



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 04:55 AM UTC

PDB ID : 5LJV / pdb_00005lvj
EMDB ID : EMD-4062
Title : MamK double helical filament
Authors : Lowe, J.
Deposited on : 2016-07-21
Resolution : 3.64 Å(reported)

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:

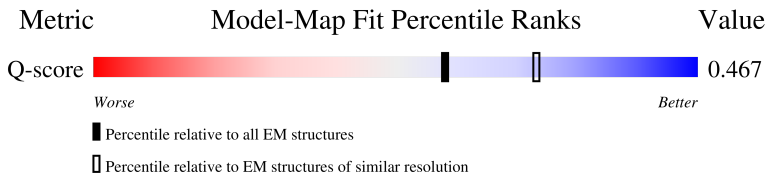
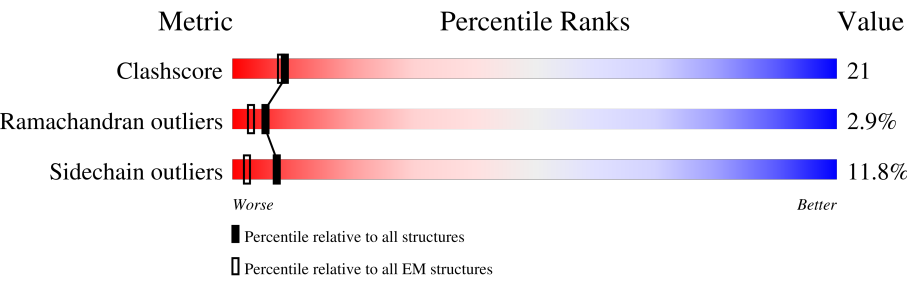
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.64 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11633 (3.14 - 4.14)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	347	 38% 35% 18% 6%
1	B	347	 40% 33% 17% 6%
1	C	347	 37% 33% 21% 6%
1	D	347	 39% 33% 19% 6%

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Mol	Chain	Length	Quality of chain
1	E	347	
1	F	347	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15000 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 Actin-like ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	325	Total	C	N	O	S	0	0
			2472	1569	425	466	12		
1	B	325	Total	C	N	O	S	0	0
			2472	1569	425	466	12		
1	C	325	Total	C	N	O	S	0	0
			2472	1569	425	466	12		
1	D	325	Total	C	N	O	S	0	0
			2472	1569	425	466	12		
1	E	325	Total	C	N	O	S	0	0
			2472	1569	425	466	12		
1	F	325	Total	C	N	O	S	0	0
			2472	1569	425	466	12		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	VAL	ILE	conflict	UNP Q2W8Q6
B	16	VAL	ILE	conflict	UNP Q2W8Q6
C	16	VAL	ILE	conflict	UNP Q2W8Q6
D	16	VAL	ILE	conflict	UNP Q2W8Q6
E	16	VAL	ILE	conflict	UNP Q2W8Q6
F	16	VAL	ILE	conflict	UNP Q2W8Q6

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

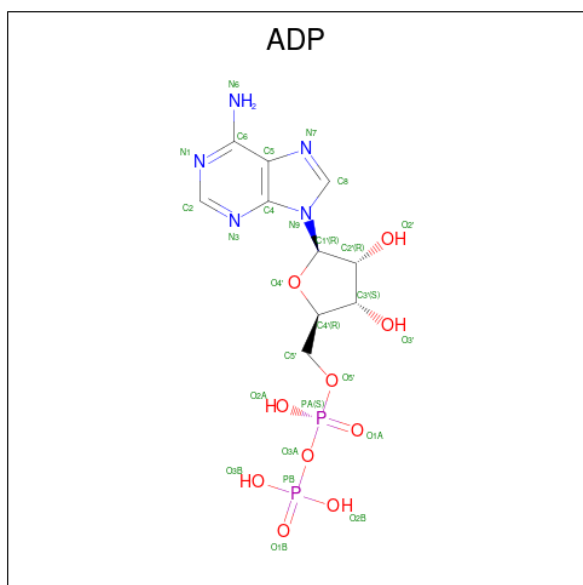
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Mg	0
			1	1	
2	B	1	Total	Mg	0
			1	1	
2	C	1	Total	Mg	0
			1	1	
2	D	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
2	E	1	Total Mg 1 1	0
2	F	1	Total Mg 1 1	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

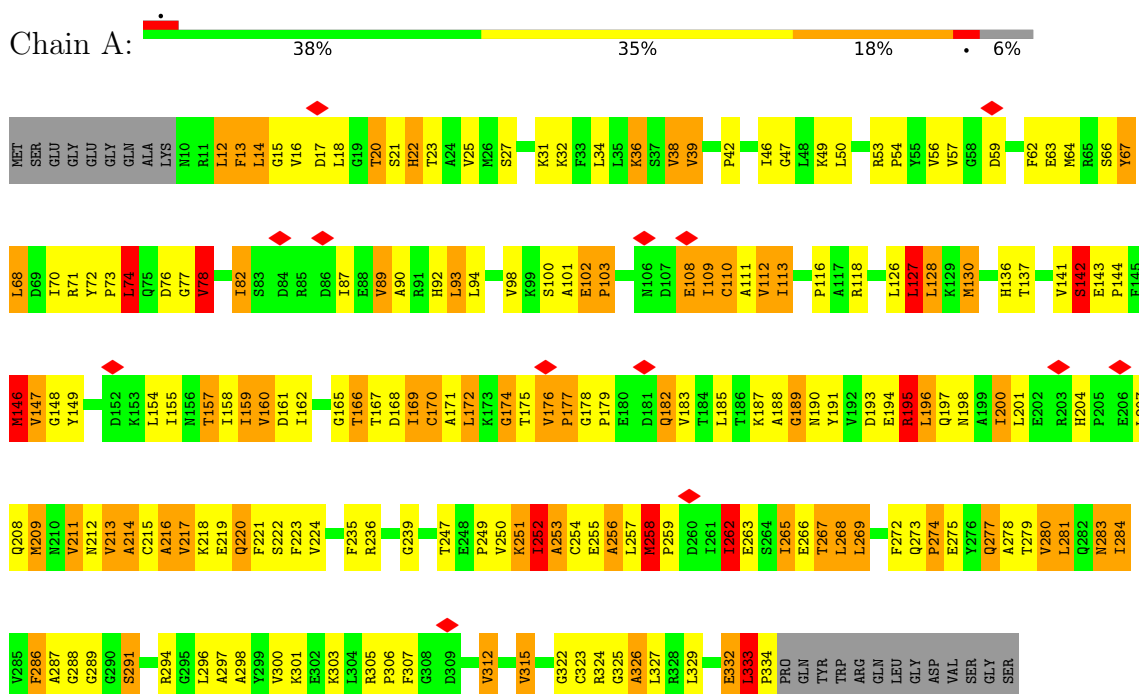


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0
3	F	1	Total 27	C 10	N 5	O 10	P 2	0

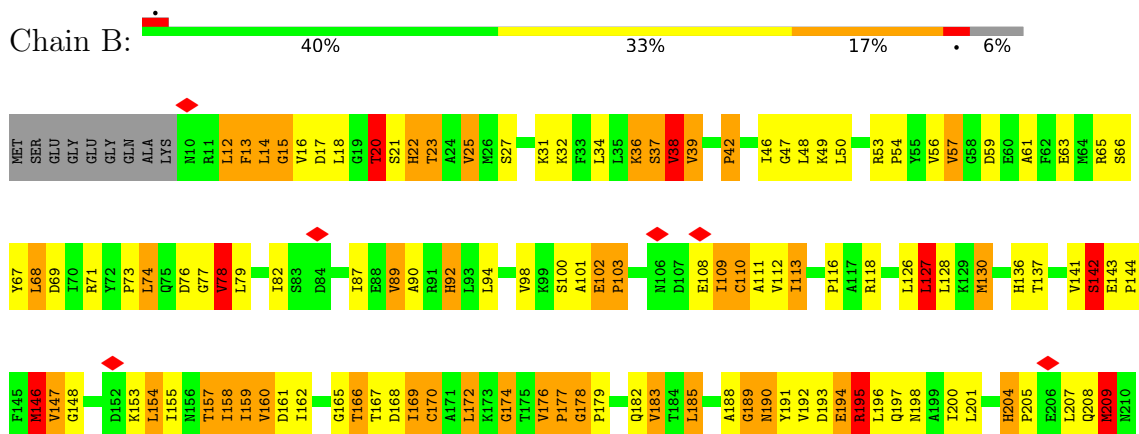
3 Residue-property plots

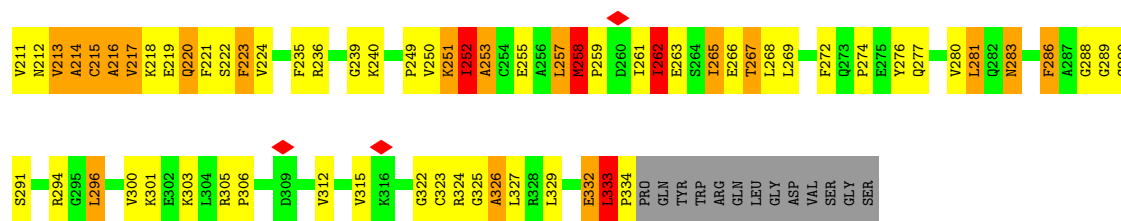
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Actin-like ATPase



