



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2024 – 11:14 PM EDT

PDB ID : 2RMA  
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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (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)	:	2.37.1

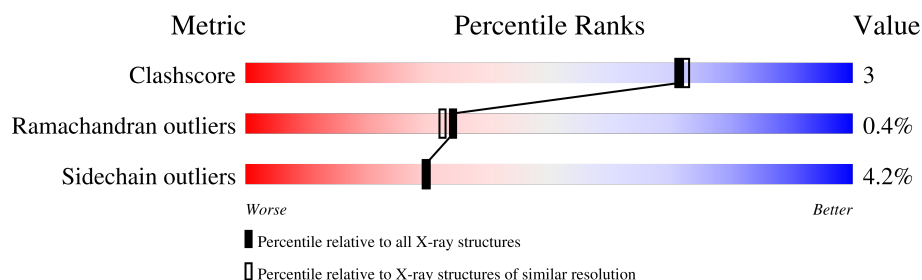
# 1 Overall quality at a glance

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)



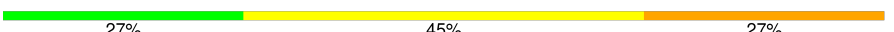
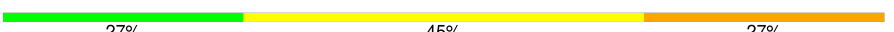
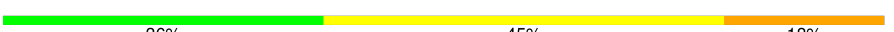

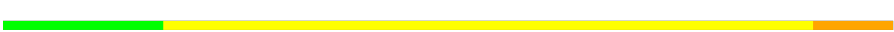





The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	165	88% 10% .
1	C	165	85% 13% .
1	E	165	91% 8% .
1	G	165	90% 9% .
1	I	165	90% 10% .
1	K	165	86% 12% .
1	M	165	89% 10% .
1	O	165	90% 8% .

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Mol	Chain	Length	Quality of chain
1	Q	165	 85% 14%
1	S	165	 87% 10%
2	B	11	 27% 45% 27%
2	D	11	 27% 45% 27%
2	F	11	 36% 45% 18%
2	H	11	 18% 45% 36%
2	J	11	 18% 73% 9%
2	L	11	 27% 45% 27%
2	N	11	 27% 55% 18%
2	P	11	 45% 55%
2	R	11	 18% 45% 36%
2	T	11	 27% 64% 9%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 18346 atoms, of which 4204 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
1	A	165	Total	C	H	N	O	S	0	0	0
			1553	802	287	218	237	9			
1	C	165	Total	C	H	N	O	S	0	0	0
			1553	802	287	218	237	9			
1	E	165	Total	C	H	N	O	S	0	0	0
			1553	802	287	218	237	9			
1	G	165	Total	C	H	N	O	S	0	0	0
			1553	802	287	218	237	9			
1	I	165	Total	C	H	N	O	S	0	0	0
			1553	802	287	218	237	9			
1	K	165	Total	C	H	N	O	S	0	0	0
			1553	802	287	218	237	9			
1	M	165	Total	C	H	N	O	S	0	0	0
			1553	802	287	218	237	9			
1	O	165	Total	C	H	N	O	S	0	0	0
			1553	802	287	218	237	9			
1	Q	165	Total	C	H	N	O	S	0	0	0
			1553	802	287	218	237	9			
1	S	165	Total	C	H	N	O	S	0	0	0
			1553	802	287	218	237	9			

