



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 19, 2020 – 07:47 pm BST

PDB ID : 2RMB
Title : Crystal structures of cyclophilin A complexed with cyclosporin A and N-methyl-4-[(E)-2-butenyl]-4,4-dimethylthreonine cyclosporin A
Authors : Ke, H.; Mayrose, D.
Deposited on : 1994-01-07
Resolution : 2.10 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

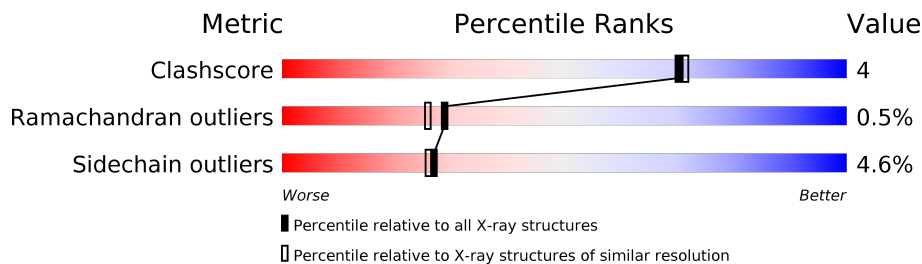
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)




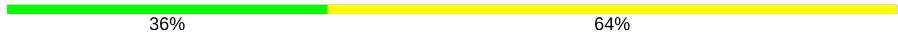

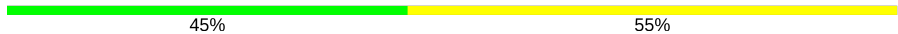



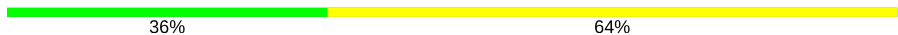


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	165	
1	C	165	
1	E	165	
1	G	165	
1	I	165	
1	K	165	
1	M	165	
1	O	165	

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Mol	Chain	Length	Quality of chain
1	Q	165	 89% 8%
1	S	165	 85% 15%
2	B	11	 64% 36%
2	D	11	 36% 64%
2	F	11	 64% 36%
2	H	11	 45% 55%
2	J	11	 82% 18%
2	L	11	 64% 36%
2	N	11	 64% 36%
2	P	11	 36% 64%
2	R	11	 64% 36%
2	T	11	 73% 27%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 18488 atoms, of which 4292 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 PEPTIDYL-PROLYL CIS-TRANS ISOMERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	165	1553	802	287	218	237	9	0	0	0
1	C	165	1553	802	287	218	237	9	0	0	0
1	E	165	1553	802	287	218	237	9	0	0	0
1	G	165	1553	802	287	218	237	9	0	0	0
1	I	165	1553	802	287	218	237	9	0	0	0
1	K	165	1553	802	287	218	237	9	0	0	0
1	M	165	1553	802	287	218	237	9	0	0	0
1	O	165	1553	802	287	218	237	9	0	0	0
1	Q	165	1553	802	287	218	237	9	0	0	0
1	S	165	1553	802	287	218	237	9	0	0	0

- Molecule 2 is a protein called CYCLOSPORIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	B	11	93	63	7	11	12	0	0	0
2	D	11	93	63	7	11	12	0	0	0
2	F	11	93	63	7	11	12	0	0	0
2	H	11	93	63	7	11	12	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	J	11	Total	C	H	N	O	0	0	0
			93	63	7	11	12			
2	L	11	Total	C	H	N	O	0	0	0
			93	63	7	11	12			
2	N	11	Total	C	H	N	O	0	0	0
			93	63	7	11	12			
2	P	11	Total	C	H	N	O	0	0	0
			93	63	7	11	12			
2	R	11	Total	C	H	N	O	0	0	0
			93	63	7	11	12			
2	T	11	Total	C	H	N	O	0	0	0
			93	63	7	11	12			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	5	DMT	BMT	ENGINEERED MUTATION	NOR NOR00033
D	5	DMT	BMT	ENGINEERED MUTATION	NOR NOR00033
F	5	DMT	BMT	ENGINEERED MUTATION	NOR NOR00033
H	5	DMT	BMT	ENGINEERED MUTATION	NOR NOR00033
J	5	DMT	BMT	ENGINEERED MUTATION	NOR NOR00033
L	5	DMT	BMT	ENGINEERED MUTATION	NOR NOR00033
N	5	DMT	BMT	ENGINEERED MUTATION	NOR NOR00033
P	5	DMT	BMT	ENGINEERED MUTATION	NOR NOR00033
R	5	DMT	BMT	ENGINEERED MUTATION	NOR NOR00033
T	5	DMT	BMT	ENGINEERED MUTATION	NOR NOR00033

