Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:44 AM GMT

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/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:

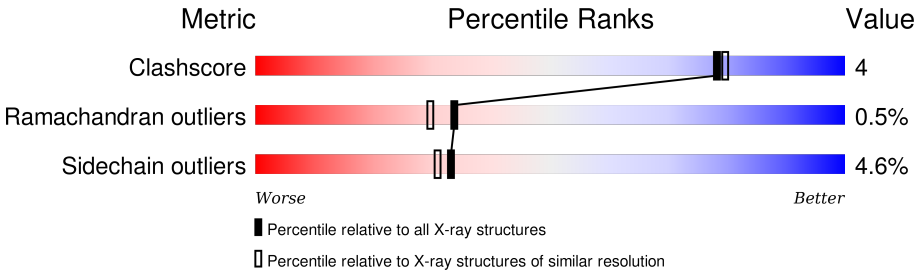
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (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. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	165	88% 10% •
1	C	165	85% 15%
1	E	165	88% 11% •
1	G	165	87% 13% •
1	I	165	88% 11% •
1	K	165	90% 8% ••
1	M	165	82% 15% ••

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Mol	Chain	Length	Quality of chain
1	O	165	92% 7%
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

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
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
			93	63	7	11	12			
2	D	11	Total	C	H	N	O	0	0	0
			93	63	7	11	12			
2	F	11	Total	C	H	N	O	0	0	0
			93	63	7	11	12			
2	H	11	Total	C	H	N	O	0	0	0
			93	63	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
			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 H O 6 4 2	0	0
3	I	68	Total H O 204 136 68	0	0
3	J	2	Total H O 6 4 2	0	0
3	K	73	Total H O 219 146 73	0	0
3	L	1	Total H O 3 2 1	0	0
3	M	52	Total H O 156 104 52	0	0
3	N	1	Total H O 3 2 1	0	0
3	O	66	Total H O 198 132 66	0	0
3	P	3	Total H O 9 6 3	0	0
3	Q	48	Total H O 144 96 48	0	0
3	R	2	Total H O 6 4 2	0	0
3	S	72	Total H O 216 144 72	0	0
3	T	2	Total H O 6 4 2	0	0

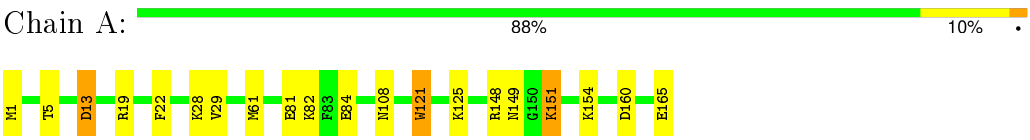
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

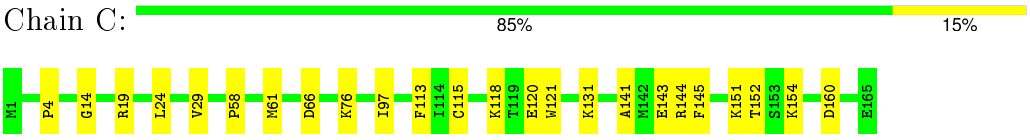
• Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

Chain A:



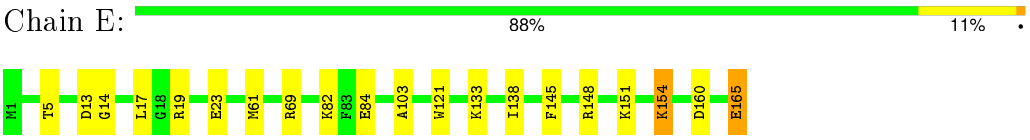
• Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

Chain C:



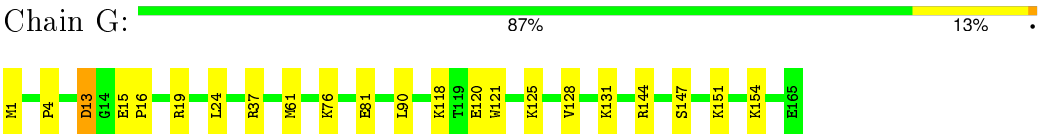
• Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

Chain E:



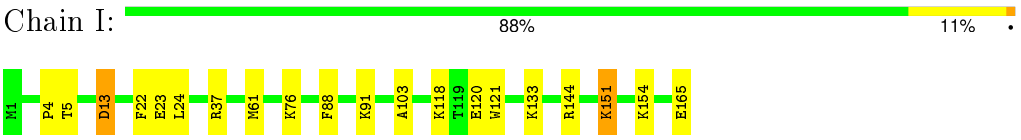
• Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

Chain G:



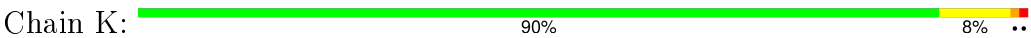
• Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

Chain I:



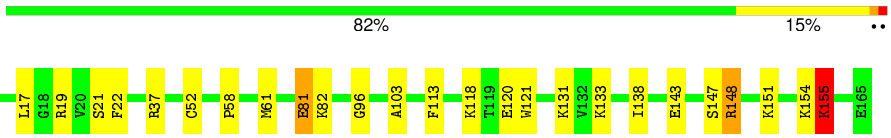
• Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

Chain K:



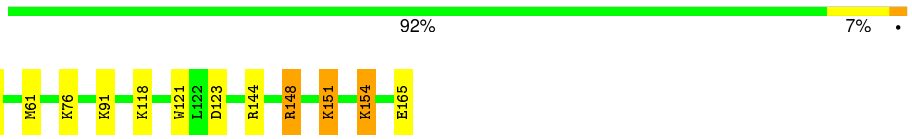
• Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

Chain M:



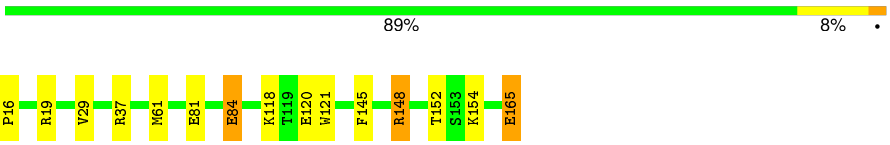
• Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

Chain O:



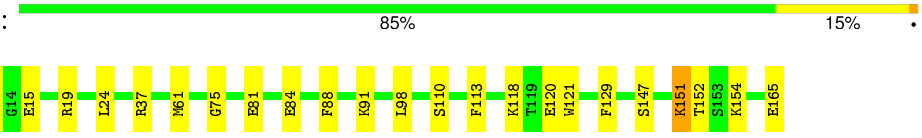
• Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

Chain Q:



• Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

Chain S:



• Molecule 2: CYCLOSPORIN A

Chain B:

• Molecule 2: CYCLOSPORIN A

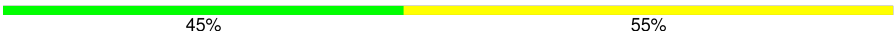
Chain D:

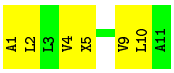
• Molecule 2: CYCLOSPORIN A

Chain F:

• Molecule 2: CYCLOSPORIN A

Chain H:





• Molecule 2: CYCLOSPORIN A

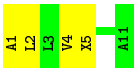
Chain J:

• Molecule 2: CYCLOSPORIN A

Chain L:

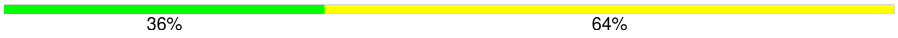
• Molecule 2: CYCLOSPORIN A

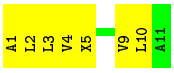
Chain N:



• Molecule 2: CYCLOSPORIN A

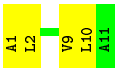
Chain P:





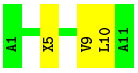
• Molecule 2: CYCLOSPORIN A

Chain R:



• Molecule 2: CYCLOSPORIN A

Chain T:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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.	Xtriage
Total number of atoms	18488	wwPDB-VP
Average B, all atoms (Å^2)	27.0	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: 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.

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
1	Q	19	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	I	121	TRP	CD1-CG-CD2	8.07	112.75	106.30
1	M	121	TRP	CD1-CG-CD2	8.03	112.72	106.30
1	A	121	TRP	CD1-CG-CD2	7.96	112.67	106.30
1	Q	121	TRP	CD1-CG-CD2	7.89	112.61	106.30
1	E	121	TRP	CD1-CG-CD2	7.59	112.37	106.30
1	C	121	TRP	CD1-CG-CD2	7.44	112.25	106.30
1	O	121	TRP	CD1-CG-CD2	7.42	112.24	106.30
1	K	121	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	S	121	TRP	CE2-CD2-CG	-7.23	101.51	107.30
1	I	144	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	I	121	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	Q	121	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	O	121	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	G	121	TRP	CD1-CG-CD2	6.96	111.87	106.30
1	E	121	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	G	76	LYS	CA-CB-CG	6.93	128.65	113.40
1	A	121	TRP	CE2-CD2-CG	-6.86	101.82	107.30
1	Q	148	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	C	121	TRP	CE2-CD2-CG	-6.61	102.01	107.30
1	M	121	TRP	CE2-CD2-CG	-6.55	102.06	107.30
1	M	19	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	G	37	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	G	121	TRP	CE2-CD2-CG	-6.50	102.10	107.30
1	A	13	ASP	CB-CG-OD1	6.34	124.01	118.30
1	E	165	GLU	CA-CB-CG	6.32	127.30	113.40
1	K	19	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	E	19	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	G	19	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	S	81	GLU	CA-CB-CG	6.14	126.91	113.40
1	Q	165	GLU	CA-CB-CG	6.08	126.77	113.40
1	G	144	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	O	19	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	Q	84	GLU	OE1-CD-OE2	-5.72	116.44	123.30
1	I	13	ASP	CB-CG-OD1	5.69	123.42	118.30
1	I	37	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	K	121	TRP	CG-CD1-NE1	-5.67	104.44	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	13	ASP	CB-CG-OD1	5.61	123.35	118.30
1	S	37	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	M	121	TRP	CG-CD1-NE1	-5.59	104.50	110.10
1	M	148	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	S	121	TRP	CG-CD1-NE1	-5.53	104.57	110.10
1	A	81	GLU	CA-CB-CG	5.47	125.44	113.40
1	K	151	LYS	CA-CB-CG	5.43	125.36	113.40
1	M	81	GLU	CA-CB-CG	5.30	125.06	113.40
1	M	155	LYS	CA-CB-CG	5.30	125.05	113.40
1	C	66	ASP	CB-CG-OD1	5.26	123.04	118.30
1	S	37	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	Q	81	GLU	CA-CB-CG	5.19	124.83	113.40
1	I	121	TRP	CG-CD1-NE1	-5.17	104.93	110.10
1	E	165	GLU	OE1-CD-OE2	-5.17	117.10	123.30
1	M	37	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	O	123	ASP	CB-CG-OD2	5.14	122.92	118.30
1	E	69	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	121	TRP	CG-CD1-NE1	-5.08	105.02	110.10
1	Q	37	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	C	121	TRP	CG-CD1-NE1	-5.04	105.06	110.10

