



## Full wwPDB EM Validation Report ⓘ

Mar 24, 2025 – 02:20 PM JST

PDB ID : 9J36  
EMDB ID : EMD-61107  
Title : Cryo-EM structure of Arabidopsis CNGC5  
Authors : Wang, J.P.; Zhang, P.; Zhang, X.  
Deposited on : 2024-08-07  
Resolution : 2.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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) : 2.41.2

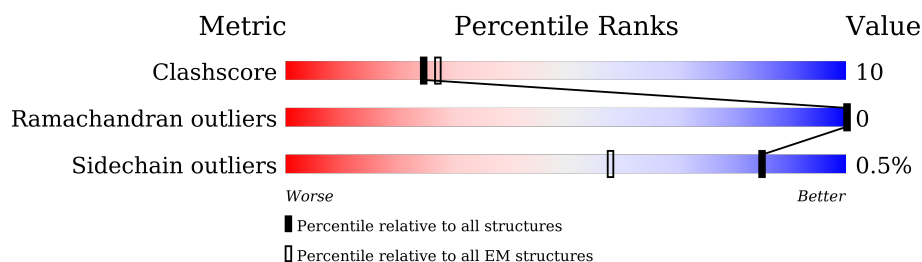
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.50 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  $\geq 3$ , 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	726	58% 14% 28%
1	B	726	58% 14% 28%
1	C	726	59% 13% 28%
1	D	726	58% 14% 28%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16960 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 Probable cyclic nucleotide-gated ion channel 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	523	Total	C	N	O	S	0	0
			4240	2752	710	753	25		
1	C	523	Total	C	N	O	S	0	0
			4240	2752	710	753	25		
1	D	523	Total	C	N	O	S	0	0
			4240	2752	710	753	25		
1	B	523	Total	C	N	O	S	0	0
			4240	2752	710	753	25		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP Q8RWS9
A	-7	ASP	-	expression tag	UNP Q8RWS9
A	-6	TYR	-	expression tag	UNP Q8RWS9
A	-5	LYS	-	expression tag	UNP Q8RWS9
A	-4	ASP	-	expression tag	UNP Q8RWS9
A	-3	ASP	-	expression tag	UNP Q8RWS9
A	-2	ASP	-	expression tag	UNP Q8RWS9
A	-1	ASP	-	expression tag	UNP Q8RWS9
A	0	LYS	-	expression tag	UNP Q8RWS9
C	-8	MET	-	initiating methionine	UNP Q8RWS9
C	-7	ASP	-	expression tag	UNP Q8RWS9
C	-6	TYR	-	expression tag	UNP Q8RWS9
C	-5	LYS	-	expression tag	UNP Q8RWS9
C	-4	ASP	-	expression tag	UNP Q8RWS9
C	-3	ASP	-	expression tag	UNP Q8RWS9
C	-2	ASP	-	expression tag	UNP Q8RWS9
C	-1	ASP	-	expression tag	UNP Q8RWS9
C	0	LYS	-	expression tag	UNP Q8RWS9
D	-8	MET	-	initiating methionine	UNP Q8RWS9
D	-7	ASP	-	expression tag	UNP Q8RWS9
D	-6	TYR	-	expression tag	UNP Q8RWS9
D	-5	LYS	-	expression tag	UNP Q8RWS9

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	ASP	-	expression tag	UNP Q8RWS9
D	-3	ASP	-	expression tag	UNP Q8RWS9
D	-2	ASP	-	expression tag	UNP Q8RWS9
D	-1	ASP	-	expression tag	UNP Q8RWS9
D	0	LYS	-	expression tag	UNP Q8RWS9
B	-8	MET	-	initiating methionine	UNP Q8RWS9
B	-7	ASP	-	expression tag	UNP Q8RWS9
B	-6	TYR	-	expression tag	UNP Q8RWS9
B	-5	LYS	-	expression tag	UNP Q8RWS9
B	-4	ASP	-	expression tag	UNP Q8RWS9
B	-3	ASP	-	expression tag	UNP Q8RWS9
B	-2	ASP	-	expression tag	UNP Q8RWS9
B	-1	ASP	-	expression tag	UNP Q8RWS9
B	0	LYS	-	expression tag	UNP Q8RWS9





PHE  
ILE  
GLN  
ALA  
ALA  
TRP  
ARG  
ARG  
TYR  
CYS  
LYS  
ARG  
LYS  
LYS  
MET  
GLU  
GLU  
ALA  
GLU  
ALA  
GLU  
ALA  
ALA  
ALA  
VAL  
SER  
SER  
SER  
THR  
ALA  
GLY  
PRO  
SER  
TYR  
SER  
SER  
ILE  
GLY  
ALA  
ALA  
PHE  
LEU  
ALA  
THR  
LYS  
PHE  
ALA  
ALA  
ASN  
ALA  
LEU  
ARG  
THR  
ILE  
HIS  
ARG  
ASN  
ARG  
ASN  
THR  
LYS

ILE  
ARG  
ASP  
LEU  
VAL  
LYS  
LEU  
GLN  
LYS  
PRO  
GLU  
PRO  
ASP  
PHE  
THR  
ALA  
ASP

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	204715	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor



## 5 Model quality

### 5.1 Standard geometry

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	0.51	5/4337 (0.1%)	0.66	5/5877 (0.1%)
1	B	0.50	4/4337 (0.1%)	0.65	5/5877 (0.1%)
1	C	0.50	4/4337 (0.1%)	0.68	6/5877 (0.1%)
1	D	0.50	4/4337 (0.1%)	0.66	7/5877 (0.1%)
All	All	0.50	17/17348 (0.1%)	0.66	23/23508 (0.1%)

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	A	0	2
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	384	GLY	CA-C	-6.00	1.42	1.51
1	C	384	GLY	CA-C	-5.94	1.42	1.51
1	D	384	GLY	CA-C	-5.93	1.42	1.51
1	A	384	GLY	CA-C	-5.89	1.42	1.51
1	D	384	GLY	C-N	-5.61	1.21	1.34
1	A	384	GLY	C-N	-5.53	1.21	1.34
1	C	569	GLU	CB-CG	5.38	1.62	1.52
1	D	569	GLU	CB-CG	5.37	1.62	1.52
1	B	569	GLU	CB-CG	5.34	1.62	1.52
1	A	569	GLU	CB-CG	5.33	1.62	1.52
1	B	384	GLY	C-N	-5.21	1.22	1.34
1	C	384	GLY	N-CA	-5.17	1.38	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	GLY	N-CA	-5.13	1.38	1.46
1	C	382	GLY	CA-C	-5.12	1.43	1.51
1	D	384	GLY	N-CA	-5.12	1.38	1.46
1	B	384	GLY	N-CA	-5.09	1.38	1.46
1	A	217	SER	C-N	-5.06	1.22	1.34

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	384	GLY	O-C-N	-11.79	103.83	122.70
1	A	218	ASP	N-CA-CB	-10.25	92.14	110.60
1	C	384	GLY	C-N-CA	10.20	147.20	121.70
1	B	218	ASP	N-CA-CB	-9.88	92.82	110.60
1	D	218	ASP	N-CA-CB	-9.51	93.47	110.60
1	C	218	ASP	N-CA-CB	-9.47	93.55	110.60
1	C	384	GLY	CA-C-N	9.02	137.03	117.20
1	A	569	GLU	CA-CB-CG	7.54	129.98	113.40
1	B	569	GLU	CA-CB-CG	7.51	129.93	113.40
1	D	569	GLU	CA-CB-CG	7.51	129.93	113.40
1	C	569	GLU	CA-CB-CG	7.50	129.90	113.40
1	A	384	GLY	C-N-CA	7.07	139.37	121.70
1	B	384	GLY	C-N-CA	7.05	139.34	121.70
1	D	384	GLY	C-N-CA	6.80	138.70	121.70
1	A	217	SER	O-C-N	-6.77	111.87	122.70
1	B	217	SER	CB-CA-C	6.71	122.84	110.10
1	D	218	ASP	CB-CA-C	6.01	122.41	110.40
1	C	217	SER	CB-CA-C	5.94	121.38	110.10
1	D	217	SER	CB-CA-C	5.93	121.38	110.10
1	A	218	ASP	N-CA-C	5.46	125.73	111.00
1	D	158	GLN	N-CA-C	-5.21	96.94	111.00
1	B	158	GLN	N-CA-C	-5.20	96.97	111.00
1	D	218	ASP	N-CA-C	5.06	124.66	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217	SER	Mainchain
1	A	256	ALA	Peptide
1	B	256	ALA	Peptide
1	C	256	ALA	Peptide
1	D	256	ALA	Peptide

## 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	4240	0	4281	97	0
1	B	4240	0	4282	99	0
1	C	4240	0	4283	94	0
1	D	4240	0	4282	99	0
All	All	16960	0	17128	355	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 10.

All (355) 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:547:THR:CG2	1:A:589:ARG:HG2	1.63	1.28
1:B:547:THR:CG2	1:B:589:ARG:HG2	1.63	1.28
1:C:547:THR:CG2	1:C:589:ARG:HG2	1.63	1.27
1:D:547:THR:CG2	1:D:589:ARG:HG2	1.63	1.27
1:C:155:MET:O	1:C:159:LEU:HG	1.34	1.27
1:C:158:GLN:HA	1:C:161:THR:CG2	1.66	1.25
1:B:158:GLN:HA	1:B:161:THR:CG2	1.72	1.18
1:B:158:GLN:HA	1:B:161:THR:HG21	1.22	1.17
1:D:158:GLN:HA	1:D:161:THR:CG2	1.75	1.15
1:C:156:ALA:HA	1:C:159:LEU:HD12	1.28	1.14
1:D:158:GLN:HA	1:D:161:THR:HG21	1.23	1.13
1:A:158:GLN:HA	1:A:161:THR:CG2	1.78	1.12
1:A:158:GLN:HA	1:A:161:THR:HG21	1.26	1.12
1:C:158:GLN:HA	1:C:161:THR:HG21	1.32	1.11
1:B:156:ALA:HA	1:B:159:LEU:CD1	1.83	1.08
1:D:156:ALA:HA	1:D:159:LEU:HD12	1.32	1.08
1:C:547:THR:HG22	1:C:589:ARG:HG2	1.33	1.07
1:C:156:ALA:HA	1:C:159:LEU:CD1	1.84	1.07
1:D:156:ALA:HA	1:D:159:LEU:CD1	1.83	1.07
1:D:547:THR:HG22	1:D:589:ARG:HG2	1.33	1.07
1:C:154:HIS:CE1	1:C:158:GLN:NE2	2.22	1.07
1:B:542:ARG:HG3	1:B:562:LYS:HG2	1.34	1.06
1:C:155:MET:O	1:C:159:LEU:CG	2.04	1.05

