Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 03:42 AM EST

PDB ID	:	4JC2
Title	:	Isolation, Cloning and Biophysical Analysis of a Novel Hexameric Green Fluorescent Protein from a Philippine Soft Coral
Authors	:	Huang, Y.C.; Emralino, F.L.; Liu, F.C.; Saloma, C.P.; Bascos, N.A.; Chen, C.J.
Deposited on	:	2013-02-21
Resolution	:	2.35 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 (i) 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 (i)) were used in the production of this report:

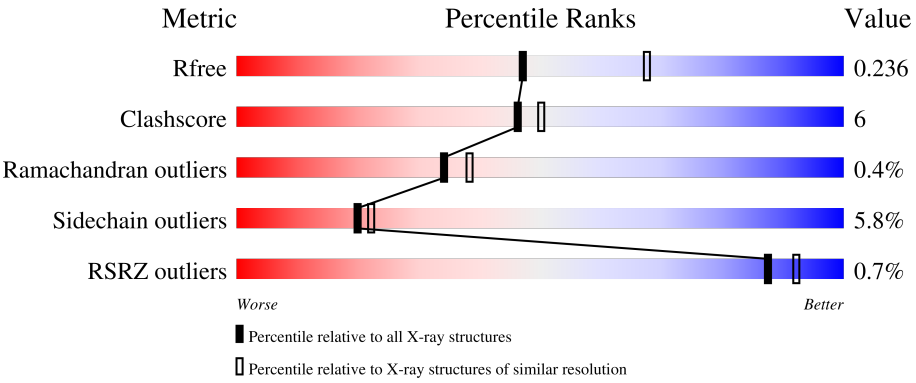
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	222	84% 14%
1	B	222	86% 11%
1	C	222	83% 14%
1	D	222	83% 13%
1	E	222	86% 11%

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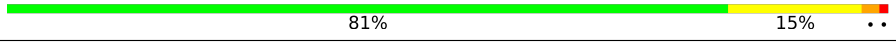
Mol	Chain	Length	Quality of chain
1	F	222	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11563 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 asFP504.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1800	1148	306	335	11			
1	B	221	Total	C	N	O	S	0	0	0
			1800	1148	306	335	11			
1	C	220	Total	C	N	O	S	0	0	0
			1795	1145	305	334	11			
1	D	221	Total	C	N	O	S	0	0	0
			1800	1148	306	335	11			
1	E	221	Total	C	N	O	S	0	0	0
			1800	1148	306	335	11			
1	F	221	Total	C	N	O	S	0	0	0
			1800	1148	306	335	11			

- Molecule 2 is water.

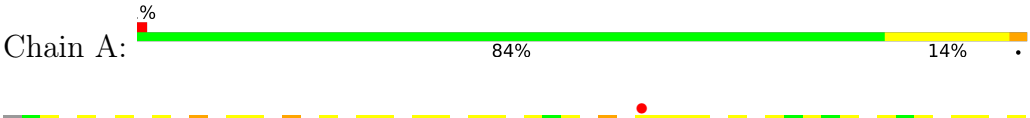
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	119	Total	O	0	0
			119	119		
2	B	151	Total	O	0	0
			151	151		
2	C	151	Total	O	0	0
			151	151		
2	D	137	Total	O	0	0
			137	137		
2	E	111	Total	O	0	0
			111	111		
2	F	99	Total	O	0	0
			99	99		

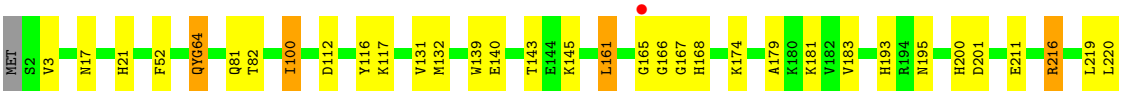
3 Residue-property plots (i)

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: asFP504

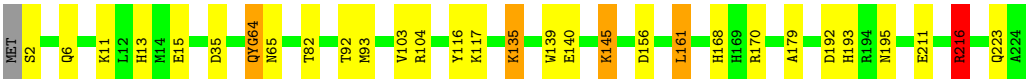
Chain A:





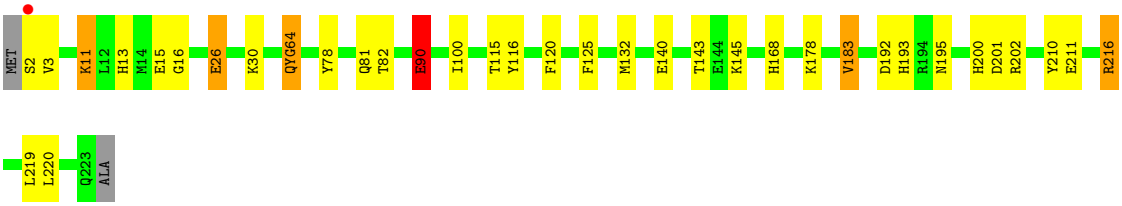
• Molecule 1: asFP504

Chain B:



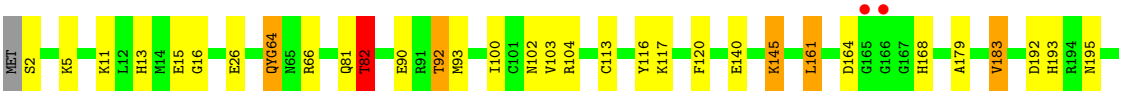
• Molecule 1: asFP504

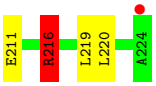
Chain C:



• Molecule 1: asFP504

Chain D:



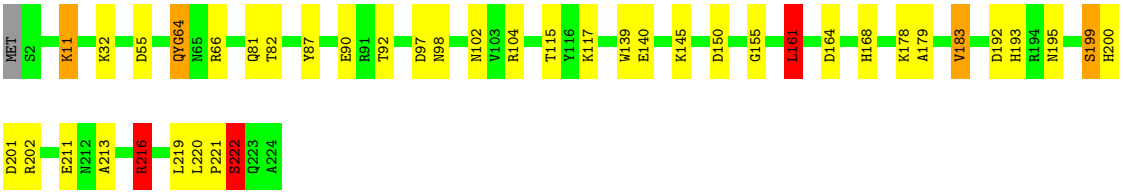


• Molecule 1: asFP504

Chain E:

• Molecule 1: asFP504

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.07Å 127.71Å 158.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.62 – 2.35 29.62 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.62-2.35) 99.8 (29.62-2.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	4.89 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.175 , 0.235 0.181 , 0.236	Depositor DCC
R_{free} test set	3292 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	18.4	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 28.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11563	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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

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	0.79	0/1822	0.93	3/2457 (0.1%)
1	B	0.82	0/1822	1.03	9/2457 (0.4%)
1	C	0.83	1/1817 (0.1%)	0.96	4/2450 (0.2%)
1	D	0.77	1/1822 (0.1%)	0.96	4/2457 (0.2%)
1	E	0.75	0/1822	0.86	2/2457 (0.1%)
1	F	0.71	0/1822	0.90	4/2457 (0.2%)
All	All	0.78	2/10927 (0.0%)	0.94	26/14735 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	90	GLU	CD-OE2	5.68	1.31	1.25
1	D	90	GLU	CD-OE2	5.63	1.31	1.25

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	216	ARG	NE-CZ-NH2	-13.33	113.63	120.30
1	B	216	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	C	216	ARG	NE-CZ-NH2	-9.46	115.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	216	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	D	216	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	A	216	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	A	216	ARG	NE-CZ-NH2	-7.99	116.30	120.30
1	E	216	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	D	216	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	F	161	LEU	CA-CB-CG	6.30	129.79	115.30
1	C	216	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	D	161	LEU	CA-CB-CG	6.17	129.50	115.30
1	F	216	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	D	82	THR	CB-CA-C	-6.03	95.32	111.60
1	E	216	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	B	170	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	C	192	ASP	CB-CG-OD1	5.82	123.54	118.30
1	A	112	ASP	CB-CG-OD1	5.64	123.38	118.30
1	B	216	ARG	CD-NE-CZ	5.59	131.42	123.60
1	B	156	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	35	ASP	CB-CG-OD1	5.45	123.20	118.30
1	B	35	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	B	104	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	F	55	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	216	ARG	CG-CD-NE	-5.11	101.07	111.80
1	C	216	ARG	CG-CD-NE	-5.11	101.07	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2	SER	Peptide
1	D	164	ASP	Peptide

