Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 01:17 PM EST

PDB ID	:	6CIU
Title	:	Structure of a Thr-rich interface in an Azami Green tetramer
Authors	:	Oi, C.; Lim, C.S.; Knecht, K.M.; Xiong, Y.; Regan, L.
Deposited on	:	2018-02-25
Resolution	:	1.70 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:

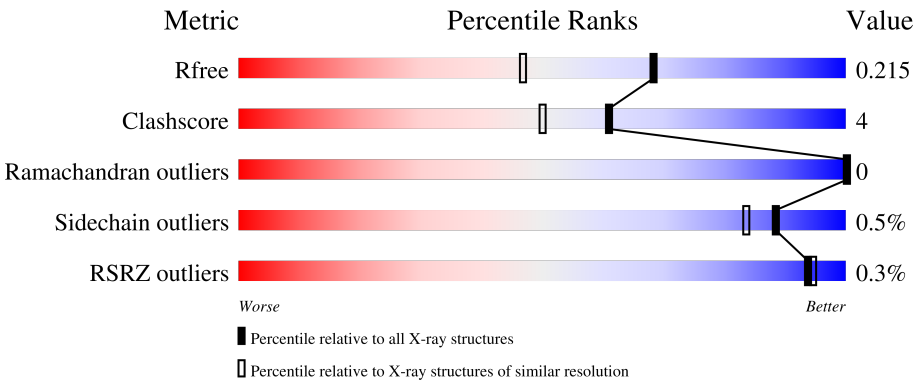
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	236	82% 11% 6%
1	B	236	81% 11% • 7%
1	C	236	79% 13% • 6%
1	D	236	79% 13% • 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7642 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 Azami-Green.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	221	1803	1155	301	335	12	0	0	0
1	B	220	1798	1152	300	334	12	0	0	0
1	C	221	1806	1158	302	334	12	0	0	0
1	D	219	1792	1149	299	332	12	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP Q60I25
A	-11	GLY	-	expression tag	UNP Q60I25
A	-10	SER	-	expression tag	UNP Q60I25
A	-9	SER	-	expression tag	UNP Q60I25
A	-8	HIS	-	expression tag	UNP Q60I25
A	-7	HIS	-	expression tag	UNP Q60I25
A	-6	HIS	-	expression tag	UNP Q60I25
A	-5	HIS	-	expression tag	UNP Q60I25
A	-4	HIS	-	expression tag	UNP Q60I25
A	-3	HIS	-	expression tag	UNP Q60I25
A	-2	SER	-	expression tag	UNP Q60I25
A	-1	GLN	-	expression tag	UNP Q60I25
A	0	MET	-	expression tag	UNP Q60I25
A	1	VAL	-	expression tag	UNP Q60I25
A	64	CRQ	GLN	chromophore	UNP Q60I25
A	64	CRQ	TYR	chromophore	UNP Q60I25
A	64	CRQ	GLY	chromophore	UNP Q60I25
A	119	THR	ARG	engineered mutation	UNP Q60I25
A	121	THR	ASP	engineered mutation	UNP Q60I25
A	123	THR	VAL	engineered mutation	UNP Q60I25
B	-12	MET	-	initiating methionine	UNP Q60I25

