Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Apr 25, 2019 – 12:53 PM EDT

PDB ID	:	6GYO
EMDB ID:	:	EMD-0094
Title	:	Structure of human HCN4 hyperpolarization-activated cyclic nucleotide-gated ion channel in complex with cAMP
Authors	:	Shintre, C.A.; Pike, A.C.W.; Tessitore, A.; Young, M.; Bushell, S.R.; Strain-Damerell, C.; Mukhopadhyay, S.; Burgess-Brown, N.A.; Huiskonen, J.T.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Carpenter, E.P.; Structural Genomics Consortium (SGC)
Deposited on	:	2018-06-30
Resolution	:	3.40 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report for a publicly released PDB/EMDB 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 (i) symbol.

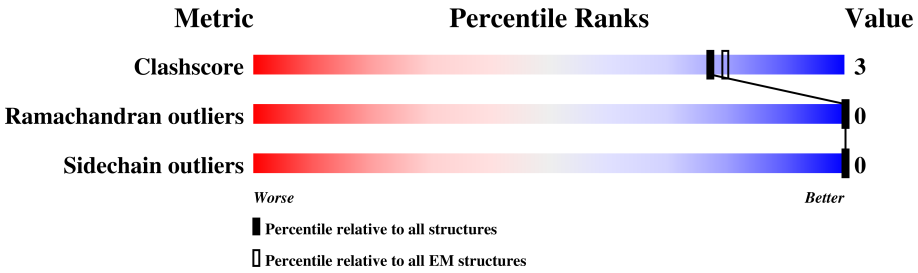
MolProbity	:	4.02b-467
Mogul	:	1.8.0 (224370), CSD as540be (2019)
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	521	88% 8% .
1	B	521	88% 8% .
1	C	521	88% 8% .
1	D	521	89% 7% .

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17540 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.

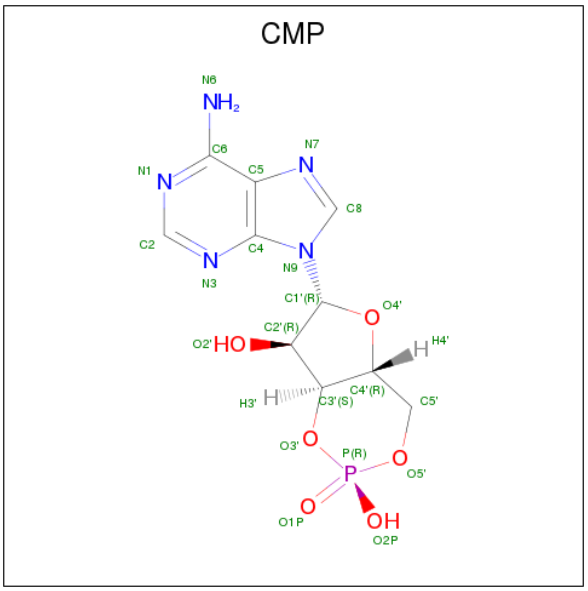
- Molecule 1 is a protein called Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	501	Total	C	N	O	S	0	0
			4047	2628	689	698	32		
1	B	501	Total	C	N	O	S	0	0
			4047	2628	689	698	32		
1	C	501	Total	C	N	O	S	0	0
			4047	2628	689	698	32		
1	D	501	Total	C	N	O	S	0	0
			4047	2628	689	698	32		

There are 8 discrepancies between the modelled and reference sequences:

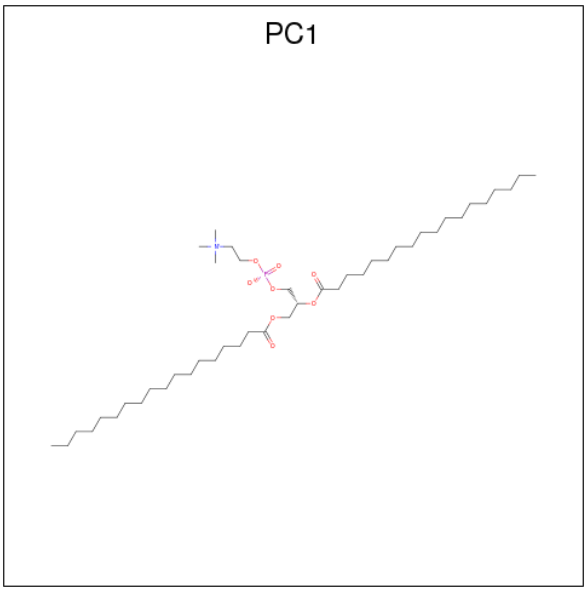
Chain	Residue	Modelled	Actual	Comment	Reference
A	199	SER	-	expression tag	UNP Q9Y3Q4
A	200	MET	-	expression tag	UNP Q9Y3Q4
B	199	SER	-	expression tag	UNP Q9Y3Q4
B	200	MET	-	expression tag	UNP Q9Y3Q4
C	199	SER	-	expression tag	UNP Q9Y3Q4
C	200	MET	-	expression tag	UNP Q9Y3Q4
D	199	SER	-	expression tag	UNP Q9Y3Q4
D	200	MET	-	expression tag	UNP Q9Y3Q4

