



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:48 PM UTC

PDB ID : 4GCH / pdb_00004gch
Title : STRUCTURE AND ACTIVITY OF TWO PHOTOREVERSIBLE CINNAMATES BOUND TO CHYMOTRYPSIN
Authors : Stoddard, B.L.; Ringe, D.; Petsko, G.A.
Deposited on : 1989-09-25
Resolution : 1.90 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

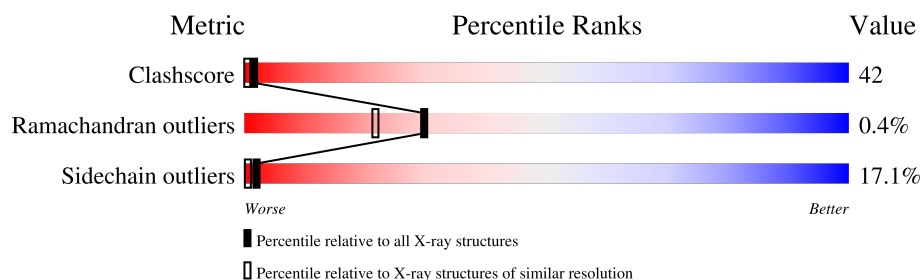
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	E	13	
2	F	131	
3	G	97	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DMC	G	246	-	X	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1826 atoms, of which 0 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 GAMMA-CHYMOTRYPSIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	11	Total	C	N	O	S	0	0	1
			69	45	12	11	1			

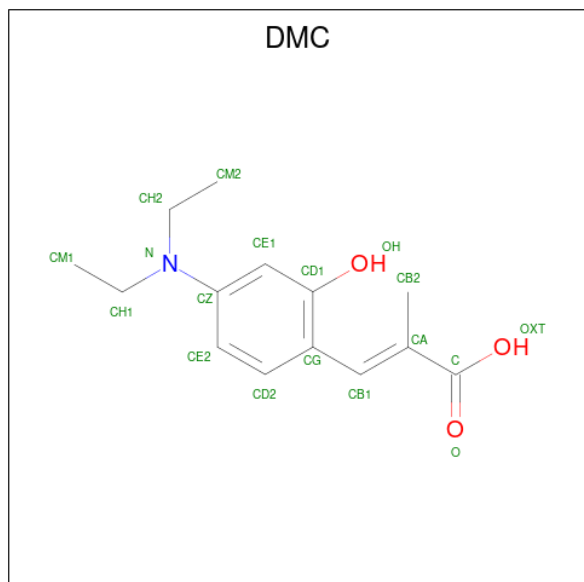
- Molecule 2 is a protein called GAMMA-CHYMOTRYPSIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	131	Total	C	N	O	S	0	0	0
			979	618	162	195	4			

- Molecule 3 is a protein called GAMMA-CHYMOTRYPSIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	95	Total	C	N	O	S	0	0	0
			688	429	120	132	7			

- Molecule 4 is 3-(4-DIETHYLAMINO-2-HYDROXY-PHENYL)-2-METHYL-PROPIONIC ACID (CCD ID: DMC) (formula: $C_{14}H_{19}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	N	O	0	0
			17	14	1	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	4	Total	O	0	0
			4	4		
5	F	50	Total	O	0	0
			50	50		
5	G	19	Total	O	0	0
			19	19		

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.

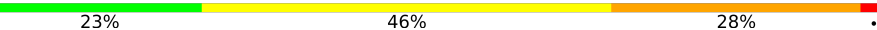
Note EDS was not executed.

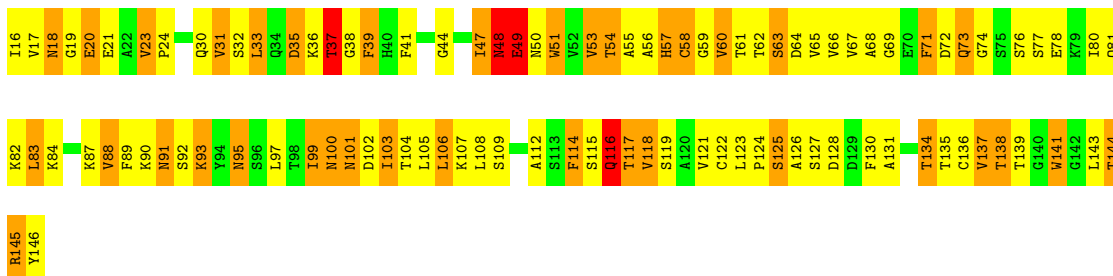
• Molecule 1: GAMMA-CHYMOTRYPSIN A

Chain E: 



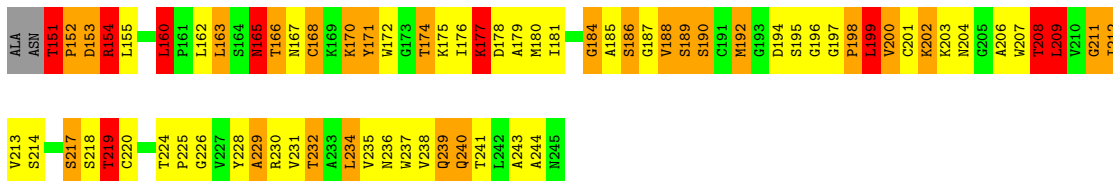
• Molecule 2: GAMMA-CHYMOTRYPSIN A

Chain F: 