- Molecule 2 is a protein called CYCLOSPORIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	H	N	O	0	0	0
			92	62	7	11	12			
2	D	11	Total	C	H	N	O	0	0	0
			92	62	7	11	12			
2	F	11	Total	C	H	N	O	0	0	0
			92	62	7	11	12			
2	H	11	Total	C	H	N	O	0	0	0
			92	62	7	11	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	11	Total	C	H	N	O	0	0	0
			92	62	7	11	12			
2	L	11	Total	C	H	N	O	0	0	0
			92	62	7	11	12			
2	N	11	Total	C	H	N	O	0	0	0
			92	62	7	11	12			
2	P	11	Total	C	H	N	O	0	0	0
			92	62	7	11	12			
2	R	11	Total	C	H	N	O	0	0	0
			92	62	7	11	12			
2	T	11	Total	C	H	N	O	0	0	0
			92	62	7	11	12			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	66	Total	H	O	0	0
			198	132	66		
3	C	57	Total	H	O	0	0
			171	114	57		
3	D	1	Total	H	O	0	0
			3	2	1		
3	E	57	Total	H	O	0	0
			171	114	57		
3	F	2	Total	H	O	0	0
			6	4	2		
3	G	64	Total	H	O	0	0
			192	128	64		
3	H	1	Total	H	O	0	0
			3	2	1		
3	I	70	Total	H	O	0	0
			210	140	70		
3	J	3	Total	H	O	0	0
			9	6	3		
3	K	68	Total	H	O	0	0
			204	136	68		
3	L	1	Total	H	O	0	0
			3	2	1		
3	M	50	Total	H	O	0	0
			150	100	50		
3	N	1	Total	H	O	0	0
			3	2	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	64	Total	H	O	0	0
			192	128	64		
3	P	2	Total	H	O	0	0
			6	4	2		
3	Q	55	Total	H	O	0	0
			165	110	55		
3	R	2	Total	H	O	0	0
			6	4	2		
3	S	65	Total	H	O	0	0
			195	130	65		
3	T	3	Total	H	O	0	0
			9	6	3		

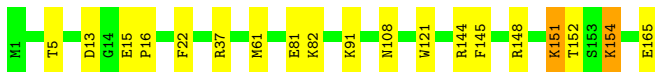
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.


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% 13%




- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

Chain E:  91% 8%




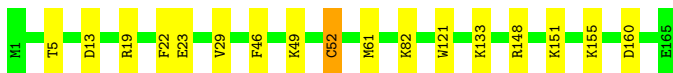
- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

Chain G:  90% 9%




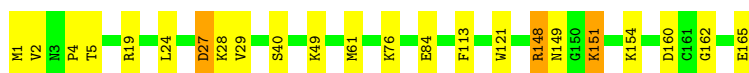
- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

Chain I:  90% 10%

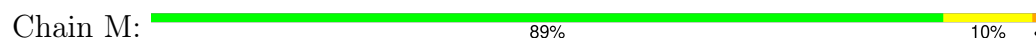


- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

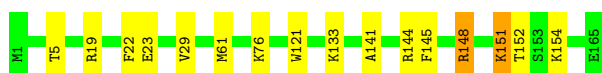
Chain K:  86% 12%



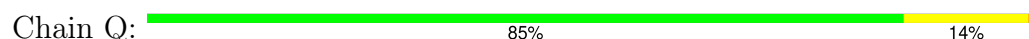
- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE



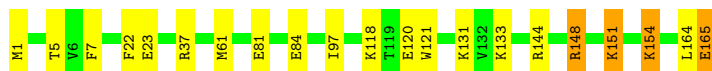
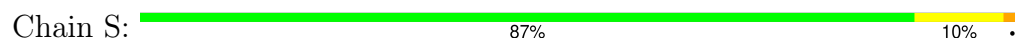
- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE



- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE



- Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE



- Molecule 2: CYCLOSPORIN A



- Molecule 2: CYCLOSPORIN A

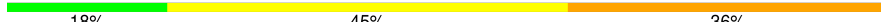


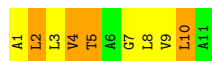
- Molecule 2: CYCLOSPORIN A



- Molecule 2: CYCLOSPORIN A



Chain H:  18% 45% 36%

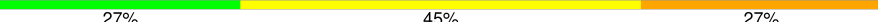


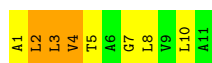
• Molecule 2: CYCLOSPORIN A

Chain J:  18% 73% 9%



• Molecule 2: CYCLOSPORIN A

Chain L:  27% 45% 27%



• Molecule 2: CYCLOSPORIN A

Chain N:  27% 55% 18%

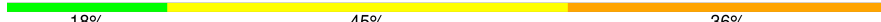


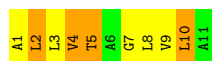
• Molecule 2: CYCLOSPORIN A

Chain P:  45% 55%



• Molecule 2: CYCLOSPORIN A

Chain R:  18% 45% 36%



• Molecule 2: CYCLOSPORIN A

Chain T:  27% 64% 9%



## 4 Data and refinement statistics

Xtriage (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, $\alpha$ , $\beta$ , $\gamma$	72.60Å 160.90Å 95.30Å 90.00° 90.60° 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, $R_{free}$	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18346	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	1.19	4/1733 (0.2%)
1	C	0.68	0/1294	1.20	9/1733 (0.5%)
1	E	0.68	0/1294	1.22	4/1733 (0.2%)
1	G	0.68	0/1294	1.25	7/1733 (0.4%)
1	I	0.67	0/1294	1.19	4/1733 (0.2%)
1	K	0.68	0/1294	1.24	7/1733 (0.4%)
1	M	0.68	0/1294	1.24	5/1733 (0.3%)
1	O	0.67	0/1294	1.19	5/1733 (0.3%)
1	Q	0.68	0/1294	1.25	8/1733 (0.5%)
1	S	0.67	0/1294	1.25	10/1733 (0.6%)
2	B	0.39	0/10	1.13	0/11
2	D	0.42	0/10	1.15	0/11
2	F	0.28	0/10	1.34	0/11
2	H	0.39	0/10	1.10	0/11
2	J	0.33	0/10	1.32	0/11
2	L	0.25	0/10	1.24	0/11
2	N	0.36	0/10	1.06	0/11
2	P	0.33	0/10	1.16	0/11
2	R	0.43	0/10	1.00	0/11
2	T	0.39	0/10	0.98	0/11
All	All	0.67	0/13040	1.22	63/17440 (0.4%)

There are no bond length outliers.

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	19	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	S	121	TRP	CD1-CG-CD2	8.29	112.93	106.30
1	O	121	TRP	CD1-CG-CD2	8.24	112.89	106.30
1	S	81	GLU	CA-CB-CG	8.18	131.40	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	19	ARG	NE-CZ-NH2	-8.10	116.25	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	11	0
1	E	1266	287	1237	4	0
1	G	1266	287	1237	4	0
1	I	1266	287	1237	6	0
1	K	1266	287	1237	10	0
1	M	1266	287	1237	8	0
1	O	1266	287	1237	6	0
1	Q	1266	287	1237	8	0
1	S	1266	287	1237	11	0
2	B	85	7	109	2	0
2	D	85	7	109	2	0
2	F	85	7	109	2	0
2	H	85	7	109	3	0
2	J	85	7	110	2	0
2	L	85	7	109	3	0
2	N	85	7	109	2	0
2	P	85	7	109	0	0
2	R	85	7	109	3	0
2	T	85	7	109	1	0
3	A	66	132	0	0	0
3	C	57	114	0	1	0
3	D	1	2	0	0	0
3	E	57	114	0	0	0
3	F	2	4	0	0	0
3	G	64	128	0	0	0
3	H	1	2	0	0	0
3	I	70	140	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	3	6	0	0	0
3	K	68	136	0	5	0
3	L	1	2	0	0	0
3	M	50	100	0	1	0
3	N	1	2	0	0	0
3	O	64	128	0	1	0
3	P	2	4	0	0	0
3	Q	55	110	0	1	0
3	R	2	4	0	0	0
3	S	65	130	0	1	0
3	T	3	6	0	0	0
All	All	14142	4204	13461	93	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.

The worst 5 of 93 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:Q:5:THR:HB	1:Q:165:GLU:HB3	1.65	0.78
1:K:40:SER:HB3	3:K:2066:HOH:O	1.89	0.73
1:E:5:THR:HB	1:E:165:GLU:HB3	1.69	0.72
1:A:5:THR:HB	1:A:165:GLU:HG2	1.72	0.71
1:S:5:THR:HB	1:S:165:GLU:HB3	1.74	0.70

