



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:12 AM UTC

PDB ID : 5EJU / pdb_00005eju
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

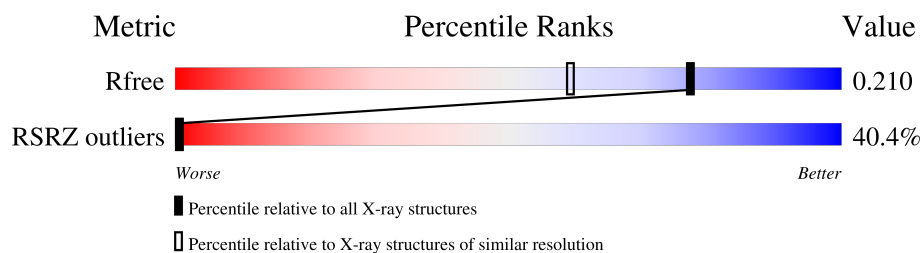
1 Overall quality at a glance

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}	180053	2563 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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			

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	75.97Å 81.09Å 39.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.27 – 1.65 28.27 – 1.65	Depositor EDS
% Data completeness (in resolution range)	97.4 (28.27-1.65) 95.6 (28.27-1.65)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.47 (at 1.65Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.151 , 0.194 0.176 , 0.210	Depositor DCC
R_{free} test set	1888 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.01 , 21.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	167541	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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	14-A	62	1	25,25,26	2.01	6 (24%)	28,34,36	1.76	8 (28%)
1	CRQ	1-A	62	1	25,25,26	1.90	5 (20%)	28,34,36	2.00	9 (32%)
1	CRQ	5-A	62	1	25,25,26	1.93	6 (24%)	28,34,36	1.58	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CRQ	29-A	62	1	25,25,26	1.96	5 (20%)	28,34,36	2.09	9 (32%)
1	CRQ	31-A	62	1	25,25,26	1.89	5 (20%)	28,34,36	1.26	5 (17%)
1	CRQ	13-A	62	1	25,25,26	2.07	6 (24%)	28,34,36	1.49	5 (17%)
1	CRQ	3-A	62	1	25,25,26	1.89	7 (28%)	28,34,36	1.59	6 (21%)
1	CRQ	20-A	62	1	25,25,26	1.77	6 (24%)	28,34,36	1.12	2 (7%)
1	CRQ	41-A	62	1	25,25,26	2.05	7 (28%)	28,34,36	1.47	6 (21%)
1	CRQ	46-A	62	1	25,25,26	2.13	6 (24%)	28,34,36	1.40	5 (17%)
1	CRQ	42-A	62	1	25,25,26	1.98	7 (28%)	28,34,36	1.42	5 (17%)
1	CRQ	35-A	62	1	25,25,26	2.03	6 (24%)	28,34,36	2.15	10 (35%)
1	CRQ	40-A	62	1	25,25,26	1.87	7 (28%)	28,34,36	1.50	8 (28%)
1	CRQ	9-A	62	1	25,25,26	1.78	5 (20%)	28,34,36	1.91	7 (25%)
1	CRQ	11-A	62	1	25,25,26	1.94	7 (28%)	28,34,36	1.49	5 (17%)
1	CRQ	2-A	62	1	25,25,26	2.00	7 (28%)	28,34,36	1.30	4 (14%)
1	CRQ	19-A	62	1	25,25,26	2.04	5 (20%)	28,34,36	2.30	11 (39%)
1	CRQ	39-A	62	1	25,25,26	2.01	7 (28%)	28,34,36	1.37	4 (14%)
1	CRQ	4-A	62	1	25,25,26	2.12	7 (28%)	28,34,36	1.64	8 (28%)
1	CRQ	30-A	62	1	25,25,26	1.86	7 (28%)	28,34,36	1.32	6 (21%)
1	CRQ	34-A	62	1	25,25,26	1.92	6 (24%)	28,34,36	1.36	3 (10%)
1	CRQ	22-A	62	1	25,25,26	1.96	6 (24%)	28,34,36	1.47	9 (32%)
1	CRQ	38-A	62	1	25,25,26	1.86	6 (24%)	28,34,36	1.64	6 (21%)
1	CRQ	12-A	62	1	25,25,26	2.06	6 (24%)	28,34,36	1.70	7 (25%)
1	CRQ	25-A	62	1	25,25,26	2.00	7 (28%)	28,34,36	1.60	6 (21%)
1	CRQ	10-A	62	1	25,25,26	1.92	6 (24%)	28,34,36	1.28	3 (10%)
1	CRQ	18-A	62	1	25,25,26	2.09	7 (28%)	28,34,36	1.46	5 (17%)
1	CRQ	26-A	62	1	25,25,26	1.72	5 (20%)	28,34,36	1.61	6 (21%)
1	CRQ	33-A	62	1	25,25,26	1.86	5 (20%)	28,34,36	1.86	8 (28%)
1	CRQ	16-A	62	1	25,25,26	1.91	6 (24%)	28,34,36	1.58	5 (17%)
1	CRQ	36-A	62	1	25,25,26	1.93	8 (32%)	28,34,36	1.65	4 (14%)
1	CRQ	17-A	62	1	25,25,26	1.75	6 (24%)	28,34,36	1.44	5 (17%)
1	CRQ	44-A	62	1	25,25,26	1.79	6 (24%)	28,34,36	1.33	5 (17%)
1	CRQ	15-A	62	1	25,25,26	2.05	6 (24%)	28,34,36	1.91	11 (39%)
1	CRQ	32-A	62	1	25,25,26	2.14	6 (24%)	28,34,36	1.94	10 (35%)
1	CRQ	21-A	62	1	25,25,26	2.02	7 (28%)	28,34,36	1.50	4 (14%)
1	CRQ	27-A	62	1	25,25,26	1.89	7 (28%)	28,34,36	1.32	4 (14%)
1	CRQ	28-A	62	1	25,25,26	1.95	6 (24%)	28,34,36	1.50	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CRQ	7-A	62	1	25,25,26	2.22	8 (32%)	28,34,36	1.57	5 (17%)
1	CRQ	24-A	62	1	25,25,26	1.76	6 (24%)	28,34,36	1.35	5 (17%)
1	CRQ	8-A	62	1	25,25,26	1.85	6 (24%)	28,34,36	1.39	7 (25%)
1	CRQ	47-A	62	1	25,25,26	1.98	5 (20%)	28,34,36	1.76	8 (28%)
1	CRQ	37-A	62	1	25,25,26	2.06	7 (28%)	28,34,36	1.52	6 (21%)
1	CRQ	43-A	62	1	25,25,26	1.99	8 (32%)	28,34,36	1.57	5 (17%)
1	CRQ	45-A	62	1	25,25,26	2.03	7 (28%)	28,34,36	1.25	3 (10%)
1	CRQ	6-A	62	1	25,25,26	2.03	6 (24%)	28,34,36	2.02	8 (28%)
1	CRQ	23-A	62	1	25,25,26	1.93	7 (28%)	28,34,36	1.42	3 (10%)

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	14-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	1-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	5-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	29-A	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	31-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	13-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	3-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	20-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	41-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	46-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	42-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	35-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	40-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	9-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	11-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	2-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	19-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	-	2/10/32/33	0/2/2/2
1	CRQ	30-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	34-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	22-A	62	1	-	2/10/32/33	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CRQ	38-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	12-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	25-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	10-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	18-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	26-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	33-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	16-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	36-A	62	1	-	5/10/32/33	0/2/2/2
1	CRQ	17-A	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	44-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	15-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	32-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	27-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	28-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	7-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	24-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	8-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	47-A	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	37-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	43-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	45-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	6-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	23-A	62	1	-	2/10/32/33	0/2/2/2