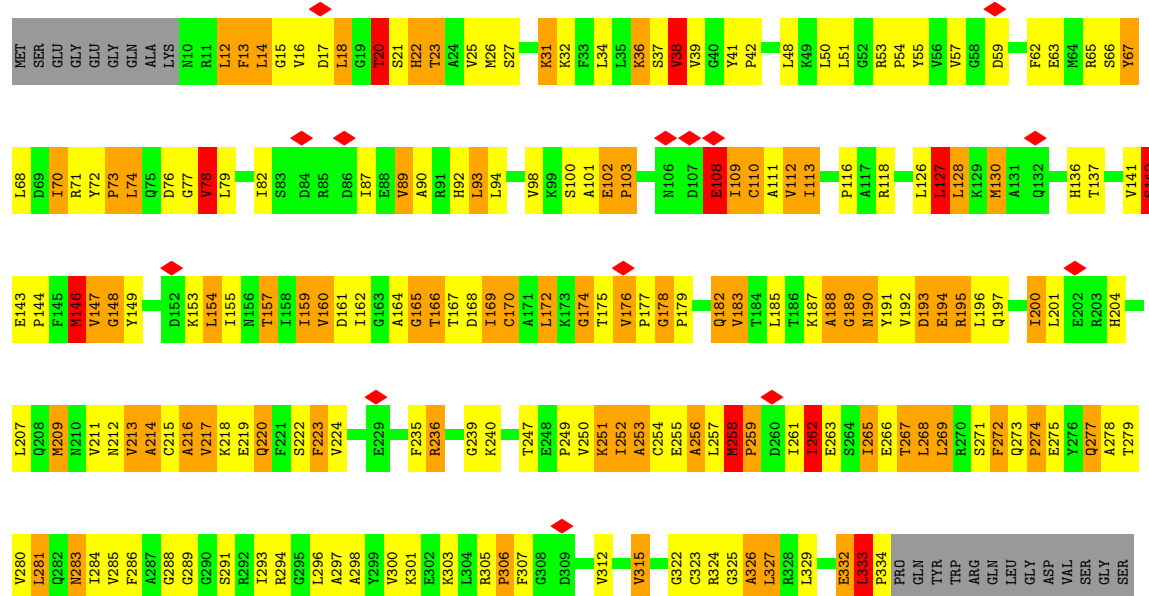
• Molecule 1: Actin-like ATPase





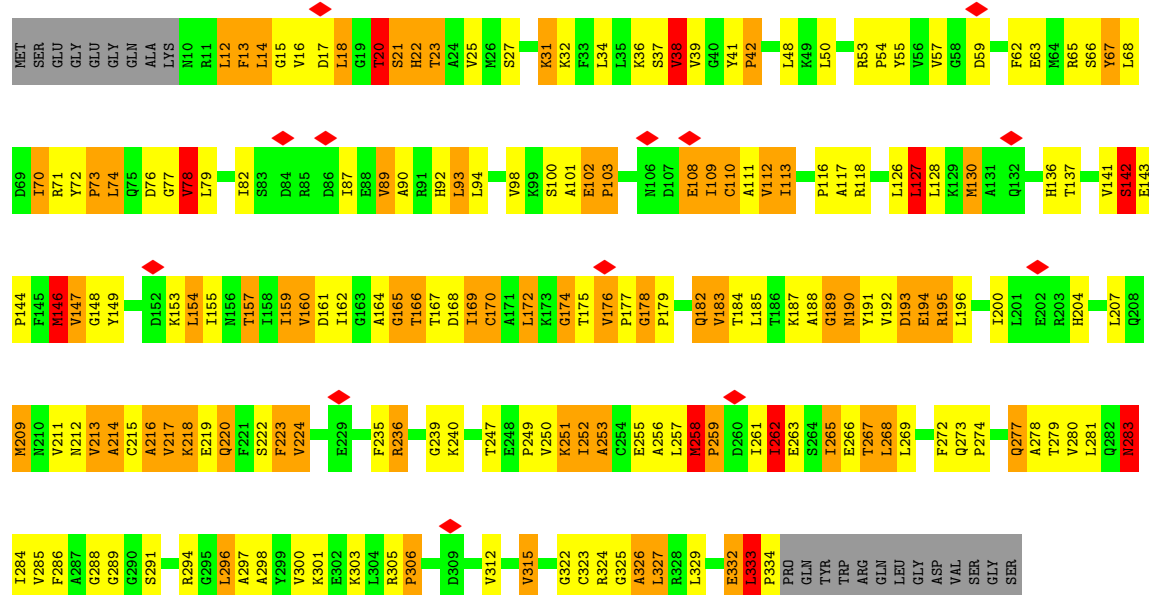
• Molecule 1: Actin-like ATPase

Chain C: 37% 33% 21% 6%



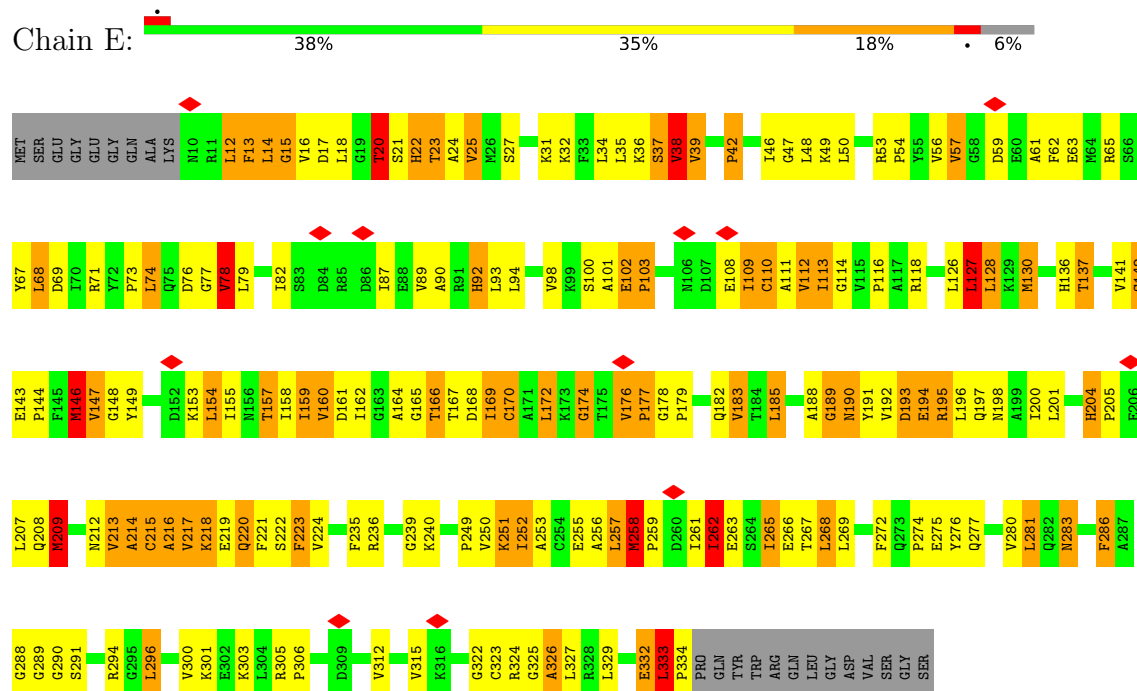
• Molecule 1: Actin-like ATPase

Chain D: 39% 33% 19% 6%



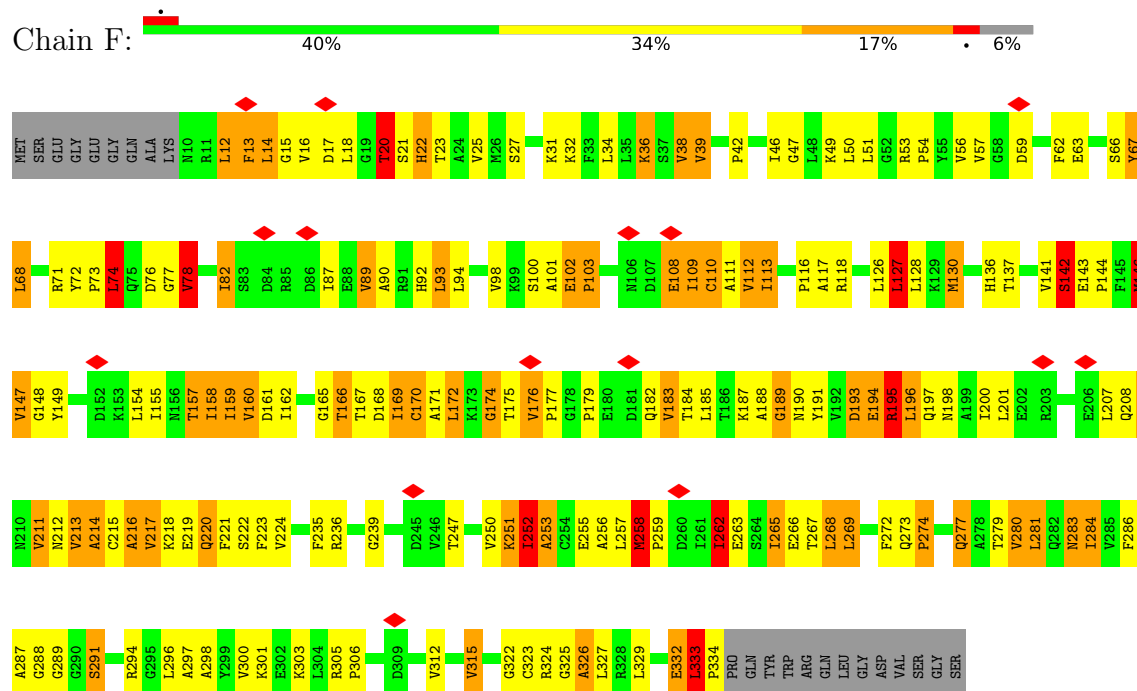
• Molecule 1: Actin-like ATPase

Chain E:



• Molecule 1: Actin-like ATPase

Chain F:



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=23.77°, rise=52.15 Å, axial sym=C2	Depositor
Number of segments used	596427	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	40	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.822	Depositor
Minimum map value	-0.418	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.155	Depositor
Map size (Å)	375.2, 375.2, 375.2	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.93	64/2514 (2.5%)	1.72	60/3411 (1.8%)
1	B	2.11	91/2514 (3.6%)	1.70	49/3411 (1.4%)
1	C	2.13	96/2514 (3.8%)	1.72	53/3411 (1.6%)
1	D	2.13	100/2514 (4.0%)	1.72	51/3411 (1.5%)
1	E	2.15	100/2514 (4.0%)	1.71	49/3411 (1.4%)
1	F	1.94	64/2514 (2.5%)	1.72	59/3411 (1.7%)
All	All	2.07	515/15084 (3.4%)	1.71	321/20466 (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	A	0	4
1	B	0	4
1	C	0	4
1	D	0	4
1	E	0	3
1	F	0	2
All	All	0	21