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ALA:HA	1:B:159:LEU:HD12	1.37	1.05
1:A:156:ALA:HA	1:A:159:LEU:HD12	1.38	1.05
1:A:547:THR:HG22	1:A:589:ARG:HG2	1.33	1.05
1:B:155:MET:O	1:B:159:LEU:HG	1.57	1.05
1:C:542:ARG:HG3	1:C:562:LYS:HG2	1.34	1.05
1:D:542:ARG:HG3	1:D:562:LYS:HG2	1.34	1.04
1:B:547:THR:HG22	1:B:589:ARG:HG2	1.33	1.04
1:A:155:MET:O	1:A:159:LEU:HG	1.57	1.04
1:A:542:ARG:HG3	1:A:562:LYS:HG2	1.34	1.04
1:D:155:MET:O	1:D:159:LEU:HG	1.56	1.03
1:D:542:ARG:HD2	1:D:562:LYS:HE2	1.40	1.02
1:A:542:ARG:HD2	1:A:562:LYS:HE2	1.41	1.02
1:C:547:THR:HG22	1:C:589:ARG:CG	1.90	1.02
1:D:547:THR:HG22	1:D:589:ARG:CG	1.90	1.02
1:B:542:ARG:HD2	1:B:562:LYS:HE2	1.41	1.01
1:A:547:THR:HG22	1:A:589:ARG:CG	1.90	1.00
1:B:158:GLN:OE1	1:B:187:TYR:CE1	2.14	1.00
1:A:383:GLN:HG2	1:B:383:GLN:HE22	1.27	0.99
1:B:547:THR:HG22	1:B:589:ARG:CG	1.90	0.99
1:C:542:ARG:HD2	1:C:562:LYS:HE2	1.40	0.99
1:D:158:GLN:OE1	1:D:187:TYR:CE1	2.15	0.99
1:C:158:GLN:HA	1:C:161:THR:HG23	1.44	0.98
1:A:383:GLN:HE22	1:D:383:GLN:HG2	1.27	0.98
1:C:383:GLN:HE22	1:B:383:GLN:HG2	1.26	0.97
1:C:547:THR:CG2	1:C:589:ARG:CG	2.43	0.96
1:D:547:THR:CG2	1:D:589:ARG:CG	2.43	0.95
1:B:547:THR:CG2	1:B:589:ARG:CG	2.43	0.95
1:A:547:THR:CG2	1:A:589:ARG:CG	2.43	0.95
1:C:383:GLN:HG2	1:D:383:GLN:HE22	1.32	0.95
1:A:154:HIS:CE1	1:A:158:GLN:NE2	2.35	0.94
1:C:542:ARG:CD	1:C:562:LYS:HE2	1.98	0.93
1:A:158:GLN:OE1	1:A:187:TYR:CE1	2.22	0.93
1:D:542:ARG:CD	1:D:562:LYS:HE2	1.98	0.92
1:B:542:ARG:CD	1:B:562:LYS:HE2	1.99	0.92
1:A:542:ARG:CD	1:A:562:LYS:HE2	1.99	0.91
1:B:533:ASP:OD1	1:B:584:LEU:HD13	1.71	0.89
1:D:154:HIS:CE1	1:D:158:GLN:NE2	2.41	0.89
1:A:155:MET:O	1:A:159:LEU:CG	2.20	0.89
1:B:154:HIS:CE1	1:B:158:GLN:NE2	2.42	0.87
1:C:158:GLN:CA	1:C:161:THR:HG23	2.05	0.86
1:C:158:GLN:CA	1:C:161:THR:CG2	2.53	0.86

