Full wwPDB X-ray Structure Validation Report ⓘ

Dec 19, 2023 – 03:46 AM EST

PDB ID	:	3CGL
Title	:	Crystal Structure and Raman Studies of dsFP483, a Cyan Fluorescent Protein from Discosoma striata
Authors	:	Malo, G.D.
Deposited on	:	2008-03-05
Resolution	:	2.09 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:

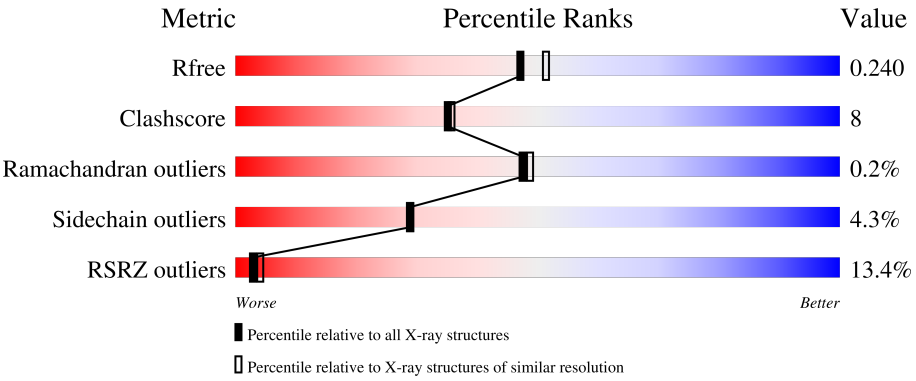
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	241	4% 79% 12% • 7%
1	B	241	8% 78% 9% • 10%
1	C	241	4% 74% 16% • 8%
1	D	241	11% 70% 20% • 9%
1	E	241	22% 76% 11% • 10%

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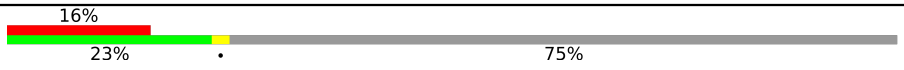
Mol	Chain	Length	Quality of chain
1	F	241	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9673 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 GFP-like fluorescent chromoprotein dsFP483.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	5	0
			1816	1172	304	326	14			
1	B	218	Total	C	N	O	S	0	4	0
			1756	1134	295	316	11			
1	C	221	Total	C	N	O	S	4	4	0
			1799	1163	302	323	11			
1	D	220	Total	C	N	O	S	3	2	0
			1764	1140	296	317	11			
1	E	216	Total	C	N	O	S	0	0	1
			1612	1039	276	288	9			
1	F	60	Total	C	N	O	S	4	0	1
			357	226	68	62	1			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP Q9U6Y7
A	-9	ARG	-	expression tag	UNP Q9U6Y7
A	-8	GLY	-	expression tag	UNP Q9U6Y7
A	-7	SER	-	expression tag	UNP Q9U6Y7
A	-6	HIS	-	expression tag	UNP Q9U6Y7
A	-5	HIS	-	expression tag	UNP Q9U6Y7
A	-4	HIS	-	expression tag	UNP Q9U6Y7
A	-3	HIS	-	expression tag	UNP Q9U6Y7
A	-2	HIS	-	expression tag	UNP Q9U6Y7
A	-1	HIS	-	expression tag	UNP Q9U6Y7
A	0	GLY	-	expression tag	UNP Q9U6Y7
B	-10	MET	-	expression tag	UNP Q9U6Y7
B	-9	ARG	-	expression tag	UNP Q9U6Y7
B	-8	GLY	-	expression tag	UNP Q9U6Y7
B	-7	SER	-	expression tag	UNP Q9U6Y7
B	-6	HIS	-	expression tag	UNP Q9U6Y7
B	-5	HIS	-	expression tag	UNP Q9U6Y7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	expression tag	UNP Q9U6Y7
B	-3	HIS	-	expression tag	UNP Q9U6Y7
B	-2	HIS	-	expression tag	UNP Q9U6Y7
B	-1	HIS	-	expression tag	UNP Q9U6Y7
B	0	GLY	-	expression tag	UNP Q9U6Y7
C	-10	MET	-	expression tag	UNP Q9U6Y7
C	-9	ARG	-	expression tag	UNP Q9U6Y7
C	-8	GLY	-	expression tag	UNP Q9U6Y7
C	-7	SER	-	expression tag	UNP Q9U6Y7
C	-6	HIS	-	expression tag	UNP Q9U6Y7
C	-5	HIS	-	expression tag	UNP Q9U6Y7
C	-4	HIS	-	expression tag	UNP Q9U6Y7
C	-3	HIS	-	expression tag	UNP Q9U6Y7
C	-2	HIS	-	expression tag	UNP Q9U6Y7
C	-1	HIS	-	expression tag	UNP Q9U6Y7
C	0	GLY	-	expression tag	UNP Q9U6Y7
D	-10	MET	-	expression tag	UNP Q9U6Y7
D	-9	ARG	-	expression tag	UNP Q9U6Y7
D	-8	GLY	-	expression tag	UNP Q9U6Y7
D	-7	SER	-	expression tag	UNP Q9U6Y7
D	-6	HIS	-	expression tag	UNP Q9U6Y7
D	-5	HIS	-	expression tag	UNP Q9U6Y7
D	-4	HIS	-	expression tag	UNP Q9U6Y7
D	-3	HIS	-	expression tag	UNP Q9U6Y7
D	-2	HIS	-	expression tag	UNP Q9U6Y7
D	-1	HIS	-	expression tag	UNP Q9U6Y7
D	0	GLY	-	expression tag	UNP Q9U6Y7
E	-10	MET	-	expression tag	UNP Q9U6Y7
E	-9	ARG	-	expression tag	UNP Q9U6Y7
E	-8	GLY	-	expression tag	UNP Q9U6Y7
E	-7	SER	-	expression tag	UNP Q9U6Y7
E	-6	HIS	-	expression tag	UNP Q9U6Y7
E	-5	HIS	-	expression tag	UNP Q9U6Y7
E	-4	HIS	-	expression tag	UNP Q9U6Y7
E	-3	HIS	-	expression tag	UNP Q9U6Y7
E	-2	HIS	-	expression tag	UNP Q9U6Y7
E	-1	HIS	-	expression tag	UNP Q9U6Y7
E	0	GLY	-	expression tag	UNP Q9U6Y7
F	-10	MET	-	expression tag	UNP Q9U6Y7
F	-9	ARG	-	expression tag	UNP Q9U6Y7
F	-8	GLY	-	expression tag	UNP Q9U6Y7
F	-7	SER	-	expression tag	UNP Q9U6Y7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-6	HIS	-	expression tag	UNP Q9U6Y7
F	-5	HIS	-	expression tag	UNP Q9U6Y7
F	-4	HIS	-	expression tag	UNP Q9U6Y7
F	-3	HIS	-	expression tag	UNP Q9U6Y7
F	-2	HIS	-	expression tag	UNP Q9U6Y7
F	-1	HIS	-	expression tag	UNP Q9U6Y7
F	0	GLY	-	expression tag	UNP Q9U6Y7