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	GLY	-	expression tag	UNP Q60I25
B	-10	SER	-	expression tag	UNP Q60I25
B	-9	SER	-	expression tag	UNP Q60I25
B	-8	HIS	-	expression tag	UNP Q60I25
B	-7	HIS	-	expression tag	UNP Q60I25
B	-6	HIS	-	expression tag	UNP Q60I25
B	-5	HIS	-	expression tag	UNP Q60I25
B	-4	HIS	-	expression tag	UNP Q60I25
B	-3	HIS	-	expression tag	UNP Q60I25
B	-2	SER	-	expression tag	UNP Q60I25
B	-1	GLN	-	expression tag	UNP Q60I25
B	0	MET	-	expression tag	UNP Q60I25
B	1	VAL	-	expression tag	UNP Q60I25
B	64	CRQ	GLN	chromophore	UNP Q60I25
B	64	CRQ	TYR	chromophore	UNP Q60I25
B	64	CRQ	GLY	chromophore	UNP Q60I25
B	119	THR	ARG	engineered mutation	UNP Q60I25
B	121	THR	ASP	engineered mutation	UNP Q60I25
B	123	THR	VAL	engineered mutation	UNP Q60I25
C	-12	MET	-	initiating methionine	UNP Q60I25
C	-11	GLY	-	expression tag	UNP Q60I25
C	-10	SER	-	expression tag	UNP Q60I25
C	-9	SER	-	expression tag	UNP Q60I25
C	-8	HIS	-	expression tag	UNP Q60I25
C	-7	HIS	-	expression tag	UNP Q60I25
C	-6	HIS	-	expression tag	UNP Q60I25
C	-5	HIS	-	expression tag	UNP Q60I25
C	-4	HIS	-	expression tag	UNP Q60I25
C	-3	HIS	-	expression tag	UNP Q60I25
C	-2	SER	-	expression tag	UNP Q60I25
C	-1	GLN	-	expression tag	UNP Q60I25
C	0	MET	-	expression tag	UNP Q60I25
C	1	VAL	-	expression tag	UNP Q60I25
C	64	CRQ	GLN	chromophore	UNP Q60I25
C	64	CRQ	TYR	chromophore	UNP Q60I25
C	64	CRQ	GLY	chromophore	UNP Q60I25
C	119	THR	ARG	engineered mutation	UNP Q60I25
C	121	THR	ASP	engineered mutation	UNP Q60I25
C	123	THR	VAL	engineered mutation	UNP Q60I25
D	-12	MET	-	initiating methionine	UNP Q60I25
D	-11	GLY	-	expression tag	UNP Q60I25
D	-10	SER	-	expression tag	UNP Q60I25

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	SER	-	expression tag	UNP Q60I25
D	-8	HIS	-	expression tag	UNP Q60I25
D	-7	HIS	-	expression tag	UNP Q60I25
D	-6	HIS	-	expression tag	UNP Q60I25
D	-5	HIS	-	expression tag	UNP Q60I25
D	-4	HIS	-	expression tag	UNP Q60I25
D	-3	HIS	-	expression tag	UNP Q60I25
D	-2	SER	-	expression tag	UNP Q60I25
D	-1	GLN	-	expression tag	UNP Q60I25
D	0	MET	-	expression tag	UNP Q60I25
D	1	VAL	-	expression tag	UNP Q60I25
D	64	CRQ	GLN	chromophore	UNP Q60I25
D	64	CRQ	TYR	chromophore	UNP Q60I25
D	64	CRQ	GLY	chromophore	UNP Q60I25
D	119	THR	ARG	engineered mutation	UNP Q60I25
D	121	THR	ASP	engineered mutation	UNP Q60I25
D	123	THR	VAL	engineered mutation	UNP Q60I25

- Molecule 2 is water.

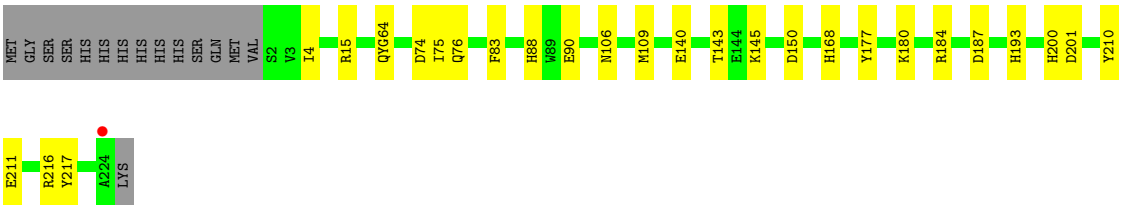
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	113	113	113	0	0
			Total	O		
2	B	116	116	116	0	0
			Total	O		
2	C	110	110	110	0	0
			Total	O		
2	D	104	104	104	0	0

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.