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:GLN:OE1	1:B:187:TYR:HE1	1.59	0.86
1:D:155:MET:O	1:D:159:LEU:CG	2.27	0.82
1:B:158:GLN:CA	1:B:161:THR:CG2	2.57	0.82
1:B:155:MET:O	1:B:159:LEU:CG	2.29	0.81
1:D:158:GLN:OE1	1:D:187:TYR:HE1	1.60	0.81
1:B:158:GLN:HA	1:B:161:THR:HG23	1.61	0.80
1:D:158:GLN:CA	1:D:161:THR:CG2	2.60	0.78
1:C:154:HIS:CE1	1:C:158:GLN:CD	2.57	0.77
1:A:158:GLN:HA	1:A:161:THR:HG23	1.66	0.77
1:D:158:GLN:HA	1:D:161:THR:HG23	1.64	0.77
1:A:155:MET:O	1:A:159:LEU:CD1	2.33	0.76
1:C:154:HIS:NE2	1:C:158:GLN:NE2	2.33	0.76
1:A:383:GLN:O	1:A:383:GLN:HG3	1.84	0.76
1:A:158:GLN:CA	1:A:161:THR:CG2	2.63	0.75
1:B:547:THR:HG21	1:B:589:ARG:HG2	1.68	0.75
1:B:383:GLN:HG3	1:B:383:GLN:O	1.84	0.75
1:D:383:GLN:HG3	1:D:383:GLN:O	1.84	0.75
1:C:383:GLN:O	1:C:383:GLN:HG3	1.84	0.74
1:A:158:GLN:OE1	1:A:187:TYR:HE1	1.66	0.74
1:B:158:GLN:CA	1:B:161:THR:HG23	2.18	0.74
1:B:158:GLN:OE1	1:B:187:TYR:CZ	2.41	0.73
1:D:158:GLN:OE1	1:D:187:TYR:CZ	2.42	0.72
1:D:158:GLN:CA	1:D:161:THR:HG23	2.20	0.71
1:C:158:GLN:OE1	1:C:187:TYR:CE1	2.44	0.71
1:C:547:THR:HG21	1:C:589:ARG:HG2	1.69	0.71
1:D:156:ALA:CA	1:D:159:LEU:HD12	2.17	0.69
1:D:547:THR:HG21	1:D:589:ARG:HG2	1.69	0.69
1:A:158:GLN:CA	1:A:161:THR:HG23	2.22	0.69
1:A:547:THR:HG21	1:A:589:ARG:HG2	1.69	0.69
1:C:155:MET:O	1:C:159:LEU:CD2	2.41	0.69
1:B:156:ALA:CA	1:B:159:LEU:HD12	2.20	0.68
1:A:158:GLN:OE1	1:A:187:TYR:CZ	2.47	0.68
1:C:383:GLN:HE22	1:B:383:GLN:CG	2.05	0.68
1:C:383:GLN:HB2	1:B:380:THR:HG21	1.76	0.68
1:A:544:GLU:OE2	1:A:546:VAL:HG13	1.95	0.67
1:D:527:ARG:HG3	1:D:530:ASP:OD2	1.95	0.66
1:B:544:GLU:OE2	1:B:546:VAL:HG13	1.95	0.66
1:D:443:ARG:HH11	1:B:173:ARG:HD2	1.60	0.66
1:D:544:GLU:OE2	1:D:546:VAL:HG13	1.95	0.66
1:B:527:ARG:HG3	1:B:530:ASP:OD2	1.95	0.66
1:C:544:GLU:OE2	1:C:546:VAL:HG13	1.95	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ALA:CA	1:C:159:LEU:HD12	2.18	0.66
1:C:383:GLN:NE2	1:B:383:GLN:HG2	2.07	0.65
1:C:154:HIS:CE1	1:C:158:GLN:HE22	2.11	0.65
1:C:527:ARG:HG3	1:C:530:ASP:OD2	1.96	0.65
1:D:173:ARG:HD2	1:B:443:ARG:HH11	1.60	0.65
1:C:542:ARG:HG3	1:C:562:LYS:CG	2.20	0.65
1:B:542:ARG:HG3	1:B:562:LYS:CG	2.21	0.65
1:A:156:ALA:HA	1:A:159:LEU:CD1	2.23	0.65
1:D:542:ARG:HD2	1:D:562:LYS:CE	2.24	0.65
1:A:527:ARG:HG3	1:A:530:ASP:OD2	1.96	0.64
1:A:542:ARG:HD2	1:A:562:LYS:CE	2.24	0.64
1:D:542:ARG:HG3	1:D:562:LYS:CG	2.20	0.64
1:C:542:ARG:HD2	1:C:562:LYS:CE	2.23	0.63
1:C:158:GLN:CA	1:C:161:THR:HG21	2.21	0.63
1:C:155:MET:C	1:C:159:LEU:HG	2.16	0.62
1:B:158:GLN:OE1	1:B:187:TYR:OH	2.15	0.62
1:A:542:ARG:HG3	1:A:562:LYS:CG	2.21	0.61
1:C:505:LYS:NZ	1:B:529:GLY:O	2.34	0.61
1:B:547:THR:HG23	1:B:589:ARG:HG2	1.77	0.60
1:C:164:ILE:HG23	1:C:174:GLY:HA3	1.84	0.60
1:A:154:HIS:CE1	1:A:158:GLN:CD	2.75	0.59
1:A:154:HIS:NE2	1:A:158:GLN:NE2	2.51	0.59
1:B:164:ILE:HG23	1:B:174:GLY:HA3	1.84	0.59