5.2 Too-close contacts (i)

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	1800	0	1733	21	0
1	B	1800	0	1733	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1795	0	1728	26	0
1	D	1800	0	1733	20	0
1	E	1800	0	1733	19	0
1	F	1800	0	1733	28	0
2	A	119	0	0	3	0
2	B	151	0	0	1	0
2	C	151	0	0	8	0
2	D	137	0	0	1	0
2	E	111	0	0	2	0
2	F	99	0	0	4	0
All	All	11563	0	10393	133	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 6.

All (133) 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:90:GLU:OE1	1:F:104:ARG:HD3	1.64	0.97
1:F:221:PRO:O	1:F:222:SER:HB2	1.68	0.93
1:B:64:CRQ:C3	1:B:65:ASN:CA	2.51	0.89
1:C:125:PHE:HB2	1:C:132:MET:HE3	1.53	0.89
1:F:81:GLN:HB3	1:F:183:VAL:HG22	1.56	0.88
1:C:2:SER:HA	2:C:426:HOH:O	1.74	0.86
1:B:93:MET:CE	1:B:103:VAL:HG21	2.06	0.86
1:E:193:HIS:HD2	1:E:211:GLU:OE1	1.66	0.78
1:F:82:THR:HG21	1:F:179:ALA:CB	2.15	0.76
1:F:82:THR:HG21	1:F:179:ALA:HB1	1.65	0.76
1:F:82:THR:CG2	1:F:179:ALA:HB1	2.16	0.75
1:C:81:GLN:HB3	1:C:183:VAL:HG22	1.69	0.74
1:A:139:TRP:CZ3	1:A:161:LEU:HD13	2.22	0.73
1:F:221:PRO:O	1:F:222:SER:CB	2.37	0.73
1:B:192:ASP:OD2	1:B:216:ARG:HD3	1.89	0.72
1:A:81:GLN:HB3	1:A:183:VAL:HG22	1.70	0.72
1:B:64:CRQ:CA3	1:B:65:ASN:N	2.53	0.70
1:D:82:THR:CG2	1:D:179:ALA:HB1	2.22	0.70
1:C:125:PHE:CB	1:C:132:MET:HE3	2.21	0.70
1:B:193:HIS:HD2	1:B:211:GLU:OE1	1.75	0.69
1:E:82:THR:HG22	1:E:179:ALA:HB1	1.75	0.69
1:F:140:GLU:OE2	1:F:168:HIS:HE1	1.75	0.68
1:A:139:TRP:CE3	1:A:161:LEU:HD13	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:HIS:HD2	2:C:342:HOH:O	1.77	0.67
1:E:41:ASN:HD21	1:E:208:LYS:NZ	1.94	0.66
1:F:199:SER:HB3	2:F:398:HOH:O	1.96	0.65
1:B:82:THR:HG21	1:B:179:ALA:CB	2.27	0.65
1:C:2:SER:CB	2:C:449:HOH:O	2.45	0.64
1:F:199:SER:CB	2:F:398:HOH:O	2.45	0.63
1:C:200:HIS:HD2	1:C:201:ASP:O	1.82	0.63
1:D:93:MET:CE	1:D:103:VAL:HG21	2.29	0.62
1:F:192:ASP:OD2	1:F:216:ARG:HD3	1.99	0.62
1:B:64:CRQ:HE2	1:B:195:ASN:HB2	1.81	0.62
1:D:82:THR:HG23	1:D:179:ALA:HB1	1.81	0.62
1:F:64:CRQ:HE2	1:F:195:ASN:HB2	1.81	0.62
1:B:82:THR:CG2	1:B:179:ALA:HB1	2.31	0.61
1:A:193:HIS:HD2	1:A:211:GLU:OE1	1.82	0.61
1:A:181:LYS:HB2	2:A:356:HOH:O	2.01	0.60
2:B:311:HOH:O	1:C:168:HIS:HD2	1.85	0.60
1:C:2:SER:HB3	2:C:449:HOH:O	2.01	0.59
