



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 11:48 am BST

PDB ID : 2IB5
Title : Structural characterization of a blue chromoprotein and its yellow mutant from the sea anemone *cnidopus japonicus*
Authors : Chan, M.C.Y.; Bosanac, I.; Ikura, M.
Deposited on : 2006-09-10
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

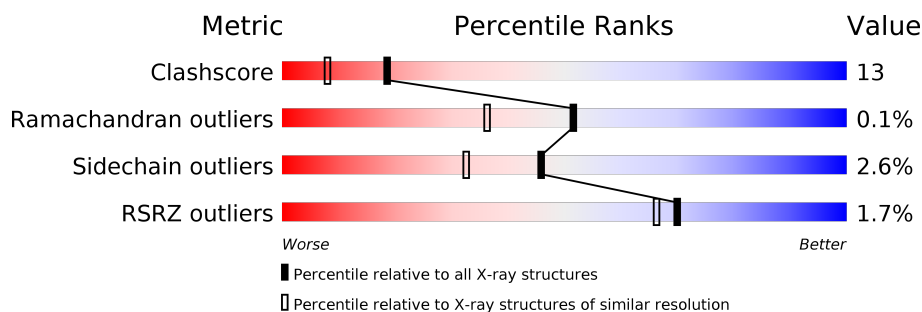
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 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	233	<div> <div></div> <div>79%16%..</div> </div>
1	B	233	<div> <div>%</div> <div>75%21%..</div> </div>
1	C	233	<div> <div>2%</div> <div>70%24%..</div> </div>
1	D	233	<div> <div>%</div> <div>71%24%..</div> </div>
1	E	233	<div> <div></div> <div>74%22%..</div> </div>
1	F	233	<div> <div>2%</div> <div>73%23%..</div> </div>
1	G	233	<div> <div>4%</div> <div>72%24%..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	233	<div> <div>%</div> <div> </div> <div>75%21%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	2001	-	-	X	-
2	PO4	H	2005	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15792 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 Chromo protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	Se	0	0	0
			1798	1132	308	340	11	7			
1	B	226	Total	C	N	O	S	Se	0	0	0
			1798	1132	308	340	11	7			
1	C	226	Total	C	N	O	S	Se	0	0	0
			1798	1132	308	340	11	7			
1	D	226	Total	C	N	O	S	Se	0	0	0
			1798	1132	308	340	11	7			
1	E	226	Total	C	N	O	S	Se	0	0	0
			1798	1132	308	340	11	7			
1	F	226	Total	C	N	O	S	Se	0	0	0
			1798	1132	308	340	11	7			
1	G	226	Total	C	N	O	S	Se	0	0	0
			1798	1132	308	340	11	7			
1	H	226	Total	C	N	O	S	Se	0	0	0
			1798	1132	308	340	11	7			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP A0AQQ7
A	-1	SER	-	EXPRESSION TAG	UNP A0AQQ7
A	0	HIS	-	EXPRESSION TAG	UNP A0AQQ7
A	65	CRQ	GLN	CHROMOPHORE	UNP A0AQQ7
A	65	CRQ	TYR	CHROMOPHORE	UNP A0AQQ7
A	65	CRQ	GLY	CHROMOPHORE	UNP A0AQQ7
B	-2	GLY	-	EXPRESSION TAG	UNP A0AQQ7
B	-1	SER	-	EXPRESSION TAG	UNP A0AQQ7
B	0	HIS	-	EXPRESSION TAG	UNP A0AQQ7
B	65	CRQ	GLN	CHROMOPHORE	UNP A0AQQ7
B	65	CRQ	TYR	CHROMOPHORE	UNP A0AQQ7
B	65	CRQ	GLY	CHROMOPHORE	UNP A0AQQ7
C	-2	GLY	-	EXPRESSION TAG	UNP A0AQQ7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	EXPRESSION TAG	UNP A0AQQ7
C	0	HIS	-	EXPRESSION TAG	UNP A0AQQ7
C	65	CRQ	GLN	CHROMOPHORE	UNP A0AQQ7
C	65	CRQ	TYR	CHROMOPHORE	UNP A0AQQ7
C	65	CRQ	GLY	CHROMOPHORE	UNP A0AQQ7
D	-2	GLY	-	EXPRESSION TAG	UNP A0AQQ7
D	-1	SER	-	EXPRESSION TAG	UNP A0AQQ7
D	0	HIS	-	EXPRESSION TAG	UNP A0AQQ7
D	65	CRQ	GLN	CHROMOPHORE	UNP A0AQQ7
D	65	CRQ	TYR	CHROMOPHORE	UNP A0AQQ7
D	65	CRQ	GLY	CHROMOPHORE	UNP A0AQQ7
E	-2	GLY	-	EXPRESSION TAG	UNP A0AQQ7
E	-1	SER	-	EXPRESSION TAG	UNP A0AQQ7
E	0	HIS	-	EXPRESSION TAG	UNP A0AQQ7
E	65	CRQ	GLN	CHROMOPHORE	UNP A0AQQ7
E	65	CRQ	TYR	CHROMOPHORE	UNP A0AQQ7
E	65	CRQ	GLY	CHROMOPHORE	UNP A0AQQ7
F	-2	GLY	-	EXPRESSION TAG	UNP A0AQQ7
F	-1	SER	-	EXPRESSION TAG	UNP A0AQQ7
F	0	HIS	-	EXPRESSION TAG	UNP A0AQQ7
F	65	CRQ	GLN	CHROMOPHORE	UNP A0AQQ7
F	65	CRQ	TYR	CHROMOPHORE	UNP A0AQQ7
F	65	CRQ	GLY	CHROMOPHORE	UNP A0AQQ7
G	-2	GLY	-	EXPRESSION TAG	UNP A0AQQ7
G	-1	SER	-	EXPRESSION TAG	UNP A0AQQ7
G	0	HIS	-	EXPRESSION TAG	UNP A0AQQ7
G	65	CRQ	GLN	CHROMOPHORE	UNP A0AQQ7
G	65	CRQ	TYR	CHROMOPHORE	UNP A0AQQ7
G	65	CRQ	GLY	CHROMOPHORE	UNP A0AQQ7
H	-2	GLY	-	EXPRESSION TAG	UNP A0AQQ7
H	-1	SER	-	EXPRESSION TAG	UNP A0AQQ7
H	0	HIS	-	EXPRESSION TAG	UNP A0AQQ7
H	65	CRQ	GLN	CHROMOPHORE	UNP A0AQQ7
H	65	CRQ	TYR	CHROMOPHORE	UNP A0AQQ7
H	65	CRQ	GLY	CHROMOPHORE	UNP A0AQQ7