All (515) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	HIS	CA-C	-12.08	1.37	1.52
1	C	160	VAL	CA-C	-11.89	1.43	1.53
1	F	22	HIS	CA-C	-11.89	1.38	1.52
1	D	160	VAL	CA-C	-11.45	1.43	1.53
1	D	183	VAL	CA-CB	-11.20	1.44	1.55
1	B	22	HIS	CA-C	-10.87	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	22	HIS	CA-C	-10.75	1.39	1.52
1	E	217	VAL	C-O	-10.41	1.11	1.24
1	C	183	VAL	CA-CB	-9.86	1.45	1.55
1	C	333	LEU	CA-C	9.80	1.65	1.52
1	C	22	HIS	CA-C	-9.60	1.40	1.52
1	D	168	ASP	CA-C	-9.41	1.41	1.52
1	D	333	LEU	CA-C	9.34	1.64	1.52
1	F	67	TYR	CA-CB	-9.32	1.39	1.53
1	A	67	TYR	CA-CB	-9.28	1.39	1.53
1	D	22	HIS	CA-C	-9.21	1.41	1.52
1	E	21	SER	CA-C	-9.11	1.40	1.52
1	B	21	SER	CA-C	-9.05	1.40	1.52
1	F	111	ALA	CA-C	-9.03	1.41	1.52
1	E	111	ALA	CA-C	-8.99	1.41	1.52
1	F	39	VAL	N-CA	-8.96	1.35	1.46
1	C	70	ILE	CA-C	-8.94	1.41	1.52
1	D	170	CYS	N-CA	-8.94	1.35	1.46
1	A	333	LEU	CA-C	8.86	1.64	1.52
1	C	168	ASP	CA-C	-8.85	1.42	1.52
1	E	274	PRO	CA-C	-8.78	1.39	1.52
1	B	111	ALA	CA-C	-8.73	1.41	1.52
1	B	169	ILE	CA-C	-8.70	1.41	1.52
1	B	160	VAL	CA-C	-8.69	1.45	1.53
1	D	277	GLN	CA-CB	-8.64	1.39	1.53
1	C	277	GLN	CA-CB	-8.62	1.39	1.53
1	C	170	CYS	N-CA	-8.60	1.35	1.46
1	E	222	SER	CA-C	-8.60	1.41	1.52
1	A	21	SER	CA-C	-8.59	1.41	1.52
1	E	169	ILE	CA-C	-8.58	1.41	1.52
1	E	128	LEU	N-CA	-8.58	1.36	1.46
1	E	39	VAL	N-CA	-8.58	1.36	1.46
1	B	162	ILE	CA-C	-8.55	1.42	1.52
1	B	280	VAL	CA-CB	-8.54	1.44	1.54
1	B	274	PRO	CA-C	-8.54	1.39	1.52
1	E	214	ALA	C-O	-8.52	1.14	1.24
1	A	111	ALA	CA-C	-8.46	1.42	1.52
1	F	333	LEU	CA-C	8.41	1.63	1.52
1	D	70	ILE	CA-C	-8.41	1.42	1.52
1	E	168	ASP	C-O	-8.40	1.13	1.23
1	E	160	VAL	CA-C	-8.39	1.46	1.53
1	F	21	SER	CA-C	-8.31	1.42	1.52
1	E	160	VAL	N-CA	-8.29	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	200	ILE	CA-CB	-8.22	1.43	1.54
1	D	164	ALA	CA-C	-8.21	1.42	1.53
1	B	333	LEU	CA-C	8.20	1.63	1.52
1	B	128	LEU	N-CA	-8.19	1.36	1.46
1	E	162	ILE	CA-C	-8.18	1.42	1.52
1	E	172	LEU	CA-C	-8.13	1.44	1.53
1	D	67	TYR	N-CA	-8.12	1.36	1.46
1	E	67	TYR	N-CA	-8.12	1.36	1.46
1	E	67	TYR	CA-CB	-8.10	1.41	1.53
1	C	164	ALA	CA-C	-8.07	1.42	1.53
1	D	128	LEU	N-CA	-8.04	1.36	1.46
1	F	274	PRO	CA-C	-8.01	1.40	1.52
1	B	167	THR	CA-C	-8.01	1.43	1.52
1	B	67	TYR	CA-CB	-7.97	1.41	1.53
1	E	333	LEU	CA-C	7.97	1.62	1.52
1	E	280	VAL	CA-CB	-7.95	1.45	1.54
1	D	39	VAL	N-CA	-7.95	1.36	1.46
1	C	272	PHE	CA-CB	-7.94	1.40	1.53
1	A	274	PRO	CA-C	-7.94	1.40	1.52
1	B	192	VAL	CA-CB	-7.91	1.44	1.54
1	B	172	LEU	CA-C	-7.91	1.45	1.53
1	E	194	GLU	CA-C	-7.87	1.42	1.52
1	A	160	VAL	CA-C	-7.86	1.46	1.53
1	B	222	SER	CA-C	-7.85	1.42	1.52
1	C	265	ILE	CA-CB	-7.84	1.45	1.54
1	D	272	PHE	CA-CB	-7.83	1.40	1.53
1	D	168	ASP	C-N	-7.83	1.24	1.33
1	E	183	VAL	CA-CB	-7.82	1.47	1.55
1	F	177	PRO	N-CA	7.76	1.57	1.47
1	C	39	VAL	CA-CB	-7.76	1.44	1.54
1	A	262	ILE	CA-C	-7.76	1.43	1.52
1	B	169	ILE	C-N	-7.75	1.23	1.33
1	B	160	VAL	N-CA	-7.74	1.38	1.46
1	E	253	ALA	CA-C	-7.73	1.43	1.52
1	E	167	THR	CA-C	-7.72	1.43	1.52
1	C	193	ASP	CA-C	-7.72	1.43	1.52
1	C	168	ASP	C-N	-7.69	1.24	1.33
1	D	217	VAL	C-O	-7.69	1.15	1.24
1	D	193	ASP	CA-C	-7.67	1.43	1.52
1	E	113	ILE	N-CA	-7.66	1.36	1.46
1	E	169	ILE	C-N	-7.65	1.23	1.33
1	F	217	VAL	C-O	-7.64	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	253	ALA	CA-C	-7.64	1.43	1.52
1	D	200	ILE	CA-CB	-7.63	1.44	1.54
1	D	67	TYR	CA-CB	-7.61	1.42	1.53
1	A	177	PRO	N-CA	7.58	1.56	1.47
1	D	265	ILE	CA-CB	-7.56	1.46	1.54
1	C	67	TYR	CA-CB	-7.55	1.42	1.53
1	C	217	VAL	N-CA	-7.55	1.38	1.46
1	C	116	PRO	CA-C	-7.54	1.43	1.52
1	B	168	ASP	CA-C	-7.53	1.43	1.52
1	B	170	CYS	N-CA	-7.53	1.37	1.46
1	A	39	VAL	N-CA	-7.53	1.37	1.46
1	D	116	PRO	CA-C	-7.52	1.43	1.52
1	C	57	VAL	CA-CB	-7.51	1.43	1.54
1	B	194	GLU	CA-C	-7.50	1.42	1.52
1	E	168	ASP	CA-C	-7.50	1.43	1.52
1	D	273	GLN	CA-C	-7.49	1.45	1.53
1	E	170	CYS	N-CA	-7.49	1.37	1.46
1	B	217	VAL	C-O	-7.48	1.15	1.24
1	D	236	ARG	CA-C	-7.48	1.43	1.52
1	A	36	LYS	C-O	-7.48	1.14	1.23
1	E	71	ARG	CA-C	-7.45	1.43	1.52
1	C	334	PRO	N-CA	7.42	1.58	1.47
1	E	192	VAL	CA-CB	-7.41	1.45	1.54
1	A	272	PHE	CA-CB	-7.40	1.41	1.53
1	B	39	VAL	N-CA	-7.38	1.37	1.46
1	B	113	ILE	N-CA	-7.34	1.37	1.46
1	A	334	PRO	N-CA	7.34	1.58	1.47
1	B	71	ARG	CA-C	-7.34	1.44	1.52
1	C	67	TYR	N-CA	-7.32	1.37	1.46
1	B	67	TYR	N-CA	-7.31	1.37	1.46
1	F	214	ALA	C-O	-7.29	1.15	1.24
1	B	277	GLN	CA-CB	-7.28	1.41	1.53
1	C	236	ARG	CA-C	-7.27	1.44	1.52
1	B	272	PHE	CA-CB	-7.27	1.41	1.53
1	B	183	VAL	CA-CB	-7.24	1.48	1.55
1	C	291	SER	CA-C	7.23	1.62	1.52
1	F	262	ILE	CA-C	-7.23	1.44	1.52
