



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 09:07 AM UTC

PDB ID : 6ZJY / pdb_00006zjy
EMDB ID : EMD-11238
Title : Respiratory complex I from *Thermus thermophilus*, NAD⁺ dataset, minor state
Authors : Kaszuba, K.; Tambalo, M.; Gallagher, G.T.; Sazanov, L.A.
Deposited on : 2020-06-29
Resolution : 5.50 Å(reported)
Based on initial model : 6Y11

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

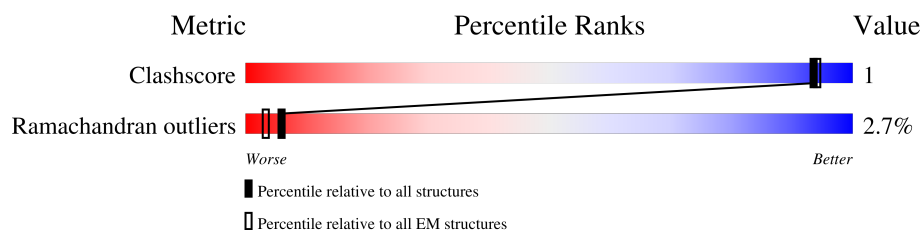
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.50 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1	438	 86% 13% .
2	2	181	 87% 10% ..
3	3	783	 79% 16% . .
4	4	409	 81% 12% 6%
5	5	207	 84% 11% 5%
6	6	181	 77% 14% . 8%
7	9	182	 79% 17% . .
8	7	129	 80% 18% . .
9	A	119	 90% 8% . .
10	J	176	 82% 9% . 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
11	K	95	 92% 8%
12	L	606	 92% 8%
13	M	469	 88% 11%
14	N	427	 91% 9%
15	H	365	 85% 11% ..

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
16	SF4	1	501	-	-	X	-
16	SF4	3	803	-	-	X	-
16	SF4	9	202	-	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 22855 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 NADH-quinone oxidoreductase subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	437	Total	C	N	O	0	0
			2136	1262	437	437		

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	2	178	Total	C	N	O	0	0
			875	519	178	178		

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	3	754	Total	C	N	O	0	0
			3714	2206	754	754		

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	4	384	Total	C	N	O	0	0
			1890	1122	384	384		

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	5	196	Total	C	N	O	0	0
			961	569	196	196		

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	6	166	Total	C	N	O	0	0
			818	486	166	166		

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	9	180	Total	C	N	O	0	0
			885	525	180	180		

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	7	127	Total	C	N	O	0	0
			628	374	127	127		

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	A	117	Total	C	N	O	0	0
			570	336	117	117		

- Molecule 10 is a protein called NADH-quinone oxidoreductase subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	160	Total	C	N	O	0	0
			783	463	160	160		

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit 11.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	95	Total	C	N	O	0	0
			467	277	95	95		

- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	605	Total	C	N	O	0	0
			2955	1745	605	605		

- Molecule 13 is a protein called NADH-quinone oxidoreductase subunit 13.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	467	Total	C	N	O	0	0
			2276	1342	467	467		

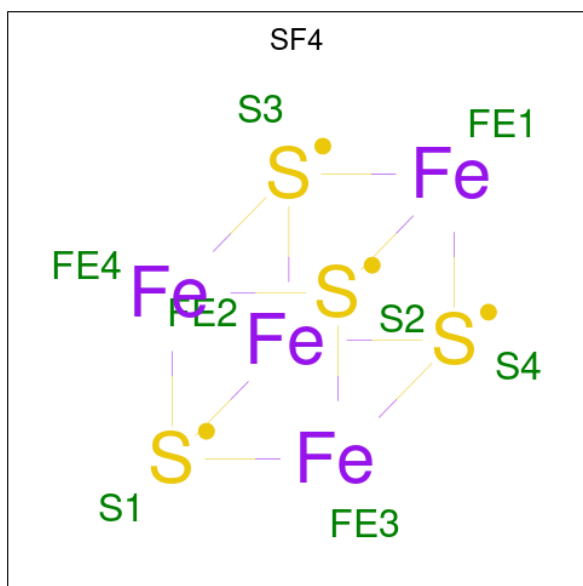
- Molecule 14 is a protein called NADH-quinone oxidoreductase subunit 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	427	Total	C	N	O	0	0
			2092	1238	427	427		

- Molecule 15 is a protein called NADH-quinone oxidoreductase subunit 8.

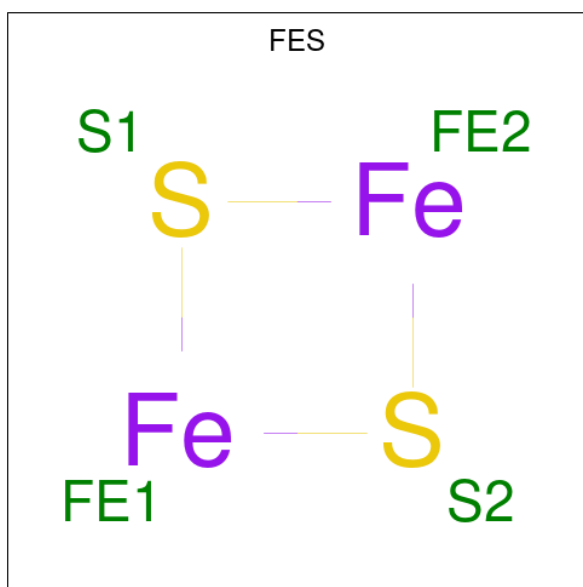
Mol	Chain	Residues	Atoms				AltConf	Trace
15	H	353	Total	C	N	O	0	0
			1741	1035	353	353		

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
16	1	1	Total	Fe	S	0
			8	4	4	
16	3	1	Total	Fe	S	0
			8	4	4	
16	3	1	Total	Fe	S	0
			8	4	4	
16	3	1	Total	Fe	S	0
			8	4	4	
16	6	1	Total	Fe	S	0
			8	4	4	
16	9	1	Total	Fe	S	0
			8	4	4	
16	9	1	Total	Fe	S	0
			8	4	4	

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

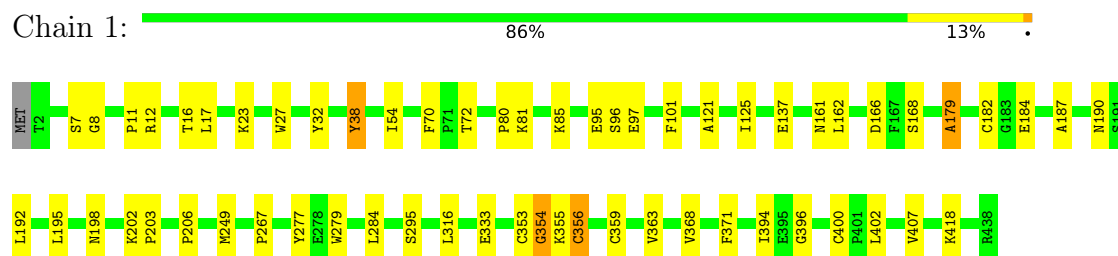


Mol	Chain	Residues	Atoms			AltConf
17	2	1	Total	Fe	S	0
			4	2	2	
17	3	1	Total	Fe	S	0
			4	2	2	

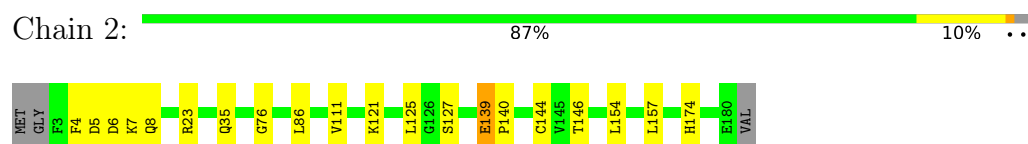
3 Residue-property plots

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.