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		

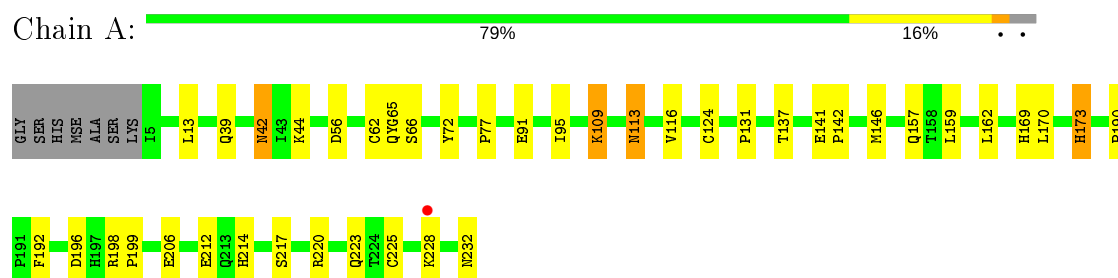
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	198	Total	O	0	0
			198	198		
3	B	174	Total	O	0	0
			174	174		
3	C	183	Total	O	0	0
			183	183		
3	D	182	Total	O	0	0
			182	182		
3	E	151	Total	O	0	0
			151	151		
3	F	136	Total	O	0	0
			136	136		
3	G	141	Total	O	0	0
			141	141		
3	H	163	Total	O	0	0
			163	163		