1	C	177	PRO	N-CA	7.22	1.56	1.47
1	C	262	ILE	CA-C	-7.22	1.44	1.52
1	E	168	ASP	C-N	-7.22	1.24	1.33
1	C	167	THR	N-CA	-7.21	1.37	1.46
1	D	222	SER	CA-C	-7.21	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	170	CYS	N-CA	-7.20	1.38	1.46
1	C	128	LEU	N-CA	-7.19	1.37	1.46
1	B	168	ASP	C-N	-7.18	1.24	1.33
1	F	272	PHE	CA-CB	-7.17	1.41	1.53
1	B	39	VAL	CA-CB	-7.17	1.45	1.54
1	F	197	GLN	CA-C	-7.16	1.43	1.52
1	A	169	ILE	C-O	-7.15	1.16	1.23
1	D	39	VAL	CA-CB	-7.14	1.45	1.54
1	E	177	PRO	N-CA	7.11	1.56	1.47
1	B	262	ILE	CA-C	-7.06	1.44	1.52
1	A	127	LEU	CA-C	-7.05	1.43	1.52
1	D	57	VAL	CA-CB	-7.04	1.44	1.54
1	E	272	PHE	CA-CB	-7.01	1.42	1.53
1	D	253	ALA	CA-C	-6.99	1.44	1.52
1	C	113	ILE	N-CA	-6.98	1.37	1.46
1	C	38	VAL	CA-C	-6.97	1.43	1.52
1	F	160	VAL	CA-C	-6.97	1.47	1.53
1	B	250	VAL	N-CA	-6.96	1.38	1.46
1	A	197	GLN	CA-C	-6.96	1.43	1.52
1	C	273	GLN	CA-C	-6.96	1.45	1.53
1	B	127	LEU	CA-C	-6.96	1.43	1.52
1	E	277	GLN	CA-CB	-6.93	1.42	1.53
1	D	79	LEU	CA-C	-6.93	1.43	1.52
1	A	277	GLN	CA-CB	-6.92	1.41	1.53
1	E	127	LEU	CA-C	-6.92	1.43	1.52
1	B	38	VAL	CA-C	-6.92	1.44	1.52
1	D	177	PRO	N-CA	6.90	1.55	1.47
1	B	265	ILE	CA-CB	-6.89	1.46	1.54
1	F	334	PRO	N-CA	6.88	1.57	1.47
1	E	39	VAL	CA-CB	-6.88	1.45	1.54
1	C	253	ALA	CA-C	-6.88	1.44	1.52
1	F	273	GLN	CA-C	-6.88	1.45	1.53
1	D	194	GLU	CA-C	-6.86	1.43	1.52
1	B	334	PRO	N-CA	6.85	1.57	1.47
1	B	177	PRO	N-CA	6.85	1.55	1.47
1	F	280	VAL	CA-C	-6.83	1.44	1.52
1	B	169	ILE	N-CA	-6.83	1.38	1.46
1	E	280	VAL	CA-C	-6.82	1.44	1.52
1	C	286	PHE	CB-CG	-6.81	1.34	1.50
1	A	170	CYS	N-CA	-6.80	1.38	1.46
1	C	79	LEU	CA-C	-6.80	1.43	1.52
1	F	168	ASP	C-O	-6.77	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	154	LEU	CA-CB	-6.77	1.43	1.53
1	C	113	ILE	CA-CB	-6.75	1.46	1.54
1	D	220	GLN	C-O	-6.74	1.15	1.24
1	D	154	LEU	CA-CB	-6.72	1.44	1.53
1	D	190	ASN	CA-C	-6.71	1.44	1.52
1	D	262	ILE	CA-C	-6.70	1.44	1.52
1	E	23	THR	N-CA	-6.70	1.38	1.46
1	E	268	LEU	CA-CB	-6.69	1.42	1.53
1	F	253	ALA	CA-C	-6.66	1.44	1.52
1	E	250	VAL	N-CA	-6.65	1.38	1.46
1	C	192	VAL	CA-CB	-6.63	1.46	1.54
1	D	113	ILE	N-CA	-6.62	1.38	1.46
1	C	220	GLN	C-O	-6.61	1.15	1.24
1	B	268	LEU	CA-CB	-6.59	1.42	1.53
1	F	298	ALA	N-CA	-6.58	1.37	1.46
1	D	167	THR	N-CA	-6.58	1.38	1.46
1	D	286	PHE	CB-CG	-6.58	1.35	1.50
1	C	222	SER	CA-C	-6.57	1.44	1.52
1	B	21	SER	N-CA	-6.57	1.37	1.46
1	F	168	ASP	CA-C	-6.56	1.44	1.52
1	B	167	THR	N-CA	-6.56	1.38	1.46
1	E	334	PRO	N-CA	6.54	1.56	1.47
1	A	253	ALA	CA-C	-6.53	1.44	1.52
1	F	277	GLN	CA-CB	-6.53	1.42	1.53
1	F	222	SER	CA-C	-6.53	1.44	1.52
1	C	39	VAL	N-CA	-6.52	1.38	1.46
1	C	285	VAL	CA-C	6.51	1.60	1.52
1	F	158	ILE	C-O	-6.51	1.16	1.24
1	D	18	LEU	CA-C	-6.49	1.44	1.53
1	F	71	ARG	CA-C	-6.48	1.45	1.52
1	D	168	ASP	C-O	-6.47	1.15	1.23
1	D	334	PRO	N-CA	6.47	1.56	1.47
1	F	128	LEU	N-CA	-6.46	1.38	1.46
1	A	298	ALA	N-CA	-6.44	1.38	1.46
1	E	265	ILE	CA-CB	-6.44	1.47	1.54
1	E	218	LYS	C-O	-6.43	1.16	1.24
1	D	291	SER	CA-C	6.42	1.61	1.52
1	E	261	ILE	CA-C	-6.42	1.45	1.52
1	E	290	GLY	N-CA	6.41	1.55	1.45
1	A	273	GLN	CA-C	-6.40	1.46	1.53
1	C	194	GLU	CA-C	-6.40	1.44	1.52
1	E	169	ILE	N-CA	-6.39	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	SER	N-CA	-6.38	1.37	1.46
1	A	196	LEU	N-CA	-6.38	1.38	1.46
1	B	214	ALA	C-O	-6.37	1.16	1.24
1	B	269	LEU	CA-C	-6.37	1.44	1.52
1	F	159	ILE	CA-CB	-6.37	1.46	1.54
1	F	127	LEU	CA-C	-6.37	1.44	1.52
1	F	67	TYR	CA-C	-6.36	1.44	1.52
1	B	25	VAL	CA-CB	-6.36	1.46	1.54
1	D	111	ALA	CA-C	-6.36	1.44	1.52
1	E	166	THR	C-N	-6.34	1.25	1.33
1	B	166	THR	C-N	-6.33	1.25	1.33
1	A	67	TYR	CA-C	-6.32	1.44	1.52
1	D	23	THR	CA-C	-6.32	1.45	1.52
1	D	214	ALA	C-O	-6.30	1.16	1.24
1	C	41	TYR	CA-CB	-6.30	1.44	1.53
1	D	217	VAL	N-CA	-6.30	1.39	1.46
1	E	21	SER	N-CA	-6.29	1.38	1.46
1	D	113	ILE	CA-CB	-6.28	1.46	1.54
1	A	159	ILE	CA-CB	-6.27	1.46	1.54
1	F	21	SER	N-CA	-6.25	1.37	1.46
1	D	192	VAL	CA-CB	-6.25	1.46	1.54
1	E	166	THR	CA-C	-6.25	1.44	1.52
1	C	190	ASN	CA-C	-6.25	1.44	1.52
1	D	67	TYR	CA-C	-6.24	1.44	1.52
1	F	74	LEU	CA-C	-6.24	1.45	1.52
1	E	262	ILE	CA-C	-6.23	1.45	1.52
1	B	200	ILE	CA-CB	-6.22	1.47	1.54
1	C	36	LYS	C-O	-6.22	1.16	1.23
1	B	79	LEU	CA-C	-6.21	1.44	1.52
1	F	154	LEU	N-CA	-6.21	1.39	1.46
1	E	92	HIS	CA-C	-6.20	1.44	1.52
1	D	285	VAL	CA-C	6.20	1.60	1.52
1	C	182	GLN	CA-CB	-6.18	1.43	1.53
1	E	215	CYS	CA-C	-6.18	1.44	1.52
1	E	193	ASP	C-O	-6.18	1.17	1.24
1	B	23	THR	N-CA	-6.16	1.38	1.46
1	D	169	ILE	C-N	-6.16	1.25	1.33
1	A	168	ASP	CA-C	-6.15	1.45	1.52
1	A	291	SER	CA-C	6.15	1.61	1.52
1	F	67	TYR	N-CA	-6.13	1.38	1.46
1	C	67	TYR	CA-C	-6.13	1.45	1.52
