



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 12:38 PM UTC

PDB ID : 6CIU / pdb_00006ciu
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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

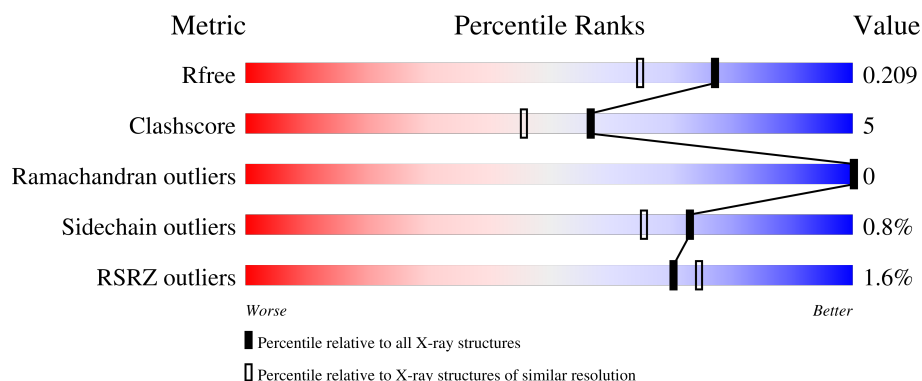
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 $\leq 5\%$. 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	236	
1	B	236	
1	C	236	
1	D	236	

2 Entry composition

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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.

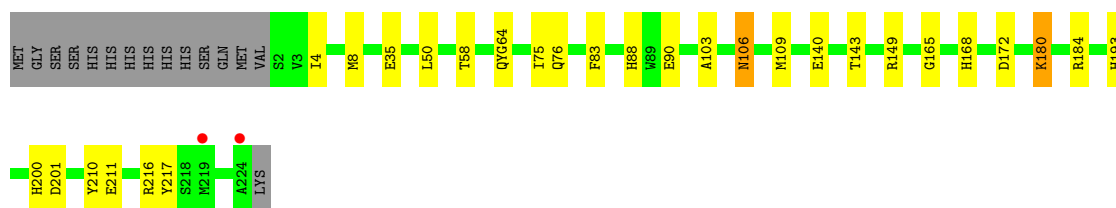
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	113	Total O 113 113	0	0
2	B	116	Total O 116 116	0	0
2	C	110	Total O 110 110	0	0
2	D	104	Total O 104 104	0	0

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.

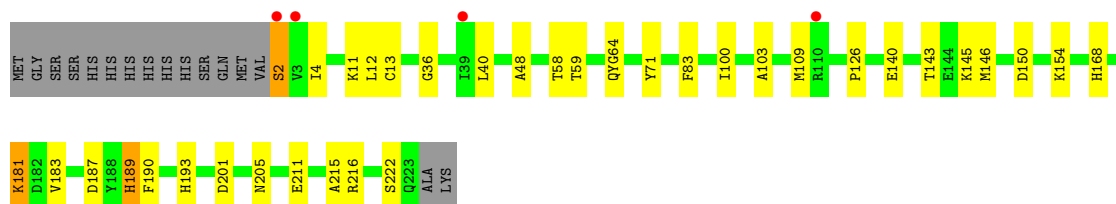
- Molecule 1: Azami-Green

Chain A: 



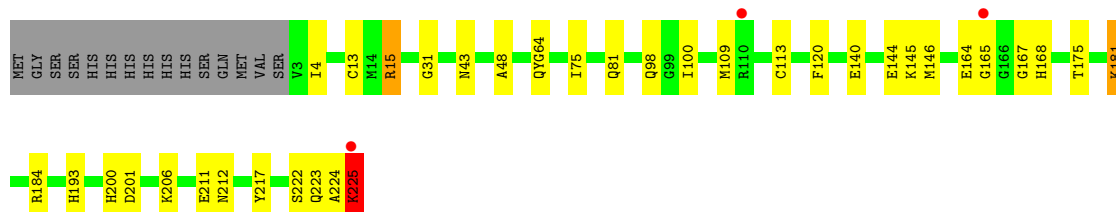
- Molecule 1: Azami-Green

Chain B: 



- Molecule 1: Azami-Green

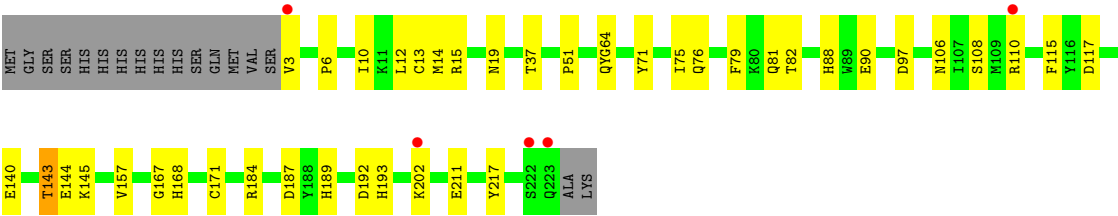
Chain C: 