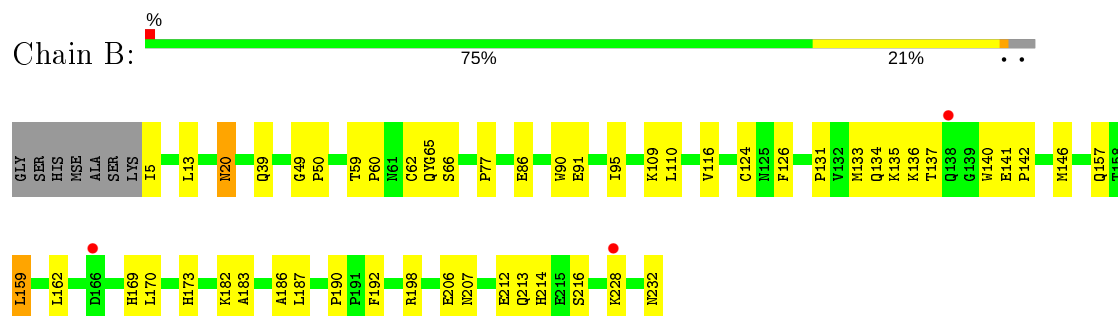
3 Residue-property plots [i](#)

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.

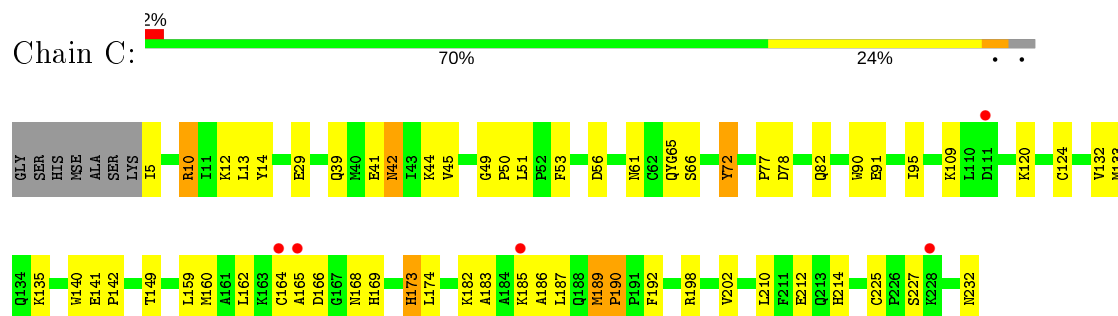
• Molecule 1: Chromo protein



• Molecule 1: Chromo protein

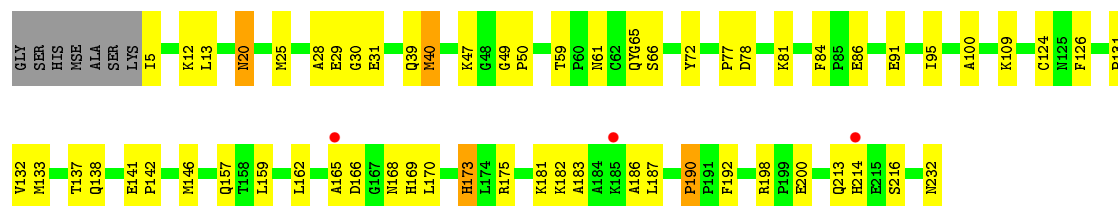


• Molecule 1: Chromo protein

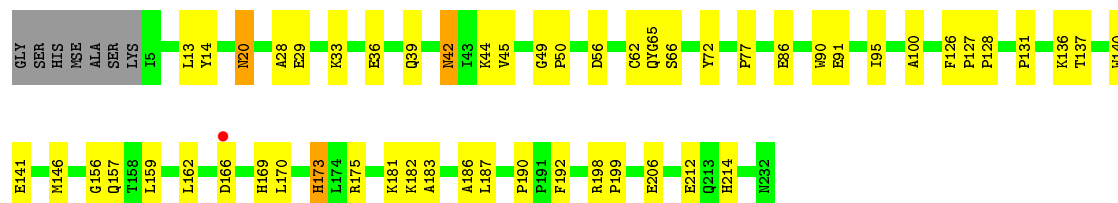