1	A	222	SER	CA-C	-6.12	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	158	ILE	C-O	-6.11	1.17	1.24
1	A	71	ARG	CA-C	-6.11	1.45	1.52
1	E	176	VAL	CA-C	6.09	1.59	1.52
1	E	24	ALA	C-O	6.09	1.30	1.23
1	B	61	ALA	C-O	-6.08	1.17	1.24
1	C	169	ILE	C-N	-6.08	1.25	1.33
1	B	280	VAL	CA-C	-6.08	1.45	1.52
1	F	193	ASP	C-O	-6.08	1.17	1.24
1	A	74	LEU	CA-C	-6.07	1.45	1.52
1	F	36	LYS	C-O	-6.07	1.16	1.23
1	D	41	TYR	CA-CB	-6.06	1.44	1.53
1	D	38	VAL	CA-C	-6.06	1.45	1.52
1	B	37	SER	CA-C	-6.06	1.45	1.52
1	B	286	PHE	CA-C	-6.06	1.45	1.52
1	B	168	ASP	C-O	-6.05	1.16	1.23
1	B	217	VAL	C-N	-6.05	1.26	1.33
1	D	21	SER	N-CA	-6.04	1.38	1.46
1	A	287	ALA	CA-CB	-6.04	1.44	1.53
1	F	209	MET	CA-C	-6.02	1.45	1.52
1	E	158	ILE	N-CA	-6.02	1.39	1.46
1	C	188	ALA	CA-CB	-6.01	1.46	1.53
1	B	290	GLY	N-CA	6.00	1.54	1.45
1	A	209	MET	CA-C	-6.00	1.45	1.52
1	F	200	ILE	C-O	-5.99	1.17	1.24
1	B	154	LEU	CA-CB	-5.99	1.45	1.53
1	E	57	VAL	CA-C	-5.99	1.45	1.52
1	C	249	PRO	CA-C	-5.98	1.43	1.52
1	D	55	TYR	CA-C	-5.97	1.45	1.52
1	E	269	LEU	CA-C	-5.96	1.45	1.52
1	E	268	LEU	CA-C	-5.96	1.44	1.52
1	B	249	PRO	CA-C	-5.96	1.43	1.52
1	C	217	VAL	C-O	-5.96	1.17	1.24
1	F	281	LEU	CA-CB	-5.95	1.43	1.53
1	F	279	THR	N-CA	-5.94	1.38	1.46
1	A	39	VAL	CA-CB	-5.93	1.47	1.54
1	B	261	ILE	CA-C	-5.92	1.45	1.52
1	E	20	THR	CA-C	-5.92	1.44	1.52
1	C	23	THR	CA-C	-5.91	1.45	1.52
1	E	249	PRO	CA-C	-5.90	1.43	1.52
1	A	66	SER	N-CA	5.90	1.53	1.46
1	E	25	VAL	CA-CB	-5.90	1.46	1.54
1	D	166	THR	CA-C	-5.90	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	146	MET	CA-C	5.88	1.60	1.52
1	A	281	LEU	CA-CB	-5.88	1.43	1.53
1	E	61	ALA	C-O	-5.87	1.17	1.24
1	E	160	VAL	CA-CB	-5.87	1.47	1.53
1	E	281	LEU	CA-CB	-5.86	1.43	1.53
1	D	284	ILE	CA-CB	-5.86	1.47	1.54
1	C	127	LEU	CA-C	-5.86	1.45	1.52
1	E	38	VAL	CA-C	-5.84	1.45	1.52
1	E	154	LEU	CA-CB	-5.83	1.45	1.53
1	A	128	LEU	N-CA	-5.83	1.39	1.46
1	F	183	VAL	CA-CB	-5.82	1.49	1.55
1	C	176	VAL	CA-C	5.82	1.59	1.52
1	C	55	TYR	CA-C	-5.81	1.45	1.52
1	C	18	LEU	CA-C	-5.80	1.45	1.53
1	D	249	PRO	CA-C	-5.80	1.43	1.52
1	C	178	GLY	N-CA	5.80	1.52	1.44
1	B	176	VAL	CA-C	5.79	1.58	1.52
1	E	167	THR	N-CA	-5.78	1.39	1.46
1	B	281	LEU	CA-CB	-5.76	1.43	1.53
1	C	172	LEU	CA-C	-5.75	1.47	1.53
1	C	165	GLY	C-O	5.75	1.30	1.24
1	B	166	THR	CA-C	-5.75	1.45	1.52
1	C	223	PHE	CA-C	-5.74	1.45	1.52
1	A	280	VAL	CA-C	-5.74	1.45	1.52
1	D	193	ASP	C-O	-5.74	1.17	1.24
1	B	42	PRO	N-CA	-5.73	1.40	1.47
1	B	116	PRO	CA-C	-5.73	1.45	1.52
1	C	20	THR	CB-CG2	5.73	1.71	1.52
1	E	116	PRO	CA-C	-5.72	1.45	1.52
1	E	296	LEU	CA-C	-5.72	1.45	1.52
1	B	261	ILE	CA-CB	-5.71	1.47	1.54
1	A	154	LEU	N-CA	-5.70	1.39	1.46
1	F	196	LEU	C-O	-5.69	1.17	1.24
1	E	196	LEU	C-O	-5.68	1.17	1.24
1	D	218	LYS	C-O	-5.68	1.17	1.24
1	C	111	ALA	CA-C	-5.68	1.45	1.52
1	E	200	ILE	CA-CB	-5.68	1.47	1.54
1	B	160	VAL	CA-CB	-5.67	1.47	1.53
1	F	196	LEU	N-CA	-5.67	1.39	1.46
1	F	142	SER	C-O	-5.66	1.17	1.23
1	D	280	VAL	CA-C	-5.66	1.46	1.52
1	E	42	PRO	N-CA	-5.66	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	158	ILE	CA-C	-5.66	1.46	1.52
1	D	178	GLY	N-CA	5.66	1.52	1.44
1	C	142	SER	C-O	-5.65	1.17	1.23
1	F	66	SER	N-CA	5.65	1.52	1.46
1	A	113	ILE	CA-CB	-5.64	1.47	1.54
1	A	279	THR	N-CA	-5.61	1.39	1.46
1	C	21	SER	N-CA	-5.60	1.38	1.46
1	E	220	GLN	C-O	-5.60	1.16	1.24
1	C	284	ILE	CA-CB	-5.60	1.47	1.54
1	E	178	GLY	N-CA	5.60	1.52	1.44
1	C	168	ASP	C-O	-5.59	1.16	1.23
1	B	158	ILE	CA-C	-5.59	1.46	1.52
1	A	169	ILE	C-N	-5.58	1.26	1.33
1	C	37	SER	CA-C	-5.58	1.45	1.52
1	D	172	LEU	CA-C	-5.58	1.47	1.53
1	F	291	SER	CA-C	5.58	1.60	1.52
1	E	154	LEU	N-CA	-5.57	1.40	1.46
1	F	113	ILE	CA-CB	-5.56	1.47	1.54
1	D	182	GLN	CA-CB	-5.55	1.44	1.53
1	D	250	VAL	N-CA	-5.55	1.40	1.46
1	A	168	ASP	C-O	-5.54	1.16	1.23
1	B	36	LYS	C-O	-5.54	1.17	1.23
1	E	216	ALA	C-N	-5.54	1.26	1.33
1	D	279	THR	N-CA	-5.53	1.39	1.46
1	E	79	LEU	CA-C	-5.52	1.45	1.52
1	C	166	THR	CA-C	-5.51	1.45	1.52
1	D	166	THR	C-N	-5.51	1.26	1.33
1	B	277	GLN	CD-OE1	5.51	1.34	1.23
1	C	166	THR	C-N	-5.51	1.26	1.33
1	D	71	ARG	CA-C	-5.51	1.46	1.52
1	B	92	HIS	CA-C	-5.50	1.45	1.52
1	E	217	VAL	C-N	-5.49	1.27	1.33
1	B	197	GLN	CA-C	-5.49	1.45	1.52
1	D	223	PHE	CA-C	-5.49	1.46	1.52
1	F	39	VAL	CA-CB	-5.48	1.47	1.54
1	D	57	VAL	CA-C	-5.48	1.45	1.52
1	B	216	ALA	C-N	-5.48	1.26	1.33
1	E	277	GLN	CD-OE1	5.48	1.33	1.23
1	B	296	LEU	CA-C	-5.48	1.46	1.52
1	A	167	THR	N-CA	-5.47	1.39	1.46
1	D	261	ILE	CA-C	-5.47	1.46	1.52
1	F	168	ASP	C-N	-5.47	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	SER	N-CA	5.46	1.53	1.46
