



wwPDB EM Validation Summary Report ⓘ

Oct 16, 2024 – 12:52 AM JST

PDB ID : 8WPZ
EMDB ID : EMD-37727
Title : Cryo-ET structure of RuBisCO at 3.9 angstroms from *Synechococcus elongatus* PCC 7942
Authors : Kong, W.W.; Jiang, Y.L.; Zhou, C.Z.
Deposited on : 2023-10-10
Resolution : 3.90 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

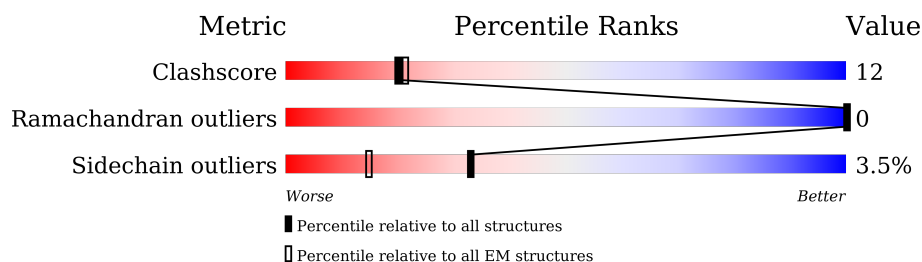
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	111	66% 23% • 10%
1	B	111	59% 31% 10%
1	E	111	65% 23% • 10%
1	F	111	62% 27% • 10%
1	I	111	62% 27% • 10%
1	L	111	62% 26% • 10%
1	M	111	64% 26% 10%
1	P	111	60% 30% 10%
2	C	472	75% 22% •

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Mol	Chain	Length	Quality of chain
2	D	472	 70% 26% ..
2	G	472	 71% 26% ..
2	H	472	 71% 25% ..
2	J	472	 69% 28% .
2	K	472	 69% 28% ..
2	N	472	 70% 27% .
2	O	472	 74% 23% ..

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 35774 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Ribulose biphosphate carboxylase small subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	100	Total	C	N	O	S	0	0
			848	544	142	156	6		
1	B	100	Total	C	N	O	S	0	0
			848	544	142	156	6		
1	E	100	Total	C	N	O	S	0	0
			848	544	142	156	6		
1	F	100	Total	C	N	O	S	0	0
			848	544	142	156	6		
1	I	100	Total	C	N	O	S	0	0
			848	544	142	156	6		
1	L	100	Total	C	N	O	S	0	0
			848	544	142	156	6		
1	M	100	Total	C	N	O	S	0	0
			848	544	142	156	6		
1	P	100	Total	C	N	O	S	0	0
			848	544	142	156	6		

- Molecule 2 is a protein called Ribulose biphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	460	Total	C	N	O	S	0	0
			3611	2299	631	663	18		
2	D	460	Total	C	N	O	S	0	0
			3611	2299	631	663	18		
2	G	462	Total	C	N	O	S	0	0
			3628	2309	634	667	18		
2	H	462	Total	C	N	O	S	0	0
			3628	2309	634	667	18		
2	J	462	Total	C	N	O	S	0	0
			3628	2309	634	667	18		
2	K	462	Total	C	N	O	S	0	0
			3628	2309	634	667	18		
2	N	462	Total	C	N	O	S	0	0
			3628	2309	634	667	18		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	462	Total	C	N	O	S	0	0
			3628	2309	634	667	18		

3 Residue-property plots

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. 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. 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: Ribulose biphosphate carboxylase small subunit

Chain A: 



- Molecule 1: Ribulose biphosphate carboxylase small subunit

Chain B: 