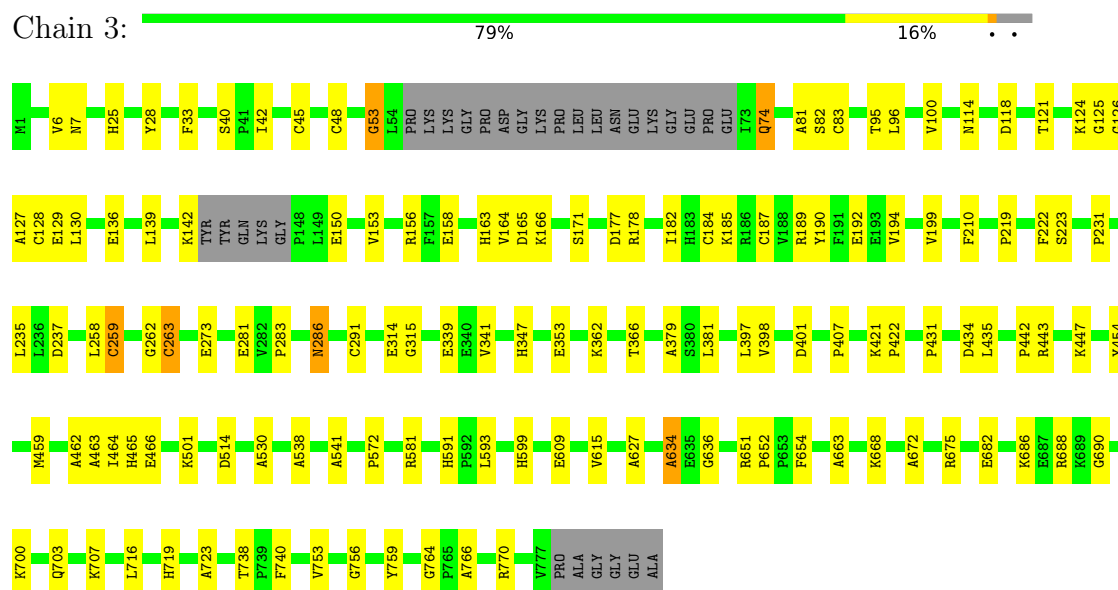
- Molecule 1: NADH-quinone oxidoreductase subunit 1



- Molecule 2: NADH-quinone oxidoreductase subunit 2

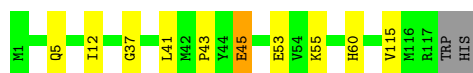


- Molecule 3: NADH-quinone oxidoreductase subunit 3



- Molecule 4: NADH-quinone oxidoreductase subunit 4





- Molecule 10: NADH-quinone oxidoreductase subunit 10

Chain J: 82% 9% 9%



- Molecule 11: NADH-quinone oxidoreductase subunit 11

Chain K: 92% 8%



- Molecule 12: NADH-quinone oxidoreductase subunit 12

Chain L: 92% 8%



- Molecule 13: NADH-quinone oxidoreductase subunit 13

Chain M: 88% 11%



- Molecule 14: NADH-quinone oxidoreductase subunit 14

Chain N: 91% 9%



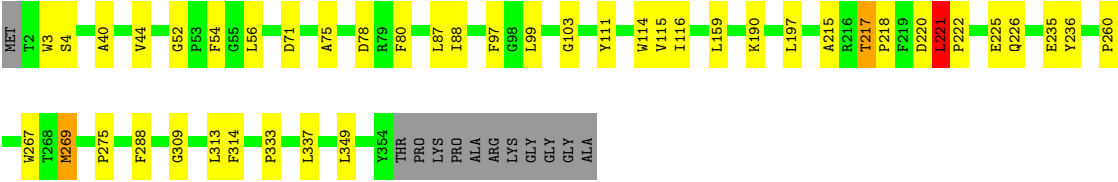
- Molecule 15: NADH-quinone oxidoreductase subunit 8

Chain H:

85%

11%

••



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	34	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, FES

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	1	1.80	10/2135 (0.5%)	1.92	50/2958 (1.7%)
2	2	1.75	1/874 (0.1%)	1.96	23/1213 (1.9%)
3	3	1.83	23/3711 (0.6%)	1.92	101/5157 (2.0%)
4	4	1.89	11/1889 (0.6%)	1.93	42/2625 (1.6%)
5	5	1.79	2/960 (0.2%)	1.89	24/1331 (1.8%)
6	6	1.95	6/817 (0.7%)	1.94	22/1135 (1.9%)
7	9	1.92	10/884 (1.1%)	1.94	26/1227 (2.1%)
8	7	1.91	4/627 (0.6%)	1.93	22/872 (2.5%)
9	A	1.62	0/569	1.81	10/786 (1.3%)
10	J	1.81	1/782 (0.1%)	1.89	18/1083 (1.7%)
11	K	1.76	0/466	1.79	7/646 (1.1%)
12	L	1.66	4/2954 (0.1%)	1.92	60/4092 (1.5%)
13	M	1.76	7/2275 (0.3%)	1.88	36/3148 (1.1%)
14	N	1.79	6/2091 (0.3%)	1.76	32/2900 (1.1%)
15	H	1.85	8/1740 (0.5%)	1.87	29/2420 (1.2%)
All	All	1.80	93/22774 (0.4%)	1.90	502/31593 (1.6%)

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	1	0	3
2	2	0	1
4	4	0	3
6	6	0	1
7	9	0	4
9	A	0	1
10	J	0	1
11	K	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
13	M	0	1
14	N	0	1
15	H	0	2
All	All	0	19

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	9	99	ILE	CA-C	-8.66	1.41	1.53
3	3	74	GLN	CA-C	-7.22	1.46	1.53
3	3	222	PHE	CA-C	-6.95	1.44	1.52
3	3	466	GLU	CA-C	-6.20	1.45	1.52
4	4	213	ILE	CA-C	-6.00	1.46	1.52
7	9	100	PHE	CA-C	-6.00	1.45	1.53
3	3	190	TYR	CA-C	-5.99	1.45	1.52
4	4	53	LEU	CA-C	-5.95	1.48	1.52
1	1	161	ASN	CA-C	-5.90	1.45	1.52
8	7	91	ILE	CA-C	-5.85	1.45	1.52
3	3	114	ASN	CA-C	-5.85	1.45	1.52
13	M	359	LEU	CA-C	-5.80	1.45	1.52
14	N	418	LEU	CA-C	-5.80	1.47	1.53
15	H	309	GLY	CA-C	-5.77	1.46	1.52
10	J	137	PHE	CA-C	-5.76	1.45	1.52
14	N	378	LEU	CA-C	-5.75	1.47	1.53
1	1	54	ILE	CA-C	-5.71	1.46	1.52
1	1	279	TRP	CA-C	-5.71	1.47	1.53
3	3	163	HIS	CA-C	-5.71	1.45	1.52
1	1	277	TYR	CA-C	-5.69	1.47	1.53
14	N	54	ALA	CA-C	-5.65	1.47	1.53
3	3	184	CYS	CA-C	-5.65	1.44	1.52
3	3	235	LEU	CA-C	-5.64	1.45	1.52
3	3	53	GLY	CA-C	-5.63	1.46	1.52
13	M	346	GLY	CA-C	-5.59	1.44	1.51
7	9	5	ALA	CA-C	-5.58	1.45	1.52
14	N	265	HIS	CA-C	-5.54	1.45	1.52
6	6	119	ASN	CA-C	-5.54	1.46	1.52
8	7	84	LEU	CA-C	-5.53	1.46	1.52
13	M	414	PHE	CA-C	-5.52	1.46	1.52
6	6	140	CYS	CA-C	-5.49	1.48	1.52
3	3	273	GLU	CA-C	-5.47	1.46	1.52
4	4	171	ASN	CA-C	-5.42	1.46	1.53
12	L	240	ILE	CA-C	-5.39	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	45	CYS	CA-C	-5.37	1.45	1.52
5	5	51	ASP	CA-C	-5.35	1.46	1.52
1	1	125	ILE	CA-C	-5.34	1.46	1.53
5	5	184	TYR	CA-C	-5.34	1.46	1.52
3	3	759	TYR	CA-C	-5.32	1.46	1.52
6	6	124	VAL	CA-C	-5.32	1.46	1.52
1	1	363	VAL	CA-C	-5.31	1.46	1.52
7	9	136	MET	CA-C	-5.29	1.46	1.52
1	1	168	SER	CA-C	-5.28	1.46	1.52
4	4	76	LEU	CA-C	-5.27	1.46	1.52
14	N	348	ALA	CA-C	-5.27	1.46	1.52
7	9	50	LEU	CA-C	-5.26	1.46	1.52
4	4	336	HIS	CA-C	-5.26	1.47	1.52
6	6	104	TRP	CA-C	-5.25	1.46	1.52
14	N	158	THR	CA-C	-5.25	1.46	1.52
3	3	281	GLU	CA-C	-5.24	1.47	1.53
4	4	252	TYR	CA-C	-5.24	1.46	1.52
8	7	93	LEU	CA-C	-5.24	1.46	1.52
12	L	293	LYS	CA-C	-5.23	1.46	1.52
15	H	3	TRP	CA-C	-5.23	1.48	1.52
8	7	82	ILE	CA-C	-5.22	1.46	1.52
12	L	253	ILE	CA-C	-5.21	1.46	1.52
3	3	464	ILE	CA-C	-5.20	1.48	1.53
12	L	11	LEU	CA-C	-5.19	1.46	1.52
3	3	33	PHE	CA-C	-5.18	1.46	1.52
4	4	234	LEU	CA-C	-5.18	1.46	1.52
7	9	101	CYS	CA-C	-5.18	1.46	1.52
15	H	99	LEU	CA-C	-5.18	1.46	1.52
13	M	198	ALA	CA-C	-5.17	1.46	1.52
15	H	116	ILE	CA-C	-5.16	1.46	1.52
2	2	154	LEU	CA-C	-5.16	1.46	1.52
4	4	85	MET	N-CA	-5.16	1.42	1.47
15	H	337	LEU	CA-C	-5.15	1.45	1.52
3	3	83	CYS	N-CA	-5.15	1.40	1.46
13	M	65	PHE	CA-C	-5.15	1.46	1.52
3	3	136	GLU	CA-C	-5.14	1.46	1.52
3	3	397	LEU	CA-C	-5.14	1.46	1.52
3	3	465	HIS	CA-C	-5.13	1.46	1.52
3	3	100	VAL	CA-C	-5.13	1.46	1.52
15	H	236	TYR	CA-C	-5.12	1.46	1.52
6	6	41	PHE	CA-C	-5.12	1.45	1.53
1	1	162	LEU	N-CA	-5.12	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	260	PRO	CA-C	-5.11	1.45	1.52
3	3	716	LEU	CA-C	-5.10	1.46	1.52
7	9	24	VAL	CA-C	-5.09	1.49	1.52
7	9	63	CYS	CA-C	-5.09	1.47	1.52
4	4	168	PHE	CA-C	-5.08	1.46	1.52
15	H	71	ASP	CA-C	-5.07	1.47	1.53
4	4	200	ARG	CA-C	-5.07	1.46	1.52
13	M	449	TYR	CA-C	-5.04	1.46	1.52
1	1	192	LEU	CA-C	-5.04	1.46	1.52
13	M	39	LEU	CA-C	-5.04	1.46	1.52
3	3	398	VAL	CA-C	-5.03	1.46	1.52
7	9	43	LEU	CA-C	-5.03	1.46	1.52
1	1	85	LYS	CA-C	-5.03	1.46	1.52
3	3	654	PHE	CA-C	-5.02	1.46	1.52
6	6	79	ILE	CA-C	-5.01	1.47	1.52
4	4	260	TYR	CA-C	-5.01	1.46	1.52
7	9	24	VAL	CA-CB	-5.01	1.50	1.54