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	74	Total	H	O	0	0
			222	148	74		
3	B	4	Total	H	O	0	0
			12	8	4		
3	C	66	Total	H	O	0	0
			198	132	66		
3	E	70	Total	H	O	0	0
			210	140	70		
3	F	2	Total	H	O	0	0
			6	4	2		
3	G	68	Total	H	O	0	0
			204	136	68		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	2	Total 6	H 4	O 2	0	0
3	I	68	Total 204	H 136	O 68	0	0
3	J	2	Total 6	H 4	O 2	0	0
3	K	73	Total 219	H 146	O 73	0	0
3	L	1	Total 3	H 2	O 1	0	0
3	M	52	Total 156	H 104	O 52	0	0
3	N	1	Total 3	H 2	O 1	0	0
3	O	66	Total 198	H 132	O 66	0	0
3	P	3	Total 9	H 6	O 3	0	0
3	Q	48	Total 144	H 96	O 48	0	0
3	R	2	Total 6	H 4	O 2	0	0
3	S	72	Total 216	H 144	O 72	0	0
3	T	2	Total 6	H 4	O 2	0	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.


Note EDS was not executed.

- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

Chain A:  88% 10%




- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

Chain C:  85% 15%



- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

Chain E:  88% 11%




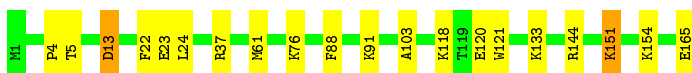
- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

Chain G:  87% 13%




- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

Chain I:  88% 11%

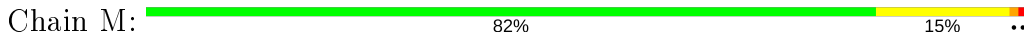


- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

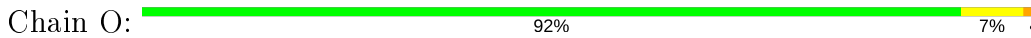
Chain K:  90% 8%



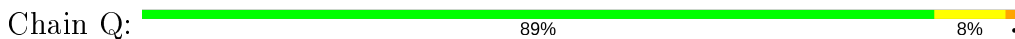
● Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE



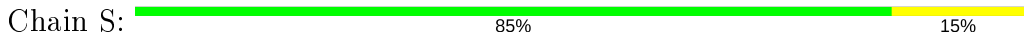
● Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE



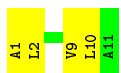
● Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE



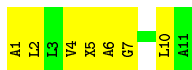
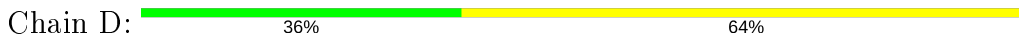
● Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE



● Molecule 2: CYCLOSPORIN A



● Molecule 2: CYCLOSPORIN A



● Molecule 2: CYCLOSPORIN A

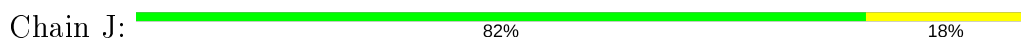




- Molecule 2: CYCLOSPORIN A



- Molecule 2: CYCLOSPORIN A



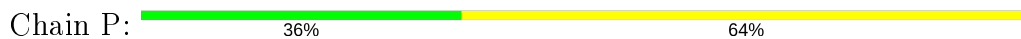
- Molecule 2: CYCLOSPORIN A



- Molecule 2: CYCLOSPORIN A



- Molecule 2: CYCLOSPORIN A



- Molecule 2: CYCLOSPORIN A



- Molecule 2: CYCLOSPORIN A





4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.60Å 160.60Å 95.30Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	18488	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ABA, MLE, DAL, MVA, DMT, SAR

