Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2017 – 09:04 AM EST

PDB ID	:	4PPL
Title	:	Crystal structure of eCGP123 H193Q variant at pH 7.5
Authors	:	Don Paul, C.; Traore, D.A.K.; Devenish, R.J.; Close, D.; Bell, T.; Bradbury, A.; Wilce, M.C.J.; Prescott, M.
Deposited on	:	unknown
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

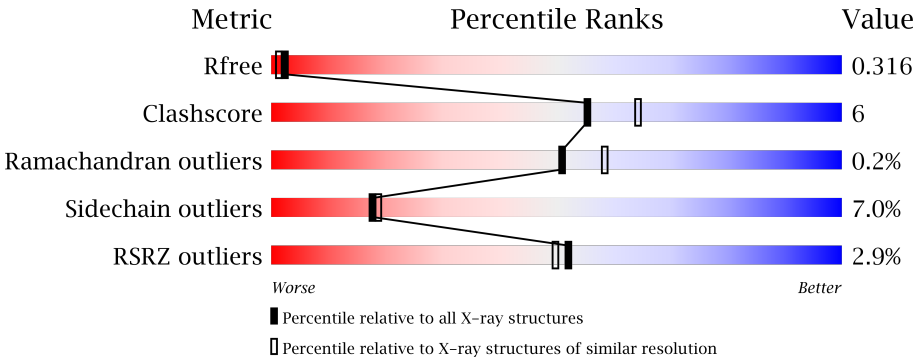
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

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 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	245	72% 14% • 13%
1	B	245	72% 16% • 12%
1	C	245	4% 67% 19% • 12%
1	D	245	6% 73% 15% 12%

2 Entry composition (i)

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.

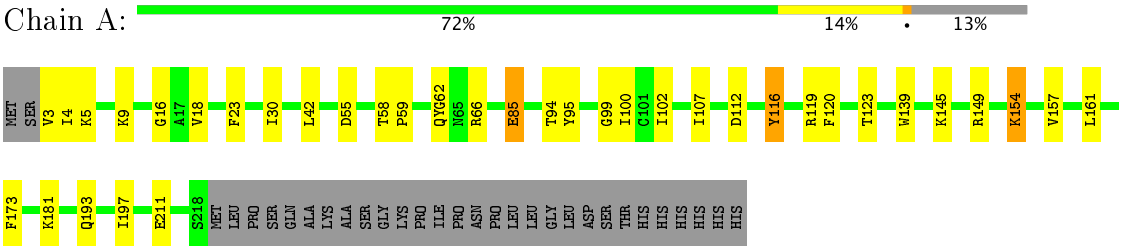
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	241	Total	O	0	0
			241	241		
2	B	203	Total	O	0	0
			203	203		
2	C	202	Total	O	0	0
			202	202		
2	D	168	Total	O	0	0
			168	168		

3 Residue-property plots (i)

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

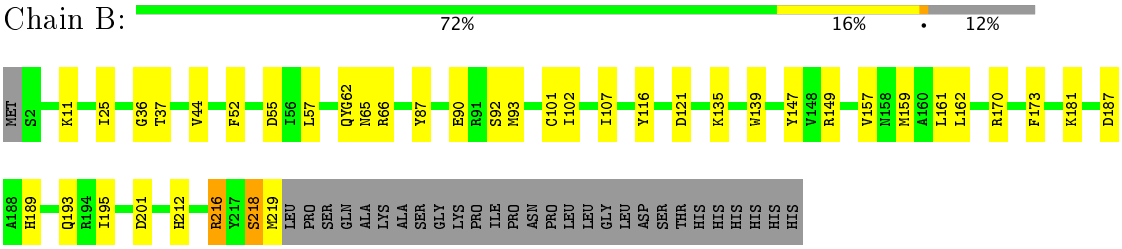
- Molecule 1: Monomeric Azami Green

Chain A:



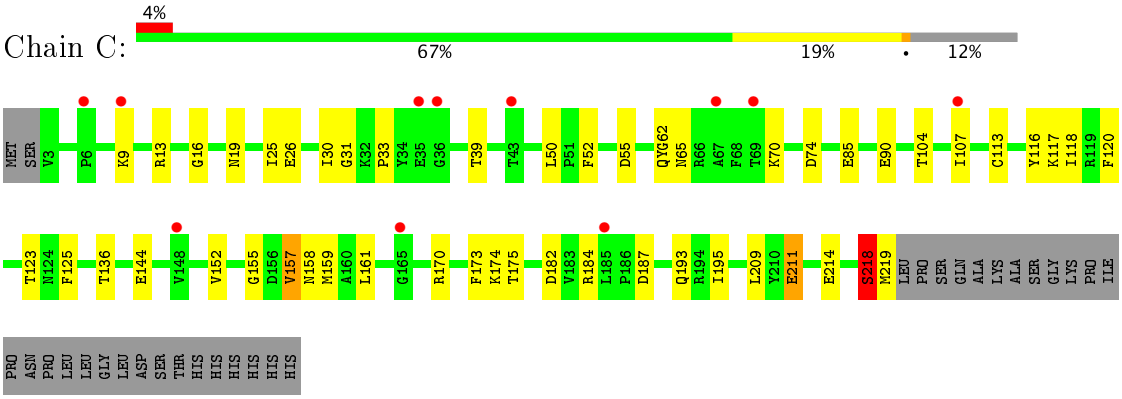
- Molecule 1: Monomeric Azami Green

Chain B:



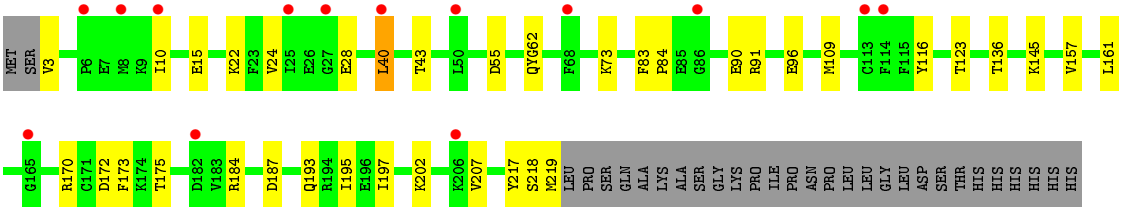
- Molecule 1: Monomeric Azami Green

Chain C:



- Molecule 1: Monomeric Azami Green

Chain D:


MET SER V3 P6 E7 M8 K9 I10 E15 K22 F23 V24 T25 E26 G27 E28 L40 T43 L50 D55 QYG62 F68 K73 F83 P84 E85 G86 E90 R91 E96 M109 C113 F114 F115 Y116 T123 T136 K145 V157 L161
G165 R170 C171 D172 F173 K174 T175 D182 V183 R184 D187 Q193 R194 I195 E196 I197 K202 K206 V207 Y217 S218 M219 LEU PRO SER GLN ALA LYS ALA SER GLY LYS PRO ILE PRO ASN PRO LEU LEU GLY LEU ASP SER THR HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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) 99.2 (46.21-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.27%)	DCC
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 91.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.046 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	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.*

[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	0.54	0/1776	0.76	0/2393
1	B	0.53	0/1790	0.78	1/2411 (0.0%)
1	C	0.44	0/1778	0.67	0/2395
1	D	0.44	0/1778	0.68	0/2395
All	All	0.49	0/7122	0.72	1/9594 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	218	SER	C-N-CA	5.47	135.38	121.70

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	1753	0	1706	26	0
1	B	1770	0	1719	21	0
1	C	1758	0	1710	25	0
1	D	1758	0	1710	15	0
2	A	241	0	0	0	0
2	B	203	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	202	0	0	3	0
2	D	168	0	0	0	0
All	All	7853	0	6845	80	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 (80) 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:CB	1:A:197:ILE:CD1	2.80	0.57
1:C:157:VAL:HG22	1:C:159:MET:HG2	1.87	0.57
1:D:62:CRQ:HD1	1:D:62:CRQ:N2	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:HD1	1:B:62:CRQ:N2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:HG2	1:A:85:GLU:H	1.63	0.41
1:A:18:VAL:HG23	1:A:23:PHE:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:CRQ:OE1	1:C:211:GLU:HB2	2.21	0.41
1:B:66:ARG:NE	1:B:66:ARG:HA	2.36	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:NH1	1:C:170:ARG:HB3	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 (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	212/245 (86%)	210 (99%)	2 (1%)	0	100	100
1	B	214/245 (87%)	208 (97%)	6 (3%)	0	100	100
1	C	212/245 (86%)	203 (96%)	7 (3%)	2 (1%)	20	18
1	D	212/245 (86%)	206 (97%)	6 (3%)	0	100	100
All	All	850/980 (87%)	827 (97%)	21 (2%)	2 (0%)	51	58