All (502) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	156	ARG	N-CA-C	-11.22	101.83	114.62
1	1	356	CYS	CA-C-N	10.56	136.60	120.97
1	1	356	CYS	C-N-CA	10.56	136.60	120.97
6	6	66	GLU	N-CA-C	-10.50	100.77	114.31
4	4	213	ILE	N-CA-C	-10.30	102.95	111.81
9	A	41	LEU	N-CA-C	-9.28	104.05	114.62
15	H	78	ASP	CA-C-N	8.92	132.04	120.44
15	H	78	ASP	C-N-CA	8.92	132.04	120.44
8	7	40	PHE	N-CA-C	-8.80	101.45	112.72
12	L	351	LYS	N-CA-C	-8.71	104.69	114.62
7	9	167	ARG	N-CA-C	-8.59	99.25	110.07
1	1	354	GLY	N-CA-C	-8.50	104.96	115.08
3	3	463	ALA	N-CA-C	-8.24	102.22	113.18
15	H	288	PHE	CB-CA-C	-8.18	97.21	110.79
3	3	599	HIS	N-CA-C	-8.10	104.54	114.75
1	1	16	THR	N-CA-C	-7.96	105.54	114.62
12	L	380	SER	CA-C-N	7.94	128.92	120.03
12	L	380	SER	C-N-CA	7.94	128.92	120.03
5	5	105	THR	CA-C-N	7.80	133.08	120.60
5	5	105	THR	C-N-CA	7.80	133.08	120.60
3	3	187	CYS	N-CA-CB	7.73	121.60	110.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	42	ARG	N-CA-C	-7.67	96.40	108.90
7	9	22	VAL	N-CA-C	-7.60	106.49	113.71
7	9	102	GLY	N-CA-C	-7.57	104.00	114.67
6	6	41	PHE	CA-C-N	7.50	127.23	120.10
6	6	41	PHE	C-N-CA	7.50	127.23	120.10
4	4	211	SER	N-CA-C	-7.45	93.34	109.81
8	7	89	ALA	N-CA-C	-7.43	106.15	114.62
15	H	3	TRP	N-CA-C	-7.42	102.82	113.21
5	5	140	ASP	N-CA-C	-7.36	104.16	113.72
15	H	235	GLU	N-CA-C	-7.35	101.86	111.71
1	1	284	LEU	N-CA-C	-7.30	106.30	114.62
13	M	395	ALA	N-CA-C	7.30	120.16	111.33
12	L	568	GLY	CA-C-N	7.29	128.07	119.98
12	L	568	GLY	C-N-CA	7.29	128.07	119.98
5	5	124	ILE	N-CA-C	7.25	118.71	108.93
3	3	339	GLU	N-CA-C	-7.24	104.30	113.72
3	3	454	TYR	CA-C-N	7.23	131.67	120.75
3	3	454	TYR	C-N-CA	7.23	131.67	120.75
13	M	140	GLY	CA-C-N	7.20	130.26	120.54
13	M	140	GLY	C-N-CA	7.20	130.26	120.54
5	5	2	ARG	CA-C-N	7.18	130.24	120.54
5	5	2	ARG	C-N-CA	7.18	130.24	120.54
15	H	71	ASP	N-CA-C	-7.15	95.29	107.23
13	M	38	TYR	CB-CA-C	-7.12	99.42	110.81
4	4	315	HIS	N-CA-C	-7.11	104.54	112.57
3	3	124	LYS	N-CA-C	-7.05	102.80	111.40
12	L	461	LEU	CA-C-N	7.03	128.63	119.84
12	L	461	LEU	C-N-CA	7.03	128.63	119.84
3	3	189	ARG	CA-C-N	7.01	129.56	120.44
3	3	189	ARG	C-N-CA	7.01	129.56	120.44
4	4	317	LEU	CA-C-N	7.00	130.60	120.38
4	4	317	LEU	C-N-CA	7.00	130.60	120.38
4	4	65	GLY	N-CA-C	-6.92	96.77	113.18
3	3	33	PHE	CB-CA-C	-6.90	100.11	109.28
1	1	137	GLU	N-CA-C	-6.88	105.42	113.88
7	9	110	THR	N-CA-C	-6.88	104.92	113.38
15	H	220	ASP	N-CA-C	-6.87	98.20	108.99
3	3	178	ARG	N-CA-C	6.85	118.75	111.28
1	1	54	ILE	N-CA-C	-6.85	103.98	110.42
3	3	353	GLU	CA-C-N	6.83	127.38	119.94
3	3	353	GLU	C-N-CA	6.83	127.38	119.94
7	9	138	VAL	N-CA-C	-6.82	104.65	111.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	7	LYS	CA-C-N	6.80	131.48	120.60
2	2	7	LYS	C-N-CA	6.80	131.48	120.60
7	9	82	SER	N-CA-C	-6.77	98.36	108.99
3	3	291	CYS	CA-C-N	6.76	129.67	120.54
3	3	291	CYS	C-N-CA	6.76	129.67	120.54
7	9	55	GLY	CA-C-N	6.75	129.32	120.28
7	9	55	GLY	C-N-CA	6.75	129.32	120.28
15	H	80	PHE	N-CA-C	-6.73	103.87	111.14
13	M	91	VAL	N-CA-C	-6.72	98.79	108.53
10	J	85	PRO	N-CA-C	-6.71	105.27	114.80
15	H	218	PRO	N-CA-C	-6.71	104.78	113.57
14	N	50	PHE	N-CA-C	-6.71	104.25	113.18
10	J	23	ARG	N-CA-C	-6.68	102.25	110.61
3	3	150	GLU	N-CA-C	-6.68	104.70	114.39
4	4	39	GLY	N-CA-C	-6.66	103.05	112.37
5	5	195	LEU	N-CA-C	-6.60	106.43	114.75
13	M	38	TYR	N-CA-CB	6.60	119.77	109.94
15	H	115	VAL	N-CA-C	-6.59	106.56	111.90
6	6	45	CYS	CB-CA-C	6.59	121.88	110.68
4	4	272	VAL	CA-C-N	6.58	129.40	120.38
4	4	272	VAL	C-N-CA	6.58	129.40	120.38
12	L	514	ARG	N-CA-C	6.57	119.00	111.11
12	L	489	ALA	CA-C-N	6.57	129.62	120.29
12	L	489	ALA	C-N-CA	6.57	129.62	120.29
14	N	337	PRO	N-CA-C	-6.57	102.69	110.70
2	2	127	SER	N-CA-C	-6.56	102.67	110.41
12	L	576	GLN	CA-C-N	6.56	127.26	119.98
12	L	576	GLN	C-N-CA	6.56	127.26	119.98
13	M	56	LEU	CA-C-N	6.56	128.04	119.84
13	M	56	LEU	C-N-CA	6.56	128.04	119.84
8	7	126	LEU	N-CA-C	-6.55	103.34	112.45
5	5	172	ALA	N-CA-C	-6.55	104.92	113.17
3	3	100	VAL	N-CA-C	-6.55	104.27	110.42
7	9	22	VAL	CA-C-N	6.54	130.43	120.82
7	9	22	VAL	C-N-CA	6.54	130.43	120.82
1	1	23	LYS	N-CA-C	-6.52	98.27	108.90
2	2	23	ARG	N-CA-C	6.51	118.38	111.28
11	K	52	ASP	N-CA-C	-6.51	104.82	112.89
3	3	127	ALA	N-CA-C	-6.47	104.69	112.59
3	3	703	GLN	N-CA-C	-6.47	105.21	113.23
15	H	87	LEU	CA-C-N	6.46	128.93	120.60
15	H	87	LEU	C-N-CA	6.46	128.93	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	8	GLN	CA-C-N	6.44	128.91	120.28
2	2	8	GLN	C-N-CA	6.44	128.91	120.28
6	6	124	VAL	N-CA-C	-6.44	99.09	108.11
15	H	314	PHE	N-CA-CB	6.42	121.80	110.37
3	3	182	ILE	N-CA-C	-6.41	106.49	112.83
15	H	269	MET	N-CA-C	-6.37	95.72	109.81
5	5	148	LYS	CA-C-N	6.35	128.79	120.28
5	5	148	LYS	C-N-CA	6.35	128.79	120.28
3	3	719	HIS	CA-C-N	6.33	127.75	119.84
3	3	719	HIS	C-N-CA	6.33	127.75	119.84
12	L	11	LEU	N-CA-C	-6.32	104.27	112.68
1	1	371	PHE	CB-CA-C	-6.32	100.88	110.92
1	1	11	PRO	N-CA-C	-6.31	105.41	114.18
3	3	443	ARG	N-CA-C	-6.31	99.56	108.96
4	4	176	GLY	N-CA-C	-6.30	106.73	114.92
4	4	337	PRO	N-CA-C	-6.29	103.02	110.70
3	3	401	ASP	CA-C-N	6.29	126.03	119.05
3	3	401	ASP	C-N-CA	6.29	126.03	119.05
10	J	83	PHE	N-CA-C	-6.29	102.88	111.56
7	9	102	GLY	CA-C-N	6.29	129.34	120.28
7	9	102	GLY	C-N-CA	6.29	129.34	120.28
3	3	347	HIS	N-CA-C	-6.28	105.47	112.57
4	4	237	GLY	N-CA-C	-6.28	106.58	115.43
3	3	231	PRO	N-CA-C	-6.27	107.46	114.92
7	9	20	LYS	N-CA-C	-6.27	101.89	109.72
3	3	291	CYS	N-CA-CB	6.24	119.78	110.29
14	N	251	GLN	N-CA-C	6.24	118.08	110.41
1	1	353	CYS	N-CA-C	-6.23	104.57	111.36
13	M	70	LEU	CA-C-N	6.22	128.94	120.54
13	M	70	LEU	C-N-CA	6.22	128.94	120.54
1	1	394	ILE	N-CA-C	-6.22	106.46	111.81
13	M	447	PRO	CA-C-N	6.20	126.98	120.03
13	M	447	PRO	C-N-CA	6.20	126.98	120.03
6	6	178	ARG	N-CA-C	-6.20	99.72	108.96
8	7	37	PHE	CA-C-N	6.20	125.42	118.97
8	7	37	PHE	C-N-CA	6.20	125.42	118.97
10	J	101	ALA	CA-C-N	6.17	126.79	119.94
10	J	101	ALA	C-N-CA	6.17	126.79	119.94
13	M	282	LYS	CA-C-N	6.17	128.46	120.44
13	M	282	LYS	C-N-CA	6.17	128.46	120.44
3	3	442	PRO	N-CA-C	6.16	120.14	111.33
14	N	21	PRO	CA-C-O	-6.15	115.87	120.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	289	THR	N-CA-C	-6.13	104.00	112.03
6	6	73	ARG	N-CA-C	-6.13	106.07	112.93
3	3	48	CYS	N-CA-C	-6.11	105.14	112.59
2	2	4	PHE	N-CA-C	-6.10	105.77	112.72
2	2	121	LYS	N-CA-C	-6.10	102.66	110.53
10	J	57	ILE	N-CA-C	6.10	116.27	110.42
1	1	206	PRO	CA-C-N	6.09	128.77	120.54
1	1	206	PRO	C-N-CA	6.09	128.77	120.54
1	1	38	TYR	CA-C-N	6.08	128.35	120.44
1	1	38	TYR	C-N-CA	6.08	128.35	120.44
4	4	171	ASN	N-CA-C	-6.08	103.21	112.99
14	N	304	PRO	N-CA-C	-6.07	106.91	114.68
1	1	359	CYS	N-CA-C	-6.07	106.42	113.88
6	6	66	GLU	N-CA-CB	6.05	118.94	110.90
12	L	108	PHE	CB-CA-C	-6.04	101.66	110.96
14	N	395	PRO	N-CA-C	-6.04	103.33	110.70
13	M	49	HIS	N-CA-C	-6.02	99.54	108.99
14	N	2	THR	N-CA-C	-6.01	104.30	111.69
12	L	25	ARG	CA-C-N	6.00	127.59	120.09
