



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:02 am GMT

PDB ID : 2C9I
Title : STRUCTURE OF THE FLUORESCENT PROTEIN ASFP499 FROM ANEMONIA SULCATA
Authors : Renzi, F.; Nienhaus, K.; Wiedenmann, J.; Vallone, B.; Nienhaus, G.U.
Deposited on : 2005-12-12
Resolution : 1.82 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

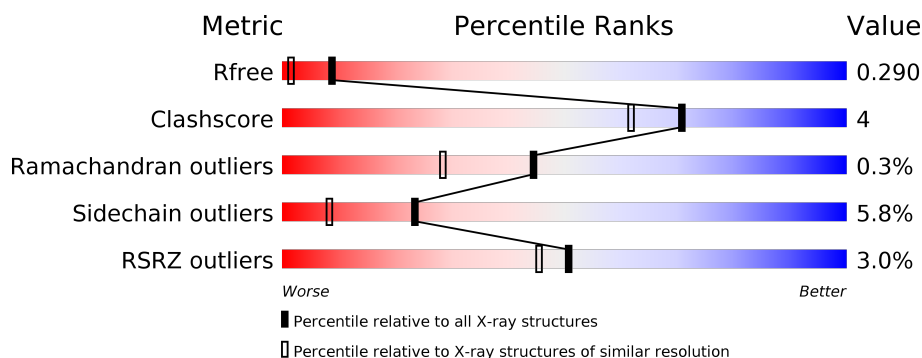
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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}	100719	5868 (1.84-1.80)
Clashscore	112137	6856 (1.84-1.80)
Ramachandran outliers	110173	6780 (1.84-1.80)
Sidechain outliers	110143	6780 (1.84-1.80)
RSRZ outliers	101464	5947 (1.84-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	A	226	<div> <div>3%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	B	226	<div> <div>4%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
1	C	226	<div> <div>6%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	D	226	<div> <div>4%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	E	226	<div> <div>2%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
1	F	226	<div> <div>%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	226	<div><div></div><div>4%</div><div>86%</div><div>12%</div><div></div></div>
1	H	226	<div><div></div><div>2%</div><div>85%</div><div>12%</div><div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15798 atoms, of which 0 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 GREEN FLUORESCENT PROTEIN ASFP499.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1781	1137	296	336	12			
1	B	225	Total	C	N	O	S	0	0	0
			1773	1132	295	335	11			
1	C	226	Total	C	N	O	S	0	0	0
			1781	1137	296	336	12			
1	D	226	Total	C	N	O	S	0	0	0
			1781	1137	296	336	12			
1	E	226	Total	C	N	O	S	0	0	0
			1781	1137	296	336	12			
1	F	225	Total	C	N	O	S	0	1	0
			1784	1138	299	336	11			
1	G	226	Total	C	N	O	S	0	0	0
			1781	1137	296	336	12			
1	H	225	Total	C	N	O	S	0	0	0
			1773	1132	295	335	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	CRQ	GLN	CHROMOPHORE	UNP Q9GPI6
A	63	CRQ	TYR	CHROMOPHORE	UNP Q9GPI6
A	63	CRQ	GLY	CHROMOPHORE	UNP Q9GPI6
B	63	CRQ	GLN	CHROMOPHORE	UNP Q9GPI6
B	63	CRQ	TYR	CHROMOPHORE	UNP Q9GPI6
B	63	CRQ	GLY	CHROMOPHORE	UNP Q9GPI6
C	63	CRQ	GLN	CHROMOPHORE	UNP Q9GPI6
C	63	CRQ	TYR	CHROMOPHORE	UNP Q9GPI6
C	63	CRQ	GLY	CHROMOPHORE	UNP Q9GPI6
D	63	CRQ	GLN	CHROMOPHORE	UNP Q9GPI6
D	63	CRQ	TYR	CHROMOPHORE	UNP Q9GPI6
D	63	CRQ	GLY	CHROMOPHORE	UNP Q9GPI6
E	63	CRQ	GLN	CHROMOPHORE	UNP Q9GPI6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	63	CRQ	TYR	CHROMOPHORE	UNP Q9GPI6
E	63	CRQ	GLY	CHROMOPHORE	UNP Q9GPI6
F	63	CRQ	GLN	CHROMOPHORE	UNP Q9GPI6
F	63	CRQ	TYR	CHROMOPHORE	UNP Q9GPI6
F	63	CRQ	GLY	CHROMOPHORE	UNP Q9GPI6
G	63	CRQ	GLN	CHROMOPHORE	UNP Q9GPI6
G	63	CRQ	TYR	CHROMOPHORE	UNP Q9GPI6
G	63	CRQ	GLY	CHROMOPHORE	UNP Q9GPI6
H	63	CRQ	GLN	CHROMOPHORE	UNP Q9GPI6
H	63	CRQ	TYR	CHROMOPHORE	UNP Q9GPI6
H	63	CRQ	GLY	CHROMOPHORE	UNP Q9GPI6