1:A:383:GLN:HB2	1:D:380:THR:HG21	1.83	0.59
1:A:164:ILE:HG23	1:A:174:GLY:HA3	1.84	0.59
1:A:548:THR:O	1:A:556:PHE:CD1	2.56	0.59
1:C:548:THR:O	1:C:556:PHE:CD1	2.56	0.59
1:D:114:ASP:OD1	1:D:144:ARG:NH1	2.36	0.58
1:D:164:ILE:HG23	1:D:174:GLY:HA3	1.84	0.58
1:B:548:THR:O	1:B:556:PHE:CD1	2.56	0.58
1:A:114:ASP:OD1	1:A:144:ARG:NH1	2.36	0.58
1:D:548:THR:O	1:D:556:PHE:CD1	2.56	0.58
1:C:106:SER:OG	1:C:147:ILE:HG23	2.04	0.58
1:A:155:MET:O	1:A:159:LEU:HD11	2.03	0.58
1:A:380:THR:HG21	1:B:383:GLN:HB2	1.85	0.58
1:D:547:THR:HG23	1:D:589:ARG:HG2	1.77	0.57
1:B:542:ARG:HD2	1:B:562:LYS:CE	2.24	0.57
1:D:158:GLN:OE1	1:D:187:TYR:OH	2.15	0.57
1:B:114:ASP:OD1	1:B:144:ARG:NH1	2.36	0.57
1:D:106:SER:OG	1:D:147:ILE:HG23	2.04	0.57
1:C:574:TRP:NE1	1:C:583:ASN:O	2.38	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:SER:OG	1:B:147:ILE:HG23	2.04	0.56
1:A:543:LEU:HB2	1:A:561:LEU:HB2	1.87	0.56
1:D:543:LEU:HB2	1:D:561:LEU:HB2	1.87	0.56
1:A:574:TRP:NE1	1:A:583:ASN:O	2.38	0.56
1:C:547:THR:HG23	1:C:589:ARG:HG2	1.77	0.56
1:B:574:TRP:NE1	1:B:583:ASN:O	2.38	0.56
1:B:547:THR:HG21	1:B:589:ARG:CG	2.31	0.56
1:A:106:SER:OG	1:A:147:ILE:HG23	2.04	0.56
1:B:543:LEU:HB2	1:B:561:LEU:HB2	1.87	0.56
1:C:543:LEU:HB2	1:C:561:LEU:HB2	1.87	0.56
1:C:423:THR:HG22	1:D:250:ARG:HA	1.88	0.55
1:C:114:ASP:OD1	1:C:144:ARG:NH1	2.36	0.55
1:D:574:TRP:NE1	1:D:583:ASN:O	2.38	0.55
1:C:158:GLN:OE1	1:C:187:TYR:HE1	1.87	0.54
1:A:158:GLN:OE1	1:A:187:TYR:OH	2.16	0.54
1:A:489:CYS:HB3	1:A:514:LEU:HD12	1.90	0.54
1:A:547:THR:HG21	1:A:589:ARG:CG	2.32	0.53
1:A:423:THR:HG22	1:B:250:ARG:HA	1.90	0.53
1:C:154:HIS:HE1	1:C:158:GLN:HE22	1.54	0.53
1:C:394:ILE:HG21	1:B:368:CYS:HB3	1.91	0.53
1:C:529:GLY:O	1:D:505:LYS:NZ	2.41	0.53
1:D:154:HIS:CE1	1:D:158:GLN:CD	2.81	0.53
1:D:489:CYS:HB3	1:D:514:LEU:HD12	1.90	0.53
1:A:547:THR:HG23	1:A:589:ARG:HG2	1.76	0.53
1:C:158:GLN:OE1	1:C:187:TYR:CZ	2.61	0.53
1:A:289:ASN:HD22	1:A:353:LEU:HD22	1.74	0.52
1:A:509:ALA:O	1:A:513:ARG:NH1	2.42	0.52
1:C:509:ALA:O	1:C:513:ARG:NH1	2.42	0.52
1:D:158:GLN:CA	1:D:161:THR:HG21	2.17	0.52
1:D:289:ASN:HD22	1:D:353:LEU:HD22	1.74	0.52
1:B:542:ARG:HD3	1:B:562:LYS:HE2	1.90	0.52
1:C:289:ASN:HD22	1:C:353:LEU:HD22	1.74	0.52
1:B:100:ASN:HA	1:B:103:PHE:HB3	1.91	0.52
1:B:489:CYS:HB3	1:B:514:LEU:HD12	1.90	0.52
1:B:154:HIS:CE1	1:B:158:GLN:CD	2.83	0.52
1:B:156:ALA:HA	1:B:159:LEU:CG	2.39	0.52
1:C:154:HIS:HE1	1:C:158:GLN:NE2	1.95	0.52
1:C:489:CYS:HB3	1:C:514:LEU:HD12	1.90	0.52
1:B:509:ALA:O	1:B:513:ARG:NH1	2.42	0.52
1:D:154:HIS:NE2	1:D:158:GLN:NE2	2.58	0.52
1:D:509:ALA:O	1:D:513:ARG:NH1	2.42	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:THR:HG23	1:A:589:ARG:HG3	1.92	0.52
1:C:100:ASN:HA	1:C:103:PHE:HB3	1.91	0.52
1:D:533:ASP:N	1:D:533:ASP:OD1	2.43	0.52
1:C:588:THR:HG23	1:C:589:ARG:HG3	1.92	0.52
1:D:588:THR:HG23	1:D:589:ARG:HG3	1.92	0.51