1:D:192:ASP:OD2	1:D:216:ARG:HD3	2.01	0.59
1:A:64:CRQ:HE2	1:A:195:ASN:HB2	1.84	0.59
1:A:168:HIS:HD2	2:E:318:HOH:O	1.85	0.58
1:E:200:HIS:HD2	1:E:201:ASP:O	1.84	0.58
1:B:139:TRP:CE3	1:B:161:LEU:HD13	2.38	0.58
1:C:193:HIS:HD2	1:C:211:GLU:OE1	1.85	0.58
1:A:200:HIS:HD2	1:A:201:ASP:O	1.86	0.57
1:A:140:GLU:OE2	1:A:168:HIS:HE1	1.88	0.57
1:A:200:HIS:HE1	2:A:345:HOH:O	1.88	0.56
1:B:93:MET:CE	1:B:103:VAL:CG2	2.81	0.56
1:B:82:THR:HG22	1:B:179:ALA:HB1	1.87	0.56
1:F:193:HIS:HD2	1:F:211:GLU:OE1	1.89	0.56
1:E:140:GLU:OE2	1:E:168:HIS:HE1	1.89	0.55
1:E:41:ASN:HD21	1:E:208:LYS:HZ2	1.53	0.55
1:D:168:HIS:HD2	2:F:320:HOH:O	1.90	0.55
1:F:139:TRP:CE3	1:F:161:LEU:HD13	2.41	0.55
1:C:140:GLU:OE2	1:C:168:HIS:HE1	1.90	0.55
1:D:140:GLU:OE2	1:D:168:HIS:HE1	1.90	0.54
1:E:216:ARG:NH2	2:E:367:HOH:O	2.39	0.54
1:B:223:GLN:HG3	1:C:210:TYR:CE2	2.42	0.54
1:F:81:GLN:HB3	1:F:183:VAL:CG2	2.34	0.54
1:D:64:CRQ:HE2	1:D:195:ASN:HB2	1.91	0.53
1:A:17:ASN:HA	1:A:21:HIS:O	2.09	0.52
2:D:301:HOH:O	1:F:168:HIS:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:MET:HE1	1:D:103:VAL:HG21	1.91	0.52
1:E:64:CRQ:HE2	1:E:195:ASN:HB2	1.90	0.52
1:C:2:SER:HB2	2:C:449:HOH:O	2.10	0.51
1:A:52:PHE:HB3	1:A:132:MET:CE	2.41	0.51
1:C:13:HIS:HE1	1:C:15:GLU:OE2	1.93	0.51
1:B:140:GLU:OE2	1:B:168:HIS:HE1	1.93	0.51
1:C:200:HIS:HE1	2:C:400:HOH:O	1.92	0.51
1:E:193:HIS:CD2	1:E:211:GLU:OE1	2.57	0.51
1:D:193:HIS:HD2	1:D:211:GLU:OE1	1.94	0.50
1:B:82:THR:CG2	1:B:179:ALA:CB	2.87	0.50
1:D:93:MET:CE	1:D:103:VAL:CG2	2.89	0.50
1:D:13:HIS:HE1	1:D:15:GLU:OE2	1.95	0.49
1:B:93:MET:HE1	1:B:103:VAL:HG21	1.93	0.49
1:A:145:LYS:NZ	1:E:143:THR:H	2.11	0.48
1:A:165:GLY:O	1:A:167:GLY:N	2.39	0.48
1:C:178:LYS:HE2	2:C:347:HOH:O	2.13	0.48
1:E:139:TRP:CE3	1:E:161:LEU:HD13	2.49	0.48
1:D:81:GLN:HB3	1:D:183:VAL:HG22	1.95	0.48
1:C:64:CRQ:HE2	1:C:195:ASN:HB2	1.97	0.47
1:D:66:ARG:NE	1:D:66:ARG:HA	2.30	0.46
1:A:131:VAL:HG12	1:A:132:MET:CE	2.45	0.46
1:E:66:ARG:NE	1:E:66:ARG:HA	2.31	0.46
2:A:326:HOH:O	1:E:168:HIS:HD2	1.97	0.46
1:B:13:HIS:HE1	1:B:15:GLU:OE2	1.99	0.46
1:C:125:PHE:CB	1:C:132:MET:CE	2.94	0.46
1:F:82:THR:HG21	1:F:179:ALA:CA	2.46	0.45
1:F:87:TYR:HB2	1:F:178:LYS:O	2.17	0.45
1:B:145:LYS:NZ	1:C:143:THR:H	2.15	0.45