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
1:I:23:GLU:HB2	1:I:133:LYS:HD2	1.90	0.54
1:Q:145:PHE:O	1:Q:152:THR:HA	2.08	0.54
1:A:5:THR:HB	1:A:165:GLU:HG2	1.90	0.53
1:E:23:GLU:HB2	1:E:133:LYS:HD2	1.92	0.51
1:G:81:GLU:HG2	2:R:10:MLE:HD23	1.91	0.51
1:Q:118:LYS:HZ2	1:Q:120:GLU:HB3	1.77	0.50
1:I:88:PHE:O	1:I:91:LYS:NZ	2.45	0.50
1:I:5:THR:HA	1:I:22:PHE:O	2.12	0.49
1:G:90:LEU:HB2	1:G:128:VAL:HB	1.94	0.49
1:A:28:LYS:NZ	3:A:2010:HOH:O	2.46	0.49
1:O:154:LYS:NZ	3:O:2061:HOH:O	2.45	0.49
1:S:5:THR:HB	1:S:165:GLU:HG2	1.95	0.48
1:A:121:TRP:O	1:A:125:LYS:NZ	2.45	0.48
1:K:5:THR:HB	1:K:165:GLU:HG2	1.95	0.48
1:A:149:ASN:HD21	1:A:151:LYS:HB3	1.80	0.47
2:P:2:MLE:HA	2:P:3:MLE:HN1	1.76	0.47
2:R:1:DAL:HA	2:R:2:MLE:HN1	1.77	0.46
2:B:9:VAL:HA	2:B:10:MLE:HN1	1.69	0.46
1:M:52:CYS:HB3	1:M:155:LYS:NZ	2.31	0.46
1:I:118:LYS:HZ2	1:I:120:GLU:HB3	1.80	0.46
1:M:118:LYS:HZ2	1:M:120:GLU:HB3	1.79	0.46
1:E:82:LYS:NZ	3:E:2033:HOH:O	2.43	0.46
1:C:145:PHE:O	1:C:152:THR:HA	2.14	0.46
1:E:145:PHE:CD1	1:E:154:LYS:HG3	2.51	0.46
2:P:9:VAL:HA	2:P:10:MLE:HN1	1.68	0.46
1:M:13:ASP:OD1	1:M:154:LYS:HB3	2.16	0.46
2:B:1:DAL:HA	2:B:2:MLE:HN1	1.76	0.46
1:E:5:THR:CB	1:E:165:GLU:HB3	2.41	0.46
1:C:118:LYS:NZ	1:C:120:GLU:HB3	2.30	0.46
1:S:147:SER:OG	1:S:151:LYS:HD3	2.16	0.45
1:G:118:LYS:NZ	1:G:120:GLU:HB3	2.32	0.45
1:S:4:PRO:HG2	1:S:24:LEU:HB2	1.97	0.45
1:I:76:LYS:HD2	3:I:2012:HOH:O	2.15	0.45
1:C:113:PHE:CD1	2:D:4:MVA:HG11	2.52	0.45
1:M:82:LYS:NZ	3:M:2020:HOH:O	2.49	0.45
1:E:103:ALA:HB1	2:P:5:DMT:HH1	1.97	0.45
1:A:151:LYS:NZ	3:A:2071:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1:DAL:HA	2:H:2:MLE:HN1	1.82	0.44
2:H:9:VAL:HA	2:H:10:MLE:HN1	1.71	0.44
2:L:5:DMT:O	2:L:7:SAR:HN1	2.16	0.44
1:O:151:LYS:NZ	1:O:151:LYS:O	2.47	0.44
1:G:15:GLU:HA	1:G:16:PRO:HD2	1.86	0.44
1:E:17:LEU:HG	1:E:138:ILE:HG23	1.99	0.44
1:O:148:ARG:NH1	3:O:2058:HOH:O	2.49	0.44
1:I:103:ALA:HB1	2:T:5:DMT:HH1	1.99	0.43
1:G:118:LYS:HZ3	1:G:120:GLU:HB3	1.82	0.43
1:C:58:PRO:HA	1:C:143:GLU:OE2	2.18	0.43
1:O:5:THR:HB	1:O:165:GLU:HG2	1.99	0.43
1:S:118:LYS:NZ	1:S:120:GLU:HB3	2.34	0.43
2:R:9:VAL:HA	2:R:10:MLE:HN1	1.73	0.43
1:Q:118:LYS:NZ	1:Q:120:GLU:HB3	2.34	0.43
1:G:125:LYS:NZ	3:G:2054:HOH:O	2.52	0.43
2:L:9:VAL:HA	2:L:10:MLE:HN1	1.80	0.43
1:I:151:LYS:O	1:I:151:LYS:NZ	2.51	0.43
1:C:131:LYS:NZ	3:C:2052:HOH:O	2.52	0.43
1:M:3:ASN:HA	1:M:4:PRO:HD3	1.94	0.42
1:M:5:THR:HA	1:M:22:PHE:O	2.18	0.42
1:Q:15:GLU:HA	1:Q:16:PRO:HD2	1.91	0.42
1:A:5:THR:HA	1:A:22:PHE:O	2.19	0.42
1:A:82:LYS:HA	1:A:108:ASN:O	2.19	0.42
1:M:113:PHE:CD1	2:N:4:MVA:HG11	2.54	0.42
2:N:1:DAL:HA	2:N:2:MLE:HN1	1.88	0.42
1:M:96:GLY:O	1:M:131:LYS:HG3	2.20	0.42
2:J:9:VAL:HA	2:J:10:MLE:HN1	1.68	0.42
1:M:58:PRO:HA	1:M:143:GLU:OE2	2.20	0.42
1:K:4:PRO:HG2	1:K:24:LEU:HB2	2.02	0.42
1:I:4:PRO:HG2	1:I:24:LEU:HB2	2.01	0.42
1:K:15:GLU:HA	1:K:16:PRO:HD2	1.87	0.41
1:M:21:SER:OG	1:M:133:LYS:HB3	2.20	0.41
1:C:141:ALA:HA	1:C:144:ARG:NH2	2.36	0.41
1:M:52:CYS:HB3	1:M:155:LYS:HZ1	1.85	0.41
2:F:1:DAL:HA	2:F:2:MLE:HN1	1.84	0.41
1:S:88:PHE:O	1:S:91:LYS:NZ	2.53	0.41
1:O:76:LYS:NZ	3:O:2029:HOH:O	2.53	0.41
2:D:1:DAL:HA	2:D:2:MLE:HN1	1.84	0.41
2:T:9:VAL:HA	2:T:10:MLE:HN1	1.67	0.41
2:F:9:VAL:HA	2:F:10:MLE:HN1	1.76	0.41
1:S:98:LEU:HG	1:S:129:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ILE:N	3:C:2031:HOH:O	2.51	0.41
2:N:4:MVA:HA	2:N:5:DMT:HCN1	1.79	0.41
2:D:6:ABA:HA	2:D:7:SAR:HN1	1.90	0.41
2:H:4:MVA:HA	2:H:5:DMT:HCN1	1.76	0.41
2:P:1:DAL:HA	2:P:2:MLE:HN1	1.80	0.40
1:O:118:LYS:NZ	3:O:2047:HOH:O	2.49	0.40
2:D:5:DMT:HH1	1:M:103:ALA:HB1	2.03	0.40
1:S:75:GLY:HA3	1:S:110:SER:OG	2.22	0.40
1:I:5:THR:HB	1:I:165:GLU:HG2	2.02	0.40
2:P:4:MVA:HA	2:P:5:DMT:HCN1	1.76	0.40
2:D:10:MLE:HD23	1:M:81:GLU:HG2	2.02	0.40
1:M:17:LEU:HG	1:M:138:ILE:HG23	2.03	0.40
1:C:4:PRO:HG2	1:C:24:LEU:HB2	2.02	0.40
1:K:76:LYS:NZ	3:K:2032:HOH:O	2.53	0.40
1:G:4:PRO:HG2	1:G:24:LEU:HB2	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 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%)	30	24
1	C	163/165 (99%)	156 (96%)	6 (4%)	1 (1%)	30	24
1	E	163/165 (99%)	155 (95%)	6 (4%)	2 (1%)	16	10
1	G	163/165 (99%)	153 (94%)	9 (6%)	1 (1%)	30	24
1	I	163/165 (99%)	155 (95%)	7 (4%)	1 (1%)	30	24
1	K	163/165 (99%)	154 (94%)	8 (5%)	1 (1%)	30	24
1	M	163/165 (99%)	151 (93%)	11 (7%)	1 (1%)	30	24
1	O	163/165 (99%)	156 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	163/165 (99%)	153 (94%)	9 (6%)	1 (1%)	30	24
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%)	34	30

