wwPDB X-ray Structure Validation Summary Report (i)

Nov 6, 2023 – 02:07 AM EST

PDB ID	:	2IB6
Title	:	Structural characterization of a blue chromoprotein and its yellow mutant from the sea anemone cnidopus japonicus
Authors	:	Chan, M.C.Y.; Bosanac, I.; Ho, D.; Prive, G.; Ikura, M.
Deposited on	:	2006-09-10
Resolution	:	2.00 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

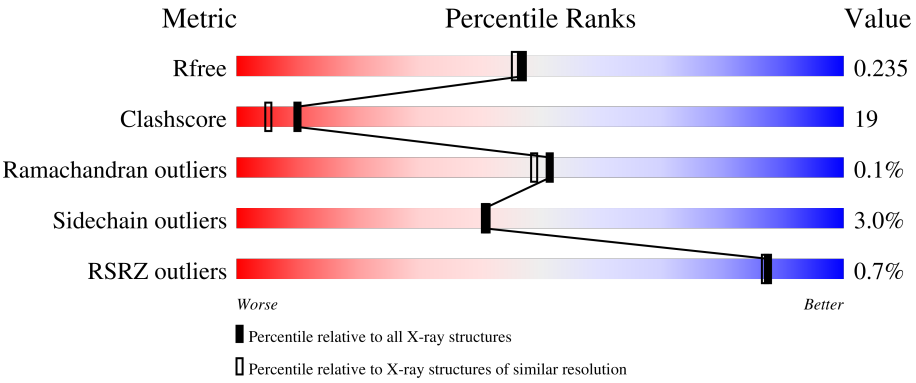
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	233	77% 19%
1	B	233	71% 24%
1	C	233	3% 72% 22%
1	D	233	74% 21%
1	E	233	73% 23%

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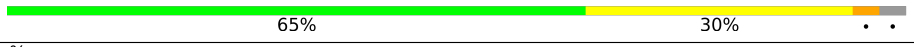
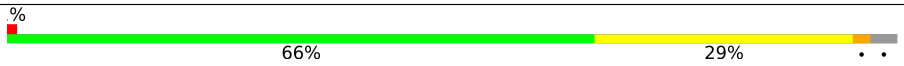
Mol	Chain	Length	Quality of chain
1	F	233	
1	G	233	
1	H	233	

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
1	QLG	A	65	-	-	X	-
1	QLG	B	65	-	-	X	-
1	QLG	C	65	-	-	X	-
1	QLG	D	65	-	-	X	-
1	QLG	E	65	-	-	X	-
1	QLG	F	65	-	-	X	-
1	QLG	G	65	-	-	X	-
1	QLG	H	65	-	-	X	-
2	PO4	A	2001	-	-	X	-
2	PO4	B	2002	-	-	X	-
2	PO4	H	2013	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15772 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 Yellow mutant chromo protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	Se	0	0	0
			1794	1129	308	339	11	7			
1	B	226	Total	C	N	O	S	Se	0	0	0
			1794	1129	308	339	11	7			
1	C	226	Total	C	N	O	S	Se	0	0	0
			1794	1129	308	339	11	7			
1	D	226	Total	C	N	O	S	Se	0	0	0
			1794	1129	308	339	11	7			
1	E	226	Total	C	N	O	S	Se	0	0	0
			1794	1129	308	339	11	7			
1	F	226	Total	C	N	O	S	Se	0	0	0
			1794	1129	308	339	11	7			
1	G	226	Total	C	N	O	S	Se	0	0	0
			1794	1129	308	339	11	7			
1	H	226	Total	C	N	O	S	Se	0	0	0
			1794	1129	308	339	11	7			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0AQQ8
A	-1	SER	-	expression tag	UNP A0AQQ8
A	0	HIS	-	expression tag	UNP A0AQQ8
A	65	QLG	GLN	chromophore	UNP A0AQQ8
A	65	QLG	LEU	chromophore	UNP A0AQQ8
A	65	QLG	GLY	chromophore	UNP A0AQQ8
B	-2	GLY	-	expression tag	UNP A0AQQ8
B	-1	SER	-	expression tag	UNP A0AQQ8
B	0	HIS	-	expression tag	UNP A0AQQ8
B	65	QLG	GLN	chromophore	UNP A0AQQ8
B	65	QLG	LEU	chromophore	UNP A0AQQ8
B	65	QLG	GLY	chromophore	UNP A0AQQ8
C	-2	GLY	-	expression tag	UNP A0AQQ8