1:D:82:THR:HG21	1:D:179:ALA:HB1	1.95	0.45
1:C:125:PHE:HB2	1:C:132:MET:CE	2.35	0.44
1:F:199:SER:HB2	2:F:398:HOH:O	2.15	0.44
1:F:81:GLN:CB	1:F:183:VAL:HG22	2.39	0.44
1:B:135:LYS:HA	1:B:135:LYS:HD2	1.76	0.44
1:D:145:LYS:N	1:D:145:LYS:HD2	2.32	0.44
1:E:82:THR:HG22	1:E:179:ALA:CB	2.46	0.43
1:F:200:HIS:HD2	1:F:201:ASP:O	2.01	0.43
1:A:82:THR:HG22	1:A:179:ALA:HB1	2.00	0.43
1:B:93:MET:HE2	1:B:103:VAL:HG21	1.98	0.43
1:B:93:MET:HE3	1:B:103:VAL:CG2	2.49	0.43
1:C:78:TYR:O	1:C:82:THR:HG23	2.17	0.43
1:B:145:LYS:HZ1	1:C:143:THR:H	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:66:ARG:NE	1:F:66:ARG:HA	2.32	0.43
1:F:220:LEU:HA	1:F:221:PRO:HD3	1.77	0.43
1:B:139:TRP:CZ3	1:B:161:LEU:HD13	2.54	0.43
1:A:81:GLN:CB	1:A:183:VAL:HG22	2.42	0.42
1:E:200:HIS:CD2	1:E:201:ASP:O	2.69	0.42
1:A:52:PHE:CB	1:A:132:MET:CE	2.98	0.42
1:A:143:THR:H	1:E:145:LYS:NZ	2.17	0.42
1:E:100:ILE:HD13	1:E:101:CYS:N	2.35	0.42
1:D:82:THR:HG21	1:D:179:ALA:CB	2.50	0.42
1:F:97:ASP:O	1:F:98:ASN:HB2	2.20	0.42
1:F:145:LYS:O	1:F:155:GLY:HA2	2.20	0.42
1:D:11:LYS:HG2	1:D:113:CYS:SG	2.61	0.41
1:C:11:LYS:O	1:C:115:THR:HA	2.20	0.41
1:C:200:HIS:CD2	1:C:201:ASP:O	2.70	0.41
1:E:11:LYS:O	1:E:115:THR:HA	2.19	0.41
1:D:92:THR:HB	1:D:102:ASN:ND2	2.36	0.41
1:B:82:THR:HG21	1:B:179:ALA:HB1	1.97	0.41
1:C:26:GLU:OE2	1:C:26:GLU:HA	2.20	0.41
1:D:82:THR:HG21	1:D:179:ALA:CA	2.51	0.41
1:F:192:ASP:O	1:F:213:ALA:HA	2.21	0.41
1:A:100:ILE:HD13	1:A:100:ILE:O	2.21	0.41
1:C:90:GLU:HG3	2:C:347:HOH:O	2.21	0.41
1:F:92:THR:HG22	1:F:102:ASN:ND2	2.36	0.41
1:C:16:GLY:HA2	1:C:120:PHE:O	2.21	0.40
1:A:52:PHE:CB	1:A:132:MET:HE2	2.51	0.40
1:D:16:GLY:HA2	1:D:120:PHE:O	2.21	0.40
1:E:82:THR:CG2	1:E:179:ALA:CB	3.00	0.40
1:F:11:LYS:O	1:F:115:THR:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	216/222 (97%)	212 (98%)	3 (1%)	1 (0%)	29 32
1	B	216/222 (97%)	213 (99%)	3 (1%)	0	100 100
1	C	215/222 (97%)	214 (100%)	1 (0%)	0	100 100
1	D	216/222 (97%)	215 (100%)	1 (0%)	0	100 100
1	E	216/222 (97%)	211 (98%)	4 (2%)	1 (0%)	29 32
1	F	216/222 (97%)	208 (96%)	5 (2%)	3 (1%)	11 9
All	All	1295/1332 (97%)	1273 (98%)	17 (1%)	5 (0%)	34 38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	164	ASP
1	F	222	SER
1	A	166	GLY
1	F	150	ASP
1	E	3	VAL

