



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:01 PM UTC

PDB ID : 2RMA / pdb_00002rma
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

<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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

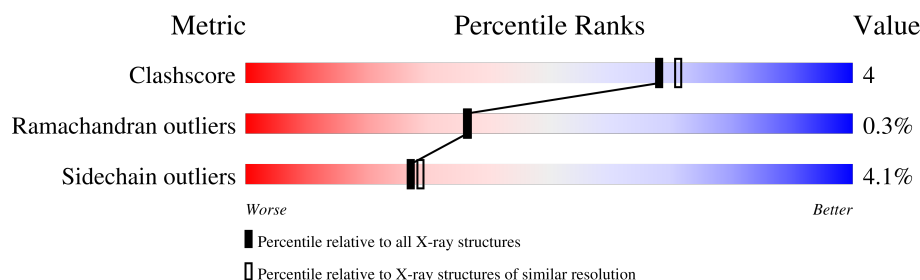
1 Overall quality at a glance

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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

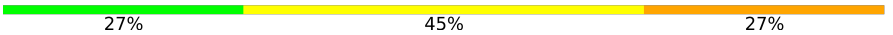
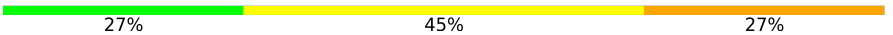
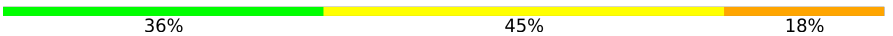
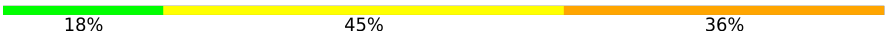
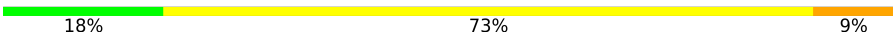
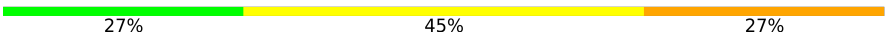
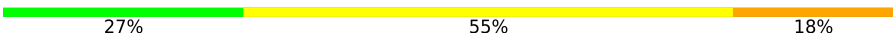
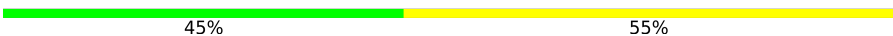
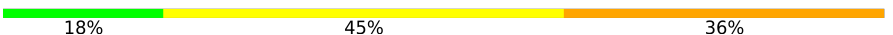
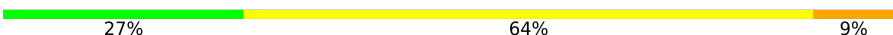
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	86% 14%
1	C	165	82% 18% .
1	E	165	85% 12% .
1	G	165	88% 12%
1	I	165	83% 16% .
1	K	165	80% 19% .
1	M	165	81% 19% .
1	O	165	85% 15% .

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Mol	Chain	Length	Quality of chain
1	Q	165	 78%21%
1	S	165	 82%15%
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		

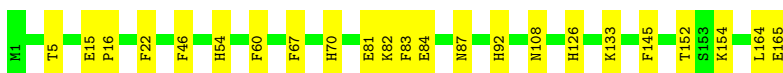
3 Residue-property plots [i](#)

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:  86% 14%



• Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

Chain C:  82% 18%



• Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

Chain E:  85% 12%



• Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

Chain G:  88% 12%



• Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

Chain I:  83% 16%

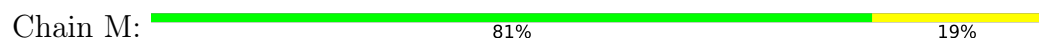


• Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE

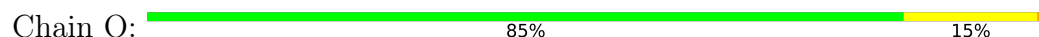
Chain K:  80% 19%



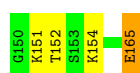
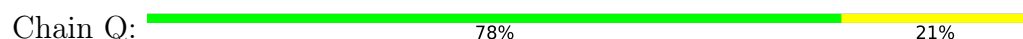
• Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE



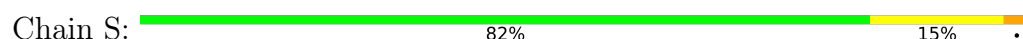
• Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE



• Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE



• Molecule 1: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE



• Molecule 2: CYCLOSPORIN A

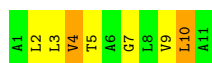


• Molecule 2: CYCLOSPORIN A

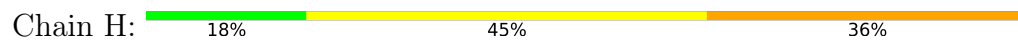


• Molecule 2: CYCLOSPORIN A





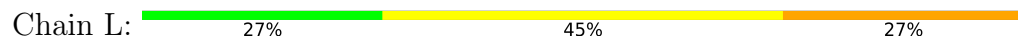
- Molecule 2: CYCLOSPORIN A



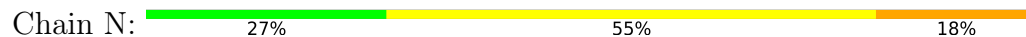
- Molecule 2: CYCLOSPORIN A



- Molecule 2: CYCLOSPORIN A



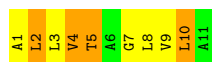
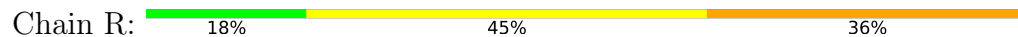
- Molecule 2: CYCLOSPORIN A



- Molecule 2: CYCLOSPORIN A



- Molecule 2: CYCLOSPORIN A



- Molecule 2: CYCLOSPORIN A



4 Data and refinement statistics

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, α , β , γ	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 ²)	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: ABA, DAL, MLE, BMT, SAR, MVA