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	0.67	0/1294	1.25	6/1733 (0.3%)
1	C	0.67	0/1294	1.21	5/1733 (0.3%)
1	E	0.71	0/1294	1.24	6/1733 (0.3%)
1	G	0.68	0/1294	1.22	6/1733 (0.3%)
1	I	0.67	0/1294	1.20	6/1733 (0.3%)
1	K	0.69	0/1294	1.23	5/1733 (0.3%)
1	M	0.69	0/1294	1.24	8/1733 (0.5%)
1	O	0.67	0/1294	1.19	5/1733 (0.3%)
1	Q	0.67	0/1294	1.27	8/1733 (0.5%)
1	S	0.67	0/1294	1.24	7/1733 (0.4%)
2	B	0.42	0/10	1.10	0/11
2	D	0.38	0/10	1.17	0/11
2	F	0.33	0/10	1.05	0/11
2	H	0.53	0/10	1.40	0/11
2	J	0.34	0/10	1.38	0/11
2	L	0.45	0/10	0.95	0/11
2	N	0.36	0/10	0.92	0/11
2	P	0.35	0/10	1.03	0/11
2	R	0.51	0/10	0.90	0/11
2	T	0.47	0/10	1.15	0/11
All	All	0.68	0/13040	1.23	62/17440 (0.4%)

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	S	0	1

There are no bond length outliers.

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	19	ARG	NE-CZ-NH2	-9.13	115.74	120.30
1	S	19	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	K	121	TRP	CD1-CG-CD2	8.52	113.11	106.30
1	S	121	TRP	CD1-CG-CD2	8.41	113.03	106.30
1	A	19	ARG	NE-CZ-NH2	-8.16	116.22	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	S	113	PHE	Sidechain

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	1266	287	1237	7	0
1	C	1266	287	1237	9	0
1	E	1266	287	1237	7	0
1	G	1266	287	1237	7	0
1	I	1266	287	1237	10	0
1	K	1266	287	1237	5	0
1	M	1266	287	1237	14	0
1	O	1266	287	1237	6	0
1	Q	1266	287	1237	5	0
1	S	1266	287	1237	7	0
2	B	86	7	111	2	0
2	D	86	7	111	5	0
2	F	86	7	111	2	0
2	H	86	7	111	3	0
2	J	86	7	111	1	0
2	L	86	7	111	2	0
2	N	86	7	111	3	0
2	P	86	7	111	5	0
2	R	86	7	111	3	0
2	T	86	7	111	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	74	148	0	2	0
3	B	4	8	0	0	0
3	C	66	132	0	3	0
3	E	70	140	0	1	0
3	F	2	4	0	0	0
3	G	68	136	0	1	0
3	H	2	4	0	0	0
3	I	68	136	0	1	0
3	J	2	4	0	0	0
3	K	73	146	0	1	0
3	L	1	2	0	0	0
3	M	52	104	0	1	0
3	N	1	2	0	0	0
3	O	66	132	0	4	0
3	P	3	6	0	0	0
3	Q	48	96	0	0	0
3	R	2	4	0	0	0
3	S	72	144	0	0	0
3	T	2	4	0	0	0
All	All	14196	4292	13480	98	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 4.

The worst 5 of 98 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:5:THR:HB	1:E:165:GLU:HB3	1.61	0.83
1:Q:5:THR:HB	1:Q:165:GLU:HB3	1.70	0.73
1:K:147:SER:OG	1:K:151:LYS:HD3	2.00	0.61
1:C:115:CYS:HB2	3:C:2031:HOH:O	2.06	0.56
1:I:118:LYS:NZ	1:I:120:GLU:HB3	2.22	0.54

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	163/165 (99%)	156 (96%)	6 (4%)	1 (1%)	25	21
1	C	163/165 (99%)	156 (96%)	6 (4%)	1 (1%)	25	21
1	E	163/165 (99%)	155 (95%)	6 (4%)	2 (1%)	13	8
1	G	163/165 (99%)	153 (94%)	9 (6%)	1 (1%)	25	21
1	I	163/165 (99%)	155 (95%)	7 (4%)	1 (1%)	25	21
1	K	163/165 (99%)	154 (94%)	8 (5%)	1 (1%)	25	21
1	M	163/165 (99%)	151 (93%)	11 (7%)	1 (1%)	25	21
1	O	163/165 (99%)	156 (96%)	7 (4%)	0	100	100
1	Q	163/165 (99%)	153 (94%)	9 (6%)	1 (1%)	25	21
1	S	163/165 (99%)	156 (96%)	7 (4%)	0	100	100
2	B	1/11 (9%)	1 (100%)	0	0	100	100
2	D	1/11 (9%)	1 (100%)	0	0	100	100
2	F	1/11 (9%)	1 (100%)	0	0	100	100
2	H	1/11 (9%)	1 (100%)	0	0	100	100
2	J	1/11 (9%)	1 (100%)	0	0	100	100
2	L	1/11 (9%)	1 (100%)	0	0	100	100
2	N	1/11 (9%)	1 (100%)	0	0	100	100
2	P	1/11 (9%)	1 (100%)	0	0	100	100
2	R	1/11 (9%)	1 (100%)	0	0	100	100
2	T	1/11 (9%)	1 (100%)	0	0	100	100
All	All	1640/1760 (93%)	1555 (95%)	76 (5%)	9 (0%)	29	26

