



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:22 PM UTC

PDB ID : 4PPL / pdb_00004ppl
Title : Crystal structure of eCGP123 H193Q variant at pH 7.5
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Deposited on : 2014-02-27
Resolution : 2.20 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

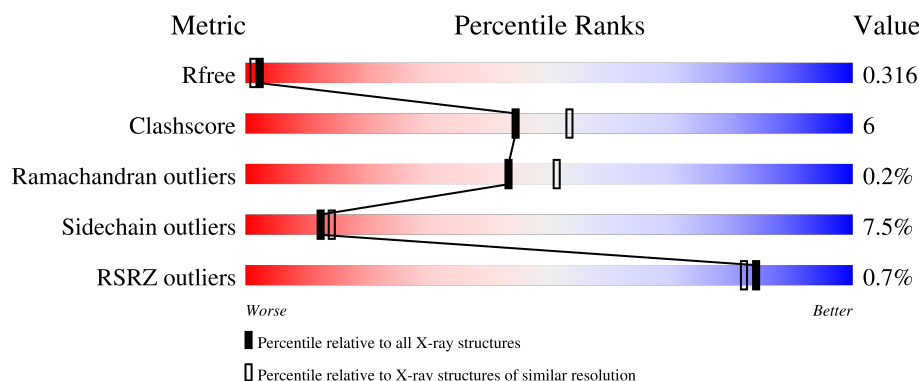
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	245	
1	B	245	
1	C	245	
1	D	245	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7853 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 Monomeric Azami Green.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	1	0
			1753	1124	291	328	10			
1	B	216	Total	C	N	O	S	3	1	0
			1770	1133	294	332	11			
1	C	215	Total	C	N	O	S	22	0	0
			1758	1127	292	328	11			
1	D	215	Total	C	N	O	S	85	0	0
			1758	1127	292	328	11			

- Molecule 2 is water.

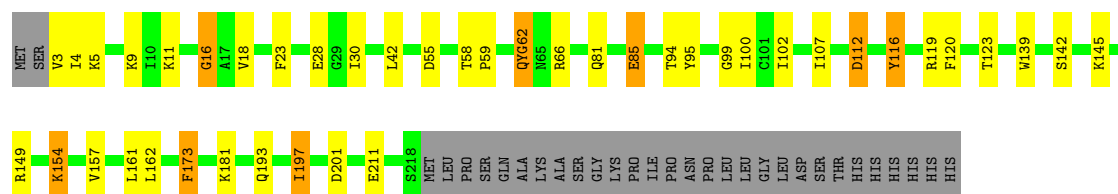
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	241	Total	O	0	0
			241	241		
2	B	203	Total	O	0	0
			203	203		
2	C	202	Total	O	0	0
			202	202		
2	D	168	Total	O	0	0
			168	168		

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.

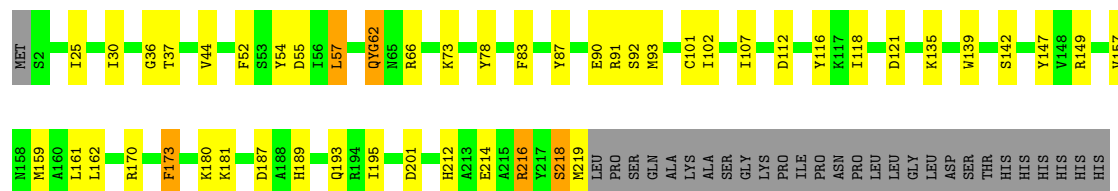
- Molecule 1: Monomeric Azami Green

Chain A: 



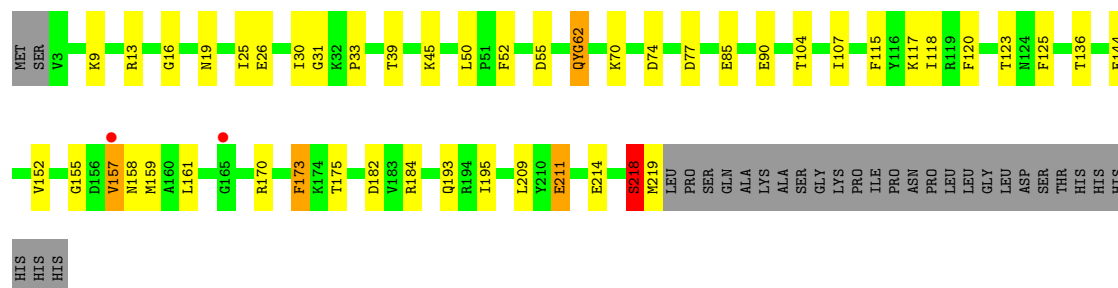
- Molecule 1: Monomeric Azami Green

Chain B: 



