



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 24, 2026 – 12:02 AM UTC

PDB ID : 5EXU / pdb_00005exu
Title : Reversibly photoswitching protein Dathail, Ensemble refinement
Authors : Close, D.W.; Langan, P.S.; Bradbury, A.R.M.
Deposited on : 2015-11-24
Resolution : 1.65 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

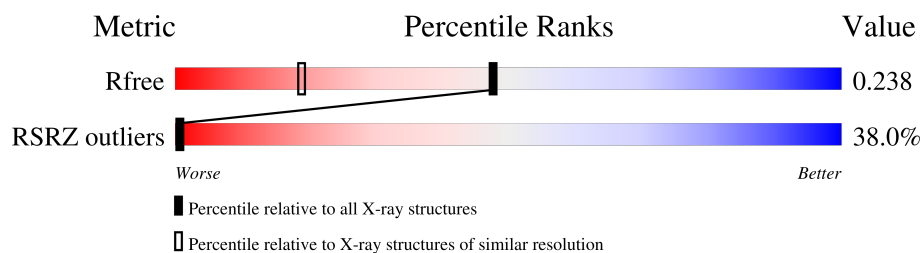
1 Overall quality at a glance

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 224314 atoms, of which 105273 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Reversibly photoswitching protein Dathail.

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

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

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

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

- Molecule 2 is water.

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

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

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

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

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	76.25Å 81.18Å 39.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.18 – 1.65 32.18 – 1.65	Depositor EDS
% Data completeness (in resolution range)	97.6 (32.18-1.65) 94.1 (32.18-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.65Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.168 , 0.210 0.193 , 0.238	Depositor DCC
R_{free} test set	2264 reflections (7.48%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.01 , 32.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	224314	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.76% 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](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CRQ	31-A	62	1	25,25,26	2.12	6 (24%)	28,34,36	3.32	14 (50%)
1	CRQ	39-A	62	1	25,25,26	2.11	8 (32%)	28,34,36	2.02	8 (28%)
1	CRQ	48-A	62	1	25,25,26	2.24	6 (24%)	28,34,36	1.76	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CRQ	28-A	62	1	25,25,26	2.04	6 (24%)	28,34,36	1.73	7 (25%)
1	CRQ	56-A	62	1	25,25,26	1.88	6 (24%)	28,34,36	3.26	7 (25%)
1	CRQ	16-A	62	1	25,25,26	1.99	8 (32%)	28,34,36	6.95	17 (60%)
1	CRQ	27-A	62	1	25,25,26	2.01	7 (28%)	28,34,36	2.13	8 (28%)
1	CRQ	46-A	62	1	25,25,26	1.99	6 (24%)	28,34,36	2.26	7 (25%)
1	CRQ	11-A	62	1	25,25,26	2.00	6 (24%)	28,34,36	2.18	9 (32%)
1	CRQ	50-A	62	1	25,25,26	2.20	6 (24%)	28,34,36	2.21	6 (21%)
1	CRQ	62-A	62	1	25,25,26	2.10	8 (32%)	28,34,36	2.78	8 (28%)
1	CRQ	25-A	62	1	25,25,26	2.13	7 (28%)	28,34,36	1.67	7 (25%)
1	CRQ	58-A	62	1	25,25,26	3.21	10 (40%)	28,34,36	3.93	16 (57%)
1	CRQ	32-A	62	1	25,25,26	2.12	6 (24%)	28,34,36	2.32	7 (25%)
1	CRQ	7-A	62	1	25,25,26	2.04	6 (24%)	28,34,36	3.85	7 (25%)
1	CRQ	23-A	62	1	25,25,26	2.17	7 (28%)	28,34,36	3.68	13 (46%)
1	CRQ	60-A	62	1	25,25,26	2.02	7 (28%)	28,34,36	2.14	8 (28%)
1	CRQ	41-A	62	1	25,25,26	2.17	6 (24%)	28,34,36	3.69	11 (39%)
1	CRQ	35-A	62	1	25,25,26	1.96	4 (16%)	28,34,36	2.40	7 (25%)
1	CRQ	9-A	62	1	25,25,26	2.64	9 (36%)	28,34,36	2.47	12 (42%)
1	CRQ	43-A	62	1	25,25,26	2.47	7 (28%)	28,34,36	4.89	13 (46%)
1	CRQ	63-A	62	1	25,25,26	2.25	5 (20%)	28,34,36	3.05	13 (46%)
1	CRQ	47-A	62	1	25,25,26	2.39	7 (28%)	28,34,36	3.70	12 (42%)
1	CRQ	18-A	62	1	25,25,26	1.86	7 (28%)	28,34,36	3.44	13 (46%)
1	CRQ	49-A	62	1	25,25,26	1.98	5 (20%)	28,34,36	2.13	7 (25%)
1	CRQ	3-A	62	1	25,25,26	2.89	8 (32%)	28,34,36	3.40	14 (50%)
1	CRQ	53-A	62	1	25,25,26	2.14	8 (32%)	28,34,36	4.12	12 (42%)
1	CRQ	15-A	62	1	25,25,26	2.17	8 (32%)	28,34,36	3.19	11 (39%)
1	CRQ	30-A	62	1	25,25,26	2.11	8 (32%)	28,34,36	2.19	11 (39%)
1	CRQ	37-A	62	1	25,25,26	2.23	6 (24%)	28,34,36	3.25	10 (35%)
1	CRQ	13-A	62	1	25,25,26	2.05	6 (24%)	28,34,36	3.57	9 (32%)
1	CRQ	21-A	62	1	25,25,26	2.23	7 (28%)	28,34,36	2.26	9 (32%)
1	CRQ	40-A	62	1	25,25,26	1.95	6 (24%)	28,34,36	1.98	7 (25%)
1	CRQ	29-A	62	1	25,25,26	2.19	5 (20%)	28,34,36	4.58	8 (28%)
1	CRQ	34-A	62	1	25,25,26	1.89	5 (20%)	28,34,36	2.15	8 (28%)
1	CRQ	4-A	62	1	25,25,26	2.27	8 (32%)	28,34,36	2.53	9 (32%)
1	CRQ	54-A	62	1	25,25,26	1.86	5 (20%)	28,34,36	4.36	16 (57%)
1	CRQ	8-A	62	1	25,25,26	2.12	5 (20%)	28,34,36	1.65	5 (17%)