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	192/193 (100%)	183 (95%)	9 (5%)	26 31
1	B	192/193 (100%)	183 (95%)	9 (5%)	26 31
1	C	192/193 (100%)	179 (93%)	13 (7%)	16 16
1	D	192/193 (100%)	177 (92%)	15 (8%)	12 12
1	E	192/193 (100%)	181 (94%)	11 (6%)	20 22
1	F	192/193 (100%)	182 (95%)	10 (5%)	23 27
All	All	1152/1158 (100%)	1085 (94%)	67 (6%)	20 22

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	100	ILE
1	A	116	TYR
1	A	117	LYS
1	A	161	LEU
1	A	174	LYS
1	A	216	ARG
1	A	219	LEU
1	A	220	LEU
1	B	6	GLN
1	B	11	LYS
1	B	92	THR
1	B	116	TYR
1	B	117	LYS
1	B	135	LYS
1	B	145	LYS
1	B	161	LEU
1	B	216	ARG
1	C	3	VAL
1	C	11	LYS
1	C	26	GLU
1	C	30	LYS
1	C	90	GLU
1	C	100	ILE
1	C	116	TYR
1	C	145	LYS
1	C	183	VAL
1	C	202	ARG
1	C	216	ARG
1	C	219	LEU
1	C	220	LEU
1	D	2	SER
1	D	5	LYS
1	D	26	GLU
1	D	82	THR
1	D	92	THR
1	D	100	ILE
1	D	104	ARG
1	D	116	TYR
1	D	117	LYS
1	D	145	LYS
1	D	161	LEU
1	D	183	VAL

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Mol	Chain	Res	Type
1	D	216	ARG
1	D	219	LEU
1	D	220	LEU
1	E	5	LYS
1	E	30	LYS
1	E	90	GLU
1	E	100	ILE
1	E	104	ARG
1	E	145	LYS
1	E	161	LEU
1	E	202	ARG
1	E	216	ARG
1	E	219	LEU
1	E	220	LEU
1	F	11	LYS
1	F	32	LYS
1	F	117	LYS
1	F	161	LEU
1	F	183	VAL
1	F	199	SER
1	F	202	ARG
1	F	216	ARG
1	F	219	LEU
1	F	222	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	168	HIS
1	A	169	HIS
1	A	193	HIS
1	A	200	HIS
1	B	6	GLN
1	B	13	HIS
1	B	128	ASN
1	B	158	ASN
1	B	168	HIS
1	B	169	HIS
1	B	193	HIS
1	B	200	HIS
1	C	13	HIS

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Mol	Chain	Res	Type
1	C	38	GLN
1	C	133	GLN
1	C	168	HIS
1	C	169	HIS
1	C	193	HIS
1	C	200	HIS
1	D	13	HIS
1	D	102	ASN
1	D	168	HIS
1	D	169	HIS
1	D	193	HIS
1	D	200	HIS
1	E	38	GLN
1	E	41	ASN
1	E	133	GLN
1	E	168	HIS
1	E	169	HIS
1	E	184	GLN
1	E	193	HIS
1	E	200	HIS
1	F	13	HIS
1	F	102	ASN
1	F	168	HIS
1	F	169	HIS
1	F	184	GLN
1	F	193	HIS
1	F	200	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 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	64	1	24,25,26	2.56	4 (16%)	27,34,36	3.19	7 (25%)
1	CRQ	E	64	1	24,25,26	3.36	5 (20%)	27,34,36	3.26	6 (22%)
1	CRQ	F	64	1	24,25,26	3.42	5 (20%)	27,34,36	3.55	5 (18%)
1	CRQ	C	64	1	24,25,26	2.89	4 (16%)	27,34,36	3.03	6 (22%)
1	CRQ	A	64	1	24,25,26	3.38	4 (16%)	27,34,36	3.29	5 (18%)
1	CRQ	D	64	1	24,25,26	3.34	5 (20%)	27,34,36	3.19	7 (25%)