- Molecule 2 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: $C_{10}H_{12}N_5O_6P$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	B	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	C	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	D	1	Total	C	N	O	P	0
			22	10	5	6	1	

- Molecule 3 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



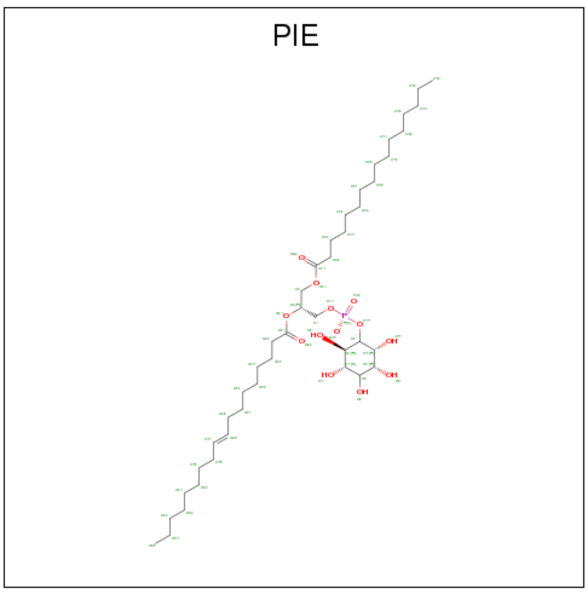
Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C N O P 197 155 2 37 3	0
3	A	1	Total C N O P 197 155 2 37 3	0
3	A	1	Total C N O P 197 155 2 37 3	0
3	A	1	Total C N O P 197 155 2 37 3	0
3	A	1	Total C N O P 197 155 2 37 3	0
3	A	1	Total C N O P 197 155 2 37 3	0
3	A	1	Total C N O P 197 155 2 37 3	0
3	B	1	Total C N O P 197 155 2 37 3	0
3	B	1	Total C N O P 197 155 2 37 3	0
3	B	1	Total C N O P 197 155 2 37 3	0
3	B	1	Total C N O P 197 155 2 37 3	0
3	B	1	Total C N O P 197 155 2 37 3	0
3	B	1	Total C N O P 197 155 2 37 3	0
3	B	1	Total C N O P 197 155 2 37 3	0
3	C	1	Total C N O P 197 155 2 37 3	0
3	C	1	Total C N O P 197 155 2 37 3	0
3	C	1	Total C N O P 197 155 2 37 3	0
3	C	1	Total C N O P 197 155 2 37 3	0
3	C	1	Total C N O P 197 155 2 37 3	0
3	C	1	Total C N O P 197 155 2 37 3	0
3	C	1	Total C N O P 197 155 2 37 3	0
3	D	1	Total C N O P 197 155 2 37 3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
3	D	1	Total C N O P 197 155 2 37 3	0
3	D	1	Total C N O P 197 155 2 37 3	0
3	D	1	Total C N O P 197 155 2 37 3	0
3	D	1	Total C N O P 197 155 2 37 3	0
3	D	1	Total C N O P 197 155 2 37 3	0
3	D	1	Total C N O P 197 155 2 37 3	0

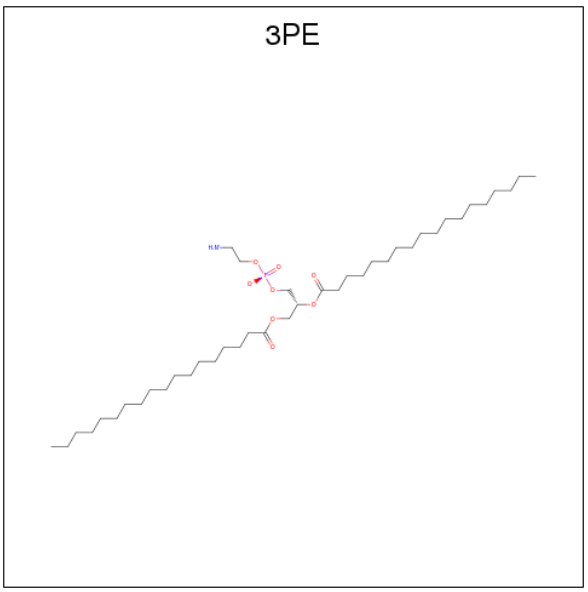
- Molecule 4 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOINOSITOL (three-letter code: PIE) (formula: $C_{43}H_{80}O_{13}P$).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C O P 32 18 13 1	0
4	B	1	Total C O P 32 18 13 1	0
4	C	1	Total C O P 32 18 13 1	0
4	D	1	Total C O P 32 18 13 1	0

