wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:41 PM BST

PDB ID	:	2W6D
EMDB ID:	:	EMD-1589
Title	:	BACTERIAL DYNAMIN-LIKE PROTEIN LIPID TUBE BOUND
Authors	:	Low, H.H.; Sachse, C.; Amos, L.A.; Lowe, J.
Deposited on	:	2008-12-18
Resolution	:	9.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

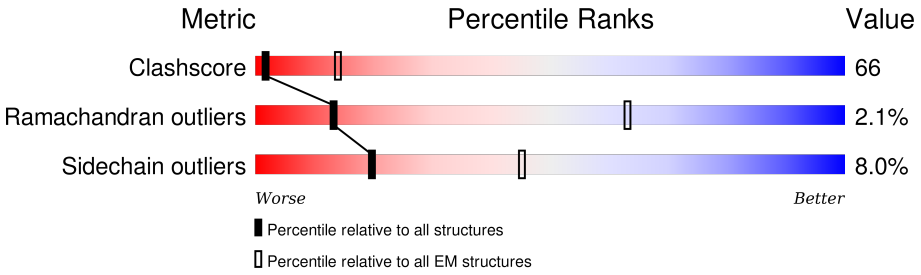
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 9.00 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	695	48% 44% 6% •
1	B	695	48% 44% 6% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CPL	A	1697	-	-	X	-
2	CPL	A	1700	-	-	X	-
2	CPL	A	1701	-	-	X	-
2	CPL	A	1702	-	-	X	-
2	CPL	A	1703	-	-	X	-
2	CPL	A	1705	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CPL	A	1707	-	-	X	-
2	CPL	A	1708	-	-	X	-
2	CPL	A	1709	-	-	X	-
2	CPL	A	1710	-	-	X	-
2	CPL	A	1718	-	-	X	-
2	CPL	A	3097	-	-	X	-
2	CPL	B	1696	-	-	X	-
2	CPL	B	1697	-	-	X	-
2	CPL	B	1700	-	-	X	-
2	CPL	B	1701	-	-	X	-
2	CPL	B	1703	-	-	X	-
2	CPL	B	1704	-	-	X	-
2	CPL	B	1705	-	-	X	-
2	CPL	B	1710	-	-	X	-
3	GDP	A	1696	-	-	X	-
3	GDP	B	1706	-	-	X	-

2 Entry composition

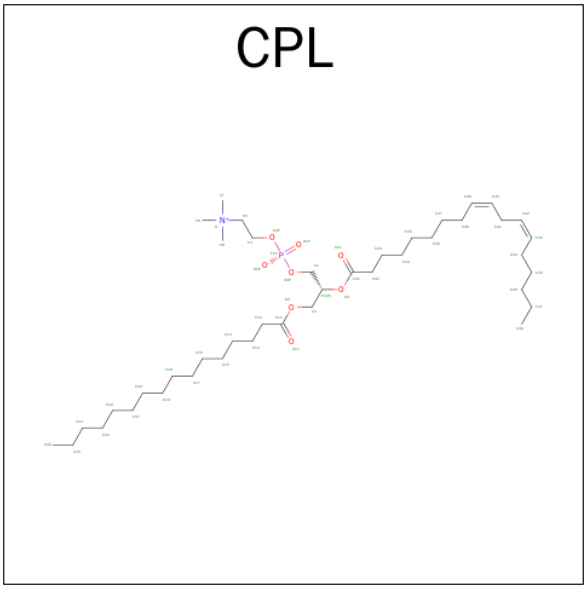
There are 3 unique types of molecules in this entry. The entry contains 13202 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DYNAMIN FAMILY PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	680	Total	C	N	O	S	0	0
			5429	3423	952	1043	11		
1	B	680	Total	C	N	O	S	0	0
			5429	3423	952	1043	11		

- Molecule 2 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: CPL) (formula: $C_{42}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	

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Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	
2	A	1	Total	C	N	O	P	0
			1352	1092	26	208	26	