12	L	25	ARG	C-N-CA	6.00	127.59	120.09
9	A	53	GLU	N-CA-C	-6.00	105.14	112.88
4	4	252	TYR	N-CA-C	-5.99	100.38	109.30
9	A	12	ILE	CA-C-N	5.98	128.62	120.54
9	A	12	ILE	C-N-CA	5.98	128.62	120.54
8	7	91	ILE	N-CA-C	-5.98	98.93	107.77
15	H	159	LEU	CA-C-N	5.96	128.63	120.46
15	H	159	LEU	C-N-CA	5.96	128.63	120.46
3	3	42	ILE	N-CA-C	-5.96	101.26	108.53
7	9	64	PRO	N-CA-C	-5.95	105.91	114.18
3	3	185	LYS	N-CA-C	-5.94	105.33	113.30
3	3	514	ASP	CA-C-N	5.94	128.55	120.54
3	3	514	ASP	C-N-CA	5.94	128.55	120.54
7	9	26	TYR	N-CA-C	-5.93	101.36	110.32
6	6	172	PRO	N-CA-C	-5.93	107.86	114.92
6	6	46	CYS	CB-CA-C	-5.92	98.64	110.42
1	1	72	THR	CA-C-N	5.92	126.51	119.94
1	1	72	THR	C-N-CA	5.92	126.51	119.94
3	3	129	GLU	CA-C-N	5.92	128.46	120.65
3	3	129	GLU	C-N-CA	5.92	128.46	120.65
13	M	197	PHE	CB-CA-C	-5.92	99.31	110.67
1	1	95	GLU	N-CA-C	-5.91	99.71	108.99
3	3	286	ASN	N-CA-C	-5.91	98.20	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	128	CYS	CA-C-N	5.90	128.77	120.28
3	3	128	CYS	C-N-CA	5.90	128.77	120.28
14	N	85	TYR	N-CA-C	-5.88	104.24	112.12
3	3	421	LYS	CA-C-N	5.86	126.42	120.38
3	3	421	LYS	C-N-CA	5.86	126.42	120.38
8	7	60	SER	CA-C-N	5.86	128.13	120.28
8	7	60	SER	C-N-CA	5.86	128.13	120.28
12	L	93	GLY	CA-C-N	5.84	128.10	120.28
12	L	93	GLY	C-N-CA	5.84	128.10	120.28
4	4	205	GLU	CA-C-N	5.84	128.68	120.28
4	4	205	GLU	C-N-CA	5.84	128.68	120.28
10	J	13	LEU	CA-C-N	5.84	128.03	120.44
10	J	13	LEU	C-N-CA	5.84	128.03	120.44
5	5	122	PHE	N-CA-C	-5.82	100.56	109.41
1	1	182	CYS	CA-C-N	5.82	126.40	120.00
1	1	182	CYS	C-N-CA	5.82	126.40	120.00
1	1	27	TRP	N-CA-C	-5.82	104.74	112.94
2	2	157	LEU	CA-C-N	5.79	128.62	120.28
2	2	157	LEU	C-N-CA	5.79	128.62	120.28
3	3	219	PRO	N-CA-C	-5.79	108.03	114.92
2	2	6	ASP	N-CA-C	-5.78	106.00	114.39
14	N	335	GLY	N-CA-C	-5.78	107.20	115.64
13	M	92	GLU	N-CA-C	-5.78	105.61	114.16
13	M	86	ALA	CA-C-N	5.77	128.29	120.44
13	M	86	ALA	C-N-CA	5.77	128.29	120.44
3	3	126	GLY	N-CA-C	-5.77	108.32	114.67
12	L	527	ALA	CA-C-N	5.76	128.00	120.28
12	L	527	ALA	C-N-CA	5.76	128.00	120.28
3	3	81	ALA	CA-C-N	5.76	128.00	120.28
3	3	81	ALA	C-N-CA	5.76	128.00	120.28
14	N	102	ARG	N-CA-C	-5.76	105.64	114.16
12	L	215	GLY	CA-C-N	5.76	127.99	120.28
12	L	215	GLY	C-N-CA	5.76	127.99	120.28
6	6	62	ARG	N-CA-C	-5.75	105.84	112.92
5	5	111	ALA	CA-C-N	5.75	128.78	120.79
5	5	111	ALA	C-N-CA	5.75	128.78	120.79
6	6	125	GLN	N-CA-C	-5.75	100.03	109.40
7	9	3	LEU	N-CA-C	5.74	117.34	111.14
3	3	210	PHE	CA-C-N	5.74	128.89	120.91
3	3	210	PHE	C-N-CA	5.74	128.89	120.91
3	3	366	THR	N-CA-C	-5.73	99.11	109.09
4	4	85	MET	N-CA-C	-5.73	105.19	113.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	60	HIS	CA-C-N	5.73	127.95	120.28
9	A	60	HIS	C-N-CA	5.73	127.95	120.28
3	3	153	VAL	N-CA-C	-5.72	99.51	108.95
3	3	435	LEU	N-CA-C	-5.72	106.84	113.88
3	3	6	VAL	N-CA-C	-5.72	99.64	107.99
7	9	48	ASN	N-CA-C	-5.71	106.16	113.02
12	L	246	VAL	CA-C-N	5.71	128.50	120.28
12	L	246	VAL	C-N-CA	5.71	128.50	120.28
3	3	381	LEU	N-CA-C	-5.70	105.66	113.30
4	4	212	PRO	N-CA-C	-5.70	107.22	114.35
8	7	97	TYR	N-CA-C	-5.70	100.42	109.59
14	N	126	ARG	CA-C-N	5.68	126.40	120.03
14	N	126	ARG	C-N-CA	5.68	126.40	120.03
2	2	5	ASP	N-CA-C	-5.68	106.57	112.93
14	N	164	GLY	N-CA-C	-5.68	106.33	115.08
1	1	187	ALA	CA-C-N	5.68	127.82	120.44
1	1	187	ALA	C-N-CA	5.68	127.82	120.44
12	L	187	GLU	CB-CA-C	-5.67	98.35	110.32
4	4	197	LEU	N-CA-C	5.67	121.32	113.45
8	7	38	PRO	CA-C-N	5.66	132.34	121.54
8	7	38	PRO	C-N-CA	5.66	132.34	121.54
8	7	82	ILE	N-CA-C	-5.65	100.04	108.46
12	L	160	ILE	N-CA-C	-5.65	105.60	110.74
6	6	164	ASN	N-CA-C	-5.65	100.90	108.86
3	3	121	THR	N-CA-C	-5.64	106.38	113.72
10	J	79	GLY	N-CA-C	-5.64	99.81	113.18
3	3	362	LYS	CA-C-N	5.62	128.61	120.79
3	3	362	LYS	C-N-CA	5.62	128.61	120.79
3	3	259	CYS	N-CA-C	-5.61	99.79	108.55
13	M	309	MET	CA-C-N	5.61	126.31	120.03
13	M	309	MET	C-N-CA	5.61	126.31	120.03
15	H	288	PHE	N-CA-CB	5.60	118.36	110.12
3	3	379	ALA	N-CA-C	-5.59	106.22	113.16
3	3	652	PRO	N-CA-C	-5.59	103.88	110.70
12	L	574	LEU	CA-C-N	5.58	126.28	120.03
12	L	574	LEU	C-N-CA	5.58	126.28	120.03
1	1	400	CYS	CA-C-N	-5.57	115.15	120.83
1	1	400	CYS	C-N-CA	-5.57	115.15	120.83
1	1	333	GLU	N-CA-C	-5.57	106.26	113.16
6	6	128	ASP	CA-C-N	5.57	127.68	120.44
6	6	128	ASP	C-N-CA	5.57	127.68	120.44
3	3	237	ASP	CA-C-N	5.56	127.73	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	237	ASP	C-N-CA	5.56	127.73	120.28
5	5	94	VAL	CB-CA-C	-5.56	104.54	110.16
12	L	420	TRP	N-CA-C	5.56	117.03	110.97
14	N	366	VAL	CB-CA-C	-5.56	104.76	111.88
3	3	82	SER	CA-C-N	5.56	127.67	120.44
3	3	82	SER	C-N-CA	5.56	127.67	120.44
10	J	62	ALA	N-CA-C	-5.55	104.13	111.96
12	L	433	HIS	N-CA-C	-5.54	100.66	109.59
2	2	35	GLN	N-CA-C	-5.54	105.16	111.14
3	3	422	PRO	N-CA-C	5.54	117.46	110.70
6	6	44	ALA	CA-C-N	5.54	127.97	120.38
6	6	44	ALA	C-N-CA	5.54	127.97	120.38
3	3	25	HIS	CB-CA-C	-5.54	101.60	110.79
12	L	144	PHE	N-CA-C	-5.53	106.04	112.89
3	3	341	VAL	CA-C-N	5.52	127.45	122.20
3	3	341	VAL	C-N-CA	5.52	127.45	122.20
4	4	311	PRO	CA-C-O	-5.52	116.92	120.90
10	J	81	ILE	N-CA-C	-5.52	100.38	108.11
1	1	121	ALA	CA-C-N	5.52	126.23	119.99
1	1	121	ALA	C-N-CA	5.52	126.23	119.99
8	7	102	GLY	N-CA-C	-5.51	103.23	110.29
15	H	190	LYS	N-CA-CB	5.51	118.22	110.12
7	9	39	GLY	N-CA-C	-5.51	106.18	112.79
13	M	13	GLY	N-CA-C	5.51	119.34	112.73
3	3	95	THR	N-CA-C	-5.50	107.81	114.75
3	3	756	GLY	N-CA-C	-5.50	107.44	115.63
8	7	116	PHE	CB-CA-C	-5.49	101.67	110.79
4	4	298	GLU	CA-C-N	5.49	125.49	119.89
4	4	298	GLU	C-N-CA	5.49	125.49	119.89
14	N	104	LEU	N-CA-C	5.49	117.26	111.28
12	L	108	PHE	N-CA-CB	5.49	117.92	109.91
13	M	462	ALA	N-CA-C	-5.49	106.26	113.12
2	2	139	GLU	CA-C-N	5.48	126.69	119.84
2	2	139	GLU	C-N-CA	5.48	126.69	119.84
4	4	341	GLU	N-CA-C	-5.48	101.65	110.14
14	N	423	LEU	N-CA-C	-5.47	104.55	113.19
3	3	615	VAL	CA-C-N	5.46	128.85	120.82
3	3	615	VAL	C-N-CA	5.46	128.85	120.82
10	J	135	TRP	CA-C-N	5.46	127.86	120.38
10	J	135	TRP	C-N-CA	5.46	127.86	120.38
15	H	111	TYR	N-CA-C	-5.46	101.45	109.81
15	H	349	LEU	N-CA-C	-5.46	104.17	112.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	250	LYS	N-CA-C	-5.44	105.44	112.68
14	N	169	GLY	CA-C-N	5.43	124.89	119.24
14	N	169	GLY	C-N-CA	5.43	124.89	119.24
3	3	753	VAL	N-CA-C	-5.43	102.27	107.76
8	7	67	PHE	N-CA-C	-5.43	106.03	113.30
1	1	198	ASN	N-CA-C	-5.43	97.82	109.81
8	7	5	SER	CA-C-N	5.42	131.89	121.54
8	7	5	SER	C-N-CA	5.42	131.89	121.54
3	3	130	LEU	N-CA-C	-5.42	105.07	110.97
3	3	651	ARG	N-CA-CB	5.42	117.33	110.23
4	4	143	LEU	CA-C-N	5.41	130.11	121.62
4	4	143	LEU	C-N-CA	5.41	130.11	121.62
13	M	313	TYR	CA-C-N	5.40	127.78	120.38
13	M	313	TYR	C-N-CA	5.40	127.78	120.38
14	N	124	TRP	N-CA-C	-5.40	106.00	112.59
10	J	156	LEU	CB-CA-C	-5.40	101.82	110.79
6	6	85	SER	CA-C-N	5.40	127.77	120.38
6	6	85	SER	C-N-CA	5.40	127.77	120.38
1	1	70	PHE	N-CA-C	-5.39	101.75	109.24