• Molecule 3: GAMMA-CHYMOTRYPSIN A

Chain G: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	69.70 Å 69.70 Å 97.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (45.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.209 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1826	wwPDB-VP
Average B, all atoms (Å ²)	8.0	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: DMC

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	E	1.72	0/70	3.23	11/97 (11.3%)
2	F	1.56	10/999 (1.0%)	2.97	120/1361 (8.8%)
3	G	1.41	2/701 (0.3%)	2.77	81/955 (8.5%)
All	All	1.51	12/1770 (0.7%)	2.91	212/2413 (8.8%)

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	E	0	1
2	F	0	1
3	G	0	1
All	All	0	3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	137	VAL	C-O	7.34	1.31	1.24
2	F	144	THR	C-N	-6.71	1.25	1.33
2	F	20	GLU	C-N	-6.44	1.25	1.33
2	F	88	VAL	N-CA	6.27	1.53	1.46
2	F	114	PHE	N-CA	6.23	1.54	1.45
2	F	20	GLU	N-CA	5.89	1.53	1.45
2	F	58	CYS	C-N	-5.72	1.27	1.33
3	G	214	SER	CA-C	-5.46	1.47	1.52
2	F	57	HIS	ND1-CE1	-5.28	1.27	1.32
3	G	211	GLY	N-CA	5.26	1.50	1.45
2	F	19	GLY	N-CA	5.08	1.50	1.45
2	F	138	THR	C-N	-5.01	1.26	1.33