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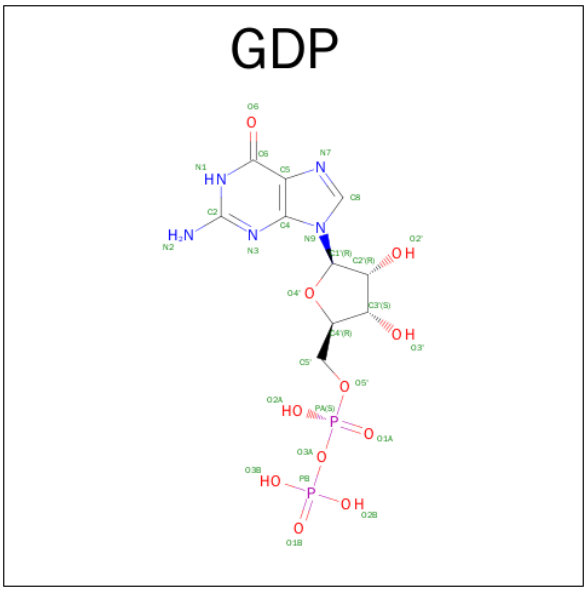
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 1352	C 1092	N 26	O 208	P 26	0
2	B	1	Total 936	C 756	N 18	O 144	P 18	0
2	B	1	Total 936	C 756	N 18	O 144	P 18	0
2	B	1	Total 936	C 756	N 18	O 144	P 18	0
2	B	1	Total 936	C 756	N 18	O 144	P 18	0
2	B	1	Total 936	C 756	N 18	O 144	P 18	0
2	B	1	Total 936	C 756	N 18	O 144	P 18	0
2	B	1	Total 936	C 756	N 18	O 144	P 18	0
2	B	1	Total 936	C 756	N 18	O 144	P 18	0
2	B	1	Total 936	C 756	N 18	O 144	P 18	0
2	B	1	Total 936	C 756	N 18	O 144	P 18	0
2	B	1	Total 936	C 756	N 18	O 144	P 18	0
2	B	1	Total 936	C 756	N 18	O 144	P 18	0
2	B	1	Total 936	C 756	N 18	O 144	P 18	0
2	B	1	Total 936	C 756	N 18	O 144	P 18	0
2	B	1	Total 936	C 756	N 18	O 144	P 18	0
2	B	1	Total 936	C 756	N 18	O 144	P 18	0
2	B	1	Total 936	C 756	N 18	O 144	P 18	0
2	B	1	Total 936	C 756	N 18	O 144	P 18	0

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



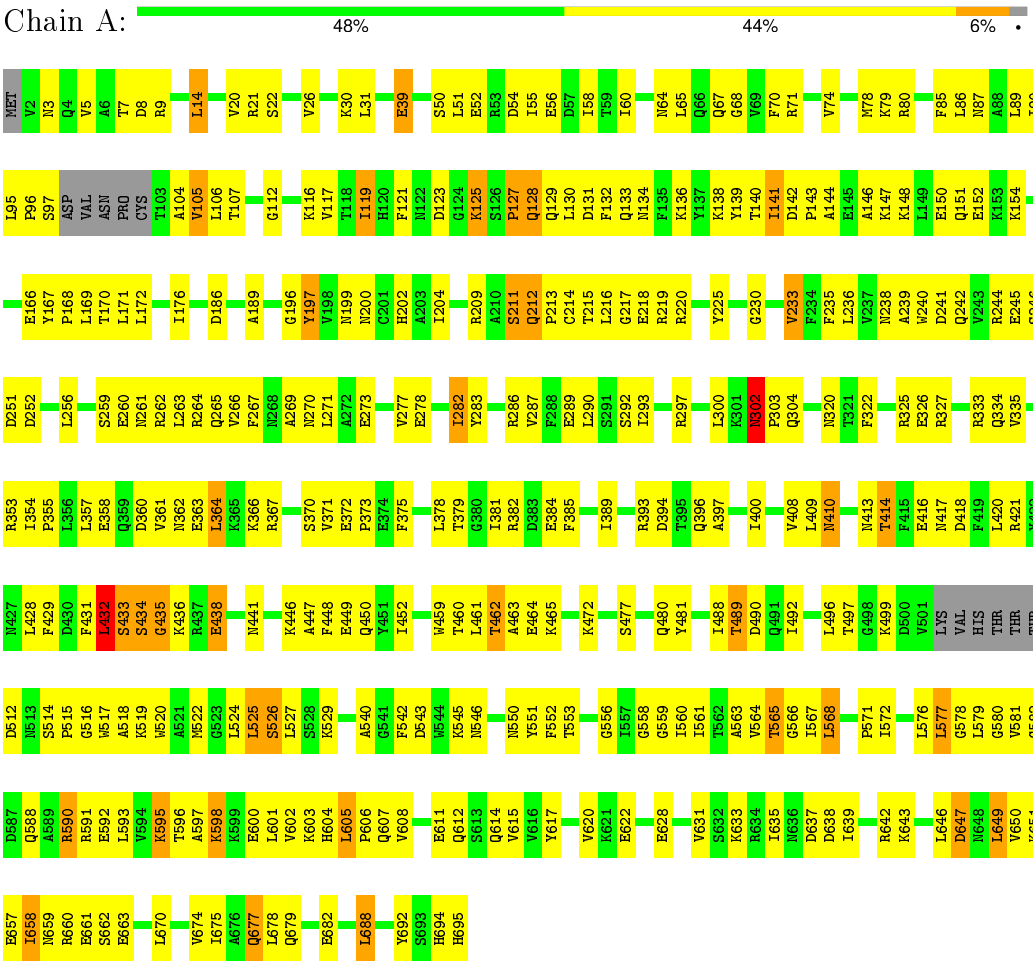
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