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	0.79	4/1294 (0.3%)	1.44	10/1733 (0.6%)
1	C	0.80	5/1294 (0.4%)	1.43	6/1733 (0.3%)
1	E	0.81	4/1294 (0.3%)	1.44	10/1733 (0.6%)
1	G	0.81	5/1294 (0.4%)	1.46	7/1733 (0.4%)
1	I	0.79	4/1294 (0.3%)	1.43	9/1733 (0.5%)
1	K	0.81	4/1294 (0.3%)	1.46	9/1733 (0.5%)
1	M	0.80	4/1294 (0.3%)	1.50	14/1733 (0.8%)
1	O	0.81	5/1294 (0.4%)	1.40	6/1733 (0.3%)
1	Q	0.81	6/1294 (0.5%)	1.47	12/1733 (0.7%)
1	S	0.79	5/1294 (0.4%)	1.44	12/1733 (0.7%)
2	B	0.30	0/10	1.06	0/11
2	D	0.39	0/10	1.10	0/11
2	F	0.24	0/10	1.35	0/11
2	H	0.37	0/10	1.10	0/11
2	J	0.28	0/10	1.18	0/11
2	L	0.26	0/10	1.25	0/11
2	N	0.34	0/10	1.05	0/11
2	P	0.33	0/10	1.25	0/11
2	R	0.37	0/10	0.96	0/11
2	T	0.33	0/10	1.01	0/11
All	All	0.80	46/13040 (0.4%)	1.45	95/17440 (0.5%)

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	70	HIS	CD2-NE2	-7.11	1.30	1.37
1	E	70	HIS	CD2-NE2	-7.01	1.30	1.37
1	M	54	HIS	CD2-NE2	-6.63	1.30	1.37
1	Q	126	HIS	CD2-NE2	-6.60	1.30	1.37
1	A	126	HIS	CD2-NE2	-6.55	1.30	1.37
1	G	70	HIS	CD2-NE2	-6.47	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	126	HIS	CD2-NE2	-6.45	1.30	1.37
1	A	70	HIS	CD2-NE2	-6.45	1.30	1.37
1	M	70	HIS	CD2-NE2	-6.45	1.30	1.37
1	K	54	HIS	CD2-NE2	-6.44	1.30	1.37
1	C	126	HIS	CD2-NE2	-6.41	1.30	1.37
1	G	126	HIS	CD2-NE2	-6.41	1.30	1.37
1	Q	54	HIS	CD2-NE2	-6.40	1.30	1.37
1	M	126	HIS	CD2-NE2	-6.40	1.30	1.37
1	S	54	HIS	CD2-NE2	-6.36	1.30	1.37
1	Q	70	HIS	CD2-NE2	-6.35	1.30	1.37
1	O	70	HIS	CD2-NE2	-6.34	1.30	1.37
1	C	70	HIS	CD2-NE2	-6.33	1.30	1.37
1	A	54	HIS	CD2-NE2	-6.29	1.30	1.37
1	O	126	HIS	CD2-NE2	-6.21	1.31	1.37
1	O	54	HIS	CD2-NE2	-6.20	1.31	1.37
1	I	126	HIS	CD2-NE2	-6.19	1.31	1.37
1	E	126	HIS	CD2-NE2	-6.18	1.31	1.37
1	K	70	HIS	CD2-NE2	-6.17	1.31	1.37
1	E	54	HIS	CD2-NE2	-6.14	1.31	1.37
1	G	54	HIS	CD2-NE2	-6.14	1.31	1.37
1	C	54	HIS	CD2-NE2	-6.03	1.31	1.37
1	Q	92	HIS	CD2-NE2	-5.99	1.31	1.37
1	G	92	HIS	CD2-NE2	-5.83	1.31	1.37
1	S	126	HIS	CD2-NE2	-5.83	1.31	1.37
1	E	92	HIS	CD2-NE2	-5.82	1.31	1.37
1	S	92	HIS	CD2-NE2	-5.81	1.31	1.37
1	I	92	HIS	CD2-NE2	-5.80	1.31	1.37
1	S	70	HIS	CD2-NE2	-5.76	1.31	1.37
1	C	92	HIS	CD2-NE2	-5.71	1.31	1.37
1	K	92	HIS	CD2-NE2	-5.63	1.31	1.37
1	I	54	HIS	CD2-NE2	-5.51	1.31	1.37
1	M	92	HIS	CD2-NE2	-5.47	1.31	1.37
1	O	92	HIS	CD2-NE2	-5.47	1.31	1.37
1	A	92	HIS	CD2-NE2	-5.40	1.31	1.37
1	G	54	HIS	CG-ND1	-5.12	1.32	1.38
1	C	70	HIS	CG-ND1	-5.11	1.32	1.38
1	Q	126	HIS	CG-ND1	-5.09	1.32	1.38
1	S	70	HIS	CG-ND1	-5.05	1.32	1.38
1	Q	54	HIS	CG-ND1	-5.05	1.32	1.38
1	O	54	HIS	CG-ND1	-5.02	1.32	1.38