1:B:588:THR:HG23	1:B:589:ARG:HG3	1.92	0.51
1:C:533:ASP:OD1	1:C:533:ASP:N	2.43	0.51
1:B:289:ASN:HD22	1:B:353:LEU:HD22	1.74	0.51
1:D:100:ASN:HA	1:D:103:PHE:HB3	1.92	0.51
1:B:155:MET:O	1:B:159:LEU:CD2	2.58	0.51
1:A:100:ASN:HA	1:A:103:PHE:HB3	1.91	0.51
1:A:154:HIS:HE1	1:A:158:GLN:NE2	2.05	0.51
1:A:157:LEU:O	1:A:161:THR:HG23	2.11	0.51
1:C:547:THR:HG21	1:C:589:ARG:CG	2.32	0.51
1:A:505:LYS:NZ	1:D:529:GLY:O	2.44	0.51
1:D:157:LEU:O	1:D:161:THR:HG23	2.12	0.50
1:B:158:GLN:CA	1:B:161:THR:HG21	2.15	0.50
1:A:394:ILE:HG21	1:D:368:CYS:HB3	1.93	0.50
1:D:258:THR:OG1	1:D:259:ALA:N	2.45	0.50
1:B:156:ALA:HA	1:B:159:LEU:HD11	1.85	0.50
1:A:440:MET:HG2	1:A:445:LEU:HD22	1.94	0.50
1:B:440:MET:HG2	1:B:445:LEU:HD22	1.94	0.50
1:D:155:MET:O	1:D:159:LEU:CD2	2.60	0.50
1:A:250:ARG:HA	1:D:423:THR:HG22	1.93	0.49
1:C:440:MET:HG2	1:C:445:LEU:HD22	1.94	0.49
1:D:440:MET:HG2	1:D:445:LEU:HD22	1.94	0.49
1:C:107:CYS:HB3	1:C:241:VAL:HG12	1.95	0.49
1:B:107:CYS:HB3	1:B:241:VAL:HG12	1.95	0.49
1:D:107:CYS:HB3	1:D:241:VAL:HG12	1.95	0.49
1:A:258:THR:OG1	1:A:259:ALA:N	2.45	0.48
1:C:210:PHE:HD1	1:C:211:LEU:HD12	1.78	0.48
1:C:258:THR:OG1	1:C:259:ALA:N	2.45	0.48
1:B:210:PHE:HD1	1:B:211:LEU:HD12	1.78	0.48
1:A:107:CYS:HB3	1:A:241:VAL:HG12	1.95	0.48
1:B:258:THR:OG1	1:B:259:ALA:N	2.45	0.48
1:C:158:GLN:C	1:C:161:THR:HG23	2.32	0.48
1:D:173:ARG:HD3	1:B:443:ARG:HA	1.94	0.48
1:D:443:ARG:HA	1:B:173:ARG:HD3	1.95	0.48
1:D:547:THR:HG21	1:D:589:ARG:CG	2.32	0.48
1:B:154:HIS:NE2	1:B:158:GLN:NE2	2.59	0.48
1:A:249:LYS:HA	1:A:249:LYS:HD3	1.70	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:GLN:NE2	1:D:383:GLN:HG2	2.11	0.48
1:A:533:ASP:N	1:A:533:ASP:OD1	2.43	0.48
1:C:383:GLN:HG2	1:D:383:GLN:NE2	2.15	0.48
1:A:542:ARG:HD3	1:A:562:LYS:HE2	1.90	0.48
1:C:156:ALA:HA	1:C:159:LEU:CG	2.43	0.48
1:C:158:GLN:OE1	1:C:187:TYR:OH	2.18	0.48
1:C:502:MET:HG3	1:C:503:ASP:HB2	1.96	0.48
1:D:502:MET:HG3	1:D:503:ASP:HB2	1.96	0.48
1:C:288:ARG:HD2	1:C:288:ARG:HA	1.73	0.47
1:D:210:PHE:HD1	1:D:211:LEU:HD12	1.79	0.47
1:A:210:PHE:HD1	1:A:211:LEU:HD12	1.78	0.47
1:D:542:ARG:HD3	1:D:562:LYS:HE2	1.89	0.47
1:C:535:MET:HE1	1:C:572:LEU:HB2	1.97	0.47
1:B:502:MET:HG3	1:B:503:ASP:HB2	1.96	0.47
1:A:502:MET:HG3	1:A:503:ASP:HB2	1.96	0.47
1:C:542:ARG:HD3	1:C:562:LYS:HE2	1.89	0.47
1:B:157:LEU:O	1:B:161:THR:HG23	2.15	0.47
1:A:357:ILE:HA	1:A:360:SER:HB2	1.97	0.46
1:A:383:GLN:HG2	1:B:383:GLN:NE2	2.11	0.46
1:A:535:MET:HE1	1:A:572:LEU:HB2	1.96	0.46
1:D:357:ILE:HA	1:D:360:SER:HB2	1.97	0.46
1:C:353:LEU:HD23	1:C:358:VAL:HG11	1.97	0.46
1:A:288:ARG:HA	1:A:288:ARG:HD2	1.72	0.46
1:D:535:MET:HE1	1:D:572:LEU:HB2	1.97	0.46
1:D:249:LYS:HA	1:D:249:LYS:HD3	1.70	0.46
1:B:353:LEU:HD23	1:B:358:VAL:HG11	1.97	0.46
1:B:357:ILE:HA	1:B:360:SER:HB2	1.97	0.46
1:A:368:CYS:HB3	1:B:394:ILE:HG21	1.98	0.46
1:A:132:ILE:HG12	1:A:219:VAL:HG13	1.98	0.46