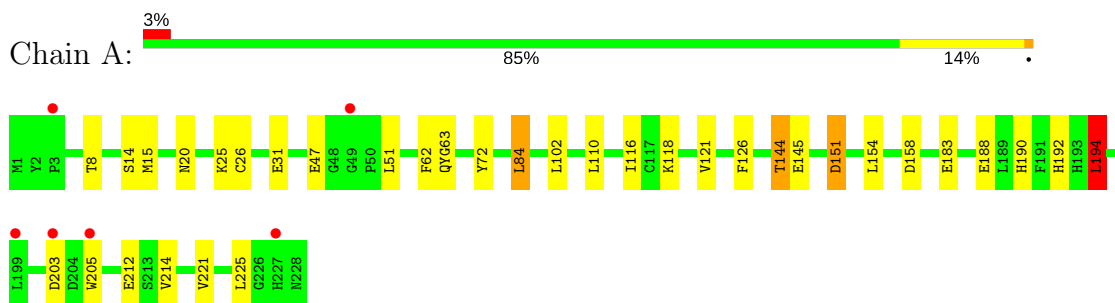
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	236	Total O 236 236	0	0
2	B	212	Total O 212 212	0	0
2	C	176	Total O 176 176	0	0
2	D	179	Total O 179 179	0	0
2	E	202	Total O 202 202	0	0
2	F	201	Total O 201 201	0	0
2	G	168	Total O 168 168	0	0
2	H	189	Total O 189 189	0	0

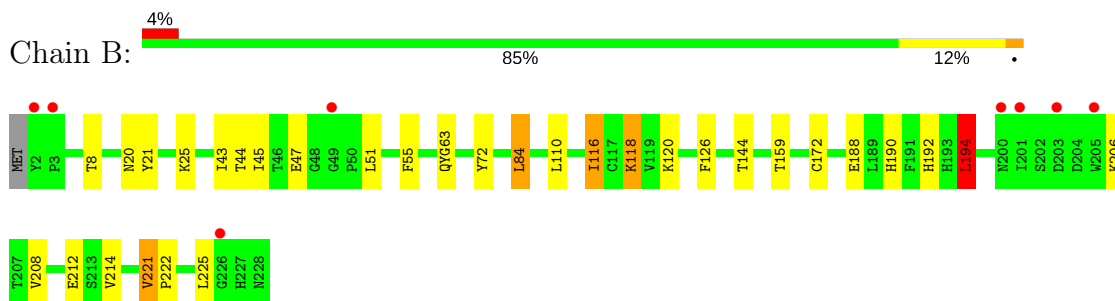
3 Residue-property plots

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

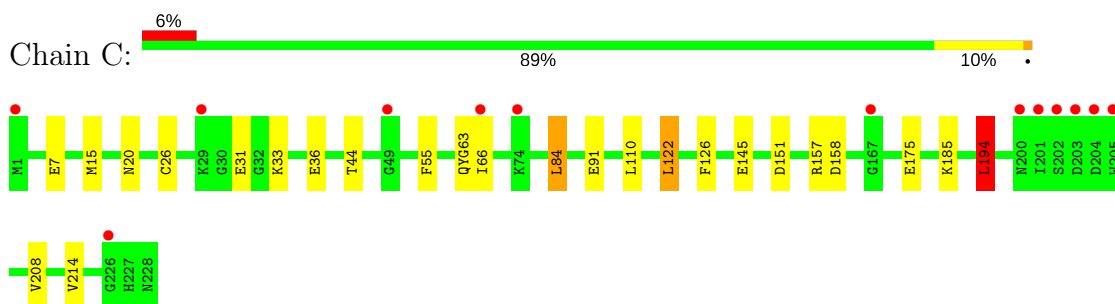
• Molecule 1: GREEN FLUORESCENT PROTEIN ASFP499



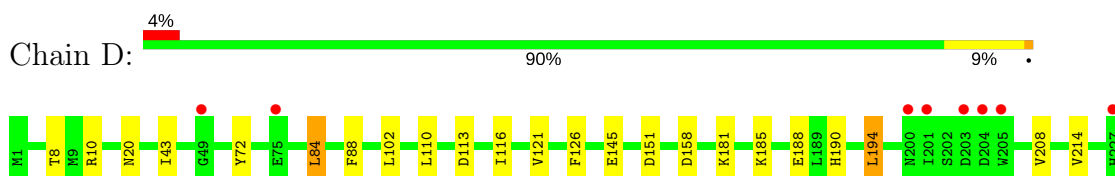
• Molecule 1: GREEN FLUORESCENT PROTEIN ASFP499