All (296) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	19-A	62	CRQ	C1-N3	6.20	1.48	1.38
1	37-A	62	CRQ	C1-N3	6.01	1.48	1.38
1	1-A	62	CRQ	C1-N3	5.90	1.48	1.38
1	32-A	62	CRQ	C1-N3	5.86	1.47	1.38
1	15-A	62	CRQ	C1-N3	5.85	1.47	1.38
1	22-A	62	CRQ	C1-N3	5.52	1.47	1.38
1	6-A	62	CRQ	C1-N3	5.52	1.47	1.38
1	10-A	62	CRQ	C1-N3	5.51	1.47	1.38
1	41-A	62	CRQ	C1-N3	5.45	1.47	1.38
1	32-A	62	CRQ	CA2-C2	-5.41	1.42	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-A	62	CRQ	CB2-CA2	5.40	1.40	1.35
1	21-A	62	CRQ	C1-N3	5.26	1.46	1.38
1	39-A	62	CRQ	C1-N3	5.23	1.46	1.38
1	7-A	62	CRQ	C1-N3	5.19	1.46	1.38
1	42-A	62	CRQ	C1-N3	5.16	1.46	1.38
1	23-A	62	CRQ	C1-N3	5.15	1.46	1.38
1	47-A	62	CRQ	CA2-C2	-5.11	1.43	1.48
1	8-A	62	CRQ	C1-N3	5.08	1.46	1.38
1	5-A	62	CRQ	C1-N3	5.06	1.46	1.38
1	47-A	62	CRQ	C1-N3	4.99	1.46	1.38
1	45-A	62	CRQ	C1-N3	4.95	1.46	1.38
1	20-A	62	CRQ	C1-N3	4.94	1.46	1.38
1	33-A	62	CRQ	CA3-N3	-4.93	1.38	1.47
1	46-A	62	CRQ	C1-N3	4.91	1.46	1.38
1	18-A	62	CRQ	C1-N3	4.91	1.46	1.38
1	35-A	62	CRQ	C1-N3	4.88	1.46	1.38
1	19-A	62	CRQ	CA2-C2	-4.85	1.43	1.48
1	7-A	62	CRQ	CB2-CA2	4.83	1.39	1.35
1	2-A	62	CRQ	CB2-CA2	4.82	1.39	1.35
1	36-A	62	CRQ	CB2-CA2	4.80	1.39	1.35
1	14-A	62	CRQ	C1-N3	4.80	1.46	1.38
1	25-A	62	CRQ	CA3-N3	-4.79	1.38	1.47
1	11-A	62	CRQ	C1-N3	4.76	1.46	1.38
1	28-A	62	CRQ	C1-N3	4.75	1.46	1.38
1	12-A	62	CRQ	CA3-N3	-4.74	1.38	1.47
1	4-A	62	CRQ	C1-N3	4.69	1.45	1.38
1	12-A	62	CRQ	C1-N3	4.67	1.45	1.38
1	46-A	62	CRQ	CA2-C2	-4.64	1.43	1.48
1	38-A	62	CRQ	C1-N3	4.64	1.45	1.38
1	3-A	62	CRQ	C1-N3	4.60	1.45	1.38
1	25-A	62	CRQ	C1-N3	4.58	1.45	1.38
1	13-A	62	CRQ	C1-N3	4.57	1.45	1.38
1	35-A	62	CRQ	CA3-N3	-4.47	1.39	1.47
1	43-A	62	CRQ	CB2-CA2	4.38	1.39	1.35
1	29-A	62	CRQ	CB2-CA2	4.36	1.39	1.35
1	4-A	62	CRQ	CA1-N1	4.35	1.37	1.27
1	18-A	62	CRQ	CA3-N3	-4.33	1.39	1.47
1	6-A	62	CRQ	CA3-N3	-4.30	1.39	1.47
1	11-A	62	CRQ	CB2-CA2	4.29	1.39	1.35
1	45-A	62	CRQ	CA3-N3	-4.29	1.39	1.47
1	30-A	62	CRQ	C1-N3	4.28	1.45	1.38
1	31-A	62	CRQ	CA3-N3	-4.28	1.39	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	34-A	62	CRQ	C1-N3	4.27	1.45	1.38
1	27-A	62	CRQ	C1-N3	4.25	1.45	1.38
1	43-A	62	CRQ	C1-N3	4.24	1.45	1.38
1	15-A	62	CRQ	CA2-C2	-4.24	1.44	1.48
1	13-A	62	CRQ	CB2-CA2	4.23	1.39	1.35
1	46-A	62	CRQ	CA3-N3	-4.22	1.39	1.47
1	18-A	62	CRQ	CA2-C2	-4.21	1.44	1.48
1	29-A	62	CRQ	CA3-N3	-4.20	1.39	1.47
1	13-A	62	CRQ	CA3-N3	-4.19	1.39	1.47
1	44-A	62	CRQ	C1-N3	4.18	1.45	1.38
1	3-A	62	CRQ	CA1-N1	4.14	1.36	1.27
1	21-A	62	CRQ	CB2-CA2	4.13	1.39	1.35
1	45-A	62	CRQ	CA2-C2	-4.13	1.44	1.48
1	26-A	62	CRQ	C1-N3	4.13	1.45	1.38
1	28-A	62	CRQ	CA1-N1	4.12	1.36	1.27
1	29-A	62	CRQ	C1-N3	4.11	1.45	1.38
1	26-A	62	CRQ	CA3-N3	-4.11	1.39	1.47
1	14-A	62	CRQ	CA2-C2	-4.11	1.44	1.48
1	21-A	62	CRQ	CA1-N1	4.10	1.36	1.27
1	6-A	62	CRQ	CA1-N1	4.08	1.36	1.27
1	7-A	62	CRQ	CA3-N3	-4.07	1.39	1.47
1	31-A	62	CRQ	CB2-CA2	4.06	1.39	1.35
1	16-A	62	CRQ	CB2-CA2	4.06	1.39	1.35
1	15-A	62	CRQ	CA1-N1	4.05	1.36	1.27
1	31-A	62	CRQ	C1-N3	4.04	1.44	1.38
1	5-A	62	CRQ	CA1-N1	4.02	1.36	1.27
1	16-A	62	CRQ	C1-N3	4.01	1.44	1.38
1	32-A	62	CRQ	CA1-N1	3.98	1.36	1.27
1	37-A	62	CRQ	CA2-C2	-3.95	1.44	1.48
1	16-A	62	CRQ	CA1-N1	3.95	1.36	1.27
1	47-A	62	CRQ	CA3-N3	-3.95	1.39	1.47
1	41-A	62	CRQ	CA1-N1	3.95	1.36	1.27
1	40-A	62	CRQ	CA3-N3	-3.94	1.40	1.47
1	10-A	62	CRQ	CA2-C2	-3.93	1.44	1.48
1	38-A	62	CRQ	CA1-N1	3.93	1.36	1.27
1	12-A	62	CRQ	CB2-CA2	3.92	1.38	1.35
1	46-A	62	CRQ	CB2-CA2	3.90	1.38	1.35
1	33-A	62	CRQ	CA1-N1	3.90	1.36	1.27
1	13-A	62	CRQ	CA1-N1	3.89	1.36	1.27
1	35-A	62	CRQ	CA2-C2	-3.89	1.44	1.48
1	33-A	62	CRQ	C1-N3	3.89	1.44	1.38
1	17-A	62	CRQ	C1-N3	3.88	1.44	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	17-A	62	CRQ	CA2-C2	-3.87	1.44	1.48
1	39-A	62	CRQ	CA3-N3	-3.84	1.40	1.47
1	40-A	62	CRQ	CA2-C2	-3.84	1.44	1.48
1	2-A	62	CRQ	CA3-N3	-3.81	1.40	1.47
1	5-A	62	CRQ	CA3-N3	-3.80	1.40	1.47
1	34-A	62	CRQ	CA1-N1	3.79	1.36	1.27
1	14-A	62	CRQ	CB2-CA2	3.78	1.38	1.35
1	24-A	62	CRQ	C1-N3	3.78	1.44	1.38
1	22-A	62	CRQ	CA1-N1	3.78	1.36	1.27
1	41-A	62	CRQ	CA3-N3	-3.77	1.40	1.47
1	34-A	62	CRQ	CA3-N3	-3.77	1.40	1.47
1	25-A	62	CRQ	CA1-N1	3.77	1.35	1.27
1	40-A	62	CRQ	CA1-N1	3.76	1.35	1.27
1	18-A	62	CRQ	CB2-CA2	3.76	1.38	1.35
1	25-A	62	CRQ	CA2-C2	-3.76	1.44	1.48
1	45-A	62	CRQ	CA1-N1	3.75	1.35	1.27
1	9-A	62	CRQ	CA1-N1	3.75	1.35	1.27
1	30-A	62	CRQ	CB2-CA2	3.75	1.38	1.35
1	42-A	62	CRQ	CB2-CA2	3.74	1.38	1.35
1	40-A	62	CRQ	C1-N3	3.73	1.44	1.38
1	9-A	62	CRQ	C1-N3	3.73	1.44	1.38
1	17-A	62	CRQ	CA3-N3	-3.73	1.40	1.47
1	29-A	62	CRQ	CA1-N1	3.72	1.35	1.27
1	28-A	62	CRQ	CB2-CA2	3.72	1.38	1.35
1	20-A	62	CRQ	CA1-N1	3.71	1.35	1.27
1	7-A	62	CRQ	CA2-C2	-3.71	1.44	1.48
1	12-A	62	CRQ	CA1-N1	3.71	1.35	1.27
1	41-A	62	CRQ	CB2-CA2	3.71	1.38	1.35
1	3-A	62	CRQ	CA2-C2	-3.71	1.44	1.48
1	30-A	62	CRQ	CA1-N1	3.71	1.35	1.27
1	27-A	62	CRQ	CA2-C2	-3.70	1.44	1.48
1	46-A	62	CRQ	CA1-N1	3.69	1.35	1.27
1	42-A	62	CRQ	CA2-C2	-3.69	1.44	1.48
1	23-A	62	CRQ	CA1-N1	3.66	1.35	1.27
1	22-A	62	CRQ	CA2-C2	-3.65	1.44	1.48
1	39-A	62	CRQ	CA1-N1	3.65	1.35	1.27
1	38-A	62	CRQ	CB2-CA2	3.63	1.38	1.35
1	2-A	62	CRQ	C1-N3	3.63	1.44	1.38
1	44-A	62	CRQ	CA3-N3	-3.63	1.40	1.47
1	33-A	62	CRQ	CA2-C2	-3.62	1.44	1.48
1	13-A	62	CRQ	CA2-C2	-3.61	1.44	1.48
1	14-A	62	CRQ	CA1-N1	3.61	1.35	1.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	36-A	62	CRQ	C1-N3	3.60	1.44	1.38
1	27-A	62	CRQ	CA3-N3	-3.59	1.40	1.47
1	17-A	62	CRQ	CA1-N1	3.57	1.35	1.27
1	1-A	62	CRQ	CA1-N1	3.57	1.35	1.27
1	34-A	62	CRQ	CA2-C2	-3.55	1.44	1.48
1	27-A	62	CRQ	CA1-N1	3.55	1.35	1.27
1	9-A	62	CRQ	CA2-C2	-3.55	1.44	1.48
1	24-A	62	CRQ	CA1-N1	3.55	1.35	1.27
1	31-A	62	CRQ	CA1-N1	3.53	1.35	1.27
1	44-A	62	CRQ	CA2-C2	-3.51	1.44	1.48
1	35-A	62	CRQ	CB2-CA2	3.51	1.38	1.35
1	8-A	62	CRQ	CA1-N1	3.51	1.35	1.27