1:B:535:MET:HE1	1:B:572:LEU:HB2	1.97	0.46
1:C:547:THR:HG22	1:C:589:ARG:HG3	1.91	0.45
1:A:135:LYS:HA	1:A:138:ILE:HG12	1.99	0.45
1:D:156:ALA:HA	1:D:159:LEU:CG	2.42	0.45
1:A:353:LEU:HD23	1:A:358:VAL:HG11	1.97	0.45
1:C:357:ILE:HA	1:C:360:SER:HB2	1.98	0.45
1:D:156:ALA:HA	1:D:159:LEU:HD11	1.88	0.45
1:D:353:LEU:HD23	1:D:358:VAL:HG11	1.97	0.45
1:B:489:CYS:HB2	1:B:511:CYS:HB2	1.99	0.45
1:C:132:ILE:HG12	1:C:219:VAL:HG13	1.98	0.45
1:A:489:CYS:HB2	1:A:511:CYS:HB2	1.99	0.45
1:B:299:ASP:OD2	1:B:332:LYS:NZ	2.50	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:ASP:OD2	1:D:332:LYS:NZ	2.50	0.45
1:C:135:LYS:HA	1:C:138:ILE:HG12	1.99	0.45
1:C:155:MET:O	1:C:159:LEU:HD21	2.14	0.45
1:B:288:ARG:HA	1:B:288:ARG:HD2	1.72	0.45
1:C:489:CYS:HB2	1:C:511:CYS:HB2	1.99	0.45
1:B:135:LYS:HA	1:B:138:ILE:HG12	1.99	0.45
1:A:299:ASP:OD2	1:A:332:LYS:NZ	2.50	0.44
1:C:155:MET:O	1:C:159:LEU:CD1	2.64	0.44
1:D:132:ILE:HG12	1:D:219:VAL:HG13	1.98	0.44
1:B:522:SER:HA	1:B:592:LYS:HE3	1.99	0.44
1:A:439:TRP:HH2	1:B:484:ILE:HD13	1.83	0.44
1:D:123:ILE:HG12	1:D:130:LEU:HD23	1.99	0.44
1:D:288:ARG:HD2	1:D:288:ARG:HA	1.72	0.44
1:B:123:ILE:HG12	1:B:130:LEU:HD23	1.99	0.44
1:A:522:SER:HA	1:A:592:LYS:HE3	1.99	0.44
1:A:547:THR:HG22	1:A:589:ARG:HA	2.00	0.44
1:B:514:LEU:HB3	1:B:600:PHE:HB3	1.99	0.44
1:A:383:GLN:HE22	1:D:383:GLN:CG	2.15	0.44
1:C:514:LEU:HB3	1:C:600:PHE:HB3	1.99	0.44
1:D:135:LYS:HA	1:D:138:ILE:HG12	1.99	0.44
1:A:123:ILE:HG12	1:A:130:LEU:HD23	1.99	0.44
1:A:547:THR:HG22	1:A:589:ARG:HG3	1.91	0.44
1:D:522:SER:HA	1:D:592:LYS:HE3	1.99	0.44
1:D:547:THR:HG22	1:D:589:ARG:HA	2.00	0.44
1:B:132:ILE:HG12	1:B:219:VAL:HG13	1.98	0.44
1:A:154:HIS:CE1	1:A:158:GLN:HE22	2.27	0.44
1:A:514:LEU:HB3	1:A:600:PHE:HB3	1.99	0.44
1:A:529:GLY:O	1:B:505:LYS:NZ	2.51	0.44
1:C:299:ASP:OD2	1:C:332:LYS:NZ	2.50	0.44
1:D:198:SER:O	1:D:237:ARG:NH1	2.51	0.44
1:D:489:CYS:HB2	1:D:511:CYS:HB2	1.99	0.44
1:B:158:GLN:C	1:B:161:THR:HG23	2.38	0.44
1:C:123:ILE:HG12	1:C:130:LEU:HD23	1.99	0.43
1:D:514:LEU:HB3	1:D:600:PHE:HB3	1.99	0.43
1:B:507:LEU:HA	1:B:510:ILE:HD12	2.00	0.43
1:B:547:THR:HG22	1:B:589:ARG:HA	2.00	0.43
1:D:154:HIS:HE1	1:D:158:GLN:NE2	2.11	0.43
1:D:507:LEU:HA	1:D:510:ILE:HD12	2.00	0.43
1:C:183:ILE:HA	1:C:186:ARG:HB3	2.01	0.43
1:C:547:THR:HG22	1:C:589:ARG:HA	2.00	0.43
1:C:522:SER:HA	1:C:592:LYS:HE3	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:ILE:HA	1:D:186:ARG:HB3	2.01	0.43
1:B:198:SER:O	1:B:237:ARG:NH1	2.51	0.43
1:B:496:VAL:HB	1:B:499:PHE:HB2	2.00	0.43
1:A:198:SER:O	1:A:237:ARG:NH1	2.51	0.43
1:B:547:THR:HG22	1:B:589:ARG:HG3	1.91	0.43
1:A:158:GLN:CA	1:A:161:THR:HG21	2.20	0.43
1:C:198:SER:O	1:C:237:ARG:NH1	2.51	0.43
1:C:249:LYS:HD3	1:C:249:LYS:HA	1.70	0.43
1:B:154:HIS:CE1	1:B:158:GLN:HE22	2.34	0.43
1:A:496:VAL:HB	1:A:499:PHE:HB2	2.00	0.42
1:A:507:LEU:HA	1:A:510:ILE:HD12	2.00	0.42