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	204	ASN	CA-CB-CG	18.74	131.34	112.60
2	F	130	PHE	CA-C-N	13.12	139.34	120.71
2	F	130	PHE	C-N-CA	13.12	139.34	120.71
3	G	153	ASP	CA-CB-CG	11.60	124.20	112.60
2	F	114	PHE	CA-CB-CG	11.36	125.16	113.80
2	F	18	ASN	OD1-CG-ND2	11.26	133.86	122.60
2	F	101	ASN	CA-C-N	11.10	138.48	122.05
2	F	101	ASN	C-N-CA	11.10	138.48	122.05
2	F	106	LEU	CA-C-O	10.64	131.52	120.24
2	F	20	GLU	CA-C-O	-10.12	109.60	121.44
2	F	117	THR	CA-C-O	-10.12	107.28	119.32
2	F	30	GLN	OE1-CD-NE2	9.66	132.26	122.60
3	G	200	VAL	N-CA-C	9.65	122.53	108.53
2	F	95	ASN	OD1-CG-ND2	9.38	131.98	122.60
1	E	7	GLN	CA-C-O	9.36	128.09	119.76
2	F	95	ASN	CA-C-O	9.35	130.42	120.33
2	F	18	ASN	CA-CB-CG	-9.30	103.30	112.60
2	F	144	THR	CA-C-N	9.15	137.19	121.64
2	F	144	THR	C-N-CA	9.15	137.19	121.64
2	F	62	THR	CA-CB-OG1	-9.09	95.96	109.60
2	F	128	ASP	CA-C-O	8.97	130.74	120.96
2	F	145	ARG	NE-CZ-NH2	8.84	127.16	119.20
2	F	21	GLU	CA-C-O	-8.84	111.47	121.19
2	F	109	SER	CA-C-N	8.74	135.53	123.11
2	F	109	SER	C-N-CA	8.74	135.53	123.11
3	G	198	PRO	CA-C-O	8.72	131.18	120.97
2	F	64	ASP	CA-CB-CG	8.71	121.31	112.60
2	F	116	GLN	CB-CG-CD	-8.60	97.98	112.60
1	E	7	GLN	CB-CA-C	8.56	123.28	109.41
2	F	101	ASN	CA-CB-CG	8.31	120.91	112.60
2	F	126	ALA	N-CA-C	-8.30	102.16	111.71
3	G	229	ALA	CA-C-O	-8.16	112.66	121.56
3	G	198	PRO	N-CA-C	8.13	123.81	110.55
2	F	131	ALA	N-CA-C	8.12	122.01	110.23
2	F	78	GLU	CB-CG-CD	8.11	126.38	112.60
3	G	192	MET	CA-C-N	-7.99	112.30	123.08
3	G	192	MET	C-N-CA	-7.99	112.30	123.08
3	G	189	SER	O-C-N	7.98	132.75	123.41
2	F	23	VAL	CA-C-O	-7.91	112.35	119.71
2	F	139	THR	CA-C-N	7.91	136.91	121.41
2	F	139	THR	C-N-CA	7.91	136.91	121.41
2	F	62	THR	CB-CA-C	7.83	123.80	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	204	ASN	OD1-CG-ND2	-7.78	114.82	122.60
3	G	175	LYS	CA-C-N	7.74	132.63	121.80
3	G	175	LYS	C-N-CA	7.74	132.63	121.80
1	E	7	GLN	CB-CG-CD	7.67	125.63	112.60
2	F	38	GLY	CA-C-N	7.64	133.59	121.66
2	F	38	GLY	C-N-CA	7.64	133.59	121.66
1	E	7	GLN	OE1-CD-NE2	-7.61	114.99	122.60
3	G	217	SER	CA-C-O	-7.59	112.88	121.07
2	F	90	LYS	O-C-N	7.54	131.87	123.04
3	G	174	THR	CB-CA-C	7.48	123.75	110.81
3	G	209	LEU	O-C-N	7.47	132.37	122.96
3	G	244	ALA	CA-C-O	-7.43	107.02	118.91
2	F	44	GLY	CA-C-O	-7.42	114.37	121.49
3	G	171	TYR	CB-CA-C	-7.37	98.70	110.86
3	G	232	THR	CA-C-O	7.35	128.56	120.63
3	G	197	GLY	CA-C-N	7.21	128.28	120.13
3	G	197	GLY	C-N-CA	7.21	128.28	120.13
2	F	83	LEU	CA-C-N	7.18	131.78	121.50
2	F	83	LEU	C-N-CA	7.18	131.78	121.50
2	F	135	THR	CA-CB-OG1	-7.18	98.83	109.60
2	F	126	ALA	O-C-N	7.18	130.62	122.22
3	G	203	LYS	CA-C-O	7.17	130.15	120.47
2	F	20	GLU	N-CA-C	-7.10	98.51	109.52
3	G	234	LEU	O-C-N	7.07	129.47	122.19
2	F	95	ASN	CA-C-N	7.07	132.52	120.72
2	F	95	ASN	C-N-CA	7.07	132.52	120.72
2	F	35	ASP	CA-C-O	-7.01	112.83	121.67
3	G	232	THR	CA-CB-CG2	7.01	122.42	110.50