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 errors 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.

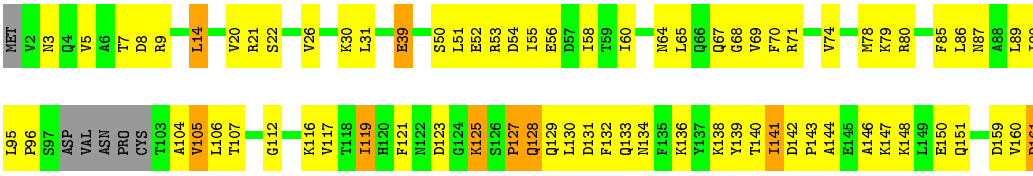
- Molecule 1: DYNAMIN FAMILY PROTEIN

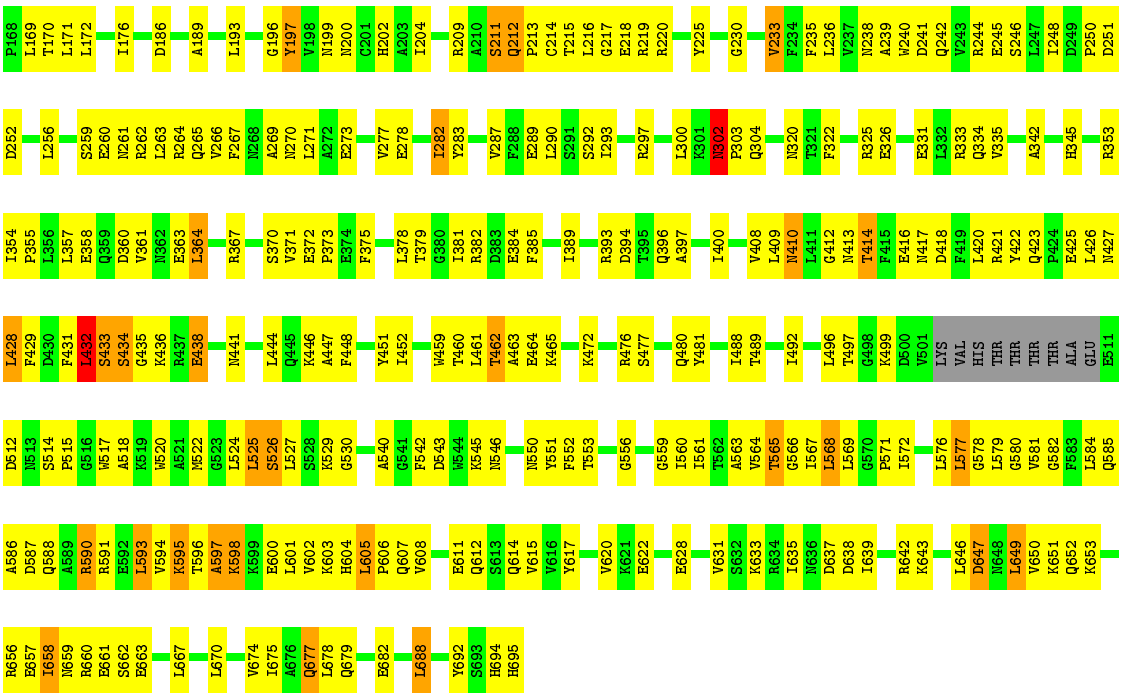
Chain A:



- Molecule 1: DYNAMIN FAMILY PROTEIN

Chain B:




P168 L169 T170 L171 L172 I176 D186 A189 L193 G196 Y197 Y198 N199 N200 C201 H202 A203 I204 R209 A210 S211 Q212 P213 C214 T215 L216 G217 E218 R219 R220 Y225 G230 V233 F234 F235 L236 Y237 N238 A239 W240 D241 Q242 Y243 R244 E245 S246 L247 I248 D249 P250 D251
D252 L256 S259 E260 N261 R262 L263 R264 Q265 V266 F267 N268 A269 N270 L271 A272 E273 V277 E278 I282 Y283 V287 F288 E289 L290 S291 S292 I293 R297 L300 K301 N302 P303 Q304 N320 T321 F322 R325 E326 E331 L332 R333 Q334 V335 A342 H345 R353
I354 P355 L356 L357 E358 Q359 D360 V361 N362 E363 L364 R367 S370 V371 E372 P373 E374 F375 L378 T379 G380 I381 R382 D383 E384 F385 I389 R393 D394 T395 Q396 A397 I400 V408 L409 N410 L411 G412 N413 T414 F415 E416 N417 D418 F419 L420 R421 Y422 Q423 P424 E425 L426 N427
L428 F429 D430 F431 L432 S433 S434 G435 K436 R437 E438 N441 L444 Q445 K446 A447 F448 Y451 I452 W459 T460 L461 T462 A463 E464 K465 K472 R476 S477 Q480 Y481 I488 T489 I492 L496 T497 G498 K499 D500 W501 LYS VAL HIS THR THR THR THR ALA GLU E511
D512 N513 S514 P515 G516 W517 A518 K519 W520 A521 M522 G523 L524 L525 S526 L527 S528 K529 G530 A540 G541 F542 D543 W544 K545 N546 N550 Y551 F552 T553 G556 G559 I560 I561 T562 A563 V564 T565 G566 I567 L568 L569 G570 P571 I572 L576 L577 G578 L579 G580 V581 G582 F583 L584 Q585
A586 D587 Q588 A589 R590 R591 E592 L593 V594 K595 T596 A597 K598 K599 E600 L601 V602 K603 H604 L605 P606 Q607 V608 E611 Q612 S613 Q614 V615 V616 Y617 V620 K621 E622 E628 V631 S632 K633 R634 I635 N636 D637 D638 I639 R642 K643 L646 D647 N648 L649 V650 K651 Q652 K653
R656 E657 I658 N659 R660 E661 S662 E663 L667 L670 V674 I675 A676 Q677 L678 Q679 E682 L688 Y692 S693 H694 H695

4 Experimental information (i)

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	59000	Depositor
Image detector	FILM	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, CPL

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	0.39	0/5509	0.61	0/7428
1	B	0.39	0/5509	0.61	0/7428
All	All	0.39	0/11018	0.61	0/14856

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	5429	0	5411	966	0
1	B	5429	0	5407	958	0
2	A	1352	0	2047	452	0
2	B	936	0	1408	366	0
3	A	28	0	9	10	0
3	B	28	0	9	11	0
All	All	13202	0	14291	1805	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 66.