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0

- Molecule 3 is water.

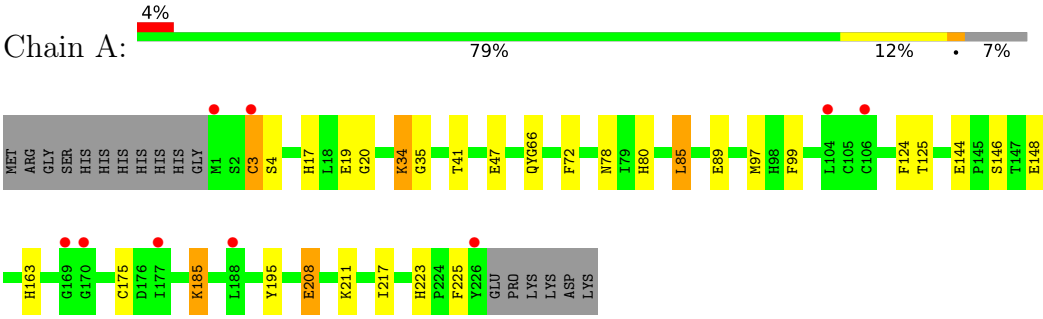
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	194	Total O 194 194	0	0
3	B	85	Total O 85 85	0	0
3	C	176	Total O 176 176	0	0
3	D	98	Total O 98 98	0	0
3	E	14	Total O 14 14	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

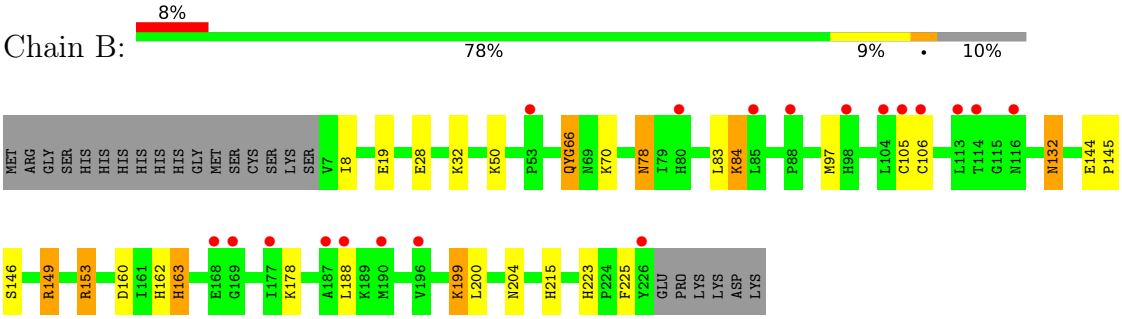
• Molecule 1: GFP-like fluorescent chromoprotein dsFP483

Chain A:



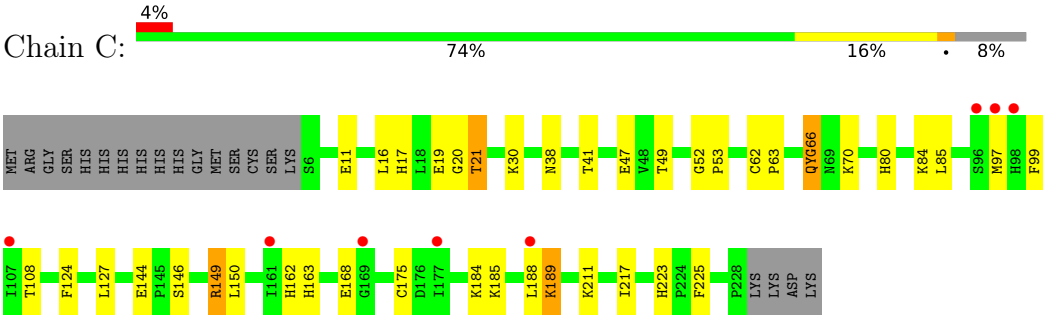
• Molecule 1: GFP-like fluorescent chromoprotein dsFP483

Chain B:



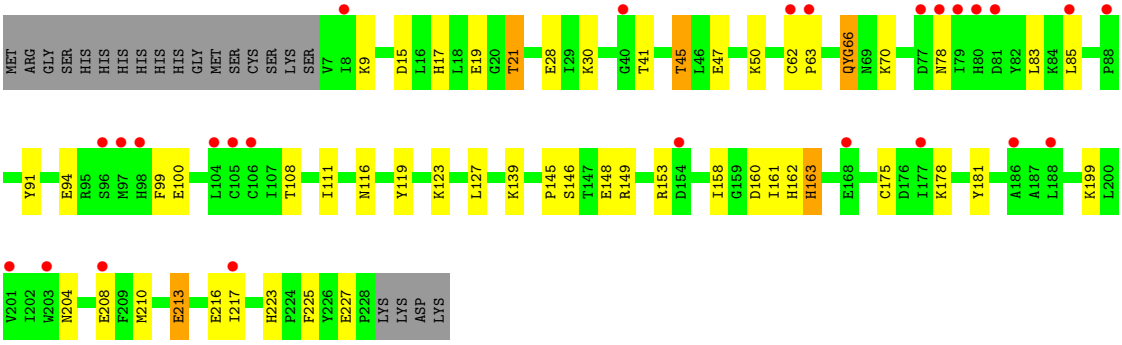
• Molecule 1: GFP-like fluorescent chromoprotein dsFP483

Chain C:



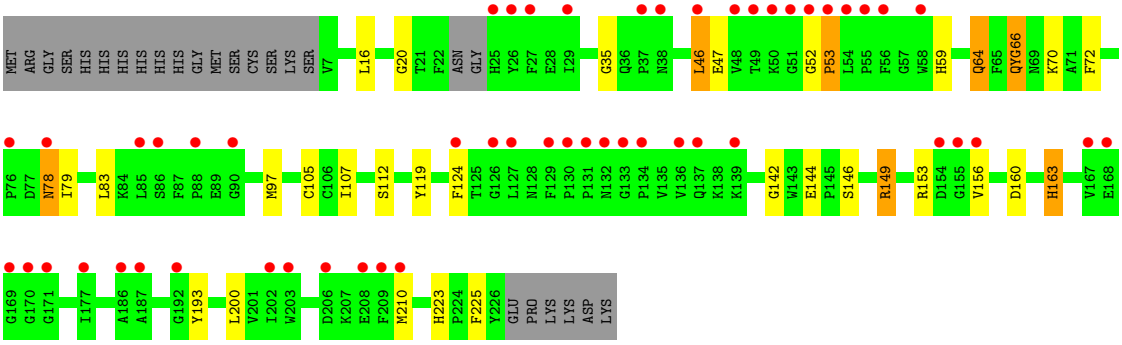
• Molecule 1: GFP-like fluorescent chromoprotein dsFP483

Chain D:



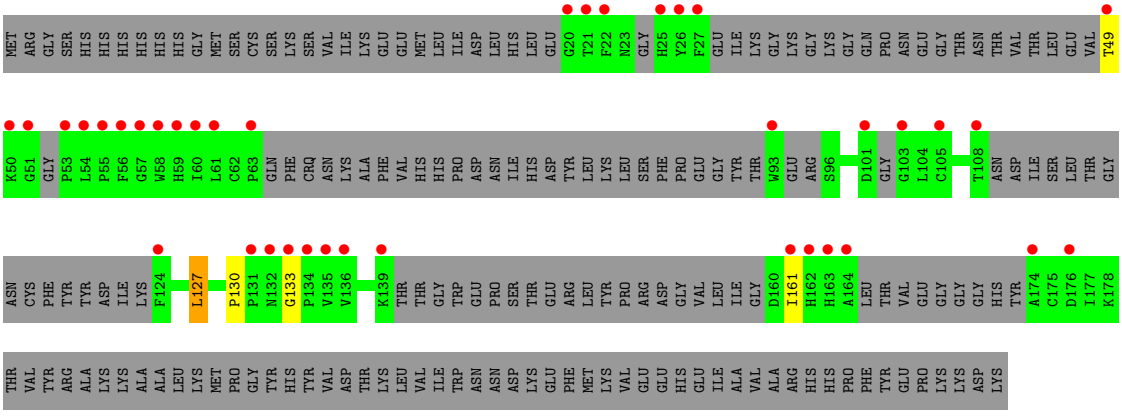
• Molecule 1: GFP-like fluorescent chromoprotein dsFP483

Chain E:



• Molecule 1: GFP-like fluorescent chromoprotein dsFP483

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	111.20Å 78.27Å 188.57Å 90.00° 91.35° 90.00°	Depositor
Resolution (Å)	40.00 – 2.09 39.13 – 2.09	Depositor EDS
% Data completeness (in resolution range)	94.8 (40.00-2.09) 94.8 (39.13-2.09)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.18 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.185 , 0.217 0.214 , 0.240	Depositor DCC
R_{free} test set	4569 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9673	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, NA

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	0.60	0/1869	0.72	0/2533
1	B	0.48	0/1805	0.64	1/2452 (0.0%)
1	C	0.67	1/1849 (0.1%)	0.72	1/2510 (0.0%)
1	D	0.58	1/1805 (0.1%)	0.67	0/2453
1	E	0.37	0/1638	0.55	0/2225
1	F	1.70	2/363 (0.6%)	0.49	0/471
All	All	0.64	4/9329 (0.0%)	0.66	2/12644 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	49	THR	CA-CB	-26.96	0.83	1.53
1	F	127	LEU	CB-CG	-16.79	1.03	1.52
1	C	168	GLU	CB-CG	8.75	1.68	1.52
1	D	116	ASN	CB-CG	-8.10	1.32	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	153	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	16	LEU	CA-CB-CG	5.08	126.97	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	1816	0	1725	30	0
1	B	1756	0	1633	30	0
1	C	1799	0	1698	39	0
1	D	1764	0	1643	41	0
1	E	1612	0	1424	21	0
1	F	357	0	230	1	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	194	0	0	0	1
3	B	85	0	0	5	0
3	C	176	0	0	5	1
3	D	98	0	0	4	0
3	E	14	0	0	0	0
All	All	9673	0	8353	144	1

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 8.