3	G	212	ILE	O-C-N	7.00	130.46	123.18
3	G	190	SER	N-CA-C	-6.98	101.13	110.55
2	F	63	SER	CA-C-O	6.96	127.70	119.28
2	F	102	ASP	N-CA-CB	-6.93	102.08	110.53
2	F	125	SER	CA-C-O	-6.91	113.66	121.81
2	F	91	ASN	N-CA-C	-6.90	99.82	110.10
2	F	19	GLY	CA-C-O	-6.83	112.93	122.36
2	F	63	SER	CB-CA-C	6.83	122.30	110.01
3	G	209	LEU	CA-C-O	-6.76	112.74	120.58
2	F	90	LYS	CA-C-O	-6.71	113.04	120.69
2	F	97	LEU	N-CA-C	-6.69	103.81	112.23
3	G	236	ASN	CA-C-N	6.62	129.69	120.29
3	G	236	ASN	C-N-CA	6.62	129.69	120.29
2	F	138	THR	CA-C-N	6.61	133.93	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	138	THR	C-N-CA	6.61	133.93	122.82
3	G	207	TRP	CB-CA-C	6.59	120.58	109.84
2	F	62	THR	N-CA-CB	-6.58	100.94	110.56
3	G	204	ASN	O-C-N	6.58	131.15	122.47
2	F	18	ASN	N-CA-C	6.56	124.78	110.80
2	F	135	THR	O-C-N	6.54	130.67	123.22
3	G	185	ALA	N-CA-C	-6.54	102.65	111.54
1	E	7	GLN	O-C-N	-6.53	114.50	121.42
3	G	160	LEU	N-CA-CB	-6.52	104.25	111.10
2	F	121	VAL	O-C-N	6.50	130.70	122.57
3	G	187	GLY	CA-C-O	6.45	126.13	118.97
1	E	2	GLY	N-CA-C	6.45	128.46	113.18
3	G	160	LEU	CB-CA-C	6.42	118.70	110.22
3	G	232	THR	CB-CA-C	6.39	121.55	110.68
2	F	145	ARG	NE-CZ-NH1	-6.36	115.14	121.50
3	G	166	THR	CA-C-O	-6.33	113.61	121.02
2	F	36	LYS	N-CA-CB	6.33	121.05	110.41
3	G	219	THR	CA-CB-OG1	-6.30	100.15	109.60
3	G	199	LEU	CA-C-O	6.26	126.97	120.40
2	F	92	SER	CA-C-O	-6.23	110.95	119.05
2	F	136	CYS	CA-C-N	6.20	131.74	122.75
2	F	136	CYS	C-N-CA	6.20	131.74	122.75
2	F	39	PHE	CA-C-N	6.19	129.61	120.95
2	F	39	PHE	C-N-CA	6.19	129.61	120.95
2	F	91	ASN	CA-C-O	-6.18	113.88	120.92
2	F	67	VAL	CB-CA-C	6.14	119.98	110.83
2	F	144	THR	CA-C-O	-6.14	112.15	119.15
3	G	226	GLY	N-CA-C	-6.13	104.36	112.82
2	F	137	VAL	CA-C-O	6.12	127.11	120.43
3	G	224	THR	CA-CB-OG1	-6.12	100.42	109.60
2	F	114	PHE	N-CA-CB	6.08	119.06	110.36
3	G	229	ALA	O-C-N	6.04	129.98	122.86
3	G	229	ALA	N-CA-C	-6.03	101.99	110.50
2	F	136	CYS	CA-C-O	-6.03	114.50	121.49
2	F	31	VAL	O-C-N	6.02	129.72	123.04
3	G	165	ASN	CA-C-N	6.02	130.76	121.19
3	G	165	ASN	C-N-CA	6.02	130.76	121.19
3	G	152	PRO	CA-C-O	-6.00	114.68	122.12
2	F	93	LYS	CB-CA-C	-5.99	98.21	109.72
3	G	234	LEU	N-CA-CB	-5.99	103.07	110.98
2	F	37	THR	CA-CB-CG2	5.97	120.65	110.50
3	G	232	THR	OG1-CB-CG2	5.97	121.24	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	112	ALA	CB-CA-C	5.97	119.61	109.53
1	E	10	LEU	O-C-N	-5.95	113.48	123.00
3	G	241	THR	O-C-N	5.95	128.43	122.12
2	F	60	VAL	CA-CB-CG2	5.92	120.47	110.40
2	F	23	VAL	N-CA-CB	-5.91	104.59	110.08
3	G	171	TYR	N-CA-C	5.85	118.79	111.24
2	F	141	TRP	CA-C-N	5.83	127.12	120.53
2	F	141	TRP	C-N-CA	5.83	127.12	120.53
2	F	71	PHE	N-CA-C	-5.82	102.67	111.34
2	F	116	GLN	OE1-CD-NE2	5.79	128.39	122.60
2	F	128	ASP	CA-CB-CG	5.78	118.38	112.60
2	F	23	VAL	N-CA-C	-5.75	103.31	108.95
3	G	208	THR	CB-CA-C	5.75	120.35	109.37
3	G	229	ALA	CA-C-N	-5.73	114.88	122.85
3	G	229	ALA	C-N-CA	-5.73	114.88	122.85