1	37-A	62	CRQ	CA3-N3	-3.51	1.40	1.47
1	44-A	62	CRQ	CA1-N1	3.50	1.35	1.27
1	39-A	62	CRQ	CA2-C2	-3.49	1.44	1.48
1	24-A	62	CRQ	CA3-N3	-3.48	1.40	1.47
1	43-A	62	CRQ	CA3-N3	-3.48	1.40	1.47
1	28-A	62	CRQ	CA2-C2	-3.47	1.44	1.48
1	19-A	62	CRQ	CA1-N1	3.47	1.35	1.27
1	12-A	62	CRQ	CA2-C2	-3.45	1.44	1.48
1	10-A	62	CRQ	CA1-N1	3.43	1.35	1.27
1	7-A	62	CRQ	CA1-N1	3.43	1.35	1.27
1	2-A	62	CRQ	CA1-N1	3.42	1.35	1.27
1	42-A	62	CRQ	CA1-N1	3.41	1.35	1.27
1	34-A	62	CRQ	CB2-CA2	3.41	1.38	1.35
1	14-A	62	CRQ	CA3-N3	-3.39	1.41	1.47
1	1-A	62	CRQ	CA2-C2	-3.38	1.44	1.48
1	43-A	62	CRQ	CA1-N1	3.36	1.35	1.27
1	23-A	62	CRQ	CB2-CA2	3.35	1.38	1.35
1	21-A	62	CRQ	CA2-C2	-3.35	1.44	1.48
1	26-A	62	CRQ	CA1-N1	3.34	1.35	1.27
1	41-A	62	CRQ	CA2-C2	-3.33	1.44	1.48
1	16-A	62	CRQ	CA3-N3	-3.33	1.41	1.47
1	9-A	62	CRQ	CA3-N3	-3.32	1.41	1.47
1	27-A	62	CRQ	CB2-CA2	3.32	1.38	1.35
1	42-A	62	CRQ	CA3-N3	-3.31	1.41	1.47
1	47-A	62	CRQ	CA1-N1	3.30	1.34	1.27
1	30-A	62	CRQ	CA3-N3	-3.29	1.41	1.47
1	35-A	62	CRQ	CA1-N1	3.28	1.34	1.27
1	24-A	62	CRQ	CA2-C2	-3.28	1.45	1.48
1	23-A	62	CRQ	CA2-C2	-3.26	1.45	1.48
1	8-A	62	CRQ	CB2-CA2	3.24	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	11-A	62	CRQ	CA1-N1	3.24	1.34	1.27
1	29-A	62	CRQ	CD3-NE1	3.24	1.43	1.32
1	22-A	62	CRQ	CB2-CA2	3.23	1.38	1.35
1	36-A	62	CRQ	CA2-C2	-3.22	1.45	1.48
1	37-A	62	CRQ	CA1-N1	3.22	1.34	1.27
1	36-A	62	CRQ	CA1-N1	3.21	1.34	1.27
1	3-A	62	CRQ	CA3-N3	-3.20	1.41	1.47
1	9-A	62	CRQ	CD3-NE1	3.20	1.43	1.32
1	1-A	62	CRQ	CA3-N3	-3.18	1.41	1.47
1	38-A	62	CRQ	CD3-NE1	3.15	1.43	1.32
1	19-A	62	CRQ	CA3-N3	-3.14	1.41	1.47
1	39-A	62	CRQ	CB2-CA2	3.11	1.38	1.35
1	14-A	62	CRQ	CD3-NE1	3.10	1.42	1.32
1	5-A	62	CRQ	CA2-C2	-3.10	1.45	1.48
1	8-A	62	CRQ	CA3-N3	-3.10	1.41	1.47
1	45-A	62	CRQ	CB2-CA2	3.09	1.38	1.35
1	32-A	62	CRQ	CB2-CA2	3.08	1.38	1.35
1	15-A	62	CRQ	CD3-NE1	3.08	1.42	1.32
1	42-A	62	CRQ	CD3-NE1	3.07	1.42	1.32
1	31-A	62	CRQ	CD3-NE1	3.07	1.42	1.32
1	6-A	62	CRQ	CD3-NE1	3.05	1.42	1.32
1	2-A	62	CRQ	CD3-NE1	3.05	1.42	1.32
1	10-A	62	CRQ	CD3-NE1	3.05	1.42	1.32
1	2-A	62	CRQ	CG2-CB2	3.05	1.52	1.46
1	16-A	62	CRQ	CD3-NE1	3.04	1.42	1.32
1	11-A	62	CRQ	CA2-C2	-3.04	1.45	1.48
1	30-A	62	CRQ	CA2-C2	-3.02	1.45	1.48
1	25-A	62	CRQ	CD3-NE1	3.02	1.42	1.32
1	43-A	62	CRQ	CD3-NE1	3.02	1.42	1.32
1	19-A	62	CRQ	CD3-NE1	3.01	1.42	1.32
1	24-A	62	CRQ	CB2-CA2	3.00	1.38	1.35
1	6-A	62	CRQ	CA2-C2	-3.00	1.45	1.48
1	39-A	62	CRQ	CD3-NE1	3.00	1.42	1.32
1	22-A	62	CRQ	CA3-N3	-2.99	1.41	1.47
1	23-A	62	CRQ	CA3-N3	-2.99	1.41	1.47
1	28-A	62	CRQ	CD3-NE1	2.97	1.42	1.32
1	45-A	62	CRQ	CD3-NE1	2.96	1.42	1.32
1	32-A	62	CRQ	CD3-NE1	2.95	1.42	1.32
1	37-A	62	CRQ	CD3-NE1	2.95	1.42	1.32
1	46-A	62	CRQ	CD3-NE1	2.94	1.42	1.32
1	21-A	62	CRQ	CA3-N3	-2.94	1.41	1.47
1	8-A	62	CRQ	CD3-NE1	2.93	1.42	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	7-A	62	CRQ	CD3-NE1	2.93	1.42	1.32
1	18-A	62	CRQ	CA1-N1	2.93	1.34	1.27
1	20-A	62	CRQ	CB2-CA2	2.93	1.38	1.35
1	10-A	62	CRQ	CA3-N3	-2.92	1.41	1.47
1	11-A	62	CRQ	CD3-NE1	2.92	1.42	1.32
1	18-A	62	CRQ	CD3-NE1	2.91	1.42	1.32
1	40-A	62	CRQ	CD3-NE1	2.91	1.42	1.32
1	34-A	62	CRQ	CD3-NE1	2.90	1.42	1.32
1	44-A	62	CRQ	CD3-NE1	2.90	1.42	1.32
1	27-A	62	CRQ	CD3-NE1	2.88	1.42	1.32
1	32-A	62	CRQ	CA3-N3	-2.87	1.41	1.47
1	35-A	62	CRQ	CD3-NE1	2.86	1.42	1.32
1	41-A	62	CRQ	CD3-NE1	2.86	1.42	1.32
1	13-A	62	CRQ	CD3-NE1	2.85	1.42	1.32
1	40-A	62	CRQ	CB2-CA2	2.85	1.37	1.35
1	5-A	62	CRQ	CB2-CA2	2.84	1.37	1.35
1	11-A	62	CRQ	CG2-CB2	2.84	1.52	1.46
1	47-A	62	CRQ	CD3-NE1	2.84	1.42	1.32
1	5-A	62	CRQ	CD3-NE1	2.84	1.42	1.32
1	4-A	62	CRQ	CA3-N3	-2.83	1.42	1.47
1	26-A	62	CRQ	CD3-NE1	2.82	1.41	1.32
1	8-A	62	CRQ	CA2-C2	-2.82	1.45	1.48
1	36-A	62	CRQ	CA3-N3	-2.82	1.42	1.47
1	21-A	62	CRQ	CD3-NE1	2.80	1.41	1.32
1	33-A	62	CRQ	CD3-NE1	2.79	1.41	1.32
1	20-A	62	CRQ	CD3-NE1	2.75	1.41	1.32
1	22-A	62	CRQ	CD3-NE1	2.75	1.41	1.32
1	12-A	62	CRQ	CD3-NE1	2.75	1.41	1.32
1	3-A	62	CRQ	CB2-CA2	2.73	1.37	1.35
1	23-A	62	CRQ	CD3-NE1	2.73	1.41	1.32
1	36-A	62	CRQ	CD3-NE1	2.73	1.41	1.32
1	44-A	62	CRQ	CB2-CA2	2.72	1.37	1.35
1	3-A	62	CRQ	CD3-NE1	2.71	1.41	1.32
1	43-A	62	CRQ	CA2-C2	-2.70	1.45	1.48
1	43-A	62	CRQ	CA2-N2	2.70	1.44	1.38
1	1-A	62	CRQ	CD3-NE1	2.69	1.41	1.32
1	28-A	62	CRQ	CA3-N3	-2.69	1.42	1.47
1	30-A	62	CRQ	CD3-NE1	2.67	1.41	1.32
1	25-A	62	CRQ	CB2-CA2	2.67	1.37	1.35
1	26-A	62	CRQ	CA2-C2	-2.66	1.45	1.48
1	24-A	62	CRQ	CD3-NE1	2.66	1.41	1.32
1	37-A	62	CRQ	CB2-CA2	2.64	1.37	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	62	CRQ	CA2-C2	-2.63	1.45	1.48
1	11-A	62	CRQ	CA3-N3	-2.63	1.42	1.47
1	6-A	62	CRQ	CB2-CA2	2.63	1.37	1.35
1	17-A	62	CRQ	CD3-NE1	2.63	1.41	1.32
1	16-A	62	CRQ	CA2-C2	-2.62	1.45	1.48
1	4-A	62	CRQ	CD3-NE1	2.60	1.41	1.32
1	20-A	62	CRQ	CA3-N3	-2.60	1.42	1.47
1	36-A	62	CRQ	CA2-N2	2.54	1.44	1.38
1	15-A	62	CRQ	CB2-CA2	2.53	1.37	1.35
1	10-A	62	CRQ	CB2-CA2	2.52	1.37	1.35
1	40-A	62	CRQ	CA2-N2	2.47	1.43	1.38
1	7-A	62	CRQ	CA2-N2	2.47	1.43	1.38
1	30-A	62	CRQ	CG2-CB2	2.45	1.51	1.46
1	7-A	62	CRQ	CG2-CB2	2.45	1.51	1.46
1	39-A	62	CRQ	CA2-N2	2.43	1.43	1.38
1	15-A	62	CRQ	CA3-N3	-2.38	1.42	1.47
1	4-A	62	CRQ	CG2-CB2	2.31	1.51	1.46
1	17-A	62	CRQ	CB2-CA2	2.27	1.37	1.35
1	38-A	62	CRQ	CG2-CB2	2.26	1.51	1.46
1	3-A	62	CRQ	CA2-N2	2.25	1.43	1.38
1	37-A	62	CRQ	CA2-N2	2.19	1.43	1.38
1	36-A	62	CRQ	CG2-CB2	2.19	1.50	1.46
1	27-A	62	CRQ	CA2-N2	2.18	1.43	1.38
1	21-A	62	CRQ	CA2-N2	2.18	1.43	1.38
1	41-A	62	CRQ	CA2-N2	2.16	1.43	1.38
1	38-A	62	CRQ	CA2-C2	-2.14	1.46	1.48
1	43-A	62	CRQ	CG2-CB2	2.12	1.50	1.46
1	20-A	62	CRQ	CA2-C2	-2.11	1.46	1.48
1	42-A	62	CRQ	CA2-N2	2.10	1.43	1.38
1	45-A	62	CRQ	CA2-N2	2.09	1.43	1.38
1	4-A	62	CRQ	OH-CZ	2.07	1.41	1.37
1	23-A	62	CRQ	CG2-CB2	2.06	1.50	1.46
1	25-A	62	CRQ	CA2-N2	2.03	1.43	1.38
1	18-A	62	CRQ	CG2-CB2	2.01	1.50	1.46