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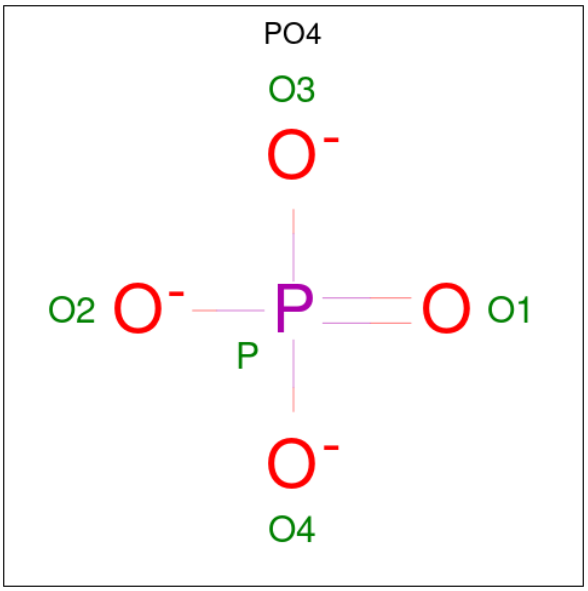
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP A0AQQ8
C	0	HIS	-	expression tag	UNP A0AQQ8
C	65	QLG	GLN	chromophore	UNP A0AQQ8
C	65	QLG	LEU	chromophore	UNP A0AQQ8
C	65	QLG	GLY	chromophore	UNP A0AQQ8
D	-2	GLY	-	expression tag	UNP A0AQQ8
D	-1	SER	-	expression tag	UNP A0AQQ8
D	0	HIS	-	expression tag	UNP A0AQQ8
D	65	QLG	GLN	chromophore	UNP A0AQQ8
D	65	QLG	LEU	chromophore	UNP A0AQQ8
D	65	QLG	GLY	chromophore	UNP A0AQQ8
E	-2	GLY	-	expression tag	UNP A0AQQ8
E	-1	SER	-	expression tag	UNP A0AQQ8
E	0	HIS	-	expression tag	UNP A0AQQ8
E	65	QLG	GLN	chromophore	UNP A0AQQ8
E	65	QLG	LEU	chromophore	UNP A0AQQ8
E	65	QLG	GLY	chromophore	UNP A0AQQ8
F	-2	GLY	-	expression tag	UNP A0AQQ8
F	-1	SER	-	expression tag	UNP A0AQQ8
F	0	HIS	-	expression tag	UNP A0AQQ8
F	65	QLG	GLN	chromophore	UNP A0AQQ8
F	65	QLG	LEU	chromophore	UNP A0AQQ8
F	65	QLG	GLY	chromophore	UNP A0AQQ8
G	-2	GLY	-	expression tag	UNP A0AQQ8
G	-1	SER	-	expression tag	UNP A0AQQ8
G	0	HIS	-	expression tag	UNP A0AQQ8
G	65	QLG	GLN	chromophore	UNP A0AQQ8
G	65	QLG	LEU	chromophore	UNP A0AQQ8
G	65	QLG	GLY	chromophore	UNP A0AQQ8
H	-2	GLY	-	expression tag	UNP A0AQQ8
H	-1	SER	-	expression tag	UNP A0AQQ8
H	0	HIS	-	expression tag	UNP A0AQQ8
H	65	QLG	GLN	chromophore	UNP A0AQQ8
H	65	QLG	LEU	chromophore	UNP A0AQQ8
H	65	QLG	GLY	chromophore	UNP A0AQQ8

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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

- Molecule 3 is water.

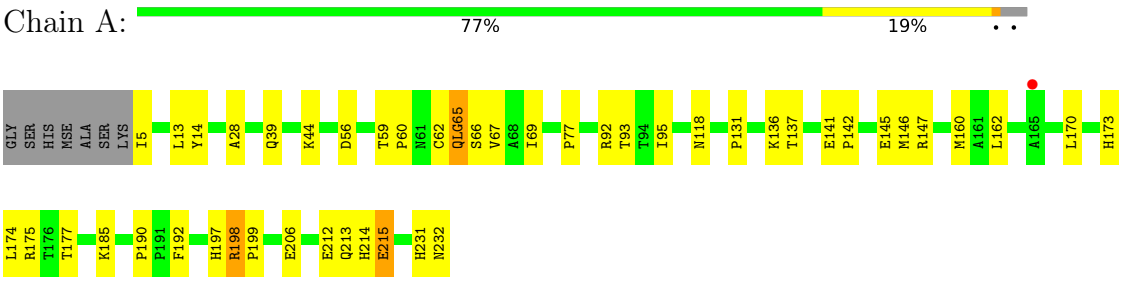
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	178	Total O 178 178	0	0
3	B	168	Total O 168 168	0	0
3	C	183	Total O 183 183	0	0
3	D	180	Total O 180 180	0	0
3	E	165	Total O 165 165	0	0
3	F	149	Total O 149 149	0	0
3	G	152	Total O 152 152	0	0
3	H	165	Total O 165 165	0	0