- Molecule 1: Azami-Green

Chain D: 





4 Data and refinement statistics

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 73.64 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.2 (73.64-1.70) 96.3 (73.64-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.165 , 0.205 0.173 , 0.209	Depositor DCC
R_{free} test set	4570 reflections (4.81%)	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 , 28.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

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	1.61	6/1825 (0.3%)	1.32	4/2465 (0.2%)
1	B	1.73	16/1820 (0.9%)	1.36	5/2458 (0.2%)
1	C	1.65	14/1828 (0.8%)	1.35	7/2468 (0.3%)
1	D	1.70	16/1814 (0.9%)	1.33	3/2450 (0.1%)
All	All	1.67	52/7287 (0.7%)	1.34	19/9841 (0.2%)

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	175	THR	C-O	7.92	1.34	1.24
1	B	146	MET	SD-CE	-7.63	1.60	1.79
1	B	103	ALA	C-O	7.37	1.32	1.23
1	D	192	ASP	CA-C	-7.28	1.43	1.52
1	D	10	ILE	N-CA	7.18	1.54	1.46
1	D	51	PRO	CA-C	7.07	1.59	1.52
1	C	100	ILE	C-O	6.62	1.31	1.24
1	A	172	ASP	C-O	-6.62	1.16	1.24
1	D	157	VAL	C-O	6.60	1.30	1.23
1	B	11	LYS	CA-C	6.34	1.60	1.52
1	C	167	GLY	N-CA	6.33	1.53	1.45
1	B	190	PHE	CA-C	-6.22	1.44	1.52
1	A	50	LEU	N-CA	6.14	1.54	1.45
1	C	165	GLY	N-CA	6.10	1.54	1.44
1	D	117	ASP	CA-C	6.07	1.60	1.52
1	C	164	GLU	N-CA	6.01	1.53	1.46
1	D	108	SER	N-CA	5.92	1.54	1.46
1	C	120	PHE	N-CA	5.91	1.53	1.46
1	D	97	ASP	N-CA	5.88	1.52	1.46
1	B	13	CYS	CA-C	5.76	1.59	1.52
1	D	37	THR	CA-C	-5.71	1.45	1.52
1	A	103	ALA	CA-C	-5.71	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	212	ASN	C-O	-5.71	1.17	1.24
1	C	31	GLY	C-O	-5.61	1.17	1.23
1	A	106	ASN	CG-ND2	-5.58	1.21	1.33
1	D	115	PHE	N-CA	-5.56	1.39	1.46
1	B	189	HIS	CA-C	-5.56	1.46	1.52
1	C	4	ILE	CA-CB	5.56	1.60	1.53
1	B	103	ALA	N-CA	-5.52	1.39	1.45
1	D	19	ASN	CG-OD1	5.51	1.34	1.23
1	D	10	ILE	CA-C	-5.50	1.45	1.52
1	B	12	LEU	N-CA	5.42	1.52	1.45
1	B	12	LEU	CA-C	-5.39	1.46	1.52
1	D	14	MET	N-CA	5.38	1.52	1.46
1	B	100	ILE	C-O	5.35	1.29	1.24
1	C	113	CYS	N-CA	5.30	1.52	1.46
1	C	109	MET	CA-C	5.29	1.58	1.52
1	C	146	MET	CA-C	5.24	1.59	1.52
1	A	35	GLU	N-CA	5.24	1.53	1.46
1	B	150	ASP	C-O	-5.16	1.17	1.23
1	D	76	GLN	C-O	5.14	1.30	1.23
1	B	183	VAL	C-O	-5.10	1.18	1.23
1	D	106	ASN	C-O	5.07	1.30	1.24
1	B	126	PRO	C-O	-5.06	1.18	1.24
1	A	180	LYS	N-CA	5.06	1.52	1.46
1	B	40	LEU	CA-C	-5.06	1.46	1.52
1	C	48	ALA	C-O	5.04	1.30	1.23
1	D	171	CYS	C-O	-5.04	1.18	1.23
1	B	36	GLY	CA-C	-5.04	1.44	1.51
1	B	201	ASP	N-CA	5.01	1.52	1.45
1	C	181	LYS	CA-CB	-5.01	1.45	1.54
1	D	143	THR	CA-C	5.00	1.58	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	GLU	CA-C-N	-9.37	109.18	122.86
1	C	164	GLU	C-N-CA	-9.37	109.18	122.86
1	C	224	ALA	CA-C-N	7.29	134.83	121.70
1	C	224	ALA	C-N-CA	7.29	134.83	121.70
1	B	58	THR	N-CA-C	7.25	119.19	111.28
1	A	165	GLY	N-CA-C	-6.57	106.09	114.37
1	A	216	ARG	NE-CZ-NH2	6.51	125.06	119.20
1	A	58	THR	N-CA-C	6.40	118.26	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2	SER	CB-CA-C	6.22	121.91	110.10
1	C	225	LYS	CB-CG-CD	5.96	125.02	111.30
1	C	15	ARG	CG-CD-NE	-5.76	99.32	112.00
1	D	202	LYS	CB-CG-CD	5.63	124.25	111.30
1	B	59	THR	N-CA-C	-5.44	106.59	113.18
1	B	181	LYS	CB-CG-CD	5.27	123.43	111.30
1	C	164	GLU	O-C-N	-5.26	116.74	123.06
1	D	110	ARG	CB-CG-CD	5.23	123.33	111.30
1	D	167	GLY	N-CA-C	-5.15	106.19	112.68
1	A	149	ARG	CA-CB-CG	-5.06	103.97	114.10
1	B	222	SER	N-CA-CB	-5.06	102.17	110.52