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	157 (96%)	5 (3%)	1 (1%)	25 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	163/165 (99%)	156 (96%)	7 (4%)	0	100	100
1	E	163/165 (99%)	155 (95%)	7 (4%)	1 (1%)	25	21
1	G	163/165 (99%)	153 (94%)	9 (6%)	1 (1%)	25	21
1	I	163/165 (99%)	153 (94%)	9 (6%)	1 (1%)	25	21
1	K	163/165 (99%)	153 (94%)	9 (6%)	1 (1%)	25	21
1	M	163/165 (99%)	152 (93%)	10 (6%)	1 (1%)	25	21
1	O	163/165 (99%)	157 (96%)	6 (4%)	0	100	100
1	Q	163/165 (99%)	153 (94%)	10 (6%)	0	100	100
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%)	79 (5%)	6 (0%)	34	32

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	13	ASP
1	G	13	ASP
1	M	13	ASP
1	A	13	ASP
1	I	46	PHE

### 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 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%)	127 (96%)	6 (4%)	27	27
1	C	133/133 (100%)	128 (96%)	5 (4%)	33	34
1	E	133/133 (100%)	128 (96%)	5 (4%)	33	34
1	G	133/133 (100%)	129 (97%)	4 (3%)	41	44
1	I	133/133 (100%)	127 (96%)	6 (4%)	27	27
1	K	133/133 (100%)	126 (95%)	7 (5%)	22	20
1	M	133/133 (100%)	128 (96%)	5 (4%)	33	34
1	O	133/133 (100%)	128 (96%)	5 (4%)	33	34
1	Q	133/133 (100%)	125 (94%)	8 (6%)	19	16
1	S	133/133 (100%)	128 (96%)	5 (4%)	33	34
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
All	All	1340/1340 (100%)	1284 (96%)	56 (4%)	30	30

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	61	MET
1	S	154	LYS
1	M	61	MET
1	S	151	LYS
1	Q	148	ARG