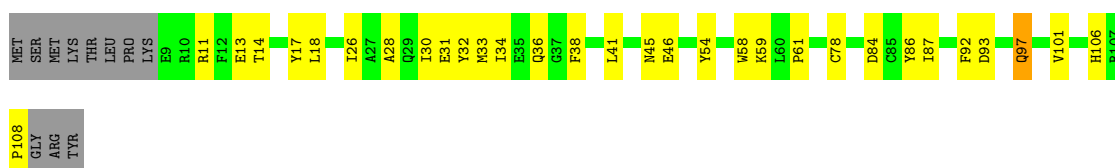
- Molecule 1: Ribulose biphosphate carboxylase small subunit

Chain E: 



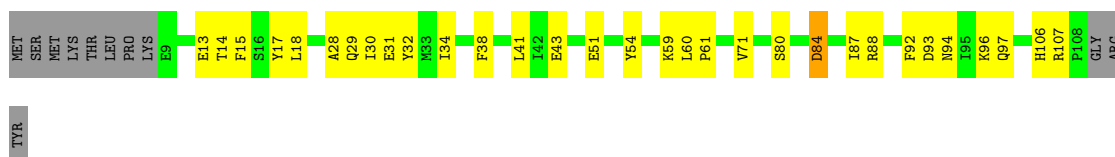
- Molecule 1: Ribulose biphosphate carboxylase small subunit

Chain F: 

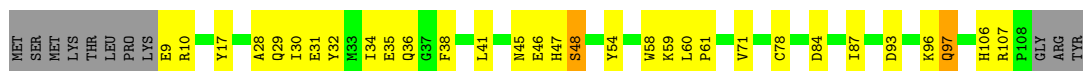


- Molecule 1: Ribulose biphosphate carboxylase small subunit

Chain I: 



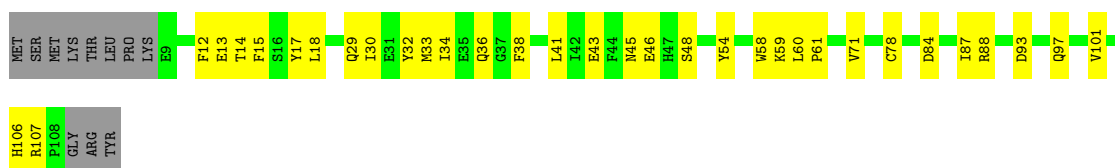
- Molecule 1: Ribulose biphosphate carboxylase small subunit



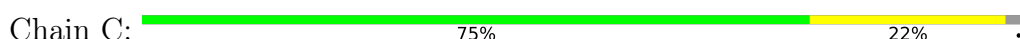
- Molecule 1: Ribulose biphosphate carboxylase small subunit