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	13	ASP

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Mol	Chain	Res	Type
1	I	13	ASP
1	K	13	ASP
1	A	13	ASP
1	G	13	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	133/133 (100%)	125 (94%)	8 (6%)	19	16
1	C	133/133 (100%)	127 (96%)	6 (4%)	27	27
1	E	133/133 (100%)	127 (96%)	6 (4%)	27	27
1	G	133/133 (100%)	126 (95%)	7 (5%)	22	20
1	I	133/133 (100%)	130 (98%)	3 (2%)	50	55
1	K	133/133 (100%)	127 (96%)	6 (4%)	27	27
1	M	133/133 (100%)	127 (96%)	6 (4%)	27	27
1	O	133/133 (100%)	127 (96%)	6 (4%)	27	27
1	Q	133/133 (100%)	127 (96%)	6 (4%)	27	27
1	S	133/133 (100%)	126 (95%)	7 (5%)	22	20
2	B	1/1 (100%)	1 (100%)	0	100	100
2	D	1/1 (100%)	1 (100%)	0	100	100
2	F	1/1 (100%)	1 (100%)	0	100	100
2	H	1/1 (100%)	1 (100%)	0	100	100
2	J	1/1 (100%)	1 (100%)	0	100	100
2	L	1/1 (100%)	1 (100%)	0	100	100
2	N	1/1 (100%)	1 (100%)	0	100	100
2	P	1/1 (100%)	1 (100%)	0	100	100
2	R	1/1 (100%)	1 (100%)	0	100	100
2	T	1/1 (100%)	1 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1340/1340 (100%)	1279 (95%)	61 (5%)	27 26

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	61	MET
1	K	151	LYS
1	S	61	MET
1	I	151	LYS
1	K	13	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