2	F	128	ASP	CA-C-N	5.72	132.36	122.64
2	F	128	ASP	C-N-CA	5.72	132.36	122.64
2	F	33	LEU	CA-C-N	5.69	131.50	122.62
2	F	33	LEU	C-N-CA	5.69	131.50	122.62
2	F	141	TRP	CA-CB-CG	5.68	124.39	113.60
3	G	199	LEU	CB-CA-C	5.65	119.83	110.74
3	G	154	ARG	CA-CB-CG	-5.63	102.84	114.10
3	G	241	THR	CA-C-O	-5.63	114.58	120.55
2	F	100	ASN	CA-C-N	5.56	130.54	122.36
2	F	100	ASN	C-N-CA	5.56	130.54	122.36
3	G	153	ASP	O-C-N	-5.56	115.01	122.23
2	F	54	THR	CA-CB-OG1	-5.55	101.28	109.60
2	F	81	GLN	CA-C-O	-5.54	114.58	120.40
3	G	206	ALA	O-C-N	5.53	130.38	123.19
2	F	119	SER	O-C-N	-5.48	117.13	122.99
3	G	165	ASN	CA-C-O	5.47	126.57	120.82
3	G	241	THR	N-CA-C	-5.46	105.33	111.28
2	F	118	VAL	CA-C-O	-5.40	114.82	120.27
2	F	73	GLN	CA-CB-CG	5.38	124.87	114.10
3	G	231	VAL	CA-C-N	5.38	127.75	120.38
3	G	231	VAL	C-N-CA	5.38	127.75	120.38
1	E	6	ILE	CB-CA-C	-5.38	103.71	111.19
2	F	20	GLU	O-C-N	5.38	130.14	123.15
2	F	61	THR	CA-C-O	-5.37	114.75	121.46
3	G	177	LYS	CB-CA-C	5.37	119.37	109.71
2	F	103	ILE	CA-CB-CG2	5.36	119.61	110.50
2	F	88	VAL	CB-CA-C	5.35	118.94	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	74	GLY	CA-C-N	5.34	129.06	121.42
2	F	74	GLY	C-N-CA	5.34	129.06	121.42
3	G	199	LEU	CD1-CG-CD2	5.33	122.54	110.80
3	G	201	CYS	N-CA-C	-5.32	101.09	109.50
2	F	18	ASN	N-CA-CB	-5.31	101.51	110.49
2	F	93	LYS	N-CA-CB	5.31	118.80	110.46
1	E	7	GLN	CG-CD-OE1	5.28	131.36	120.80
3	G	186	SER	N-CA-CB	-5.27	103.60	110.88
1	E	5	ALA	N-CA-C	-5.27	105.59	112.23
2	F	49	GLU	CA-CB-CG	5.26	124.63	114.10
3	G	184	GLY	O-C-N	5.23	129.50	122.70
2	F	47	ILE	N-CA-CB	5.22	120.00	112.07
2	F	67	VAL	O-C-N	-5.21	117.71	123.18
3	G	196	GLY	N-CA-C	-5.20	108.89	115.08
2	F	134	THR	CA-CB-OG1	-5.19	101.81	109.60
2	F	123	LEU	CA-C-N	5.17	125.64	120.52
2	F	123	LEU	C-N-CA	5.17	125.64	120.52
2	F	87	LYS	CA-C-N	-5.14	116.47	123.10
2	F	87	LYS	C-N-CA	-5.14	116.47	123.10
1	E	10	LEU	CA-C-N	-5.13	105.93	116.20
2	F	64	ASP	CB-CG-OD1	5.13	130.21	118.40
2	F	119	SER	CA-C-O	5.13	126.80	121.31
2	F	49	GLU	CA-C-O	-5.12	112.55	119.11
3	G	178	ASP	CA-C-O	-5.12	115.11	120.63
2	F	36	LYS	CA-CB-CG	5.11	124.31	114.10
3	G	194	ASP	CA-CB-CG	5.11	117.70	112.60
2	F	32	SER	CA-C-N	5.09	128.78	121.50
2	F	32	SER	C-N-CA	5.09	128.78	121.50
3	G	207	TRP	CA-CB-CG	5.08	123.26	113.60
2	F	20	GLU	CG-CD-OE2	-5.07	106.74	118.40
2	F	83	LEU	CA-C-O	5.07	125.90	120.38
3	G	151	THR	N-CA-CB	-5.06	102.89	111.50
3	G	154	ARG	CA-C-N	5.05	127.95	120.82
3	G	154	ARG	C-N-CA	5.05	127.95	120.82
3	G	155	LEU	N-CA-C	5.03	117.60	110.10
3	G	192	MET	O-C-N	5.03	129.13	122.89
2	F	103	ILE	CB-CA-C	5.01	119.47	110.65
3	G	202	LYS	CA-C-O	5.01	126.31	120.49
3	G	189	SER	N-CA-CB	5.01	120.20	111.13
2	F	51	TRP	CA-C-O	5.01	126.31	120.20
3	G	219	THR	N-CA-CB	-5.01	103.05	110.61
3	G	243	ALA	CA-C-O	-5.01	115.74	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	168	CYS	CA-C-N	5.00	127.69	120.38
3	G	168	CYS	C-N-CA	5.00	127.69	120.38