The worst 5 of 1805 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:446:LYS:CD	2:A:1708:CPL:HC72	1.26	1.65
1:B:585:GLN:CG	2:B:1696:CPL:H261	1.14	1.61
1:A:432:LEU:CB	2:A:1709:CPL:H322	1.14	1.61
1:B:581:VAL:CA	2:B:1699:CPL:H461	1.16	1.61
1:A:579:LEU:CD2	2:A:1705:CPL:H462	1.26	1.60

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	666/695 (96%)	571 (86%)	81 (12%)	14 (2%)	9 50
1	B	666/695 (96%)	570 (86%)	82 (12%)	14 (2%)	9 50
All	All	1332/1390 (96%)	1141 (86%)	163 (12%)	28 (2%)	13 50

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	197	TYR
1	B	128	GLN
1	B	197	TYR
1	A	125	LYS

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	587/601 (98%)	540 (92%)	47 (8%)	15 50
1	B	587/601 (98%)	540 (92%)	47 (8%)	15 50
All	All	1174/1202 (98%)	1080 (92%)	94 (8%)	20 50

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	658	ILE
1	B	119	ILE
1	B	622	GLU
1	A	661	GLU
1	B	7	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	618	ASN
1	B	67	GLN
1	B	588	GLN
1	A	659	ASN
1	B	4	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

46 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	$\#\|Z\| > 2$
3	GDP	A	1696	-	24,30,30	1.27	2 (8%)	26,47,47	1.94	7 (26%)
2	CPL	A	1697	-	51,51,51	0.84	2 (3%)	55,59,59	0.85	2 (3%)
2	CPL	A	1698	-	51,51,51	0.85	2 (3%)	55,59,59	0.92	2 (3%)
2	CPL	A	1699	-	51,51,51	0.84	2 (3%)	55,59,59	0.92	3 (5%)
2	CPL	A	1700	-	51,51,51	0.88	3 (5%)	55,59,59	0.94	4 (7%)
2	CPL	A	1701	-	51,51,51	0.87	3 (5%)	55,59,59	1.06	2 (3%)
2	CPL	A	1702	-	51,51,51	0.85	3 (5%)	55,59,59	1.05	3 (5%)
2	CPL	A	1703	-	51,51,51	0.84	3 (5%)	55,59,59	1.05	3 (5%)
2	CPL	A	1704	-	51,51,51	0.87	3 (5%)	55,59,59	1.05	2 (3%)
2	CPL	A	1705	-	51,51,51	0.87	3 (5%)	55,59,59	1.06	2 (3%)
2	CPL	A	1706	-	51,51,51	0.88	3 (5%)	55,59,59	0.93	4 (7%)
2	CPL	A	1707	-	51,51,51	0.85	3 (5%)	55,59,59	0.92	3 (5%)
2	CPL	A	1708	-	51,51,51	0.85	3 (5%)	55,59,59	1.05	3 (5%)
2	CPL	A	1709	-	51,51,51	0.86	3 (5%)	55,59,59	1.08	2 (3%)
2	CPL	A	1710	-	51,51,51	0.85	3 (5%)	55,59,59	1.05	3 (5%)
2	CPL	A	1711	-	51,51,51	0.84	2 (3%)	55,59,59	0.85	2 (3%)
2	CPL	A	1712	-	51,51,51	0.88	3 (5%)	55,59,59	0.92	4 (7%)
2	CPL	A	1713	-	51,51,51	0.89	3 (5%)	55,59,59	0.96	4 (7%)
2	CPL	A	1714	-	51,51,51	0.85	3 (5%)	55,59,59	0.92	3 (5%)
2	CPL	A	1715	-	51,51,51	0.84	2 (3%)	55,59,59	0.81	2 (3%)
2	CPL	A	1716	-	51,51,51	0.87	3 (5%)	55,59,59	1.07	2 (3%)
2	CPL	A	1717	-	51,51,51	0.85	3 (5%)	55,59,59	1.05	3 (5%)
2	CPL	A	1718	-	51,51,51	0.84	2 (3%)	55,59,59	0.85	2 (3%)
2	CPL	A	3077	-	51,51,51	0.83	2 (3%)	55,59,59	0.95	3 (5%)
2	CPL	A	3094	-	51,51,51	0.88	3 (5%)	55,59,59	0.94	4 (7%)
2	CPL	A	3097	-	51,51,51	0.83	2 (3%)	55,59,59	0.95	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CPL	A	3181	-	51,51,51	0.87	3 (5%)	55,59,59	1.07	2 (3%)
2	CPL	B	1696	-	51,51,51	0.84	3 (5%)	55,59,59	1.05	3 (5%)
2	CPL	B	1697	-	51,51,51	0.88	3 (5%)	55,59,59	0.93	4 (7%)
2	CPL	B	1698	-	51,51,51	0.85	3 (5%)	55,59,59	1.05	3 (5%)
2	CPL	B	1699	-	51,51,51	0.88	3 (5%)	55,59,59	0.93	4 (7%)
2	CPL	B	1700	-	51,51,51	0.88	3 (5%)	55,59,59	0.93	4 (7%)
2	CPL	B	1701	-	51,51,51	0.85	3 (5%)	55,59,59	1.04	3 (5%)
2	CPL	B	1702	-	51,51,51	0.85	2 (3%)	55,59,59	0.85	2 (3%)
2	CPL	B	1703	-	51,51,51	0.87	3 (5%)	55,59,59	1.06	2 (3%)
2	CPL	B	1704	-	51,51,51	0.88	3 (5%)	55,59,59	0.93	4 (7%)
2	CPL	B	1705	-	51,51,51	0.85	2 (3%)	55,59,59	0.93	3 (5%)
3	GDP	B	1706	-	24,30,30	1.28	3 (12%)	26,47,47	1.93	7 (26%)
2	CPL	B	1707	-	51,51,51	0.87	3 (5%)	55,59,59	1.06	2 (3%)
2	CPL	B	1708	-	51,51,51	0.88	3 (5%)	55,59,59	0.93	4 (7%)
2	CPL	B	1709	-	51,51,51	0.86	3 (5%)	55,59,59	1.08	2 (3%)
2	CPL	B	1710	-	51,51,51	0.84	3 (5%)	55,59,59	1.05	3 (5%)
2	CPL	B	1711	-	51,51,51	0.84	2 (3%)	55,59,59	0.85	2 (3%)
2	CPL	B	1712	-	51,51,51	0.84	3 (5%)	55,59,59	1.05	3 (5%)
2	CPL	B	1713	-	51,51,51	0.88	3 (5%)	55,59,59	0.95	4 (7%)
2	CPL	B	1714	-	51,51,51	0.84	2 (3%)	55,59,59	0.85	2 (3%)