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	ABA	T	6	2	4,5,6	0.73	0	1,5,7	0.39	0
2	MVA	R	4	2	6,7,8	0.94	0	6,8,10	1.35	1 (16%)
2	MLE	T	10	2	7,8,9	0.87	0	7,9,11	1.53	2 (28%)
2	MLE	H	3	2	7,8,9	1.05	0	7,9,11	1.80	1 (14%)
2	MVA	T	4	2	6,7,8	1.11	0	6,8,10	2.07	3 (50%)
2	MLE	H	10	2	7,8,9	0.86	0	7,9,11	1.74	2 (28%)
2	MVA	N	4	2	6,7,8	0.98	0	6,8,10	1.67	1 (16%)
2	BMT	R	5	2	11,12,13	1.24	1 (9%)	11,14,16	1.46	1 (9%)
2	MLE	B	8	2	7,8,9	0.77	0	7,9,11	1.12	1 (14%)
2	MLE	R	10	2	7,8,9	0.93	0	7,9,11	1.36	2 (28%)
2	SAR	F	7	2	3,4,5	0.68	0	1,3,5	2.68	1 (100%)
2	MLE	B	2	2	7,8,9	1.15	1 (14%)	7,9,11	1.47	2 (28%)
2	MLE	N	8	2	7,8,9	0.73	0	7,9,11	0.92	0
2	ABA	P	6	2	4,5,6	0.85	0	1,5,7	0.06	0
2	BMT	N	5	2	11,12,13	1.21	0	11,14,16	1.38	2 (18%)
2	BMT	P	5	2	11,12,13	1.19	0	11,14,16	1.25	1 (9%)
2	SAR	L	7	2	3,4,5	0.72	0	1,3,5	2.65	1 (100%)
2	MLE	L	2	2	7,8,9	0.73	0	7,9,11	1.21	1 (14%)
2	MLE	P	3	2	7,8,9	1.18	1 (14%)	7,9,11	1.70	1 (14%)
2	MLE	P	10	2	7,8,9	0.85	0	7,9,11	1.60	2 (28%)
2	ABA	J	6	2	4,5,6	0.82	0	1,5,7	0.56	0
2	MLE	D	3	2	7,8,9	0.99	0	7,9,11	1.55	1 (14%)
2	MLE	R	8	2	7,8,9	0.70	0	7,9,11	1.13	1 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MLE	D	2	2	7,8,9	0.80	0	7,9,11	1.42	2 (28%)
2	MVA	F	4	2	6,7,8	0.97	0	6,8,10	1.60	2 (33%)
2	MLE	D	10	2	7,8,9	0.92	0	7,9,11	1.61	2 (28%)
2	MLE	T	3	2	7,8,9	1.05	0	7,9,11	1.47	2 (28%)
2	MLE	F	3	2	7,8,9	0.96	0	7,9,11	1.30	1 (14%)
2	MLE	J	2	2	7,8,9	0.72	0	7,9,11	1.28	0
2	SAR	N	7	2	3,4,5	0.83	0	1,3,5	2.21	1 (100%)
2	SAR	R	7	2	3,4,5	0.78	0	1,3,5	2.02	1 (100%)
2	MLE	R	2	2	7,8,9	0.80	0	7,9,11	1.36	2 (28%)
2	MLE	T	8	2	7,8,9	0.81	0	7,9,11	1.09	1 (14%)
2	MLE	T	2	2	7,8,9	0.70	0	7,9,11	1.16	1 (14%)
2	SAR	T	7	2	3,4,5	0.74	0	1,3,5	2.49	1 (100%)
2	MLE	L	3	2	7,8,9	0.95	0	7,9,11	1.63	1 (14%)
2	ABA	D	6	2	4,5,6	0.84	0	1,5,7	0.58	0
2	MLE	D	8	2	7,8,9	0.76	0	7,9,11	1.10	1 (14%)
2	BMT	D	5	2	11,12,13	1.14	0	11,14,16	1.50	3 (27%)
2	MLE	B	10	2	7,8,9	0.80	0	7,9,11	1.58	2 (28%)
2	BMT	L	5	2	11,12,13	1.19	1 (9%)	11,14,16	1.27	1 (9%)
2	SAR	B	7	2	3,4,5	0.77	0	1,3,5	2.30	1 (100%)
2	MLE	J	3	2	7,8,9	0.92	0	7,9,11	1.74	2 (28%)
2	MLE	J	10	2	7,8,9	0.78	0	7,9,11	1.58	2 (28%)
2	ABA	H	6	2	4,5,6	0.72	0	1,5,7	0.06	0
2	BMT	H	5	2	11,12,13	1.25	1 (9%)	11,14,16	1.23	1 (9%)
2	ABA	B	6	2	4,5,6	0.80	0	1,5,7	0.36	0
2	MLE	F	10	2	7,8,9	0.80	0	7,9,11	1.83	3 (42%)
2	MLE	P	8	2	7,8,9	0.87	0	7,9,11	1.13	1 (14%)
2	MVA	P	4	2	6,7,8	1.01	0	6,8,10	1.46	1 (16%)
2	MVA	H	4	2	6,7,8	1.10	0	6,8,10	1.46	2 (33%)
2	BMT	B	5	2	11,12,13	1.16	0	11,14,16	1.48	2 (18%)
2	MLE	L	8	2	7,8,9	0.65	0	7,9,11	1.02	1 (14%)
2	BMT	J	5	2	11,12,13	1.26	1 (9%)	11,14,16	1.32	1 (9%)
2	ABA	R	6	2	4,5,6	0.77	0	1,5,7	0.47	0
2	MLE	B	3	2	7,8,9	0.92	0	7,9,11	1.59	2 (28%)
2	ABA	L	6	2	4,5,6	0.77	0	1,5,7	0.28	0
2	MLE	R	3	2	7,8,9	0.96	0	7,9,11	1.70	1 (14%)
2	SAR	P	7	2	3,4,5	0.76	0	1,3,5	2.34	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MLE	N	10	2	7,8,9	0.71	0	7,9,11	1.51	2 (28%)
2	MLE	N	2	2	7,8,9	0.75	0	7,9,11	1.39	1 (14%)
2	MVA	B	4	2	6,7,8	0.97	0	6,8,10	1.69	3 (50%)
2	SAR	J	7	2	3,4,5	0.74	0	1,3,5	2.09	1 (100%)
2	MLE	P	2	2	7,8,9	0.70	0	7,9,11	1.05	0
2	MLE	L	10	2	7,8,9	0.81	0	7,9,11	1.64	2 (28%)
2	MVA	L	4	2	6,7,8	0.94	0	6,8,10	1.46	2 (33%)
2	ABA	F	6	2	4,5,6	0.83	0	1,5,7	0.34	0
2	MLE	H	8	2	7,8,9	0.72	0	7,9,11	1.18	1 (14%)
2	BMT	F	5	2	11,12,13	1.34	1 (9%)	11,14,16	1.09	1 (9%)
2	SAR	D	7	2	3,4,5	0.88	0	1,3,5	2.06	1 (100%)
2	MLE	J	8	2	7,8,9	0.83	0	7,9,11	1.19	1 (14%)
2	MLE	N	3	2	7,8,9	1.12	0	7,9,11	1.55	1 (14%)
2	MVA	D	4	2	6,7,8	0.93	0	6,8,10	1.63	2 (33%)
2	ABA	N	6	2	4,5,6	0.87	0	1,5,7	0.23	0
2	BMT	T	5	2	11,12,13	1.03	0	11,14,16	1.19	1 (9%)
2	MLE	F	8	2	7,8,9	0.74	0	7,9,11	1.04	0
2	MLE	F	2	2	7,8,9	0.87	0	7,9,11	1.30	1 (14%)
2	SAR	H	7	2	3,4,5	0.75	0	1,3,5	2.66	1 (100%)
2	MLE	H	2	2	7,8,9	0.74	0	7,9,11	1.11	1 (14%)
2	MVA	J	4	2	6,7,8	0.89	0	6,8,10	1.60	2 (33%)