- Molecule 5 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter

code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			86	66	2	16	2	
5	A	1	Total	C	N	O	P	0
			86	66	2	16	2	
5	B	1	Total	C	N	O	P	0
			86	66	2	16	2	
5	B	1	Total	C	N	O	P	0
			86	66	2	16	2	
5	C	1	Total	C	N	O	P	0
			86	66	2	16	2	
5	C	1	Total	C	N	O	P	0
			86	66	2	16	2	
5	D	1	Total	C	N	O	P	0
			86	66	2	16	2	
5	D	1	Total	C	N	O	P	0
			86	66	2	16	2	

- Molecule 6 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	X	0
			1	1	
6	A	1	Total	X	0
			1	1	
6	D	1	Total	X	0
			1	1	

Continued on next page...

Continued from previous page...

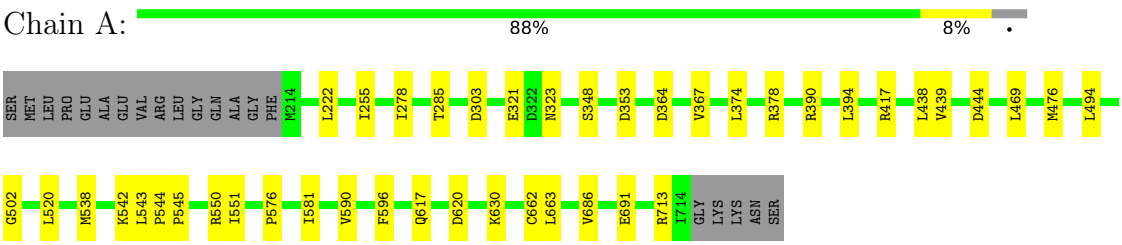
Mol	Chain	Residues	Atoms	AltConf
6	C	1	Total X 1 1	0

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. 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.

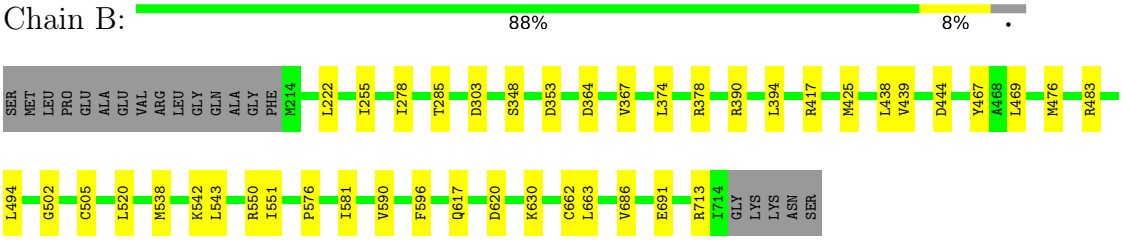
• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 4

Chain A:



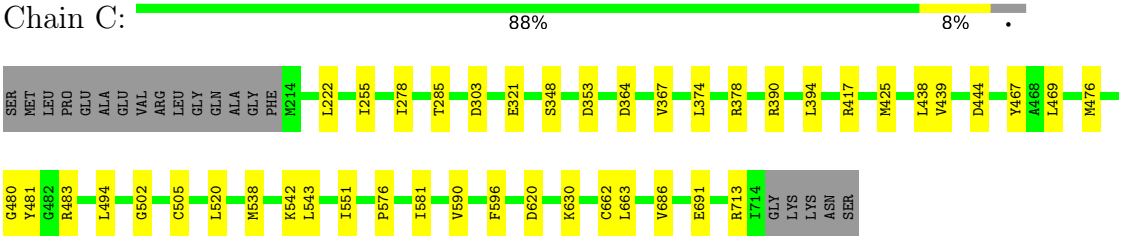
• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 4

Chain B:



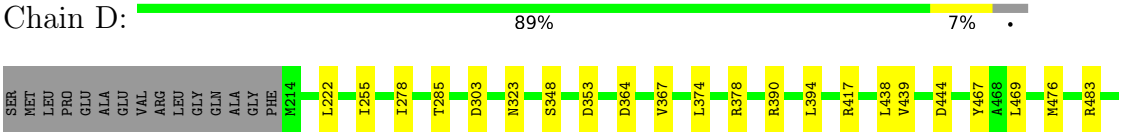
• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 4