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	13	ASP
1	I	13	ASP
1	K	13	ASP
1	A	13	ASP
1	G	13	ASP
1	E	13	ASP
1	C	14	GLY
1	M	13	ASP
1	E	14	GLY

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	133/133 (100%)	125 (94%)	8 (6%)	24	20
1	C	133/133 (100%)	127 (96%)	6 (4%)	34	32
1	E	133/133 (100%)	127 (96%)	6 (4%)	34	32
1	G	133/133 (100%)	126 (95%)	7 (5%)	28	25
1	I	133/133 (100%)	130 (98%)	3 (2%)	58	62
1	K	133/133 (100%)	127 (96%)	6 (4%)	34	32
1	M	133/133 (100%)	127 (96%)	6 (4%)	34	32
1	O	133/133 (100%)	127 (96%)	6 (4%)	34	32
1	Q	133/133 (100%)	127 (96%)	6 (4%)	34	32
1	S	133/133 (100%)	126 (95%)	7 (5%)	28	25
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%)	1279 (95%)	61 (5%)	33	31

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	29	VAL
1	A	61	MET
1	A	84	GLU
1	A	148	ARG
1	A	151	LYS
1	A	154	LYS
1	A	160	ASP

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Mol	Chain	Res	Type
1	C	29	VAL
1	C	61	MET
1	C	76	LYS
1	C	151	LYS
1	C	154	LYS
1	C	160	ASP
1	E	61	MET
1	E	84	GLU
1	E	148	ARG
1	E	151	LYS
1	E	154	LYS
1	E	160	ASP
1	G	1	MET
1	G	13	ASP
1	G	61	MET
1	G	131	LYS
1	G	147	SER
1	G	151	LYS
1	G	154	LYS
1	I	61	MET
1	I	151	LYS
1	I	154	LYS
1	K	13	ASP
1	K	29	VAL
1	K	61	MET
1	K	148	ARG
1	K	151	LYS
1	K	154	LYS
1	M	13	ASP
1	M	61	MET
1	M	147	SER
1	M	148	ARG
1	M	151	LYS
1	M	155	LYS
1	O	61	MET
1	O	91	LYS
1	O	144	ARG
1	O	148	ARG
1	O	151	LYS
1	O	154	LYS
1	Q	13	ASP
1	Q	29	VAL

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Mol	Chain	Res	Type
1	Q	61	MET
1	Q	84	GLU
1	Q	148	ARG
1	Q	154	LYS
1	S	13	ASP
1	S	15	GLU
1	S	61	MET
1	S	84	GLU
1	S	151	LYS
1	S	152	THR
1	S	154	LYS