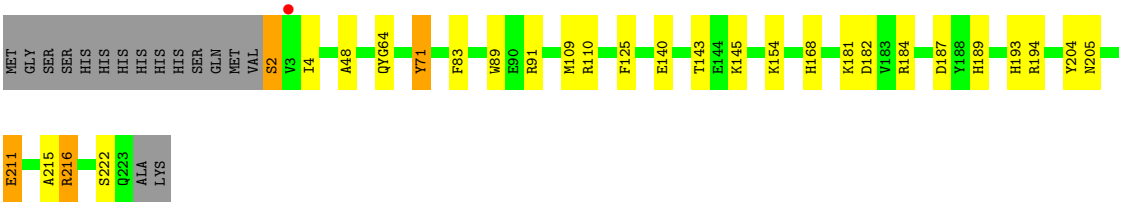
• Molecule 1: Azami-Green

Chain A: 82% 11% 6%



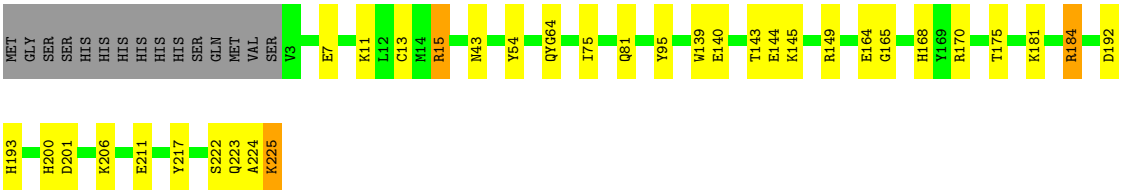
• Molecule 1: Azami-Green

Chain B: 81% 11% • 7%



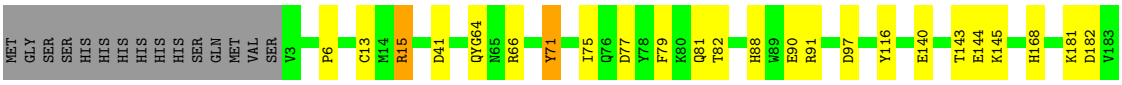
• Molecule 1: Azami-Green

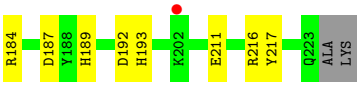
Chain C: 79% 13% • 6%



• Molecule 1: Azami-Green

Chain D: 79% 13% • 7%




R184
D187
Y188
H189
D192
H193
K202
E211
R216
Y217
Q223
ALA
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.50Å 86.18Å 141.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.64 – 1.70 43.24 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.2 (73.64-1.70) 96.3 (43.24-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.165 , 0.205 0.180 , 0.215	Depositor DCC
R_{free} test set	4570 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 36.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7642	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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 (i)

5.1 Standard geometry (i)

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	1.28	1/1825 (0.1%)	1.24	6/2465 (0.2%)
1	B	1.38	5/1820 (0.3%)	1.27	10/2458 (0.4%)
1	C	1.34	5/1828 (0.3%)	1.24	12/2468 (0.5%)
1	D	1.33	1/1814 (0.1%)	1.26	13/2450 (0.5%)
All	All	1.33	12/7287 (0.2%)	1.25	41/9841 (0.4%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	54	TYR	CE1-CZ	7.40	1.48	1.38
1	C	139	TRP	CE3-CZ3	5.73	1.48	1.38
1	B	71	TYR	CB-CG	5.73	1.60	1.51
1	C	165	GLY	N-CA	5.68	1.54	1.46
1	C	175	THR	C-O	5.67	1.34	1.23
1	D	71	TYR	CE1-CZ	-5.64	1.31	1.38
1	B	89	TRP	CZ3-CH2	5.50	1.48	1.40
1	B	125	PHE	CG-CD1	5.47	1.47	1.38
1	A	177	TYR	CG-CD1	5.36	1.46	1.39
1	B	204	TYR	CE1-CZ	-5.17	1.31	1.38
1	B	2	SER	CA-CB	5.12	1.60	1.52
1	C	7	GLU	CD-OE1	-5.05	1.20	1.25

