106	ASP
1	16-A	116	TYR
1	16-A	149	GLU
1	16-A	150	ASP
1	16-A	152	VAL
1	16-A	154	LYS
1	16-A	157	VAL
1	16-A	180	LYS
1	16-A	194	ARG
1	16-A	212	HIS

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Mol	Chain	Res	Type
1	16-A	216	ARG
1	16-A	217	TYR
1	17-A	9	LYS
1	17-A	19	ASN
1	17-A	28	GLU
1	17-A	41	ASP
1	17-A	50	LEU
1	17-A	70	LYS
1	17-A	73	GLU
1	17-A	78	TYR
1	17-A	98	GLN
1	17-A	116	TYR
1	17-A	123	THR
1	17-A	138	LYS
1	17-A	145	LYS
1	17-A	152	VAL
1	17-A	156	ASP
1	17-A	161	LEU
1	17-A	180	LYS
1	17-A	182	ASP
1	17-A	190	GLU
1	17-A	202	LYS
1	17-A	206	LYS
1	17-A	217	TYR
1	18-A	2	SER
1	18-A	3	VAL
1	18-A	19	ASN
1	18-A	35	GLU
1	18-A	39	THR
1	18-A	43	THR
1	18-A	50	LEU
1	18-A	51	PRO
1	18-A	73	GLU
1	18-A	74	ASP
1	18-A	78	TYR
1	18-A	100	ILE
1	18-A	116	TYR
1	18-A	124	ASN
1	18-A	138	LYS
1	18-A	146	MET
1	18-A	149	GLU
1	18-A	150	ASP

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Mol	Chain	Res	Type
1	18-A	152	VAL
1	18-A	153	LEU
1	18-A	154	LYS
1	18-A	168	HIS
1	18-A	178	LYS
1	18-A	185	LEU
1	18-A	193	HIS
1	18-A	205	ASN
1	18-A	214	GLU
1	19-A	5	LYS
1	19-A	7	GLU
1	19-A	9	LYS
1	19-A	28	GLU
1	19-A	39	THR
1	19-A	74	ASP
1	19-A	81	GLN
1	19-A	96	GLU
1	19-A	112	ASP
1	19-A	116	TYR
1	19-A	117	GLU
1	19-A	123	THR
1	19-A	124	ASN
1	19-A	138	LYS
1	19-A	147	TYR
1	19-A	149	GLU
1	19-A	150	ASP
1	19-A	158	GLU
1	19-A	181	LYS
1	19-A	192	ASP
1	19-A	211	GLU
1	19-A	212	HIS
1	20-A	2	SER
1	20-A	3	VAL
1	20-A	7	GLU
1	20-A	32	LYS
1	20-A	98	GLN
1	20-A	102	ILE
1	20-A	110	GLU
1	20-A	116	TYR
1	20-A	117	GLU
1	20-A	135	LYS
1	20-A	147	TYR

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Mol	Chain	Res	Type
1	20-A	149	GLU
1	20-A	156	ASP
1	20-A	161	LEU
1	20-A	176	THR
1	20-A	194	ARG
1	20-A	196	GLU
1	20-A	202	LYS
1	20-A	203	ASP
1	20-A	216	ARG
1	20-A	217	TYR
1	21-A	9	LYS
1	21-A	30	ILE
1	21-A	35	GLU
1	21-A	39	THR
1	21-A	41	ASP
1	21-A	50	LEU
1	21-A	70	LYS
1	21-A	90	GLU
1	21-A	116	TYR
1	21-A	145	LYS
1	21-A	147	TYR
1	21-A	148	VAL
1	21-A	149	GLU
1	21-A	153	LEU
1	21-A	161	LEU
1	21-A	172	ASP
1	21-A	181	LYS
1	21-A	202	LYS
1	21-A	212	HIS
1	21-A	216	ARG
1	21-A	217	TYR
1	22-A	3	VAL
1	22-A	5	LYS
1	22-A	39	THR
1	22-A	41	ASP
1	22-A	50	LEU
1	22-A	73	GLU
1	22-A	74	ASP
1	22-A	100	ILE
1	22-A	116	TYR
1	22-A	138	LYS
1	22-A	141	SER

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Mol	Chain	Res	Type
1	22-A	147	TYR
1	22-A	150	ASP
1	22-A	170	ARG
1	22-A	174	LYS
1	22-A	176	THR
1	22-A	185	LEU
1	22-A	194	ARG
1	22-A	202	LYS
1	22-A	208	ARG
1	22-A	216	ARG
1	22-A	217	TYR
1	23-A	2	SER
1	23-A	5	LYS
1	23-A	7	GLU
1	23-A	22	LYS
1	23-A	28	GLU
1	23-A	73	GLU
1	23-A	96	GLU
1	23-A	106	ASP
1	23-A	109	MET
1	23-A	112	ASP
1	23-A	116	TYR
1	23-A	145	LYS
1	23-A	152	VAL
1	23-A	153	LEU
1	23-A	156	ASP
1	23-A	157	VAL
1	23-A	168	HIS
1	23-A	174	LYS
1	23-A	180	LYS
1	23-A	194	ARG
1	23-A	196	GLU
1	23-A	202	LYS
1	24-A	7	GLU
1	24-A	21	HIS
1	24-A	22	LYS
1	24-A	106	ASP
1	24-A	110	GLU
1	24-A	116	TYR
1	24-A	134	LYS
1	24-A	138	LYS
1	24-A	147	TYR

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Mol	Chain	Res	Type
1	24-A	150	ASP
1	24-A	153	LEU
1	24-A	161	LEU
1	24-A	172	ASP
1	24-A	178	LYS
1	24-A	180	LYS
1	24-A	190	GLU
1	25-A	3	VAL
1	25-A	28	GLU
1	25-A	41	ASP
1	25-A	50	LEU
1	25-A	74	ASP
1	25-A	100	ILE
1	25-A	116	TYR
1	25-A	117	GLU
1	25-A	123	THR
1	25-A	127	PRO
1	25-A	148	VAL
1	25-A	156	ASP
1	25-A	161	LEU
1	25-A	192	ASP
1	25-A	193	HIS
1	25-A	194	ARG
1	25-A	206	LYS
1	25-A	216	ARG
1	26-A	21	HIS
1	26-A	116	TYR
1	26-A	126	PRO
1	26-A	143	THR
1	26-A	149	GLU
1	26-A	154	LYS
1	26-A	190	GLU
1	26-A	192	ASP
1	26-A	194	ARG
1	26-A	196	GLU
1	26-A	202	LYS
1	26-A	205	ASN
1	26-A	206	LYS
1	26-A	216	ARG
1	26-A	217	TYR
1	27-A	3	VAL
1	27-A	28	GLU

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Mol	Chain	Res	Type
1	27-A	43	THR
1	27-A	45	GLU
1	27-A	50	LEU
1	27-A	98	GLN
1	27-A	109	MET
1	27-A	116	TYR
1	27-A	124	ASN
1	27-A	132	MET
1	27-A	143	THR
1	27-A	148	VAL
1	27-A	153	LEU
1	27-A	156	ASP
1	27-A	176	THR
1	27-A	193	HIS
1	27-A	206	LYS
1	27-A	216	ARG
1	28-A	2	SER
1	28-A	4	ILE
1	28-A	7	GLU
1	28-A	28	GLU
1	28-A	32	LYS
1	28-A	41	ASP
1	28-A	43	THR
1	28-A	50	LEU
1	28-A	73	GLU
1	28-A	90	GLU
1	28-A	109	MET
1	28-A	116	TYR
1	28-A	125	PHE
1	28-A	145	LYS
1	28-A	148	VAL
1	28-A	149	GLU
1	28-A	161	LEU
1	28-A	176	THR
1	28-A	178	LYS
1	28-A	192	ASP
1	28-A	206	LYS
1	28-A	212	HIS
1	28-A	216	ARG
1	29-A	2	SER
1	29-A	3	VAL
1	29-A	7	GLU

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Mol	Chain	Res	Type
1	29-A	13	ARG
1	29-A	30	ILE
1	29-A	32	LYS
1	29-A	39	THR
1	29-A	50	LEU
1	29-A	73	GLU
1	29-A	100	ILE
1	29-A	116	TYR
1	29-A	138	LYS
1	29-A	149	GLU
1	29-A	150	ASP
1	29-A	153	LEU
1	29-A	156	ASP
1	29-A	157	VAL
1	29-A	161	LEU
1	29-A	168	HIS
1	29-A	170	ARG
1	29-A	174	LYS
1	29-A	176	THR
1	29-A	178	LYS
1	29-A	182	ASP
1	29-A	187	ASP
1	29-A	193	HIS
1	29-A	194	ARG
1	29-A	201	ASP
1	29-A	202	LYS
1	29-A	211	GLU
1	29-A	212	HIS
1	30-A	2	SER
1	30-A	11	LYS
1	30-A	13	ARG
1	30-A	93	MET
1	30-A	115	PHE
1	30-A	116	TYR
1	30-A	123	THR
1	30-A	132	MET
1	30-A	134	LYS
1	30-A	138	LYS
1	30-A	143	THR
1	30-A	152	VAL
1	30-A	153	LEU
1	30-A	170	ARG

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Mol	Chain	Res	Type
1	30-A	176	THR
1	30-A	178	LYS
1	30-A	181	LYS
1	30-A	185	LEU
1	30-A	193	HIS
1	30-A	194	ARG
1	30-A	202	LYS
1	30-A	203	ASP
1	30-A	206	LYS
1	30-A	211	GLU
1	30-A	216	ARG
1	31-A	3	VAL
1	31-A	5	LYS
1	31-A	8	MET
1	31-A	11	LYS
1	31-A	13	ARG
1	31-A	22	LYS
1	31-A	41	ASP
1	31-A	50	LEU
1	31-A	106	ASP
1	31-A	116	TYR
1	31-A	136	THR
1	31-A	149	GLU
1	31-A	153	LEU
1	31-A	156	ASP
1	31-A	158	GLU
1	31-A	161	LEU
1	31-A	174	LYS
1	31-A	185	LEU
1	31-A	190	GLU
1	31-A	192	ASP
1	31-A	203	ASP
1	31-A	208	ARG
1	31-A	217	TYR
1	32-A	5	LYS
1	32-A	13	ARG
1	32-A	22	LYS
1	32-A	35	GLU
1	32-A	41	ASP
1	32-A	45	GLU
1	32-A	74	ASP
1	32-A	116	TYR