Chain C:



• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 4

Chain D:




L494
G502
L520
M538
L543
I551
P576
I581
V590
F596
D620
K630
C662
L663
V686
E691
R713
T714
GLY
LYS
LYS
ASN
SER

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	55829	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	37313	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UNX, PC1, CMP, 3PE, PIE

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	$\#\|Z\| > 2$	RMSZ	$\#\|Z\| > 2$
1	A	0.49	0/4143	0.53	0/5608
1	B	0.49	0/4143	0.53	0/5608
1	C	0.49	0/4143	0.53	0/5608
1	D	0.48	0/4143	0.53	0/5608
All	All	0.49	0/16572	0.53	0/22432

There are no bond length outliers.

There are no bond angle outliers.

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	4047	0	4034	31	0
1	B	4047	0	4034	30	0
1	C	4047	0	4034	32	0
1	D	4047	0	4034	28	0
2	A	22	0	11	3	0
2	B	22	0	11	3	0
2	C	22	0	11	3	0
2	D	22	0	11	3	0
3	A	197	0	243	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	197	0	243	2	0
3	C	197	0	243	2	0
3	D	197	0	243	2	0
4	A	32	0	26	0	0
4	B	32	0	26	0	0
4	C	32	0	26	0	0
4	D	32	0	26	0	0
5	A	86	0	120	5	0
5	B	86	0	120	5	0
5	C	86	0	120	5	0
5	D	86	0	120	5	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
All	All	17540	0	17736	113	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 3.