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
3	GDP	A	1696	-	-	0/12/32/32	0/3/3/3
2	CPL	A	1697	-	-	0/55/55/55	0/0/0/0
2	CPL	A	1698	-	-	0/55/55/55	0/0/0/0
2	CPL	A	1699	-	-	0/55/55/55	0/0/0/0
2	CPL	A	1700	-	-	0/55/55/55	0/0/0/0
2	CPL	A	1701	-	-	0/55/55/55	0/0/0/0
2	CPL	A	1702	-	-	0/55/55/55	0/0/0/0
2	CPL	A	1703	-	-	0/55/55/55	0/0/0/0
2	CPL	A	1704	-	-	0/55/55/55	0/0/0/0
2	CPL	A	1705	-	-	0/55/55/55	0/0/0/0
2	CPL	A	1706	-	-	0/55/55/55	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CPL	A	1707	-	-	0/55/55/55	0/0/0/0
2	CPL	A	1708	-	-	0/55/55/55	0/0/0/0
2	CPL	A	1709	-	-	0/55/55/55	0/0/0/0
2	CPL	A	1710	-	-	0/55/55/55	0/0/0/0
2	CPL	A	1711	-	-	0/55/55/55	0/0/0/0
2	CPL	A	1712	-	-	0/55/55/55	0/0/0/0
2	CPL	A	1713	-	-	0/55/55/55	0/0/0/0
2	CPL	A	1714	-	-	0/55/55/55	0/0/0/0
2	CPL	A	1715	-	-	0/55/55/55	0/0/0/0
2	CPL	A	1716	-	-	0/55/55/55	0/0/0/0
2	CPL	A	1717	-	-	0/55/55/55	0/0/0/0
2	CPL	A	1718	-	-	0/55/55/55	0/0/0/0
2	CPL	A	3077	-	-	0/55/55/55	0/0/0/0
2	CPL	A	3094	-	-	0/55/55/55	0/0/0/0
2	CPL	A	3097	-	-	0/55/55/55	0/0/0/0
2	CPL	A	3181	-	-	0/55/55/55	0/0/0/0
2	CPL	B	1696	-	-	0/55/55/55	0/0/0/0
2	CPL	B	1697	-	-	0/55/55/55	0/0/0/0
2	CPL	B	1698	-	-	0/55/55/55	0/0/0/0
2	CPL	B	1699	-	-	0/55/55/55	0/0/0/0
2	CPL	B	1700	-	-	0/55/55/55	0/0/0/0
2	CPL	B	1701	-	-	0/55/55/55	0/0/0/0
2	CPL	B	1702	-	-	0/55/55/55	0/0/0/0
2	CPL	B	1703	-	-	0/55/55/55	0/0/0/0
2	CPL	B	1704	-	-	0/55/55/55	0/0/0/0
2	CPL	B	1705	-	-	0/55/55/55	0/0/0/0
3	GDP	B	1706	-	-	0/12/32/32	0/3/3/3
2	CPL	B	1707	-	-	0/55/55/55	0/0/0/0
2	CPL	B	1708	-	-	0/55/55/55	0/0/0/0
2	CPL	B	1709	-	-	0/55/55/55	0/0/0/0
2	CPL	B	1710	-	-	0/55/55/55	0/0/0/0
2	CPL	B	1711	-	-	0/55/55/55	0/0/0/0
2	CPL	B	1712	-	-	0/55/55/55	0/0/0/0
2	CPL	B	1713	-	-	0/55/55/55	0/0/0/0
2	CPL	B	1714	-	-	0/55/55/55	0/0/0/0