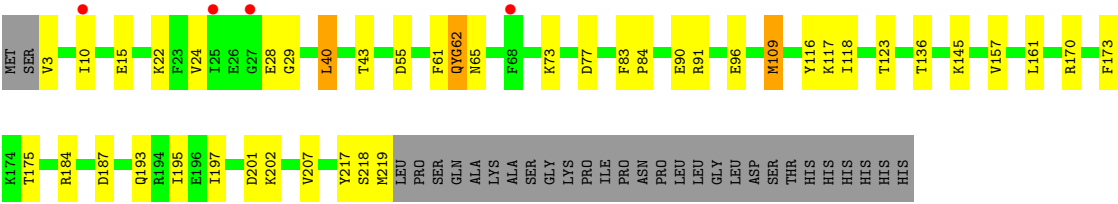
- Molecule 1: Monomeric Azami Green

Chain C: 



- Molecule 1: Monomeric Azami Green

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.56Å 83.39Å 74.65Å 90.00° 102.19° 90.00°	Depositor
Resolution (Å)	46.21 – 2.20 46.21 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.21-2.20) 99.1 (46.21-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.190 , 0.287 0.208 , 0.316	Depositor DCC
R_{free} test set	2195 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 113.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.046 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7853	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.89	1/1776 (0.1%)	1.25	6/2393 (0.3%)
1	B	0.90	2/1790 (0.1%)	1.30	12/2411 (0.5%)
1	C	0.79	0/1778	1.17	4/2395 (0.2%)
1	D	0.81	0/1778	1.23	7/2395 (0.3%)
All	All	0.85	3/7122 (0.0%)	1.24	29/9594 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	197	ILE	CG1-CD1	8.02	1.83	1.51
1	B	214	GLU	CA-C	5.76	1.59	1.52
1	B	91	ARG	CA-C	-5.01	1.46	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	PHE	CA-CB-CG	7.72	121.52	113.80
1	B	218	SER	CA-C-N	7.60	135.38	121.70
1	B	218	SER	C-N-CA	7.60	135.38	121.70
1	B	54	TYR	CA-C-N	7.60	130.79	120.38
1	B	54	TYR	C-N-CA	7.60	130.79	120.38
1	C	77	ASP	CA-C-N	6.44	128.91	120.28
1	C	77	ASP	C-N-CA	6.44	128.91	120.28
1	B	57	LEU	CA-C-N	6.16	127.42	119.78
1	B	57	LEU	C-N-CA	6.16	127.42	119.78
1	C	173	PHE	CA-CB-CG	6.13	119.93	113.80
1	D	77	ASP	CA-C-N	6.07	128.74	120.54
1	D	77	ASP	C-N-CA	6.07	128.74	120.54
1	D	65	ASN	CA-CB-CG	5.79	118.39	112.60
1	C	115	PHE	CA-CB-CG	5.58	119.38	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	29	GLY	CA-C-N	5.51	128.28	122.11
1	D	29	GLY	C-N-CA	5.51	128.28	122.11
1	A	201	ASP	CA-C-N	5.50	129.08	120.82
1	A	201	ASP	C-N-CA	5.50	129.08	120.82
1	A	142	SER	N-CA-C	5.46	117.09	108.96
1	D	201	ASP	CA-CB-CG	5.40	118.00	112.60
1	B	142	SER	N-CA-C	5.34	117.52	109.41
1	B	78	TYR	CA-C-N	5.23	127.72	120.29
1	B	78	TYR	C-N-CA	5.23	127.72	120.29
1	A	112	ASP	CA-CB-CG	5.21	117.81	112.60
1	D	61	PHE	CA-CB-CG	5.12	118.92	113.80
1	A	16	GLY	N-CA-C	5.10	117.99	110.80
1	A	173	PHE	CA-CB-CG	5.07	118.87	113.80
1	B	83	PHE	CA-CB-CG	-5.04	108.76	113.80
1	B	112	ASP	CA-CB-CG	5.03	117.63	112.60