90 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
2	MVA	F	4	2	6,7,8	0.95	0	7,8,10	1.84	3 (42%)
2	MLE	R	10	2	7,8,9	0.88	0	6,9,11	0.98	1 (16%)
2	MLE	H	8	2	7,8,9	0.72	0	6,9,11	1.07	1 (16%)
2	ABA	N	6	2	4,5,6	0.86	0	1,5,7	0.21	0
2	MVA	H	4	2	6,7,8	1.12	0	7,8,10	2.27	3 (42%)
2	MVA	T	4	2	6,7,8	0.95	0	7,8,10	1.45	1 (14%)
2	DMT	P	5	2	12,13,14	1.23	1 (8%)	13,17,19	0.92	0
2	DMT	J	5	2	12,13,14	1.18	0	13,17,19	1.24	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MLE	J	3	2	7,8,9	0.78	0	6,9,11	1.29	0
2	MLE	B	2	2	7,8,9	0.77	0	6,9,11	1.25	1 (16%)
2	MLE	T	3	2	7,8,9	0.85	0	6,9,11	1.47	1 (16%)
2	MLE	N	10	2	7,8,9	0.75	0	6,9,11	1.24	1 (16%)
2	MLE	P	10	2	7,8,9	0.77	0	6,9,11	1.31	1 (16%)
2	DMT	R	5	2	12,13,14	1.30	1 (8%)	13,17,19	0.87	0
2	MLE	P	8	2	7,8,9	0.82	0	6,9,11	1.08	1 (16%)
2	MLE	H	2	2	7,8,9	0.74	0	6,9,11	1.37	1 (16%)
2	MLE	N	8	2	7,8,9	0.66	0	6,9,11	1.01	1 (16%)
2	MLE	N	3	2	7,8,9	0.90	0	6,9,11	1.23	0
2	MLE	L	8	2	7,8,9	0.65	0	6,9,11	1.09	1 (16%)
2	MVA	L	4	2	6,7,8	0.92	0	7,8,10	1.54	3 (42%)
2	MLE	D	3	2	7,8,9	0.87	0	6,9,11	1.23	0
2	DMT	N	5	2	12,13,14	1.11	0	13,17,19	0.94	0
2	MLE	H	3	2	7,8,9	0.92	0	6,9,11	1.22	0
2	MVA	N	4	2	6,7,8	0.86	0	7,8,10	1.84	2 (28%)
2	MLE	H	10	2	7,8,9	0.76	0	6,9,11	1.19	1 (16%)
2	MLE	L	3	2	7,8,9	0.90	0	6,9,11	1.08	0
2	SAR	H	7	2	4,4,5	0.76	0	1,3,5	3.17	1 (100%)
2	ABA	R	6	2	4,5,6	0.74	0	1,5,7	0.43	0
2	ABA	L	6	2	4,5,6	0.78	0	1,5,7	0.98	0
2	MLE	B	10	2	7,8,9	0.75	0	6,9,11	1.21	1 (16%)
2	ABA	F	6	2	4,5,6	0.78	0	1,5,7	0.65	0
2	MLE	T	8	2	7,8,9	0.76	0	6,9,11	0.97	1 (16%)
2	ABA	P	6	2	4,5,6	0.86	0	1,5,7	0.82	0
2	MLE	J	10	2	7,8,9	0.74	0	6,9,11	1.19	1 (16%)
2	MLE	B	3	2	7,8,9	0.93	0	6,9,11	1.36	0
2	MLE	J	2	2	7,8,9	0.69	0	6,9,11	1.48	1 (16%)
2	SAR	J	7	2	4,4,5	0.72	0	1,3,5	3.05	1 (100%)
2	MVA	D	4	2	6,7,8	0.83	0	7,8,10	1.58	2 (28%)
2	SAR	R	7	2	4,4,5	0.74	0	1,3,5	3.24	1 (100%)
2	ABA	D	6	2	4,5,6	0.80	0	1,5,7	0.12	0
2	MLE	P	2	2	7,8,9	0.73	0	6,9,11	1.24	0
2	SAR	D	7	2	4,4,5	0.73	0	1,3,5	2.92	1 (100%)
2	MLE	R	2	2	7,8,9	0.72	0	6,9,11	1.70	2 (33%)
2	SAR	P	7	2	4,4,5	0.69	0	1,3,5	2.82	1 (100%)
2	MLE	D	8	2	7,8,9	0.64	0	6,9,11	1.26	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MLE	P	3	2	7,8,9	0.91	0	6,9,11	1.18	0
2	DMT	B	5	2	12,13,14	1.16	0	13,17,19	0.99	1 (7%)
2	MVA	J	4	2	6,7,8	0.83	0	7,8,10	1.61	3 (42%)
2	ABA	B	6	2	4,5,6	0.76	0	1,5,7	0.59	0
2	MLE	D	2	2	7,8,9	0.70	0	6,9,11	1.33	1 (16%)
2	ABA	T	6	2	4,5,6	0.73	0	1,5,7	0.01	0
2	MLE	L	10	2	7,8,9	0.79	0	6,9,11	1.18	1 (16%)
2	MLE	F	8	2	7,8,9	0.72	0	6,9,11	1.23	1 (16%)
2	SAR	T	7	2	4,4,5	0.81	0	1,3,5	2.93	1 (100%)
2	MLE	N	2	2	7,8,9	0.68	0	6,9,11	1.08	0
2	SAR	N	7	2	4,4,5	0.78	0	1,3,5	2.93	1 (100%)
2	MLE	R	8	2	7,8,9	0.66	0	6,9,11	1.14	1 (16%)
2	MLE	D	10	2	7,8,9	0.82	0	6,9,11	1.32	1 (16%)
2	SAR	F	7	2	4,4,5	0.86	0	1,3,5	2.66	1 (100%)
2	MLE	J	8	2	7,8,9	0.74	0	6,9,11	1.18	1 (16%)
2	SAR	L	7	2	4,4,5	0.76	0	1,3,5	3.34	1 (100%)
2	DMT	D	5	2	12,13,14	1.36	1 (8%)	13,17,19	1.06	1 (7%)
2	SAR	B	7	2	4,4,5	0.91	0	1,3,5	2.86	1 (100%)
2	MLE	T	10	2	7,8,9	0.74	0	6,9,11	1.34	1 (16%)
2	DMT	H	5	2	12,13,14	1.25	1 (8%)	13,17,19	1.22	2 (15%)
2	DMT	L	5	2	12,13,14	1.27	2 (16%)	13,17,19	1.26	2 (15%)
2	MLE	R	3	2	7,8,9	0.94	0	6,9,11	1.25	0
2	ABA	H	6	2	4,5,6	0.69	0	1,5,7	0.54	0
2	MVA	P	4	2	6,7,8	0.84	0	7,8,10	1.31	0
2	MLE	F	10	2	7,8,9	0.73	0	6,9,11	1.21	1 (16%)
2	MLE	B	8	2	7,8,9	0.72	0	6,9,11	1.09	0
2	MLE	F	2	2	7,8,9	0.70	0	6,9,11	1.02	0
2	MVA	R	4	2	6,7,8	0.85	0	7,8,10	1.64	2 (28%)
2	DMT	F	5	2	12,13,14	1.27	1 (8%)	13,17,19	1.02	1 (7%)
2	MLE	L	2	2	7,8,9	0.67	0	6,9,11	1.39	1 (16%)
2	MLE	F	3	2	7,8,9	0.88	0	6,9,11	1.28	1 (16%)
2	MVA	B	4	2	6,7,8	0.86	0	7,8,10	1.50	2 (28%)
2	DMT	T	5	2	12,13,14	1.32	1 (8%)	13,17,19	0.93	0
2	ABA	J	6	2	4,5,6	0.72	0	1,5,7	0.96	0
2	MLE	T	2	2	7,8,9	0.65	0	6,9,11	1.38	1 (16%)