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Mol	Chain	Res	Type
1	32-A	138	LYS
1	32-A	143	THR
1	32-A	145	LYS
1	32-A	150	ASP
1	32-A	153	LEU
1	32-A	161	LEU
1	32-A	174	LYS
1	32-A	176	THR
1	32-A	185	LEU
1	32-A	192	ASP
1	32-A	193	HIS
1	32-A	194	ARG
1	32-A	202	LYS
1	32-A	212	HIS
1	32-A	217	TYR
1	33-A	3	VAL
1	33-A	9	LYS
1	33-A	11	LYS
1	33-A	30	ILE
1	33-A	32	LYS
1	33-A	50	LEU
1	33-A	116	TYR
1	33-A	124	ASN
1	33-A	141	SER
1	33-A	142	PRO
1	33-A	145	LYS
1	33-A	148	VAL
1	33-A	152	VAL
1	33-A	153	LEU
1	33-A	168	HIS
1	33-A	176	THR
1	33-A	180	LYS
1	33-A	190	GLU
1	33-A	193	HIS
1	33-A	194	ARG
1	33-A	216	ARG
1	34-A	7	GLU
1	34-A	11	LYS
1	34-A	13	ARG
1	34-A	39	THR
1	34-A	98	GLN
1	34-A	116	TYR

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Mol	Chain	Res	Type
1	34-A	133	GLN
1	34-A	135	LYS
1	34-A	145	LYS
1	34-A	148	VAL
1	34-A	149	GLU
1	34-A	150	ASP
1	34-A	152	VAL
1	34-A	153	LEU
1	34-A	156	ASP
1	34-A	164	GLU
1	34-A	180	LYS
1	34-A	187	ASP
1	34-A	196	GLU
1	34-A	202	LYS
1	34-A	216	ARG
1	35-A	2	SER
1	35-A	5	LYS
1	35-A	11	LYS
1	35-A	13	ARG
1	35-A	28	GLU
1	35-A	50	LEU
1	35-A	70	LYS
1	35-A	73	GLU
1	35-A	90	GLU
1	35-A	109	MET
1	35-A	112	ASP
1	35-A	116	TYR
1	35-A	123	THR
1	35-A	128	ASN
1	35-A	133	GLN
1	35-A	134	LYS
1	35-A	138	LYS
1	35-A	145	LYS
1	35-A	150	ASP
1	35-A	157	VAL
1	35-A	161	LEU
1	35-A	172	ASP
1	35-A	176	THR
1	35-A	178	LYS
1	35-A	180	LYS
1	35-A	181	LYS
1	35-A	193	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	35-A	194	ARG
1	35-A	202	LYS
1	36-A	2	SER
1	36-A	5	LYS
1	36-A	13	ARG
1	36-A	21	HIS
1	36-A	73	GLU
1	36-A	81	GLN
1	36-A	98	GLN
1	36-A	116	TYR
1	36-A	124	ASN
1	36-A	133	GLN
1	36-A	143	THR
1	36-A	152	VAL
1	36-A	153	LEU
1	36-A	187	ASP
1	36-A	192	ASP
1	36-A	198	LEU
1	36-A	202	LYS
1	36-A	216	ARG
1	36-A	217	TYR
1	37-A	5	LYS
1	37-A	7	GLU
1	37-A	11	LYS
1	37-A	39	THR
1	37-A	50	LEU
1	37-A	53	SER
1	37-A	81	GLN
1	37-A	90	GLU
1	37-A	98	GLN
1	37-A	109	MET
1	37-A	116	TYR
1	37-A	128	ASN
1	37-A	150	ASP
1	37-A	152	VAL
1	37-A	158	GLU
1	37-A	174	LYS
1	37-A	176	THR
1	37-A	185	LEU
1	37-A	196	GLU
1	37-A	198	LEU
1	37-A	202	LYS

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Mol	Chain	Res	Type
1	37-A	208	ARG
1	37-A	211	GLU
1	37-A	216	ARG
1	37-A	217	TYR
1	38-A	3	VAL
1	38-A	11	LYS
1	38-A	21	HIS
1	38-A	28	GLU
1	38-A	45	GLU
1	38-A	50	LEU
1	38-A	74	ASP
1	38-A	90	GLU
1	38-A	98	GLN
1	38-A	100	ILE
1	38-A	116	TYR
1	38-A	138	LYS
1	38-A	142	PRO
1	38-A	143	THR
1	38-A	150	ASP
1	38-A	154	LYS
1	38-A	156	ASP
1	38-A	161	LEU
1	38-A	178	LYS
1	38-A	185	LEU
1	38-A	187	ASP
1	38-A	202	LYS
1	38-A	216	ARG
1	39-A	2	SER
1	39-A	3	VAL
1	39-A	5	LYS
1	39-A	28	GLU
1	39-A	35	GLU
1	39-A	41	ASP
1	39-A	50	LEU
1	39-A	70	LYS
1	39-A	88	SER
1	39-A	90	GLU
1	39-A	98	GLN
1	39-A	100	ILE
1	39-A	106	ASP
1	39-A	116	TYR
1	39-A	143	THR

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Mol	Chain	Res	Type
1	39-A	148	VAL
1	39-A	153	LEU
1	39-A	154	LYS
1	39-A	158	GLU
1	39-A	161	LEU
1	39-A	168	HIS
1	39-A	185	LEU
1	39-A	193	HIS
1	39-A	203	ASP
1	39-A	206	LYS
1	40-A	2	SER
1	40-A	5	LYS
1	40-A	7	GLU
1	40-A	21	HIS
1	40-A	81	GLN
1	40-A	90	GLU
1	40-A	100	ILE
1	40-A	116	TYR
1	40-A	149	GLU
1	40-A	153	LEU
1	40-A	158	GLU
1	40-A	174	LYS
1	40-A	178	LYS
1	40-A	180	LYS
1	40-A	181	LYS
1	40-A	185	LEU
1	40-A	196	GLU
1	40-A	203	ASP
1	40-A	216	ARG
1	40-A	217	TYR
1	41-A	5	LYS
1	41-A	21	HIS
1	41-A	39	THR
1	41-A	73	GLU
1	41-A	78	TYR
1	41-A	81	GLN
1	41-A	116	TYR
1	41-A	117	GLU
1	41-A	124	ASN
1	41-A	134	LYS
1	41-A	143	THR
1	41-A	153	LEU

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Mol	Chain	Res	Type
1	41-A	174	LYS
1	41-A	185	LEU
1	41-A	194	ARG
1	41-A	196	GLU
1	41-A	203	ASP
1	42-A	2	SER
1	42-A	13	ARG
1	42-A	28	GLU
1	42-A	30	ILE
1	42-A	41	ASP
1	42-A	50	LEU
1	42-A	81	GLN
1	42-A	90	GLU
1	42-A	100	ILE
1	42-A	102	ILE
1	42-A	106	ASP
1	42-A	116	TYR
1	42-A	117	GLU
1	42-A	124	ASN
1	42-A	128	ASN
1	42-A	138	LYS
1	42-A	143	THR
1	42-A	148	VAL
1	42-A	149	GLU
1	42-A	150	ASP
1	42-A	153	LEU
1	42-A	154	LYS
1	42-A	156	ASP
1	42-A	161	LEU
1	42-A	185	LEU
1	42-A	193	HIS
1	42-A	206	LYS
1	43-A	8	MET
1	43-A	11	LYS
1	43-A	41	ASP
1	43-A	74	ASP
1	43-A	98	GLN
1	43-A	109	MET
1	43-A	116	TYR
1	43-A	142	PRO
1	43-A	148	VAL
1	43-A	149	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	43-A	150	ASP
1	43-A	161	LEU
1	43-A	185	LEU
1	43-A	190	GLU
1	43-A	192	ASP
1	43-A	193	HIS
1	43-A	194	ARG
1	43-A	206	LYS
1	43-A	211	GLU
1	43-A	212	HIS
1	44-A	2	SER
1	44-A	3	VAL
1	44-A	11	LYS
1	44-A	13	ARG
1	44-A	30	ILE
1	44-A	39	THR
1	44-A	41	ASP
1	44-A	50	LEU
1	44-A	55	ASP
1	44-A	73	GLU
1	44-A	98	GLN
1	44-A	110	GLU
1	44-A	112	ASP
1	44-A	116	TYR
1	44-A	128	ASN
1	44-A	134	LYS
1	44-A	141	SER
1	44-A	150	ASP
1	44-A	153	LEU
1	44-A	154	LYS
1	44-A	156	ASP
1	44-A	177	TYR
1	44-A	178	LYS
1	44-A	185	LEU
1	44-A	190	GLU
1	44-A	212	HIS
1	44-A	217	TYR
1	45-A	7	GLU
1	45-A	11	LYS
1	45-A	50	LEU
1	45-A	81	GLN
1	45-A	110	GLU

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Mol	Chain	Res	Type
1	45-A	112	ASP
1	45-A	116	TYR
1	45-A	134	LYS
1	45-A	143	THR
1	45-A	181	LYS
1	45-A	202	LYS
1	45-A	216	ARG
1	46-A	3	VAL
1	46-A	11	LYS
1	46-A	19	ASN
1	46-A	35	GLU
1	46-A	53	SER
1	46-A	81	GLN
1	46-A	123	THR
1	46-A	128	ASN
1	46-A	132	MET
1	46-A	143	THR
1	46-A	146	MET
1	46-A	150	ASP
1	46-A	161	LEU
1	46-A	168	HIS
1	46-A	170	ARG
1	46-A	181	LYS
1	46-A	185	LEU
1	46-A	187	ASP
1	46-A	192	ASP
1	46-A	193	HIS
1	46-A	194	ARG
1	46-A	216	ARG
1	46-A	217	TYR
1	47-A	11	LYS
1	47-A	19	ASN
1	47-A	35	GLU
1	47-A	53	SER
1	47-A	116	TYR
1	47-A	124	ASN
1	47-A	132	MET
1	47-A	141	SER
1	47-A	145	LYS
1	47-A	150	ASP
1	47-A	152	VAL
1	47-A	154	LYS

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Mol	Chain	Res	Type
1	47-A	156	ASP
1	47-A	161	LEU
1	47-A	178	LYS
1	47-A	181	LYS
1	47-A	185	LEU
1	47-A	194	ARG
1	47-A	196	GLU
1	47-A	214	GLU
1	47-A	216	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (142) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	19	ASN
1	1-A	81	GLN
1	1-A	193	HIS
1	2-A	19	ASN
1	2-A	81	GLN
1	2-A	133	GLN
1	2-A	193	HIS
1	3-A	19	ASN
1	3-A	81	GLN
1	3-A	133	GLN
1	4-A	19	ASN
1	4-A	168	HIS
1	5-A	19	ASN
1	6-A	19	ASN
1	6-A	81	GLN
1	6-A	212	HIS
1	7-A	19	ASN
1	7-A	128	ASN
1	7-A	205	ASN
1	8-A	19	ASN
1	8-A	81	GLN
1	8-A	98	GLN
1	8-A	128	ASN
1	8-A	168	HIS
1	8-A	193	HIS
1	8-A	205	ASN
1	9-A	19	ASN
1	9-A	81	GLN
1	9-A	128	ASN