All (144) 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:C:17:HIS:HD2	1:C:30:LYS:HE3	1.21	1.01
1:C:223:HIS:HD2	1:C:225:PHE:H	1.09	0.94
1:C:17:HIS:CD2	1:C:30:LYS:HE3	2.05	0.90
1:B:223:HIS:HD2	1:B:225:PHE:H	1.16	0.89
1:D:223:HIS:HD2	1:D:225:PHE:H	1.22	0.87
1:B:153:ARG:NH2	1:D:100:GLU:OE1	2.13	0.82
1:C:223:HIS:CD2	1:C:225:PHE:H	1.98	0.81
1:B:223:HIS:CD2	1:B:225:PHE:H	1.99	0.81
1:B:215:HIS:HB2	3:B:301:HOH:O	1.81	0.80
1:A:34:LYS:HB2	1:A:34:LYS:NZ	1.97	0.79
1:E:223:HIS:HD2	1:E:225:PHE:H	1.31	0.78
1:A:223:HIS:HD2	1:A:225:PHE:H	1.30	0.76
1:C:80[B]:HIS:HE1	3:C:474:HOH:O	1.68	0.76
1:B:223:HIS:HE1	1:D:146:SER:O	1.71	0.73
1:D:223:HIS:CD2	1:D:225:PHE:H	2.07	0.73
1:A:41:THR:HG22	1:A:217[A]:ILE:HG22	1.72	0.72
1:E:223:HIS:CD2	1:E:225:PHE:H	2.08	0.71
1:B:66:CRQ:HG12	3:B:300:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80[A]:HIS:NE2	1:C:189:LYS:NZ	2.41	0.68
1:D:70:LYS:HG3	3:D:403:HOH:O	1.94	0.67
1:A:47:GLU:HG2	1:A:211:LYS:HG2	1.77	0.65
1:A:223:HIS:CD2	1:A:225:PHE:H	2.11	0.65
1:A:208:GLU:H	1:A:208:GLU:CD	2.00	0.65
1:A:34:LYS:NZ	1:A:34:LYS:CB	2.60	0.65
1:C:17:HIS:CE1	1:C:19:GLU:HG3	2.32	0.64
1:D:146:SER:HB3	1:D:163:HIS:CE1	2.32	0.64
1:A:34:LYS:HB2	1:A:34:LYS:HZ3	1.62	0.63
1:A:17:HIS:CE1	1:A:19:GLU:HG2	2.35	0.62
1:C:80[B]:HIS:CD2	1:C:189:LYS:HG3	2.34	0.62
1:B:146:SER:O	1:D:223:HIS:HE1	1.84	0.61
1:D:62:CYS:HB2	1:D:63:PRO:HD3	1.83	0.61
1:E:64:GLN:HG3	1:E:107:ILE:HG21	1.83	0.60
1:A:146:SER:O	1:C:223:HIS:HE1	1.85	0.60
1:C:17:HIS:HD2	1:C:30:LYS:CE	2.06	0.60
1:A:223:HIS:HE1	1:C:146:SER:O	1.84	0.59
1:E:35:GLY:HA3	1:E:72:PHE:CE2	2.36	0.59
1:C:21:THR:HG21	1:D:108:THR:HG21	1.83	0.59
1:A:89:GLU:HG2	1:A:185:LYS:HE3	1.85	0.59
1:E:66:CRQ:HE1	1:E:200:LEU:HB2	1.86	0.58
1:A:17:HIS:HE1	1:A:19:GLU:HG2	1.69	0.58
1:C:146:SER:HB3	1:C:163:HIS:CE1	2.40	0.57
1:B:145:PRO:HB3	1:B:199:LYS:HG2	1.86	0.56
1:C:80[B]:HIS:NE2	1:C:85:LEU:HD12	2.21	0.56
1:E:16:LEU:HD11	1:E:46:LEU:HD12	1.88	0.56
1:E:146:SER:HB3	1:E:163:HIS:CE1	2.39	0.56
1:D:145:PRO:HG3	1:D:199:LYS:HD3	1.88	0.56
1:E:149:ARG:HD2	1:E:193:TYR:CZ	2.41	0.56
1:A:17:HIS:CE1	1:A:19:GLU:CG	2.89	0.55
1:A:146:SER:HB3	1:A:163:HIS:CE1	2.41	0.55
1:D:30:LYS:HZ3	1:D:47:GLU:HB2	1.70	0.55
1:D:99:PHE:CD1	1:D:175[B]:CYS:HB3	2.43	0.54
1:C:97:MET:HB3	1:C:175[B]:CYS:SG	2.47	0.54
1:A:17:HIS:HE1	1:A:19:GLU:CG	2.20	0.54
1:A:89:GLU:HG2	1:A:185:LYS:CE	2.38	0.53
1:E:144:GLU:O	1:E:163:HIS:HE1	1.91	0.53
1:D:66:CRQ:N2	1:D:66:CRQ:HD1	2.23	0.53
1:D:208:GLU:HG2	1:D:210:MET:HG2	1.91	0.53
1:B:144:GLU:O	1:B:163:HIS:HE1	1.92	0.53
1:A:34:LYS:HB2	1:A:34:LYS:HZ2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:ASN:HD22	1:E:79:ILE:HG13	1.74	0.52
1:A:80:HIS:CE1	1:A:85:LEU:HD23	2.44	0.52
1:C:223:HIS:HD2	1:C:225:PHE:N	1.93	0.51
1:D:153:ARG:HB3	1:D:158:ILE:HD12	1.90	0.51
1:C:149:ARG:HD2	1:C:149:ARG:C	2.30	0.51
1:D:21:THR:CG2	3:D:310:HOH:O	2.59	0.51
1:D:45:THR:HB	1:D:213:GLU:HG2	1.92	0.51
1:D:227:GLU:HG3	1:E:119:TYR:CE1	2.46	0.51
1:A:99:PHE:CD1	1:A:175[B]:CYS:HB3	2.46	0.50
1:C:184:LYS:C	1:C:185:LYS:HD2	2.32	0.50
1:D:148:GLU:HB2	1:D:161:ILE:HG12	1.94	0.50
1:C:108:THR:HG21	1:D:21:THR:HG21	1.93	0.50