• Molecule 1: GREEN FLUORESCENT PROTEIN ASFP499




• Molecule 1: GREEN FLUORESCENT PROTEIN ASFP499




N228


• Molecule 1: GREEN FLUORESCENT PROTEIN ASFP499

Chain E:  87% 12% 2%G226
H227
N228


• Molecule 1: GREEN FLUORESCENT PROTEIN ASFP499

Chain F:  82% 15% 3%S180
K181
K185
E188
L189
H190
F191
H192
H193
L194
R195
V208
V221
L225
N228

• Molecule 1: GREEN FLUORESCENT PROTEIN ASFP499

Chain G:  86% 12% 4%V208
V214
S219
Q220
V221
L225
G226
H227
N228

• Molecule 1: GREEN FLUORESCENT PROTEIN ASFP499

Chain H:  85% 12% 2%V208
V214
V221
P222
H227
N228

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.88Å 135.13Å 95.07Å 90.00° 106.93° 90.00°	Depositor
Resolution (Å)	50.00 – 1.82 29.94 – 1.82	Depositor EDS
% Data completeness (in resolution range)	87.3 (50.00-1.82) 87.3 (29.94-1.82)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.245 , 0.292 0.244 , 0.290	Depositor DCC
R_{free} test set	6741 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15798	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CRQ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.33	0/1801	0.51	1/2433 (0.0%)
1	B	0.33	0/1793	0.51	1/2423 (0.0%)
1	C	0.32	0/1801	0.50	1/2433 (0.0%)
1	D	0.33	0/1801	0.51	0/2433
1	E	0.34	0/1801	0.51	0/2433
1	F	0.33	0/1804	0.52	1/2437 (0.0%)
1	G	0.33	0/1801	0.51	0/2433
1	H	0.33	0/1793	0.52	1/2423 (0.0%)
All	All	0.33	0/14395	0.51	5/19448 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	LEU	CA-CB-CG	6.37	129.96	115.30
1	B	194	LEU	CA-CB-CG	6.22	129.60	115.30
1	H	194	LEU	CA-CB-CG	5.63	128.25	115.30
1	F	194	LEU	CA-CB-CG	5.57	128.10	115.30
1	C	194	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

There are no planarity outliers.