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	216	ARG	NE-CZ-NH1	10.69	125.64	120.30
1	A	216	ARG	NE-CZ-NH2	9.53	125.06	120.30
1	D	192	ASP	CB-CG-OD1	8.11	125.60	118.30
1	B	110	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	C	164	GLU	OE1-CD-OE2	7.52	132.32	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	15	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	D	97	ASP	CB-CG-OD1	7.39	124.95	118.30
1	D	216	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	B	182	ASP	CB-CG-OD1	6.82	124.43	118.30
1	D	77	ASP	CB-CG-OD1	6.69	124.32	118.30
1	B	91	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	D	182	ASP	CB-CG-OD1	6.25	123.93	118.30
1	C	164	GLU	C-N-CA	-6.25	109.18	122.30
1	B	2	SER	CB-CA-C	6.22	121.91	110.10
1	B	211	GLU	OE1-CD-OE2	-6.12	115.95	123.30
1	D	66	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	C	149	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	D	15	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	C	15	ARG	CG-CD-NE	-5.94	99.32	111.80
1	C	15	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	D	216	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	74	ASP	CB-CG-OD1	5.86	123.57	118.30
1	C	170	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	C	184	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	B	184	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	216	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	D	41	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	184	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	B	222	SER	N-CA-CB	-5.55	102.17	110.50
1	D	181	LYS	CD-CE-NZ	-5.38	99.33	111.70
1	A	150	ASP	CB-CG-OD2	5.35	123.12	118.30
1	D	91	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	C	192	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	187	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	C	224	ALA	C-N-CA	5.25	134.83	121.70
1	B	194	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	164	GLU	CG-CD-OE2	-5.21	107.88	118.30
1	D	116	TYR	CB-CG-CD1	5.19	124.11	121.00
1	D	66	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	C	225	LYS	CB-CG-CD	5.16	125.02	111.60
1	C	95	TYR	CB-CG-CD1	5.02	124.01	121.00

There are no chirality outliers.

There are no planarity outliers.