3	3	142	LYS	N-CA-C	-5.39	95.92	111.00
12	L	64	PRO	CA-C-N	5.38	130.33	122.41
12	L	64	PRO	C-N-CA	5.38	130.33	122.41
8	7	62	GLY	N-CA-C	-5.38	100.42	113.18
12	L	2	ALA	CA-C-N	5.38	127.80	120.54
12	L	2	ALA	C-N-CA	5.38	127.80	120.54
15	H	103	GLY	CA-C-N	5.38	125.92	120.38
15	H	103	GLY	C-N-CA	5.38	125.92	120.38
3	3	682	GLU	N-CA-C	-5.37	99.94	109.06
1	1	7	SER	N-CA-C	-5.36	101.14	108.38
12	L	6	THR	CA-C-N	5.36	128.03	120.42
12	L	6	THR	C-N-CA	5.36	128.03	120.42
2	2	111	VAL	N-CA-C	-5.35	100.77	108.48
3	3	142	LYS	N-CA-CB	5.35	119.60	110.50
15	H	313	LEU	N-CA-C	5.35	117.11	111.28
13	M	113	ARG	N-CA-C	-5.34	105.74	113.21
14	N	135	LYS	CA-C-N	5.34	127.43	120.28
14	N	135	LYS	C-N-CA	5.34	127.43	120.28
1	1	12	ARG	N-CA-C	-5.33	106.79	113.72
1	1	316	LEU	CA-C-N	5.33	128.82	120.82
1	1	316	LEU	C-N-CA	5.33	128.82	120.82
3	3	591	HIS	CA-C-N	5.33	126.50	119.84
3	3	591	HIS	C-N-CA	5.33	126.50	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	688	ARG	N-CA-C	-5.32	101.22	109.14
1	1	162	LEU	N-CA-C	-5.32	97.18	107.44
8	7	85	ARG	N-CA-CB	5.32	119.55	110.57
2	2	146	THR	N-CA-C	-5.31	101.68	109.81
9	A	5	GLN	N-CA-C	5.31	117.75	111.33
10	J	5	GLU	CA-C-N	5.31	125.99	119.99
10	J	5	GLU	C-N-CA	5.31	125.99	119.99
12	L	308	LEU	CA-C-N	5.31	127.65	120.65
12	L	308	LEU	C-N-CA	5.31	127.65	120.65
4	4	83	PRO	N-CA-C	-5.29	107.28	114.80
14	N	174	LEU	CA-C-N	5.29	127.68	120.54
14	N	174	LEU	C-N-CA	5.29	127.68	120.54
14	N	79	SER	N-CA-C	-5.29	99.71	108.75
12	L	371	LEU	CA-C-N	5.28	127.35	120.28
12	L	371	LEU	C-N-CA	5.28	127.35	120.28
1	1	407	VAL	N-CA-CB	5.28	118.49	110.58
3	3	663	ALA	CA-C-N	5.28	127.30	120.44
3	3	663	ALA	C-N-CA	5.28	127.30	120.44
13	M	164	LEU	CA-C-N	5.27	125.95	119.99
13	M	164	LEU	C-N-CA	5.27	125.95	119.99
7	9	103	LEU	N-CA-C	-5.27	105.65	111.71
1	1	17	LEU	N-CA-C	-5.26	106.72	112.72
3	3	192	GLU	CB-CA-C	-5.26	102.59	110.90
3	3	178	ARG	CB-CA-C	-5.26	102.06	110.79
7	9	103	LEU	CA-C-N	5.25	128.09	120.79
7	9	103	LEU	C-N-CA	5.25	128.09	120.79
13	M	416	GLU	N-CA-C	-5.25	103.76	110.53
12	L	151	TYR	N-CA-CB	5.25	117.06	110.45
10	J	124	PRO	CA-C-N	5.24	128.07	120.79
10	J	124	PRO	C-N-CA	5.24	128.07	120.79
9	A	45	GLU	N-CA-CB	5.24	119.34	110.49
1	1	96	SER	N-CA-C	-5.23	99.65	110.80
3	3	171	SER	CB-CA-C	-5.23	99.86	110.17
3	3	675	ARG	N-CA-C	-5.23	101.18	109.76
13	M	215	PRO	CA-C-O	-5.23	112.98	120.56
14	N	71	LEU	N-CA-C	-5.23	105.49	111.14
14	N	320	PRO	CA-C-N	5.23	127.23	120.44
14	N	320	PRO	C-N-CA	5.23	127.23	120.44
5	5	166	ILE	CA-C-N	5.22	124.67	119.24
5	5	166	ILE	C-N-CA	5.22	124.67	119.24
9	A	37	GLY	CA-C-N	5.22	127.27	120.28
9	A	37	GLY	C-N-CA	5.22	127.27	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	144	HIS	CA-C-N	5.21	125.50	119.92
5	5	144	HIS	C-N-CA	5.21	125.50	119.92
15	H	197	LEU	CA-C-N	5.21	127.79	120.28
15	H	197	LEU	C-N-CA	5.21	127.79	120.28
4	4	144	THR	N-CA-C	5.21	120.65	113.77
12	L	112	ILE	CB-CA-C	-5.21	105.30	111.97
3	3	237	ASP	N-CA-CB	5.20	118.10	110.35
5	5	94	VAL	CA-C-N	5.20	125.50	119.93
5	5	94	VAL	C-N-CA	5.20	125.50	119.93
11	K	1	MET	CA-C-N	5.20	127.56	120.54
11	K	1	MET	C-N-CA	5.20	127.56	120.54
11	K	53	GLY	N-CA-C	-5.19	108.96	114.67
3	3	28	TYR	N-CA-C	-5.19	101.41	109.24
3	3	397	LEU	N-CA-C	-5.19	100.72	109.07
4	4	61	TYR	N-CA-C	-5.18	106.64	113.17
7	9	100	PHE	N-CA-C	-5.18	104.24	111.39
12	L	444	TRP	N-CA-CB	5.18	115.31	110.39
1	1	394	ILE	CA-C-N	5.18	127.99	120.79
1	1	394	ILE	C-N-CA	5.18	127.99	120.79
1	1	32	TYR	CA-C-N	5.18	127.53	120.54
1	1	32	TYR	C-N-CA	5.18	127.53	120.54
12	L	22	LYS	N-CA-C	-5.18	106.97	113.28
14	N	418	LEU	N-CA-C	-5.18	104.66	111.96
3	3	164	VAL	CA-C-N	5.17	131.41	121.54
3	3	164	VAL	C-N-CA	5.17	131.41	121.54
4	4	225	PRO	CA-C-N	5.17	126.30	119.84
4	4	225	PRO	C-N-CA	5.17	126.30	119.84
1	1	8	GLY	N-CA-C	-5.17	100.94	113.18
1	1	190	ASN	CB-CA-C	-5.17	102.77	110.88
1	1	184	GLU	N-CA-CB	5.16	117.48	109.48
14	N	400	ALA	CA-C-N	5.16	127.51	120.54
14	N	400	ALA	C-N-CA	5.16	127.51	120.54
3	3	190	TYR	N-CA-C	-5.16	105.55	111.07
4	4	262	PHE	N-CA-C	-5.16	99.81	110.80
12	L	177	TRP	N-CA-C	-5.16	99.81	110.80
2	2	7	LYS	N-CA-C	-5.15	104.33	110.41
13	M	175	PHE	N-CA-CB	5.15	119.16	110.92
3	3	96	LEU	N-CA-C	-5.15	106.84	113.02
11	K	2	SER	CA-C-N	5.15	127.18	120.28
11	K	2	SER	C-N-CA	5.15	127.18	120.28
15	H	88	ILE	N-CA-CB	-5.15	104.80	110.51
12	L	438	ALA	CA-C-N	5.14	125.68	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	438	ALA	C-N-CA	5.14	125.68	120.38
13	M	393	ALA	N-CA-C	-5.14	105.57	111.07
4	4	66	PHE	CA-C-N	5.13	127.88	120.38
4	4	66	PHE	C-N-CA	5.13	127.88	120.38
7	9	74	GLU	N-CA-CB	5.13	118.78	110.42
3	3	723	ALA	CA-C-N	5.12	129.34	121.19
3	3	723	ALA	C-N-CA	5.12	129.34	121.19
5	5	107	LEU	N-CA-C	-5.12	107.70	114.31
15	H	114	TRP	N-CA-C	-5.12	101.47	108.38
5	5	20	ASN	N-CA-C	-5.12	101.93	110.17
6	6	22	THR	CA-C-N	5.12	127.90	120.79
6	6	22	THR	C-N-CA	5.12	127.90	120.79
13	M	9	PRO	CA-C-N	5.11	127.00	120.56
13	M	9	PRO	C-N-CA	5.11	127.00	120.56
2	2	76	GLY	CA-C-N	5.11	127.84	120.38
2	2	76	GLY	C-N-CA	5.11	127.84	120.38
13	M	352	PRO	N-CA-C	-5.11	107.38	114.27
3	3	634	ALA	N-CA-C	-5.11	99.92	110.80
3	3	707	LYS	N-CA-C	-5.11	106.21	112.90
12	L	242	ALA	N-CA-C	-5.11	99.92	110.80
2	2	125	LEU	N-CA-C	-5.10	106.47	113.30
8	7	22	GLU	CA-C-N	5.10	127.36	120.38
8	7	22	GLU	C-N-CA	5.10	127.36	120.38
3	3	572	PRO	CA-C-N	5.10	126.21	119.84
3	3	572	PRO	C-N-CA	5.10	126.21	119.84
5	5	51	ASP	N-CA-C	5.10	117.90	109.85
11	K	89	ASP	N-CA-C	-5.09	106.84	113.16
12	L	526	ALA	CA-C-N	5.09	127.42	120.54
12	L	526	ALA	C-N-CA	5.09	127.42	120.54
4	4	242	SER	N-CA-C	-5.09	106.38	112.59
4	4	271	ASP	CA-C-N	5.09	126.97	120.56
4	4	271	ASP	C-N-CA	5.09	126.97	120.56
3	3	615	VAL	N-CA-C	-5.08	99.85	107.37
8	7	125	ALA	N-CA-CB	5.08	117.64	110.13
12	L	355	LEU	N-CA-C	-5.08	107.06	114.12
5	5	133	ARG	N-CA-C	-5.07	101.03	108.79
3	3	501	LYS	N-CA-C	-5.07	107.27	113.50
12	L	147	LYS	N-CA-C	-5.07	106.41	112.59
14	N	158	THR	N-CA-C	-5.07	101.04	108.79
1	1	179	ALA	N-CA-CB	5.06	119.04	110.49
12	L	327	PHE	N-CA-CB	5.05	117.50	110.07
4	4	273	PHE	N-CA-CB	-5.05	102.48	110.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	6	21	PHE	N-CA-C	-5.05	100.12	108.75
1	1	368	VAL	N-CA-C	5.05	115.66	110.36
15	H	40	ALA	CA-C-N	5.04	127.35	120.54
15	H	40	ALA	C-N-CA	5.04	127.35	120.54
7	9	46	HIS	CA-C-N	5.03	125.71	120.12
7	9	46	HIS	C-N-CA	5.03	125.71	120.12
4	4	406	ASP	CB-CA-C	-5.03	102.98	110.88
12	L	474	LYS	CA-C-N	5.03	124.81	119.28
12	L	474	LYS	C-N-CA	5.03	124.81	119.28
1	1	402	LEU	N-CA-C	5.02	116.44	111.07
4	4	144	THR	CA-C-N	5.02	124.68	119.56
4	4	144	THR	C-N-CA	5.02	124.68	119.56
13	M	93	GLY	N-CA-C	-5.02	107.75	115.73
14	N	263	ILE	N-CA-C	-5.02	105.53	111.00
2	2	174	HIS	CA-C-N	5.02	127.00	120.28
2	2	174	HIS	C-N-CA	5.02	127.00	120.28
12	L	315	TYR	CA-C-N	5.01	127.49	120.28
12	L	315	TYR	C-N-CA	5.01	127.49	120.28
7	9	159	VAL	CB-CA-C	-5.00	105.75	110.70