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	A	1781	0	1752	16	0
1	B	1773	0	1739	18	0
1	C	1781	0	1750	12	0
1	D	1781	0	1751	11	0
1	E	1781	0	1751	14	0
1	F	1784	0	1750	23	0
1	G	1781	0	1751	15	0
1	H	1773	0	1738	18	0
2	A	236	0	0	1	0
2	B	212	0	0	0	0
2	C	176	0	0	0	0
2	D	179	0	0	2	0
2	E	202	0	0	1	0
2	F	201	0	0	2	0
2	G	168	0	0	2	0
2	H	189	0	0	0	0
All	All	15798	0	13982	116	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (116) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:CRQ:C	1:F:66:ILE:N	2.21	1.02
1:A:62:PHE:C	1:A:63:CRQ:N	2.24	0.91
1:C:63:CRQ:C	1:C:66:ILE:N	2.38	0.87
1:A:183:GLU:H	1:F:129:ASN:HD21	1.23	0.86
1:E:144:THR:HG21	1:F:144:THR:HG21	1.67	0.76
1:G:144:THR:HG21	1:H:144:THR:HG21	1.74	0.69
1:H:63:CRQ:C	1:H:66:ILE:N	2.60	0.65
1:E:212:GLU:HG3	2:E:2168:HOH:O	1.97	0.65
1:E:219:SER:OG	1:E:221:VAL:HG12	1.98	0.63
1:F:179:LYS:NZ	2:F:2137:HOH:O	2.09	0.60
1:G:192:HIS:HB3	1:G:194:LEU:HD11	1.85	0.59
1:F:62:PHE:C	1:F:63:CRQ:N	2.56	0.59
1:G:25:LYS:HB2	1:G:47:GLU:HB2	1.85	0.59
1:D:84:LEU:HD22	1:D:110:LEU:HB2	1.84	0.58
1:B:116:ILE:HD11	1:B:118:LYS:HE2	1.85	0.58
1:F:188:GLU:O	1:F:190:HIS:HD2	1.87	0.56
1:F:63:CRQ:CA3	1:F:66:ILE:N	2.68	0.56
1:C:33:LYS:HB2	1:C:36:GLU:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:LYS:HB2	1:F:47:GLU:HB2	1.90	0.53
1:F:145:GLU:HG3	1:F:158:ASP:HB2	1.90	0.53
1:A:183:GLU:H	1:F:129:ASN:ND2	2.01	0.53
1:C:145:GLU:HG3	1:C:158:ASP:HB2	1.91	0.53
1:G:145:GLU:HG3	1:G:158:ASP:HB2	1.92	0.52
2:G:2123:HOH:O	1:H:173:PHE:HZ	1.92	0.52
1:D:102:LEU:HD21	1:D:121:VAL:HG13	1.91	0.51
1:B:43:ILE:HB	1:B:208:VAL:HG13	1.92	0.51
1:E:25:LYS:HB2	1:E:47:GLU:HB2	1.92	0.51
1:F:20:ASN:HD21	1:F:126:PHE:H	1.58	0.50
1:G:84:LEU:HD22	1:G:110:LEU:HB2	1.94	0.50
1:H:63:CRQ:CA3	1:H:66:ILE:N	2.74	0.50
1:H:188:GLU:O	1:H:190:HIS:HD2	1.95	0.50
1:B:84:LEU:HD13	1:B:110:LEU:HD22	1.94	0.50
1:F:34:PRO:HA	1:F:69:PHE:HA	1.94	0.50
1:H:25:LYS:HB2	1:H:47:GLU:HB2	1.95	0.49
2:A:2164:HOH:O	1:B:159:THR:HB	2.12	0.48
1:A:194:LEU:HD13	1:A:214:VAL:HG13	1.93	0.48
1:C:15:MET:HB3	1:C:26:CYS:HB2	1.94	0.48
1:C:84:LEU:HD22	1:C:110:LEU:HB2	1.94	0.48
1:D:84:LEU:HD13	1:D:110:LEU:HD22	1.94	0.48
1:E:84:LEU:HD22	1:E:110:LEU:HB2	1.94	0.48
1:B:188:GLU:O	1:B:190:HIS:HD2	1.95	0.48
1:H:20:ASN:HD21	1:H:126:PHE:H	1.62	0.47
1:E:188:GLU:O	1:E:190:HIS:HD2	1.97	0.47
1:B:25:LYS:HB2	1:B:47:GLU:HB2	1.97	0.47
1:A:102:LEU:HD21	1:A:121:VAL:HG13	1.94	0.47
1:B:116:ILE:HD11	1:B:118:LYS:CE	2.45	0.47
1:D:113:ASP:HB2	2:D:2007:HOH:O	2.15	0.47
1:G:194:LEU:HD12	1:G:214:VAL:HG22	1.97	0.47
1:E:157:ARG:HG2	1:E:175:GLU:HG2	1.97	0.46
1:D:88:PHE:HZ	2:D:2048:HOH:O	1.97	0.46
1:A:63:CRQ:HB12	1:A:212:GLU:OE1	2.15	0.46
1:F:9:MET:HE1	1:F:113:ASP:HB2	1.97	0.46
1:G:157:ARG:HG2	2:G:2123:HOH:O	2.15	0.46
1:E:55:PHE:CZ	1:E:208:VAL:HG11	2.51	0.46
1:H:221:VAL:HA	1:H:222:PRO:HD3	1.84	0.46
1:A:188:GLU:O	1:A:190:HIS:HD2	1.99	0.45
1:G:84:LEU:HD11	1:G:115:ILE:HG12	1.99	0.45
1:G:156:LEU:HB2	1:G:176:THR:HG23	1.98	0.45
1:C:55:PHE:CZ	1:C:208:VAL:HG11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:ASN:HD21	1:E:126:PHE:H	1.65	0.45
1:B:55:PHE:CZ	1:B:208:VAL:HG11	2.51	0.45
1:H:12:GLN:HB3	1:H:116:ILE:HD13	1.98	0.45
1:F:63:CRQ:CE1	1:F:194:LEU:HG	2.47	0.45
1:B:20:ASN:HD21	1:B:126:PHE:H	1.64	0.45
1:G:219:SER:OG	1:G:221:VAL:HG12	2.17	0.45
1:G:20:ASN:HD21	1:G:126:PHE:H	1.63	0.44
1:A:25:LYS:HB2	1:A:47:GLU:HB2	1.99	0.44
1:H:157:ARG:HG2	1:H:175:GLU:HG2	2.00	0.44
1:D:188:GLU:O	1:D:190:HIS:HD2	2.01	0.44
1:A:72:TYR:OH	1:A:190:HIS:HE1	2.01	0.44
1:D:194:LEU:HD13	1:D:214:VAL:HG13	1.99	0.44
1:E:221:VAL:HG13	1:F:195:ARG:HB2	2.00	0.44
1:A:84:LEU:HD13	1:A:110:LEU:HD22	1.99	0.44
1:B:221:VAL:HA	1:B:222:PRO:HD3	1.87	0.44
1:B:45:ILE:HD13	1:B:51:LEU:HD13	2.00	0.44
1:B:72:TYR:OH	1:B:190:HIS:HE1	2.01	0.43
1:G:201:ILE:HG23	1:G:208:VAL:HG22	1.98	0.43
1:D:43:ILE:HB	1:D:208:VAL:HG13	2.01	0.43
1:C:63:CRQ:CA3	1:C:66:ILE:N	2.81	0.43
1:F:154:LEU:HB2	1:F:178:TYR:HB2	2.00	0.43
1:D:145:GLU:HG3	1:D:158:ASP:HB2	1.99	0.43
1:H:34:PRO:HA	1:H:69:PHE:HA	2.01	0.43
1:A:145:GLU:HG3	1:A:158:ASP:HB2	2.01	0.43
1:F:188:GLU:HG2	2:F:2197:HOH:O	2.18	0.43
1:D:72:TYR:OH	1:D:190:HIS:HE1	2.02	0.42
1:E:221:VAL:HA	1:E:222:PRO:HD3	1.94	0.42
1:F:84:LEU:HD22	1:F:110:LEU:HB2	2.00	0.42
1:C:20:ASN:HD21	1:C:126:PHE:H	1.68	0.42
1:H:63:CRQ:HA31	1:H:66:ILE:N	2.34	0.42
1:D:20:ASN:HD21	1:D:126:PHE:H	1.68	0.42
1:B:84:LEU:HD22	1:B:110:LEU:HB2	2.02	0.42
1:B:192:HIS:HB3	1:B:194:LEU:HD11	2.01	0.42
1:G:141:GLU:OE1	1:H:227:HIS:HE1	2.03	0.42
1:F:72:TYR:OH	1:F:190:HIS:HE1	2.03	0.42
1:G:188:GLU:O	1:G:190:HIS:HD2	2.03	0.42
1:B:120:LYS:HD2	1:C:122:LEU:HD23	2.02	0.42
1:H:145:GLU:HG3	1:H:158:ASP:HB2	2.02	0.42
1:C:157:ARG:HG2	1:C:175:GLU:HG2	2.02	0.41
1:E:221:VAL:CG1	1:F:195:ARG:HB2	2.49	0.41
1:C:194:LEU:HD12	1:C:214:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:CRQ:HB11	1:B:212:GLU:OE1	2.20	0.41
1:A:144:THR:HA	1:A:192:HIS:O	2.20	0.41
1:F:63:CRQ:O2	1:F:92:ARG:NH1	2.52	0.41
1:E:77:PRO:HG3	1:E:185:LYS:HE3	2.03	0.41
1:A:14:SER:OG	1:A:118:LYS:HD3	2.21	0.41
1:E:120:LYS:HD2	1:H:122:LEU:HD23	2.03	0.41
1:H:83:SER:HB3	1:H:88:PHE:HB3	2.03	0.41
1:A:63:CRQ:CE1	1:A:194:LEU:HG	2.51	0.41
1:B:21:TYR:CE2	1:C:91:GLU:HG3	2.56	0.41
1:F:63:CRQ:O	1:F:66:ILE:N	2.51	0.41
1:A:20:ASN:HD21	1:A:126:PHE:H	1.68	0.40
1:A:15:MET:HB3	1:A:26:CYS:HB2	2.03	0.40
1:H:194:LEU:HD13	1:H:214:VAL:HG13	2.03	0.40
1:B:194:LEU:HD12	1:B:214:VAL:HG22	2.03	0.40
1:F:144:THR:HA	1:F:192:HIS:O	2.20	0.40
1:G:144:THR:CG2	1:H:144:THR:HG21	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	222/226 (98%)	218 (98%)	3 (1%)	1 (0%)	32	17
1	B	222/226 (98%)	219 (99%)	3 (1%)	0	100	100
1	C	222/226 (98%)	220 (99%)	1 (0%)	1 (0%)	32	17
1	D	223/226 (99%)	220 (99%)	2 (1%)	1 (0%)	38	22
1	E	223/226 (99%)	220 (99%)	3 (1%)	0	100	100
1	F	221/226 (98%)	218 (99%)	2 (1%)	1 (0%)	32	17
1	G	223/226 (99%)	219 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	221/226 (98%)	219 (99%)	1 (0%)	1 (0%)	32	17
All	All	1777/1808 (98%)	1753 (99%)	19 (1%)	5 (0%)	44	28