All (2) Ramachandran outliers are listed below:

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

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	186/212 (88%)	179 (96%)	7 (4%)	38 47
1	B	188/212 (89%)	176 (94%)	12 (6%)	20 23
1	C	186/212 (88%)	167 (90%)	19 (10%)	8 8
1	D	186/212 (88%)	172 (92%)	14 (8%)	16 16
All	All	746/848 (88%)	694 (93%)	52 (7%)	18 19

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LEU
1	A	85	GLU
1	A	116	TYR
1	A	145	LYS
1	A	154	LYS
1	A	181	LYS
1	A	193	GLN
1	B	11	LYS
1	B	37	THR
1	B	65	ASN
1	B	116	TYR
1	B	135	LYS
1	B	162	LEU
1	B	170	ARG
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	65	ASN
1	C	74	ASP
1	C	85	GLU
1	C	113	CYS
1	C	116	TYR
1	C	117	LYS

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Mol	Chain	Res	Type
1	C	118	ILE
1	C	152	VAL
1	C	157	VAL
1	C	174	LYS
1	C	175	THR
1	C	182	ASP
1	C	187	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
1	D	43	THR
1	D	55	ASP
1	D	73	LYS
1	D	116	TYR
1	D	123	THR
1	D	145	LYS
1	D	172	ASP
1	D	184	ARG
1	D	187	ASP
1	D	193	GLN
1	D	202	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	81	GLN
1	A	193	GLN
1	B	158	ASN
1	C	19	ASN
1	C	65	ASN
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	A	62	1	24,25,26	4.00	5 (20%)	26,34,36	3.30	7 (26%)
1	CRQ	B	62	1	24,25,26	3.80	6 (25%)	26,34,36	2.75	6 (23%)
1	CRQ	C	62	1	24,25,26	4.05	6 (25%)	26,34,36	3.55	8 (30%)
1	CRQ	D	62	1	24,25,26	4.05	6 (25%)	26,34,36	3.41	9 (34%)

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

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	62	CRQ	CA2-C2	-11.99	1.36	1.48
1	D	62	CRQ	CA2-C2	-11.70	1.36	1.48
1	A	62	CRQ	CA2-C2	-11.67	1.36	1.48
1	B	62	CRQ	CA2-C2	-10.50	1.38	1.48
1	C	62	CRQ	CD3-NE1	-9.38	1.02	1.32
1	D	62	CRQ	CD3-NE1	-9.25	1.02	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	CRQ	CD3-NE1	-9.03	1.03	1.32
1	B	62	CRQ	CD3-NE1	-8.99	1.03	1.32
1	A	62	CRQ	CG2-CB2	-5.46	1.35	1.46
1	D	62	CRQ	CG2-CB2	-5.18	1.36	1.46
1	C	62	CRQ	CG2-CB2	-4.85	1.37	1.46
1	B	62	CRQ	CG2-CB2	-4.73	1.37	1.46
1	D	62	CRQ	CB2-CA2	2.01	1.36	1.35
1	C	62	CRQ	CB2-CA2	2.07	1.37	1.35
1	B	62	CRQ	CB2-CA2	2.54	1.37	1.35
1	C	62	CRQ	O2-C2	5.38	1.34	1.23
1	A	62	CRQ	O2-C2	5.49	1.35	1.23
1	D	62	CRQ	O2-C2	5.61	1.35	1.23
1	B	62	CRQ	O2-C2	6.03	1.36	1.23
1	B	62	CRQ	CA1-N	8.52	1.48	1.27
1	A	62	CRQ	CA1-N	9.22	1.50	1.27
1	C	62	CRQ	CA1-N	9.23	1.50	1.27
1	D	62	CRQ	CA1-N	9.33	1.50	1.27