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	166	ASP	Peptide
1	1	203	PRO	Peptide
1	1	396	GLY	Peptide
2	2	139	GLU	Peptide
4	4	142	ALA	Peptide
4	4	254	TYR	Peptide
4	4	36	SER	Peptide
6	6	55	ASP	Peptide
7	9	100	PHE	Mainchain
7	9	178	GLU	Peptide
7	9	20	LYS	Peptide
7	9	21	PRO	Peptide
9	A	115	VAL	Peptide
15	H	217	THR	Peptide
15	H	221	LEU	Peptide
10	J	83	PHE	Peptide
11	K	50	GLY	Peptide
13	M	71	SER	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
14	N	169	GLY	Peptide

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	1	2136	0	989	7	0
2	2	875	0	398	0	0
3	3	3714	0	1785	16	0
4	4	1890	0	833	2	0
5	5	961	0	427	1	0
6	6	818	0	388	2	0
7	9	885	0	406	9	0
8	7	628	0	300	1	0
9	A	570	0	280	0	0
10	J	783	0	409	0	0
11	K	467	0	248	0	0
12	L	2955	0	1499	0	0
13	M	2276	0	1200	2	0
14	N	2092	0	1120	1	0
15	H	1741	0	818	3	0
16	1	8	0	0	6	0
16	3	24	0	0	7	0
16	6	8	0	0	1	0
16	9	16	0	0	8	0
17	2	4	0	0	0	0
17	3	4	0	0	0	0
All	All	22855	0	11100	43	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 1.