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	151	ASP
1	F	151	ASP
1	H	151	ASP
1	A	151	ASP
1	C	151	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	196/196 (100%)	183 (93%)	13 (7%)	19	6
1	B	195/196 (100%)	184 (94%)	11 (6%)	25	9
1	C	196/196 (100%)	189 (96%)	7 (4%)	40	23
1	D	196/196 (100%)	189 (96%)	7 (4%)	40	23
1	E	196/196 (100%)	184 (94%)	12 (6%)	22	7
1	F	196/196 (100%)	181 (92%)	15 (8%)	15	4
1	G	196/196 (100%)	183 (93%)	13 (7%)	19	6
1	H	195/196 (100%)	183 (94%)	12 (6%)	21	7
All	All	1566/1568 (100%)	1476 (94%)	90 (6%)	23	9

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	31	GLU
1	A	51	LEU

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Mol	Chain	Res	Type
1	A	84	LEU
1	A	116	ILE
1	A	144	THR
1	A	151	ASP
1	A	154	LEU
1	A	194	LEU
1	A	203	ASP
1	A	205	TRP
1	A	221	VAL
1	A	225	LEU
1	B	8	THR
1	B	44	THR
1	B	84	LEU
1	B	116	ILE
1	B	118	LYS
1	B	144	THR
1	B	172	CYS
1	B	194	LEU
1	B	206	LYS
1	B	221	VAL
1	B	225	LEU
1	C	7	GLU
1	C	31	GLU
1	C	44	THR
1	C	84	LEU
1	C	122	LEU
1	C	185	LYS
1	C	194	LEU
1	D	8	THR
1	D	10	ARG
1	D	84	LEU
1	D	116	ILE
1	D	181	LYS
1	D	185	LYS
1	D	194	LEU
1	E	1	MET
1	E	44	THR
1	E	84	LEU
1	E	113	ASP
1	E	116	ILE
1	E	155	LEU
1	E	172	CYS

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Mol	Chain	Res	Type
1	E	182	LYS
1	E	185	LYS
1	E	188	GLU
1	E	194	LEU
1	E	200	ASN
1	F	10	ARG
1	F	31	GLU
1	F	51	LEU
1	F	75	GLU
1	F	84	LEU
1	F	116	ILE
1	F	144	THR
1	F	172	CYS
1	F	181	LYS
1	F	185	LYS
1	F	188	GLU
1	F	194	LEU
1	F	208	VAL
1	F	221	VAL
1	F	225	LEU
1	G	10	ARG
1	G	20	ASN
1	G	44	THR
1	G	84	LEU
1	G	116	ILE
1	G	122	LEU
1	G	151	ASP
1	G	155	LEU
1	G	172	CYS
1	G	188	GLU
1	G	194	LEU
1	G	203	ASP
1	G	225	LEU
1	H	20	ASN
1	H	31	GLU
1	H	51	LEU
1	H	84	LEU
1	H	122	LEU
1	H	144	THR
1	H	182	LYS
1	H	185	LYS
1	H	188	GLU