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	MVA	F	4	2	-	1/6/8/10	-
2	MLE	R	10	2	-	0/5/8/10	-
2	MLE	H	8	2	-	2/5/8/10	-
2	ABA	N	6	2	-	1/3/4/6	-
2	MVA	H	4	2	-	2/6/8/10	-
2	MVA	T	4	2	-	2/6/8/10	-
2	DMT	P	5	2	-	1/16/19/21	-
2	DMT	J	5	2	-	2/16/19/21	-
2	MLE	J	3	2	-	0/5/8/10	-
2	MLE	B	2	2	-	0/5/8/10	-
2	MLE	T	3	2	-	0/5/8/10	-
2	MLE	N	10	2	-	0/5/8/10	-
2	MLE	P	10	2	-	0/5/8/10	-
2	DMT	R	5	2	-	2/16/19/21	-
2	MLE	P	8	2	-	1/5/8/10	-
2	MLE	H	2	2	-	0/5/8/10	-
2	MLE	N	8	2	-	1/5/8/10	-
2	MLE	N	3	2	-	0/5/8/10	-
2	MLE	L	8	2	-	1/5/8/10	-
2	MVA	L	4	2	-	2/6/8/10	-
2	MLE	D	3	2	-	0/5/8/10	-
2	DMT	N	5	2	-	2/16/19/21	-
2	MLE	H	3	2	-	0/5/8/10	-
2	MVA	N	4	2	-	2/6/8/10	-
2	MLE	H	10	2	-	0/5/8/10	-
2	MLE	L	3	2	-	0/5/8/10	-
2	SAR	H	7	2	-	1/1/2/3	-
2	ABA	R	6	2	-	1/3/4/6	-
2	ABA	L	6	2	-	1/3/4/6	-
2	MLE	B	10	2	-	0/5/8/10	-
2	ABA	F	6	2	-	1/3/4/6	-
2	MLE	T	8	2	-	1/5/8/10	-
2	ABA	P	6	2	-	1/3/4/6	-
2	MLE	J	10	2	-	0/5/8/10	-
2	MLE	B	3	2	-	0/5/8/10	-
2	MLE	J	2	2	-	0/5/8/10	-
2	SAR	J	7	2	-	1/1/2/3	-
2	MVA	D	4	2	-	2/6/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAR	R	7	2	-	1/1/2/3	-
2	ABA	D	6	2	-	1/3/4/6	-
2	MLE	P	2	2	-	0/5/8/10	-
2	SAR	D	7	2	-	1/1/2/3	-
2	MLE	R	2	2	-	0/5/8/10	-
2	SAR	P	7	2	-	1/1/2/3	-
2	MLE	D	8	2	-	1/5/8/10	-
2	MLE	P	3	2	-	0/5/8/10	-
2	DMT	B	5	2	-	2/16/19/21	-
2	MVA	J	4	2	-	1/6/8/10	-
2	ABA	B	6	2	-	1/3/4/6	-
2	MLE	D	2	2	-	0/5/8/10	-
2	ABA	T	6	2	-	1/3/4/6	-
2	MLE	L	10	2	-	0/5/8/10	-
2	MLE	F	8	2	-	1/5/8/10	-
2	SAR	T	7	2	-	1/1/2/3	-
2	MLE	N	2	2	-	0/5/8/10	-
2	SAR	N	7	2	-	1/1/2/3	-
2	MLE	R	8	2	-	1/5/8/10	-
2	MLE	D	10	2	-	0/5/8/10	-
2	SAR	F	7	2	-	1/1/2/3	-
2	MLE	J	8	2	-	1/5/8/10	-
2	SAR	L	7	2	-	1/1/2/3	-
2	DMT	D	5	2	-	1/16/19/21	-
2	SAR	B	7	2	-	1/1/2/3	-
2	MLE	T	10	2	-	0/5/8/10	-
2	DMT	H	5	2	-	2/16/19/21	-
2	DMT	L	5	2	-	3/16/19/21	-
2	MLE	R	3	2	-	0/5/8/10	-
2	ABA	H	6	2	-	1/3/4/6	-
2	MVA	P	4	2	-	1/6/8/10	-
2	MLE	F	10	2	-	0/5/8/10	-
2	MLE	B	8	2	-	1/5/8/10	-
2	MLE	F	2	2	-	0/5/8/10	-
2	MVA	R	4	2	-	2/6/8/10	-
2	DMT	F	5	2	-	2/16/19/21	-
2	MLE	L	2	2	-	0/5/8/10	-
2	MLE	F	3	2	-	0/5/8/10	-
2	MVA	B	4	2	-	1/6/8/10	-
2	DMT	T	5	2	-	1/16/19/21	-
2	ABA	J	6	2	-	1/3/4/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLE	T	2	2	-	0/5/8/10	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5	DMT	CB-CA	2.80	1.60	1.53
2	T	5	DMT	CB-CA	2.80	1.60	1.53
2	L	5	DMT	CB-CA	2.43	1.59	1.53
2	R	5	DMT	CB-CA	2.42	1.59	1.53
2	F	5	DMT	CB-CA	2.39	1.59	1.53