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	62	CRQ	O2-C2-CA2	-11.32	124.87	130.97
1	A	62	CRQ	O2-C2-CA2	-10.63	125.24	130.97
1	C	62	CRQ	O2-C2-CA2	-10.57	125.27	130.97
1	B	62	CRQ	O2-C2-CA2	-7.05	127.17	130.97
1	C	62	CRQ	N3-C1-N2	-3.92	108.28	113.31
1	D	62	CRQ	N3-C1-N2	-3.75	108.49	113.31
1	A	62	CRQ	N3-C1-N2	-3.73	108.53	113.31
1	C	62	CRQ	C2-CA2-N2	-3.47	106.39	108.93
1	A	62	CRQ	CG2-CB2-CA2	-3.40	126.24	130.19
1	A	62	CRQ	O-C-CA3	-3.21	115.75	126.38
1	C	62	CRQ	O-C-CA3	-3.14	116.00	126.38
1	B	62	CRQ	O-C-CA3	-3.10	116.14	126.38
1	B	62	CRQ	N3-C1-N2	-3.04	109.40	113.31
1	A	62	CRQ	CB1-CA1-N	-2.76	115.83	125.34
1	D	62	CRQ	O-C-CA3	-2.68	117.51	126.38
1	D	62	CRQ	CA3-N3-C1	-2.65	122.86	128.19
1	D	62	CRQ	C2-CA2-N2	-2.65	106.99	108.93
1	B	62	CRQ	CB1-CA1-N	-2.45	116.88	125.34
1	C	62	CRQ	CB1-CA1-N	-2.11	118.06	125.34
1	A	62	CRQ	CA2-N2-C1	2.09	108.12	104.21
1	B	62	CRQ	CB2-CA2-C2	2.34	125.26	122.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	62	CRQ	CA3-N3-C2	2.46	129.39	123.94
1	D	62	CRQ	CB2-CA2-C2	2.48	125.44	122.32
1	D	62	CRQ	CA2-N2-C1	2.48	108.84	104.21
1	C	62	CRQ	CA2-N2-C1	2.84	109.51	104.21
1	C	62	CRQ	CB2-CA2-C2	3.54	126.78	122.32
1	B	62	CRQ	CA2-C2-N3	9.76	107.65	103.30
1	A	62	CRQ	CA2-C2-N3	10.21	107.86	103.30
1	D	62	CRQ	CA2-C2-N3	10.24	107.87	103.30
1	C	62	CRQ	CA2-C2-N3	11.83	108.58	103.30

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	62	CRQ	C-CA3-N3-C2

There are no ring outliers.

4 monomers are involved in 11 short contacts:

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

5.5 Carbohydrates (i)

There are no carbohydrates 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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	213/245 (86%)	-0.23	0	100	100	22, 44, 70, 93	0
1	B	215/245 (87%)	-0.18	0	100	100	24, 45, 74, 94	2 (0%)
1	C	214/245 (87%)	0.50	11 (5%)	29	27	48, 72, 100, 123	5 (2%)
1	D	214/245 (87%)	0.46	14 (6%)	20	18	48, 70, 92, 102	18 (8%)
All	All	856/980 (87%)	0.14	25 (2%)	52	50	22, 59, 92, 123	25 (2%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	10	ILE	4.2
1	C	185	LEU	3.8
1	C	36	GLY	3.8
1	C	165	GLY	3.8
1	D	40	LEU	3.7
1	D	165	GLY	3.4
1	D	8	MET	3.3
1	D	68	PHE	3.1
1	C	67	ALA	3.1
1	C	148	VAL	3.0
1	C	35	GLU	2.8
1	C	6	PRO	2.7
1	D	6	PRO	2.6
1	D	113	CYS	2.5
1	D	182	ASP	2.5
1	D	27	GLY	2.5
1	D	86	GLY	2.4
1	D	206	LYS	2.4
1	C	107	ILE	2.3
1	C	9	LYS	2.2
1	C	69	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	43	THR	2.2
1	D	25	ILE	2.2
1	D	50	LEU	2.1
1	D	114	PHE	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
1	CRQ	A	62	24/25	0.96	0.11	-	24,36,45,48	0
1	CRQ	C	62	24/25	0.88	0.17	-	58,61,72,74	0
1	CRQ	B	62	24/25	0.97	0.11	-	24,32,40,43	0
1	CRQ	D	62	24/25	0.92	0.14	-	65,68,70,70	0

6.3 Carbohydrates (i)

There are no carbohydrates 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.