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.

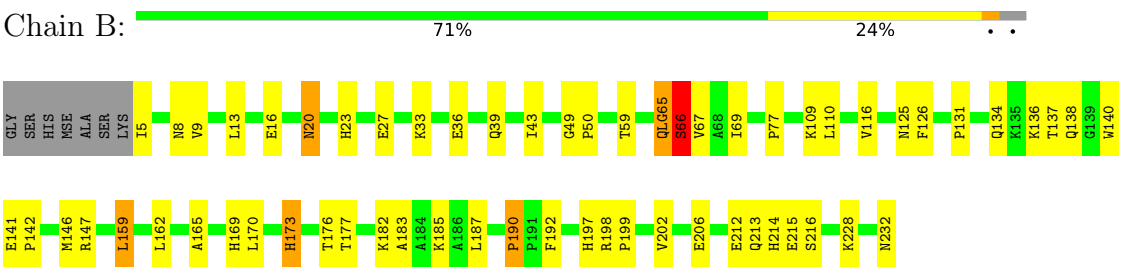
• Molecule 1: Yellow mutant chromo protein

Chain A:



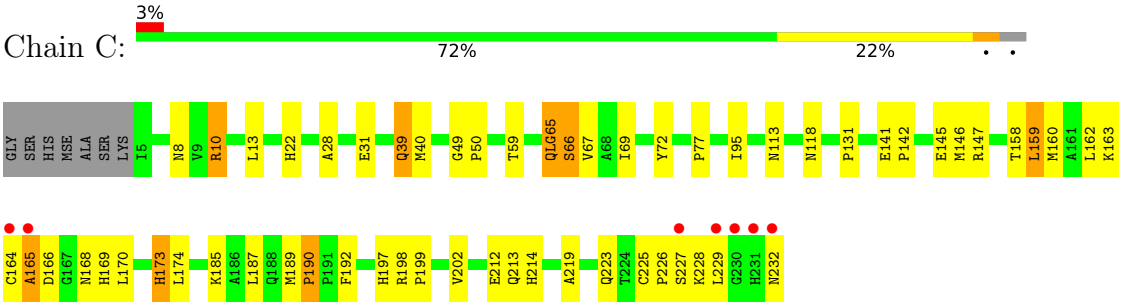
• Molecule 1: Yellow mutant chromo protein

Chain B:



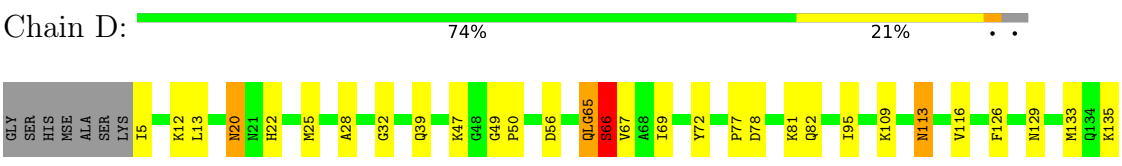
• Molecule 1: Yellow mutant chromo protein

Chain C:



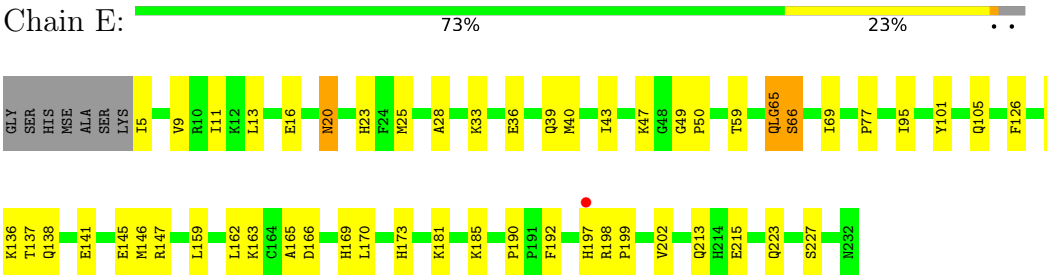
• Molecule 1: Yellow mutant chromo protein