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	ABA	T	6	2	-	1/3/4/6	-
2	MVA	R	4	2	-	0/6/8/10	-
2	MLE	T	10	2	-	0/5/8/10	-
2	MLE	H	3	2	-	0/5/8/10	-
2	MVA	T	4	2	-	0/6/8/10	-
2	MLE	H	10	2	-	0/5/8/10	-
2	MVA	N	4	2	-	0/6/8/10	-
2	BMT	R	5	2	-	0/14/16/18	-
2	MLE	B	8	2	-	1/5/8/10	-
2	MLE	R	10	2	-	0/5/8/10	-
2	SAR	F	7	2	-	1/1/2/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLE	B	2	2	-	0/5/8/10	-
2	MLE	N	8	2	-	1/5/8/10	-
2	ABA	P	6	2	-	0/3/4/6	-
2	BMT	N	5	2	-	0/14/16/18	-
2	BMT	P	5	2	-	0/14/16/18	-
2	SAR	L	7	2	-	1/1/2/3	-
2	MLE	L	2	2	-	0/5/8/10	-
2	MLE	P	3	2	-	0/5/8/10	-
2	MLE	P	10	2	-	0/5/8/10	-
2	ABA	J	6	2	-	1/3/4/6	-
2	MLE	D	3	2	-	0/5/8/10	-
2	MLE	R	8	2	-	1/5/8/10	-
2	MLE	D	2	2	-	0/5/8/10	-
2	MVA	F	4	2	-	1/6/8/10	-
2	MLE	D	10	2	-	0/5/8/10	-
2	MLE	T	3	2	-	0/5/8/10	-
2	MLE	F	3	2	-	0/5/8/10	-
2	MLE	J	2	2	-	0/5/8/10	-
2	SAR	N	7	2	-	1/1/2/3	-
2	SAR	R	7	2	-	1/1/2/3	-
2	MLE	R	2	2	-	0/5/8/10	-
2	MLE	T	8	2	-	1/5/8/10	-
2	MLE	T	2	2	-	0/5/8/10	-
2	SAR	T	7	2	-	1/1/2/3	-
2	MLE	L	3	2	-	0/5/8/10	-
2	ABA	D	6	2	-	1/3/4/6	-
2	MLE	D	8	2	-	1/5/8/10	-
2	BMT	D	5	2	-	0/14/16/18	-
2	MLE	B	10	2	-	0/5/8/10	-
2	BMT	L	5	2	-	0/14/16/18	-
2	SAR	B	7	2	-	1/1/2/3	-
2	MLE	J	3	2	-	0/5/8/10	-
2	MLE	J	10	2	-	0/5/8/10	-
2	ABA	H	6	2	-	1/3/4/6	-
2	BMT	H	5	2	-	0/14/16/18	-
2	ABA	B	6	2	-	1/3/4/6	-
2	MLE	F	10	2	-	0/5/8/10	-
2	MLE	P	8	2	-	1/5/8/10	-
2	MVA	P	4	2	-	0/6/8/10	-
2	MVA	H	4	2	-	0/6/8/10	-
2	BMT	B	5	2	-	0/14/16/18	-
2	MLE	L	8	2	-	1/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMT	J	5	2	-	0/14/16/18	-
2	ABA	R	6	2	-	1/3/4/6	-
2	MLE	B	3	2	-	0/5/8/10	-
2	ABA	L	6	2	-	1/3/4/6	-
2	MLE	R	3	2	-	0/5/8/10	-
2	SAR	P	7	2	-	1/1/2/3	-
2	MLE	N	10	2	-	0/5/8/10	-
2	MLE	N	2	2	-	0/5/8/10	-
2	MVA	B	4	2	-	0/6/8/10	-
2	SAR	J	7	2	-	1/1/2/3	-
2	MLE	P	2	2	-	0/5/8/10	-
2	MLE	L	10	2	-	0/5/8/10	-
2	MVA	L	4	2	-	0/6/8/10	-
2	ABA	F	6	2	-	0/3/4/6	-
2	MLE	H	8	2	-	1/5/8/10	-
2	BMT	F	5	2	-	0/14/16/18	-
2	SAR	D	7	2	-	1/1/2/3	-
2	MLE	J	8	2	-	1/5/8/10	-
2	MLE	N	3	2	-	0/5/8/10	-
2	MVA	D	4	2	-	0/6/8/10	-
2	ABA	N	6	2	-	1/3/4/6	-
2	BMT	T	5	2	-	0/14/16/18	-
2	MLE	F	8	2	-	1/5/8/10	-
2	MLE	F	2	2	-	0/5/8/10	-
2	SAR	H	7	2	-	1/1/2/3	-
2	MLE	H	2	2	-	0/5/8/10	-
2	MVA	J	4	2	-	0/6/8/10	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	5	BMT	CG2-CB	2.59	1.58	1.53
2	R	5	BMT	CG2-CB	2.38	1.57	1.53
2	H	5	BMT	CG2-CB	2.37	1.57	1.53
2	J	5	BMT	CG2-CB	2.31	1.57	1.53
2	B	2	MLE	CB-CA	2.28	1.56	1.53