• Molecule 1: Chromo protein

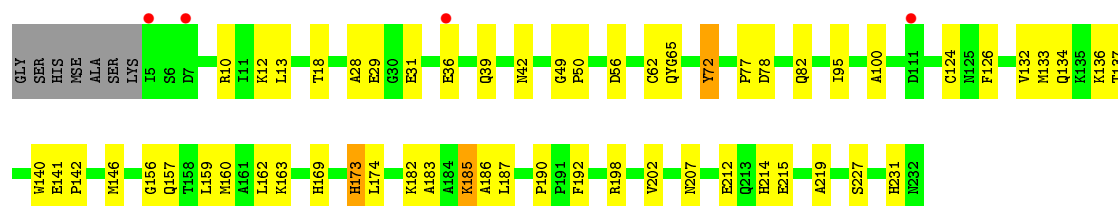
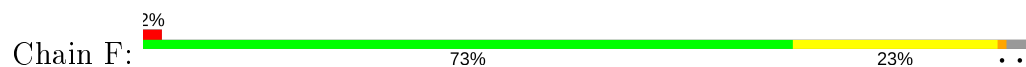




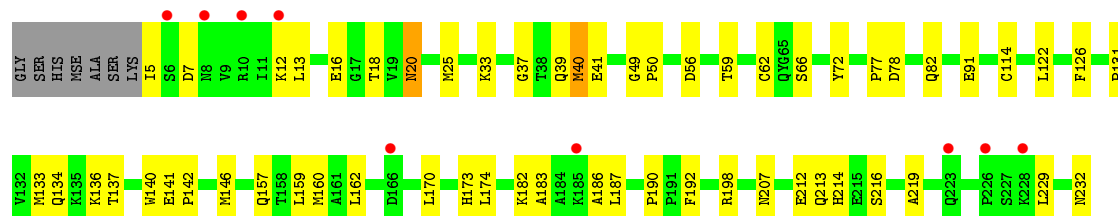
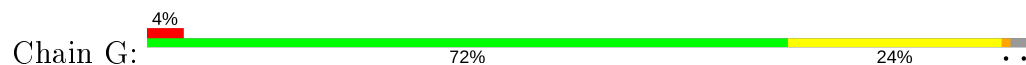
• Molecule 1: Chromo protein



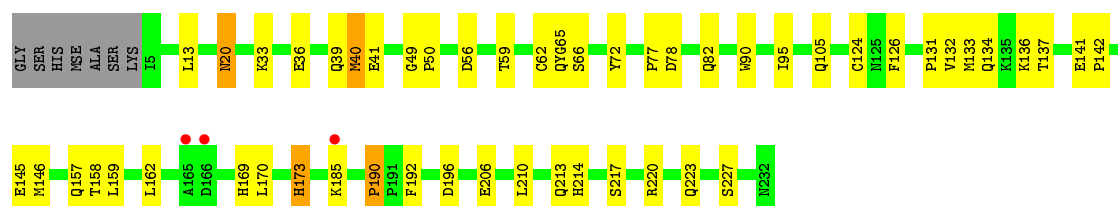
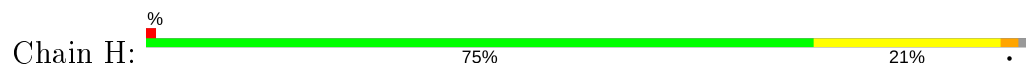
• Molecule 1: Chromo protein