All (113) 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:C:801:CMP:C2	2:C:801:CMP:H2	0.97	1.50
2:B:801:CMP:H2	2:B:801:CMP:C2	0.97	1.49
2:D:801:CMP:H2	2:D:801:CMP:C2	0.97	1.49
2:A:801:CMP:C2	2:A:801:CMP:H2	0.97	1.47
1:B:285:THR:HG22	1:B:438:LEU:HD13	1.83	0.60
1:C:303:ASP:OD1	1:C:390:ARG:NH2	2.35	0.60
1:D:303:ASP:OD1	1:D:390:ARG:NH2	2.35	0.60
1:A:285:THR:HG22	1:A:438:LEU:HD13	1.83	0.60
1:B:303:ASP:OD1	1:B:390:ARG:NH2	2.35	0.59
1:A:303:ASP:OD1	1:A:390:ARG:NH2	2.35	0.59
1:D:285:THR:HG22	1:D:438:LEU:HD13	1.83	0.59
1:C:285:THR:HG22	1:C:438:LEU:HD13	1.83	0.59
1:C:222:LEU:HD22	1:C:255:ILE:HG12	1.87	0.56
1:D:222:LEU:HD22	1:D:255:ILE:HG12	1.87	0.56
1:A:222:LEU:HD22	1:A:255:ILE:HG12	1.87	0.55
1:D:417:ARG:NH1	5:D:811:3PE:O12	2.39	0.55
1:A:417:ARG:NH1	5:A:811:3PE:O12	2.39	0.55
1:C:417:ARG:NH1	5:C:810:3PE:O12	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:LEU:HD22	1:B:255:ILE:HG12	1.87	0.55
1:B:417:ARG:NH1	5:B:810:3PE:O12	2.39	0.55
1:B:469:LEU:HD21	5:B:811:3PE:H3E2	1.89	0.55
1:C:469:LEU:HD21	5:C:811:3PE:H3E2	1.89	0.54
1:A:469:LEU:HD21	5:A:810:3PE:H3E2	1.89	0.54
1:D:469:LEU:HD21	5:D:810:3PE:H3E2	1.89	0.54
1:D:378:ARG:NH2	1:D:444:ASP:OD1	2.41	0.54
1:C:378:ARG:NH2	1:C:444:ASP:OD1	2.41	0.53
1:B:378:ARG:NH2	1:B:444:ASP:OD1	2.41	0.52
1:B:476:MET:HA	1:B:502:GLY:HA3	1.92	0.52
1:A:476:MET:HA	1:A:502:GLY:HA3	1.92	0.52
1:C:476:MET:HA	1:C:502:GLY:HA3	1.92	0.52
1:A:576:PRO:HG2	1:D:620:ASP:HB3	1.92	0.51
1:D:476:MET:HA	1:D:502:GLY:HA3	1.92	0.51
1:A:378:ARG:NH2	1:A:444:ASP:OD1	2.41	0.50
1:D:663:LEU:HG	1:D:686:VAL:HG22	1.93	0.50
1:B:374:LEU:HD21	1:B:378:ARG:HH21	1.77	0.50
1:B:663:LEU:HG	1:B:686:VAL:HG22	1.93	0.50
3:C:807:PC1:H321	5:C:810:3PE:H31	1.94	0.50
3:A:805:PC1:H321	5:A:811:3PE:H31	1.94	0.49
3:D:808:PC1:H321	5:D:811:3PE:H31	1.94	0.49
1:A:374:LEU:HD21	1:A:378:ARG:HH21	1.77	0.49
1:D:374:LEU:HD21	1:D:378:ARG:HH21	1.77	0.49
3:B:807:PC1:H321	5:B:810:3PE:H31	1.94	0.49
1:C:663:LEU:HG	1:C:686:VAL:HG22	1.93	0.49
1:A:663:LEU:HG	1:A:686:VAL:HG22	1.93	0.49
1:C:620:ASP:HB3	1:D:576:PRO:HG2	1.95	0.49
1:C:374:LEU:HD21	1:C:378:ARG:HH21	1.77	0.49
1:A:620:ASP:HB3	1:B:576:PRO:HG2	1.95	0.47
1:B:620:ASP:HB3	1:C:576:PRO:HG2	1.95	0.47
1:A:538:MET:HG2	1:A:543:LEU:HD12	1.97	0.47
1:D:538:MET:HG2	1:D:543:LEU:HD12	1.97	0.46
1:B:364:ASP:HB3	1:B:367:VAL:HB	1.98	0.46
1:D:364:ASP:HB3	1:D:367:VAL:HB	1.98	0.46
1:A:364:ASP:HB3	1:A:367:VAL:HB	1.98	0.46
1:A:520:LEU:HD11	3:B:806:PC1:H31	1.98	0.46
1:C:364:ASP:HB3	1:C:367:VAL:HB	1.98	0.46
1:B:538:MET:HG2	1:B:543:LEU:HD12	1.97	0.46
1:B:590:VAL:HG13	1:B:596:PHE:HB3	1.99	0.45
1:C:590:VAL:HG13	1:C:596:PHE:HB3	1.99	0.45
1:C:538:MET:HG2	1:C:543:LEU:HD12	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:ILE:HD11	1:D:551:ILE:HD11	1.98	0.45
1:C:520:LEU:HD11	3:D:807:PC1:H31	1.98	0.45
1:D:590:VAL:HG13	1:D:596:PHE:HB3	1.99	0.45
1:A:713:ARG:NH1	2:A:801:CMP:N1	2.65	0.45
1:C:713:ARG:NH1	2:C:801:CMP:N1	2.65	0.45
1:A:590:VAL:HG13	1:A:596:PHE:HB3	1.99	0.45
1:B:713:ARG:NH1	2:B:801:CMP:N1	2.65	0.44
1:C:439:VAL:HB	1:C:494:LEU:HD11	2.00	0.44
3:A:804:PC1:H31	1:D:520:LEU:HD11	1.99	0.44
1:B:439:VAL:HB	1:B:494:LEU:HD11	1.99	0.44
1:D:394:LEU:HD21	5:D:811:3PE:H362	2.00	0.44
1:B:394:LEU:HD21	5:B:810:3PE:H362	2.00	0.44
1:B:520:LEU:HD11	3:C:806:PC1:H31	1.99	0.44
1:D:713:ARG:NH1	2:D:801:CMP:N1	2.65	0.44
1:A:691:GLU:OE2	1:D:630:LYS:NZ	2.50	0.43
1:C:394:LEU:HD21	5:C:810:3PE:H362	2.00	0.43
1:C:630:LYS:NZ	1:D:691:GLU:OE2	2.51	0.43
1:A:394:LEU:HD21	5:A:811:3PE:H362	2.00	0.43
1:D:439:VAL:HB	1:D:494:LEU:HD11	2.00	0.43
1:A:278:ILE:HD11	5:A:811:3PE:H3B2	2.01	0.43
1:A:353:ASP:OD1	1:A:353:ASP:N	2.52	0.43
1:D:353:ASP:OD1	1:D:353:ASP:N	2.52	0.43
1:B:353:ASP:OD1	1:B:353:ASP:N	2.52	0.43
1:D:278:ILE:HD11	5:D:811:3PE:H3B2	2.01	0.43
1:A:439:VAL:HB	1:A:494:LEU:HD11	2.00	0.43
1:D:662:CYS:SG	2:D:801:CMP:O2P	2.71	0.43
1:B:550:ARG:O	1:B:617:GLN:NE2	2.42	0.43
1:B:542:LYS:NZ	1:D:323:ASN:O	2.48	0.42
1:B:278:ILE:HD11	5:B:810:3PE:H3B2	2.01	0.42
1:B:630:LYS:NZ	1:C:691:GLU:OE2	2.52	0.42
1:C:278:ILE:HD11	5:C:810:3PE:H3B2	2.01	0.42
1:B:551:ILE:HD11	1:C:581:ILE:HD11	2.00	0.42
1:A:630:LYS:NZ	1:B:691:GLU:OE2	2.52	0.42
1:C:662:CYS:SG	2:C:801:CMP:O2P	2.71	0.42
1:C:551:ILE:HD11	1:D:581:ILE:HD11	2.01	0.42
1:B:662:CYS:SG	2:B:801:CMP:O2P	2.71	0.42
1:C:480:GLY:HA2	1:C:481:TYR:HA	1.86	0.42
1:B:467:TYR:OH	1:B:483:ARG:N	2.53	0.41
1:C:348:SER:HB2	1:C:390:ARG:HG3	2.02	0.41
1:C:467:TYR:OH	1:C:483:ARG:N	2.53	0.41
1:D:348:SER:HB2	1:D:390:ARG:HG3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:ILE:HD11	1:B:581:ILE:HD11	2.01	0.41
1:A:321:GLU:HA	1:C:542:LYS:HE2	2.03	0.41
1:A:323:ASN:O	1:C:542:LYS:NZ	2.46	0.41
1:A:544:PRO:HA	1:A:545:PRO:HD3	1.93	0.41
1:C:353:ASP:OD1	1:C:353:ASP:N	2.52	0.41
1:B:348:SER:HB2	1:B:390:ARG:HG3	2.02	0.41
1:A:550:ARG:O	1:A:617:GLN:NE2	2.42	0.41
1:A:662:CYS:SG	2:A:801:CMP:O2P	2.71	0.41
1:A:348:SER:HB2	1:A:390:ARG:HG3	2.02	0.41
1:A:542:LYS:HE2	1:C:321:GLU:HA	2.02	0.40
1:B:425:MET:HG2	1:B:505:CYS:HB3	2.03	0.40
1:D:467:TYR:OH	1:D:483:ARG:N	2.53	0.40
1:C:425:MET:HG2	1:C:505:CYS:HB3	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	499/521 (96%)	476 (95%)	23 (5%)	0	100	100
1	B	499/521 (96%)	476 (95%)	23 (5%)	0	100	100
1	C	499/521 (96%)	476 (95%)	23 (5%)	0	100	100
1	D	499/521 (96%)	476 (95%)	23 (5%)	0	100	100
All	All	1996/2084 (96%)	1904 (95%)	92 (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	432/469 (92%)	432 (100%)	0	100	100
1	B	432/469 (92%)	432 (100%)	0	100	100
1	C	432/469 (92%)	432 (100%)	0	100	100
1	D	432/469 (92%)	432 (100%)	0	100	100
All	All	1728/1876 (92%)	1728 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	ASN
1	B	299	ASN
1	C	299	ASN
1	D	299	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 48 ligands modelled in this entry, 4 are unknown - leaving 44 for Mogul analysis.