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Mol	Chain	Res	Type
1	H	194	LEU
1	H	208	VAL
1	H	221	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	190	HIS
1	A	210	GLN
1	A	228	ASN
1	B	20	ASN
1	B	129	ASN
1	B	190	HIS
1	B	210	GLN
1	C	20	ASN
1	C	125	ASN
1	C	190	HIS
1	C	210	GLN
1	D	20	ASN
1	D	190	HIS
1	D	210	GLN
1	D	211	HIS
1	E	20	ASN
1	E	22	HIS
1	E	111	GLN
1	E	190	HIS
1	E	210	GLN
1	E	227	HIS
1	F	20	ASN
1	F	129	ASN
1	F	190	HIS
1	F	210	GLN
1	F	227	HIS
1	G	20	ASN
1	G	190	HIS
1	G	210	GLN
1	G	227	HIS
1	H	20	ASN
1	H	190	HIS
1	H	210	GLN
1	H	227	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	A	63	1	24,25,26	3.41	9 (37%)	26,34,36	2.69	6 (23%)
1	CRQ	B	63	1	24,25,26	3.20	8 (33%)	26,34,36	2.81	6 (23%)
1	CRQ	C	63	1	24,25,26	3.34	8 (33%)	26,34,36	3.37	10 (38%)
1	CRQ	D	63	1	24,25,26	3.30	8 (33%)	26,34,36	3.02	8 (30%)
1	CRQ	E	63	1	24,25,26	3.32	9 (37%)	26,34,36	2.88	8 (30%)
1	CRQ	F	63	-	24,25,26	3.47	8 (33%)	26,34,36	3.20	9 (34%)
1	CRQ	G	63	1	24,25,26	3.45	10 (41%)	26,34,36	2.68	6 (23%)
1	CRQ	H	63	1	24,25,26	3.23	9 (37%)	26,34,36	3.01	8 (30%)

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	A	63	1	-	0/10/32/33	0/2/2/2
1	CRQ	B	63	1	-	0/10/32/33	0/2/2/2
1	CRQ	C	63	1	-	0/10/32/33	0/2/2/2
1	CRQ	D	63	1	-	0/10/32/33	0/2/2/2
1	CRQ	E	63	1	-	0/10/32/33	0/2/2/2
1	CRQ	F	63	-	-	2/10/32/33	0/2/2/2
1	CRQ	G	63	1	-	0/10/32/33	0/2/2/2
1	CRQ	H	63	1	-	0/10/32/33	0/2/2/2

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	63	CRQ	CA2-C2	-12.11	1.36	1.48
1	C	63	CRQ	CA2-C2	-11.51	1.37	1.48
1	E	63	CRQ	CA2-C2	-11.16	1.37	1.48
1	D	63	CRQ	CA2-C2	-11.10	1.37	1.48
1	B	63	CRQ	CA2-C2	-10.73	1.37	1.48
1	G	63	CRQ	CA2-C2	-10.70	1.37	1.48
1	A	63	CRQ	CA2-C2	-10.57	1.37	1.48
1	H	63	CRQ	CA2-C2	-10.55	1.38	1.48
1	F	63	CRQ	CG2-CB2	-8.66	1.29	1.46
1	E	63	CRQ	CG2-CB2	-8.31	1.29	1.46
1	D	63	CRQ	CG2-CB2	-8.29	1.30	1.46
1	H	63	CRQ	CG2-CB2	-8.23	1.30	1.46
1	A	63	CRQ	CG2-CB2	-8.17	1.30	1.46
1	G	63	CRQ	CG2-CB2	-8.11	1.30	1.46
1	B	63	CRQ	CG2-CB2	-8.07	1.30	1.46
1	C	63	CRQ	CG2-CB2	-8.04	1.30	1.46
1	D	63	CRQ	CA3-N3	-4.57	1.37	1.47
1	E	63	CRQ	CA3-N3	-4.56	1.37	1.47
1	G	63	CRQ	CA3-N3	-4.54	1.37	1.47
1	A	63	CRQ	CA3-N3	-4.52	1.37	1.47
1	B	63	CRQ	CA3-N3	-4.40	1.37	1.47
1	F	63	CRQ	CA3-N3	-4.39	1.37	1.47
1	C	63	CRQ	CA3-N3	-4.35	1.37	1.47
1	H	63	CRQ	CA3-N3	-4.30	1.38	1.47
1	F	63	CRQ	C2-N3	-3.53	1.31	1.39
1	A	63	CRQ	C2-N3	-3.31	1.31	1.39
1	C	63	CRQ	C2-N3	-3.31	1.31	1.39
1	D	63	CRQ	C2-N3	-3.22	1.32	1.39
1	E	63	CRQ	C2-N3	-3.18	1.32	1.39
1	B	63	CRQ	C2-N3	-3.02	1.32	1.39
1	G	63	CRQ	C2-N3	-2.92	1.32	1.39
1	H	63	CRQ	C2-N3	-2.84	1.32	1.39
1	F	63	CRQ	OH-CZ	-2.82	1.30	1.37
1	E	63	CRQ	OH-CZ	-2.78	1.30	1.37
1	H	63	CRQ	OH-CZ	-2.78	1.30	1.37
1	G	63	CRQ	OH-CZ	-2.77	1.30	1.37
1	D	63	CRQ	OH-CZ	-2.76	1.30	1.37
1	C	63	CRQ	OH-CZ	-2.71	1.30	1.37
1	A	63	CRQ	OH-CZ	-2.70	1.30	1.37
1	B	63	CRQ	OH-CZ	-2.67	1.30	1.37
1	A	63	CRQ	C1-N3	-2.49	1.33	1.38
1	H	63	CRQ	C1-N3	-2.48	1.33	1.38
1	E	63	CRQ	C1-N3	-2.23	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	63	CRQ	CA1-N	2.35	1.33	1.27
1	G	63	CRQ	OE1-CD3	2.36	1.31	1.24
1	D	63	CRQ	CA1-N	2.44	1.33	1.27
1	B	63	CRQ	CA1-N	2.47	1.33	1.27
1	A	63	CRQ	O2-C2	2.47	1.28	1.23
1	E	63	CRQ	CA1-N	2.55	1.33	1.27
1	A	63	CRQ	C1-N2	2.57	1.38	1.33
1	B	63	CRQ	O2-C2	2.59	1.28	1.23
1	C	63	CRQ	O2-C2	2.60	1.28	1.23
1	D	63	CRQ	O2-C2	2.66	1.28	1.23
1	F	63	CRQ	O2-C2	2.68	1.29	1.23
1	H	63	CRQ	C1-N2	2.69	1.38	1.33
1	G	63	CRQ	O2-C2	2.69	1.29	1.23
1	H	63	CRQ	O2-C2	2.71	1.29	1.23
1	E	63	CRQ	O2-C2	2.72	1.29	1.23
1	H	63	CRQ	CA1-N	2.73	1.34	1.27
1	C	63	CRQ	CA1-N	2.77	1.34	1.27
1	B	63	CRQ	C1-N2	2.88	1.38	1.33
1	F	63	CRQ	C1-N2	2.91	1.38	1.33
1	G	63	CRQ	CG1-CB1	3.08	1.61	1.51
1	E	63	CRQ	C1-N2	3.08	1.39	1.33
1	D	63	CRQ	C1-N2	3.17	1.39	1.33
1	C	63	CRQ	C1-N2	3.25	1.39	1.33
1	G	63	CRQ	C1-N2	3.34	1.39	1.33
1	G	63	CRQ	CA1-N	4.75	1.39	1.27
1	A	63	CRQ	CA1-N	6.19	1.43	1.27