• Molecule 1: Chromo protein



• Molecule 1: Chromo protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.86Å 126.85Å 100.51Å 90.00° 102.10° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 45.82 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-1.80) 99.4 (45.82-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.73 (at 1.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.195 , 0.225 0.199 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.5	Xtriage
Anisotropy	0.776	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15792	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.60% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	0.38	0/1811	0.72	1/2436 (0.0%)
1	B	0.35	0/1811	0.69	1/2436 (0.0%)
1	C	0.36	0/1811	0.75	4/2436 (0.2%)
1	D	0.37	0/1811	0.73	1/2436 (0.0%)
1	E	0.34	0/1811	0.68	1/2436 (0.0%)
1	F	0.33	0/1811	0.66	1/2436 (0.0%)
1	G	0.33	0/1811	0.64	1/2436 (0.0%)
1	H	0.37	0/1811	0.69	2/2436 (0.1%)
All	All	0.35	0/14488	0.70	12/19488 (0.1%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	61	ASN	O-C-N	-7.17	111.23	122.70
1	C	72	TYR	N-CA-CB	-6.87	98.23	110.60
1	C	90	TRP	CA-CB-CG	6.59	126.22	113.70
1	H	90	TRP	CA-CB-CG	6.24	125.55	113.70
1	B	62	CYS	N-CA-C	5.81	126.70	111.00

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	1798	0	1730	42	0
1	B	1798	0	1730	57	0
1	C	1798	0	1730	59	0
1	D	1798	0	1730	60	0
1	E	1798	0	1730	54	0
1	F	1798	0	1730	56	0
1	G	1798	0	1730	55	0
1	H	1798	0	1730	49	0
2	A	15	0	0	2	0
2	B	15	0	0	1	0
2	D	10	0	0	0	0
2	E	5	0	0	1	0
2	F	15	0	0	1	0
2	G	10	0	0	0	0
2	H	10	0	0	2	0
3	A	198	0	0	4	0
3	B	174	0	0	2	1
3	C	183	0	0	5	0
3	D	182	0	0	4	1
3	E	151	0	0	5	0
3	F	136	0	0	2	0
3	G	141	0	0	9	0
3	H	163	0	0	4	0
All	All	15792	0	13840	373	1

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 13.

The worst 5 of 373 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:G:160:MSE:CE	3:G:2155:HOH:O	1.78	1.26
3:G:2046:HOH:O	1:H:124:CYS:HB3	1.53	1.04
1:E:182:LYS:HB3	1:E:187:LEU:HD11	1.44	0.97
1:F:160:MSE:HE2	1:F:174:LEU:HD11	1.47	0.95
1:C:182:LYS:HB3	1:C:187:LEU:HD21	1.46	0.95

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2184:HOH:O	3:D:2192:HOH:O[2_645]	0.17	2.03

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	223/233 (96%)	221 (99%)	2 (1%)	0	100	100
1	B	223/233 (96%)	221 (99%)	2 (1%)	0	100	100
1	C	223/233 (96%)	218 (98%)	3 (1%)	2 (1%)	17	6
1	D	223/233 (96%)	220 (99%)	3 (1%)	0	100	100
1	E	223/233 (96%)	221 (99%)	2 (1%)	0	100	100
1	F	223/233 (96%)	220 (99%)	3 (1%)	0	100	100
1	G	223/233 (96%)	219 (98%)	4 (2%)	0	100	100
1	H	223/233 (96%)	219 (98%)	4 (2%)	0	100	100
All	All	1784/1864 (96%)	1759 (99%)	23 (1%)	2 (0%)	51	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	165	ALA
1	C	166	ASP

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	197/195 (101%)	191 (97%)	6 (3%)	41	27
1	B	197/195 (101%)	193 (98%)	4 (2%)	55	44
1	C	197/195 (101%)	191 (97%)	6 (3%)	41	27
1	D	197/195 (101%)	190 (96%)	7 (4%)	35	20
1	E	197/195 (101%)	192 (98%)	5 (2%)	47	34
1	F	197/195 (101%)	193 (98%)	4 (2%)	55	44
1	G	197/195 (101%)	193 (98%)	4 (2%)	55	44
1	H	197/195 (101%)	192 (98%)	5 (2%)	47	34
All	All	1576/1560 (101%)	1535 (97%)	41 (3%)	46	32