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	CMP	A	801	-	20,25,25	1.06	2 (10%)	21,39,39	1.14	2 (9%)
3	PC1	A	803	-	28,28,53	0.40	0	31,33,61	0.51	0
3	PC1	A	804	-	26,26,53	0.25	0	28,28,61	0.32	0
3	PC1	A	805	-	17,17,53	0.30	0	17,17,61	0.22	0
3	PC1	A	806	-	27,27,53	0.82	1 (3%)	26,26,61	0.43	1 (3%)
3	PC1	A	807	-	31,31,53	0.42	0	34,36,61	0.70	1 (2%)
3	PC1	A	808	-	19,19,53	0.29	0	21,21,61	0.22	0
3	PC1	A	809	-	41,41,53	0.35	0	44,46,61	0.32	0
5	3PE	A	810	-	45,45,50	0.31	0	48,50,55	0.27	0
5	3PE	A	811	-	39,39,50	0.33	0	42,44,55	0.33	0
4	PIE	A	812	-	32,32,57	0.98	1 (3%)	42,44,69	0.62	0
2	CMP	B	801	-	20,25,25	1.06	2 (10%)	21,39,39	1.15	2 (9%)
3	PC1	B	803	-	27,27,53	0.82	1 (3%)	26,26,61	0.44	1 (3%)
3	PC1	B	804	-	41,41,53	0.35	0	44,46,61	0.32	0
3	PC1	B	805	-	28,28,53	0.41	0	31,33,61	0.51	0
3	PC1	B	806	-	26,26,53	0.25	0	28,28,61	0.32	0
3	PC1	B	807	-	17,17,53	0.30	0	17,17,61	0.22	0
3	PC1	B	808	-	31,31,53	0.42	0	34,36,61	0.70	1 (2%)
3	PC1	B	809	-	19,19,53	0.28	0	21,21,61	0.22	0
5	3PE	B	810	-	39,39,50	0.33	0	42,44,55	0.32	0
5	3PE	B	811	-	45,45,50	0.31	0	48,50,55	0.28	0
4	PIE	B	812	-	32,32,57	0.98	1 (3%)	42,44,69	0.62	0
2	CMP	C	801	-	20,25,25	1.07	2 (10%)	21,39,39	1.15	2 (9%)
3	PC1	C	803	-	27,27,53	0.82	1 (3%)	26,26,61	0.44	1 (3%)
3	PC1	C	804	-	41,41,53	0.35	0	44,46,61	0.32	0
3	PC1	C	805	-	28,28,53	0.41	0	31,33,61	0.51	0
3	PC1	C	806	-	26,26,53	0.25	0	28,28,61	0.32	0
3	PC1	C	807	-	17,17,53	0.31	0	17,17,61	0.22	0
3	PC1	C	808	-	31,31,53	0.42	0	34,36,61	0.70	1 (2%)
3	PC1	C	809	-	19,19,53	0.29	0	21,21,61	0.22	0
5	3PE	C	810	-	39,39,50	0.33	0	42,44,55	0.33	0
5	3PE	C	811	-	45,45,50	0.31	0	48,50,55	0.28	0
4	PIE	C	812	-	32,32,57	0.98	1 (3%)	42,44,69	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CMP	D	801	-	20,25,25	1.05	2 (10%)	21,39,39	1.15	2 (9%)
3	PC1	D	803	-	19,19,53	0.28	0	21,21,61	0.21	0
3	PC1	D	804	-	27,27,53	0.82	1 (3%)	26,26,61	0.44	1 (3%)
3	PC1	D	805	-	41,41,53	0.35	0	44,46,61	0.32	0
3	PC1	D	806	-	28,28,53	0.40	0	31,33,61	0.51	0
3	PC1	D	807	-	26,26,53	0.25	0	28,28,61	0.32	0
3	PC1	D	808	-	17,17,53	0.31	0	17,17,61	0.22	0
3	PC1	D	809	-	31,31,53	0.42	0	34,36,61	0.70	1 (2%)
5	3PE	D	810	-	45,45,50	0.30	0	48,50,55	0.28	0
5	3PE	D	811	-	39,39,50	0.33	0	42,44,55	0.33	0
4	PIE	D	812	-	32,32,57	0.98	1 (3%)	42,44,69	0.62	0