Chain D:



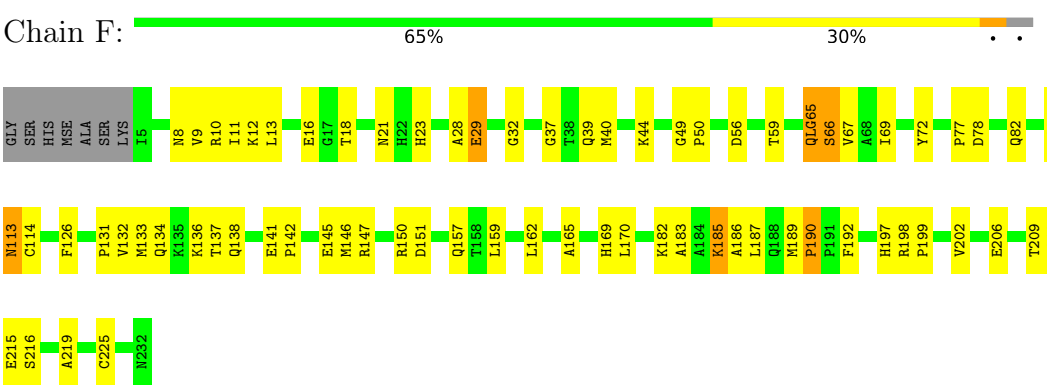
• Molecule 1: Yellow mutant chromo protein

Chain E:



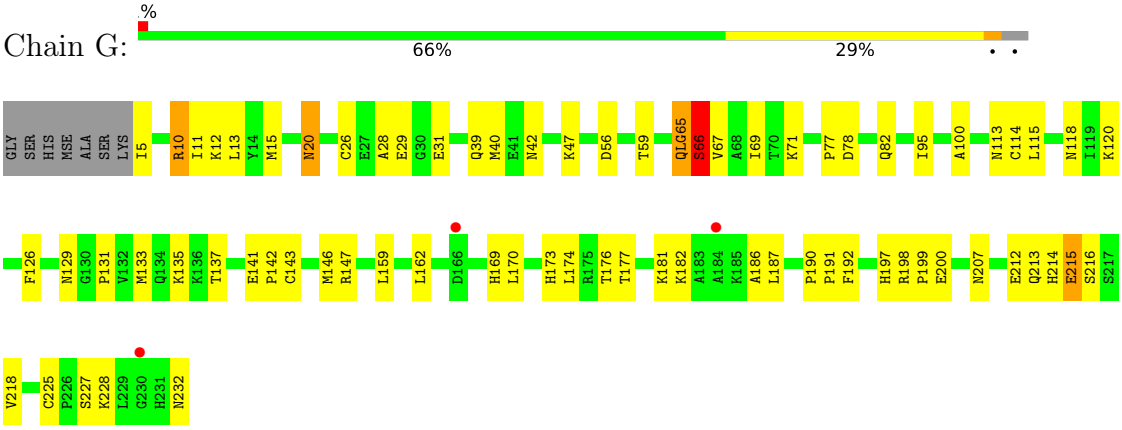
• Molecule 1: Yellow mutant chromo protein

Chain F:



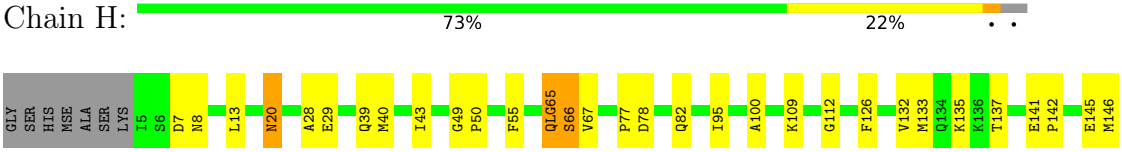
• Molecule 1: Yellow mutant chromo protein

Chain G:



• Molecule 1: Yellow mutant chromo protein

Chain H:




R147
G156
Q157
T158
L159
L162
D166
G167
N168
H173
T176
T177
K185
P190
H197
R198
P199
E206
L210
Q213
H214
E215
Q223
K228
H231
N232