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	64	1	-	2/10/32/33	0/2/2/2
1	CRQ	E	64	1	-	2/10/32/33	0/2/2/2
1	CRQ	F	64	1	-	2/10/32/33	0/2/2/2
1	CRQ	C	64	1	-	2/10/32/33	0/2/2/2
1	CRQ	A	64	1	-	2/10/32/33	0/2/2/2
1	CRQ	D	64	1	-	3/10/32/33	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	64	CRQ	CB2-CA2	15.10	1.47	1.35
1	A	64	CRQ	CB2-CA2	15.10	1.47	1.35
1	E	64	CRQ	CB2-CA2	14.91	1.47	1.35
1	D	64	CRQ	CB2-CA2	14.13	1.46	1.35
1	C	64	CRQ	CB2-CA2	12.72	1.45	1.35
1	B	64	CRQ	CB2-CA2	10.64	1.44	1.35
1	D	64	CRQ	CA2-C2	-5.45	1.43	1.48
1	B	64	CRQ	CA2-C2	-4.07	1.44	1.48
1	F	64	CRQ	CA2-C2	-4.05	1.44	1.48
1	E	64	CRQ	O2-C2	3.71	1.30	1.23
1	D	64	CRQ	C2-N3	-3.68	1.31	1.39
1	C	64	CRQ	CA2-C2	-3.63	1.45	1.48
1	A	64	CRQ	C2-N3	-3.57	1.31	1.39
1	E	64	CRQ	CA2-C2	-3.37	1.45	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	64	CRQ	C2-N3	-3.37	1.31	1.39
1	F	64	CRQ	C2-N3	-3.27	1.32	1.39
1	A	64	CRQ	O2-C2	3.24	1.29	1.23
1	F	64	CRQ	CA2-N2	-2.71	1.32	1.38
1	D	64	CRQ	CA2-N2	-2.55	1.33	1.38
1	F	64	CRQ	O2-C2	2.54	1.28	1.23
1	E	64	CRQ	CA2-N2	-2.49	1.33	1.38
1	C	64	CRQ	O2-C2	2.46	1.28	1.23
1	D	64	CRQ	O2-C2	2.44	1.28	1.23
1	E	64	CRQ	C2-N3	-2.35	1.34	1.39
1	B	64	CRQ	C2-N3	-2.26	1.34	1.39
1	A	64	CRQ	CG2-CB2	2.14	1.51	1.46
1	B	64	CRQ	CA2-N2	-2.09	1.34	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	64	CRQ	CA2-C2-N3	12.18	109.13	103.37
1	D	64	CRQ	CA2-C2-N3	11.17	108.65	103.37
1	E	64	CRQ	O2-C2-CA2	-11.07	124.74	130.96
1	F	64	CRQ	O2-C2-CA2	-11.00	124.78	130.96
1	A	64	CRQ	CA2-C2-N3	10.95	108.55	103.37
1	B	64	CRQ	O2-C2-CA2	-10.56	125.03	130.96
1	B	64	CRQ	CA2-C2-N3	10.38	108.28	103.37
1	A	64	CRQ	O2-C2-CA2	-10.32	125.16	130.96
1	C	64	CRQ	CA2-C2-N3	10.21	108.20	103.37
1	E	64	CRQ	CA2-C2-N3	10.21	108.20	103.37
1	C	64	CRQ	O2-C2-CA2	-10.00	125.34	130.96
1	D	64	CRQ	O2-C2-CA2	-8.89	125.97	130.96
1	D	64	CRQ	CB2-CA2-C2	4.88	128.10	122.28
1	F	64	CRQ	CB2-CA2-C2	4.24	127.34	122.28
1	A	64	CRQ	CB2-CA2-C2	4.17	127.26	122.28
1	E	64	CRQ	O3-C3-CA3	-4.11	113.99	126.39
1	F	64	CRQ	O3-C3-CA3	-3.76	115.03	126.39
1	A	64	CRQ	C2-CA2-N2	-3.76	106.30	108.93
1	A	64	CRQ	O3-C3-CA3	-3.61	115.49	126.39
1	F	64	CRQ	C2-CA2-N2	-3.41	106.54	108.93
1	C	64	CRQ	CB2-CA2-C2	3.32	126.24	122.28
1	B	64	CRQ	CB2-CA2-C2	3.31	126.23	122.28
1	D	64	CRQ	CB2-CA2-N2	-3.02	124.64	128.83
1	C	64	CRQ	O3-C3-CA3	-2.91	117.61	126.39
1	E	64	CRQ	C2-CA2-N2	-2.89	106.91	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	64	CRQ	CB2-CA2-C2	2.78	125.59	122.28
1	D	64	CRQ	CG2-CB2-CA2	-2.61	126.74	129.94
1	E	64	CRQ	CE2-CD2-CG2	-2.60	117.85	121.25
1	B	64	CRQ	CD1-CG2-CB2	-2.57	112.47	121.22
1	B	64	CRQ	O3-C3-CA3	-2.54	118.72	126.39
1	D	64	CRQ	C2-CA2-N2	-2.48	107.19	108.93
1	B	64	CRQ	CB2-CA2-N2	-2.29	125.65	128.83
1	D	64	CRQ	CD1-CG2-CB2	-2.17	113.82	121.22
1	B	64	CRQ	CG2-CB2-CA2	-2.12	127.35	129.94
1	C	64	CRQ	CD1-CG2-CB2	-2.10	114.06	121.22
1	C	64	CRQ	CB2-CA2-N2	-2.00	126.05	128.83