All (284) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	19-A	62	CRQ	O2-C2-CA2	-7.13	126.47	131.02
1	35-A	62	CRQ	CG2-CB2-CA2	-6.28	122.40	129.87
1	9-A	62	CRQ	CG2-CB2-CA2	5.68	136.62	129.87
1	43-A	62	CRQ	C3-CA3-N3	5.12	124.07	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	62	CRQ	O2-C2-CA2	-5.07	127.79	131.02
1	16-A	62	CRQ	C3-CA3-N3	4.73	123.18	112.43
1	6-A	62	CRQ	C2-CA2-N2	4.62	112.26	108.95
1	36-A	62	CRQ	CG2-CB2-CA2	-4.54	124.47	129.87
1	29-A	62	CRQ	CG2-CB2-CA2	-4.48	124.54	129.87
1	32-A	62	CRQ	CA2-C2-N3	4.46	107.24	103.50
1	21-A	62	CRQ	C3-CA3-N3	4.45	122.55	112.43
1	38-A	62	CRQ	O2-C2-CA2	-4.44	128.19	131.02
1	29-A	62	CRQ	CA3-N3-C1	-4.39	119.74	128.39
1	28-A	62	CRQ	CG2-CB2-CA2	4.29	134.97	129.87
1	39-A	62	CRQ	C3-CA3-N3	4.23	122.06	112.43
1	47-A	62	CRQ	C2-CA2-N2	4.23	111.98	108.95
1	3-A	62	CRQ	C3-CA3-N3	4.16	121.89	112.43
1	36-A	62	CRQ	C3-CA3-N3	4.10	121.75	112.43
1	18-A	62	CRQ	C3-CA3-N3	4.07	121.70	112.43
1	15-A	62	CRQ	CB2-CA2-C2	-4.03	117.47	122.36
1	4-A	62	CRQ	CD1-CE1-CZ	3.98	124.09	119.88
1	12-A	62	CRQ	C2-CA2-N2	3.98	111.81	108.95
1	7-A	62	CRQ	C3-CA3-N3	3.94	121.39	112.43
1	14-A	62	CRQ	O2-C2-CA2	-3.90	128.53	131.02
1	16-A	62	CRQ	O2-C2-CA2	3.84	133.47	131.02
1	15-A	62	CRQ	O2-C2-CA2	-3.84	128.57	131.02
1	19-A	62	CRQ	CB2-CA2-C2	-3.81	117.74	122.36
1	13-A	62	CRQ	C3-CA3-N3	3.80	121.07	112.43
1	29-A	62	CRQ	CA3-N3-C2	3.79	132.00	123.67
1	7-A	62	CRQ	O2-C2-CA2	-3.74	128.63	131.02
1	19-A	62	CRQ	C2-CA2-N2	3.73	111.63	108.95
1	27-A	62	CRQ	C3-CA3-N3	3.71	120.87	112.43
1	6-A	62	CRQ	C3-CA3-N3	3.71	120.87	112.43
1	23-A	62	CRQ	CG2-CB2-CA2	3.70	134.26	129.87
1	19-A	62	CRQ	C3-CA3-N3	3.68	120.81	112.43
1	2-A	62	CRQ	C3-CA3-N3	3.62	120.67	112.43
1	6-A	62	CRQ	CE1-CD1-CG2	-3.62	116.55	121.22
1	34-A	62	CRQ	C3-CA3-N3	3.55	120.50	112.43
1	9-A	62	CRQ	C3-CA3-N3	3.51	120.42	112.43
1	32-A	62	CRQ	CG2-CB2-CA2	3.50	134.02	129.87
1	42-A	62	CRQ	C3-CA3-N3	3.49	120.37	112.43
1	41-A	62	CRQ	C3-CA3-N3	3.48	120.34	112.43
1	5-A	62	CRQ	C3-CA3-N3	3.46	120.31	112.43
1	35-A	62	CRQ	O2-C2-CA2	-3.42	128.84	131.02
1	46-A	62	CRQ	C3-CA3-N3	3.38	120.12	112.43
1	6-A	62	CRQ	CD1-CE1-CZ	3.38	123.45	119.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	25-A	62	CRQ	C2-CA2-N2	3.37	111.36	108.95
1	35-A	62	CRQ	C2-CA2-N2	3.37	111.36	108.95
1	5-A	62	CRQ	C2-CA2-N2	3.36	111.36	108.95
1	33-A	62	CRQ	CA3-N3-C1	-3.34	121.81	128.39
1	33-A	62	CRQ	C2-CA2-N2	3.34	111.34	108.95
1	29-A	62	CRQ	CD1-CE1-CZ	3.32	123.39	119.88
1	1-A	62	CRQ	CE1-CD1-CG2	-3.31	116.94	121.22
1	47-A	62	CRQ	CB2-CA2-C2	-3.31	118.34	122.36
1	1-A	62	CRQ	C2-CA2-N2	3.30	111.31	108.95
1	29-A	62	CRQ	CB2-CA2-N2	-3.27	124.32	128.76
1	35-A	62	CRQ	CD2-CG2-CD1	3.25	122.48	117.65
1	26-A	62	CRQ	CG2-CB2-CA2	3.25	133.73	129.87
1	28-A	62	CRQ	C3-CA3-N3	3.24	119.80	112.43
1	32-A	62	CRQ	O2-C2-CA2	-3.23	128.96	131.02
1	4-A	62	CRQ	C3-CA3-N3	3.17	119.64	112.43
1	12-A	62	CRQ	CG2-CB2-CA2	-3.15	126.12	129.87
1	22-A	62	CRQ	O2-C2-CA2	-3.13	129.02	131.02
1	37-A	62	CRQ	C2-CA2-N2	3.13	111.19	108.95
1	47-A	62	CRQ	CD2-CG2-CD1	3.12	122.27	117.65
1	32-A	62	CRQ	CB2-CA2-N2	3.11	132.99	128.76
1	14-A	62	CRQ	CG2-CB2-CA2	3.11	133.56	129.87
1	32-A	62	CRQ	N3-C1-N2	-3.10	108.94	112.62
1	32-A	62	CRQ	CB2-CA2-C2	-3.10	118.60	122.36
1	8-A	62	CRQ	O2-C2-CA2	3.09	132.99	131.02
1	26-A	62	CRQ	C2-CA2-N2	3.09	111.16	108.95
1	33-A	62	CRQ	CG2-CB2-CA2	-3.08	126.21	129.87
1	9-A	62	CRQ	CD2-CG2-CB2	-3.08	110.64	121.22
1	38-A	62	CRQ	CA2-N2-C1	3.08	109.75	104.09
1	1-A	62	CRQ	CD1-CE1-CZ	3.07	123.13	119.88
1	33-A	62	CRQ	CE1-CD1-CG2	-3.06	117.27	121.22
1	15-A	62	CRQ	CG2-CB2-CA2	3.05	133.49	129.87
1	1-A	62	CRQ	C3-CA3-N3	3.04	119.35	112.43
1	3-A	62	CRQ	CG1-CB1-CA1	-3.04	104.29	113.51
1	37-A	62	CRQ	C3-CA3-N3	3.04	119.34	112.43
1	33-A	62	CRQ	CG1-CB1-CA1	-3.02	104.35	113.51
1	11-A	62	CRQ	O2-C2-CA2	3.00	132.94	131.02
1	29-A	62	CRQ	CB2-CA2-C2	2.99	125.99	122.36
1	19-A	62	CRQ	CD2-CG2-CD1	2.98	122.07	117.65
1	42-A	62	CRQ	CA2-C2-N3	2.95	105.98	103.50
1	6-A	62	CRQ	O2-C2-CA2	-2.93	129.15	131.02
1	32-A	62	CRQ	CA2-N2-C1	2.93	109.48	104.09
1	41-A	62	CRQ	C2-CA2-N2	2.93	111.05	108.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	37-A	62	CRQ	CE1-CD1-CG2	-2.92	117.45	121.22
1	25-A	62	CRQ	C3-CA3-N3	2.91	119.06	112.43
1	47-A	62	CRQ	CE1-CD1-CG2	-2.91	117.47	121.22
1	47-A	62	CRQ	C3-CA3-N3	2.90	119.03	112.43
1	38-A	62	CRQ	CG2-CB2-CA2	2.89	133.31	129.87
1	40-A	62	CRQ	C2-CA2-N2	2.89	111.02	108.95
1	30-A	62	CRQ	C3-CA3-N3	2.88	118.99	112.43
1	12-A	62	CRQ	O3-C3-CA3	-2.88	112.53	125.47
1	15-A	62	CRQ	CD2-CG2-CD1	2.86	121.90	117.65
1	39-A	62	CRQ	C2-CA2-N2	2.83	110.98	108.95
1	40-A	62	CRQ	CE1-CD1-CG2	-2.81	117.59	121.22
1	3-A	62	CRQ	O2-C2-CA2	2.80	132.81	131.02
1	16-A	62	CRQ	O3-C3-CA3	-2.78	112.95	125.47
1	15-A	62	CRQ	CE2-CD2-CG2	-2.78	117.63	121.22
1	14-A	62	CRQ	N3-C1-N2	-2.78	109.32	112.62
1	30-A	62	CRQ	O3-C3-CA3	-2.77	113.00	125.47
1	6-A	62	CRQ	O3-C3-CA3	-2.77	113.01	125.47
1	33-A	62	CRQ	CD2-CG2-CD1	2.74	121.71	117.65
1	17-A	62	CRQ	O3-C3-CA3	-2.73	113.17	125.47
1	15-A	62	CRQ	N3-C1-N2	-2.73	109.38	112.62
1	5-A	62	CRQ	O3-C3-CA3	-2.71	113.26	125.47
1	17-A	62	CRQ	C2-CA2-N2	2.71	110.89	108.95
1	38-A	62	CRQ	CA2-C2-N3	2.70	105.77	103.50
1	41-A	62	CRQ	CG1-CB1-CA1	-2.70	105.32	113.51
1	14-A	62	CRQ	CB2-CA2-C2	-2.70	119.09	122.36
1	17-A	62	CRQ	CG1-CB1-CA1	-2.69	105.34	113.51
1	13-A	62	CRQ	C2-CA2-N2	2.69	110.88	108.95
1	47-A	62	CRQ	O3-C3-CA3	-2.69	113.37	125.47
1	25-A	62	CRQ	O3-C3-CA3	-2.67	113.47	125.47
1	9-A	62	CRQ	CG1-CB1-CA1	-2.66	105.45	113.51
1	27-A	62	CRQ	CG1-CB1-CA1	-2.66	105.46	113.51
1	23-A	62	CRQ	C3-CA3-N3	2.65	118.46	112.43
1	4-A	62	CRQ	OH-CZ-CE2	2.64	127.36	120.00
1	25-A	62	CRQ	CB2-CA2-C2	-2.62	119.19	122.36
1	8-A	62	CRQ	C3-CA3-N3	2.61	118.38	112.43
1	19-A	62	CRQ	N3-C1-N2	-2.61	109.52	112.62
1	11-A	62	CRQ	C3-CA3-N3	2.61	118.38	112.43
1	40-A	62	CRQ	CG2-CB2-CA2	-2.61	126.77	129.87
1	41-A	62	CRQ	CB2-CA2-C2	-2.60	119.20	122.36
1	10-A	62	CRQ	C2-CA2-N2	2.60	110.81	108.95
1	24-A	62	CRQ	CG2-CB2-CA2	-2.60	126.78	129.87
1	14-A	62	CRQ	O3-C3-CA3	-2.60	113.79	125.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	29-A	62	CRQ	CA2-N2-C1	2.59	108.86	104.09
1	39-A	62	CRQ	O3-C3-CA3	-2.59	113.81	125.47
1	44-A	62	CRQ	C3-CA3-N3	2.58	118.29	112.43
1	18-A	62	CRQ	CA2-N2-C1	2.57	108.82	104.09
1	19-A	62	CRQ	O2-C2-N3	2.57	129.67	124.31
1	2-A	62	CRQ	CA2-N2-C1	2.56	108.81	104.09
1	44-A	62	CRQ	O3-C3-CA3	-2.56	113.96	125.47
1	45-A	62	CRQ	CG1-CB1-CA1	-2.54	105.80	113.51
1	17-A	62	CRQ	C3-CA3-N3	2.54	118.21	112.43
1	1-A	62	CRQ	CB2-CA2-C2	-2.54	119.28	122.36
1	4-A	62	CRQ	CA2-N2-C1	2.54	108.76	104.09