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	81	GLU	CA-CB-CG	8.65	131.40	114.10
1	G	81	GLU	CA-CB-CG	7.89	129.87	114.10
1	Q	81	GLU	CA-CB-CG	7.83	129.77	114.10
1	Q	8	PHE	CA-CB-CG	7.68	121.48	113.80
1	M	87	ASN	CA-CB-CG	7.25	119.85	112.60
1	G	8	PHE	CA-CB-CG	7.25	121.05	113.80
1	K	8	PHE	CA-CB-CG	7.20	121.00	113.80
1	M	81	GLU	CA-CB-CG	6.98	128.05	114.10
1	C	8	PHE	CA-CB-CG	6.95	120.75	113.80
1	E	165	GLU	CA-CB-CG	6.69	127.47	114.10
1	M	2	VAL	N-CA-C	-6.65	98.46	108.17
1	K	87	ASN	CA-CB-CG	6.62	119.22	112.60
1	M	83	PHE	CA-CB-CG	6.53	120.33	113.80
1	I	8	PHE	CA-CB-CG	6.51	120.31	113.80
1	A	83	PHE	CA-CB-CG	6.43	120.23	113.80
1	G	76	LYS	CA-CB-CG	6.40	126.89	114.10
1	Q	81	GLU	CB-CA-C	-6.39	100.58	110.81
1	C	165	GLU	CA-CB-CG	6.37	126.84	114.10
1	G	81	GLU	CB-CA-C	-6.37	100.63	110.81
1	I	83	PHE	CA-CB-CG	6.35	120.15	113.80
1	E	83	PHE	CA-CB-CG	6.34	120.14	113.80
1	K	13	ASP	CA-CB-CG	6.32	118.92	112.60
1	G	2	VAL	N-CA-C	-6.26	99.03	108.17
1	C	83	PHE	CA-CB-CG	6.21	120.01	113.80
1	Q	165	GLU	CA-CB-CG	6.16	126.41	114.10
1	K	27	ASP	CA-CB-CG	6.15	118.75	112.60
1	S	8	PHE	CA-CB-CG	6.08	119.88	113.80
1	S	75	GLY	N-CA-C	-6.06	105.00	112.33
1	I	113	PHE	CA-CB-CG	6.05	119.85	113.80
1	S	165	GLU	CA-CB-CG	6.04	126.19	114.10
1	S	133	LYS	N-CA-C	-6.00	103.50	111.96
1	K	83	PHE	CA-CB-CG	6.00	119.80	113.80
1	M	67	PHE	CA-CB-CG	5.98	119.78	113.80
1	C	87	ASN	CA-CB-CG	5.92	118.52	112.60
1	A	81	GLU	CA-CB-CG	5.90	125.90	114.10
1	S	102	ASN	CA-CB-CG	5.88	118.48	112.60
1	A	81	GLU	CB-CA-C	-5.84	101.04	110.74
1	S	87	ASN	CA-CB-CG	5.84	118.44	112.60
1	O	2	VAL	N-CA-C	-5.83	99.72	108.12
1	Q	149	ASN	CA-CB-CG	5.78	118.38	112.60
1	O	83	PHE	CA-CB-CG	5.76	119.56	113.80
1	I	57	ILE	CA-C-N	5.75	126.08	119.93
1	I	57	ILE	C-N-CA	5.75	126.08	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	83	PHE	CA-CB-CG	5.67	119.47	113.80
1	S	81	GLU	CB-CA-C	-5.64	101.79	110.81
1	S	143	GLU	CB-CA-C	-5.63	101.11	110.68
1	M	8	PHE	CA-CB-CG	5.63	119.43	113.80
1	M	94	GLY	CA-C-N	5.63	125.57	119.78
1	M	94	GLY	C-N-CA	5.63	125.57	119.78
1	C	71	ASN	OD1-CG-ND2	-5.61	116.99	122.60
1	I	147	SER	CA-CB-OG	5.61	122.33	111.10
1	E	57	ILE	CA-C-N	5.61	125.93	119.93
1	E	57	ILE	C-N-CA	5.61	125.93	119.93
1	E	87	ASN	CA-CB-CG	5.60	118.20	112.60
1	Q	67	PHE	CA-CB-CG	5.60	119.40	113.80
1	M	81	GLU	CB-CA-C	-5.59	101.87	110.81
1	M	102	ASN	CA-CB-CG	5.56	118.16	112.60
1	Q	87	ASN	CA-CB-CG	5.55	118.15	112.60
1	E	12	VAL	N-CA-C	-5.55	99.16	107.37
1	A	87	ASN	CA-CB-CG	5.53	118.13	112.60
1	Q	102	ASN	CA-CB-CG	5.48	118.08	112.60
1	A	84	GLU	N-CA-C	5.48	117.81	110.35
1	S	23	GLU	CA-CB-CG	-5.46	103.18	114.10
1	K	102	ASN	CA-CB-CG	5.44	118.04	112.60
1	Q	83	PHE	CA-CB-CG	5.43	119.23	113.80
1	A	164	LEU	N-CA-C	-5.41	104.72	112.13
1	K	71	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	G	83	PHE	CA-CB-CG	5.35	119.15	113.80
1	G	71	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	I	87	ASN	CA-CB-CG	5.33	117.93	112.60
1	M	60	PHE	CA-CB-CG	5.33	119.13	113.80
1	Q	106	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	A	60	PHE	CA-CB-CG	5.28	119.08	113.80
1	M	75	GLY	N-CA-C	-5.27	105.95	112.33
1	E	8	PHE	CA-CB-CG	5.25	119.06	113.80
1	E	60	PHE	CA-CB-CG	5.24	119.04	113.80
1	K	164	LEU	N-CA-C	-5.23	105.97	112.93
1	O	8	PHE	CA-CB-CG	5.20	119.00	113.80
1	I	164	LEU	N-CA-C	-5.19	106.89	113.43
1	A	46	PHE	CA-CB-CG	5.17	118.97	113.80
1	E	118	LYS	CG-CD-CE	-5.16	99.44	111.30
1	O	67	PHE	CA-CB-CG	5.16	118.96	113.80
1	K	137	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	A	133	LYS	N-CA-C	-5.14	104.63	112.04
1	M	71	ASN	OD1-CG-ND2	-5.12	117.48	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	102	ASN	CA-CB-CG	5.12	117.72	112.60
1	M	101	ALA	N-CA-C	-5.11	102.95	110.52
1	O	114	ILE	N-CA-C	-5.08	100.44	107.80
1	O	137	ASN	OD1-CG-ND2	-5.08	117.53	122.60
1	A	67	PHE	CA-CB-CG	5.07	118.86	113.80
1	I	102	ASN	CA-CB-CG	5.03	117.63	112.60
1	Q	48	TYR	N-CA-C	5.03	119.12	112.89
1	E	15	GLU	CA-CB-CG	5.02	124.15	114.10
1	Q	2	VAL	N-CA-C	-5.02	100.84	108.17
1	S	101	ALA	N-CA-C	-5.00	103.80	110.55