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	10	LEU	Mainchain
2	F	145	ARG	Sidechain
3	G	154	ARG	Sidechain

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	E	69	0	76	8	1
2	F	979	0	951	84	1
3	G	688	0	686	71	7
4	G	17	0	15	30	0
5	E	4	0	0	1	5
5	F	50	0	0	15	5
5	G	19	0	0	4	1
All	All	1826	0	1728	147	11

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 42.

All (147) 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)
4:G:246:DMC:CM2	4:G:246:DMC:CH2	1.77	1.55
3:G:217:SER:O	4:G:246:DMC:CH1	1.73	1.36
4:G:246:DMC:CH2	4:G:246:DMC:N	1.86	1.35
4:G:246:DMC:CM2	4:G:246:DMC:HE1	1.63	1.26
2:F:48:ASN:C	2:F:48:ASN:HD22	1.58	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:246:DMC:HE1	4:G:246:DMC:HM23	1.35	1.06
2:F:57:HIS:HE2	4:G:246:DMC:C	1.71	1.03
3:G:218:SER:HA	4:G:246:DMC:HM12	1.35	1.02
2:F:143:LEU:HD12	3:G:192:MET:HE2	1.40	1.01
2:F:117:THR:O	5:F:278:HOH:O	1.79	0.99
3:G:217:SER:O	4:G:246:DMC:N	1.93	0.98
3:G:192:MET:SD	4:G:246:DMC:HM13	2.03	0.98
3:G:180:MET:O	5:G:316:HOH:O	1.81	0.97
3:G:218:SER:C	4:G:246:DMC:CM1	2.38	0.97
3:G:218:SER:CA	4:G:246:DMC:HM12	1.96	0.95
3:G:218:SER:C	4:G:246:DMC:HM11	1.91	0.95
2:F:58:CYS:N	5:F:271:HOH:O	1.98	0.95
2:F:143:LEU:CD1	3:G:192:MET:HE2	1.97	0.94
1:E:9:VAL:O	1:E:9:VAL:HG12	1.70	0.90
2:F:143:LEU:HD12	3:G:192:MET:HB2	1.55	0.88
4:G:246:DMC:CM2	4:G:246:DMC:CE1	2.53	0.87
4:G:246:DMC:CH2	4:G:246:DMC:CZ	2.52	0.87
2:F:55:ALA:O	5:F:271:HOH:O	1.94	0.85
2:F:57:HIS:NE2	4:G:246:DMC:O	2.11	0.84
3:G:239:GLN:HE21	3:G:239:GLN:HA	1.44	0.83
2:F:69:GLY:HA2	5:F:278:HOH:O	1.81	0.81
2:F:144:THR:HG23	3:G:152:PRO:HG3	1.63	0.81
3:G:165:ASN:ND2	3:G:230:ARG:NH1	2.30	0.79
2:F:49:GLU:C	5:F:272:HOH:O	2.25	0.78
4:G:246:DMC:CH2	4:G:246:DMC:CE1	2.63	0.77
4:G:246:DMC:CH2	4:G:246:DMC:HE1	2.15	0.77
3:G:218:SER:C	4:G:246:DMC:HM12	2.06	0.76
2:F:146:TYR:CD2	3:G:219:THR:HA	2.22	0.74
2:F:57:HIS:NE2	4:G:246:DMC:C	2.50	0.74
2:F:31:VAL:HG12	2:F:68:ALA:HB2	1.69	0.74
2:F:144:THR:CG2	3:G:152:PRO:HG3	2.19	0.72
2:F:48:ASN:O	5:F:272:HOH:O	2.08	0.69
1:E:6:ILE:HD11	2:F:116:GLN:HG2	1.74	0.69
2:F:16:ILE:HA	3:G:189:SER:O	1.92	0.69
2:F:84:LYS:HG3	5:F:283:HOH:O	1.93	0.68
2:F:95:ASN:O	2:F:99:ILE:N	2.27	0.67
4:G:246:DMC:HE1	4:G:246:DMC:HM22	1.73	0.67
3:G:218:SER:CA	4:G:246:DMC:CM1	2.69	0.67
2:F:35:ASP:OD2	2:F:37:THR:HB	1.94	0.66
2:F:47:ILE:HG23	2:F:53:VAL:HG23	1.77	0.66
3:G:167:ASN:OD1	3:G:170:LYS:HD3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:180:MET:C	5:G:316:HOH:O	2.33	0.66
3:G:218:SER:O	4:G:246:DMC:CM1	2.43	0.65
3:G:220:CYS:HA	4:G:246:DMC:HH22	1.79	0.63
1:E:3:VAL:CG2	1:E:3:VAL:O	2.47	0.63
2:F:48:ASN:C	2:F:48:ASN:ND2	2.36	0.63
2:F:47:ILE:HG23	2:F:53:VAL:CG2	2.29	0.63
2:F:17:VAL:O	2:F:18:ASN:CB	2.47	0.62
2:F:114:PHE:CD1	2:F:118:VAL:HG12	2.35	0.62
2:F:88:VAL:HG13	2:F:106:LEU:HD23	1.83	0.61
3:G:213:VAL:HG22	3:G:228:TYR:HE2	1.65	0.60
3:G:165:ASN:ND2	3:G:230:ARG:HH12	1.98	0.60
3:G:219:THR:N	4:G:246:DMC:HM11	2.16	0.60
2:F:116:GLN:HE21	2:F:116:GLN:CA	2.15	0.59
2:F:122:CYS:O	3:G:208:THR:HA	2.03	0.59
2:F:47:ILE:CG2	2:F:53:VAL:CG2	2.81	0.58
2:F:116:GLN:O	2:F:116:GLN:HG3	2.02	0.58
2:F:88:VAL:HG13	2:F:106:LEU:CD2	2.34	0.57
2:F:143:LEU:CD1	3:G:192:MET:CE	2.79	0.57
2:F:141:TRP:O	3:G:151:THR:HG22	2.04	0.57
2:F:33:LEU:HD13	2:F:60:VAL:HG22	1.86	0.57
2:F:56:ALA:C	5:F:271:HOH:O	2.47	0.57
3:G:218:SER:O	4:G:246:DMC:HM11	2.04	0.56
1:E:5:ALA:N	5:E:296:HOH:O	2.35	0.56
2:F:122:CYS:O	3:G:209:LEU:N	2.31	0.56
2:F:33:LEU:HD13	2:F:60:VAL:CG2	2.35	0.55
3:G:167:ASN:O	3:G:170:LYS:HB2	2.06	0.55
2:F:51:TRP:HH2	2:F:89:PHE:CE1	2.25	0.55
3:G:239:GLN:HA	3:G:239:GLN:NE2	2.16	0.55
2:F:17:VAL:O	2:F:18:ASN:HB2	2.07	0.54