All (43) 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)
3:3:262:GLY:N	16:3:803:SF4:S2	2.05	1.26

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:355:LYS:N	16:1:501:SF4:S3	2.36	0.97
3:3:262:GLY:CA	16:3:803:SF4:S2	2.52	0.96
1:1:354:GLY:C	16:1:501:SF4:S3	2.49	0.96
1:1:356:CYS:O	16:1:501:SF4:S3	2.27	0.91
7:9:112:ALA:HB3	16:9:202:SF4:S4	2.15	0.86
7:9:55:GLY:CA	16:9:202:SF4:S1	2.64	0.85
7:9:55:GLY:HA2	16:9:202:SF4:S1	2.17	0.84
3:3:259:CYS:N	16:3:803:SF4:S3	2.61	0.73
7:9:55:GLY:C	16:9:202:SF4:S1	2.63	0.71
3:3:609:GLU:HA	3:3:627:ALA:H	1.55	0.69
1:1:354:GLY:N	16:1:501:SF4:S3	2.66	0.68
3:3:262:GLY:HA2	16:3:803:SF4:S2	2.33	0.67
3:3:459:MET:HA	3:3:462:ALA:HB3	1.80	0.63
3:3:700:LYS:HA	3:3:764:GLY:H	1.63	0.62
3:3:538:ALA:HB3	3:3:541:ALA:HB2	1.81	0.61
1:1:354:GLY:CA	16:1:501:SF4:S3	2.92	0.58
7:9:108:CYS:HA	16:9:202:SF4:S3	2.46	0.56
7:9:108:CYS:CB	16:9:202:SF4:S3	2.95	0.55
7:9:112:ALA:CB	16:9:202:SF4:S4	2.92	0.55
8:7:60:SER:HA	8:7:66:PRO:HA	1.90	0.54
3:3:263:CYS:N	16:3:803:SF4:S2	2.81	0.53
7:9:53:CYS:HA	16:9:202:SF4:S2	2.50	0.52
3:3:166:LYS:HA	3:3:177:ASP:HA	1.93	0.50
1:1:249:MET:HA	1:1:267:PRO:HA	1.94	0.50
15:H:221:LEU:H	15:H:222:PRO:HA	1.75	0.50
1:1:355:LYS:CB	16:1:501:SF4:S2	3.01	0.49
6:6:111:CYS:N	16:6:201:SF4:S3	2.83	0.48
3:3:125:GLY:N	16:3:801:SF4:S3	2.77	0.47
13:M:268:ALA:HB2	13:M:294:GLY:HA3	1.98	0.46
13:M:139:GLU:C	13:M:141:ARG:H	2.24	0.46
6:6:71:SER:C	6:6:73:ARG:H	2.22	0.45
15:H:221:LEU:H	15:H:222:PRO:CA	2.29	0.45
7:9:101:CYS:C	7:9:103:LEU:H	2.24	0.44
3:3:40:SER:HA	3:3:434:ASP:H	1.82	0.44
15:H:52:GLY:HA2	15:H:56:LEU:H	1.82	0.44
3:3:738:THR:C	3:3:740:PHE:H	2.26	0.44
3:3:258:LEU:C	16:3:803:SF4:S3	3.01	0.44
3:3:53:GLY:HA2	3:3:74:GLN:O	2.19	0.43
3:3:690:GLY:H	3:3:770:ARG:CB	2.32	0.42
4:4:211:SER:C	4:4:213:ILE:H	2.29	0.41
4:4:60:GLY:HA3	5:5:136:LEU:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:315:LEU:H	14:N:382:VAL:HA	1.85	0.41