The worst 5 of 125 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1710	CPL	P-O2P	-2.40	1.44	1.55
2	B	1701	CPL	P-O2P	-2.38	1.45	1.55
2	A	1717	CPL	P-O2P	-2.36	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1698	CPL	P-O2P	-2.36	1.45	1.55
2	A	1708	CPL	P-O2P	-2.36	1.45	1.55

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1696	GDP	N3-C2-N1	-4.85	120.96	127.56
3	B	1706	GDP	N3-C2-N1	-4.83	120.98	127.56
3	A	1696	GDP	C5-C6-N1	-4.17	118.07	123.52
3	B	1706	GDP	C5-C6-N1	-4.12	118.14	123.52
3	B	1706	GDP	C6-C5-C4	-2.81	117.64	120.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

45 monomers are involved in 834 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1696	GDP	10	0
2	A	1697	CPL	37	0
2	A	1698	CPL	15	0
2	A	1699	CPL	14	0
2	A	1700	CPL	41	0
2	A	1701	CPL	53	0
2	A	1702	CPL	27	0
2	A	1703	CPL	32	0
2	A	1704	CPL	17	0
2	A	1705	CPL	53	0
2	A	1706	CPL	6	0
2	A	1707	CPL	48	0
2	A	1708	CPL	58	0
2	A	1709	CPL	53	0
2	A	1710	CPL	21	0
2	A	1711	CPL	10	0
2	A	1712	CPL	4	0
2	A	1713	CPL	4	0
2	A	1714	CPL	14	0
2	A	1715	CPL	14	0
2	A	1716	CPL	7	0
2	A	1717	CPL	4	0
2	A	1718	CPL	24	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3077	CPL	6	0
2	A	3094	CPL	7	0
2	A	3097	CPL	24	0
2	A	3181	CPL	7	0
2	B	1696	CPL	24	0
2	B	1697	CPL	82	0
2	B	1698	CPL	7	0
2	B	1699	CPL	18	0
2	B	1700	CPL	34	0
2	B	1701	CPL	36	0
2	B	1702	CPL	7	0
2	B	1703	CPL	74	0
2	B	1704	CPL	28	0
2	B	1705	CPL	42	0
3	B	1706	GDP	11	0
2	B	1707	CPL	7	0
2	B	1708	CPL	2	0
2	B	1709	CPL	6	0
2	B	1710	CPL	26	0
2	B	1711	CPL	9	0
2	B	1712	CPL	18	0
2	B	1714	CPL	16	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.