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	63	CRQ	O2-C2-CA2	-10.15	125.50	130.97
1	E	63	CRQ	O2-C2-CA2	-8.44	126.42	130.97
1	D	63	CRQ	O2-C2-CA2	-8.22	126.54	130.97
1	C	63	CRQ	O2-C2-CA2	-7.89	126.72	130.97
1	B	63	CRQ	O2-C2-CA2	-7.87	126.73	130.97
1	F	63	CRQ	O2-C2-CA2	-7.77	126.78	130.97
1	G	63	CRQ	O2-C2-CA2	-7.60	126.87	130.97
1	A	63	CRQ	O2-C2-CA2	-7.09	127.15	130.97
1	A	63	CRQ	CB1-CA1-N	-6.18	104.03	125.34
1	G	63	CRQ	N3-C1-N2	-5.73	105.96	113.31
1	C	63	CRQ	N3-C1-N2	-5.61	106.11	113.31
1	B	63	CRQ	CB1-CA1-N	-5.32	106.98	125.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	63	CRQ	CB1-CA1-N	-5.27	107.14	125.34
1	F	63	CRQ	N3-C1-N2	-5.13	106.72	113.31
1	D	63	CRQ	N3-C1-N2	-4.82	107.12	113.31
1	E	63	CRQ	N3-C1-N2	-4.64	107.35	113.31
1	B	63	CRQ	N3-C1-N2	-4.49	107.54	113.31
1	H	63	CRQ	CA3-N3-C1	-4.44	119.26	128.19
1	C	63	CRQ	CB1-CA1-N	-4.16	111.00	125.34
1	H	63	CRQ	CB1-CA1-N	-3.91	111.84	125.34
1	H	63	CRQ	N3-C1-N2	-3.85	108.37	113.31
1	F	63	CRQ	CA3-N3-C2	-3.71	115.72	123.94
1	A	63	CRQ	N3-C1-N2	-3.66	108.61	113.31
1	E	63	CRQ	CB1-CA1-N	-3.55	113.10	125.34
1	F	63	CRQ	O-C-CA3	-3.52	114.75	126.38
1	C	63	CRQ	CA3-N3-C2	-3.52	116.15	123.94
1	D	63	CRQ	CB1-CA1-N	-3.38	113.67	125.34
1	E	63	CRQ	O-C-CA3	-3.34	115.34	126.38
1	D	63	CRQ	O-C-CA3	-3.30	115.48	126.38
1	C	63	CRQ	O-C-CA3	-3.20	115.81	126.38
1	A	63	CRQ	O-C-CA3	-3.18	115.86	126.38
1	G	63	CRQ	O-C-CA3	-3.12	116.06	126.38
1	H	63	CRQ	O-C-CA3	-2.99	116.50	126.38
1	B	63	CRQ	O-C-CA3	-2.95	116.62	126.38
1	D	63	CRQ	CB2-CA2-C2	-2.78	118.83	122.32
1	E	63	CRQ	CA3-N3-C1	-2.63	122.90	128.19
1	E	63	CRQ	CB2-CA2-C2	-2.55	119.12	122.32
1	F	63	CRQ	CB2-CA2-C2	-2.40	119.30	122.32
1	G	63	CRQ	CA3-N3-C1	-2.40	123.36	128.19
1	A	63	CRQ	CA3-N3-C1	-2.27	123.62	128.19
1	G	63	CRQ	CB1-CA1-N	-2.27	117.51	125.34
1	C	63	CRQ	CB2-CA2-C2	-2.12	119.65	122.32
1	F	63	CRQ	CG2-CB2-CA2	2.12	132.65	130.19
1	C	63	CRQ	CB2-CA2-N2	2.15	132.04	128.79
1	D	63	CRQ	CB2-CA2-N2	2.24	132.18	128.79
1	H	63	CRQ	CG2-CB2-CA2	2.39	132.97	130.19
1	C	63	CRQ	CA3-N3-C1	2.55	133.32	128.19
1	B	63	CRQ	CG2-CB2-CA2	2.62	133.23	130.19
1	H	63	CRQ	CA3-N3-C2	2.78	130.10	123.94
1	F	63	CRQ	CA3-N3-C1	2.85	133.91	128.19
1	E	63	CRQ	CG2-CB2-CA2	3.58	134.36	130.19
1	C	63	CRQ	CG2-CB2-CA2	4.40	135.30	130.19
1	D	63	CRQ	CG2-CB2-CA2	4.77	135.73	130.19
1	H	63	CRQ	CA2-C2-N3	6.74	106.30	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	63	CRQ	CA2-C2-N3	7.33	106.57	103.30
1	A	63	CRQ	CA2-C2-N3	7.60	106.69	103.30
1	G	63	CRQ	CA2-C2-N3	7.87	106.81	103.30
1	B	63	CRQ	CA2-C2-N3	8.03	106.88	103.30
1	D	63	CRQ	CA2-C2-N3	8.29	107.00	103.30
1	F	63	CRQ	CA2-C2-N3	9.58	107.57	103.30
1	C	63	CRQ	CA2-C2-N3	10.79	108.11	103.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	63	CRQ	C-CA3-N3-C2
1	F	63	CRQ	C-CA3-N3-C1