1	B	215	CYS	CA-C	-5.46	1.45	1.52
1	D	176	VAL	CA-C	5.45	1.58	1.52
1	F	67	TYR	CB-CG	-5.45	1.39	1.51
1	C	113	ILE	CA-C	5.44	1.59	1.52
1	F	169	ILE	CA-CB	-5.44	1.47	1.54
1	F	68	LEU	CA-C	-5.43	1.46	1.52
1	D	142	SER	C-O	-5.43	1.17	1.24
1	C	217	VAL	C-N	-5.43	1.27	1.33
1	E	261	ILE	CA-CB	-5.42	1.48	1.54
1	F	169	ILE	C-N	-5.42	1.26	1.33
1	D	267	THR	N-CA	-5.40	1.39	1.46
1	E	212	ASN	C-O	-5.40	1.17	1.24
1	A	176	VAL	CA-C	5.40	1.58	1.52
1	E	146	MET	CA-C	5.40	1.60	1.52
1	B	178	GLY	N-CA	5.39	1.52	1.44
1	C	267	THR	N-CA	-5.39	1.39	1.46
1	E	276	TYR	CA-C	-5.39	1.45	1.52
1	B	158	ILE	N-CA	-5.38	1.39	1.46
1	E	37	SER	CA-C	-5.37	1.46	1.52
1	E	192	VAL	C-O	-5.37	1.17	1.24
1	A	265	ILE	CA-CB	-5.37	1.48	1.54
1	B	66	SER	N-CA	5.36	1.52	1.46
1	B	268	LEU	CA-C	-5.35	1.45	1.52
1	C	167	THR	CA-C	-5.35	1.46	1.52
1	B	190	ASN	CA-C	-5.34	1.45	1.52
1	A	182	GLN	CA-CB	-5.34	1.45	1.53
1	B	240	LYS	CA-C	-5.34	1.46	1.52
1	A	197	GLN	CA-CB	-5.34	1.45	1.53
1	D	224	VAL	CA-C	-5.34	1.46	1.52
1	F	62	PHE	N-CA	-5.33	1.39	1.46
1	D	72	TYR	CA-C	-5.33	1.47	1.53
1	D	296	LEU	CA-C	-5.33	1.46	1.52
1	A	168	ASP	C-N	-5.32	1.27	1.33
1	E	209	MET	CA-C	-5.32	1.46	1.52
1	A	217	VAL	N-CA	-5.31	1.40	1.46
1	B	20	THR	CA-C	-5.31	1.45	1.52
1	E	68	LEU	CA-C	-5.30	1.46	1.52
1	D	159	ILE	CA-CB	-5.29	1.47	1.54
1	A	68	LEU	CA-C	-5.28	1.46	1.52
1	B	276	TYR	CA-C	-5.28	1.45	1.52
1	C	247	THR	CA-C	-5.28	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	70	ILE	CA-CB	-5.28	1.47	1.54
1	E	137	THR	C-O	-5.28	1.18	1.24
1	C	62	PHE	N-CA	-5.27	1.39	1.46
1	C	71	ARG	CA-C	-5.27	1.46	1.52
1	E	286	PHE	CA-C	-5.27	1.46	1.52
1	B	209	MET	CA-C	-5.26	1.46	1.52
1	C	250	VAL	N-CA	-5.26	1.40	1.46
1	E	240	LYS	CA-C	-5.26	1.47	1.52
1	C	298	ALA	N-CA	-5.26	1.39	1.46
1	C	279	THR	N-CA	-5.25	1.40	1.46
1	A	249	PRO	C-O	-5.25	1.17	1.24
1	D	298	ALA	N-CA	-5.24	1.39	1.46
1	D	217	VAL	C-N	-5.24	1.27	1.33
1	D	37	SER	CA-C	-5.24	1.45	1.52
1	F	116	PRO	CA-C	-5.23	1.46	1.52
1	D	240	LYS	CA-C	-5.23	1.47	1.52
1	A	67	TYR	CB-CG	-5.22	1.40	1.51
1	C	240	LYS	CA-C	-5.22	1.47	1.52
1	D	280	VAL	CA-CB	-5.21	1.48	1.54
1	A	172	LEU	CA-C	-5.21	1.47	1.53
1	C	26	MET	CA-C	-5.21	1.46	1.52
1	D	20	THR	CB-CG2	5.20	1.69	1.52
1	D	39	VAL	CA-C	-5.20	1.46	1.52
1	D	62	PHE	N-CA	-5.19	1.39	1.46
1	D	165	GLY	C-O	5.19	1.30	1.24
1	D	247	THR	CA-C	-5.19	1.46	1.52
1	E	56	VAL	CA-CB	-5.18	1.46	1.54
1	C	169	ILE	N-CA	-5.17	1.40	1.46
1	B	68	LEU	CA-C	-5.17	1.46	1.52
1	D	66	SER	N-CA	5.17	1.52	1.46
1	E	197	GLN	CA-C	-5.17	1.46	1.52
1	D	216	ALA	C-N	-5.17	1.27	1.33
1	E	252	ILE	CA-CB	-5.17	1.48	1.54
1	A	70	ILE	CA-C	-5.16	1.46	1.52
1	D	42	PRO	N-CA	-5.16	1.40	1.47
1	B	159	ILE	C-N	-5.16	1.26	1.33
1	D	236	ARG	CZ-NH2	5.16	1.40	1.33
1	F	169	ILE	C-O	-5.16	1.18	1.23
1	C	21	SER	CA-C	-5.15	1.46	1.52
1	C	259	PRO	N-CA	-5.15	1.40	1.47
1	F	287	ALA	CA-CB	-5.15	1.45	1.53
1	A	64	MET	CA-CB	-5.15	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	PRO	N-CA	-5.15	1.40	1.47
1	D	73	PRO	N-CA	-5.14	1.40	1.47
1	D	281	LEU	CA-CB	-5.14	1.44	1.53
1	E	190	ASN	CA-C	-5.13	1.46	1.52
1	F	92	HIS	CA-C	-5.13	1.46	1.52
1	D	216	ALA	C-O	-5.13	1.18	1.24
1	C	20	THR	CA-C	-5.12	1.45	1.52
1	C	216	ALA	C-N	-5.12	1.27	1.33
1	A	214	ALA	C-O	-5.12	1.18	1.24
1	F	194	GLU	CA-C	-5.12	1.45	1.52
1	C	280	VAL	CA-CB	-5.12	1.48	1.54
1	E	185	LEU	CA-CB	-5.12	1.44	1.53
1	D	259	PRO	N-CA	-5.11	1.40	1.47
1	C	281	LEU	CA-CB	-5.11	1.44	1.53
1	A	116	PRO	CA-C	-5.11	1.46	1.52
1	E	164	ALA	CA-C	-5.10	1.46	1.53
1	F	284	ILE	CA-CB	-5.09	1.48	1.54
1	A	284	ILE	CA-CB	-5.09	1.48	1.54
1	C	293	ILE	CA-C	5.09	1.59	1.52
1	C	197	GLN	C-N	-5.08	1.27	1.34
1	F	20	THR	CA-C	-5.08	1.45	1.52
1	C	327	LEU	CA-C	-5.08	1.46	1.52
1	D	196	LEU	C-O	-5.08	1.18	1.24
1	C	93	LEU	N-CA	-5.08	1.40	1.46
1	D	92	HIS	CA-C	-5.07	1.46	1.52
1	A	312	VAL	CA-CB	-5.06	1.48	1.54
1	E	159	ILE	C-N	-5.06	1.27	1.33
1	A	62	PHE	N-CA	-5.06	1.39	1.46
1	A	249	PRO	CA-C	-5.05	1.45	1.52
1	A	142	SER	C-O	-5.05	1.17	1.23
1	D	327	LEU	CA-C	-5.05	1.46	1.52
1	B	185	LEU	CA-CB	-5.05	1.45	1.53
1	A	286	PHE	CB-CG	-5.05	1.39	1.50
1	D	93	LEU	N-CA	-5.03	1.40	1.46
1	B	223	PHE	CA-C	-5.03	1.46	1.52
1	E	62	PHE	N-CA	-5.02	1.39	1.46
1	B	57	VAL	CA-CB	-5.02	1.47	1.54
1	C	196	LEU	CA-C	-5.02	1.46	1.52
1	F	176	VAL	CA-C	5.02	1.58	1.52
1	A	67	TYR	N-CA	-5.02	1.40	1.46
1	B	252	ILE	CA-CB	-5.02	1.48	1.54
1	F	277	GLN	CA-C	-5.02	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	127	LEU	CA-C	-5.01	1.46	1.52
1	F	265	ILE	CA-CB	-5.01	1.48	1.54
1	C	70	ILE	CA-CB	-5.01	1.48	1.54
1	C	274	PRO	CA-C	-5.01	1.44	1.52
1	B	128	LEU	CA-C	-5.00	1.46	1.52