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	4	MVA	CG1-CB-CA	-3.71	105.53	111.21
2	L	5	DMT	CG2-CB-CA	3.48	122.46	116.88
2	N	4	MVA	CG1-CB-CA	-3.48	105.88	111.21
2	L	7	SAR	O-C-CA	-3.34	115.76	125.42
2	R	7	SAR	O-C-CA	-3.24	116.04	125.42

There are no chirality outliers.

5 of 65 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	5	DMT	CG2-CD1-CE-CZ
2	P	8	MLE	O-C-CA-CB
2	N	8	MLE	O-C-CA-CB
2	L	8	MLE	O-C-CA-CB
2	N	5	DMT	CG2-CD1-CE-CZ

There are no ring outliers.

30 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	10	MLE	2	0
2	H	4	MVA	1	0
2	P	5	DMT	2	0
2	B	2	MLE	1	0
2	P	10	MLE	1	0
2	H	2	MLE	1	0
2	N	5	DMT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	4	MVA	2	0
2	H	10	MLE	1	0
2	B	10	MLE	1	0
2	J	10	MLE	1	0
2	D	4	MVA	1	0
2	D	6	ABA	1	0
2	P	2	MLE	2	0
2	D	7	SAR	1	0
2	R	2	MLE	1	0
2	P	3	MLE	1	0
2	D	2	MLE	1	0
2	L	10	MLE	1	0
2	N	2	MLE	1	0
2	D	10	MLE	1	0
2	L	7	SAR	1	0
2	D	5	DMT	1	0
2	T	10	MLE	1	0
2	H	5	DMT	1	0
2	L	5	DMT	1	0
2	P	4	MVA	1	0
2	F	10	MLE	1	0
2	F	2	MLE	1	0
2	T	5	DMT	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.