2:F:47:ILE:HG21	2:F:53:VAL:HG21	1.89	0.54
2:F:65:VAL:CG2	5:F:265:HOH:O	2.55	0.54
2:F:91:ASN:HA	3:G:237:TRP:CZ2	2.42	0.54
2:F:143:LEU:HD13	3:G:192:MET:HE2	1.89	0.53
2:F:73:GLN:HG3	3:G:153:ASP:O	2.07	0.53
3:G:213:VAL:HG22	3:G:228:TYR:CE2	2.44	0.53
2:F:59:GLY:HA2	5:F:288:HOH:O	2.08	0.53
2:F:138:THR:HA	3:G:198:PRO:O	2.08	0.53
2:F:116:GLN:HE21	2:F:116:GLN:HA	1.73	0.52
2:F:114:PHE:HD1	2:F:118:VAL:HG12	1.73	0.52
3:G:217:SER:HB3	4:G:246:DMC:HH21	1.92	0.52
3:G:174:THR:O	3:G:177:LYS:HE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:212:ILE:HB	3:G:229:ALA:HB3	1.93	0.51
3:G:217:SER:O	4:G:246:DMC:CM1	2.50	0.50
3:G:165:ASN:ND2	3:G:230:ARG:HH11	2.08	0.50
3:G:220:CYS:SG	4:G:246:DMC:CH1	3.00	0.49
3:G:160:LEU:HD12	3:G:184:GLY:HA2	1.92	0.49
1:E:3:VAL:O	1:E:3:VAL:HG23	2.12	0.49
2:F:66:VAL:HG21	2:F:108:LEU:HD21	1.95	0.49
3:G:165:ASN:HD21	3:G:230:ARG:NH1	2.05	0.48
2:F:73:GLN:HG3	3:G:153:ASP:HA	1.95	0.48
2:F:51:TRP:CH2	2:F:89:PHE:CE1	3.02	0.48
1:E:9:VAL:HB	2:F:23:VAL:HG21	1.95	0.48
2:F:58:CYS:CA	5:F:271:HOH:O	2.56	0.48
3:G:230:ARG:NE	5:G:316:HOH:O	1.72	0.48
2:F:48:ASN:ND2	2:F:50:ASN:H	2.12	0.47
2:F:146:TYR:CE2	3:G:219:THR:HA	2.49	0.47
3:G:217:SER:OG	3:G:219:THR:HG23	2.14	0.47
2:F:66:VAL:HG12	2:F:83:LEU:HD12	1.95	0.47
2:F:146:TYR:C	2:F:146:TYR:CD1	2.85	0.47
2:F:47:ILE:CG2	2:F:53:VAL:HG21	2.44	0.47
2:F:146:TYR:CD1	3:G:192:MET:HE1	2.50	0.47
2:F:124:PRO:O	3:G:235:VAL:HG21	2.15	0.47
3:G:160:LEU:HD12	3:G:184:GLY:CA	2.45	0.47
2:F:125:SER:C	2:F:127:SER:N	2.72	0.46
3:G:234:LEU:O	3:G:238:VAL:HG23	2.17	0.45
2:F:51:TRP:HH2	2:F:89:PHE:CD1	2.34	0.45
2:F:65:VAL:HG21	5:F:265:HOH:O	2.15	0.45
2:F:58:CYS:HB2	5:F:271:HOH:O	2.17	0.45
3:G:172:TRP:HB2	3:G:176:ILE:CG1	2.47	0.45
3:G:199:LEU:HD23	3:G:211:GLY:N	2.32	0.45
3:G:192:MET:HE2	3:G:192:MET:HB2	1.85	0.45
2:F:39:PHE:CE2	2:F:41:PHE:HB3	2.52	0.45
1:E:5:ALA:HB3	2:F:116:GLN:HG3	1.98	0.44
3:G:239:GLN:HE21	3:G:239:GLN:CA	2.23	0.44
2:F:31:VAL:HG12	2:F:68:ALA:CB	2.43	0.44
2:F:50:ASN:N	5:F:272:HOH:O	2.45	0.44
2:F:100:ASN:HD22	2:F:100:ASN:HA	1.51	0.44
3:G:168:CYS:O	3:G:171:TYR:HB2	2.18	0.44
2:F:73:GLN:CG	3:G:153:ASP:O	2.67	0.43
2:F:137:VAL:O	3:G:200:VAL:HG22	2.18	0.43
3:G:163:LEU:HD11	3:G:225:PRO:HB3	2.01	0.43
2:F:100:ASN:HD21	3:G:179:ALA:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:186:SER:OG	3:G:188:VAL:CG2	2.67	0.43
2:F:134:THR:HB	3:G:162:LEU:HD12	2.00	0.43
2:F:51:TRP:CH2	2:F:107:LYS:HB2	2.54	0.42
3:G:235:VAL:O	3:G:239:GLN:HB2	2.19	0.42
2:F:65:VAL:HG22	5:F:265:HOH:O	2.17	0.42
2:F:24:PRO:HB3	2:F:71:PHE:CG	2.55	0.42
2:F:51:TRP:CZ3	2:F:105:LEU:HB3	2.55	0.41
2:F:54:THR:OG1	2:F:55:ALA:N	2.50	0.41
3:G:172:TRP:HB2	3:G:176:ILE:HG12	2.01	0.41
3:G:230:ARG:HG3	5:G:301:HOH:O	2.20	0.41
2:F:72:ASP:C	2:F:72:ASP:OD2	2.62	0.41
4:G:246:DMC:CE1	4:G:246:DMC:HM22	2.41	0.41
2:F:115:SER:HB2	2:F:116:GLN:H	1.54	0.41
3:G:190:SER:O	4:G:246:DMC:HM22	2.20	0.41
1:E:4:PRO:CG	1:E:8:PRO:HD3	2.50	0.41
3:G:165:ASN:O	3:G:168:CYS:HB3	2.21	0.40
2:F:93:LYS:O	2:F:101:ASN:ND2	2.51	0.40
3:G:181:ILE:HG23	3:G:228:TYR:HB2	2.02	0.40
2:F:51:TRP:CH2	2:F:89:PHE:CD1	3.10	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:274:HOH:O	5:F:286:HOH:O[2_675]	0.35	1.85
3:G:240:GLN:CG	5:E:251:HOH:O[5_646]	1.08	1.12
3:G:240:GLN:CD	5:E:251:HOH:O[5_646]	1.11	1.09
3:G:240:GLN:CB	5:E:251:HOH:O[5_646]	1.66	0.54
5:F:308:HOH:O	5:F:308:HOH:O[8_777]	1.67	0.53
3:G:240:GLN:NE2	5:E:251:HOH:O[5_646]	1.74	0.46
2:F:82:LYS:NZ	5:F:302:HOH:O[6_476]	1.92	0.28
5:F:305:HOH:O	5:G:319:HOH:O[8_777]	1.95	0.25
3:G:240:GLN:OE1	5:E:251:HOH:O[5_646]	2.14	0.06
3:G:170:LYS:CD	5:F:303:HOH:O[8_777]	2.14	0.06
1:E:5:ALA:O	3:G:240:GLN:OE1[5_656]	2.15	0.05