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1266	287	1237	6	0
1	C	1266	287	1237	11	0
1	E	1266	287	1237	5	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	9	0
1	O	1266	287	1237	7	0
1	Q	1266	287	1237	10	0
1	S	1266	287	1237	12	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	2	0
3	R	2	4	0	0	0
3	S	65	130	0	2	0
3	T	3	6	0	0	0
All	All	14142	4204	13461	97	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 (97) 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
1:G:118:LYS:HZ2	1:G:120:GLU:HB3	1.67	0.59
1:I:52:CYS:HB2	3:I:2029:HOH:O	2.03	0.59
1:C:23:GLU:HB2	1:C:133:LYS:HD2	1.89	0.55
1:M:118:LYS:HZ2	1:M:120:GLU:HB3	1.72	0.54
1:G:118:LYS:NZ	1:G:120:GLU:HB3	2.23	0.54
1:M:5:THR:HB	1:M:165:GLU:HG2	1.90	0.54
1:C:5:THR:HB	1:C:165:GLU:HB3	1.90	0.53
1:C:118:LYS:HZ2	1:C:120:GLU:HB3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:GLU:HG3	1:C:82:LYS:HG2	1.91	0.52
1:C:118:LYS:NZ	1:C:120:GLU:HB3	2.24	0.52
1:S:151:LYS:NZ	1:S:151:LYS:O	2.43	0.52
1:O:151:LYS:NZ	1:O:151:LYS:O	2.43	0.52
1:O:141:ALA:HA	1:O:144:ARG:NH1	2.26	0.51
1:Q:97:ILE:HD13	1:Q:131:LYS:HG3	1.92	0.50
1:S:118:LYS:HZ2	1:S:120:GLU:HB3	1.77	0.50
1:K:28:LYS:HE2	3:K:2009:HOH:O	2.12	0.50
1:O:121:TRP:HH2	1:Q:1:MET:HE1	1.77	0.49
1:S:154:LYS:NZ	3:S:2061:HOH:O	2.46	0.49
1:K:149:ASN:OD1	1:K:151:LYS:HD3	2.13	0.48
1:O:5:THR:HA	1:O:22:PHE:O	2.12	0.48
1:I:5:THR:HA	1:I:22:PHE:O	2.14	0.48
1:K:49:LYS:NZ	1:K:160:ASP:OD1	2.47	0.47
1:Q:23:GLU:HB2	1:Q:133:LYS:HD2	1.96	0.47
1:M:131:LYS:NZ	3:M:2046:HOH:O	2.47	0.47
1:O:23:GLU:HB2	1:O:133:LYS:HD2	1.95	0.47
1:S:23:GLU:HB2	1:S:133:LYS:HD2	1.96	0.47
1:I:82:LYS:NZ	3:I:2037:HOH:O	2.47	0.47
1:S:97:ILE:HD13	1:S:131:LYS:HG2	1.96	0.47
1:I:23:GLU:HB2	1:I:133:LYS:HD2	1.97	0.47
1:M:118:LYS:NZ	1:M:120:GLU:HB3	2.30	0.46
1:Q:49:LYS:NZ	3:Q:2011:HOH:O	2.48	0.46
1:E:13:ASP:CG	1:E:154:LYS:HZ2	2.23	0.46
1:M:5:THR:HA	1:M:22:PHE:O	2.15	0.46
2:H:1:DAL:HA	2:H:2:MLE:HN1	1.80	0.46
1:M:3:ASN:HA	1:M:4:PRO:HD3	1.86	0.46
1:C:145:PHE:O	1:C:152:THR:HA	2.16	0.45
1:M:82:LYS:HA	1:M:108:ASN:O	2.16	0.45
1:C:141:ALA:HA	1:C:144:ARG:CZ	2.47	0.45
2:F:9:VAL:HA	2:F:10:MLE:HN1	1.79	0.45
1:K:5:THR:HB	1:K:165:GLU:HG2	1.99	0.45
1:K:162:GLY:N	3:K:2066:HOH:O	2.50	0.44
2:L:1:DAL:HA	2:L:2:MLE:HN1	1.74	0.44
1:K:28:LYS:NZ	3:K:2011:HOH:O	2.48	0.44
1:Q:76:LYS:NZ	3:Q:2023:HOH:O	2.49	0.44
2:R:1:DAL:HA	2:R:2:MLE:HN1	1.76	0.44
2:T:9:VAL:HA	2:T:10:MLE:HN1	1.73	0.44
1:C:5:THR:CB	1:C:165:GLU:HB3	2.47	0.44
1:Q:141:ALA:HA	1:Q:144:ARG:CZ	2.48	0.44
1:Q:145:PHE:O	1:Q:152:THR:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:9:VAL:HA	2:R:10:MLE:HN1	1.69	0.44
1:M:5:THR:HB	1:M:165:GLU:CG	2.48	0.44
2:N:9:VAL:HA	2:N:10:MLE:HN1	1.68	0.43
2:B:4:MVA:HA	2:B:5:BMT:HN1	1.86	0.43
2:R:4:MVA:HA	2:R:5:BMT:HN1	1.89	0.43
1:A:82:LYS:HA	1:A:108:ASN:O	2.19	0.43
1:E:15:GLU:HA	1:E:16:PRO:HD2	1.85	0.43
1:S:142:MET:HE3	1:S:156:ILE:HG21	2.00	0.43
1:S:155:LYS:NZ	3:S:2063:HOH:O	2.52	0.43
1:Q:118:LYS:NZ	1:Q:120:GLU:HB3	2.34	0.43
2:D:9:VAL:HA	2:D:10:MLE:HN1	1.71	0.42
1:K:4:PRO:HG2	1:K:24:LEU:HB2	2.01	0.42
2:H:9:VAL:HA	2:H:10:MLE:HN1	1.71	0.42
2:J:9:VAL:HA	2:J:10:MLE:HN1	1.65	0.42
2:N:1:DAL:HA	2:N:2:MLE:HN1	1.85	0.42
1:S:5:THR:CB	1:S:165:GLU:HB3	2.48	0.42
1:G:82:LYS:HA	1:G:108:ASN:O	2.20	0.42
1:S:5:THR:HA	1:S:22:PHE:O	2.20	0.42
1:O:145:PHE:O	1:O:152:THR:HA	2.20	0.41
2:D:2:MLE:HA	2:D:3:MLE:HN1	1.86	0.41
1:E:113:PHE:CD1	2:F:4:MVA:HG11	2.55	0.41
1:K:113:PHE:CD1	2:L:4:MVA:HG11	2.55	0.41
2:B:9:VAL:HA	2:B:10:MLE:HN1	1.65	0.41
1:A:5:THR:HA	1:A:22:PHE:O	2.20	0.41
1:C:125:LYS:NZ	3:C:2050:HOH:O	2.53	0.41
1:I:52:CYS:SG	1:I:155:LYS:NZ	2.84	0.41
1:S:118:LYS:NZ	1:S:120:GLU:HB3	2.35	0.41
1:A:15:GLU:HA	1:A:16:PRO:HD2	1.91	0.41
2:J:1:DAL:HA	2:J:2:MLE:HN1	1.79	0.41
2:L:3:MLE:HA	2:L:4:MVA:HN1	1.84	0.41
1:A:145:PHE:O	1:A:152:THR:HA	2.21	0.40
1:C:5:THR:HA	1:C:22:PHE:O	2.21	0.40
1:K:27:ASP:HB3	3:K:2001:HOH:O	2.21	0.40
1:C:82:LYS:HA	1:C:108:ASN:O	2.20	0.40
2:H:4:MVA:HA	2:H:5:BMT:HN1	1.87	0.40
1:E:23:GLU:HB2	1:E:133:LYS:HD2	2.03	0.40
1:G:6:VAL:HG23	1:G:22:PHE:HD2	1.86	0.40
1:M:1:MET:HE3	1:M:1:MET:HA	2.03	0.40
1:A:154:LYS:NZ	1:A:154:LYS:HA	2.37	0.40
1:I:49:LYS:NZ	1:I:160:ASP:OD1	2.49	0.40
1:Q:5:THR:CB	1:Q:165:GLU:HB3	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:76:LYS:NZ	3:O:2022:HOH:O	2.51	0.40
1:S:7:PHE:HD2	1:S:164:LEU:HG	1.87	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	58/165 (35%)	57 (98%)	1 (2%)	0	100	100
1	C	163/165 (99%)	156 (96%)	7 (4%)	0	100	100
1	E	163/165 (99%)	155 (95%)	7 (4%)	1 (1%)	21	18
1	G	163/165 (99%)	153 (94%)	9 (6%)	1 (1%)	21	18
1	I	163/165 (99%)	153 (94%)	9 (6%)	1 (1%)	21	18
1	K	163/165 (99%)	153 (94%)	9 (6%)	1 (1%)	21	18
1	M	163/165 (99%)	152 (93%)	10 (6%)	1 (1%)	21	18
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	R	1/11 (9%)	1 (100%)	0	0	100	100
2	T	1/11 (9%)	1 (100%)	0	0	100	100
All	All	1535/1760 (87%)	1455 (95%)	75 (5%)	5 (0%)	36	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	13	ASP
1	G	13	ASP
1	M	13	ASP
1	I	46	PHE
1	K	2	VAL