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	1753	0	1703	26	0
1	B	1770	0	1716	21	0
1	C	1758	0	1707	25	0
1	D	1758	0	1707	16	0
2	A	241	0	0	0	0
2	B	203	0	0	0	0
2	C	202	0	0	3	0
2	D	168	0	0	0	0
All	All	7853	0	6833	81	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 (81) 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:A:197:ILE:CG1	1:A:197:ILE:CD1	1.83	1.56
1:A:100:ILE:HD11	1:B:92:SER:HB2	1.56	0.85
1:D:3:VAL:HG21	1:D:84:PRO:HG3	1.71	0.70
1:B:25:ILE:HG12	1:B:44:VAL:HG22	1.79	0.65
1:A:102:ILE:HG12	1:B:102:ILE:HD11	1.80	0.64
1:A:62:CRQ:HD1	1:A:62:CRQ:N2	2.12	0.64
1:C:19:ASN:HD21	1:C:125:PHE:HB2	1.64	0.62
1:C:70:LYS:HB3	1:C:214:GLU:HG3	1.84	0.60
1:C:62:CRQ:N2	1:C:62:CRQ:HD1	2.18	0.58
1:A:55:ASP:HB3	1:A:161:LEU:HD21	1.85	0.58
1:A:123:THR:OG1	1:B:90:GLU:HB3	2.03	0.58
1:A:197:ILE:CD1	1:A:197:ILE:CB	2.80	0.57
1:C:157:VAL:HG22	1:C:159:MET:HG2	1.87	0.57
1:D:62:CRQ:N2	1:D:62:CRQ:HD1	2.19	0.57
1:D:218:SER:N	1:D:219:MET:HA	2.19	0.56
1:C:144:GLU:OE2	1:C:155:GLY:HA3	2.06	0.56
1:D:157:VAL:HG13	1:D:173:PHE:HB2	1.88	0.56
1:D:96:GLU:HB3	1:D:170:ARG:HB2	1.87	0.55
1:C:158:ASN:HB3	1:C:170:ARG:HH21	1.71	0.55
1:A:100:ILE:CD1	1:B:92:SER:HB2	2.35	0.54
1:C:16:GLY:HA3	1:C:120:PHE:O	2.08	0.53
1:C:90:GLU:HG2	1:C:104:THR:HG22	1.89	0.53
1:D:83:PHE:CD1	1:D:109:MET:HG2	2.43	0.53
1:B:62:CRQ:N2	1:B:62:CRQ:HD1	2.23	0.52
1:A:16:GLY:HA3	1:A:120:PHE:O	2.09	0.52
1:A:102:ILE:HD11	1:B:121:ASP:HB3	1.92	0.51
1:A:58:THR:OG1	1:A:59:PRO:HD3	2.11	0.50
1:A:62:CRQ:OE1	1:A:211:GLU:HB2	2.12	0.49
1:B:139:TRP:CZ3	1:B:159:MET:HB3	2.47	0.49
1:B:218:SER:HA	1:B:219:MET:HB2	1.95	0.49
1:A:16:GLY:HA2	1:A:119:ARG:CZ	2.43	0.48
1:A:157:VAL:HG13	1:A:173:PHE:HB2	1.95	0.48
1:A:102:ILE:HD11	1:B:121:ASP:CB	2.43	0.48
1:B:157:VAL:HG13	1:B:173:PHE:HB2	1.96	0.48
1:C:157:VAL:HG13	1:C:173:PHE:HB2	1.95	0.48
1:A:95:TYR:HB2	1:A:99:GLY:O	2.15	0.47
1:B:62:CRQ:HE1	1:B:195:ILE:HB	1.97	0.47
1:C:13:ARG:HG3	1:C:26:GLU:HG2	1.97	0.47
1:D:84:PRO:HB3	1:D:109:MET:HE2	1.96	0.47
1:D:10:ILE:HG21	1:D:40:LEU:HD11	1.97	0.46
1:A:94:THR:HA	1:A:100:ILE:HG22	1.97	0.46