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	1803	0	1745	18	0
1	B	1798	0	1739	18	0
1	C	1806	0	1752	15	0
1	D	1792	0	1734	18	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	65	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 5.

All (65) 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:B:4:ILE:CD1	1:B:109:MET:HE1	2.08	0.83

Continued on next page...

Continued from previous page...

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:B:4:ILE:HD13	1:B:109:MET:HE1	1.65	0.76
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:A:4:ILE:HD13	1:A:109:MET:HE1	1.82	0.60
1:D:193:HIS:HD2	1:D:211:GLU:OE2	1.84	0.60
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:193:HIS:HD2	1:B:211:GLU:OE2	1.87	0.58
1:B:4:ILE:HD11	1:B:109:MET:HE1	1.85	0.58
1:B:83:PHE:CD1	1:B:109:MET:HE3	2.40	0.57
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:A:76:GLN:NE2	1:A:184:ARG:HE	2.05	0.55
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: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:B:4:ILE:CD1	1:B:109:MET:CE	2.85	0.50
1:A:83:PHE:CD1	1:A:109:MET:HE3	2.46	0.50
1:A:8:MET:HE2	1:A:109:MET:HE2	1.93	0.50
1:A:4:ILE:CD1	1:A:109:MET:HE1	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:144:GLU:OE1	1:C:193:HIS:CE1	2.67	0.47
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: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:A:4:ILE:HD13	1:A:109:MET:CE	2.46	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:12:LEU:C	1:D:12:LEU:HD12	2.43	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:B:143:THR:H	1:D:145:LYS:HZ1	1.66	0.42
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: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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	81	76
1	C	193/207 (93%)	190 (98%)	3 (2%)	55	41
1	D	192/207 (93%)	190 (99%)	2 (1%)	68	58
All	All	771/828 (93%)	765 (99%)	6 (1%)	73	65

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2	SER
1	C	98	GLN
1	C	181	LYS
1	C	225	LYS
1	D	3	VAL
1	D	6	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	76	GLN
1	A	88	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	106	ASN
1	A	128	ASN
1	A	133	GLN
1	A	158	ASN
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	81	GLN
1	C	106	ASN
1	C	128	ASN
1	C	133	GLN
1	C	158	ASN
1	C	168	HIS
1	C	193	HIS
1	C	200	HIS
1	D	19	ASN
1	D	81	GLN
1	D	88	HIS
1	D	128	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 ⓘ

There are no RNA molecules in this entry.

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

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	25,25,26	2.50	8 (32%)	28,34,36	2.21	8 (28%)
1	CRQ	D	64	1	25,25,26	1.93	4 (16%)	28,34,36	1.95	5 (17%)
1	CRQ	A	64	1	25,25,26	2.38	5 (20%)	28,34,36	2.83	7 (25%)
1	CRQ	B	64	1	25,25,26	2.89	7 (28%)	28,34,36	2.81	8 (28%)