All (321) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	147	VAL	CB-CA-C	-10.24	98.86	111.97
1	B	147	VAL	CB-CA-C	-10.07	99.08	111.97
1	D	147	VAL	CB-CA-C	-9.86	99.35	111.97
1	C	147	VAL	CB-CA-C	-9.67	99.72	111.81
1	F	147	VAL	CB-CA-C	-9.29	100.08	111.97
1	A	147	VAL	CB-CA-C	-9.10	100.32	111.97
1	A	17	ASP	N-CA-C	-9.09	91.91	107.99
1	B	128	LEU	N-CA-C	-8.96	101.46	111.14
1	E	128	LEU	N-CA-C	-8.77	101.67	111.14
1	F	146	MET	N-CA-C	-8.58	101.87	111.82
1	F	17	ASP	N-CA-C	-8.46	93.01	107.99
1	C	17	ASP	N-CA-C	-8.36	93.19	107.99
1	B	17	ASP	N-CA-C	-8.21	93.45	107.99
1	A	146	MET	N-CA-C	-8.13	102.39	111.82
1	E	162	ILE	CB-CA-C	-8.12	100.84	110.91
1	D	213	VAL	CB-CA-C	-8.10	101.42	111.87
1	B	161	ASP	CA-C-N	-8.10	111.93	122.37
1	B	161	ASP	C-N-CA	-8.10	111.93	122.37
1	E	214	ALA	N-CA-C	-8.05	102.50	111.28
1	E	161	ASP	CA-C-N	-8.05	111.99	122.37
1	E	161	ASP	C-N-CA	-8.05	111.99	122.37
1	B	214	ALA	N-CA-C	-8.01	102.55	111.28
1	B	162	ILE	CB-CA-C	-7.89	101.12	110.91
1	F	161	ASP	CA-C-N	-7.86	112.54	122.37
1	F	161	ASP	C-N-CA	-7.86	112.54	122.37
1	E	146	MET	N-CA-C	-7.85	102.71	111.82
1	D	17	ASP	N-CA-C	-7.77	94.23	107.99
1	F	128	LEU	N-CA-C	-7.77	102.75	111.14
1	A	128	LEU	N-CA-C	-7.76	102.75	111.14
1	D	128	LEU	N-CA-C	-7.76	102.76	111.07
1	C	213	VAL	CB-CA-C	-7.75	101.88	111.87
1	E	17	ASP	N-CA-C	-7.73	94.31	107.99
1	C	128	LEU	N-CA-C	-7.64	102.88	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ASP	CA-C-N	-7.58	112.60	122.37
1	A	161	ASP	C-N-CA	-7.58	112.60	122.37
1	A	32	LYS	N-CA-C	-7.51	96.97	109.07
1	B	167	THR	N-CA-C	-7.49	97.02	109.07
1	B	146	MET	N-CA-C	-7.46	103.17	111.82
1	E	16	VAL	N-CA-C	-7.46	94.71	107.24
1	E	332	GLU	N-CA-C	7.44	122.42	112.30
1	A	93	LEU	N-CA-C	-7.43	103.12	111.07
1	C	32	LYS	N-CA-C	-7.41	97.13	109.07
1	E	167	THR	N-CA-C	-7.36	97.22	109.07
1	A	214	ALA	N-CA-C	-7.32	103.39	111.36
1	C	159	ILE	CB-CA-C	-7.30	100.28	111.31
1	D	146	MET	N-CA-C	-7.30	103.36	111.82
1	D	332	GLU	N-CA-C	7.27	122.19	112.30
1	F	32	LYS	N-CA-C	-7.26	97.38	109.07
1	B	332	GLU	N-CA-C	7.26	122.17	112.30
1	D	159	ILE	CB-CA-C	-7.25	100.36	111.31
1	D	32	LYS	N-CA-C	-7.18	97.51	109.07
1	F	214	ALA	N-CA-C	-7.17	103.47	111.28
1	A	167	THR	N-CA-C	-7.14	97.57	109.07
1	B	32	LYS	N-CA-C	-7.11	97.62	109.07
1	C	332	GLU	N-CA-C	7.09	121.94	112.30
1	E	127	LEU	CB-CA-C	-7.08	98.81	110.85
1	A	198	ASN	N-CA-C	7.00	119.76	111.71
1	A	159	ILE	CB-CA-C	-6.99	99.69	110.95
1	A	159	ILE	CA-C-N	-6.97	116.33	122.96
1	A	159	ILE	C-N-CA	-6.97	116.33	122.96
1	E	283	ASN	N-CA-C	6.93	122.72	112.94
1	F	332	GLU	N-CA-C	6.93	121.72	112.30
1	E	32	LYS	N-CA-C	-6.91	97.94	109.07
1	E	159	ILE	CB-CA-C	-6.91	100.88	111.31
1	F	159	ILE	CB-CA-C	-6.90	99.83	110.95
1	E	251	LYS	N-CA-C	-6.89	103.46	110.97
1	E	250	VAL	N-CA-C	6.88	117.63	110.62
1	B	283	ASN	N-CA-C	6.83	122.58	112.94
1	C	93	LEU	N-CA-C	-6.83	103.76	111.07
1	F	127	LEU	CB-CA-C	-6.83	99.24	110.85
1	C	146	MET	N-CA-C	-6.83	103.90	111.82
1	B	250	VAL	N-CA-C	6.82	117.58	110.62
1	B	127	LEU	CB-CA-C	-6.80	99.29	110.85
1	B	159	ILE	CB-CA-C	-6.79	101.05	111.31
1	D	127	LEU	CB-CA-C	-6.75	99.58	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	GLU	N-CA-C	6.75	121.48	112.30
1	C	127	LEU	CB-CA-C	-6.74	99.60	110.79
1	C	283	ASN	N-CA-C	6.74	122.45	112.94
1	F	265	ILE	CB-CA-C	-6.73	103.39	111.81
1	F	16	VAL	N-CA-C	-6.71	95.97	107.24
1	F	198	ASN	N-CA-C	6.70	119.42	111.71
1	E	56	VAL	CB-CA-C	-6.69	101.27	110.90
1	F	159	ILE	CA-C-N	-6.67	116.62	122.96
1	F	159	ILE	C-N-CA	-6.67	116.62	122.96
1	A	127	LEU	CB-CA-C	-6.67	99.52	110.85
1	A	157	THR	CA-C-N	-6.66	114.51	123.10
1	A	157	THR	C-N-CA	-6.66	114.51	123.10
1	F	213	VAL	CB-CA-C	-6.64	103.30	111.87
1	B	16	VAL	N-CA-C	-6.63	96.09	107.24
1	A	82	ILE	N-CA-C	-6.61	106.35	112.43
1	C	161	ASP	CA-C-N	-6.59	114.13	122.37
1	C	161	ASP	C-N-CA	-6.59	114.13	122.37
1	F	167	THR	N-CA-C	-6.59	98.46	109.07
1	D	161	ASP	CA-C-N	-6.55	114.19	122.37
1	D	161	ASP	C-N-CA	-6.55	114.19	122.37
1	B	251	LYS	N-CA-C	-6.54	103.03	111.02
1	E	147	VAL	N-CA-C	6.54	116.70	110.42
1	F	93	LEU	N-CA-C	-6.54	104.07	111.07
1	F	157	THR	CA-C-N	-6.52	114.69	123.10
1	F	157	THR	C-N-CA	-6.52	114.69	123.10
1	C	167	THR	N-CA-C	-6.49	98.63	109.07
1	A	211	VAL	CB-CA-C	-6.48	103.28	112.22
1	F	82	ILE	N-CA-C	-6.47	106.48	112.43
1	C	157	THR	CA-C-N	-6.47	114.76	123.10
1	C	157	THR	C-N-CA	-6.47	114.76	123.10
1	D	283	ASN	N-CA-C	6.47	122.06	112.94
1	B	147	VAL	N-CA-C	6.43	116.60	110.42
1	C	251	LYS	N-CA-C	-6.41	103.20	111.02