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

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Mol	Chain	Res	Type
1	21-A	212	HIS
1	22-A	193	HIS
1	23-A	81	GLN
1	23-A	168	HIS
1	24-A	81	GLN
1	26-A	98	GLN
1	26-A	124	ASN
1	26-A	168	HIS
1	26-A	205	ASN
1	27-A	21	HIS
1	27-A	124	ASN
1	27-A	205	ASN
1	28-A	21	HIS
1	28-A	124	ASN
1	28-A	128	ASN
1	28-A	133	GLN
1	29-A	124	ASN
1	29-A	128	ASN
1	29-A	205	ASN
1	29-A	212	HIS
1	30-A	21	HIS
1	30-A	81	GLN
1	30-A	205	ASN
1	31-A	21	HIS
1	31-A	81	GLN
1	31-A	128	ASN
1	31-A	133	GLN
1	31-A	212	HIS
1	32-A	133	GLN
1	33-A	212	HIS
1	34-A	21	HIS
1	34-A	133	GLN
1	35-A	21	HIS
1	35-A	98	GLN
1	35-A	133	GLN
1	35-A	193	HIS
1	36-A	98	GLN
1	36-A	124	ASN
1	37-A	21	HIS
1	37-A	124	ASN
1	37-A	128	ASN
1	37-A	193	HIS

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Mol	Chain	Res	Type
1	39-A	21	HIS
1	39-A	133	GLN
1	40-A	81	GLN
1	40-A	193	HIS
1	40-A	205	ASN
1	41-A	81	GLN
1	41-A	124	ASN
1	42-A	98	GLN
1	42-A	124	ASN
1	42-A	193	HIS
1	43-A	38	GLN
1	43-A	124	ASN
1	43-A	128	ASN
1	43-A	133	GLN
1	43-A	212	HIS
1	44-A	133	GLN
1	45-A	19	ASN
1	45-A	133	GLN
1	45-A	193	HIS
1	45-A	212	HIS
1	46-A	19	ASN
1	46-A	81	GLN
1	46-A	133	GLN
1	46-A	168	HIS
1	47-A	19	ASN
1	47-A	38	GLN
1	47-A	81	GLN
1	47-A	98	GLN
1	47-A	212	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	1-A	62	1	24,25,26	1.67	5 (20%)	24,34,36	2.16	9 (37%)
1	CRQ	10-A	62	1	24,25,26	1.73	6 (25%)	24,34,36	1.44	4 (16%)
1	CRQ	11-A	62	1	24,25,26	1.81	7 (29%)	24,34,36	1.62	5 (20%)
1	CRQ	12-A	62	1	24,25,26	1.89	6 (25%)	24,34,36	1.72	6 (25%)
1	CRQ	13-A	62	1	24,25,26	1.92	7 (29%)	24,34,36	1.60	4 (16%)
1	CRQ	14-A	62	1	24,25,26	1.86	6 (25%)	24,34,36	1.79	7 (29%)
1	CRQ	15-A	62	1	24,25,26	1.84	6 (25%)	24,34,36	2.04	9 (37%)
1	CRQ	16-A	62	1	24,25,26	1.76	7 (29%)	24,34,36	1.86	4 (16%)
1	CRQ	17-A	62	1	24,25,26	1.60	6 (25%)	24,34,36	1.43	6 (25%)
1	CRQ	18-A	62	1	24,25,26	1.93	5 (20%)	24,34,36	1.65	5 (20%)
1	CRQ	19-A	62	1	24,25,26	1.83	5 (20%)	24,34,36	2.57	10 (41%)
1	CRQ	2-A	62	1	24,25,26	1.89	8 (33%)	24,34,36	1.46	4 (16%)
1	CRQ	20-A	62	1	24,25,26	1.57	6 (25%)	24,34,36	1.18	2 (8%)
1	CRQ	21-A	62	1	24,25,26	1.84	7 (29%)	24,34,36	1.85	5 (20%)
1	CRQ	22-A	62	1	24,25,26	1.77	6 (25%)	24,34,36	1.63	7 (29%)
1	CRQ	23-A	62	1	24,25,26	1.75	6 (25%)	24,34,36	1.54	5 (20%)
1	CRQ	24-A	62	1	24,25,26	1.61	6 (25%)	24,34,36	1.30	3 (12%)
1	CRQ	25-A	62	1	24,25,26	1.81	7 (29%)	24,34,36	1.62	5 (20%)
1	CRQ	26-A	62	1	24,25,26	1.54	6 (25%)	24,34,36	1.64	4 (16%)
1	CRQ	27-A	62	1	24,25,26	1.74	7 (29%)	24,34,36	1.37	3 (12%)
1	CRQ	28-A	62	1	24,25,26	1.78	6 (25%)	24,34,36	1.54	4 (16%)
1	CRQ	29-A	62	1	24,25,26	1.81	5 (20%)	24,34,36	1.92	9 (37%)
1	CRQ	3-A	62	1	24,25,26	1.71	7 (29%)	24,34,36	1.96	5 (20%)
1	CRQ	30-A	62	1	24,25,26	1.70	7 (29%)	24,34,36	1.41	3 (12%)
1	CRQ	31-A	62	1	24,25,26	1.74	5 (20%)	24,34,36	1.09	2 (8%)
1	CRQ	32-A	62	1	24,25,26	1.95	6 (25%)	24,34,36	2.35	7 (29%)
1	CRQ	33-A	62	1	24,25,26	1.66	5 (20%)	24,34,36	1.83	8 (33%)
1	CRQ	34-A	62	1	24,25,26	1.76	6 (25%)	24,34,36	1.46	3 (12%)
1	CRQ	35-A	62	1	24,25,26	1.86	6 (25%)	24,34,36	2.26	8 (33%)
1	CRQ	36-A	62	1	24,25,26	1.85	8 (33%)	24,34,36	1.89	5 (20%)
1	CRQ	37-A	62	1	24,25,26	1.87	7 (29%)	24,34,36	1.64	6 (25%)
1	CRQ	38-A	62	1	24,25,26	1.69	6 (25%)	24,34,36	1.84	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CRQ	39-A	62	1	24,25,26	1.82	7 (29%)	24,34,36	1.50	4 (16%)
1	CRQ	4-A	62	1	24,25,26	1.97	6 (25%)	24,34,36	1.87	7 (29%)
1	CRQ	40-A	62	1	24,25,26	1.71	7 (29%)	24,34,36	1.50	6 (25%)
1	CRQ	41-A	62	1	24,25,26	1.86	7 (29%)	24,34,36	1.55	6 (25%)
1	CRQ	42-A	62	1	24,25,26	1.81	7 (29%)	24,34,36	1.78	4 (16%)
1	CRQ	43-A	62	1	24,25,26	1.85	7 (29%)	24,34,36	1.90	7 (29%)
1	CRQ	44-A	62	1	24,25,26	1.63	6 (25%)	24,34,36	1.53	3 (12%)
1	CRQ	45-A	62	1	24,25,26	1.85	7 (29%)	24,34,36	1.43	4 (16%)
1	CRQ	46-A	62	1	24,25,26	1.97	6 (25%)	24,34,36	1.55	4 (16%)
1	CRQ	47-A	62	1	24,25,26	1.80	6 (25%)	24,34,36	2.49	8 (33%)
1	CRQ	5-A	62	1	24,25,26	1.72	6 (25%)	24,34,36	1.70	5 (20%)
1	CRQ	6-A	62	1	24,25,26	1.80	6 (25%)	24,34,36	2.11	8 (33%)
1	CRQ	7-A	62	1	24,25,26	2.07	8 (33%)	24,34,36	1.78	4 (16%)
1	CRQ	8-A	62	1	24,25,26	1.67	6 (25%)	24,34,36	1.51	4 (16%)
1	CRQ	9-A	62	1	24,25,26	1.60	5 (20%)	24,34,36	2.00	7 (29%)

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	-	0/10/32/33	0/2/2/2
1	CRQ	17-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	18-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	19-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	2-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	20-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	21-A	62	1	-	0/10/32/33	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	-	0/10/32/33	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CRQ	25-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	26-A	62	1	-	0/10/32/33	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	-	0/10/32/33	0/2/2/2
1	CRQ	4-A	62	1	-	0/10/32/33	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	-	0/10/32/33	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	5-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	7-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	8-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	9-A	62	1	-	0/10/32/33	0/2/2/2