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	1.92	6 (24%)	28,34,36	3.67	12 (42%)
1	CRQ	6-A	62	1	25,25,26	2.12	5 (20%)	28,34,36	2.95	10 (35%)
1	CRQ	52-A	62	1	25,25,26	2.11	5 (20%)	28,34,36	3.23	12 (42%)
1	CRQ	24-A	62	1	25,25,26	1.86	4 (16%)	28,34,36	2.91	10 (35%)
1	CRQ	10-A	62	1	25,25,26	1.92	7 (28%)	28,34,36	3.62	11 (39%)
1	CRQ	59-A	62	1	25,25,26	2.07	7 (28%)	28,34,36	3.80	13 (46%)
1	CRQ	26-A	62	1	25,25,26	2.12	7 (28%)	28,34,36	2.32	7 (25%)
1	CRQ	17-A	62	1	25,25,26	1.88	5 (20%)	28,34,36	4.03	11 (39%)
1	CRQ	19-A	62	1	25,25,26	2.60	10 (40%)	28,34,36	2.90	17 (60%)
1	CRQ	44-A	62	1	25,25,26	2.35	7 (28%)	28,34,36	3.87	14 (50%)
1	CRQ	1-A	62	1	25,25,26	2.02	7 (28%)	28,34,36	1.92	6 (21%)
1	CRQ	57-A	62	1	25,25,26	2.07	9 (36%)	28,34,36	3.12	8 (28%)
1	CRQ	51-A	62	1	25,25,26	2.38	6 (24%)	28,34,36	3.66	9 (32%)
1	CRQ	38-A	62	1	25,25,26	2.18	7 (28%)	28,34,36	2.05	7 (25%)
1	CRQ	22-A	62	1	25,25,26	2.04	5 (20%)	28,34,36	2.81	10 (35%)
1	CRQ	55-A	62	1	25,25,26	2.25	8 (32%)	28,34,36	3.38	12 (42%)
1	CRQ	2-A	62	1	25,25,26	1.95	6 (24%)	28,34,36	2.43	11 (39%)
1	CRQ	33-A	62	1	25,25,26	2.08	6 (24%)	28,34,36	2.83	13 (46%)
1	CRQ	61-A	62	1	25,25,26	1.96	6 (24%)	28,34,36	2.16	10 (35%)
1	CRQ	42-A	62	1	25,25,26	2.05	6 (24%)	28,34,36	3.51	7 (25%)
1	CRQ	45-A	62	1	25,25,26	1.87	6 (24%)	28,34,36	1.82	6 (21%)
1	CRQ	12-A	62	1	25,25,26	2.44	9 (36%)	28,34,36	2.47	6 (21%)
1	CRQ	36-A	62	1	25,25,26	2.31	8 (32%)	28,34,36	2.65	9 (32%)
1	CRQ	5-A	62	1	25,25,26	2.24	7 (28%)	28,34,36	3.90	15 (53%)
1	CRQ	20-A	62	1	25,25,26	2.87	10 (40%)	28,34,36	3.73	14 (50%)

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	31-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	39-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	48-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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CRQ	56-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	16-A	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	27-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	46-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	11-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	50-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	62-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	25-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	58-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	32-A	62	1	-	0/10/32/33	0/2/2/2
1	CRQ	7-A	62	1	-	5/10/32/33	0/2/2/2
1	CRQ	23-A	62	1	-	6/10/32/33	0/2/2/2
1	CRQ	60-A	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	41-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	35-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	9-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	43-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	63-A	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	47-A	62	1	-	6/10/32/33	0/2/2/2
1	CRQ	18-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	49-A	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	3-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	53-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	15-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	30-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	37-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	13-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	21-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	40-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	34-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	4-A	62	1	-	5/10/32/33	0/2/2/2
1	CRQ	54-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	8-A	62	1	-	5/10/32/33	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CRQ	14-A	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	6-A	62	1	-	6/10/32/33	0/2/2/2
1	CRQ	52-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	24-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	10-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	59-A	62	1	-	6/10/32/33	0/2/2/2
1	CRQ	26-A	62	1	-	5/10/32/33	0/2/2/2
1	CRQ	17-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	19-A	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	44-A	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	1-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	57-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	51-A	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	38-A	62	1	-	5/10/32/33	0/2/2/2
1	CRQ	22-A	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	55-A	62	1	-	6/10/32/33	0/2/2/2
1	CRQ	2-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	33-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	61-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	42-A	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	45-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	12-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	36-A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	5-A	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	20-A	62	1	-	6/10/32/33	0/2/2/2