- Molecule 1: Ribulose biphosphate carboxylase small subunit

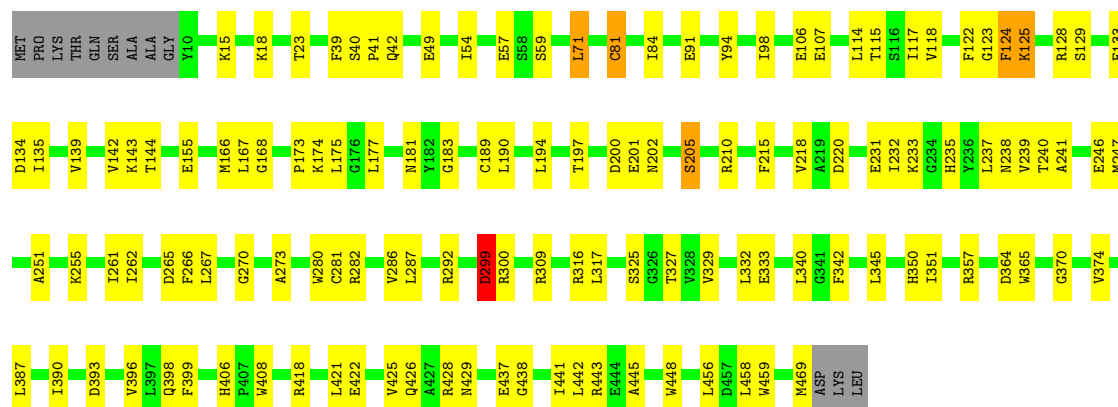


- Molecule 2: Ribulose biphosphate carboxylase large chain



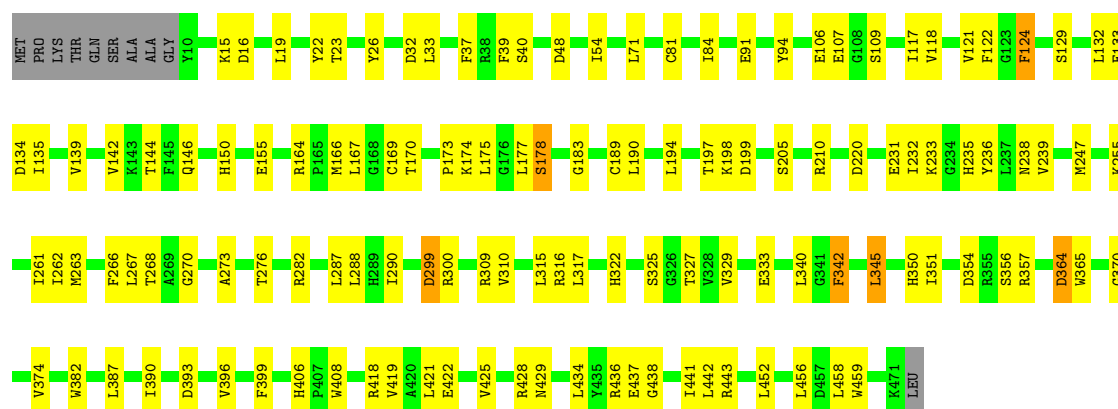
- Molecule 2: Ribulose biphosphate carboxylase large chain





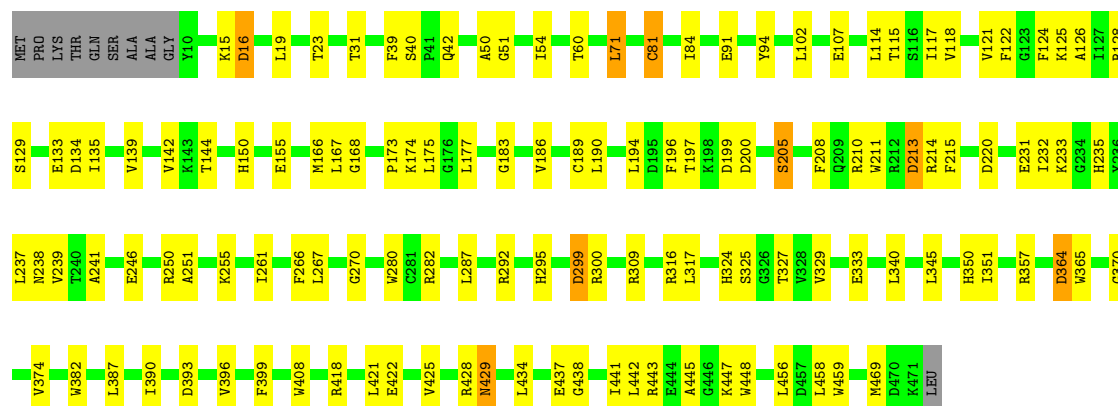
• Molecule 2: Ribulose biphosphate carboxylase large chain

Chain G: 71% 26% ..