All (296) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	32-A	62	CRQ	CA2-C2	-5.47	1.42	1.48
1	47-A	62	CRQ	CA2-C2	-5.17	1.43	1.48
1	19-A	62	CRQ	CA2-C2	-4.90	1.43	1.48
1	46-A	62	CRQ	CA2-C2	-4.69	1.43	1.48
1	33-A	62	CRQ	CA3-N3	-4.30	1.38	1.47
1	15-A	62	CRQ	CA2-C2	-4.27	1.44	1.48
1	18-A	62	CRQ	CA2-C2	-4.24	1.44	1.48
1	25-A	62	CRQ	CA3-N3	-4.17	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	45-A	62	CRQ	CA2-C2	-4.16	1.44	1.48
1	14-A	62	CRQ	CA2-C2	-4.14	1.44	1.48
1	12-A	62	CRQ	CA3-N3	-4.14	1.38	1.47
1	37-A	62	CRQ	CA2-C2	-3.98	1.44	1.48
1	10-A	62	CRQ	CA2-C2	-3.96	1.44	1.48
1	35-A	62	CRQ	CA2-C2	-3.92	1.44	1.48
1	35-A	62	CRQ	CA3-N3	-3.90	1.39	1.47
1	17-A	62	CRQ	CA2-C2	-3.90	1.44	1.48
1	40-A	62	CRQ	CA2-C2	-3.86	1.44	1.48
1	25-A	62	CRQ	CA2-C2	-3.78	1.44	1.48
1	18-A	62	CRQ	CA3-N3	-3.78	1.39	1.47
1	6-A	62	CRQ	CA3-N3	-3.75	1.39	1.47
1	45-A	62	CRQ	CA3-N3	-3.74	1.39	1.47
1	7-A	62	CRQ	CA2-C2	-3.73	1.44	1.48
1	31-A	62	CRQ	CA3-N3	-3.73	1.39	1.47
1	3-A	62	CRQ	CA2-C2	-3.73	1.44	1.48
1	27-A	62	CRQ	CA2-C2	-3.72	1.44	1.48
1	42-A	62	CRQ	CA2-C2	-3.71	1.44	1.48
1	46-A	62	CRQ	CA3-N3	-3.68	1.39	1.47
1	22-A	62	CRQ	CA2-C2	-3.67	1.44	1.48
1	29-A	62	CRQ	CA3-N3	-3.67	1.39	1.47
1	13-A	62	CRQ	CA3-N3	-3.65	1.39	1.47
1	33-A	62	CRQ	CA2-C2	-3.64	1.44	1.48
1	13-A	62	CRQ	CA2-C2	-3.63	1.44	1.48
1	26-A	62	CRQ	CA3-N3	-3.59	1.39	1.47
1	34-A	62	CRQ	CA2-C2	-3.57	1.44	1.48
1	9-A	62	CRQ	CA2-C2	-3.57	1.44	1.48
1	7-A	62	CRQ	CA3-N3	-3.55	1.39	1.47
1	44-A	62	CRQ	CA2-C2	-3.53	1.44	1.48
1	39-A	62	CRQ	CA2-C2	-3.51	1.44	1.48
1	28-A	62	CRQ	CA2-C2	-3.49	1.44	1.48
1	12-A	62	CRQ	CA2-C2	-3.47	1.44	1.48
1	47-A	62	CRQ	CA3-N3	-3.45	1.39	1.47
1	40-A	62	CRQ	CA3-N3	-3.44	1.40	1.47
1	1-A	62	CRQ	CA2-C2	-3.39	1.44	1.48
1	21-A	62	CRQ	CA2-C2	-3.36	1.44	1.48
1	39-A	62	CRQ	CA3-N3	-3.35	1.40	1.47
1	41-A	62	CRQ	CA2-C2	-3.34	1.44	1.48
1	2-A	62	CRQ	CA3-N3	-3.33	1.40	1.47
1	5-A	62	CRQ	CA3-N3	-3.32	1.40	1.47
1	41-A	62	CRQ	CA3-N3	-3.30	1.40	1.47
1	34-A	62	CRQ	CA3-N3	-3.29	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	24-A	62	CRQ	CA2-C2	-3.29	1.45	1.48
1	23-A	62	CRQ	CA2-C2	-3.27	1.45	1.48
1	17-A	62	CRQ	CA3-N3	-3.26	1.40	1.47
1	36-A	62	CRQ	CA2-C2	-3.23	1.45	1.48
1	44-A	62	CRQ	CA3-N3	-3.17	1.40	1.47
1	27-A	62	CRQ	CA3-N3	-3.14	1.40	1.47
1	5-A	62	CRQ	CA2-C2	-3.11	1.45	1.48
1	37-A	62	CRQ	CA3-N3	-3.07	1.40	1.47
1	11-A	62	CRQ	CA2-C2	-3.05	1.45	1.48
1	24-A	62	CRQ	CA3-N3	-3.04	1.40	1.47
1	43-A	62	CRQ	CA3-N3	-3.04	1.40	1.47
1	30-A	62	CRQ	CA2-C2	-3.03	1.45	1.48
1	6-A	62	CRQ	CA2-C2	-3.01	1.45	1.48
1	14-A	62	CRQ	CA3-N3	-2.97	1.41	1.47
1	16-A	62	CRQ	CA3-N3	-2.91	1.41	1.47
1	9-A	62	CRQ	CA3-N3	-2.91	1.41	1.47
1	42-A	62	CRQ	CA3-N3	-2.89	1.41	1.47
1	30-A	62	CRQ	CA3-N3	-2.87	1.41	1.47
1	8-A	62	CRQ	CA2-C2	-2.82	1.45	1.48
1	3-A	62	CRQ	CA3-N3	-2.80	1.41	1.47
1	1-A	62	CRQ	CA3-N3	-2.78	1.41	1.47
1	19-A	62	CRQ	CA3-N3	-2.75	1.41	1.47
1	8-A	62	CRQ	CA3-N3	-2.71	1.41	1.47
1	43-A	62	CRQ	CA2-C2	-2.69	1.45	1.48
1	26-A	62	CRQ	CA2-C2	-2.66	1.45	1.48
1	2-A	62	CRQ	CA2-C2	-2.63	1.45	1.48
1	16-A	62	CRQ	CA2-C2	-2.62	1.45	1.48
1	22-A	62	CRQ	CA3-N3	-2.62	1.41	1.47
1	23-A	62	CRQ	CA3-N3	-2.61	1.41	1.47
1	21-A	62	CRQ	CA3-N3	-2.57	1.41	1.47
1	10-A	62	CRQ	CA3-N3	-2.56	1.41	1.47
1	32-A	62	CRQ	CA3-N3	-2.51	1.41	1.47
1	4-A	62	CRQ	CA3-N3	-2.48	1.42	1.47
1	36-A	62	CRQ	CA3-N3	-2.47	1.42	1.47
1	28-A	62	CRQ	CA3-N3	-2.35	1.42	1.47
1	11-A	62	CRQ	CA3-N3	-2.31	1.42	1.47
1	20-A	62	CRQ	CA3-N3	-2.28	1.42	1.47
1	38-A	62	CRQ	CA2-C2	-2.13	1.46	1.48
1	20-A	62	CRQ	CA2-C2	-2.10	1.46	1.48
1	15-A	62	CRQ	CA3-N3	-2.09	1.42	1.47
1	16-A	62	CRQ	CA2-N2	2.02	1.42	1.38
1	2-A	62	CRQ	CA2-N2	2.02	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	47-A	62	CRQ	CA2-N2	2.03	1.42	1.38
1	13-A	62	CRQ	CA2-N2	2.03	1.42	1.38
1	25-A	62	CRQ	CA2-N2	2.06	1.43	1.38
1	36-A	62	CRQ	CG2-CB2	2.07	1.50	1.46
1	26-A	62	CRQ	CB2-CA2	2.08	1.37	1.35
1	45-A	62	CRQ	CA2-N2	2.12	1.43	1.38
1	38-A	62	CRQ	CG2-CB2	2.13	1.51	1.46
1	42-A	62	CRQ	CA2-N2	2.13	1.43	1.38
1	4-A	62	CRQ	CG2-CB2	2.18	1.51	1.46
1	41-A	62	CRQ	CA2-N2	2.19	1.43	1.38
1	36-A	62	CRQ	CA1-N	2.20	1.34	1.27
1	21-A	62	CRQ	CA2-N2	2.21	1.43	1.38
1	27-A	62	CRQ	CA2-N2	2.21	1.43	1.38
1	37-A	62	CRQ	CA1-N	2.21	1.34	1.27
1	37-A	62	CRQ	CA2-N2	2.22	1.43	1.38
1	11-A	62	CRQ	CA1-N	2.23	1.34	1.27
1	35-A	62	CRQ	CA1-N	2.26	1.34	1.27
1	47-A	62	CRQ	CA1-N	2.27	1.34	1.27
1	3-A	62	CRQ	CA2-N2	2.28	1.43	1.38
1	26-A	62	CRQ	CA1-N	2.30	1.35	1.27
1	7-A	62	CRQ	CG2-CB2	2.31	1.51	1.46
1	43-A	62	CRQ	CA1-N	2.31	1.35	1.27
1	30-A	62	CRQ	CG2-CB2	2.31	1.51	1.46
1	42-A	62	CRQ	CA1-N	2.35	1.35	1.27
1	2-A	62	CRQ	CA1-N	2.36	1.35	1.27
1	7-A	62	CRQ	CA1-N	2.36	1.35	1.27
1	10-A	62	CRQ	CA1-N	2.37	1.35	1.27
1	19-A	62	CRQ	CA1-N	2.39	1.35	1.27
1	44-A	62	CRQ	CA1-N	2.42	1.35	1.27
1	8-A	62	CRQ	CA1-N	2.42	1.35	1.27
1	31-A	62	CRQ	CA1-N	2.43	1.35	1.27
1	17-A	62	CRQ	CB2-CA2	2.45	1.37	1.35
1	24-A	62	CRQ	CA1-N	2.45	1.35	1.27
1	27-A	62	CRQ	CA1-N	2.45	1.35	1.27
1	39-A	62	CRQ	CA2-N2	2.45	1.43	1.38
1	1-A	62	CRQ	CA1-N	2.47	1.35	1.27
1	17-A	62	CRQ	CA1-N	2.47	1.35	1.27
1	7-A	62	CRQ	CA2-N2	2.49	1.43	1.38
1	40-A	62	CRQ	CA2-N2	2.49	1.43	1.38
1	14-A	62	CRQ	CA1-N	2.50	1.35	1.27
1	39-A	62	CRQ	CA1-N	2.52	1.35	1.27
1	23-A	62	CRQ	CA1-N	2.54	1.35	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	46-A	62	CRQ	CA1-N	2.55	1.35	1.27
1	36-A	62	CRQ	CA2-N2	2.56	1.44	1.38
1	30-A	62	CRQ	CA1-N	2.57	1.35	1.27
1	12-A	62	CRQ	CA1-N	2.57	1.35	1.27
1	20-A	62	CRQ	CA1-N	2.57	1.35	1.27
1	29-A	62	CRQ	CA1-N	2.58	1.35	1.27
1	4-A	62	CRQ	CD3-NE1	2.58	1.41	1.32
1	9-A	62	CRQ	CA1-N	2.60	1.35	1.27
1	45-A	62	CRQ	CA1-N	2.60	1.35	1.27
1	17-A	62	CRQ	CD3-NE1	2.61	1.41	1.32
1	40-A	62	CRQ	CA1-N	2.61	1.35	1.27
1	25-A	62	CRQ	CA1-N	2.61	1.35	1.27