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	36/133 (27%)	36 (100%)	0	100	100
1	C	127/133 (96%)	121 (95%)	6 (5%)	23	24
1	E	133/133 (100%)	128 (96%)	5 (4%)	29	32
1	G	133/133 (100%)	130 (98%)	3 (2%)	44	51
1	I	133/133 (100%)	126 (95%)	7 (5%)	20	19
1	K	133/133 (100%)	125 (94%)	8 (6%)	17	15
1	M	133/133 (100%)	128 (96%)	5 (4%)	29	32
1	O	133/133 (100%)	128 (96%)	5 (4%)	29	32
1	Q	133/133 (100%)	124 (93%)	9 (7%)	14	12
1	S	133/133 (100%)	130 (98%)	3 (2%)	44	51
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	1236/1339 (92%)	1185 (96%)	51 (4%)	27	29

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	29	VAL
1	C	76	LYS
1	C	110	SER
1	C	143	GLU
1	C	151	LYS
1	C	154	LYS
1	E	143	GLU
1	E	147	SER
1	E	148	ARG
1	E	151	LYS
1	E	154	LYS
1	G	148	ARG
1	G	151	LYS
1	G	154	LYS
1	I	1	MET
1	I	13	ASP
1	I	29	VAL
1	I	52	CYS
1	I	148	ARG
1	I	151	LYS
1	I	154	LYS
1	K	1	MET
1	K	29	VAL
1	K	76	LYS
1	K	143	GLU
1	K	148	ARG
1	K	151	LYS
1	K	154	LYS
1	K	157	THR

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Mol	Chain	Res	Type
1	M	13	ASP
1	M	15	GLU
1	M	147	SER
1	M	151	LYS
1	M	154	LYS
1	O	29	VAL
1	O	143	GLU
1	O	148	ARG
1	O	151	LYS
1	O	154	LYS
1	Q	13	ASP
1	Q	15	GLU
1	Q	29	VAL
1	Q	110	SER
1	Q	131	LYS
1	Q	143	GLU
1	Q	148	ARG
1	Q	151	LYS
1	Q	154	LYS
1	S	1	MET
1	S	151	LYS
1	S	154	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	111	GLN