1	45-A	62	CRQ	O3-C3-CA3	-2.53	114.10	125.47
1	9-A	62	CRQ	C2-CA2-N2	2.52	110.76	108.95
1	26-A	62	CRQ	CA3-N3-C1	-2.52	123.42	128.39
1	14-A	62	CRQ	C3-CA3-N3	2.51	118.15	112.43
1	18-A	62	CRQ	O3-C3-CA3	-2.51	114.16	125.47
1	21-A	62	CRQ	CA2-C2-N3	2.51	105.61	103.50
1	11-A	62	CRQ	O3-C3-CA3	-2.51	114.17	125.47
1	24-A	62	CRQ	CD1-CE1-CZ	2.50	122.52	119.88
1	42-A	62	CRQ	O3-C3-CA3	-2.50	114.22	125.47
1	29-A	62	CRQ	CG1-CB1-CA1	-2.49	105.95	113.51
1	13-A	62	CRQ	O3-C3-CA3	-2.49	114.25	125.47
1	43-A	62	CRQ	CA2-C2-N3	2.49	105.59	103.50
1	1-A	62	CRQ	CG1-CB1-CA1	-2.49	105.96	113.51
1	24-A	62	CRQ	CG1-CB1-CA1	-2.48	105.98	113.51
1	44-A	62	CRQ	N3-C1-N2	-2.47	109.69	112.62
1	5-A	62	CRQ	CE1-CD1-CG2	-2.47	118.03	121.22
1	26-A	62	CRQ	O3-C3-CA3	-2.47	114.35	125.47
1	1-A	62	CRQ	CG2-CB2-CA2	2.47	132.80	129.87
1	21-A	62	CRQ	CG1-CB1-CA1	-2.46	106.04	113.51
1	19-A	62	CRQ	O3-C3-CA3	-2.46	114.41	125.47
1	41-A	62	CRQ	O3-C3-CA3	-2.46	114.41	125.47
1	17-A	62	CRQ	CD2-CG2-CD1	2.45	121.29	117.65
1	22-A	62	CRQ	CB2-CA2-C2	-2.45	119.39	122.36
1	47-A	62	CRQ	CD2-CE2-CZ	-2.44	117.29	119.88
1	15-A	62	CRQ	C2-CA2-N2	2.44	110.70	108.95
1	35-A	62	CRQ	CE1-CD1-CG2	-2.43	118.09	121.22
1	9-A	62	CRQ	O3-C3-CA3	-2.42	114.57	125.47
1	33-A	62	CRQ	CA3-N3-C2	2.42	128.99	123.67
1	32-A	62	CRQ	CA3-N3-C1	2.42	133.16	128.39
1	33-A	62	CRQ	O3-C3-CA3	-2.42	114.59	125.47
1	4-A	62	CRQ	O3-C3-CA3	-2.41	114.62	125.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	46-A	62	CRQ	O3-C3-CA3	-2.41	114.62	125.47
1	22-A	62	CRQ	CD2-CG2-CD1	2.41	121.22	117.65
1	36-A	62	CRQ	CA2-C2-N3	2.40	105.52	103.50
1	34-A	62	CRQ	O3-C3-CA3	-2.39	114.71	125.47
1	15-A	62	CRQ	C3-CA3-N3	2.39	117.86	112.43
1	27-A	62	CRQ	C2-CA2-N2	2.38	110.66	108.95
1	8-A	62	CRQ	O3-C3-CA3	-2.38	114.76	125.47
1	35-A	62	CRQ	N3-C1-N2	-2.37	109.80	112.62
1	5-A	62	CRQ	CG1-CB1-CA1	-2.37	106.33	113.51
1	32-A	62	CRQ	O3-C3-CA3	-2.35	114.88	125.47
1	25-A	62	CRQ	CA3-N3-C1	-2.34	123.77	128.39
1	35-A	62	CRQ	CG1-CB1-CA1	-2.34	106.41	113.51
1	37-A	62	CRQ	CB2-CA2-C2	-2.33	119.53	122.36
1	14-A	62	CRQ	CA2-N2-C1	2.33	108.37	104.09
1	46-A	62	CRQ	N3-C1-N2	-2.32	109.86	112.62
1	43-A	62	CRQ	CD1-CE1-CZ	2.32	122.33	119.88
1	18-A	62	CRQ	N3-C1-N2	-2.32	109.87	112.62
1	45-A	62	CRQ	C3-CA3-N3	2.32	117.70	112.43
1	7-A	62	CRQ	N3-C1-N2	-2.31	109.87	112.62
1	11-A	62	CRQ	CG1-CB1-CA1	-2.30	106.53	113.51
1	15-A	62	CRQ	CA2-N2-C1	2.30	108.33	104.09
1	34-A	62	CRQ	CG1-CB1-CA1	-2.30	106.53	113.51
1	20-A	62	CRQ	CA2-N2-C1	2.30	108.33	104.09
1	6-A	62	CRQ	CG1-CB1-CA1	-2.29	106.56	113.51
1	35-A	62	CRQ	CA3-N3-C1	-2.29	123.88	128.39
1	10-A	62	CRQ	CB2-CA2-C2	-2.28	119.59	122.36
1	31-A	62	CRQ	O3-C3-CA3	-2.28	115.20	125.47
1	3-A	62	CRQ	O3-C3-CA3	-2.28	115.20	125.47
1	44-A	62	CRQ	CG2-CB2-CA2	2.28	132.57	129.87
1	2-A	62	CRQ	O3-C3-CA3	-2.27	115.25	125.47
1	26-A	62	CRQ	CG1-CB1-CA1	-2.27	106.63	113.51
1	31-A	62	CRQ	CG2-CB2-CA2	-2.26	127.17	129.87
1	44-A	62	CRQ	CA2-N2-C1	2.26	108.26	104.09
1	37-A	62	CRQ	CD1-CE1-CZ	2.26	122.27	119.88
1	19-A	62	CRQ	CE2-CD2-CG2	-2.26	118.31	121.22
1	8-A	62	CRQ	CG1-CB1-CA1	-2.26	106.67	113.51
1	13-A	62	CRQ	N3-C1-N2	-2.25	109.95	112.62
1	30-A	62	CRQ	CG2-CB2-CA2	2.25	132.54	129.87
1	40-A	62	CRQ	CD2-CG2-CD1	2.25	120.99	117.65
1	32-A	62	CRQ	CG1-CB1-CA1	-2.24	106.72	113.51
1	10-A	62	CRQ	O3-C3-CA3	-2.23	115.42	125.47
1	24-A	62	CRQ	CE1-CD1-CG2	-2.23	118.34	121.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	22-A	62	CRQ	N3-C1-N2	-2.23	109.97	112.62
1	12-A	62	CRQ	N3-C1-N2	-2.22	109.99	112.62
1	22-A	62	CRQ	O3-C3-CA3	-2.21	115.50	125.47
1	42-A	62	CRQ	CG1-CB1-CA1	-2.21	106.81	113.51
1	40-A	62	CRQ	CD2-CE2-CZ	-2.21	117.54	119.88
1	4-A	62	CRQ	CA2-C2-N3	2.21	105.35	103.50
1	41-A	62	CRQ	CD2-CG2-CD1	2.20	120.92	117.65
1	28-A	62	CRQ	CG1-CB1-CA1	-2.20	106.84	113.51
1	2-A	62	CRQ	N3-C1-N2	-2.20	110.01	112.62
1	25-A	62	CRQ	CG1-CB1-CA1	-2.19	106.86	113.51
1	26-A	62	CRQ	CA3-N3-C2	2.19	128.49	123.67
1	30-A	62	CRQ	CA2-N2-C1	2.19	108.13	104.09
1	12-A	62	CRQ	CG1-CB1-CA1	-2.19	106.87	113.51
1	22-A	62	CRQ	C3-CA3-N3	2.19	117.41	112.43
1	22-A	62	CRQ	C2-CA2-N2	2.19	110.52	108.95
1	9-A	62	CRQ	CD1-CG2-CB2	2.19	128.73	121.22
1	23-A	62	CRQ	O3-C3-CA3	-2.19	115.63	125.47
1	35-A	62	CRQ	O3-C3-CA3	-2.18	115.64	125.47
1	28-A	62	CRQ	O3-C3-CA3	-2.18	115.64	125.47
1	31-A	62	CRQ	CB2-CA2-N2	-2.18	125.80	128.76
1	7-A	62	CRQ	O3-C3-CA3	-2.18	115.67	125.47
1	8-A	62	CRQ	C2-CA2-N2	2.17	110.51	108.95
1	35-A	62	CRQ	CD2-CE2-CZ	-2.17	117.59	119.88
1	12-A	62	CRQ	O2-C2-CA2	-2.16	129.64	131.02
1	22-A	62	CRQ	CA2-N2-C1	2.16	108.07	104.09
1	31-A	62	CRQ	CG1-CB1-CA1	-2.16	106.95	113.51
1	47-A	62	CRQ	N3-C1-N2	-2.15	110.06	112.62
1	40-A	62	CRQ	CA3-N3-C1	-2.15	124.16	128.39
1	12-A	62	CRQ	CA3-N3-C1	-2.14	124.17	128.39
1	4-A	62	CRQ	CE2-CZ-CE1	-2.14	116.36	119.77
1	3-A	62	CRQ	N3-C1-N2	-2.13	110.09	112.62
1	15-A	62	CRQ	CB2-CA2-N2	2.12	131.64	128.76
1	15-A	62	CRQ	O3-C3-CA3	-2.12	115.94	125.47
1	39-A	62	CRQ	CG1-CB1-CA1	-2.12	107.09	113.51
1	8-A	62	CRQ	N3-C1-N2	-2.11	110.11	112.62
1	43-A	62	CRQ	O3-C3-CA3	-2.11	115.96	125.47
1	29-A	62	CRQ	O3-C3-CA3	-2.11	115.97	125.47
1	30-A	62	CRQ	CA2-C2-N3	2.10	105.26	103.50
1	30-A	62	CRQ	CG1-CB1-CA1	-2.10	107.16	113.51
1	19-A	62	CRQ	CA2-N2-C1	2.09	107.95	104.09
1	14-A	62	CRQ	CE2-CD2-CG2	-2.09	118.52	121.22
1	18-A	62	CRQ	CA2-C2-N3	2.08	105.25	103.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	20-A	62	CRQ	CG1-CB1-CA1	-2.08	107.21	113.51
1	38-A	62	CRQ	N3-C1-N2	-2.08	110.16	112.62
1	27-A	62	CRQ	O3-C3-CA3	-2.07	116.13	125.47
1	3-A	62	CRQ	CA2-C2-N3	2.07	105.24	103.50
1	11-A	62	CRQ	CA2-N2-C1	2.07	107.89	104.09
1	28-A	62	CRQ	CB2-CA2-C2	-2.06	119.86	122.36
1	37-A	62	CRQ	O3-C3-CA3	-2.06	116.20	125.47
1	46-A	62	CRQ	CB2-CA2-C2	-2.05	119.87	122.36
1	42-A	62	CRQ	N3-C1-N2	-2.05	110.19	112.62
1	19-A	62	CRQ	CD2-CG2-CB2	-2.04	114.20	121.22
1	16-A	62	CRQ	N3-C1-N2	-2.04	110.20	112.62
1	4-A	62	CRQ	CG1-CB1-CA1	-2.03	107.36	113.51
1	21-A	62	CRQ	CD2-CG2-CD1	2.03	120.66	117.65
1	46-A	62	CRQ	CA2-C2-N3	2.03	105.20	103.50
1	6-A	62	CRQ	O2-C2-N3	2.03	128.54	124.31
1	13-A	62	CRQ	CG1-CB1-CA1	-2.03	107.37	113.51
1	7-A	62	CRQ	C2-CA2-N2	2.02	110.40	108.95
1	24-A	62	CRQ	C3-CA3-N3	2.02	117.03	112.43
1	40-A	62	CRQ	CG1-CB1-CA1	-2.02	107.37	113.51
1	8-A	62	CRQ	CA2-N2-C1	2.02	107.81	104.09
1	43-A	62	CRQ	O2-C2-CA2	2.01	132.31	131.02
1	22-A	62	CRQ	CG1-CB1-CA1	-2.01	107.41	113.51
1	31-A	62	CRQ	CA3-N3-C1	-2.01	124.43	128.39
1	38-A	62	CRQ	O3-C3-CA3	-2.01	116.43	125.47
1	16-A	62	CRQ	CA2-N2-C1	2.01	107.78	104.09
1	36-A	62	CRQ	CG1-CB1-CA1	-2.00	107.44	113.51
1	40-A	62	CRQ	C3-CA3-N3	2.00	116.98	112.43
1	1-A	62	CRQ	N3-C1-N2	-2.00	110.25	112.62