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	1803	0	1745	17	0
1	B	1798	0	1739	18	0
1	C	1806	0	1752	16	0
1	D	1792	0	1734	17	0
2	A	113	0	0	2	0
2	B	116	0	0	6	0
2	C	110	0	0	1	0
2	D	104	0	0	2	0
All	All	7642	0	6970	63	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 (63) 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:D:140:GLU:OE2	1:D:168:HIS:HE1	1.67	0.78
1:A:106:ASN:HD21	1:A:180:LYS:NZ	1.81	0.77
1:A:106:ASN:HD21	1:A:180:LYS:HZ1	1.33	0.74
2:A:349:HOH:O	1:C:168:HIS:HD2	1.71	0.74
1:A:168:HIS:HD2	2:C:338:HOH:O	1.73	0.71
1:A:193:HIS:HD2	1:A:211:GLU:OE2	1.75	0.69
1:B:140:GLU:OE2	1:B:168:HIS:HE1	1.76	0.69
1:A:140:GLU:OE2	1:A:168:HIS:HE1	1.76	0.69
1:C:193:HIS:HD2	1:C:211:GLU:OE1	1.77	0.68
1:B:168:HIS:HD2	2:D:330:HOH:O	1.77	0.68
1:A:88:HIS:HD2	2:A:378:HOH:O	1.75	0.67
1:D:13:CYS:SG	1:D:15:ARG:NH1	2.68	0.67
1:C:140:GLU:OE2	1:C:168:HIS:HE1	1.77	0.67
1:D:88:HIS:HD2	2:D:372:HOH:O	1.78	0.67
1:B:181:LYS:HG2	2:B:389:HOH:O	1.95	0.65
1:D:81:GLN:HE22	1:D:184:ARG:H	1.45	0.65
1:C:81:GLN:HE22	1:C:184:ARG:H	1.45	0.63
1:D:88:HIS:HE1	1:D:90:GLU:OE2	1.83	0.61
1:D:193:HIS:HD2	1:D:211:GLU:OE2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:HIS:HE1	1:A:90:GLU:OE2	1.86	0.59
1:B:215:ALA:HB1	2:B:304:HOH:O	2.01	0.58
1:A:200:HIS:HD2	1:A:201:ASP:O	1.84	0.58
1:B:4:ILE:CD1	1:B:109:MET:HE1	2.34	0.58
1:B:193:HIS:HD2	1:B:211:GLU:OE2	1.87	0.58
2:B:310:HOH:O	1:D:168:HIS:HD2	1.86	0.57
1:D:187:ASP:O	1:D:189:HIS:HD2	1.88	0.57
1:C:43:ASN:OD1	1:C:206:LYS:HG2	2.05	0.56
1:A:210:TYR:CE2	1:C:223:GLN:HG3	2.41	0.55
1:B:187:ASP:O	1:B:189:HIS:HD2	1.88	0.55
1:B:4:ILE:CD1	1:B:109:MET:CE	2.85	0.55
1:A:76:GLN:NE2	1:A:184:ARG:HE	2.05	0.55
1:B:4:ILE:HD11	1:B:109:MET:HE1	1.90	0.53
1:C:144:GLU:OE1	1:C:193:HIS:HE1	1.91	0.53
1:C:222:SER:O	1:C:225:LYS:CE	2.56	0.53
1:A:4:ILE:HD13	1:A:109:MET:HE2	1.89	0.52
1:A:76:GLN:HE22	1:A:184:ARG:HE	1.58	0.52
1:B:154:LYS:HD3	2:B:331:HOH:O	2.11	0.51
1:A:75:ILE:HG12	1:A:217:TYR:CZ	2.48	0.48
1:D:79:PHE:O	1:D:82:THR:HG22	2.14	0.48
1:A:83:PHE:HB3	1:A:109:MET:HE1	1.95	0.47
1:C:144:GLU:OE1	1:C:193:HIS:CE1	2.67	0.47
1:B:4:ILE:HD13	1:B:109:MET:CE	2.45	0.47
1:B:143:THR:H	1:D:145:LYS:HZ1	1.63	0.46
1:C:222:SER:OG	1:C:225:LYS:HG3	2.16	0.46
1:D:81:GLN:NE2	1:D:184:ARG:H	2.11	0.45
1:D:144:GLU:OE1	1:D:193:HIS:HE1	1.99	0.45
1:A:4:ILE:HD13	1:A:109:MET:CE	2.46	0.45
1:C:75:ILE:HG12	1:C:217:TYR:CZ	2.51	0.45
1:A:143:THR:H	1:C:145:LYS:NZ	2.15	0.44
1:C:200:HIS:HD2	1:C:201:ASP:O	2.01	0.44
1:B:216:ARG:N	2:B:304:HOH:O	2.50	0.44
1:D:140:GLU:OE2	1:D:168:HIS:CE1	2.59	0.43
1:D:71:TYR:OH	1:D:189:HIS:HE1	2.02	0.43
1:D:144:GLU:OE1	1:D:193:HIS:CE1	2.72	0.43
1:B:181:LYS:CG	2:B:389:HOH:O	2.60	0.43
1:C:81:GLN:NE2	1:C:184:ARG:H	2.15	0.42
1:B:48:ALA:HB1	1:B:205:ASN:HD21	1.84	0.42
1:D:75:ILE:HG12	1:D:217:TYR:CZ	2.55	0.42
1:A:145:LYS:HZ1	1:C:143:THR:H	1.68	0.41
1:B:83:PHE:HB3	1:B:109:MET:HE1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:CYS:SG	1:C:15:ARG:NH1	2.94	0.40
1:B:71:TYR:OH	1:B:189:HIS:HE1	2.04	0.40
1:B:145:LYS:NZ	1:D:143:THR:H	2.19	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	216/236 (92%)	215 (100%)	1 (0%)	0	100	100
1	B	215/236 (91%)	215 (100%)	0	0	100	100
1	C	216/236 (92%)	215 (100%)	1 (0%)	0	100	100
1	D	214/236 (91%)	214 (100%)	0	0	100	100
All	All	861/944 (91%)	859 (100%)	2 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	193/207 (93%)	193 (100%)	0	100	100
1	B	193/207 (93%)	192 (100%)	1 (0%)	88	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	193/207 (93%)	191 (99%)	2 (1%)	76	67
1	D	192/207 (93%)	191 (100%)	1 (0%)	88	83
All	All	771/828 (93%)	767 (100%)	4 (0%)	88	83