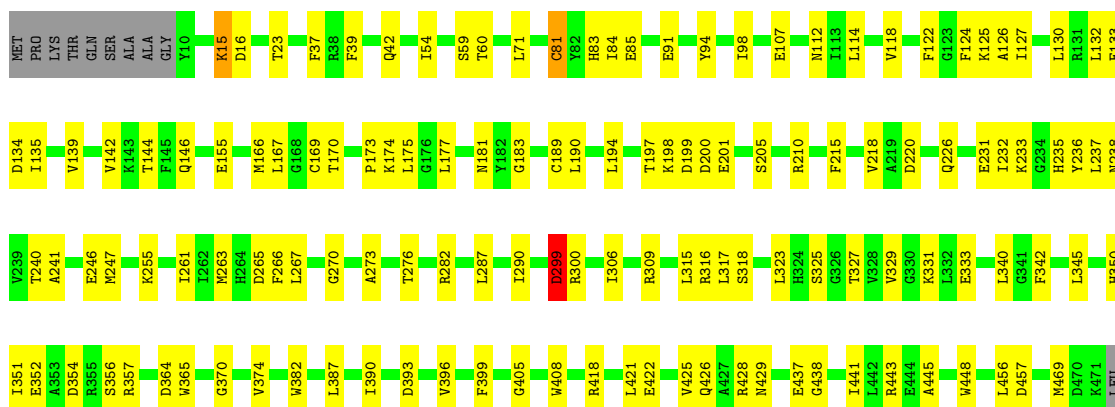
• Molecule 2: Ribulose biphosphate carboxylase large chain

Chain H: 71% 25% ..



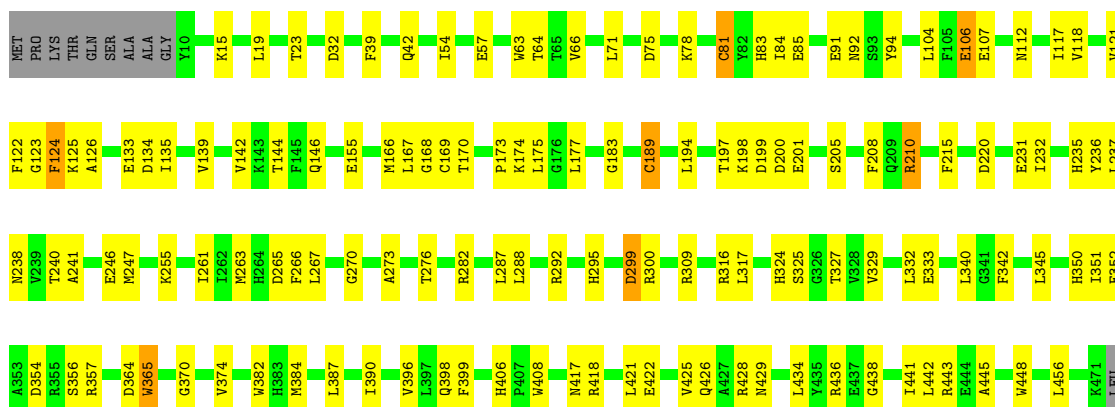
• Molecule 2: Ribulose biphosphate carboxylase large chain

Chain J: 69% 28% .



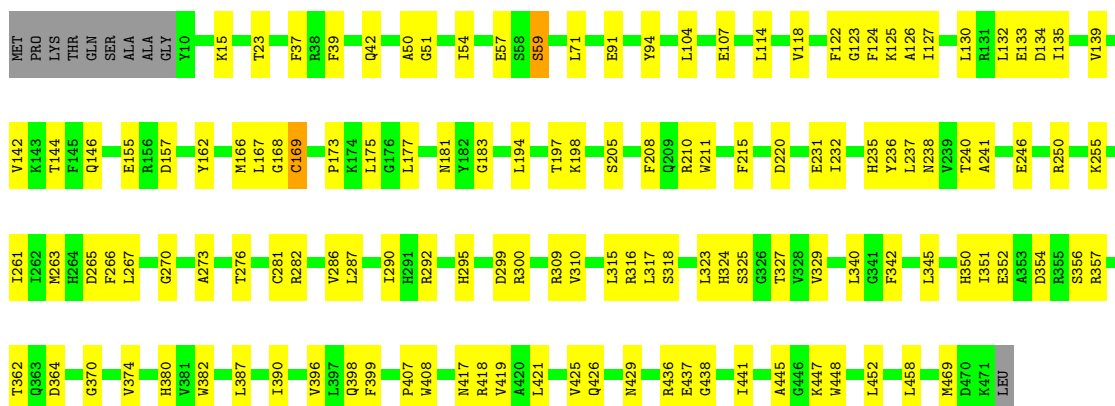
• Molecule 2: Ribulose biphosphate carboxylase large chain

Chain K: 69% 28% ..