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	3-A	62	CRQ	C2-CA2-CB2-CG2
1	4-A	62	CRQ	N2-CA2-CB2-CG2
1	4-A	62	CRQ	C2-CA2-CB2-CG2
1	6-A	62	CRQ	C3-CA3-N3-C2
1	10-A	62	CRQ	N2-CA2-CB2-CG2
1	10-A	62	CRQ	C2-CA2-CB2-CG2
1	12-A	62	CRQ	C3-CA3-N3-C2
1	14-A	62	CRQ	N2-CA2-CB2-CG2
1	14-A	62	CRQ	C2-CA2-CB2-CG2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	15-A	62	CRQ	N2-CA2-CB2-CG2
1	15-A	62	CRQ	C2-CA2-CB2-CG2
1	17-A	62	CRQ	C1-CA1-CB1-CG1
1	20-A	62	CRQ	N2-CA2-CB2-CG2
1	20-A	62	CRQ	C2-CA2-CB2-CG2
1	22-A	62	CRQ	N2-CA2-CB2-CG2
1	22-A	62	CRQ	C2-CA2-CB2-CG2
1	23-A	62	CRQ	C2-CA2-CB2-CG2
1	24-A	62	CRQ	C3-CA3-N3-C2
1	25-A	62	CRQ	C3-CA3-N3-C2
1	26-A	62	CRQ	C3-CA3-N3-C2
1	27-A	62	CRQ	C3-CA3-N3-C2
1	28-A	62	CRQ	C2-CA2-CB2-CG2
1	29-A	62	CRQ	C3-CA3-N3-C1
1	29-A	62	CRQ	C3-CA3-N3-C2
1	30-A	62	CRQ	C2-CA2-CB2-CG2
1	31-A	62	CRQ	C3-CA3-N3-C1
1	31-A	62	CRQ	C3-CA3-N3-C2
1	33-A	62	CRQ	C3-CA3-N3-C2
1	34-A	62	CRQ	C3-CA3-N3-C2
1	35-A	62	CRQ	C3-CA3-N3-C2
1	36-A	62	CRQ	C2-CA2-CB2-CG2
1	38-A	62	CRQ	N2-CA2-CB2-CG2
1	38-A	62	CRQ	C2-CA2-CB2-CG2
1	40-A	62	CRQ	C3-CA3-N3-C2
1	43-A	62	CRQ	C3-CA3-N3-C2
1	47-A	62	CRQ	C1-CA1-CB1-CG1
1	3-A	62	CRQ	N2-CA2-CB2-CG2
1	11-A	62	CRQ	N2-CA2-CB2-CG2
1	17-A	62	CRQ	N2-CA2-CB2-CG2
1	23-A	62	CRQ	N2-CA2-CB2-CG2
1	28-A	62	CRQ	N2-CA2-CB2-CG2
1	30-A	62	CRQ	N2-CA2-CB2-CG2
1	36-A	62	CRQ	N2-CA2-CB2-CG2
1	37-A	62	CRQ	N2-CA2-CB2-CG2
1	41-A	62	CRQ	N2-CA2-CB2-CG2
1	47-A	62	CRQ	N2-CA2-CB2-CG2
1	36-A	62	CRQ	CA2-CB2-CG2-CD2
1	2-A	62	CRQ	C3-CA3-N3-C2
1	5-A	62	CRQ	C3-CA3-N3-C2
1	9-A	62	CRQ	C3-CA3-N3-C2
1	13-A	62	CRQ	C3-CA3-N3-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	17-A	62	CRQ	C3-CA3-N3-C2
1	11-A	62	CRQ	C2-CA2-CB2-CG2
1	47-A	62	CRQ	C2-CA2-CB2-CG2
1	24-A	62	CRQ	C3-CA3-N3-C1
1	33-A	62	CRQ	C3-CA3-N3-C1
1	40-A	62	CRQ	C3-CA3-N3-C1
1	7-A	62	CRQ	C3-CA3-N3-C2
1	36-A	62	CRQ	C3-CA3-N3-C2
1	36-A	62	CRQ	CA2-CB2-CG2-CD1
1	8-A	62	CRQ	N2-CA2-CB2-CG2
1	41-A	62	CRQ	C2-CA2-CB2-CG2
1	6-A	62	CRQ	C3-CA3-N3-C1
1	26-A	62	CRQ	C3-CA3-N3-C1
1	35-A	62	CRQ	C3-CA3-N3-C1
1	18-A	62	CRQ	C3-CA3-N3-C2
1	45-A	62	CRQ	C3-CA3-N3-C2
1	25-A	62	CRQ	C3-CA3-N3-C1
1	29-A	62	CRQ	N2-CA2-CB2-CG2