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	MLE	J	10	2	7,8,9	0.78	0	7,9,11	1.58	2 (28%)
2	MLE	H	8	2	7,8,9	0.72	0	7,9,11	1.18	1 (14%)
2	MLE	F	8	2	7,8,9	0.74	0	7,9,11	1.04	0
2	MLE	B	8	2	7,8,9	0.77	0	7,9,11	1.12	1 (14%)
2	MLE	N	2	2	7,8,9	0.75	0	7,9,11	1.39	1 (14%)
2	BMT	D	5	2	11,12,13	1.14	0	11,14,16	1.50	3 (27%)
2	MLE	D	8	2	7,8,9	0.76	0	7,9,11	1.10	1 (14%)
2	MLE	P	10	2	7,8,9	0.85	0	7,9,11	1.60	2 (28%)
2	SAR	P	7	2	3,4,5	0.76	0	1,3,5	2.34	1 (100%)
2	MLE	P	2	2	7,8,9	0.70	0	7,9,11	1.05	0
2	ABA	T	6	2	4,5,6	0.73	0	1,5,7	0.39	0
2	MVA	T	4	2	6,7,8	1.11	0	6,8,10	2.07	3 (50%)
2	MLE	J	2	2	7,8,9	0.72	0	7,9,11	1.28	0
2	MVA	F	4	2	6,7,8	0.97	0	6,8,10	1.60	2 (33%)
2	SAR	J	7	2	3,4,5	0.74	0	1,3,5	2.09	1 (100%)
2	ABA	F	6	2	4,5,6	0.83	0	1,5,7	0.34	0
2	ABA	J	6	2	4,5,6	0.82	0	1,5,7	0.56	0
2	MLE	D	10	2	7,8,9	0.92	0	7,9,11	1.61	2 (28%)
2	MLE	N	10	2	7,8,9	0.71	0	7,9,11	1.51	2 (28%)
2	MLE	H	10	2	7,8,9	0.86	0	7,9,11	1.74	2 (28%)
2	MLE	T	8	2	7,8,9	0.81	0	7,9,11	1.09	1 (14%)
2	MLE	N	3	2	7,8,9	1.12	0	7,9,11	1.55	1 (14%)
2	SAR	R	7	2	3,4,5	0.78	0	1,3,5	2.02	1 (100%)
2	ABA	N	6	2	4,5,6	0.87	0	1,5,7	0.23	0
2	MVA	L	4	2	6,7,8	0.94	0	6,8,10	1.46	2 (33%)
2	BMT	L	5	2	11,12,13	1.19	1 (9%)	11,14,16	1.27	1 (9%)
2	BMT	T	5	2	11,12,13	1.03	0	11,14,16	1.19	1 (9%)
2	MLE	P	3	2	7,8,9	1.18	1 (14%)	7,9,11	1.70	1 (14%)
2	MLE	J	3	2	7,8,9	0.92	0	7,9,11	1.74	2 (28%)
2	BMT	R	5	2	11,12,13	1.24	1 (9%)	11,14,16	1.46	1 (9%)
2	ABA	P	6	2	4,5,6	0.85	0	1,5,7	0.06	0
2	SAR	B	7	2	3,4,5	0.77	0	1,3,5	2.30	1 (100%)
2	MVA	J	4	2	6,7,8	0.89	0	6,8,10	1.60	2 (33%)
2	MVA	B	4	2	6,7,8	0.97	0	6,8,10	1.69	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ABA	B	6	2	4,5,6	0.80	0	1,5,7	0.36	0
2	ABA	L	6	2	4,5,6	0.77	0	1,5,7	0.28	0
2	SAR	F	7	2	3,4,5	0.68	0	1,3,5	2.68	1 (100%)
2	MVA	H	4	2	6,7,8	1.10	0	6,8,10	1.46	2 (33%)
2	SAR	T	7	2	3,4,5	0.74	0	1,3,5	2.49	1 (100%)
2	MLE	H	3	2	7,8,9	1.05	0	7,9,11	1.80	1 (14%)
2	MLE	L	3	2	7,8,9	0.95	0	7,9,11	1.63	1 (14%)
2	MLE	F	3	2	7,8,9	0.96	0	7,9,11	1.30	1 (14%)
2	MLE	N	8	2	7,8,9	0.73	0	7,9,11	0.92	0
2	SAR	D	7	2	3,4,5	0.88	0	1,3,5	2.06	1 (100%)
2	MVA	R	4	2	6,7,8	0.94	0	6,8,10	1.35	1 (16%)
2	MLE	L	8	2	7,8,9	0.65	0	7,9,11	1.02	1 (14%)
2	MLE	F	10	2	7,8,9	0.80	0	7,9,11	1.83	3 (42%)