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	E	9/13 (69%)	9 (100%)	0	0	100	100
2	F	129/131 (98%)	119 (92%)	9 (7%)	1 (1%)	16	8
3	G	93/97 (96%)	84 (90%)	9 (10%)	0	100	100
All	All	231/241 (96%)	212 (92%)	18 (8%)	1 (0%)	30	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	48	ASN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	8/10 (80%)	6 (75%)	2 (25%)	0	0
2	F	109/109 (100%)	96 (88%)	13 (12%)	5	2
3	G	76/77 (99%)	58 (76%)	18 (24%)	1	0
All	All	193/196 (98%)	160 (83%)	33 (17%)	2	0

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	3	VAL
1	E	9	VAL

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Mol	Chain	Res	Type
2	F	20	GLU
2	F	37	THR
2	F	48	ASN
2	F	49	GLU
2	F	53	VAL
2	F	63	SER
2	F	76	SER
2	F	77	SER
2	F	80	ILE
2	F	99	ILE
2	F	103	ILE
2	F	104	THR
2	F	116	GLN
3	G	151	THR
3	G	154	ARG
3	G	160	LEU
3	G	163	LEU
3	G	165	ASN
3	G	166	THR
3	G	170	LYS
3	G	177	LYS
3	G	188	VAL
3	G	195	SER
3	G	199	LEU
3	G	202	LYS
3	G	208	THR
3	G	209	LEU
3	G	219	THR
3	G	232	THR
3	G	239	GLN
3	G	240	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	48	ASN
2	F	73	GLN
2	F	100	ASN
2	F	101	ASN
2	F	116	GLN
3	G	165	ASN
3	G	239	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
4	DMC	G	246	-	17,17,18	9.68	10 (58%)	21,22,24	4.64	12 (57%)

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
4	DMC	G	246	-	-	4/14/14/16	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	246	DMC	CB1-CA	29.11	1.66	1.35
4	G	246	DMC	CG-CB1	15.73	1.72	1.46
4	G	246	DMC	OH-CD1	-14.74	1.06	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	246	DMC	C-CA	9.56	1.57	1.46
4	G	246	DMC	CH2-N	9.08	1.86	1.47
4	G	246	DMC	CZ-N	-5.92	1.22	1.38
4	G	246	DMC	CM2-CH2	5.14	1.77	1.50
4	G	246	DMC	CM1-CH1	-3.98	1.28	1.50
4	G	246	DMC	CB2-CA	-3.71	1.43	1.50
4	G	246	DMC	CD2-CE2	-2.71	1.34	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	246	DMC	CM1-CH1-N	11.61	168.35	112.22
4	G	246	DMC	CB2-CA-CB1	9.68	144.18	124.69
4	G	246	DMC	CH2-N-CZ	-9.25	107.77	121.39
4	G	246	DMC	CB2-CA-C	-5.58	111.31	117.23
4	G	246	DMC	CH2-N-CH1	5.21	126.16	116.31
4	G	246	DMC	OH-CD1-CG	4.70	129.63	121.21
4	G	246	DMC	O-C-CA	4.04	129.23	125.11
4	G	246	DMC	CE1-CD1-CG	-3.18	117.77	120.72
4	G	246	DMC	CM2-CH2-N	2.79	125.70	112.22
4	G	246	DMC	OH-CD1-CE1	-2.54	112.59	119.45
4	G	246	DMC	CG-CB1-CA	-2.39	123.20	127.37
4	G	246	DMC	CE2-CZ-N	-2.01	118.60	121.39

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	246	DMC	CM1-CH1-N-CZ
4	G	246	DMC	CM2-CH2-N-CZ
4	G	246	DMC	CM2-CH2-N-CH1
4	G	246	DMC	CM1-CH1-N-CH2

There are no ring outliers.

1 monomer is involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	246	DMC	30	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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.