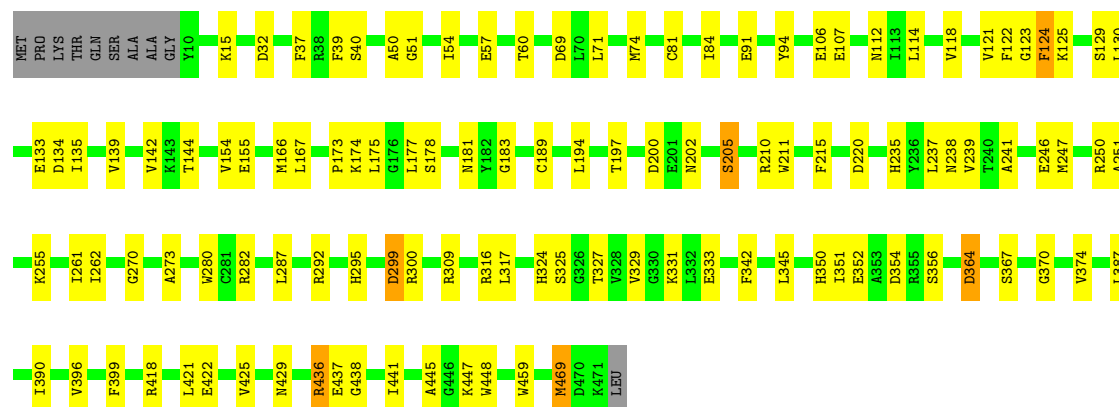
• Molecule 2: Ribulose biphosphate carboxylase large chain

Chain N: 70% 27% .



• Molecule 2: Ribulose biphosphate carboxylase large chain

Chain O: 74% 23% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, Not provided	
Number of subtomograms used	2700	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	145	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.29	0/874	0.61	3/1184 (0.3%)
1	B	0.28	0/874	0.53	0/1184
1	E	0.37	0/874	0.61	1/1184 (0.1%)
1	F	0.41	0/874	0.62	0/1184
1	I	0.30	0/874	0.53	0/1184
1	L	0.32	0/874	0.54	0/1184
1	M	0.28	0/874	0.52	0/1184
1	P	0.33	0/874	0.54	0/1184
2	C	0.27	0/3703	0.52	1/5016 (0.0%)
2	D	0.27	0/3703	0.51	1/5016 (0.0%)
2	G	0.28	0/3720	0.52	1/5038 (0.0%)
2	H	0.28	0/3720	0.53	1/5038 (0.0%)
2	J	0.28	0/3720	0.53	1/5038 (0.0%)
2	K	0.28	0/3720	0.52	1/5038 (0.0%)
2	N	0.30	1/3720 (0.0%)	0.52	1/5038 (0.0%)
2	O	0.28	0/3720	0.53	1/5038 (0.0%)
All	All	0.29	1/36718 (0.0%)	0.53	12/49732 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	169	CYS	CB-SG	-5.91	1.72	1.81

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	PRO	CA-N-CD	-7.71	100.70	111.50
1	A	106	HIS	C-N-CA	6.33	137.52	121.70
2	C	299	ASP	CB-CG-OD1	5.82	123.54	118.30
2	D	299	ASP	CB-CG-OD1	5.79	123.51	118.30
1	E	50	PRO	CA-N-CD	-5.63	103.61	111.50

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	848	0	797	19	0
1	B	848	0	797	32	0
1	E	848	0	797	33	0
1	F	848	0	797	31	0
1	I	848	0	797	25	0
1	L	848	0	797	31	0
1	M	848	0	797	22	0
1	P	848	0	797	33	0
2	C	3611	0	3527	78	0
2	D	3611	0	3527	101	0
2	G	3628	0	3544	97	0
2	H	3628	0	3544	96	0
2	J	3628	0	3544	92	0
2	K	3628	0	3544	92	0
2	N	3628	0	3544	84	0
2	O	3628	0	3544	88	0
All	All	35774	0	34694	851	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 12.