Some 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	DAL	B	1	2	3,4,5	0.79	0	0,4,6	0.00	-
2	MLE	B	10	2	7,8,9	0.70	0	4,9,11	0.98	0
2	MLE	B	2	2	7,8,9	0.71	0	4,9,11	0.99	0
2	MLE	B	3	2	7,8,9	0.87	0	4,9,11	1.16	1 (25%)
2	MVA	B	4	2	6,7,8	0.81	0	6,8,10	1.81	2 (33%)
2	DMT	B	5	2	11,13,14	1.41	2 (18%)	11,17,19	1.55	4 (36%)
2	ABA	B	6	2	4,5,6	0.69	0	3,5,7	1.22	1 (33%)
2	SAR	B	7	2	4,4,5	0.81	0	2,3,5	1.62	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MLE	B	8	2	7,8,9	0.68	0	4,9,11	1.03	0
2	DAL	D	1	2	3,4,5	0.78	0	0,4,6	0.00	-
2	MLE	D	10	2	7,8,9	0.77	0	4,9,11	1.25	1 (25%)
2	MLE	D	2	2	7,8,9	0.65	0	4,9,11	0.90	0
2	MLE	D	3	2	7,8,9	0.81	0	4,9,11	0.98	0
2	MVA	D	4	2	6,7,8	0.78	0	6,8,10	1.78	2 (33%)
2	DMT	D	5	2	11,13,14	1.63	2 (18%)	11,17,19	1.96	3 (27%)
2	ABA	D	6	2	4,5,6	0.72	0	3,5,7	1.17	0
2	SAR	D	7	2	4,4,5	0.78	0	2,3,5	1.64	1 (50%)
2	MLE	D	8	2	7,8,9	0.60	0	4,9,11	1.15	1 (25%)
2	DAL	F	1	2	3,4,5	0.81	0	0,4,6	0.00	-
2	MLE	F	10	2	7,8,9	0.69	0	4,9,11	0.98	0
2	MLE	F	2	2	7,8,9	0.66	0	4,9,11	1.00	0
2	MLE	F	3	2	7,8,9	0.82	0	4,9,11	1.18	1 (25%)
2	MVA	F	4	2	6,7,8	1.02	0	6,8,10	1.92	2 (33%)
2	DMT	F	5	2	11,13,14	1.64	2 (18%)	11,17,19	1.60	4 (36%)
2	ABA	F	6	2	4,5,6	0.70	0	3,5,7	1.07	0
2	SAR	F	7	2	4,4,5	0.79	0	2,3,5	1.48	1 (50%)
2	MLE	F	8	2	7,8,9	0.68	0	4,9,11	1.15	1 (25%)
2	DAL	H	1	2	3,4,5	0.72	0	0,4,6	0.00	-
2	MLE	H	10	2	7,8,9	0.71	0	4,9,11	0.97	0
2	MLE	H	2	2	7,8,9	0.70	0	4,9,11	0.95	0
2	MLE	H	3	2	7,8,9	0.85	0	4,9,11	1.08	1 (25%)
2	MVA	H	4	2	6,7,8	1.32	1 (16%)	6,8,10	2.38	4 (66%)
2	DMT	H	5	2	11,13,14	1.60	2 (18%)	11,17,19	1.76	4 (36%)
2	ABA	H	6	2	4,5,6	0.62	0	3,5,7	1.50	1 (33%)
2	SAR	H	7	2	4,4,5	0.92	0	2,3,5	1.76	1 (50%)
2	MLE	H	8	2	7,8,9	0.68	0	4,9,11	0.81	0
2	DAL	J	1	2	3,4,5	0.75	0	0,4,6	0.00	-
2	MLE	J	10	2	7,8,9	0.69	0	4,9,11	0.83	0
2	MLE	J	2	2	7,8,9	0.65	0	4,9,11	1.04	0
2	MLE	J	3	2	7,8,9	0.72	0	4,9,11	1.17	1 (25%)
2	MVA	J	4	2	6,7,8	0.83	0	6,8,10	1.62	2 (33%)
2	DMT	J	5	2	11,13,14	1.52	1 (9%)	11,17,19	1.65	4 (36%)
2	ABA	J	6	2	4,5,6	0.65	0	3,5,7	1.55	1 (33%)
2	SAR	J	7	2	4,4,5	0.75	0	2,3,5	1.71	1 (50%)
2	MLE	J	8	2	7,8,9	0.70	0	4,9,11	0.82	0
2	DAL	L	1	2	3,4,5	0.74	0	0,4,6	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MLE	L	10	2	7,8,9	0.74	0	4,9,11	0.97	0
2	MLE	L	2	2	7,8,9	0.62	0	4,9,11	1.00	0
2	MLE	L	3	2	7,8,9	0.83	0	4,9,11	0.95	0
2	MVA	L	4	2	6,7,8	0.96	0	6,8,10	1.71	2 (33%)
2	DMT	L	5	2	11,13,14	1.54	3 (27%)	11,17,19	1.21	1 (9%)
2	ABA	L	6	2	4,5,6	0.69	0	3,5,7	1.51	1 (33%)
2	SAR	L	7	2	4,4,5	0.77	0	2,3,5	1.87	1 (50%)
2	MLE	L	8	2	7,8,9	0.61	0	4,9,11	0.76	0
2	DAL	N	1	2	3,4,5	0.67	0	0,4,6	0.00	-