1	22-A	62	CRQ	CA1-N	2.62	1.36	1.27
1	34-A	62	CRQ	CA1-N	2.63	1.36	1.27
1	24-A	62	CRQ	CD3-NE1	2.63	1.41	1.32
1	30-A	62	CRQ	CD3-NE1	2.65	1.41	1.32
1	1-A	62	CRQ	CD3-NE1	2.67	1.41	1.32
1	11-A	62	CRQ	CG2-CB2	2.67	1.52	1.46
1	36-A	62	CRQ	C1-N3	2.68	1.44	1.38
1	3-A	62	CRQ	CD3-NE1	2.69	1.41	1.32
1	2-A	62	CRQ	C1-N3	2.70	1.44	1.38
1	13-A	62	CRQ	CA1-N	2.70	1.36	1.27
1	36-A	62	CRQ	CD3-NE1	2.70	1.41	1.32
1	33-A	62	CRQ	CA1-N	2.71	1.36	1.27
1	23-A	62	CRQ	CD3-NE1	2.71	1.41	1.32
1	10-A	62	CRQ	CB2-CA2	2.71	1.37	1.35
1	43-A	62	CRQ	CA2-N2	2.71	1.44	1.38
1	15-A	62	CRQ	CB2-CA2	2.72	1.37	1.35
1	12-A	62	CRQ	CD3-NE1	2.72	1.41	1.32
1	22-A	62	CRQ	CD3-NE1	2.73	1.41	1.32
1	38-A	62	CRQ	CA1-N	2.73	1.36	1.27
1	20-A	62	CRQ	CD3-NE1	2.73	1.41	1.32
1	41-A	62	CRQ	CA1-N	2.74	1.36	1.27
1	16-A	62	CRQ	CA1-N	2.75	1.36	1.27
1	33-A	62	CRQ	CD3-NE1	2.76	1.41	1.32
1	32-A	62	CRQ	CA1-N	2.77	1.36	1.27
1	21-A	62	CRQ	CD3-NE1	2.78	1.41	1.32
1	9-A	62	CRQ	C1-N3	2.79	1.44	1.38
1	40-A	62	CRQ	C1-N3	2.79	1.44	1.38
1	26-A	62	CRQ	CD3-NE1	2.80	1.41	1.32
1	5-A	62	CRQ	CA1-N	2.80	1.36	1.27
1	5-A	62	CRQ	CD3-NE1	2.81	1.42	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	47-A	62	CRQ	CD3-NE1	2.81	1.42	1.32
1	15-A	62	CRQ	CA1-N	2.82	1.36	1.27
1	13-A	62	CRQ	CD3-NE1	2.83	1.42	1.32
1	24-A	62	CRQ	C1-N3	2.83	1.44	1.38
1	6-A	62	CRQ	CB2-CA2	2.83	1.37	1.35
1	41-A	62	CRQ	CD3-NE1	2.83	1.42	1.32
1	35-A	62	CRQ	CD3-NE1	2.84	1.42	1.32
1	37-A	62	CRQ	CB2-CA2	2.84	1.37	1.35
1	6-A	62	CRQ	CA1-N	2.84	1.36	1.27
1	21-A	62	CRQ	CA1-N	2.86	1.36	1.27
1	27-A	62	CRQ	CD3-NE1	2.86	1.42	1.32
1	25-A	62	CRQ	CB2-CA2	2.87	1.37	1.35
1	28-A	62	CRQ	CA1-N	2.87	1.36	1.27
1	2-A	62	CRQ	CG2-CB2	2.87	1.52	1.46
1	44-A	62	CRQ	CD3-NE1	2.87	1.42	1.32
1	34-A	62	CRQ	CD3-NE1	2.88	1.42	1.32
1	40-A	62	CRQ	CD3-NE1	2.88	1.42	1.32
1	3-A	62	CRQ	CA1-N	2.88	1.36	1.27
1	18-A	62	CRQ	CD3-NE1	2.88	1.42	1.32
1	11-A	62	CRQ	CD3-NE1	2.89	1.42	1.32
1	7-A	62	CRQ	CD3-NE1	2.90	1.42	1.32
1	8-A	62	CRQ	CD3-NE1	2.91	1.42	1.32
1	17-A	62	CRQ	C1-N3	2.91	1.44	1.38
1	46-A	62	CRQ	CD3-NE1	2.91	1.42	1.32
1	33-A	62	CRQ	C1-N3	2.92	1.44	1.38
1	44-A	62	CRQ	CB2-CA2	2.92	1.37	1.35
1	37-A	62	CRQ	CD3-NE1	2.92	1.42	1.32
1	32-A	62	CRQ	CD3-NE1	2.93	1.42	1.32
1	3-A	62	CRQ	CB2-CA2	2.94	1.37	1.35
1	45-A	62	CRQ	CD3-NE1	2.94	1.42	1.32
1	28-A	62	CRQ	CD3-NE1	2.95	1.42	1.32
1	39-A	62	CRQ	CD3-NE1	2.97	1.42	1.32
1	19-A	62	CRQ	CD3-NE1	2.99	1.42	1.32
1	43-A	62	CRQ	CD3-NE1	2.99	1.42	1.32
1	25-A	62	CRQ	CD3-NE1	3.00	1.42	1.32
1	16-A	62	CRQ	C1-N3	3.01	1.44	1.38
1	16-A	62	CRQ	CD3-NE1	3.02	1.42	1.32
1	10-A	62	CRQ	CD3-NE1	3.02	1.42	1.32
1	2-A	62	CRQ	CD3-NE1	3.02	1.42	1.32
1	6-A	62	CRQ	CD3-NE1	3.03	1.42	1.32
1	31-A	62	CRQ	C1-N3	3.04	1.44	1.38
1	4-A	62	CRQ	CA1-N	3.04	1.37	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	31-A	62	CRQ	CD3-NE1	3.04	1.42	1.32
1	42-A	62	CRQ	CD3-NE1	3.04	1.42	1.32
1	5-A	62	CRQ	CB2-CA2	3.05	1.37	1.35
1	40-A	62	CRQ	CB2-CA2	3.06	1.37	1.35
1	15-A	62	CRQ	CD3-NE1	3.06	1.42	1.32
1	14-A	62	CRQ	CD3-NE1	3.08	1.42	1.32
1	29-A	62	CRQ	C1-N3	3.10	1.45	1.38
1	26-A	62	CRQ	C1-N3	3.11	1.45	1.38
1	38-A	62	CRQ	CD3-NE1	3.12	1.43	1.32
1	20-A	62	CRQ	CB2-CA2	3.14	1.38	1.35
1	44-A	62	CRQ	C1-N3	3.15	1.45	1.38
1	9-A	62	CRQ	CD3-NE1	3.17	1.43	1.32
1	43-A	62	CRQ	C1-N3	3.21	1.45	1.38
1	27-A	62	CRQ	C1-N3	3.21	1.45	1.38
1	29-A	62	CRQ	CD3-NE1	3.22	1.43	1.32
1	24-A	62	CRQ	CB2-CA2	3.22	1.38	1.35
1	34-A	62	CRQ	C1-N3	3.23	1.45	1.38
1	30-A	62	CRQ	C1-N3	3.24	1.45	1.38
1	32-A	62	CRQ	CB2-CA2	3.31	1.38	1.35
1	45-A	62	CRQ	CB2-CA2	3.32	1.38	1.35
1	39-A	62	CRQ	CB2-CA2	3.34	1.38	1.35
1	22-A	62	CRQ	CB2-CA2	3.46	1.38	1.35
1	8-A	62	CRQ	CB2-CA2	3.47	1.38	1.35
1	13-A	62	CRQ	C1-N3	3.48	1.45	1.38
1	25-A	62	CRQ	C1-N3	3.49	1.45	1.38
1	3-A	62	CRQ	C1-N3	3.50	1.45	1.38
1	38-A	62	CRQ	C1-N3	3.54	1.45	1.38
1	27-A	62	CRQ	CB2-CA2	3.56	1.38	1.35
1	12-A	62	CRQ	C1-N3	3.56	1.45	1.38
1	4-A	62	CRQ	C1-N3	3.58	1.45	1.38
1	23-A	62	CRQ	CB2-CA2	3.58	1.38	1.35
1	28-A	62	CRQ	C1-N3	3.62	1.46	1.38
1	11-A	62	CRQ	C1-N3	3.64	1.46	1.38
1	34-A	62	CRQ	CB2-CA2	3.65	1.38	1.35
1	14-A	62	CRQ	C1-N3	3.67	1.46	1.38
1	35-A	62	CRQ	C1-N3	3.74	1.46	1.38
1	35-A	62	CRQ	CB2-CA2	3.76	1.38	1.35
1	18-A	62	CRQ	C1-N3	3.76	1.46	1.38
1	46-A	62	CRQ	C1-N3	3.76	1.46	1.38
1	20-A	62	CRQ	C1-N3	3.78	1.46	1.38
1	45-A	62	CRQ	C1-N3	3.80	1.46	1.38
1	47-A	62	CRQ	C1-N3	3.83	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	38-A	62	CRQ	CB2-CA2	3.88	1.38	1.35
1	5-A	62	CRQ	C1-N3	3.88	1.46	1.38
1	8-A	62	CRQ	C1-N3	3.90	1.46	1.38
1	23-A	62	CRQ	C1-N3	3.96	1.46	1.38
1	41-A	62	CRQ	CB2-CA2	3.96	1.38	1.35
1	42-A	62	CRQ	C1-N3	3.96	1.46	1.38
1	28-A	62	CRQ	CB2-CA2	3.97	1.38	1.35
1	7-A	62	CRQ	C1-N3	3.99	1.46	1.38
1	42-A	62	CRQ	CB2-CA2	3.99	1.38	1.35
1	30-A	62	CRQ	CB2-CA2	4.00	1.38	1.35
1	18-A	62	CRQ	CB2-CA2	4.01	1.38	1.35
1	39-A	62	CRQ	C1-N3	4.02	1.46	1.38
1	14-A	62	CRQ	CB2-CA2	4.04	1.38	1.35
1	21-A	62	CRQ	C1-N3	4.05	1.46	1.38
1	46-A	62	CRQ	CB2-CA2	4.17	1.38	1.35
1	12-A	62	CRQ	CB2-CA2	4.18	1.38	1.35
1	41-A	62	CRQ	C1-N3	4.21	1.47	1.38
1	10-A	62	CRQ	C1-N3	4.25	1.47	1.38
1	6-A	62	CRQ	C1-N3	4.26	1.47	1.38
1	22-A	62	CRQ	C1-N3	4.27	1.47	1.38
1	16-A	62	CRQ	CB2-CA2	4.33	1.39	1.35
1	31-A	62	CRQ	CB2-CA2	4.33	1.39	1.35
1	21-A	62	CRQ	CB2-CA2	4.41	1.39	1.35
1	13-A	62	CRQ	CB2-CA2	4.51	1.39	1.35
1	15-A	62	CRQ	C1-N3	4.54	1.47	1.38
1	32-A	62	CRQ	C1-N3	4.54	1.47	1.38
1	11-A	62	CRQ	CB2-CA2	4.58	1.39	1.35
1	1-A	62	CRQ	C1-N3	4.58	1.48	1.38
1	29-A	62	CRQ	CB2-CA2	4.64	1.39	1.35
1	37-A	62	CRQ	C1-N3	4.67	1.48	1.38
1	43-A	62	CRQ	CB2-CA2	4.67	1.39	1.35
1	19-A	62	CRQ	C1-N3	4.82	1.48	1.38
1	36-A	62	CRQ	CB2-CA2	5.11	1.39	1.35
1	2-A	62	CRQ	CB2-CA2	5.13	1.39	1.35
1	7-A	62	CRQ	CB2-CA2	5.14	1.39	1.35
1	4-A	62	CRQ	CB2-CA2	5.74	1.40	1.35