3:C:507:HOH:O	1:D:127:LEU:HD13	2.12	0.50
1:C:80[B]:HIS:NE2	1:C:85:LEU:CD1	2.75	0.49
1:E:47:GLU:HA	1:E:210:MET:O	2.13	0.49
1:A:125:THR:HG21	1:B:106[A]:CYS:SG	2.53	0.49
1:B:78:ASN:HD22	1:B:78:ASN:H	1.58	0.49
1:B:153:ARG:HH22	1:D:100:GLU:CD	2.11	0.49
1:B:215:HIS:HD2	3:B:299:HOH:O	1.94	0.48
1:B:199:LYS:HD3	3:B:265:HOH:O	2.13	0.48
1:B:66:CRQ:HD1	1:B:66:CRQ:N2	2.29	0.48
1:E:52:GLY:O	1:E:53:PRO:C	2.52	0.47
1:E:153:ARG:O	1:E:156:VAL:HG22	2.14	0.47
1:D:9:LYS:HD3	3:D:395:HOH:O	2.14	0.47
1:C:106[A]:CYS:SG	1:D:127:LEU:HD21	2.55	0.47
1:C:144:GLU:O	1:C:163:HIS:HE1	1.97	0.47
1:B:162:HIS:CD2	1:D:160:ASP:HB3	2.50	0.47
1:A:148:GLU:O	1:A:195:TYR:HA	2.14	0.47
1:B:146:SER:HB3	1:B:163:HIS:CE1	2.50	0.47
1:C:80[B]:HIS:NE2	1:C:189:LYS:HG3	2.30	0.47
1:A:149:ARG:HD2	1:A:149:ARG:C	2.36	0.46
1:B:19:GLU:OE2	3:B:312:HOH:O	2.20	0.46
1:B:70:LYS:HB2	1:B:83:LEU:CD1	2.45	0.46
1:D:17:HIS:CE1	1:D:19:GLU:HG3	2.50	0.46
1:C:38:ASN:ND2	1:C:84:LYS:HE2	2.31	0.46
1:D:149:ARG:HD2	1:D:149:ARG:C	2.36	0.46
1:A:20:GLY:HA2	1:A:124:PHE:O	2.16	0.46
1:B:8:ILE:HG21	1:B:84:LYS:HD3	1.99	0.45
1:B:149:ARG:HD2	1:B:149:ARG:C	2.36	0.45
1:C:99:PHE:CD1	1:C:175[A]:CYS:HB3	2.52	0.45
3:C:516:HOH:O	1:D:123:LYS:HD3	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:GLU:CG	1:D:210:MET:HG2	2.46	0.45
1:A:97:MET:HB3	1:A:175[A]:CYS:SG	2.56	0.45
1:E:59:HIS:CD2	1:E:142:GLY:HA2	2.51	0.45
1:E:97:MET:HB2	1:E:105:CYS:HB2	1.98	0.45
1:E:149:ARG:NH2	1:E:160:ASP:OD2	2.49	0.45
1:F:130:PRO:HG2	1:F:133:GLY:HA3	1.99	0.45
1:C:127:LEU:HB2	1:D:94:GLU:HG3	1.99	0.45
1:C:70:LYS:HG2	3:C:371:HOH:O	2.16	0.45
1:D:199:LYS:HD2	3:D:381:HOH:O	2.17	0.45
1:D:15:ASP:O	1:D:119:TYR:HA	2.17	0.45
1:D:223:HIS:HD2	1:D:225:PHE:N	2.03	0.45
1:B:223:HIS:HD2	1:B:225:PHE:N	1.97	0.44
1:E:20:GLY:HA3	1:E:124:PHE:HB3	2.00	0.44
1:C:106[A]:CYS:SG	1:D:127:LEU:CD2	3.05	0.44
1:C:11:GLU:CD	3:C:515:HOH:O	2.57	0.44
1:A:35:GLY:HA3	1:A:72:PHE:CE2	2.52	0.43
1:B:160:ASP:HB3	1:D:162:HIS:CD2	2.53	0.43
1:C:66:CRQ:HD1	1:C:66:CRQ:N2	2.33	0.43
1:C:52:GLY:HA2	1:C:53:PRO:C	2.39	0.43
1:B:66:CRQ:HE1	1:B:200:LEU:HB2	2.00	0.43
1:C:38:ASN:HD22	1:C:84:LYS:HE2	1.84	0.43
1:C:62:CYS:HB2	1:C:63:PRO:HD3	2.00	0.43
1:E:78:ASN:ND2	1:E:79:ILE:HG13	2.34	0.43
1:A:160:ASP:HB3	1:C:162:HIS:CD2	2.54	0.42
1:B:162:HIS:CG	1:D:160:ASP:HB3	2.54	0.42
1:C:30:LYS:HG2	1:C:49:THR:HG21	2.00	0.42
1:A:34:LYS:CB	1:A:34:LYS:HZ3	2.28	0.42
1:B:28:GLU:HB2	1:B:50:LYS:HB2	2.01	0.41
1:C:20:GLY:HA2	1:C:124:PHE:O	2.20	0.41
1:C:47:GLU:HG2	1:C:211:LYS:HG2	2.02	0.41
1:E:223:HIS:HD2	1:E:225:PHE:N	2.10	0.41
1:D:91:TYR:CZ	1:D:111:ILE:HD13	2.55	0.41
1:A:144:GLU:O	1:A:163:HIS:HE1	2.04	0.41
1:C:80[A]:HIS:CE1	1:C:189:LYS:NZ	2.89	0.41
1:B:97:MET:HB2	1:B:105:CYS:HB2	2.02	0.41
1:D:41:THR:HA	1:D:216:GLU:O	2.21	0.41
1:D:83:LEU:HD21	1:D:181:TYR:HB3	2.02	0.40
1:E:70:LYS:HB2	1:E:83:LEU:CD1	2.51	0.40
1:C:41:THR:HG22	1:C:217[A]:ILE:HG12	2.02	0.40
1:D:28:GLU:HB2	1:D:50:LYS:HB2	2.03	0.40
1:A:3[A]:CYS:SG	1:A:4:SER:N	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:HIS:CE1	1:D:146:SER:O	2.61	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:423:HOH:O	3:C:421:HOH:O[3_445]	2.02	0.18