2	MLE	N	10	2	7,8,9	0.70	0	4,9,11	0.86	0
2	MLE	N	2	2	7,8,9	0.64	0	4,9,11	1.04	0
2	MLE	N	3	2	7,8,9	0.84	0	4,9,11	1.11	1 (25%)
2	MVA	N	4	2	6,7,8	0.80	0	6,8,10	2.08	2 (33%)
2	DMT	N	5	2	11,13,14	1.33	1 (9%)	11,17,19	1.56	3 (27%)
2	ABA	N	6	2	4,5,6	0.78	0	3,5,7	1.39	1 (33%)
2	SAR	N	7	2	4,4,5	0.76	0	2,3,5	1.63	1 (50%)
2	MLE	N	8	2	7,8,9	0.62	0	4,9,11	0.72	0
2	DAL	P	1	2	3,4,5	0.80	0	0,4,6	0.00	-
2	MLE	P	10	2	7,8,9	0.72	0	4,9,11	1.03	0
2	MLE	P	2	2	7,8,9	0.68	0	4,9,11	1.05	0
2	MLE	P	3	2	7,8,9	0.85	0	4,9,11	1.20	1 (25%)
2	MVA	P	4	2	6,7,8	0.81	0	6,8,10	1.47	0
2	DMT	P	5	2	11,13,14	1.59	2 (18%)	11,17,19	1.75	4 (36%)
2	ABA	P	6	2	4,5,6	0.77	0	3,5,7	1.39	1 (33%)
2	SAR	P	7	2	4,4,5	0.76	0	2,3,5	1.63	1 (50%)
2	MLE	P	8	2	7,8,9	0.77	0	4,9,11	0.87	0
2	DAL	R	1	2	3,4,5	0.82	0	0,4,6	0.00	-
2	MLE	R	10	2	7,8,9	0.83	0	4,9,11	0.61	0
2	MLE	R	2	2	7,8,9	0.67	0	4,9,11	1.26	1 (25%)
2	MLE	R	3	2	7,8,9	0.88	0	4,9,11	1.16	1 (25%)
2	MVA	R	4	2	6,7,8	0.83	0	6,8,10	1.63	2 (33%)
2	DMT	R	5	2	11,13,14	1.67	2 (18%)	11,17,19	1.57	3 (27%)
2	ABA	R	6	2	4,5,6	0.66	0	3,5,7	1.52	1 (33%)
2	SAR	R	7	2	4,4,5	0.83	0	2,3,5	1.86	1 (50%)
2	MLE	R	8	2	7,8,9	0.62	0	4,9,11	1.03	0
2	DAL	T	1	2	3,4,5	0.76	0	0,4,6	0.00	-
2	MLE	T	10	2	7,8,9	0.70	0	4,9,11	0.85	0
2	MLE	T	2	2	7,8,9	0.61	0	4,9,11	1.14	1 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MLE	T	3	2	7,8,9	0.79	0	4,9,11	1.21	1 (25%)
2	MVA	T	4	2	6,7,8	0.98	0	6,8,10	1.61	2 (33%)
2	DMT	T	5	2	11,13,14	1.64	2 (18%)	11,17,19	1.86	3 (27%)
2	ABA	T	6	2	4,5,6	0.65	0	3,5,7	1.38	1 (33%)
2	SAR	T	7	2	4,4,5	0.89	0	2,3,5	1.67	1 (50%)
2	MLE	T	8	2	7,8,9	0.71	0	4,9,11	0.55	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	DAL	B	1	2	-	0/0/2/4	0/0/0/0
2	MLE	B	10	2	-	0/4/8/10	0/0/0/0
2	MLE	B	2	2	-	0/4/8/10	0/0/0/0
2	MLE	B	3	2	-	0/4/8/10	0/0/0/0
2	MVA	B	4	2	-	0/5/8/10	0/0/0/0
2	DMT	B	5	2	-	0/16/19/21	0/0/0/0
2	ABA	B	6	2	-	0/2/4/6	0/0/0/0
2	SAR	B	7	2	-	0/1/2/3	0/0/0/0
2	MLE	B	8	2	-	0/4/8/10	0/0/0/0
2	DAL	D	1	2	-	0/0/2/4	0/0/0/0
2	MLE	D	10	2	-	0/4/8/10	0/0/0/0
2	MLE	D	2	2	-	0/4/8/10	0/0/0/0
2	MLE	D	3	2	-	0/4/8/10	0/0/0/0
2	MVA	D	4	2	-	0/5/8/10	0/0/0/0
2	DMT	D	5	2	-	0/16/19/21	0/0/0/0
2	ABA	D	6	2	-	0/2/4/6	0/0/0/0
2	SAR	D	7	2	-	0/1/2/3	0/0/0/0
2	MLE	D	8	2	-	0/4/8/10	0/0/0/0
2	DAL	F	1	2	-	0/0/2/4	0/0/0/0
2	MLE	F	10	2	-	0/4/8/10	0/0/0/0
2	MLE	F	2	2	-	0/4/8/10	0/0/0/0
2	MLE	F	3	2	-	0/4/8/10	0/0/0/0
2	MVA	F	4	2	-	0/5/8/10	0/0/0/0
2	DMT	F	5	2	-	0/16/19/21	0/0/0/0
2	ABA	F	6	2	-	0/2/4/6	0/0/0/0
2	SAR	F	7	2	-	0/1/2/3	0/0/0/0
2	MLE	F	8	2	-	0/4/8/10	0/0/0/0
2	DAL	H	1	2	-	0/0/2/4	0/0/0/0