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.08Å 126.93Å 100.08Å 90.00° 101.97° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 77.52 – 1.90	Depositor EDS
% Data completeness (in resolution range)	80.3 (50.00-2.00) 89.3 (77.52-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.71 (at 1.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.244 0.191 , 0.235	Depositor DCC
R_{free} test set	6148 reflections (4.43%)	wwPDB-VP
Wilson B-factor (Å^2)	10.2	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 61.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15772	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.68% 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: PO4, QLG

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	0.35	0/1811	0.69	0/2436
1	B	0.36	0/1811	0.77	5/2436 (0.2%)
1	C	0.35	0/1811	0.70	1/2436 (0.0%)
1	D	0.44	1/1811 (0.1%)	0.69	0/2436
1	E	0.35	0/1811	0.67	0/2436
1	F	0.33	0/1811	0.65	0/2436
1	G	0.44	1/1811 (0.1%)	0.68	1/2436 (0.0%)
1	H	0.36	0/1811	0.66	0/2436
All	All	0.37	2/14488 (0.0%)	0.69	7/19488 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	66	SER	N-CA	-11.83	1.22	1.46
1	D	66	SER	N-CA	-10.63	1.25	1.46

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	66	SER	C-N-CA	8.31	142.48	121.70
1	B	66	SER	N-CA-CB	8.09	122.63	110.50
1	G	66	SER	N-CA-CB	6.42	120.14	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	66	SER	N-CA-C	6.16	127.64	111.00
1	B	67	VAL	CA-CB-CG1	-6.01	101.88	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	66	SER	Peptide

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	1794	0	1729	65	0
1	B	1794	0	1729	72	0
1	C	1794	0	1729	70	0
1	D	1794	0	1729	64	0
1	E	1794	0	1729	69	0
1	F	1794	0	1729	88	0
1	G	1794	0	1729	96	0
1	H	1794	0	1729	65	0
2	A	15	0	0	2	0
2	B	10	0	0	3	0
2	C	5	0	0	0	0
2	D	10	0	0	0	0
2	F	15	0	0	1	0
2	G	10	0	0	0	0
2	H	15	0	0	2	0
3	A	178	0	0	8	0
3	B	168	0	0	9	0
3	C	183	0	0	13	0
3	D	180	0	0	14	0
3	E	165	0	0	8	0
3	F	149	0	0	5	0
3	G	152	0	0	14	0
3	H	165	0	0	16	0
All	All	15772	0	13832	537	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 19.

The worst 5 of 537 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:E:65:QLG:HD13	3:E:292:HOH:O	1.33	1.23
1:A:39:GLN:HG2	1:A:215:GLU:OE2	1.42	1.17
1:C:65:QLG:HD13	3:C:2041:HOH:O	1.45	1.16
1:E:65:QLG:HB2	1:E:197:HIS:CE1	1.82	1.15
1:F:65:QLG:HD13	3:F:2058:HOH:O	1.47	1.15

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	221/233 (95%)	218 (99%)	3 (1%)	0	100	100
1	B	221/233 (95%)	218 (99%)	3 (1%)	0	100	100
1	C	221/233 (95%)	213 (96%)	6 (3%)	2 (1%)	17	11
1	D	221/233 (95%)	218 (99%)	3 (1%)	0	100	100
1	E	221/233 (95%)	218 (99%)	3 (1%)	0	100	100
1	F	221/233 (95%)	218 (99%)	3 (1%)	0	100	100
1	G	221/233 (95%)	216 (98%)	5 (2%)	0	100	100
1	H	221/233 (95%)	216 (98%)	5 (2%)	0	100	100
All	All	1768/1864 (95%)	1735 (98%)	31 (2%)	2 (0%)	51	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	165	ALA

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Mol	Chain	Res	Type
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%)	194 (98%)	3 (2%)	65	69
1	B	197/195 (101%)	190 (96%)	7 (4%)	35	34
1	C	197/195 (101%)	187 (95%)	10 (5%)	24	19
1	D	197/195 (101%)	190 (96%)	7 (4%)	35	34
1	E	197/195 (101%)	194 (98%)	3 (2%)	65	69
1	F	197/195 (101%)	190 (96%)	7 (4%)	35	34
1	G	197/195 (101%)	190 (96%)	7 (4%)	35	34
1	H	197/195 (101%)	194 (98%)	3 (2%)	65	69
All	All	1576/1560 (101%)	1529 (97%)	47 (3%)	41	41