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2	SER
1	C	11	LYS
1	C	181	LYS
1	D	6	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	76	GLN
1	A	88	HIS
1	A	106	ASN
1	A	133	GLN
1	A	168	HIS
1	A	193	HIS
1	A	200	HIS
1	B	38	GLN
1	B	43	ASN
1	B	88	HIS
1	B	168	HIS
1	B	189	HIS
1	B	193	HIS
1	B	205	ASN
1	C	38	GLN
1	C	81	GLN
1	C	106	ASN
1	C	128	ASN
1	C	133	GLN
1	C	168	HIS
1	C	193	HIS
1	C	200	HIS
1	D	19	ASN
1	D	32	ASN

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Mol	Chain	Res	Type
1	D	81	GLN
1	D	88	HIS
1	D	158	ASN
1	D	168	HIS
1	D	189	HIS
1	D	193	HIS
1	D	205	ASN
1	D	223	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	C	64	1	24,25,26	2.76	8 (33%)	27,34,36	2.37	6 (22%)
1	CRQ	D	64	1	24,25,26	2.11	5 (20%)	27,34,36	1.81	6 (22%)
1	CRQ	B	64	1	24,25,26	3.18	7 (29%)	27,34,36	3.29	7 (25%)
1	CRQ	A	64	1	24,25,26	2.52	5 (20%)	27,34,36	3.38	6 (22%)

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	C	64	1	-	1/10/32/33	0/2/2/2
1	CRQ	D	64	1	-	1/10/32/33	0/2/2/2
1	CRQ	B	64	1	-	1/10/32/33	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CRQ	A	64	1	-	0/10/32/33	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	CRQ	CB2-CA2	10.98	1.44	1.35
1	C	64	CRQ	CB2-CA2	9.47	1.43	1.35
1	D	64	CRQ	CB2-CA2	7.72	1.41	1.35
1	B	64	CRQ	CA2-C2	-7.15	1.41	1.48
1	A	64	CRQ	CA2-C2	-7.09	1.41	1.48
1	A	64	CRQ	CB2-CA2	6.03	1.40	1.35
1	A	64	CRQ	CA1-N1	5.58	1.41	1.27
1	C	64	CRQ	CA2-C2	-5.46	1.43	1.48
1	B	64	CRQ	C2-N3	-3.86	1.30	1.39
1	A	64	CRQ	C2-N3	-3.83	1.30	1.39
1	D	64	CRQ	O2-C2	3.59	1.30	1.23
1	C	64	CRQ	C1-N3	-3.55	1.32	1.38
1	B	64	CRQ	O2-C2	3.52	1.30	1.23
1	B	64	CRQ	CE2-CZ	-3.44	1.32	1.38
1	D	64	CRQ	CA2-C2	-3.23	1.45	1.48
1	B	64	CRQ	CA1-N1	3.21	1.35	1.27
1	B	64	CRQ	CD2-CG2	-3.19	1.33	1.39
1	A	64	CRQ	O2-C2	2.77	1.28	1.23
1	C	64	CRQ	C2-N3	-2.73	1.33	1.39
1	C	64	CRQ	CG2-CB2	-2.67	1.41	1.46
1	C	64	CRQ	O2-C2	2.63	1.28	1.23
1	C	64	CRQ	CE2-CZ	2.43	1.43	1.38
1	D	64	CRQ	C1-N3	-2.19	1.34	1.38
1	C	64	CRQ	CA1-N1	2.18	1.32	1.27
1	D	64	CRQ	CA1-N1	2.00	1.32	1.27