The worst 5 of 420 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3-A	62	CRQ	CB2-CA2	10.38	1.45	1.35
1	58-A	62	CRQ	CB2-CA2	9.81	1.44	1.35
1	20-A	62	CRQ	C1-CA1	8.24	1.60	1.48
1	63-A	62	CRQ	C1-N3	7.65	1.50	1.38
1	9-A	62	CRQ	CB2-CA2	7.49	1.42	1.35

The worst 5 of 631 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16-A	62	CRQ	O2-C2-CA2	21.99	145.05	131.02
1	29-A	62	CRQ	CG2-CB2-CA2	-17.75	108.77	129.87
1	54-A	62	CRQ	CG2-CB2-CA2	-17.36	109.23	129.87
1	17-A	62	CRQ	CG2-CB2-CA2	-17.30	109.30	129.87
1	16-A	62	CRQ	CB2-CA2-N2	-17.02	105.65	128.76

There are no chirality outliers.

5 of 219 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1-A	62	CRQ	C3-CA3-N3-C2
1	1-A	62	CRQ	N2-CA2-CB2-CG2
1	1-A	62	CRQ	C2-CA2-CB2-CG2
1	2-A	62	CRQ	C3-CA3-N3-C1
1	2-A	62	CRQ	C3-CA3-N3-C2

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	52-A	1
1	15-A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
52	A	62:CRQ	C3	65:ASN	N	1.19
15	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%)	2.06	81 (38%) 1 1	0, 0, 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	-	-	-	-

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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	-	-	-	-
1	48-A	0/229	-	-	-	-
1	49-A	0/229	-	-	-	-
1	50-A	0/229	-	-	-	-
1	51-A	0/229	-	-	-	-
1	52-A	0/229	-	-	-	-
1	53-A	0/229	-	-	-	-
1	54-A	0/229	-	-	-	-
1	55-A	0/229	-	-	-	-
1	56-A	0/229	-	-	-	-
1	57-A	0/229	-	-	-	-
1	58-A	0/229	-	-	-	-
1	59-A	0/229	-	-	-	-
1	60-A	0/229	-	-	-	-
1	61-A	0/229	-	-	-	-
1	62-A	0/229	-	-	-	-
1	63-A	0/229	-	-	-	-
All	All	213/14427 (1%)	2.06	81 (38%) 1 1	0, 0, 1, 1	213 (100%)

The worst 5 of 81 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	192	ASP	7.6
1	1-A	159	MET	6.9
1	1-A	155	GLY	6.6
1	1-A	210	TYR	6.3
1	1-A	217	TYR	6.2

5.2 Non-standard residues in protein, DNA, RNA chains

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CRQ	1-A	62	24/25	0.66	0.19	19,20,22,23	24
1	CRQ	2-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	3-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	4-A	62	24/25	-	-	19,20,22,24	24
1	CRQ	5-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	6-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	7-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	8-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	9-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	10-A	62	24/25	-	-	20,20,22,24	24
1	CRQ	11-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	12-A	62	24/25	-	-	20,20,22,23	24
1	CRQ	13-A	62	24/25	-	-	19,20,22,24	24
1	CRQ	14-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	15-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	16-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	17-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	18-A	62	24/25	-	-	20,20,22,23	24
1	CRQ	19-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	20-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	21-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	22-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	23-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	24-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	25-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	26-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	27-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	28-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	29-A	62	24/25	-	-	20,20,22,23	24
1	CRQ	30-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	31-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	32-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	33-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	34-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	35-A	62	24/25	-	-	20,20,22,23	24
1	CRQ	36-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	37-A	62	24/25	-	-	19,20,22,23	24

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CRQ	38-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	39-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	40-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	41-A	62	24/25	-	-	20,20,22,23	24
1	CRQ	42-A	62	24/25	-	-	19,20,22,24	24
1	CRQ	43-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	44-A	62	24/25	-	-	19,20,22,24	24
1	CRQ	45-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	46-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	47-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	48-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	49-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	50-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	51-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	52-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	53-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	54-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	55-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	56-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	57-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	58-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	59-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	60-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	61-A	62	24/25	-	-	20,20,22,23	24
1	CRQ	62-A	62	24/25	-	-	19,20,22,23	24
1	CRQ	63-A	62	24/25	-	-	19,20,22,23	24

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

There are no ligands in this entry.

5.5 Other polymers [i](#)

There are no such residues in this entry.