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	66	SER
1	F	189	MSE
1	E	173	HIS
1	F	66	SER
1	G	10	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	22	HIS
1	G	169	HIS
1	F	39	GLN
1	F	223	GLN

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Mol	Chain	Res	Type
1	G	232	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	QLG	C	65	1	18,20,21	2.79	3 (16%)	20,27,29	4.88	13 (65%)
1	QLG	F	65	1	18,20,21	1.63	3 (16%)	20,27,29	4.89	13 (65%)
1	QLG	E	65	1	18,20,21	2.86	3 (16%)	20,27,29	4.89	13 (65%)
1	QLG	G	65	1	18,20,21	2.81	3 (16%)	20,27,29	4.88	13 (65%)
1	QLG	A	65	1	18,20,21	1.55	3 (16%)	20,27,29	4.87	13 (65%)
1	QLG	B	65	1	18,20,21	2.41	3 (16%)	20,27,29	4.88	13 (65%)
1	QLG	D	65	1	18,20,21	3.54	3 (16%)	20,27,29	4.88	13 (65%)
1	QLG	H	65	1	18,20,21	3.14	3 (16%)	20,27,29	4.87	13 (65%)

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	QLG	C	65	1	-	7/10/32/33	0/1/1/1
1	QLG	F	65	1	-	7/10/32/33	0/1/1/1
1	QLG	E	65	1	-	7/10/32/33	0/1/1/1
1	QLG	G	65	1	-	7/10/32/33	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	QLG	A	65	1	-	7/10/32/33	0/1/1/1
1	QLG	B	65	1	-	7/10/32/33	0/1/1/1
1	QLG	D	65	1	-	7/10/32/33	0/1/1/1
1	QLG	H	65	1	-	7/10/32/33	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	65	QLG	CA1-N1	14.32	1.62	1.27
1	H	65	QLG	CA1-N1	12.52	1.57	1.27
1	E	65	QLG	CA1-N1	11.25	1.54	1.27
1	G	65	QLG	CA1-N1	11.00	1.54	1.27
1	C	65	QLG	CA1-N1	10.92	1.53	1.27

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	65	QLG	CG1-CB1-CA1	12.20	151.36	113.53
1	E	65	QLG	CG1-CB1-CA1	12.20	151.36	113.53
1	C	65	QLG	CG1-CB1-CA1	12.19	151.32	113.53
1	A	65	QLG	CG1-CB1-CA1	12.19	151.31	113.53
1	B	65	QLG	CG1-CB1-CA1	12.19	151.31	113.53

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	65	QLG	C2-CA2-CB2-CG2
1	A	65	QLG	N2-CA2-CB2-CG2
1	A	65	QLG	C3-CA3-N3-C1
1	A	65	QLG	CA2-CB2-CG2-CD2
1	B	65	QLG	C2-CA2-CB2-CG2

There are no ring outliers.

8 monomers are involved in 110 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	65	QLG	14	0
1	F	65	QLG	15	0
1	E	65	QLG	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	65	QLG	13	0
1	A	65	QLG	15	0
1	B	65	QLG	13	0
1	D	65	QLG	12	0
1	H	65	QLG	15	0

5.5 Carbohydrates (i)

There are no monosaccharides 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	B	2002	-	4,4,4	1.73	1 (25%)	6,6,6	0.43	0
2	PO4	H	2013	-	4,4,4	1.64	0	6,6,6	0.43	0
2	PO4	A	2009	-	4,4,4	1.59	0	6,6,6	0.44	0
2	PO4	F	2007	-	4,4,4	1.72	1 (25%)	6,6,6	0.43	0
2	PO4	A	2001	-	4,4,4	1.65	0	6,6,6	0.42	0
2	PO4	D	2003	-	4,4,4	1.72	1 (25%)	6,6,6	0.44	0
2	PO4	G	2006	-	4,4,4	1.65	1 (25%)	6,6,6	0.43	0
2	PO4	D	2012	-	4,4,4	1.61	0	6,6,6	0.42	0
2	PO4	F	2015	-	4,4,4	1.63	0	6,6,6	0.43	0
2	PO4	G	2016	-	4,4,4	1.63	0	6,6,6	0.44	0
2	PO4	H	2014	-	4,4,4	1.64	0	6,6,6	0.42	0
2	PO4	B	2010	-	4,4,4	1.58	0	6,6,6	0.42	0
2	PO4	C	2011	-	4,4,4	1.64	0	6,6,6	0.42	0
2	PO4	H	2005	-	4,4,4	1.64	1 (25%)	6,6,6	0.43	0
2	PO4	F	2008	-	4,4,4	1.80	1 (25%)	6,6,6	0.43	0
2	PO4	A	2004	-	4,4,4	1.64	1 (25%)	6,6,6	0.42	0