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
2	CMP	A	801	-	-	0/0/31/31	0/4/4/4
3	PC1	A	803	-	-	0/32/32/57	0/0/0/0
3	PC1	A	804	-	-	0/27/27/57	0/0/0/0
3	PC1	A	805	-	-	0/16/16/57	0/0/0/0
3	PC1	A	806	-	-	0/24/24/57	0/0/0/0
3	PC1	A	807	-	-	0/35/35/57	0/0/0/0
3	PC1	A	808	-	-	0/20/20/57	0/0/0/0
3	PC1	A	809	-	-	0/45/45/57	0/0/0/0
5	3PE	A	810	-	-	0/49/49/54	0/0/0/0
5	3PE	A	811	-	-	0/43/43/54	0/0/0/0
4	PIE	A	812	-	-	0/27/51/76	0/1/1/1
2	CMP	B	801	-	-	0/0/31/31	0/4/4/4
3	PC1	B	803	-	-	0/24/24/57	0/0/0/0
3	PC1	B	804	-	-	0/45/45/57	0/0/0/0
3	PC1	B	805	-	-	0/32/32/57	0/0/0/0
3	PC1	B	806	-	-	0/27/27/57	0/0/0/0
3	PC1	B	807	-	-	0/16/16/57	0/0/0/0
3	PC1	B	808	-	-	0/35/35/57	0/0/0/0
3	PC1	B	809	-	-	0/20/20/57	0/0/0/0
5	3PE	B	810	-	-	0/43/43/54	0/0/0/0
5	3PE	B	811	-	-	0/49/49/54	0/0/0/0
4	PIE	B	812	-	-	0/27/51/76	0/1/1/1
2	CMP	C	801	-	-	0/0/31/31	0/4/4/4
3	PC1	C	803	-	-	0/24/24/57	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PC1	C	804	-	-	0/45/45/57	0/0/0/0
3	PC1	C	805	-	-	0/32/32/57	0/0/0/0
3	PC1	C	806	-	-	0/27/27/57	0/0/0/0
3	PC1	C	807	-	-	0/16/16/57	0/0/0/0
3	PC1	C	808	-	-	0/35/35/57	0/0/0/0
3	PC1	C	809	-	-	0/20/20/57	0/0/0/0
5	3PE	C	810	-	-	0/43/43/54	0/0/0/0
5	3PE	C	811	-	-	0/49/49/54	0/0/0/0
4	PIE	C	812	-	-	0/27/51/76	0/1/1/1
2	CMP	D	801	-	-	0/0/31/31	0/4/4/4
3	PC1	D	803	-	-	0/20/20/57	0/0/0/0
3	PC1	D	804	-	-	0/24/24/57	0/0/0/0
3	PC1	D	805	-	-	0/45/45/57	0/0/0/0
3	PC1	D	806	-	-	0/32/32/57	0/0/0/0
3	PC1	D	807	-	-	0/27/27/57	0/0/0/0
3	PC1	D	808	-	-	0/16/16/57	0/0/0/0
3	PC1	D	809	-	-	0/35/35/57	0/0/0/0
5	3PE	D	810	-	-	0/49/49/54	0/0/0/0
5	3PE	D	811	-	-	0/43/43/54	0/0/0/0
4	PIE	D	812	-	-	0/27/51/76	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	804	PC1	O21-C21	-4.18	1.20	1.42
3	B	803	PC1	O21-C21	-4.18	1.20	1.42
3	C	803	PC1	O21-C21	-4.17	1.20	1.42
3	A	806	PC1	O21-C21	-4.16	1.20	1.42
2	C	801	CMP	O5'-C5'	-2.54	1.42	1.46
2	B	801	CMP	O5'-C5'	-2.50	1.42	1.46
2	A	801	CMP	O5'-C5'	-2.50	1.42	1.46
2	D	801	CMP	O5'-C5'	-2.42	1.42	1.46
2	B	801	CMP	O3'-C3'	-2.18	1.41	1.44
2	C	801	CMP	O3'-C3'	-2.16	1.41	1.44
2	A	801	CMP	O3'-C3'	-2.12	1.41	1.44
2	D	801	CMP	O3'-C3'	-2.11	1.41	1.44
4	B	812	PIE	P-O14	5.13	1.74	1.60
4	C	812	PIE	P-O14	5.14	1.74	1.60
4	A	812	PIE	P-O14	5.14	1.74	1.60
4	D	812	PIE	P-O14	5.15	1.74	1.60