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	5-A	1
1	1-A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
5	A	62:CRQ	C3	65:ASN	N	1.20
1	A	62:CRQ	C3	65:ASN	N	1.18

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	213/229 (93%)	2.09	86 (40%) 0 0	0, 1, 1, 1	213 (100%)
1	2-A	0/229	-	-	-	-
1	3-A	0/229	-	-	-	-
1	4-A	0/229	-	-	-	-
1	5-A	0/229	-	-	-	-
1	6-A	0/229	-	-	-	-
1	7-A	0/229	-	-	-	-
1	8-A	0/229	-	-	-	-
1	9-A	0/229	-	-	-	-
1	10-A	0/229	-	-	-	-
1	11-A	0/229	-	-	-	-
1	12-A	0/229	-	-	-	-
1	13-A	0/229	-	-	-	-
1	14-A	0/229	-	-	-	-
1	15-A	0/229	-	-	-	-
1	16-A	0/229	-	-	-	-
1	17-A	0/229	-	-	-	-
1	18-A	0/229	-	-	-	-
1	19-A	0/229	-	-	-	-
1	20-A	0/229	-	-	-	-
1	21-A	0/229	-	-	-	-
1	22-A	0/229	-	-	-	-
1	23-A	0/229	-	-	-	-
1	24-A	0/229	-	-	-	-
1	25-A	0/229	-	-	-	-
1	26-A	0/229	-	-	-	-
1	27-A	0/229	-	-	-	-
1	28-A	0/229	-	-	-	-
1	29-A	0/229	-	-	-	-
1	30-A	0/229	-	-	-	-
1	31-A	0/229	-	-	-	-
1	32-A	0/229	-	-	-	-