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2008	PO4	P-O3	-2.17	1.48	1.54
2	A	2004	PO4	P-O2	-2.10	1.48	1.54
2	D	2003	PO4	P-O3	-2.10	1.48	1.54
2	B	2002	PO4	P-O3	-2.05	1.48	1.54
2	F	2007	PO4	P-O4	-2.03	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.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2002	PO4	2	0
2	H	2013	PO4	1	0
2	F	2007	PO4	1	0
2	A	2001	PO4	2	0
2	B	2010	PO4	1	0
2	H	2005	PO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	65:QLG	C3	66:SER	N	1.11
1	A	65:QLG	C3	66:SER	N	1.02

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	218/233 (93%)	-0.39	1 (0%) 91 90	5, 11, 24, 34	0
1	B	218/233 (93%)	-0.36	0 100 100	5, 13, 25, 37	0
1	C	218/233 (93%)	-0.25	7 (3%) 47 46	4, 11, 25, 51	0
1	D	218/233 (93%)	-0.37	0 100 100	4, 11, 22, 34	0
1	E	218/233 (93%)	-0.29	1 (0%) 91 90	4, 14, 26, 33	0
1	F	218/233 (93%)	-0.22	0 100 100	4, 16, 27, 38	0
1	G	218/233 (93%)	-0.14	3 (1%) 75 74	6, 16, 31, 41	0
1	H	218/233 (93%)	-0.16	1 (0%) 91 90	6, 16, 28, 39	0
All	All	1744/1864 (93%)	-0.27	13 (0%) 87 87	4, 13, 27, 51	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	230	GLY	4.7
1	C	165	ALA	4.1
1	C	231	HIS	3.9
1	C	227	SER	3.8
1	G	184	ALA	3.6

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, 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	B-factors(Å^2)	Q<0.9
1	QLG	H	65	20/21	0.78	0.24	10,38,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	QLG	C	65	20/21	0.80	0.28	10,38,54,54	0
1	QLG	E	65	20/21	0.82	0.28	10,38,54,54	0
1	QLG	B	65	20/21	0.82	0.27	10,38,54,54	0
1	QLG	F	65	20/21	0.83	0.23	10,38,54,54	0
1	QLG	D	65	20/21	0.83	0.24	10,38,54,54	0
1	QLG	A	65	20/21	0.84	0.23	10,38,54,54	0
1	QLG	G	65	20/21	0.86	0.28	10,38,54,54	0

6.3 Carbohydrates (i)

There are no monosaccharides 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(Å^2)	Q<0.9
2	PO4	H	2013	5/5	0.59	0.61	76,77,77,77	0
2	PO4	B	2010	5/5	0.72	0.33	38,39,42,43	0
2	PO4	F	2015	5/5	0.73	0.26	52,52,53,53	0
2	PO4	G	2016	5/5	0.77	0.23	51,51,53,54	0
2	PO4	D	2012	5/5	0.79	0.22	37,37,41,41	0
2	PO4	A	2009	5/5	0.83	0.21	25,26,30,31	0
2	PO4	C	2011	5/5	0.84	0.21	40,41,42,44	0
2	PO4	H	2014	5/5	0.84	0.21	38,38,39,41	0
2	PO4	H	2005	5/5	0.95	0.09	18,19,20,22	0
2	PO4	A	2001	5/5	0.96	0.12	23,24,24,26	0
2	PO4	B	2002	5/5	0.96	0.11	20,22,23,23	0
2	PO4	A	2004	5/5	0.96	0.10	15,15,17,18	0
2	PO4	G	2006	5/5	0.96	0.08	11,15,16,18	0
2	PO4	F	2007	5/5	0.97	0.10	22,23,23,24	0
2	PO4	D	2003	5/5	0.98	0.09	17,19,20,20	0
2	PO4	F	2008	5/5	0.98	0.09	15,15,17,18	0

6.5 Other polymers (i)

There are no such residues in this entry.