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/241 (93%)	220 (98%)	4 (2%)	0	100	100
1	B	217/241 (90%)	213 (98%)	4 (2%)	0	100	100
1	C	220/241 (91%)	218 (99%)	2 (1%)	0	100	100
1	D	217/241 (90%)	210 (97%)	7 (3%)	0	100	100
1	E	207/241 (86%)	197 (95%)	9 (4%)	1 (0%)	29	26
1	F	40/241 (17%)	34 (85%)	5 (12%)	1 (2%)	5	2
All	All	1125/1446 (78%)	1092 (97%)	31 (3%)	2 (0%)	47	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	53	PRO
1	F	161	ILE

5.3.2 Protein sidechains (i)

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	193/208 (93%)	185 (96%)	8 (4%)	30	31
1	B	182/208 (88%)	171 (94%)	11 (6%)	19	16
1	C	191/208 (92%)	186 (97%)	5 (3%)	46	50
1	D	182/208 (88%)	172 (94%)	10 (6%)	21	19
1	E	151/208 (73%)	145 (96%)	6 (4%)	31	32
1	F	23/208 (11%)	22 (96%)	1 (4%)	29	29
All	All	922/1248 (74%)	881 (96%)	41 (4%)	29	28

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3[A]	CYS
1	A	3[B]	CYS
1	A	34	LYS
1	A	78	ASN
1	A	85	LEU
1	A	150	LEU
1	A	185	LYS
1	A	208	GLU
1	B	32	LYS
1	B	78	ASN
1	B	84	LYS
1	B	132[A]	ASN
1	B	132[B]	ASN
1	B	149	ARG
1	B	163	HIS
1	B	178	LYS
1	B	188	LEU
1	B	199	LYS
1	B	204	ASN
1	C	21	THR
1	C	149	ARG
1	C	150	LEU

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Mol	Chain	Res	Type
1	C	188	LEU
1	C	189	LYS
1	D	21	THR
1	D	45	THR
1	D	78	ASN
1	D	85	LEU
1	D	139	LYS
1	D	163	HIS
1	D	178	LYS
1	D	204	ASN
1	D	213	GLU
1	D	217	ILE
1	E	46	LEU
1	E	64	GLN
1	E	78	ASN
1	E	112	SER
1	E	149	ARG
1	E	163	HIS
1	F	127	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	80	HIS
1	A	222	HIS
1	A	223	HIS
1	B	78	ASN
1	B	204	ASN
1	B	222	HIS
1	B	223	HIS
1	C	17	HIS
1	C	36	GLN
1	C	38	ASN
1	C	132	ASN
1	C	222	HIS
1	C	223	HIS
1	D	17	HIS
1	D	78	ASN
1	D	132	ASN
1	D	204	ASN
1	D	223	HIS

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Mol	Chain	Res	Type
1	E	78	ASN
1	E	116	ASN
1	E	223	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

5 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	B	66	1	24,25,26	2.25	6 (25%)	27,34,36	3.06	5 (18%)
1	CRQ	C	66	1	24,25,26	2.33	5 (20%)	27,34,36	3.54	8 (29%)
1	CRQ	D	66	1	24,25,26	2.33	6 (25%)	27,34,36	3.14	6 (22%)
1	CRQ	A	66	1	24,25,26	2.38	5 (20%)	27,34,36	2.30	7 (25%)
1	CRQ	E	66	1	24,25,26	2.40	6 (25%)	27,34,36	3.27	5 (18%)