1:B:183:ILE:HA	1:B:186:ARG:HB3	2.01	0.42
1:A:505:LYS:HE3	1:D:531:PRO:HD3	2.01	0.42
1:D:547:THR:HG22	1:D:589:ARG:HG3	1.91	0.42
1:A:183:ILE:HA	1:A:186:ARG:HB3	2.01	0.42
1:C:496:VAL:HB	1:C:499:PHE:HB2	2.00	0.42
1:C:118:PHE:HB2	1:C:279:ALA:HB1	2.02	0.42
1:B:249:LYS:HA	1:B:249:LYS:HD3	1.70	0.42
1:D:496:VAL:HB	1:D:499:PHE:HB2	2.00	0.42
1:A:210:PHE:HD2	1:A:218:ASP:HB3	1.85	0.42
1:D:158:GLN:C	1:D:161:THR:HG23	2.40	0.42
1:C:507:LEU:HA	1:C:510:ILE:HD12	2.00	0.41
1:C:570:GLU:H	1:C:570:GLU:HG2	1.69	0.41
1:D:525:LEU:HD23	1:D:536:LEU:HD13	2.02	0.41
1:D:118:PHE:HB2	1:D:279:ALA:HB1	2.02	0.41
1:C:525:LEU:HD23	1:C:536:LEU:HD13	2.02	0.41
1:A:340:ASN:ND2	1:D:338:ASP:HB3	2.36	0.41
1:A:443:ARG:HH11	1:C:173:ARG:HD2	1.86	0.41
1:A:571:LEU:HG	1:A:607:LEU:HD23	2.03	0.41
1:B:118:PHE:HB2	1:B:279:ALA:HB1	2.01	0.41
1:C:210:PHE:HD2	1:C:218:ASP:HB3	1.85	0.41
1:B:608:LYS:HE3	1:B:608:LYS:HB3	1.87	0.41
1:A:158:GLN:C	1:A:161:THR:HG23	2.41	0.41
1:C:443:ARG:NH2	1:D:469:GLU:OE1	2.47	0.41
1:B:210:PHE:HD2	1:B:218:ASP:HB3	1.85	0.41
1:B:390:TYR:HA	1:B:391:PRO:HD3	1.94	0.41
1:D:210:PHE:HD2	1:D:218:ASP:HB3	1.85	0.41
1:D:570:GLU:H	1:D:570:GLU:HG2	1.69	0.40
1:A:118:PHE:HB2	1:A:279:ALA:HB1	2.02	0.40
1:A:525:LEU:HD23	1:A:536:LEU:HD13	2.02	0.40
1:B:525:LEU:HD23	1:B:536:LEU:HD13	2.02	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ASP:HB3	1:B:340:ASN:ND2	2.36	0.40
1:A:484:ILE:HD13	1:D:439:TRP:HH2	1.87	0.40
1:B:571:LEU:HG	1:B:607:LEU:HD23	2.03	0.40
1:D:571:LEU:HG	1:D:607:LEU:HD23	2.03	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 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	519/726 (72%)	484 (93%)	35 (7%)	0	100	100
1	B	519/726 (72%)	485 (93%)	34 (7%)	0	100	100
1	C	519/726 (72%)	485 (93%)	34 (7%)	0	100	100
1	D	519/726 (72%)	485 (93%)	34 (7%)	0	100	100
All	All	2076/2904 (72%)	1939 (93%)	137 (7%)	0	100	100

There are no Ramachandran outliers to report.

### 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 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	463/631 (73%)	461 (100%)	2 (0%)	89	96
1	B	463/631 (73%)	461 (100%)	2 (0%)	89	96

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	463/631 (73%)	460 (99%)	3 (1%)	84	94
1	D	463/631 (73%)	461 (100%)	2 (0%)	89	96
All	All	1852/2524 (73%)	1843 (100%)	9 (0%)	85	95

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	381	LEU
1	A	501	SER
1	C	214	SER
1	C	381	LEU
1	C	501	SER
1	D	381	LEU
1	D	501	SER
1	B	381	LEU
1	B	501	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	HIS
1	A	289	ASN
1	A	340	ASN
1	A	383	GLN
1	A	414	ASN
1	C	154	HIS
1	C	289	ASN
1	C	383	GLN
1	C	416	GLN
1	D	154	HIS
1	D	289	ASN
1	D	340	ASN
1	D	383	GLN
1	B	154	HIS
1	B	289	ASN
1	B	340	ASN
1	B	383	GLN
1	B	414	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](#)

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.