All (252) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	47-A	62	CRQ	CB1-CA1-N	-8.71	107.62	124.73
1	19-A	62	CRQ	O2-C2-CA2	-7.83	126.47	130.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	35-A	62	CRQ	CG2-CB2-CA2	-6.22	122.40	130.27
1	1-A	62	CRQ	O2-C2-CA2	-5.54	127.79	130.97
1	38-A	62	CRQ	O2-C2-CA2	-4.84	128.19	130.97
1	3-A	62	CRQ	CB1-CA1-N	-4.73	115.44	124.73
1	36-A	62	CRQ	CG2-CB2-CA2	-4.58	124.47	130.27
1	29-A	62	CRQ	CG2-CB2-CA2	-4.53	124.54	130.27
1	44-A	62	CRQ	CB1-CA1-N	-4.29	116.30	124.73
1	14-A	62	CRQ	O2-C2-CA2	-4.24	128.53	130.97
1	16-A	62	CRQ	CB1-CA1-N	-4.19	116.49	124.73
1	15-A	62	CRQ	O2-C2-CA2	-4.17	128.57	130.97
1	7-A	62	CRQ	O2-C2-CA2	-4.06	128.63	130.97
1	26-A	62	CRQ	CB1-CA1-N	-3.97	116.93	124.73
1	32-A	62	CRQ	N3-C1-N2	-3.94	108.94	113.16
1	5-A	62	CRQ	CB1-CA1-N	-3.90	117.08	124.73
1	6-A	62	CRQ	CE1-CD1-CG2	-3.84	116.55	121.29
1	10-A	62	CRQ	CB1-CA1-N	-3.76	117.35	124.73
1	19-A	62	CRQ	CB1-CA1-N	-3.74	117.38	124.73
1	35-A	62	CRQ	O2-C2-CA2	-3.70	128.84	130.97
1	21-A	62	CRQ	CB1-CA1-N	-3.66	117.54	124.73
1	9-A	62	CRQ	CB1-CA1-N	-3.59	117.67	124.73
1	14-A	62	CRQ	N3-C1-N2	-3.58	109.32	113.16
1	32-A	62	CRQ	CB1-CA1-N	-3.58	117.70	124.73
1	42-A	62	CRQ	CB1-CA1-N	-3.56	117.74	124.73
1	15-A	62	CRQ	N3-C1-N2	-3.53	109.38	113.16
1	1-A	62	CRQ	CE1-CD1-CG2	-3.53	116.94	121.29
1	1-A	62	CRQ	CB1-CA1-N	-3.50	117.86	124.73
1	22-A	62	CRQ	CB1-CA1-N	-3.49	117.87	124.73
1	32-A	62	CRQ	O2-C2-CA2	-3.49	128.96	130.97
1	13-A	62	CRQ	CB1-CA1-N	-3.43	117.99	124.73
1	11-A	62	CRQ	CB1-CA1-N	-3.42	118.02	124.73
1	19-A	62	CRQ	N3-C1-N2	-3.40	109.52	113.16
1	15-A	62	CRQ	CB2-CA2-C2	-3.40	117.47	122.24
1	22-A	62	CRQ	O2-C2-CA2	-3.39	129.02	130.97
1	7-A	62	CRQ	CB1-CA1-N	-3.35	118.14	124.73
1	25-A	62	CRQ	CB1-CA1-N	-3.35	118.15	124.73
1	2-A	62	CRQ	CB1-CA1-N	-3.30	118.25	124.73
1	12-A	62	CRQ	CG2-CB2-CA2	-3.28	126.12	130.27
1	33-A	62	CRQ	CE1-CD1-CG2	-3.26	117.27	121.29
1	4-A	62	CRQ	CB1-CA1-N	-3.25	118.35	124.73
1	44-A	62	CRQ	N3-C1-N2	-3.25	109.69	113.16
1	45-A	62	CRQ	CB1-CA1-N	-3.23	118.39	124.73
1	33-A	62	CRQ	CG2-CB2-CA2	-3.21	126.21	130.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	19-A	62	CRQ	CB2-CA2-C2	-3.20	117.74	122.24
1	41-A	62	CRQ	CB1-CA1-N	-3.19	118.46	124.73
1	6-A	62	CRQ	O2-C2-CA2	-3.16	129.15	130.97
1	35-A	62	CRQ	N3-C1-N2	-3.14	109.80	113.16
1	6-A	62	CRQ	CB1-CA1-N	-3.12	118.60	124.73
1	8-A	62	CRQ	CB1-CA1-N	-3.12	118.61	124.73
1	37-A	62	CRQ	CE1-CD1-CG2	-3.11	117.45	121.29
1	9-A	62	CRQ	CD2-CG2-CB2	-3.11	110.64	121.24
1	47-A	62	CRQ	CE1-CD1-CG2	-3.10	117.47	121.29
1	46-A	62	CRQ	N3-C1-N2	-3.08	109.86	113.16
1	18-A	62	CRQ	N3-C1-N2	-3.07	109.87	113.16
1	7-A	62	CRQ	N3-C1-N2	-3.07	109.87	113.16
1	33-A	62	CRQ	CB1-CA1-N	-3.06	118.72	124.73
1	39-A	62	CRQ	CB1-CA1-N	-3.05	118.74	124.73
1	35-A	62	CRQ	CB1-CA1-N	-3.04	118.75	124.73
1	15-A	62	CRQ	CB1-CA1-N	-3.03	118.77	124.73
1	13-A	62	CRQ	N3-C1-N2	-3.00	109.95	113.16
1	40-A	62	CRQ	CE1-CD1-CG2	-3.00	117.59	121.29
1	22-A	62	CRQ	N3-C1-N2	-2.97	109.97	113.16
1	20-A	62	CRQ	CB1-CA1-N	-2.97	118.90	124.73
1	15-A	62	CRQ	CE2-CD2-CG2	-2.97	117.63	121.29
1	12-A	62	CRQ	N3-C1-N2	-2.96	109.99	113.16
1	23-A	62	CRQ	CB1-CA1-N	-2.96	118.92	124.73
1	34-A	62	CRQ	CB1-CA1-N	-2.95	118.93	124.73
1	2-A	62	CRQ	N3-C1-N2	-2.94	110.01	113.16
1	43-A	62	CRQ	CB1-CA1-N	-2.92	118.99	124.73
1	37-A	62	CRQ	CB1-CA1-N	-2.91	119.02	124.73
1	47-A	62	CRQ	N3-C1-N2	-2.89	110.06	113.16
1	3-A	62	CRQ	N3-C1-N2	-2.86	110.09	113.16
1	8-A	62	CRQ	N3-C1-N2	-2.85	110.11	113.16
1	38-A	62	CRQ	N3-C1-N2	-2.81	110.16	113.16
1	17-A	62	CRQ	CB1-CA1-N	-2.78	119.26	124.73
1	42-A	62	CRQ	N3-C1-N2	-2.77	110.19	113.16
1	47-A	62	CRQ	CB2-CA2-C2	-2.77	118.34	122.24
1	40-A	62	CRQ	CG2-CB2-CA2	-2.77	126.77	130.27
1	16-A	62	CRQ	N3-C1-N2	-2.76	110.20	113.16
1	24-A	62	CRQ	CG2-CB2-CA2	-2.76	126.78	130.27
1	1-A	62	CRQ	N3-C1-N2	-2.72	110.25	113.16
1	12-A	62	CRQ	CB1-CA1-N	-2.67	119.48	124.73
1	37-A	62	CRQ	N3-C1-N2	-2.67	110.30	113.16
1	29-A	62	CRQ	N3-C1-N2	-2.65	110.32	113.16
1	4-A	62	CRQ	N3-C1-N2	-2.65	110.32	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5-A	62	CRQ	CE1-CD1-CG2	-2.64	118.03	121.29
1	11-A	62	CRQ	N3-C1-N2	-2.61	110.37	113.16
1	35-A	62	CRQ	CE1-CD1-CG2	-2.60	118.09	121.29
1	25-A	62	CRQ	N3-C1-N2	-2.60	110.38	113.16
1	32-A	62	CRQ	CB2-CA2-C2	-2.59	118.60	122.24
1	30-A	62	CRQ	N3-C1-N2	-2.58	110.40	113.16
1	33-A	62	CRQ	N3-C1-N2	-2.56	110.42	113.16
1	10-A	62	CRQ	N3-C1-N2	-2.54	110.44	113.16
1	29-A	62	CRQ	CB1-CA1-N	-2.50	119.82	124.73
1	4-A	62	CRQ	CE2-CZ-CE1	-2.49	116.36	119.78
1	29-A	62	CRQ	CB2-CA2-N2	-2.48	124.32	128.71
1	27-A	62	CRQ	CB1-CA1-N	-2.47	119.89	124.73
1	6-A	62	CRQ	N3-C1-N2	-2.46	110.53	113.16
1	31-A	62	CRQ	CG2-CB2-CA2	-2.45	127.17	130.27
1	41-A	62	CRQ	N3-C1-N2	-2.44	110.55	113.16
1	5-A	62	CRQ	N3-C1-N2	-2.43	110.56	113.16
1	34-A	62	CRQ	N3-C1-N2	-2.42	110.57	113.16
1	19-A	62	CRQ	CE2-CD2-CG2	-2.42	118.31	121.29
1	18-A	62	CRQ	CB1-CA1-N	-2.39	120.03	124.73
1	24-A	62	CRQ	CE1-CD1-CG2	-2.39	118.34	121.29
1	12-A	62	CRQ	CA2-C2-N3	-2.37	102.19	103.37
1	14-A	62	CRQ	CB1-CA1-N	-2.35	120.11	124.73
1	21-A	62	CRQ	N3-C1-N2	-2.35	110.65	113.16
1	31-A	62	CRQ	N3-C1-N2	-2.34	110.66	113.16
1	23-A	62	CRQ	N3-C1-N2	-2.31	110.69	113.16
1	12-A	62	CRQ	O2-C2-CA2	-2.31	129.64	130.97
1	39-A	62	CRQ	N3-C1-N2	-2.29	110.71	113.16
1	46-A	62	CRQ	CB1-CA1-N	-2.26	120.29	124.73
1	28-A	62	CRQ	N3-C1-N2	-2.26	110.74	113.16
1	45-A	62	CRQ	N3-C1-N2	-2.26	110.75	113.16
1	43-A	62	CRQ	CE2-CZ-CE1	-2.24	116.70	119.78
1	14-A	62	CRQ	CB2-CA2-C2	-2.24	119.09	122.24
1	14-A	62	CRQ	CE2-CD2-CG2	-2.24	118.52	121.29
1	47-A	62	CRQ	CD2-CE2-CZ	-2.24	117.29	119.86
1	20-A	62	CRQ	N3-C1-N2	-2.20	110.81	113.16
1	36-A	62	CRQ	N3-C1-N2	-2.18	110.83	113.16
1	25-A	62	CRQ	CB2-CA2-C2	-2.17	119.19	122.24
1	41-A	62	CRQ	CB2-CA2-C2	-2.16	119.20	122.24