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	40	MSE
1	D	190	PRO
1	H	40	MSE
1	D	72	TYR
1	D	173	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	138	GLN
1	E	157	GLN
1	H	157	GLN
1	D	168	ASN
1	D	232	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	65	1	24,25,26	3.86	5 (20%)	27,34,36	5.21	8 (29%)
1	CRQ	G	65	1	24,25,26	4.41	4 (16%)	27,34,36	6.00	9 (33%)
1	CRQ	E	65	1	24,25,26	3.90	4 (16%)	27,34,36	6.16	9 (33%)
1	CRQ	D	65	1	24,25,26	2.63	4 (16%)	27,34,36	5.98	9 (33%)
1	CRQ	B	65	1	24,25,26	4.03	6 (25%)	27,34,36	6.50	9 (33%)
1	CRQ	H	65	1	24,25,26	4.71	4 (16%)	27,34,36	5.43	8 (29%)
1	CRQ	F	65	1	24,25,26	4.66	4 (16%)	27,34,36	6.49	8 (29%)
1	CRQ	C	65	1	24,25,26	3.51	5 (20%)	27,34,36	5.47	8 (29%)

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	65	1	-	5/10/32/33	0/2/2/2
1	CRQ	G	65	1	-	5/10/32/33	0/2/2/2
1	CRQ	E	65	1	-	5/10/32/33	0/2/2/2
1	CRQ	D	65	1	-	5/10/32/33	0/2/2/2
1	CRQ	B	65	1	-	3/10/32/33	0/2/2/2
1	CRQ	H	65	1	-	5/10/32/33	0/2/2/2
1	CRQ	F	65	1	-	5/10/32/33	0/2/2/2
1	CRQ	C	65	1	-	5/10/32/33	0/2/2/2

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	65	CRQ	CB2-CA2	21.16	1.52	1.35
1	F	65	CRQ	CB2-CA2	20.72	1.52	1.35
1	G	65	CRQ	CB2-CA2	19.29	1.51	1.35
1	B	65	CRQ	CB2-CA2	16.82	1.49	1.35
1	E	65	CRQ	CB2-CA2	16.74	1.49	1.35

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	65	CRQ	CB2-CA2-N2	-17.62	104.39	128.83
1	E	65	CRQ	CB2-CA2-C2	17.33	142.96	122.28
1	D	65	CRQ	CB2-CA2-C2	16.88	142.43	122.28
1	B	65	CRQ	CB2-CA2-N2	-16.75	105.59	128.83
1	B	65	CRQ	CB2-CA2-C2	16.75	142.27	122.28

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	65	CRQ	C-CA3-N3-C1
1	A	65	CRQ	C-CA3-N3-C2
1	G	65	CRQ	C-CA3-N3-C1
1	G	65	CRQ	C-CA3-N3-C2
1	E	65	CRQ	C-CA3-N3-C1

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	65	CRQ	2	0
1	E	65	CRQ	3	0
1	D	65	CRQ	2	0
1	B	65	CRQ	6	0
1	H	65	CRQ	4	0
1	F	65	CRQ	1	0
1	C	65	CRQ	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 ligands 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	$\# Z > 2$
2	PO4	G	2006	-	4,4,4	1.70	1 (25%)	6,6,6	0.44	0
2	PO4	F	2008	-	4,4,4	1.74	2 (50%)	6,6,6	0.43	0
2	PO4	A	2001	-	4,4,4	1.73	0	6,6,6	0.42	0
2	PO4	E	2013	-	4,4,4	1.64	0	6,6,6	0.43	0
2	PO4	H	2005	-	4,4,4	1.68	1 (25%)	6,6,6	0.45	0
2	PO4	B	2002	-	4,4,4	1.72	1 (25%)	6,6,6	0.42	0
2	PO4	B	2010	-	4,4,4	1.62	0	6,6,6	0.42	0
2	PO4	B	2011	-	4,4,4	1.62	0	6,6,6	0.44	0
2	PO4	D	2012	-	4,4,4	1.60	0	6,6,6	0.44	0
2	PO4	H	2014	-	4,4,4	1.60	0	6,6,6	0.41	0
2	PO4	F	2015	-	4,4,4	1.60	0	6,6,6	0.42	0
2	PO4	F	2007	-	4,4,4	1.72	1 (25%)	6,6,6	0.42	0
2	PO4	G	2016	-	4,4,4	1.64	0	6,6,6	0.44	0
2	PO4	A	2009	-	4,4,4	1.61	0	6,6,6	0.43	0
2	PO4	A	2004	-	4,4,4	1.71	1 (25%)	6,6,6	0.42	0
2	PO4	D	2003	-	4,4,4	1.70	2 (50%)	6,6,6	0.45	0