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	63	CRQ	3	0
1	B	63	CRQ	1	0
1	C	63	CRQ	2	0
1	F	63	CRQ	6	0
1	H	63	CRQ	3	0

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	225/226 (99%)	0.13	6 (2%) 55 50	14, 19, 28, 36	0
1	B	224/226 (99%)	0.20	8 (3%) 43 38	13, 19, 26, 31	0
1	C	225/226 (99%)	0.39	13 (5%) 24 19	17, 23, 34, 38	0
1	D	225/226 (99%)	0.31	8 (3%) 43 38	16, 22, 31, 37	0
1	E	225/226 (99%)	0.24	4 (1%) 69 65	17, 21, 28, 37	0
1	F	224/226 (99%)	0.33	3 (1%) 77 74	18, 23, 32, 37	0
1	G	225/226 (99%)	0.42	8 (3%) 43 38	19, 25, 35, 42	0
1	H	224/226 (99%)	0.20	4 (1%) 69 65	16, 21, 29, 32	0
All	All	1797/1808 (99%)	0.28	54 (3%) 51 45	13, 22, 31, 42	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	3	PRO	6.6
1	D	203	ASP	4.4
1	A	203	ASP	4.4
1	F	49	GLY	4.4
1	C	1	MET	4.3
1	B	205	TRP	4.2
1	D	49	GLY	4.2
1	C	205	TRP	4.2
1	B	203	ASP	4.1
1	H	49	GLY	3.8
1	A	205	TRP	3.8
1	G	3	PRO	3.8
1	E	1	MET	3.8
1	G	205	TRP	3.7
1	C	203	ASP	3.6
1	E	49	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	49	GLY	3.6
1	F	3	PRO	3.5
1	B	201	ILE	3.3
1	A	49	GLY	3.2
1	C	49	GLY	3.2
1	D	204	ASP	3.2
1	E	226	GLY	3.1
1	C	200	ASN	3.1
1	H	199	LEU	3.1
1	G	1	MET	3.0
1	C	226	GLY	2.8
1	B	49	GLY	2.8
1	C	204	ASP	2.8
1	G	74	LYS	2.8
1	B	3	PRO	2.7
1	E	3	PRO	2.6
1	C	66	ILE	2.6
1	D	205	TRP	2.6
1	G	227	HIS	2.6
1	B	226	GLY	2.6
1	D	227	HIS	2.5
1	C	202	SER	2.5
1	D	200	ASN	2.5
1	A	3	PRO	2.5
1	G	111	GLN	2.3
1	H	66	ILE	2.3
1	B	2	TYR	2.2
1	B	200	ASN	2.2
1	C	167	GLY	2.2
1	A	227	HIS	2.2
1	F	6	LYS	2.1
1	D	75	GLU	2.1
1	D	201	ILE	2.1
1	A	199	LEU	2.1
1	G	202	SER	2.1
1	C	74	LYS	2.1
1	C	29	LYS	2.0
1	C	201	ILE	2.0

6.2 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. 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, 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	LLDF	B-factors(Å ²)	Q<0.9
1	CRQ	F	63	24/25	0.81	0.21	-	25,26,27,27	0
1	CRQ	D	63	24/25	0.89	0.16	-	18,19,21,21	0
1	CRQ	H	63	24/25	0.85	0.20	-	18,20,21,22	0
1	CRQ	A	63	24/25	0.89	0.16	-	16,17,17,18	0
1	CRQ	E	63	24/25	0.88	0.17	-	19,19,21,21	0
1	CRQ	C	63	24/25	0.86	0.18	-	20,21,23,24	0
1	CRQ	G	63	24/25	0.89	0.16	-	21,23,23,24	0
1	CRQ	B	63	24/25	0.91	0.18	-	15,16,18,19	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.