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAR	P	7	2	-	0/1/2/3	0/0/0/0
2	MLE	P	8	2	-	0/4/8/10	0/0/0/0
2	DAL	R	1	2	-	0/0/2/4	0/0/0/0
2	MLE	R	10	2	-	0/4/8/10	0/0/0/0
2	MLE	R	2	2	-	0/4/8/10	0/0/0/0
2	MLE	R	3	2	-	0/4/8/10	0/0/0/0
2	MVA	R	4	2	-	0/5/8/10	0/0/0/0
2	DMT	R	5	2	-	0/16/19/21	0/0/0/0
2	ABA	R	6	2	-	0/2/4/6	0/0/0/0
2	SAR	R	7	2	-	0/1/2/3	0/0/0/0
2	MLE	R	8	2	-	0/4/8/10	0/0/0/0
2	DAL	T	1	2	-	0/0/2/4	0/0/0/0
2	MLE	T	10	2	-	0/4/8/10	0/0/0/0
2	MLE	T	2	2	-	0/4/8/10	0/0/0/0
2	MLE	T	3	2	-	0/4/8/10	0/0/0/0
2	MVA	T	4	2	-	0/5/8/10	0/0/0/0
2	DMT	T	5	2	-	0/16/19/21	0/0/0/0
2	ABA	T	6	2	-	0/2/4/6	0/0/0/0
2	SAR	T	7	2	-	0/1/2/3	0/0/0/0
2	MLE	T	8	2	-	0/4/8/10	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	5	DMT	CG2-CB	2.06	1.57	1.53
2	B	5	DMT	CB-CA	2.17	1.58	1.54
2	N	5	DMT	CG2-CB	2.26	1.57	1.53
2	L	5	DMT	CD1-CE	2.29	1.53	1.50
2	B	5	DMT	CG2-CB	2.51	1.57	1.53
2	H	4	MVA	CB-CA	2.65	1.57	1.54
2	H	5	DMT	CB-CA	2.68	1.58	1.54
2	P	5	DMT	CB-CA	2.78	1.59	1.54
2	D	5	DMT	CG2-CB	2.81	1.58	1.53
2	F	5	DMT	CB-CA	2.81	1.59	1.54
2	R	5	DMT	CB-CA	2.86	1.59	1.54
2	L	5	DMT	CB-CA	2.87	1.59	1.54
2	T	5	DMT	CG2-CB	3.01	1.58	1.53
2	H	5	DMT	CG2-CB	3.04	1.58	1.53
2	P	5	DMT	CG2-CB	3.05	1.58	1.53
2	R	5	DMT	CG2-CB	3.13	1.59	1.53
2	J	5	DMT	CG2-CB	3.30	1.59	1.53
2	F	5	DMT	CG2-CB	3.30	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	5	DMT	CB-CA	3.32	1.60	1.54
2	D	5	DMT	CB-CA	3.32	1.60	1.54