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	64	CRQ	C3-CA3-N3-C2
1	C	64	CRQ	C3-CA3-N3-C2
1	D	64	CRQ	C3-CA3-N3-C2
1	E	64	CRQ	C3-CA3-N3-C2
1	F	64	CRQ	C3-CA3-N3-C2
1	A	64	CRQ	C3-CA3-N3-C2
1	D	64	CRQ	CA1-CB1-CG1-CD3
1	F	64	CRQ	CA1-CB1-CG1-CD3
1	C	64	CRQ	C3-CA3-N3-C1
1	D	64	CRQ	C3-CA3-N3-C1
1	E	64	CRQ	C3-CA3-N3-C1
1	B	64	CRQ	C1-CA1-CB1-CG1
1	A	64	CRQ	CA1-CB1-CG1-CD3

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	64	CRQ	3	0
1	E	64	CRQ	1	0
1	F	64	CRQ	1	0
1	C	64	CRQ	1	0
1	A	64	CRQ	1	0
1	D	64	CRQ	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	C	1
1	D	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	64:CRQ	C3	65:ASN	N	1.68
1	C	64:CRQ	C3	65:ASN	N	1.66
1	D	61:PHE	C	64:CRQ	N1	1.64
1	E	64:CRQ	C3	65:ASN	N	1.62

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	220/222 (99%)	-0.40	2 (0%) 84 90	8, 14, 29, 56	0
1	B	220/222 (99%)	-0.44	0 100 100	6, 12, 26, 46	0
1	C	219/222 (98%)	-0.46	1 (0%) 91 95	6, 12, 27, 46	0
1	D	220/222 (99%)	-0.37	3 (1%) 75 83	9, 16, 31, 59	0
1	E	220/222 (99%)	-0.28	3 (1%) 75 83	11, 18, 35, 63	0
1	F	220/222 (99%)	-0.13	0 100 100	10, 22, 41, 56	0
All	All	1319/1332 (99%)	-0.35	9 (0%) 87 92	6, 16, 34, 63	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	224	ALA	4.7
1	D	165	GLY	3.7
1	E	2	SER	3.2
1	E	224	ALA	3.1
1	D	224	ALA	3.0
1	C	2	SER	2.9
1	D	166	GLY	2.7
1	A	165	GLY	2.5
1	E	3	VAL	2.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B	64	24/25	0.96	0.14	5,6,6,7	0
1	CRQ	E	64	24/25	0.96	0.16	10,12,13,14	0
1	CRQ	C	64	24/25	0.97	0.13	6,6,7,7	0
1	CRQ	D	64	24/25	0.97	0.12	10,11,12,12	0
1	CRQ	A	64	24/25	0.97	0.11	7,8,9,10	0
1	CRQ	F	64	24/25	0.97	0.22	13,14,17,18	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.