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	3	MLE	CB-CA-N	-3.63	105.09	110.59
2	T	4	MVA	CG1-CB-CA	-3.58	105.71	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	10	MLE	CB-CA-N	-3.30	105.59	110.59
2	L	3	MLE	CB-CA-N	-3.27	105.63	110.59
2	F	10	MLE	CB-CA-N	-3.27	105.63	110.59

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	6	ABA	O-C-CA-CB
2	D	6	ABA	O-C-CA-CB
2	H	6	ABA	O-C-CA-CB
2	J	6	ABA	O-C-CA-CB
2	L	6	ABA	O-C-CA-CB

There are no ring outliers.

24 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	4	MVA	1	0
2	T	10	MLE	1	0
2	H	10	MLE	1	0
2	R	5	BMT	1	0
2	R	10	MLE	1	0
2	L	2	MLE	1	0
2	D	3	MLE	1	0
2	D	2	MLE	1	0
2	F	4	MVA	1	0
2	D	10	MLE	1	0
2	J	2	MLE	1	0
2	R	2	MLE	1	0
2	L	3	MLE	1	0
2	B	10	MLE	1	0
2	J	10	MLE	1	0
2	H	5	BMT	1	0
2	F	10	MLE	1	0
2	H	4	MVA	1	0
2	B	5	BMT	1	0
2	N	10	MLE	1	0
2	N	2	MLE	1	0
2	B	4	MVA	1	0
2	L	4	MVA	2	0
2	H	2	MLE	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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.