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	806	PC1	O21-C21-C22	2.02	125.11	111.68
3	D	804	PC1	O21-C21-C22	2.03	125.17	111.68
3	B	803	PC1	O21-C21-C22	2.03	125.17	111.68
3	C	803	PC1	O21-C21-C22	2.03	125.17	111.68
2	A	801	CMP	C5-C6-N6	2.08	123.64	120.38
2	D	801	CMP	C5-C6-N6	2.08	123.65	120.38
2	B	801	CMP	C5-C6-N6	2.09	123.66	120.38
2	C	801	CMP	C5-C6-N6	2.09	123.66	120.38
3	B	808	PC1	C2-O21-C21	2.41	123.83	117.82
3	A	807	PC1	C2-O21-C21	2.41	123.83	117.82
3	C	808	PC1	C2-O21-C21	2.42	123.84	117.82
3	D	809	PC1	C2-O21-C21	2.43	123.88	117.82
2	A	801	CMP	O2P-P-O1P	3.49	119.66	108.62
2	B	801	CMP	O2P-P-O1P	3.50	119.67	108.62
2	D	801	CMP	O2P-P-O1P	3.50	119.68	108.62
2	C	801	CMP	O2P-P-O1P	3.51	119.70	108.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	CMP	3	0
3	A	804	PC1	1	0
3	A	805	PC1	1	0
5	A	810	3PE	1	0
5	A	811	3PE	4	0
2	B	801	CMP	3	0
3	B	806	PC1	1	0
3	B	807	PC1	1	0
5	B	810	3PE	4	0
5	B	811	3PE	1	0
2	C	801	CMP	3	0
3	C	806	PC1	1	0
3	C	807	PC1	1	0
5	C	810	3PE	4	0
5	C	811	3PE	1	0
2	D	801	CMP	3	0
3	D	807	PC1	1	0
3	D	808	PC1	1	0
5	D	810	3PE	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	811	3PE	4	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.