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	5	DMT	CD3-CG2-CD1	-4.42	100.91	109.62
2	H	4	MVA	CG1-CB-CA	-4.17	105.53	111.68
2	T	5	DMT	CD3-CG2-CD1	-4.13	101.47	109.62
2	N	4	MVA	CG1-CB-CA	-3.93	105.88	111.68
2	P	5	DMT	CD3-CG2-CD1	-3.54	102.65	109.62
2	H	5	DMT	CD3-CG2-CD1	-3.47	102.77	109.62
2	F	4	MVA	CG1-CB-CA	-3.34	106.74	111.68
2	T	5	DMT	CD1-CE-CZ	-3.24	118.72	124.90
2	D	4	MVA	CG1-CB-CA	-2.96	107.31	111.68
2	D	5	DMT	CD1-CE-CZ	-2.89	119.39	124.90
2	N	5	DMT	CD3-CG2-CD1	-2.84	104.02	109.62
2	J	5	DMT	CD1-CE-CZ	-2.79	119.58	124.90
2	N	5	DMT	CD1-CE-CZ	-2.78	119.61	124.90
2	R	4	MVA	CG1-CB-CA	-2.75	107.62	111.68
2	B	4	MVA	O-C-CA	-2.71	117.43	125.74
2	F	5	DMT	CD3-CG2-CD1	-2.70	104.29	109.62
2	P	5	DMT	CD1-CE-CZ	-2.65	119.85	124.90
2	B	5	DMT	CD1-CE-CZ	-2.65	119.86	124.90
2	R	5	DMT	CD3-CG2-CD1	-2.64	104.41	109.62
2	L	4	MVA	CG1-CB-CA	-2.63	107.80	111.68
2	L	7	SAR	O-C-CA	-2.63	115.76	125.23
2	J	4	MVA	CG1-CB-CA	-2.62	107.81	111.68
2	F	5	DMT	CD1-CE-CZ	-2.60	119.95	124.90
2	R	6	ABA	O-C-CA	-2.57	118.79	125.49
2	H	6	ABA	O-C-CA	-2.56	118.83	125.49
2	R	7	SAR	O-C-CA	-2.55	116.04	125.23
2	B	5	DMT	CD3-CG2-CD1	-2.54	104.61	109.62
2	R	5	DMT	CD1-CE-CZ	-2.54	120.06	124.90
2	H	7	SAR	O-C-CA	-2.49	116.25	125.23
2	J	6	ABA	O-C-CA	-2.47	119.05	125.49
2	B	4	MVA	CG1-CB-CA	-2.45	108.06	111.68
2	H	5	DMT	CD3-CG2-CD2	-2.45	104.36	109.28
2	T	4	MVA	O-C-CA	-2.43	118.27	125.74
2	F	4	MVA	O-C-CA	-2.43	118.28	125.74
2	D	4	MVA	O-C-CA	-2.42	118.31	125.74
2	J	5	DMT	CD3-CG2-CD2	-2.41	104.44	109.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	7	SAR	O-C-CA	-2.40	116.59	125.23
2	T	6	ABA	O-C-CA	-2.38	119.28	125.49
2	L	6	ABA	O-C-CA	-2.38	119.29	125.49
2	N	6	ABA	O-C-CA	-2.37	119.31	125.49
2	L	5	DMT	CD3-CG2-CD2	-2.36	104.55	109.28
2	L	4	MVA	O-C-CA	-2.34	118.55	125.74
2	D	5	DMT	CD3-CG2-CD2	-2.32	104.63	109.28
2	F	3	MLE	O-C-CA	-2.31	119.33	125.44
2	J	5	DMT	CD3-CG2-CD1	-2.30	105.08	109.62
2	N	7	SAR	O-C-CA	-2.30	116.93	125.23
2	T	7	SAR	O-C-CA	-2.30	116.95	125.23
2	D	7	SAR	O-C-CA	-2.29	116.97	125.23
2	H	5	DMT	CD1-CE-CZ	-2.27	120.57	124.90
2	B	5	DMT	CD3-CG2-CD2	-2.25	104.75	109.28
2	B	7	SAR	O-C-CA	-2.24	117.14	125.23
2	P	6	ABA	O-C-CA	-2.24	119.66	125.49
2	D	8	MLE	O-C-CA	-2.23	119.54	125.44
2	R	3	MLE	O-C-CA	-2.23	119.56	125.44
2	B	3	MLE	O-C-CA	-2.23	119.56	125.44
2	F	5	DMT	CD3-CG2-CD2	-2.22	104.82	109.28
2	P	7	SAR	O-C-CA	-2.22	117.25	125.23
2	D	10	MLE	O-C-CA	-2.21	119.59	125.44
2	P	3	MLE	O-C-CA	-2.20	119.62	125.44
2	R	2	MLE	O-C-CA	-2.18	119.67	125.44
2	T	3	MLE	O-C-CA	-2.16	119.73	125.44
2	J	3	MLE	O-C-CA	-2.16	119.73	125.44
2	J	4	MVA	O-C-CA	-2.15	119.13	125.74
2	N	4	MVA	O-C-CA	-2.15	119.13	125.74
2	F	8	MLE	O-C-CA	-2.15	119.75	125.44
2	N	3	MLE	O-C-CA	-2.14	119.80	125.44
2	T	4	MVA	CG1-CB-CA	-2.13	108.54	111.68
2	F	7	SAR	O-C-CA	-2.09	117.71	125.23
2	R	4	MVA	O-C-CA	-2.08	119.36	125.74
2	H	3	MLE	O-C-CA	-2.08	119.95	125.44
2	T	2	MLE	O-C-CA	-2.07	119.98	125.44
2	P	5	DMT	CD3-CG2-CD2	-2.05	105.17	109.28
2	H	4	MVA	O-C-CA	-2.05	119.46	125.74
2	B	6	ABA	O-C-CA	-2.04	120.17	125.49
2	H	4	MVA	CN-N-CA	2.00	119.82	113.65
2	J	5	DMT	CN-N-CA	2.07	120.02	113.65
2	F	5	DMT	CN-N-CA	2.09	120.09	113.65
2	B	5	DMT	CN-N-CA	2.16	120.30	113.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	5	DMT	CN-N-CA	2.16	120.31	113.65
2	N	5	DMT	CN-N-CA	2.27	120.66	113.65
2	H	5	DMT	CN-N-CA	2.34	120.86	113.65
2	R	5	DMT	CN-N-CA	2.48	121.29	113.65
2	H	4	MVA	CG2-CB-CA	2.50	115.36	111.68
2	P	5	DMT	CN-N-CA	2.59	121.63	113.65

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	5	DMT	CD1-CE-CZ-CH

There are no ring outliers.

37 monomers are involved in 28 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	4	MVA	2	0
2	N	5	DMT	1	0
2	P	1	DAL	1	0
2	P	10	MLE	1	0
2	P	2	MLE	2	0
2	P	3	MLE	1	0
2	P	4	MVA	1	0
2	P	5	DMT	2	0
2	R	1	DAL	1	0
2	R	10	MLE	2	0
2	R	2	MLE	1	0
2	T	10	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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.