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	B	66	1	-	2/10/32/33	0/2/2/2
1	CRQ	C	66	1	-	2/10/32/33	0/2/2/2
1	CRQ	D	66	1	-	3/10/32/33	0/2/2/2
1	CRQ	A	66	1	-	2/10/32/33	0/2/2/2
1	CRQ	E	66	1	-	1/10/32/33	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	CRQ	CA1-N1	7.64	1.46	1.27
1	E	66	CRQ	CA1-N1	7.48	1.45	1.27
1	A	66	CRQ	CA1-N1	7.48	1.45	1.27
1	D	66	CRQ	CA1-N1	7.38	1.45	1.27
1	C	66	CRQ	CA1-N1	7.21	1.44	1.27
1	E	66	CRQ	CB2-CA2	6.85	1.40	1.35
1	D	66	CRQ	CB2-CA2	6.23	1.40	1.35
1	A	66	CRQ	CB2-CA2	5.94	1.40	1.35
1	B	66	CRQ	CB2-CA2	5.32	1.39	1.35
1	C	66	CRQ	CB2-CA2	5.18	1.39	1.35
1	C	66	CRQ	CA2-C2	-4.43	1.44	1.48
1	A	66	CRQ	C2-N3	-3.70	1.31	1.39
1	C	66	CRQ	C2-N3	-3.55	1.31	1.39
1	D	66	CRQ	O2-C2	3.23	1.29	1.23
1	A	66	CRQ	CA2-C2	-3.09	1.45	1.48
1	E	66	CRQ	C2-N3	-3.07	1.32	1.39
1	B	66	CRQ	O2-C2	3.05	1.29	1.23
1	A	66	CRQ	O2-C2	2.99	1.29	1.23
1	E	66	CRQ	O2-C2	2.93	1.29	1.23
1	B	66	CRQ	C2-N3	-2.88	1.33	1.39
1	D	66	CRQ	CA2-C2	-2.83	1.45	1.48
1	B	66	CRQ	CA2-C2	-2.65	1.46	1.48
1	D	66	CRQ	C2-N3	-2.62	1.33	1.39
1	E	66	CRQ	CA2-C2	-2.39	1.46	1.48
1	E	66	CRQ	C1-N2	2.28	1.38	1.33
1	D	66	CRQ	C1-N2	2.17	1.38	1.33
1	C	66	CRQ	O2-C2	2.16	1.27	1.23
1	B	66	CRQ	C1-N2	2.07	1.37	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	66	CRQ	O2-C2-CA2	-13.57	123.34	130.96
1	E	66	CRQ	CA2-C2-N3	11.78	108.94	103.37
1	D	66	CRQ	O2-C2-CA2	-11.50	124.50	130.96
1	B	66	CRQ	O2-C2-CA2	-11.18	124.69	130.96
1	E	66	CRQ	O2-C2-CA2	-10.59	125.02	130.96
1	C	66	CRQ	CA2-C2-N3	9.39	107.81	103.37
1	B	66	CRQ	CA2-C2-N3	9.00	107.62	103.37
1	D	66	CRQ	CA2-C2-N3	8.69	107.48	103.37
1	A	66	CRQ	CA2-C2-N3	7.04	106.70	103.37
1	A	66	CRQ	O2-C2-CA2	-6.82	127.13	130.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	66	CRQ	CB2-CA2-C2	3.31	126.22	122.28
1	D	66	CRQ	CB2-CA2-C2	3.20	126.10	122.28
1	D	66	CRQ	CG2-CB2-CA2	-3.12	126.12	129.94
1	B	66	CRQ	CB2-CA2-C2	2.97	125.82	122.28
1	A	66	CRQ	CB2-CA2-C2	2.96	125.81	122.28
1	C	66	CRQ	CD2-CG2-CD1	2.90	121.93	117.64
1	C	66	CRQ	CB2-CA2-C2	2.89	125.72	122.28
1	C	66	CRQ	CA3-N3-C1	-2.85	122.64	128.22
1	E	66	CRQ	C2-CA2-N2	-2.81	106.97	108.93
1	C	66	CRQ	CE1-CD1-CG2	-2.75	117.66	121.25
1	A	66	CRQ	CD2-CG2-CD1	2.46	121.28	117.64
1	A	66	CRQ	CB2-CA2-N2	-2.32	125.61	128.83
1	C	66	CRQ	CA3-N3-C2	2.31	129.10	123.80
1	B	66	CRQ	CD2-CG2-CD1	2.30	121.05	117.64
1	D	66	CRQ	CD2-CG2-CD1	2.27	120.99	117.64
1	B	66	CRQ	CE1-CD1-CG2	-2.24	118.33	121.25
1	C	66	CRQ	O2-C2-N3	2.23	128.79	124.35
1	A	66	CRQ	CA3-N3-C1	-2.12	124.07	128.22
1	A	66	CRQ	CE1-CD1-CG2	-2.11	118.50	121.25
1	D	66	CRQ	CG1-CB1-CA1	-2.04	107.20	113.53
1	E	66	CRQ	O3-C3-CA3	-2.04	120.24	126.39

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	CRQ	C3-CA3-N3-C2
1	B	66	CRQ	C3-CA3-N3-C2
1	C	66	CRQ	C3-CA3-N3-C2
1	D	66	CRQ	C3-CA3-N3-C2
1	E	66	CRQ	C3-CA3-N3-C2
1	D	66	CRQ	C3-CA3-N3-C1
1	D	66	CRQ	C1-CA1-CB1-CG1
1	B	66	CRQ	C3-CA3-N3-C1
1	C	66	CRQ	C3-CA3-N3-C1
1	A	66	CRQ	C3-CA3-N3-C1

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	66	CRQ	3	0
1	C	66	CRQ	1	0
1	D	66	CRQ	1	0
1	E	66	CRQ	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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, 95^{th} 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	223/241 (92%)	0.42	9 (4%) 38 44	13, 17, 24, 35	1 (0%)
1	B	217/241 (90%)	0.66	19 (8%) 10 12	13, 18, 24, 30	0
1	C	220/241 (91%)	0.43	10 (4%) 33 38	12, 17, 24, 33	1 (0%)
1	D	219/241 (90%)	0.79	26 (11%) 4 5	12, 18, 25, 30	1 (0%)
1	E	215/241 (89%)	1.34	53 (24%) 0 0	13, 19, 22, 26	0
1	F	60/241 (24%)	2.82	38 (63%) 0 0	15, 24, 33, 33	2 (3%)
All	All	1154/1446 (79%)	0.83	155 (13%) 3 4	12, 18, 25, 35	5 (0%)

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	93	TRP	12.8
1	F	136	VAL	8.3
1	E	51	GLY	7.8
1	F	27	PHE	7.7
1	E	53	PRO	6.7
1	F	139	LYS	6.5
1	E	25	HIS	6.4
1	E	186	ALA	6.2
1	E	27	PHE	5.8
1	E	48	VAL	5.5
1	E	55	PRO	5.4
1	D	188	LEU	5.4
1	B	188	LEU	5.3
1	E	208	GLU	5.3
1	E	132	ASN	5.2
1	A	169	GLY	5.2
1	E	170	GLY	5.1
1	A	188	LEU	5.1
1	E	210	MET	5.0