1	17-A	62	CRQ	CE1-CD1-CG2	-2.14	118.65	121.29
1	6-A	62	CRQ	CA2-C2-N3	-2.14	102.31	103.37
1	43-A	62	CRQ	CG2-CB2-CA2	-2.14	127.56	130.27
1	33-A	62	CRQ	CA2-C2-N3	-2.13	102.31	103.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	29-A	62	CRQ	O2-C2-CA2	-2.11	129.75	130.97
1	1-A	62	CRQ	CB2-CA2-C2	-2.11	119.28	122.24
1	17-A	62	CRQ	N3-C1-N2	-2.10	110.91	113.16
1	19-A	62	CRQ	CD2-CG2-CB2	-2.07	114.20	121.24
1	29-A	62	CRQ	CE1-CD1-CG2	-2.06	118.75	121.29
1	22-A	62	CRQ	CB2-CA2-C2	-2.03	119.39	122.24
1	40-A	62	CRQ	CB1-CA1-N	-2.03	120.75	124.73
1	40-A	62	CRQ	CD2-CE2-CZ	-2.02	117.54	119.86
1	18-A	62	CRQ	O2-C2-CA2	-2.01	129.81	130.97
1	36-A	62	CRQ	O2-C2-CA2	2.00	132.12	130.97
1	1-A	62	CRQ	CG2-CB2-CA2	2.00	132.80	130.27
1	22-A	62	CRQ	CA2-C2-N3	2.01	104.36	103.37
1	21-A	62	CRQ	CD2-CG2-CD1	2.03	120.66	117.62
1	9-A	62	CRQ	O2-C2-CA2	2.06	132.15	130.97
1	26-A	62	CRQ	CA3-N3-C2	2.07	128.49	124.21
1	37-A	62	CRQ	CD1-CE1-CZ	2.10	122.27	119.86
1	11-A	62	CRQ	CA2-C2-N3	2.12	104.42	103.37
1	27-A	62	CRQ	C2-CA2-N2	2.13	110.66	109.03
1	22-A	62	CRQ	C-CA3-N3	2.15	117.41	112.97
1	43-A	62	CRQ	CD1-CE1-CZ	2.15	122.33	119.86
1	15-A	62	CRQ	C2-CA2-N2	2.19	110.70	109.03
1	9-A	62	CRQ	CD1-CG2-CB2	2.20	128.73	121.24
1	41-A	62	CRQ	CD2-CG2-CD1	2.20	120.92	117.62
1	40-A	62	CRQ	CD2-CG2-CD1	2.24	120.99	117.62
1	35-A	62	CRQ	CE2-CZ-CE1	2.26	122.89	119.78
1	9-A	62	CRQ	C2-CA2-N2	2.26	110.76	109.03
1	19-A	62	CRQ	O2-C2-N3	2.28	129.67	124.70
1	45-A	62	CRQ	C-CA3-N3	2.29	117.70	112.97
1	33-A	62	CRQ	CA3-N3-C2	2.31	128.99	124.21
1	24-A	62	CRQ	CD1-CE1-CZ	2.32	122.52	119.86
1	10-A	62	CRQ	CA2-C2-N3	2.33	104.52	103.37
1	43-A	62	CRQ	O2-C2-CA2	2.33	132.31	130.97
1	10-A	62	CRQ	C2-CA2-N2	2.34	110.81	109.03
1	15-A	62	CRQ	C-CA3-N3	2.37	117.86	112.97
1	38-A	62	CRQ	CG2-CB2-CA2	2.40	133.31	130.27
1	22-A	62	CRQ	CD2-CG2-CD1	2.40	121.22	117.62
1	32-A	62	CRQ	CB2-CA2-N2	2.41	132.99	128.71
1	13-A	62	CRQ	C2-CA2-N2	2.42	110.88	109.03
1	17-A	62	CRQ	C2-CA2-N2	2.44	110.89	109.03
1	17-A	62	CRQ	CD2-CG2-CD1	2.45	121.29	117.62
1	14-A	62	CRQ	C-CA3-N3	2.51	118.15	112.97
1	17-A	62	CRQ	C-CA3-N3	2.54	118.21	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	15-A	62	CRQ	CG2-CB2-CA2	2.55	133.49	130.27
1	39-A	62	CRQ	C2-CA2-N2	2.55	110.98	109.03
1	44-A	62	CRQ	C-CA3-N3	2.58	118.29	112.97
1	4-A	62	CRQ	OH-CZ-CE2	2.59	127.36	120.04
1	14-A	62	CRQ	CG2-CB2-CA2	2.60	133.56	130.27
1	40-A	62	CRQ	C2-CA2-N2	2.61	111.02	109.03
1	11-A	62	CRQ	C-CA3-N3	2.62	118.38	112.97
1	8-A	62	CRQ	C-CA3-N3	2.62	118.38	112.97
1	41-A	62	CRQ	C2-CA2-N2	2.64	111.05	109.03
1	23-A	62	CRQ	C-CA3-N3	2.66	118.46	112.97
1	29-A	62	CRQ	CB2-CA2-C2	2.66	125.99	122.24
1	33-A	62	CRQ	CD2-CG2-CD1	2.73	121.71	117.62
1	26-A	62	CRQ	CG2-CB2-CA2	2.73	133.73	130.27
1	26-A	62	CRQ	C2-CA2-N2	2.79	111.16	109.03
1	37-A	62	CRQ	C2-CA2-N2	2.83	111.19	109.03
1	1-A	62	CRQ	CD1-CE1-CZ	2.85	123.13	119.86
1	15-A	62	CRQ	CD2-CG2-CD1	2.85	121.90	117.62
1	23-A	62	CRQ	CA2-C2-N3	2.87	104.79	103.37
1	2-A	62	CRQ	CA2-C2-N3	2.89	104.80	103.37
1	30-A	62	CRQ	C-CA3-N3	2.91	118.99	112.97
1	47-A	62	CRQ	C-CA3-N3	2.94	119.03	112.97
1	25-A	62	CRQ	C-CA3-N3	2.95	119.06	112.97
1	32-A	62	CRQ	CG2-CB2-CA2	2.97	134.02	130.27
1	19-A	62	CRQ	CD2-CG2-CD1	2.97	122.07	117.62
1	1-A	62	CRQ	C2-CA2-N2	2.99	111.31	109.03
1	33-A	62	CRQ	C2-CA2-N2	3.03	111.34	109.03
1	5-A	62	CRQ	C2-CA2-N2	3.05	111.36	109.03
1	25-A	62	CRQ	C2-CA2-N2	3.06	111.36	109.03
1	35-A	62	CRQ	C2-CA2-N2	3.06	111.36	109.03
1	29-A	62	CRQ	CD1-CE1-CZ	3.08	123.39	119.86
1	37-A	62	CRQ	C-CA3-N3	3.08	119.34	112.97
1	1-A	62	CRQ	C-CA3-N3	3.09	119.35	112.97
1	47-A	62	CRQ	CD2-CG2-CD1	3.10	122.27	117.62
1	6-A	62	CRQ	CD1-CE1-CZ	3.12	123.45	119.86
1	23-A	62	CRQ	CG2-CB2-CA2	3.16	134.26	130.27
1	3-A	62	CRQ	O2-C2-CA2	3.21	132.81	130.97
1	4-A	62	CRQ	C-CA3-N3	3.23	119.64	112.97
1	35-A	62	CRQ	CD2-CG2-CD1	3.24	122.48	117.62
1	28-A	62	CRQ	CA2-C2-N3	3.26	104.98	103.37
1	28-A	62	CRQ	C-CA3-N3	3.31	119.80	112.97
1	19-A	62	CRQ	C2-CA2-N2	3.40	111.63	109.03
1	11-A	62	CRQ	O2-C2-CA2	3.43	132.94	130.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	46-A	62	CRQ	C-CA3-N3	3.46	120.12	112.97
1	8-A	62	CRQ	O2-C2-CA2	3.53	132.99	130.97
1	5-A	62	CRQ	C-CA3-N3	3.55	120.31	112.97
1	41-A	62	CRQ	C-CA3-N3	3.57	120.34	112.97
1	42-A	62	CRQ	C-CA3-N3	3.58	120.37	112.97
1	9-A	62	CRQ	C-CA3-N3	3.61	120.42	112.97
1	45-A	62	CRQ	CA2-C2-N3	3.63	105.16	103.37
1	12-A	62	CRQ	C2-CA2-N2	3.64	111.81	109.03
1	34-A	62	CRQ	C-CA3-N3	3.65	120.50	112.97
1	4-A	62	CRQ	CD1-CE1-CZ	3.69	124.09	119.86
1	46-A	62	CRQ	CA2-C2-N3	3.71	105.20	103.37
1	28-A	62	CRQ	CG2-CB2-CA2	3.72	134.97	130.27
1	2-A	62	CRQ	C-CA3-N3	3.73	120.67	112.97
1	29-A	62	CRQ	CA3-N3-C2	3.76	132.00	124.21
1	3-A	62	CRQ	CA2-C2-N3	3.78	105.24	103.37
1	19-A	62	CRQ	C-CA3-N3	3.80	120.81	112.97
1	18-A	62	CRQ	CA2-C2-N3	3.80	105.25	103.37
1	6-A	62	CRQ	C-CA3-N3	3.82	120.87	112.97
1	27-A	62	CRQ	C-CA3-N3	3.82	120.87	112.97
1	30-A	62	CRQ	CA2-C2-N3	3.83	105.26	103.37
1	47-A	62	CRQ	C2-CA2-N2	3.87	111.98	109.03
1	13-A	62	CRQ	C-CA3-N3	3.92	121.07	112.97
1	4-A	62	CRQ	CA2-C2-N3	4.01	105.35	103.37
1	7-A	62	CRQ	C-CA3-N3	4.07	121.39	112.97
1	18-A	62	CRQ	C-CA3-N3	4.23	121.70	112.97
1	6-A	62	CRQ	C2-CA2-N2	4.24	112.26	109.03
1	36-A	62	CRQ	C-CA3-N3	4.25	121.75	112.97
1	3-A	62	CRQ	C-CA3-N3	4.32	121.89	112.97
1	36-A	62	CRQ	CA2-C2-N3	4.34	105.52	103.37
1	16-A	62	CRQ	O2-C2-CA2	4.37	133.47	130.97
1	39-A	62	CRQ	C-CA3-N3	4.40	122.06	112.97
1	43-A	62	CRQ	CA2-C2-N3	4.50	105.59	103.37
1	21-A	62	CRQ	CA2-C2-N3	4.53	105.61	103.37
1	21-A	62	CRQ	C-CA3-N3	4.64	122.55	112.97
1	38-A	62	CRQ	CA2-C2-N3	4.86	105.77	103.37
1	16-A	62	CRQ	C-CA3-N3	4.94	123.18	112.97
1	9-A	62	CRQ	CG2-CB2-CA2	5.02	136.62	130.27
1	42-A	62	CRQ	CA2-C2-N3	5.28	105.98	103.37
1	43-A	62	CRQ	C-CA3-N3	5.37	124.07	112.97
1	32-A	62	CRQ	CA2-C2-N3	7.83	107.24	103.37