1:A:9:LYS:HG2	1:A:30:ILE:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:SER:HB3	1:C:219:MET:H	1.53	0.46
1:D:83:PHE:HD1	1:D:109:MET:HG2	1.82	0.45
1:A:107:ILE:HG12	1:A:116:TYR:CD1	2.51	0.45
1:B:147:TYR:HE2	1:B:149:ARG:HE	1.65	0.45
1:C:13:ARG:HG2	2:C:402:HOH:O	2.16	0.45
1:A:149:ARG:HD2	1:A:154:LYS:HE3	1.98	0.45
1:B:93:MET:HG2	1:B:173:PHE:CE1	2.52	0.45
1:A:3:VAL:HG13	1:A:4:ILE:HG12	2.00	0.44
1:D:62:CRQ:HE1	1:D:195:ILE:HB	1.99	0.44
1:D:91:ARG:HB2	1:D:175:THR:HG23	2.00	0.44
1:C:157:VAL:HG13	1:C:173:PHE:CB	2.47	0.44
1:B:189:HIS:HB2	1:B:216:ARG:O	2.18	0.44
1:B:36:GLY:O	1:B:212:HIS:HA	2.17	0.43
1:B:87:TYR:CZ	1:B:107:ILE:HD13	2.54	0.43
1:C:55:ASP:HB3	1:C:161:LEU:HD21	2.00	0.43
1:D:136:THR:HB	1:D:161:LEU:HD22	2.01	0.43
1:C:62:CRQ:CD3	1:C:211:GLU:HB2	2.49	0.42
1:C:136:THR:HB	1:C:161:LEU:HD22	2.01	0.42
1:D:217:TYR:HB3	1:D:219:MET:HA	2.02	0.42
1:B:55:ASP:HB3	1:B:161:LEU:HD21	2.02	0.42
1:C:31:GLY:O	1:C:33:PRO:HD3	2.20	0.42
1:B:52:PHE:HE1	1:B:57:LEU:HD11	1.84	0.42
1:A:66:ARG:NE	1:A:66:ARG:HA	2.35	0.42
1:C:107:ILE:HG23	2:C:464:HOH:O	2.19	0.41
1:C:62:CRQ:HB12	1:C:195:ILE:HD12	2.02	0.41
1:D:197:ILE:HG23	1:D:207:VAL:HG13	2.03	0.41
1:B:93:MET:HB2	1:B:101:CYS:HB2	2.02	0.41
1:A:5:LYS:HE2	1:A:112:ASP:HB3	2.01	0.41
1:D:15:GLU:HG3	1:D:24:VAL:HG22	2.02	0.41
1:A:85:GLU:H	1:A:85:GLU:HG2	1.63	0.41
1:A:18:VAL:HG23	1:A:23:PHE:HE2	1.86	0.41
1:B:66:ARG:HA	1:B:66:ARG:NE	2.36	0.41
1:C:62:CRQ:OE1	1:C:211:GLU:HB2	2.21	0.41
1:C:62:CRQ:OE1	1:C:209:LEU:HG	2.21	0.41
1:C:123:THR:OG1	1:D:90:GLU:HB3	2.21	0.40
1:C:170:ARG:HB3	1:C:170:ARG:NH1	2.36	0.40
1:A:139:TRP:CE3	1:A:161:LEU:HG	2.56	0.40
1:C:25:ILE:HG22	2:C:486:HOH:O	2.21	0.40
1:C:50:LEU:HD22	1:C:52:PHE:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	210/245 (86%)	208 (99%)	2 (1%)	0	100	100
1	B	212/245 (86%)	206 (97%)	6 (3%)	0	100	100
1	C	210/245 (86%)	201 (96%)	7 (3%)	2 (1%)	12	11
1	D	210/245 (86%)	204 (97%)	6 (3%)	0	100	100
All	All	842/980 (86%)	819 (97%)	21 (2%)	2 (0%)	43	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	218	SER
1	C	184	ARG