2	MVA	P	4	2	6,7,8	1.01	0	6,8,10	1.46	1 (16%)
2	BMT	P	5	2	11,12,13	1.19	0	11,14,16	1.25	1 (9%)
2	MLE	D	3	2	7,8,9	0.99	0	7,9,11	1.55	1 (14%)
2	MLE	D	2	2	7,8,9	0.80	0	7,9,11	1.42	2 (28%)
2	MLE	B	2	2	7,8,9	1.15	1 (14%)	7,9,11	1.47	2 (28%)
2	SAR	L	7	2	3,4,5	0.72	0	1,3,5	2.65	1 (100%)
2	MVA	D	4	2	6,7,8	0.93	0	6,8,10	1.63	2 (33%)
2	MLE	L	2	2	7,8,9	0.73	0	7,9,11	1.21	1 (14%)
2	BMT	J	5	2	11,12,13	1.26	1 (9%)	11,14,16	1.32	1 (9%)
2	BMT	B	5	2	11,12,13	1.16	0	11,14,16	1.48	2 (18%)
2	MVA	N	4	2	6,7,8	0.98	0	6,8,10	1.67	1 (16%)
2	MLE	T	10	2	7,8,9	0.87	0	7,9,11	1.53	2 (28%)
2	MLE	R	8	2	7,8,9	0.70	0	7,9,11	1.13	1 (14%)
2	MLE	B	3	2	7,8,9	0.92	0	7,9,11	1.59	2 (28%)
2	MLE	F	2	2	7,8,9	0.87	0	7,9,11	1.30	1 (14%)
2	BMT	F	5	2	11,12,13	1.34	1 (9%)	11,14,16	1.09	1 (9%)
2	MLE	B	10	2	7,8,9	0.80	0	7,9,11	1.58	2 (28%)
2	MLE	R	2	2	7,8,9	0.80	0	7,9,11	1.36	2 (28%)
2	SAR	N	7	2	3,4,5	0.83	0	1,3,5	2.21	1 (100%)
2	MLE	T	3	2	7,8,9	1.05	0	7,9,11	1.47	2 (28%)
2	MLE	L	10	2	7,8,9	0.81	0	7,9,11	1.64	2 (28%)
2	MLE	R	10	2	7,8,9	0.93	0	7,9,11	1.36	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MLE	T	2	2	7,8,9	0.70	0	7,9,11	1.16	1 (14%)
2	BMT	N	5	2	11,12,13	1.21	0	11,14,16	1.38	2 (18%)
2	ABA	H	6	2	4,5,6	0.72	0	1,5,7	0.06	0
2	MLE	P	8	2	7,8,9	0.87	0	7,9,11	1.13	1 (14%)
2	MLE	R	3	2	7,8,9	0.96	0	7,9,11	1.70	1 (14%)
2	MLE	J	8	2	7,8,9	0.83	0	7,9,11	1.19	1 (14%)
2	MLE	H	2	2	7,8,9	0.74	0	7,9,11	1.11	1 (14%)
2	SAR	H	7	2	3,4,5	0.75	0	1,3,5	2.66	1 (100%)
2	BMT	H	5	2	11,12,13	1.25	1 (9%)	11,14,16	1.23	1 (9%)
2	ABA	R	6	2	4,5,6	0.77	0	1,5,7	0.47	0
2	ABA	D	6	2	4,5,6	0.84	0	1,5,7	0.58	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	MLE	J	10	2	-	0/5/8/10	-
2	MLE	H	8	2	-	1/5/8/10	-
2	MLE	F	8	2	-	1/5/8/10	-
2	MLE	B	8	2	-	1/5/8/10	-
2	MLE	N	2	2	-	0/5/8/10	-
2	BMT	D	5	2	-	0/14/16/18	-
2	MLE	D	8	2	-	1/5/8/10	-
2	MLE	P	10	2	-	0/5/8/10	-
2	SAR	P	7	2	-	1/1/2/3	-
2	MLE	P	2	2	-	0/5/8/10	-
2	ABA	T	6	2	-	1/3/4/6	-
2	MVA	T	4	2	-	0/6/8/10	-
2	MLE	J	2	2	-	0/5/8/10	-
2	MVA	F	4	2	-	1/6/8/10	-
2	SAR	J	7	2	-	1/1/2/3	-
2	ABA	F	6	2	-	0/3/4/6	-
2	ABA	J	6	2	-	1/3/4/6	-
2	MLE	D	10	2	-	0/5/8/10	-
2	MLE	N	10	2	-	0/5/8/10	-
2	MLE	H	10	2	-	0/5/8/10	-
2	MLE	T	8	2	-	1/5/8/10	-
2	MLE	N	3	2	-	0/5/8/10	-
2	SAR	R	7	2	-	1/1/2/3	-