The worst 5 of 851 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)
2:J:261:ILE:HG13	2:J:287:LEU:HB2	1.41	1.01
2:N:261:ILE:HG13	2:N:287:LEU:HB2	1.44	0.99
2:G:261:ILE:HG13	2:G:287:LEU:HB2	1.46	0.97
1:L:29:GLN:OE1	2:O:429:ASN:ND2	2.01	0.94
1:F:17:TYR:CE2	2:G:418:ARG:HG2	2.06	0.89

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 PDB entries followed by that with respect to all EM entries.

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	98/111 (88%)	90 (92%)	8 (8%)	0	100	100
1	B	98/111 (88%)	89 (91%)	9 (9%)	0	100	100
1	E	98/111 (88%)	90 (92%)	8 (8%)	0	100	100
1	F	98/111 (88%)	92 (94%)	6 (6%)	0	100	100
1	I	98/111 (88%)	93 (95%)	5 (5%)	0	100	100
1	L	98/111 (88%)	91 (93%)	7 (7%)	0	100	100
1	M	98/111 (88%)	91 (93%)	7 (7%)	0	100	100
1	P	98/111 (88%)	94 (96%)	4 (4%)	0	100	100
2	C	458/472 (97%)	438 (96%)	20 (4%)	0	100	100
2	D	458/472 (97%)	442 (96%)	16 (4%)	0	100	100
2	G	460/472 (98%)	440 (96%)	20 (4%)	0	100	100
2	H	460/472 (98%)	442 (96%)	18 (4%)	0	100	100
2	J	460/472 (98%)	439 (95%)	21 (5%)	0	100	100
2	K	460/472 (98%)	444 (96%)	16 (4%)	0	100	100
2	N	460/472 (98%)	443 (96%)	17 (4%)	0	100	100
2	O	460/472 (98%)	438 (95%)	22 (5%)	0	100	100
All	All	4460/4664 (96%)	4256 (95%)	204 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	94/104 (90%)	91 (97%)	3 (3%)	34	56
1	B	94/104 (90%)	94 (100%)	0	100	100
1	E	94/104 (90%)	93 (99%)	1 (1%)	70	79
1	F	94/104 (90%)	93 (99%)	1 (1%)	70	79
1	I	94/104 (90%)	91 (97%)	3 (3%)	34	56
1	L	94/104 (90%)	91 (97%)	3 (3%)	34	56
1	M	94/104 (90%)	93 (99%)	1 (1%)	70	79
1	P	94/104 (90%)	94 (100%)	0	100	100
2	C	374/383 (98%)	364 (97%)	10 (3%)	40	60
2	D	374/383 (98%)	359 (96%)	15 (4%)	27	51
2	G	376/383 (98%)	359 (96%)	17 (4%)	23	48
2	H	376/383 (98%)	360 (96%)	16 (4%)	25	49
2	J	376/383 (98%)	360 (96%)	16 (4%)	25	49
2	K	376/383 (98%)	357 (95%)	19 (5%)	20	45
2	N	376/383 (98%)	364 (97%)	12 (3%)	34	56
2	O	376/383 (98%)	361 (96%)	15 (4%)	27	51
All	All	3756/3896 (96%)	3624 (96%)	132 (4%)	33	54

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	447	LYS
2	O	112	ASN
2	O	459	TRP
2	H	71	LEU
2	H	16	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	97	GLN
2	N	429	ASN
1	P	36	GLN
2	O	429	ASN
2	G	406	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

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.