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	64	CRQ	O2-C2-CA2	-11.99	124.23	130.96
1	A	64	CRQ	CA2-C2-N3	10.62	108.39	103.37
1	B	64	CRQ	CA2-C2-N3	9.54	107.88	103.37
1	B	64	CRQ	O2-C2-CA2	-9.42	125.67	130.96
1	C	64	CRQ	O2-C2-CA2	-7.69	126.64	130.96
1	D	64	CRQ	O2-C2-CA2	-6.17	127.49	130.96
1	B	64	CRQ	CD1-CE1-CZ	-5.81	113.50	119.88
1	B	64	CRQ	CD2-CE2-CZ	5.54	125.95	119.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	64	CRQ	CA2-C2-N3	5.51	105.98	103.37
1	B	64	CRQ	CE2-CD2-CG2	-4.04	115.99	121.25
1	C	64	CRQ	CE2-CZ-CE1	-3.45	113.95	119.77
1	D	64	CRQ	CD2-CE2-CZ	3.26	123.45	119.88
1	A	64	CRQ	CG2-CB2-CA2	3.06	133.70	129.94
1	C	64	CRQ	CD1-CE1-CZ	2.98	123.14	119.88
1	A	64	CRQ	CB2-CA2-N2	-2.92	124.78	128.83
1	D	64	CRQ	O3-C3-CA3	-2.79	117.98	126.39
1	D	64	CRQ	CE2-CD2-CG2	-2.63	117.82	121.25
1	C	64	CRQ	O3-C3-CA3	-2.62	118.47	126.39
1	B	64	CRQ	N3-C1-N2	-2.62	109.82	113.28
1	D	64	CRQ	CA2-C2-N3	2.53	104.57	103.37
1	C	64	CRQ	CB2-CA2-N2	-2.34	125.58	128.83
1	A	64	CRQ	CB2-CA2-C2	2.25	124.96	122.28
1	A	64	CRQ	CD2-CE2-CZ	2.20	122.29	119.88
1	D	64	CRQ	CB2-CA2-C2	-2.13	119.73	122.28
1	B	64	CRQ	CA3-N3-C1	-2.07	124.16	128.22

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	64	CRQ	C3-CA3-N3-C2
1	D	64	CRQ	C3-CA3-N3-C2
1	C	64	CRQ	N2-CA2-CB2-CG2

There are no ring outliers.

No monomer is involved in short contacts.

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)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	220/236 (93%)	-0.16	1 (0%)	91	92	18, 26, 43, 61	0
1	B	219/236 (92%)	-0.07	1 (0%)	91	92	19, 29, 48, 64	0
1	C	220/236 (93%)	-0.14	0	100	100	17, 26, 44, 65	0
1	D	218/236 (92%)	0.02	1 (0%)	91	92	20, 31, 54, 69	0
All	All	877/944 (92%)	-0.09	3 (0%)	94	94	17, 28, 48, 69	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	VAL	3.0
1	D	202	LYS	2.2
1	A	224	ALA	2.2

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CRQ	D	64	24/25	0.94	0.09	22,25,30,33	0
1	CRQ	B	64	24/25	0.96	0.08	20,21,27,29	0
1	CRQ	C	64	24/25	0.96	0.07	16,18,22,24	0
1	CRQ	A	64	24/25	0.96	0.07	16,18,21,24	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.