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

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

All (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
2	P	3	MLE	CB-CA	2.09	1.56	1.53
2	L	5	BMT	CG2-CB	2.03	1.57	1.53

All (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
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
2	J	3	MLE	CB-CA-N	-3.26	105.64	110.59
2	P	3	MLE	CB-CA-N	-3.19	105.75	110.59
2	R	5	BMT	CD2-CG2-CB	3.16	117.23	110.73
2	R	3	MLE	CB-CA-N	-3.15	105.81	110.59
2	D	3	MLE	CB-CA-N	-3.06	105.95	110.59
2	N	3	MLE	CB-CA-N	-2.97	106.09	110.59
2	B	5	BMT	CD1-CG2-CB	2.88	116.68	111.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	10	MLE	CB-CA-N	-2.84	106.28	110.59
2	B	3	MLE	CB-CA-N	-2.83	106.31	110.59
2	L	10	MLE	CB-CA-N	-2.81	106.33	110.59
2	D	10	MLE	CB-CA-N	-2.80	106.35	110.59
2	F	4	MVA	CG1-CB-CA	-2.79	106.93	111.18
2	J	10	MLE	CB-CA-N	-2.78	106.38	110.59
2	N	10	MLE	CB-CA-N	-2.74	106.44	110.59
2	B	10	MLE	CB-CA-N	-2.70	106.50	110.59
2	F	7	SAR	O-C-CA	-2.68	115.95	125.17
2	T	10	MLE	CB-CA-N	-2.67	106.54	110.59
2	H	7	SAR	O-C-CA	-2.66	116.01	125.17
2	L	7	SAR	O-C-CA	-2.65	116.05	125.17
2	N	5	BMT	CD2-CG2-CB	2.62	116.12	110.73
2	N	4	MVA	CG1-CB-CA	-2.61	107.20	111.18
2	D	4	MVA	CG1-CB-CA	-2.57	107.26	111.18
2	B	5	BMT	CD2-CG2-CB	2.53	115.94	110.73
2	R	2	MLE	CN-N-CA	2.53	121.26	113.70
2	P	4	MVA	CG1-CB-CA	-2.50	107.37	111.18
2	T	7	SAR	O-C-CA	-2.49	116.60	125.17
2	J	8	MLE	CN-N-CA	2.49	121.15	113.70
2	T	3	MLE	CB-CA-N	-2.48	106.83	110.59
2	L	5	BMT	CD2-CG2-CB	2.47	115.81	110.73
2	D	5	BMT	CD1-CG2-CB	2.45	115.89	111.45
2	D	2	MLE	CN-N-CA	2.42	120.93	113.70
2	B	10	MLE	CN-N-CA	2.42	120.92	113.70
2	J	4	MVA	CB-CA-C	-2.42	109.84	112.96
2	H	8	MLE	CN-N-CA	2.40	120.86	113.70
2	J	5	BMT	CD1-CG2-CB	2.38	115.77	111.45
2	R	8	MLE	CN-N-CA	2.38	120.81	113.70
2	P	5	BMT	CD2-CG2-CB	2.37	115.60	110.73
2	T	10	MLE	CN-N-CA	2.37	120.77	113.70
2	B	4	MVA	CG1-CB-CA	-2.35	107.59	111.18
2	H	10	MLE	CN-N-CA	2.35	120.71	113.70
2	P	7	SAR	O-C-CA	-2.34	117.12	125.17
2	B	4	MVA	O-C-CA	-2.32	118.72	124.86
2	R	10	MLE	CB-CA-N	-2.31	107.09	110.59
2	B	7	SAR	O-C-CA	-2.30	117.27	125.17
2	T	4	MVA	O-C-CA	-2.29	118.80	124.86
2	T	5	BMT	CD2-CG2-CB	2.29	115.43	110.73
2	P	10	MLE	CN-N-CA	2.27	120.48	113.70
2	L	8	MLE	CN-N-CA	2.27	120.48	113.70
2	L	10	MLE	CN-N-CA	2.26	120.47	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	10	MLE	CN-N-CA	2.26	120.47	113.70
2	D	10	MLE	CN-N-CA	2.26	120.46	113.70
2	F	5	BMT	CD2-CG2-CB	2.26	115.38	110.73
2	F	10	MLE	CB-CA-C	2.26	114.47	110.99
2	L	2	MLE	CN-N-CA	2.25	120.43	113.70
2	B	2	MLE	CB-CA-N	-2.25	107.18	110.59
2	J	3	MLE	O-C-CA	-2.25	118.99	124.77
2	H	4	MVA	CG1-CB-CA	-2.25	107.75	111.18
2	D	5	BMT	CD2-CG2-CB	2.24	115.33	110.73
2	B	8	MLE	CN-N-CA	2.23	120.37	113.70
2	N	2	MLE	CB-CA-N	-2.22	107.23	110.59
2	L	4	MVA	O-C-CA	-2.22	118.99	124.86
2	N	7	SAR	O-C-CA	-2.21	117.56	125.17
2	J	4	MVA	CG1-CB-CA	-2.21	107.81	111.18
2	D	8	MLE	CN-N-CA	2.21	120.30	113.70
2	R	2	MLE	O-C-CA	-2.21	119.10	124.77
2	D	5	BMT	CD1-CG2-CD2	2.20	113.98	110.48
2	F	4	MVA	O-C-CA	-2.20	119.05	124.86
2	N	10	MLE	CN-N-CA	2.19	120.26	113.70
2	F	10	MLE	CN-N-CA	2.19	120.26	113.70
2	D	2	MLE	CB-CA-N	-2.19	107.27	110.59
2	T	4	MVA	CG2-CB-CA	2.19	114.52	111.18
2	F	3	MLE	CB-CA-N	-2.18	107.29	110.59
2	F	2	MLE	CB-CA-N	-2.16	107.32	110.59
2	B	4	MVA	CB-CA-C	-2.15	110.18	112.96
2	P	8	MLE	CN-N-CA	2.13	120.08	113.70
2	L	4	MVA	CG1-CB-CA	-2.11	107.96	111.18
2	B	3	MLE	O-C-CA	-2.10	119.37	124.77
2	N	5	BMT	CD1-CG2-CB	2.10	115.26	111.45
2	J	7	SAR	O-C-CA	-2.09	117.97	125.17
2	D	4	MVA	O-C-CA	-2.08	119.35	124.86
2	T	3	MLE	O-C-CA	-2.07	119.45	124.77
2	R	10	MLE	CN-N-CA	2.07	119.89	113.70
2	T	8	MLE	CN-N-CA	2.07	119.89	113.70
2	D	7	SAR	O-C-CA	-2.06	118.07	125.17
2	R	4	MVA	O-C-CA	-2.05	119.44	124.86
2	T	2	MLE	CN-N-CA	2.04	119.78	113.70
2	H	5	BMT	CD2-CG2-CB	2.03	114.89	110.73
2	R	7	SAR	O-C-CA	-2.02	118.23	125.17
2	H	2	MLE	CN-N-CA	2.01	119.70	113.70
2	H	4	MVA	O-C-CA	-2.01	119.55	124.86
2	B	2	MLE	CN-N-CA	2.00	119.69	113.70

There are no chirality outliers.

All (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
2	N	6	ABA	O-C-CA-CB
2	R	6	ABA	O-C-CA-CB
2	T	6	ABA	O-C-CA-CB
2	B	8	MLE	O-C-CA-CB
2	D	8	MLE	O-C-CA-CB
2	F	8	MLE	O-C-CA-CB
2	H	8	MLE	O-C-CA-CB
2	J	8	MLE	O-C-CA-CB
2	L	8	MLE	O-C-CA-CB
2	N	8	MLE	O-C-CA-CB
2	P	8	MLE	O-C-CA-CB
2	R	8	MLE	O-C-CA-CB
2	T	8	MLE	O-C-CA-CB
2	F	4	MVA	O-C-CA-CB
2	B	7	SAR	C-CA-N-CN
2	D	7	SAR	C-CA-N-CN
2	F	7	SAR	C-CA-N-CN
2	H	7	SAR	C-CA-N-CN
2	J	7	SAR	C-CA-N-CN
2	L	7	SAR	C-CA-N-CN
2	N	7	SAR	C-CA-N-CN
2	P	7	SAR	C-CA-N-CN
2	R	7	SAR	C-CA-N-CN
2	T	7	SAR	C-CA-N-CN

There are no ring outliers.

24 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	10	MLE	1	0
2	N	2	MLE	1	0
2	J	2	MLE	1	0
2	F	4	MVA	1	0
2	D	10	MLE	1	0
2	N	10	MLE	1	0

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.