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	186/212 (88%)	175 (94%)	11 (6%)	18	22
1	B	188/212 (89%)	174 (93%)	14 (7%)	13	14
1	C	186/212 (88%)	171 (92%)	15 (8%)	11	12
1	D	186/212 (88%)	170 (91%)	16 (9%)	10	10
All	All	746/848 (88%)	690 (92%)	56 (8%)	12	14

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	28	GLU
1	A	42	LEU
1	A	81	GLN
1	A	85	GLU
1	A	116	TYR
1	A	145	LYS
1	A	154	LYS
1	A	162	LEU
1	A	181	LYS
1	A	193	GLN
1	B	30	ILE
1	B	37	THR
1	B	73	LYS
1	B	116	TYR
1	B	118	ILE
1	B	135	LYS
1	B	162	LEU
1	B	170	ARG
1	B	180	LYS
1	B	181	LYS
1	B	187	ASP
1	B	193	GLN
1	B	201	ASP
1	B	216	ARG
1	C	9	LYS
1	C	30	ILE
1	C	39	THR
1	C	45	LYS
1	C	74	ASP
1	C	85	GLU
1	C	117	LYS
1	C	118	ILE
1	C	152	VAL
1	C	157	VAL
1	C	175	THR
1	C	182	ASP
1	C	193	GLN
1	C	211	GLU
1	C	218	SER
1	D	22	LYS
1	D	28	GLU
1	D	40	LEU

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Mol	Chain	Res	Type
1	D	43	THR
1	D	55	ASP
1	D	73	LYS
1	D	109	MET
1	D	116	TYR
1	D	117	LYS
1	D	118	ILE
1	D	123	THR
1	D	145	LYS
1	D	184	ARG
1	D	187	ASP
1	D	193	GLN
1	D	202	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	GLN
1	B	65	ASN
1	B	205	ASN
1	C	19	ASN
1	C	65	ASN
1	C	205	ASN
1	D	19	ASN
1	D	38	GLN
1	D	65	ASN
1	D	98	GLN
1	D	158	ASN
1	D	193	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	B	62	1	25,25,26	3.81	6 (24%)	28,34,36	2.00	6 (21%)
1	CRQ	C	62	1	25,25,26	4.04	5 (20%)	28,34,36	2.66	8 (28%)
1	CRQ	A	62	1	25,25,26	4.00	6 (24%)	28,34,36	2.48	8 (28%)
1	CRQ	D	62	1	25,25,26	4.04	5 (20%)	28,34,36	2.59	9 (32%)