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 PDB entries followed by that with respect to all EM entries.

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	1	435/438 (99%)	387 (89%)	38 (9%)	10 (2%)	5	27
2	2	176/181 (97%)	160 (91%)	13 (7%)	3 (2%)	7	35
3	3	748/783 (96%)	650 (87%)	73 (10%)	25 (3%)	3	20
4	4	382/409 (93%)	339 (89%)	30 (8%)	13 (3%)	3	20
5	5	194/207 (94%)	173 (89%)	15 (8%)	6 (3%)	3	21
6	6	164/181 (91%)	134 (82%)	25 (15%)	5 (3%)	3	22
7	9	178/182 (98%)	155 (87%)	18 (10%)	5 (3%)	4	24
8	7	125/129 (97%)	109 (87%)	12 (10%)	4 (3%)	3	21
9	A	115/119 (97%)	104 (90%)	8 (7%)	3 (3%)	4	25
10	J	158/176 (90%)	133 (84%)	23 (15%)	2 (1%)	9	41
11	K	93/95 (98%)	85 (91%)	6 (6%)	2 (2%)	5	28
12	L	603/606 (100%)	540 (90%)	55 (9%)	8 (1%)	9	41
13	M	465/469 (99%)	408 (88%)	41 (9%)	16 (3%)	3	20
14	N	425/427 (100%)	378 (89%)	40 (9%)	7 (2%)	7	37
15	H	351/365 (96%)	306 (87%)	31 (9%)	14 (4%)	2	18
All	All	4612/4767 (97%)	4061 (88%)	428 (9%)	123 (3%)	6	25

All (123) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	101	PHE
1	1	179	ALA
3	3	165	ASP
3	3	263	CYS
3	3	634	ALA
3	3	672	ALA
4	4	211	SER
4	4	262	PHE
4	4	335	PHE
6	6	43	LEU
9	A	43	PRO
12	L	122	ASP
13	M	72	ALA
13	M	349	GLN
13	M	424	ASP
14	N	425	ALA
15	H	217	THR
15	H	221	LEU
15	H	225	GLU
2	2	86	LEU
3	3	7	ASN
3	3	139	LEU
3	3	158	GLU
3	3	314	GLU
3	3	668	LYS
3	3	766	ALA
4	4	41	LEU
4	4	63	HIS
4	4	88	LEU
4	4	89	HIS
5	5	103	THR
5	5	146	LEU
6	6	57	ARG
6	6	116	GLY
6	6	128	ASP
7	9	156	PRO
8	7	45	GLU
8	7	63	LEU
10	J	78	GLN
12	L	462	PRO
13	M	90	ARG
13	M	224	SER
13	M	426	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	H	4	SER
15	H	54	PHE
15	H	215	ALA
15	H	226	GLN
1	1	80	PRO
1	1	195	LEU
1	1	295	SER
2	2	140	PRO
3	3	199	VAL
3	3	315	GLY
3	3	447	LYS
3	3	593	LEU
4	4	50	GLU
4	4	178	VAL
4	4	246	TYR
4	4	268	GLU
5	5	179	PRO
7	9	122	ALA
8	7	39	ASP
11	K	94	ARG
12	L	399	GLY
13	M	89	ALA
14	N	393	PRO
15	H	97	PHE
15	H	267	TRP
15	H	333	PRO
2	2	144	CYS
3	3	283	PRO
3	3	286	ASN
3	3	407	PRO
3	3	431	PRO
3	3	530	ALA
3	3	581	ARG
5	5	136	LEU
6	6	17	GLU
8	7	44	MET
9	A	55	LYS
10	J	84	ASP
11	K	92	GLU
12	L	245	MET
12	L	519	ALA
13	M	387	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	404	ALA
14	N	385	ARG
15	H	75	ALA
15	H	275	PRO
1	1	81	LYS
1	1	97	GLU
1	1	418	LYS
3	3	118	ASP
3	3	223	SER
3	3	636	GLY
3	3	686	LYS
4	4	169	HIS
4	4	401	ASP
5	5	131	ASP
7	9	109	PRO
7	9	173	PHE
9	A	45	GLU
12	L	102	SER
12	L	198	ASN
13	M	304	THR
14	N	169	GLY
14	N	397	TRP
14	N	417	GLY
1	1	38	TYR
3	3	194	VAL
5	5	99	PRO
12	L	440	PRO
13	M	236	VAL
13	M	344	TYR
15	H	269	MET
1	1	202	LYS
7	9	166	VAL
13	M	57	PRO
13	M	360	ILE
14	N	302	ILE
13	M	422	VAL
15	H	44	VAL
13	M	208	PHE

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 ligands 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	$\# Z > 2$
16	SF4	1	501	1	0,12,12	-	-	-		
17	FES	2	201	-	0,4,4	-	-	-		
17	FES	3	804	-	0,4,4	-	-	-		
16	SF4	9	201	7	0,12,12	-	-	-		
16	SF4	6	201	-	0,12,12	-	-	-		
16	SF4	3	802	3	0,12,12	-	-	-		
16	SF4	9	202	7	0,12,12	-	-	-		
16	SF4	3	801	-	0,12,12	-	-	-		
16	SF4	3	803	-	0,12,12	-	-	-		

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
16	SF4	1	501	1	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	FES	2	201	-	-	-	0/1/1/1
17	FES	3	804	-	-	-	0/1/1/1
16	SF4	9	201	7	-	-	0/6/5/5
16	SF4	6	201	-	-	-	0/6/5/5
16	SF4	3	802	3	-	-	0/6/5/5
16	SF4	9	202	7	-	-	0/6/5/5
16	SF4	3	801	-	-	-	0/6/5/5
16	SF4	3	803	-	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	1	501	SF4	6	0
16	6	201	SF4	1	0
16	9	202	SF4	8	0
16	3	801	SF4	1	0
16	3	803	SF4	6	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 Map visualisation

This section contains visualisations of the EMDB entry EMD-11238. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section was not generated.