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	33-A	0/229	-	-	-	-
1	34-A	0/229	-	-	-	-
1	35-A	0/229	-	-	-	-
1	36-A	0/229	-	-	-	-
1	37-A	0/229	-	-	-	-
1	38-A	0/229	-	-	-	-
1	39-A	0/229	-	-	-	-
1	40-A	0/229	-	-	-	-
1	41-A	0/229	-	-	-	-
1	42-A	0/229	-	-	-	-
1	43-A	0/229	-	-	-	-
1	44-A	0/229	-	-	-	-
1	45-A	0/229	-	-	-	-
1	46-A	0/229	-	-	-	-
1	47-A	0/229	-	-	-	-
All	All	213/10763 (1%)	2.09	86 (40%) 0 0	0, 1, 1, 1	213 (100%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	151	GLY	11.0
1	1-A	217	TYR	8.6
1	1-A	74	ASP	7.3
1	1-A	2	SER	6.6
1	1-A	152	VAL	5.4
1	1-A	133	GLN	5.3
1	1-A	150	ASP	5.2
1	1-A	147	TYR	5.1
1	1-A	85	GLU	5.1
1	1-A	73	GLU	4.9
1	1-A	178	LYS	4.8
1	1-A	127	PRO	4.8
1	1-A	185	LEU	4.7
1	1-A	39	THR	4.5
1	1-A	196	GLU	4.3
1	1-A	102	ILE	4.2
1	1-A	149	GLU	4.2
1	1-A	3	VAL	4.2
1	1-A	148	VAL	4.1
1	1-A	176	THR	4.1
1	1-A	81	GLN	4.0
1	1-A	35	GLU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-A	191	VAL	3.8
1	1-A	134	LYS	3.8
1	1-A	157	VAL	3.5
1	1-A	174	LYS	3.5
1	1-A	48	ALA	3.4
1	1-A	156	ASP	3.4
1	1-A	7	GLU	3.3
1	1-A	180	LYS	3.3
1	1-A	183	VAL	3.3
1	1-A	34	TYR	3.3
1	1-A	154	LYS	3.3
1	1-A	142	PRO	3.2
1	1-A	212	HIS	3.2
1	1-A	28	GLU	3.2
1	1-A	141	SER	3.2
1	1-A	194	ARG	3.2
1	1-A	203	ASP	3.2
1	1-A	123	THR	3.2
1	1-A	132	MET	3.1
1	1-A	84	PRO	3.0
1	1-A	75	ILE	3.0
1	1-A	202	LYS	3.0
1	1-A	211	GLU	3.0
1	1-A	216	ARG	2.9
1	1-A	44	VAL	2.9
1	1-A	118	ILE	2.9
1	1-A	145	LYS	2.8
1	1-A	13	ARG	2.8
1	1-A	51	PRO	2.8
1	1-A	15	GLU	2.8
1	1-A	182	ASP	2.7
1	1-A	43	THR	2.7
1	1-A	98	GLN	2.6
1	1-A	215	ALA	2.6
1	1-A	111	GLY	2.5
1	1-A	162	LEU	2.5
1	1-A	112	ASP	2.5
1	1-A	5	LYS	2.5
1	1-A	210	TYR	2.5
1	1-A	17	ALA	2.5
1	1-A	83	PHE	2.5
1	1-A	124	ASN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-A	187	ASP	2.4
1	1-A	6	PRO	2.4
1	1-A	125	PHE	2.4
1	1-A	193	HIS	2.4
1	1-A	165	GLY	2.4
1	1-A	128	ASN	2.4
1	1-A	106	ASP	2.3
1	1-A	206	LYS	2.3
1	1-A	115	PHE	2.3
1	1-A	177	TYR	2.3
1	1-A	30	ILE	2.3
1	1-A	114	PHE	2.3
1	1-A	164	GLU	2.2
1	1-A	117	GLU	2.2
1	1-A	18	VAL	2.2
1	1-A	161	LEU	2.2
1	1-A	192	ASP	2.1
1	1-A	78	TYR	2.1
1	1-A	197	ILE	2.1
1	1-A	11	LYS	2.1
1	1-A	36	GLY	2.0
1	1-A	99	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CRQ	1-A	62	24/25	0.76	0.16	22,22,24,25	24
1	CRQ	2-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	3-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	4-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	5-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	6-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	7-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	8-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	9-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	10-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	11-A	62	24/25	-	-	22,22,24,25	24

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CRQ	12-A	62	24/25	-	-	22,23,24,25	24
1	CRQ	13-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	14-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	15-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	16-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	17-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	18-A	62	24/25	-	-	22,23,24,25	24
1	CRQ	19-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	20-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	21-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	22-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	23-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	24-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	25-A	62	24/25	-	-	22,23,24,25	24
1	CRQ	26-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	27-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	28-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	29-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	30-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	31-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	32-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	33-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	34-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	35-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	36-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	37-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	38-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	39-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	40-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	41-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	42-A	62	24/25	-	-	22,23,24,25	24
1	CRQ	43-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	44-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	45-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	46-A	62	24/25	-	-	22,22,24,25	24
1	CRQ	47-A	62	24/25	-	-	22,22,24,25	24

5.3 Carbohydrates

There are no oligosaccharides in this entry.

5.4 Ligands

There are no ligands in this entry.

5.5 Other polymers

There are no such residues in this entry.