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	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	C	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	D	62	1	-	2/10/32/33	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	62	CRQ	CA2-C2	-11.14	1.36	1.48
1	D	62	CRQ	CA2-C2	-10.86	1.36	1.48
1	A	62	CRQ	CA2-C2	-10.83	1.36	1.48
1	D	62	CRQ	CA1-N1	10.36	1.50	1.27
1	C	62	CRQ	CA1-N1	10.24	1.50	1.27
1	A	62	CRQ	CA1-N1	10.23	1.50	1.27
1	B	62	CRQ	CA2-C2	-9.76	1.38	1.48
1	C	62	CRQ	CD3-NE1	-9.50	1.02	1.32
1	B	62	CRQ	CA1-N1	9.46	1.48	1.27
1	D	62	CRQ	CD3-NE1	-9.37	1.02	1.32
1	A	62	CRQ	CD3-NE1	-9.14	1.03	1.32
1	B	62	CRQ	CD3-NE1	-9.10	1.03	1.32
1	B	62	CRQ	O2-C2	6.46	1.36	1.23
1	A	62	CRQ	CG2-CB2	-6.05	1.35	1.46
1	D	62	CRQ	O2-C2	6.01	1.35	1.23
1	A	62	CRQ	O2-C2	5.89	1.35	1.23
1	C	62	CRQ	O2-C2	5.76	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	62	CRQ	CG2-CB2	-5.75	1.36	1.46
1	C	62	CRQ	CG2-CB2	-5.38	1.37	1.46
1	B	62	CRQ	CG2-CB2	-5.24	1.37	1.46
1	B	62	CRQ	CB2-CA2	2.31	1.37	1.35
1	A	62	CRQ	CE1-CD1	-2.10	1.35	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	62	CRQ	O2-C2-CA2	-9.64	124.87	131.02
1	A	62	CRQ	O2-C2-CA2	-9.06	125.24	131.02
1	C	62	CRQ	O2-C2-CA2	-9.01	125.27	131.02
1	C	62	CRQ	CA2-C2-N3	6.04	108.58	103.50
1	B	62	CRQ	O2-C2-CA2	-6.03	127.17	131.02
1	D	62	CRQ	CA2-C2-N3	5.20	107.87	103.50
1	A	62	CRQ	CA2-C2-N3	5.19	107.86	103.50
1	B	62	CRQ	CA2-C2-N3	4.94	107.65	103.50
1	C	62	CRQ	N3-C1-N2	-3.66	108.28	112.62
1	C	62	CRQ	CB2-CA2-C2	3.65	126.78	122.36
1	C	62	CRQ	C2-CA2-N2	-3.57	106.39	108.95
1	D	62	CRQ	N3-C1-N2	-3.48	108.49	112.62
1	A	62	CRQ	N3-C1-N2	-3.45	108.53	112.62
1	A	62	CRQ	C3-CA3-N3	3.38	120.12	112.43
1	B	62	CRQ	C3-CA3-N3	3.30	119.94	112.43
1	C	62	CRQ	C3-CA3-N3	3.25	119.83	112.43
1	A	62	CRQ	CG2-CB2-CA2	-3.05	126.24	129.87
1	C	62	CRQ	CA2-N2-C1	2.94	109.51	104.09
1	D	62	CRQ	CA3-N3-C1	-2.81	122.86	128.39
1	D	62	CRQ	C2-CA2-N2	-2.73	106.99	108.95
1	B	62	CRQ	N3-C1-N2	-2.71	109.40	112.62
1	D	62	CRQ	CA3-N3-C2	2.60	129.39	123.67
1	D	62	CRQ	CA2-N2-C1	2.58	108.84	104.09
1	D	62	CRQ	CB2-CA2-C2	2.54	125.44	122.36
1	B	62	CRQ	CB2-CA2-C2	2.40	125.26	122.36
1	D	62	CRQ	C3-CA3-N3	2.36	117.81	112.43
1	A	62	CRQ	CA2-N2-C1	2.19	108.12	104.09
1	A	62	CRQ	O3-C3-CA3	-2.16	115.75	125.47
1	C	62	CRQ	O3-C3-CA3	-2.10	116.00	125.47
1	A	62	CRQ	CA3-N3-C1	-2.08	124.30	128.39
1	B	62	CRQ	O3-C3-CA3	-2.07	116.14	125.47

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	62	CRQ	C3-CA3-N3-C2
1	B	62	CRQ	C3-CA3-N3-C2
1	C	62	CRQ	C3-CA3-N3-C2
1	D	62	CRQ	C3-CA3-N3-C2
1	A	62	CRQ	C3-CA3-N3-C1
1	D	62	CRQ	C3-CA3-N3-C1
1	B	62	CRQ	C3-CA3-N3-C1
1	C	62	CRQ	C3-CA3-N3-C1

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	62	CRQ	2	0
1	C	62	CRQ	5	0
1	A	62	CRQ	2	0
1	D	62	CRQ	2	0

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	213/245 (86%)	-0.19	0	100 100	22, 44, 70, 93	1 (0%)
1	B	215/245 (87%)	-0.21	0	100 100	14, 45, 74, 94	3 (1%)
1	C	214/245 (87%)	0.65	2 (0%)	81 79	34, 72, 100, 123	5 (2%)
1	D	214/245 (87%)	0.52	4 (1%)	66 63	26, 68, 91, 102	18 (8%)
All	All	856/980 (87%)	0.19	6 (0%)	84 82	14, 58, 92, 123	27 (3%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	165	GLY	3.1
1	C	157	VAL	2.6
1	D	10	ILE	2.4
1	D	68	PHE	2.3
1	D	25	ILE	2.3
1	D	27	GLY	2.1

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	C	62	24/25	0.88	0.11	58,61,72,74	0
1	CRQ	D	62	24/25	0.91	0.09	65,68,70,70	0
1	CRQ	A	62	24/25	0.95	0.08	24,36,45,48	0
1	CRQ	B	62	24/25	0.95	0.07	24,32,40,43	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.