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

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	CRQ	CB2-CA2	9.49	1.44	1.35
1	C	64	CRQ	CB2-CA2	8.18	1.43	1.35
1	D	64	CRQ	CB2-CA2	6.66	1.41	1.35
1	B	64	CRQ	CA2-C2	-6.45	1.41	1.48
1	A	64	CRQ	CA2-C2	-6.39	1.41	1.48
1	A	64	CRQ	CA1-N1	6.02	1.41	1.27
1	A	64	CRQ	CB2-CA2	5.18	1.40	1.35
1	C	64	CRQ	CA2-C2	-4.91	1.43	1.48
1	B	64	CRQ	C2-N3	-4.01	1.30	1.40
1	A	64	CRQ	C2-N3	-3.98	1.30	1.40
1	D	64	CRQ	O2-C2	3.74	1.30	1.23
1	B	64	CRQ	O2-C2	3.67	1.30	1.23
1	B	64	CRQ	CE2-CZ	-3.53	1.32	1.39
1	B	64	CRQ	CA1-N1	3.47	1.35	1.27
1	C	64	CRQ	C1-N3	-3.24	1.32	1.38
1	B	64	CRQ	CD2-CG2	-3.08	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	CRQ	O2-C2	2.88	1.28	1.23
1	D	64	CRQ	CA2-C2	-2.87	1.45	1.48
1	C	64	CRQ	C2-N3	-2.85	1.33	1.40
1	C	64	CRQ	CG2-CB2	-2.80	1.41	1.46
1	C	64	CRQ	O2-C2	2.74	1.28	1.23
1	C	64	CRQ	CE2-CZ	2.44	1.43	1.39
1	C	64	CRQ	CA1-N1	2.35	1.32	1.27
1	D	64	CRQ	CA1-N1	2.17	1.32	1.27

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	CRQ	O2-C2-CA2	-10.64	124.23	131.02
1	B	64	CRQ	O2-C2-CA2	-8.38	125.67	131.02
1	C	64	CRQ	O2-C2-CA2	-6.86	126.64	131.02
1	B	64	CRQ	CD1-CE1-CZ	-6.03	113.50	119.88
1	A	64	CRQ	CA2-C2-N3	5.82	108.39	103.50
1	D	64	CRQ	C3-CA3-N3	5.78	125.58	112.43
1	B	64	CRQ	CD2-CE2-CZ	5.74	125.95	119.88
1	D	64	CRQ	O2-C2-CA2	-5.53	127.49	131.02
1	B	64	CRQ	CA2-C2-N3	5.22	107.88	103.50
1	A	64	CRQ	C3-CA3-N3	4.86	123.49	112.43
1	C	64	CRQ	C3-CA3-N3	4.34	122.31	112.43
1	B	64	CRQ	CE2-CD2-CG2	-4.05	115.99	121.22
1	C	64	CRQ	CE2-CZ-CE1	-3.66	113.95	119.77
1	D	64	CRQ	CD2-CE2-CZ	3.37	123.45	119.88
1	A	64	CRQ	CG2-CB2-CA2	3.22	133.70	129.87
1	C	64	CRQ	CD1-CE1-CZ	3.09	123.14	119.88
1	B	64	CRQ	C3-CA3-N3	2.96	119.17	112.43
1	C	64	CRQ	CA2-C2-N3	2.95	105.98	103.50
1	A	64	CRQ	CB2-CA2-N2	-2.94	124.78	128.76
1	D	64	CRQ	CE2-CD2-CG2	-2.63	117.82	121.22
1	B	64	CRQ	N3-C1-N2	-2.36	109.82	112.62
1	C	64	CRQ	CB2-CA2-N2	-2.34	125.58	128.76
1	A	64	CRQ	CD2-CE2-CZ	2.28	122.29	119.88
1	C	64	CRQ	N3-C1-N2	2.25	115.29	112.62
1	D	64	CRQ	CB2-CA2-C2	-2.16	119.73	122.36
1	A	64	CRQ	CB2-CA2-C2	2.15	124.96	122.36
1	B	64	CRQ	CA3-N3-C1	-2.14	124.16	128.39
1	C	64	CRQ	CE2-CD2-CG2	2.02	123.83	121.22

There are no chirality outliers.

All (4) 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	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 oligosaccharides 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%)	-0.02	2 (0%) 81 83	18, 26, 43, 61	0
1	B	219/236 (92%)	0.15	4 (1%) 67 72	19, 29, 48, 64	0
1	C	220/236 (93%)	0.02	3 (1%) 73 77	17, 26, 44, 65	0
1	D	218/236 (92%)	0.34	5 (2%) 61 65	20, 31, 54, 69	0
All	All	877/944 (92%)	0.12	14 (1%) 70 75	17, 28, 48, 69	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	224	ALA	4.0
1	D	3	VAL	3.4
1	C	225	LYS	3.0
1	D	223	GLN	2.7
1	B	3	VAL	2.7
1	C	165	GLY	2.6
1	C	110	ARG	2.4
1	B	2	SER	2.3
1	B	39	ILE	2.3
1	D	202	LYS	2.1
1	D	110	ARG	2.0
1	A	219	MET	2.0
1	B	110	ARG	2.0
1	D	222	SER	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, 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($\text{\AA}^2$)	Q<0.9
1	CRQ	A	64	24/25	0.97	0.06	16,18,21,24	0
1	CRQ	B	64	24/25	0.97	0.06	20,21,27,29	0
1	CRQ	C	64	24/25	0.97	0.05	16,18,22,24	0
1	CRQ	D	64	24/25	0.97	0.06	22,25,30,33	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.