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2005	PO4	P-O2	-2.20	1.48	1.54
2	B	2002	PO4	P-O3	-2.17	1.48	1.54
2	D	2003	PO4	P-O3	-2.12	1.48	1.54
2	F	2008	PO4	P-O3	-2.11	1.48	1.54
2	F	2007	PO4	P-O4	-2.09	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	PO4	2	0
2	E	2013	PO4	1	0
2	H	2005	PO4	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2002	PO4	1	0
2	F	2007	PO4	1	0

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 ⓘ

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, 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	218/233 (93%)	-0.33	1 (0%) 91 89	8, 13, 26, 39	0
1	B	218/233 (93%)	-0.24	3 (1%) 75 72	9, 15, 29, 43	0
1	C	218/233 (93%)	-0.19	5 (2%) 60 56	8, 14, 28, 40	0
1	D	218/233 (93%)	-0.29	3 (1%) 75 72	8, 14, 28, 41	0
1	E	218/233 (93%)	-0.12	1 (0%) 91 89	11, 19, 31, 37	0
1	F	218/233 (93%)	0.00	4 (1%) 68 64	10, 20, 32, 42	0
1	G	218/233 (93%)	0.13	9 (4%) 37 31	12, 22, 36, 46	0
1	H	218/233 (93%)	-0.18	3 (1%) 75 72	10, 17, 31, 48	0
All	All	1744/1864 (93%)	-0.15	29 (1%) 70 66	8, 17, 31, 48	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	165	ALA	5.5
1	C	164	CYS	4.9
1	C	165	ALA	4.6
1	D	165	ALA	4.1
1	H	166	ASP	3.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	F	65	24/25	0.82	0.14	11,19,29,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	CRQ	E	65	24/25	0.84	0.14	11,19,29,30	0
1	CRQ	D	65	24/25	0.85	0.16	11,19,29,30	0
1	CRQ	A	65	24/25	0.85	0.14	11,19,29,30	0
1	CRQ	H	65	24/25	0.86	0.14	11,19,29,30	0
1	CRQ	G	65	24/25	0.86	0.14	11,19,29,30	0
1	CRQ	B	65	24/25	0.87	0.12	11,19,29,30	0
1	CRQ	C	65	24/25	0.87	0.13	11,19,29,30	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [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(\AA^2)	Q<0.9
2	PO4	E	2013	5/5	0.66	0.34	58,60,61,61	0
2	PO4	F	2015	5/5	0.78	0.27	38,40,45,45	0
2	PO4	B	2011	5/5	0.79	0.24	27,32,37,37	0
2	PO4	G	2016	5/5	0.87	0.18	47,48,52,52	0
2	PO4	H	2014	5/5	0.89	0.18	22,22,30,31	0
2	PO4	H	2005	5/5	0.91	0.13	22,23,24,25	0
2	PO4	B	2010	5/5	0.93	0.12	23,27,32,32	0
2	PO4	D	2012	5/5	0.94	0.18	22,26,29,31	0
2	PO4	F	2007	5/5	0.95	0.14	21,23,26,26	0
2	PO4	A	2009	5/5	0.95	0.14	17,24,27,27	0
2	PO4	B	2002	5/5	0.96	0.11	20,20,24,25	0
2	PO4	A	2001	5/5	0.97	0.12	20,20,25,27	0
2	PO4	F	2008	5/5	0.98	0.11	16,16,19,21	0
2	PO4	G	2006	5/5	0.99	0.12	16,16,20,20	0
2	PO4	A	2004	5/5	0.99	0.09	14,14,18,19	0
2	PO4	D	2003	5/5	0.99	0.11	13,13,15,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.