There are no chirality outliers.

There are no torsion outliers.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	2-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	3-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	4-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	5-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	6-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	7-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	8-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	9-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	10-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	11-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	12-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	13-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	14-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	15-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	16-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	17-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	18-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	19-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	20-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	21-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	22-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	23-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	24-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	25-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	26-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	27-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	28-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	29-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	30-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	31-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	32-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	33-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	34-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	35-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	36-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	37-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	38-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	39-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	40-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	41-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	42-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	43-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	44-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	45-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	46-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
1	47-A	213/229 (93%)	-0.25	4 (1%) 70 73	22, 29, 37, 41	213 (100%)
All	All	10011/10763 (93%)	-0.25	188 (1%) 65 73	22, 29, 37, 41	10011 (100%)

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	217	TYR	6.0
1	2-A	217	TYR	6.0
1	3-A	217	TYR	6.0
1	4-A	217	TYR	6.0
1	5-A	217	TYR	6.0
1	6-A	217	TYR	6.0

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Mol	Chain	Res	Type	RSRZ
1	7-A	217	TYR	6.0
1	8-A	217	TYR	6.0
1	9-A	217	TYR	6.0
1	10-A	217	TYR	6.0
1	11-A	217	TYR	6.0
1	12-A	217	TYR	6.0
1	13-A	217	TYR	6.0
1	14-A	217	TYR	6.0
1	15-A	217	TYR	6.0
1	16-A	217	TYR	6.0
1	17-A	217	TYR	6.0
1	18-A	217	TYR	6.0
1	19-A	217	TYR	6.0
1	20-A	217	TYR	6.0
1	21-A	217	TYR	6.0
1	22-A	217	TYR	6.0
1	23-A	217	TYR	6.0
1	24-A	217	TYR	6.0
1	25-A	217	TYR	6.0
1	26-A	217	TYR	6.0
1	27-A	217	TYR	6.0
1	28-A	217	TYR	6.0
1	29-A	217	TYR	6.0
1	30-A	217	TYR	6.0
1	31-A	217	TYR	6.0
1	32-A	217	TYR	6.0
1	33-A	217	TYR	6.0
1	34-A	217	TYR	6.0
1	35-A	217	TYR	6.0
1	36-A	217	TYR	6.0
1	37-A	217	TYR	6.0
1	38-A	217	TYR	6.0
1	39-A	217	TYR	6.0
1	40-A	217	TYR	6.0
1	41-A	217	TYR	6.0
1	42-A	217	TYR	6.0
1	43-A	217	TYR	6.0
1	44-A	217	TYR	6.0
1	45-A	217	TYR	6.0
1	46-A	217	TYR	6.0
1	47-A	217	TYR	6.0
1	1-A	6	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	2-A	6	PRO	2.5
1	3-A	6	PRO	2.5
1	4-A	6	PRO	2.5
1	5-A	6	PRO	2.5
1	6-A	6	PRO	2.5
1	7-A	6	PRO	2.5
1	8-A	6	PRO	2.5
1	9-A	6	PRO	2.5
1	10-A	6	PRO	2.5
1	11-A	6	PRO	2.5
1	12-A	6	PRO	2.5
1	13-A	6	PRO	2.5
1	14-A	6	PRO	2.5
1	15-A	6	PRO	2.5
1	16-A	6	PRO	2.5
1	17-A	6	PRO	2.5
1	18-A	6	PRO	2.5
1	19-A	6	PRO	2.5
1	20-A	6	PRO	2.5
1	21-A	6	PRO	2.5
1	22-A	6	PRO	2.5
1	23-A	6	PRO	2.5
1	24-A	6	PRO	2.5
1	25-A	6	PRO	2.5
1	26-A	6	PRO	2.5
1	27-A	6	PRO	2.5
1	28-A	6	PRO	2.5
1	29-A	6	PRO	2.5
1	30-A	6	PRO	2.5
1	31-A	6	PRO	2.5
1	32-A	6	PRO	2.5
1	33-A	6	PRO	2.5
1	34-A	6	PRO	2.5
1	35-A	6	PRO	2.5
1	36-A	6	PRO	2.5
1	37-A	6	PRO	2.5
1	38-A	6	PRO	2.5
1	39-A	6	PRO	2.5
1	40-A	6	PRO	2.5
1	41-A	6	PRO	2.5
1	42-A	6	PRO	2.5
1	43-A	6	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	44-A	6	PRO	2.5
1	45-A	6	PRO	2.5
1	46-A	6	PRO	2.5
1	47-A	6	PRO	2.5
1	1-A	110	GLU	2.3
1	2-A	110	GLU	2.3
1	3-A	110	GLU	2.3
1	4-A	110	GLU	2.3
1	5-A	110	GLU	2.3
1	6-A	110	GLU	2.3
1	7-A	110	GLU	2.3
1	8-A	110	GLU	2.3
1	9-A	110	GLU	2.3
1	10-A	110	GLU	2.3
1	11-A	110	GLU	2.3
1	12-A	110	GLU	2.3
1	13-A	110	GLU	2.3
1	14-A	110	GLU	2.3
1	15-A	110	GLU	2.3
1	16-A	110	GLU	2.3
1	17-A	110	GLU	2.3
1	18-A	110	GLU	2.3
1	19-A	110	GLU	2.3
1	20-A	110	GLU	2.3
1	21-A	110	GLU	2.3
1	22-A	110	GLU	2.3
1	23-A	110	GLU	2.3
1	24-A	110	GLU	2.3
1	25-A	110	GLU	2.3
1	26-A	110	GLU	2.3
1	27-A	110	GLU	2.3
1	28-A	110	GLU	2.3
1	29-A	110	GLU	2.3
1	30-A	110	GLU	2.3
1	31-A	110	GLU	2.3
1	32-A	110	GLU	2.3
1	33-A	110	GLU	2.3
1	34-A	110	GLU	2.3
1	35-A	110	GLU	2.3
1	36-A	110	GLU	2.3
1	37-A	110	GLU	2.3
1	38-A	110	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	39-A	110	GLU	2.3
1	40-A	110	GLU	2.3
1	41-A	110	GLU	2.3
1	42-A	110	GLU	2.3
1	43-A	110	GLU	2.3
1	44-A	110	GLU	2.3
1	45-A	110	GLU	2.3
1	46-A	110	GLU	2.3
1	47-A	110	GLU	2.3
1	1-A	152	VAL	2.2
1	2-A	152	VAL	2.2
1	3-A	152	VAL	2.2
1	4-A	152	VAL	2.2
1	5-A	152	VAL	2.2
1	6-A	152	VAL	2.2
1	7-A	152	VAL	2.2
1	8-A	152	VAL	2.2
1	9-A	152	VAL	2.2
1	10-A	152	VAL	2.2
1	11-A	152	VAL	2.2
1	12-A	152	VAL	2.2
1	13-A	152	VAL	2.2
1	14-A	152	VAL	2.2
1	15-A	152	VAL	2.2
1	16-A	152	VAL	2.2
1	17-A	152	VAL	2.2
1	18-A	152	VAL	2.2
1	19-A	152	VAL	2.2
1	20-A	152	VAL	2.2
1	21-A	152	VAL	2.2
1	22-A	152	VAL	2.2
1	23-A	152	VAL	2.2
1	24-A	152	VAL	2.2
1	25-A	152	VAL	2.2
1	26-A	152	VAL	2.2
1	27-A	152	VAL	2.2
1	28-A	152	VAL	2.2
1	29-A	152	VAL	2.2
1	30-A	152	VAL	2.2
1	31-A	152	VAL	2.2
1	32-A	152	VAL	2.2
1	33-A	152	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	34-A	152	VAL	2.2
1	35-A	152	VAL	2.2
1	36-A	152	VAL	2.2
1	37-A	152	VAL	2.2
1	38-A	152	VAL	2.2
1	39-A	152	VAL	2.2
1	40-A	152	VAL	2.2
1	41-A	152	VAL	2.2
1	42-A	152	VAL	2.2
1	43-A	152	VAL	2.2
1	44-A	152	VAL	2.2
1	45-A	152	VAL	2.2
1	46-A	152	VAL	2.2
1	47-A	152	VAL	2.2

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CRQ	29-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	16-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	25-A	62	24/25	0.95	0.08	-	22,23,24,25	24
1	CRQ	31-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	30-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	35-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	24-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	3-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	2-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	7-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	18-A	62	24/25	0.95	0.08	-	22,23,24,25	24
1	CRQ	4-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	23-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	13-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	27-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	22-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	21-A	62	24/25	0.95	0.08	-	22,22,24,25	24

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CRQ	41-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	47-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	20-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	36-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	6-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	33-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	37-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	1-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	39-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	19-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	10-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	44-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	45-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	40-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	11-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	28-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	8-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	26-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	38-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	5-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	17-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	12-A	62	24/25	0.95	0.08	-	22,23,24,25	24
1	CRQ	9-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	14-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	34-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	32-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	15-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	43-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	46-A	62	24/25	0.95	0.08	-	22,22,24,25	24
1	CRQ	42-A	62	24/25	0.95	0.08	-	22,23,24,25	24

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.