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Mol	Chain	Res	Type	RSRZ
1	E	26	TYR	5.0
1	F	56	PHE	5.0
1	E	131	PRO	5.0
1	C	188	LEU	4.9
1	F	164	ALA	4.9
1	F	58	TRP	4.8
1	F	162	HIS	4.8
1	E	130	PRO	4.6
1	F	55	PRO	4.6
1	E	49	THR	4.6
1	E	187	ALA	4.5
1	F	26	TYR	4.5
1	F	59	HIS	4.3
1	B	169	GLY	4.3
1	E	209	PHE	4.2
1	F	54	LEU	4.2
1	F	60	ILE	4.2
1	E	50	LYS	4.2
1	E	56	PHE	4.1
1	F	21	THR	4.1
1	F	25	HIS	3.9
1	E	168	GLU	3.9
1	F	134	PRO	3.8
1	E	206	ASP	3.8
1	E	136	VAL	3.8
1	E	38	ASN	3.7
1	F	22	PHE	3.7
1	F	103	GLY	3.6
1	F	53	PRO	3.6
1	E	203	TRP	3.6
1	F	163	HIS	3.5
1	B	104	LEU	3.4
1	A	3[A]	CYS	3.4
1	B	187	ALA	3.3
1	F	20	GLY	3.3
1	C	169	GLY	3.3
1	E	129	PHE	3.3
1	F	101	ASP	3.2
1	E	58	TRP	3.2
1	B	53	PRO	3.1
1	D	80	HIS	3.1
1	D	168	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	88	PRO	3.1
1	E	155	GLY	3.1
1	D	78	ASN	3.1
1	A	1	MET	3.1
1	E	177	ILE	3.1
1	E	133	GLY	3.1
1	E	171	GLY	3.1
1	D	177	ILE	3.1
1	B	116	ASN	3.0
1	B	177	ILE	3.0
1	D	77	ASP	3.0
1	E	167	VAL	2.9
1	D	81	ASP	2.9
1	E	127	LEU	2.9
1	F	135	VAL	2.8
1	C	177	ILE	2.8
1	E	86	SER	2.8
1	D	106[A]	CYS	2.8
1	A	226	TYR	2.8
1	D	8	ILE	2.8
1	B	80	HIS	2.8
1	F	131	PRO	2.8
1	F	133	GLY	2.8
1	E	156	VAL	2.8
1	D	208	GLU	2.8
1	B	114	THR	2.7
1	E	202	ILE	2.7
1	E	85	LEU	2.7
1	F	57	GLY	2.7
1	E	137	GLN	2.7
1	A	170	GLY	2.7
1	F	105	CYS	2.7
1	F	124	PHE	2.7
1	D	79	ILE	2.6
1	D	186	ALA	2.6
1	C	161	ILE	2.6
1	B	85	LEU	2.6
1	C	104	LEU	2.6
1	E	46	LEU	2.6
1	E	52	GLY	2.5
1	B	190	MET	2.5
1	E	29	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	37	PRO	2.5
1	E	139	LYS	2.5
1	B	168	GLU	2.5
1	D	96	SER	2.5
1	A	177	ILE	2.5
1	D	88	PRO	2.4
1	F	51	GLY	2.4
1	D	203	TRP	2.4
1	D	104	LEU	2.4
1	F	50	LYS	2.4
1	E	134	PRO	2.4
1	F	161	ILE	2.4
1	E	126	GLY	2.3
1	D	85	LEU	2.3
1	D	105	CYS	2.3
1	D	98	HIS	2.3
1	D	40	GLY	2.3
1	E	192	GLY	2.3
1	D	97	MET	2.3
1	A	106[A]	CYS	2.3
1	A	104	LEU	2.2
1	B	226	TYR	2.2
1	E	124	PHE	2.2
1	F	132	ASN	2.2
1	C	105	CYS	2.2
1	C	107	ILE	2.2
1	B	113	LEU	2.2
1	B	88	PRO	2.2
1	B	98	HIS	2.2
1	C	98	HIS	2.2
1	F	49	THR	2.2
1	F	108	THR	2.2
1	F	63	PRO	2.2
1	E	169	GLY	2.2
1	F	174	ALA	2.2
1	E	90	GLY	2.1
1	E	76	PRO	2.1
1	F	61	LEU	2.1
1	B	105	CYS	2.1
1	C	97	MET	2.1
1	D	154	ASP	2.1
1	B	106[A]	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	62	CYS	2.1
1	E	78	ASN	2.1
1	D	217	ILE	2.1
1	B	196	VAL	2.1
1	D	201	VAL	2.1
1	C	96	SER	2.1
1	F	176	ASP	2.0
1	E	154	ASP	2.0
1	D	63	PRO	2.0
1	E	54	LEU	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. The B-factors column lists the minimum, median, 95^{th} 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	E	66	24/25	0.86	0.15	16,19,20,20	0
1	CRQ	D	66	24/25	0.91	0.16	18,21,22,22	0
1	CRQ	B	66	24/25	0.94	0.15	17,20,21,22	0
1	CRQ	C	66	24/25	0.94	0.16	11,19,21,21	0
1	CRQ	A	66	24/25	0.95	0.17	13,18,19,20	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (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, 95^{th} 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
2	NA	B	233	1/1	0.90	0.11	11,11,11,11	0
2	NA	A	233	1/1	0.97	0.09	12,12,12,12	0

6.5 Other polymers (i)

There are no such residues in this entry.