1	A	283	ASN	N-CA-C	6.40	121.97	112.94
1	C	267	THR	N-CA-C	6.39	118.25	111.28
1	C	14	LEU	N-CA-C	6.38	119.29	108.90
1	B	160	VAL	CB-CA-C	-6.36	104.81	111.23
1	F	211	VAL	CB-CA-C	-6.34	103.47	112.22
1	A	213	VAL	CB-CA-C	-6.33	103.70	111.87
1	A	265	ILE	CB-CA-C	-6.33	103.90	111.81
1	C	258	MET	CA-CB-CG	-6.32	101.47	114.10
1	A	14	LEU	N-CA-C	6.30	119.17	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	MET	CB-CG-SD	6.28	131.54	112.70
1	D	157	THR	CA-C-N	-6.26	115.02	123.10
1	D	157	THR	C-N-CA	-6.26	115.02	123.10
1	E	146	MET	CB-CG-SD	6.25	131.44	112.70
1	D	258	MET	CA-CB-CG	-6.23	101.64	114.10
1	A	146	MET	CB-CG-SD	6.23	131.38	112.70
1	A	251	LYS	N-CA-C	-6.20	103.46	111.02
1	A	252	ILE	N-CA-C	6.19	116.86	110.36
1	D	256	ALA	N-CA-C	-6.19	106.33	114.31
1	F	146	MET	CB-CG-SD	6.18	131.25	112.70
1	F	283	ASN	N-CA-C	6.18	121.65	112.94
1	C	65	ARG	N-CA-C	-6.17	104.66	111.82
1	C	256	ALA	N-CA-C	-6.16	106.36	114.31
1	B	142	SER	N-CA-C	6.16	119.28	110.10
1	D	267	THR	N-CA-C	6.15	117.98	111.28
1	D	14	LEU	N-CA-C	6.14	118.90	108.90
1	B	56	VAL	CB-CA-C	-6.13	102.08	110.90
1	D	251	LYS	N-CA-C	-6.11	103.56	111.02
1	F	89	VAL	CB-CA-C	-6.11	104.18	111.81
1	F	258	MET	CA-CB-CG	-6.11	101.89	114.10
1	C	172	LEU	CA-CB-CG	-6.10	94.94	116.30
1	C	146	MET	CB-CG-SD	6.10	131.00	112.70
1	A	258	MET	CA-CB-CG	-6.07	101.96	114.10
1	D	172	LEU	CA-CB-CG	-6.05	95.13	116.30
1	D	146	MET	CB-CG-SD	6.05	130.84	112.70
1	A	72	TYR	N-CA-C	-6.04	102.44	109.93
1	B	157	THR	CA-C-N	-6.03	115.32	123.10
1	B	157	THR	C-N-CA	-6.03	115.32	123.10
1	C	204	HIS	N-CA-C	-6.00	100.19	109.79
1	F	162	ILE	CB-CA-C	-5.99	103.71	110.96
1	D	216	ALA	CA-C-N	-5.97	112.90	120.60
1	D	216	ALA	C-N-CA	-5.97	112.90	120.60
1	E	213	VAL	CB-CA-C	-5.97	104.17	111.87
1	F	14	LEU	N-CA-C	5.97	118.63	108.90
1	D	89	VAL	CB-CA-C	-5.96	104.35	111.81
1	C	250	VAL	N-CA-C	5.95	116.69	110.62
1	E	157	THR	CA-C-N	-5.95	115.42	123.10
1	E	157	THR	C-N-CA	-5.95	115.42	123.10
1	C	159	ILE	CA-C-N	-5.94	117.32	122.96
1	C	159	ILE	C-N-CA	-5.94	117.32	122.96
1	F	216	ALA	CA-C-N	-5.92	112.96	120.60
1	F	216	ALA	C-N-CA	-5.92	112.96	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	16	VAL	N-CA-C	-5.91	97.30	107.24
1	F	56	VAL	CB-CA-C	-5.91	102.40	110.90
1	F	252	ILE	N-CA-C	5.89	116.55	110.36
1	C	216	ALA	CA-C-N	-5.89	113.01	120.60
1	C	216	ALA	C-N-CA	-5.89	113.01	120.60
1	D	93	LEU	N-CA-C	-5.87	104.79	111.07
1	D	265	ILE	CB-CA-C	-5.87	104.48	111.81
1	D	183	VAL	CB-CA-C	-5.83	103.69	111.80
1	D	204	HIS	N-CA-C	-5.80	100.51	109.79
1	D	167	THR	N-CA-C	-5.80	99.73	109.07
1	B	204	HIS	N-CA-C	-5.79	100.52	109.79
1	D	65	ARG	N-CA-C	-5.79	105.10	111.82
1	E	296	LEU	N-CA-C	-5.79	104.89	111.14
1	A	16	VAL	N-CA-C	-5.78	97.53	107.24
1	E	142	SER	N-CA-C	5.76	118.69	110.10
1	E	69	ASP	N-CA-C	-5.76	99.13	108.41
1	E	183	VAL	CB-CA-C	-5.76	103.80	111.80
1	E	216	ALA	CA-C-N	-5.72	111.68	121.97
1	E	216	ALA	C-N-CA	-5.72	111.68	121.97
1	F	251	LYS	N-CA-C	-5.71	104.06	111.02
1	A	108	GLU	N-CA-C	-5.70	99.43	108.73
1	A	216	ALA	CA-C-N	-5.70	113.25	120.60
1	A	216	ALA	C-N-CA	-5.70	113.25	120.60
1	C	89	VAL	CB-CA-C	-5.69	104.70	111.81
1	A	89	VAL	CB-CA-C	-5.68	104.70	111.81
1	C	169	ILE	N-CA-C	-5.68	100.49	108.27
1	A	102	GLU	CA-C-N	-5.67	112.75	119.84
1	A	102	GLU	C-N-CA	-5.67	112.75	119.84
1	B	213	VAL	CB-CA-C	-5.67	104.55	111.87
1	D	50	LEU	CB-CA-C	-5.67	101.38	110.79
1	B	89	VAL	N-CA-C	-5.67	104.80	110.30
1	E	220	GLN	N-CA-C	5.65	119.43	112.54
1	E	160	VAL	CB-CA-C	-5.64	105.53	111.23
1	D	159	ILE	CA-C-N	-5.63	117.61	122.96
1	D	159	ILE	C-N-CA	-5.63	117.61	122.96
1	D	102	GLU	CA-C-N	-5.63	112.80	119.84
1	D	102	GLU	C-N-CA	-5.63	112.80	119.84
1	E	204	HIS	N-CA-C	-5.63	100.79	109.79
1	B	220	GLN	N-CA-C	5.62	119.40	112.54
1	D	195	ARG	CG-CD-NE	-5.61	99.65	112.00
1	B	258	MET	CA-CB-CG	-5.61	102.89	114.10
1	F	281	LEU	N-CA-C	5.60	118.92	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	102	GLU	CA-C-N	-5.60	112.84	119.84
1	F	102	GLU	C-N-CA	-5.60	112.84	119.84
1	D	200	ILE	N-CA-C	-5.60	106.25	111.45
1	E	50	LEU	CB-CA-C	-5.59	101.17	110.68
1	A	113	ILE	N-CA-C	5.59	116.35	108.36
1	C	220	GLN	N-CA-C	5.58	119.35	112.54
1	A	222	SER	CB-CA-C	-5.58	101.48	109.84
1	D	250	VAL	N-CA-C	5.57	116.30	110.62
1	C	102	GLU	CA-C-N	-5.56	112.89	119.84
1	C	102	GLU	C-N-CA	-5.56	112.89	119.84
1	C	265	ILE	CB-CA-C	-5.56	104.86	111.81
1	E	258	MET	CA-CB-CG	-5.56	102.99	114.10
1	E	65	ARG	N-CA-C	-5.54	105.39	111.82
1	B	216	ALA	CA-C-N	-5.53	112.01	121.97
1	B	216	ALA	C-N-CA	-5.53	112.01	121.97
1	B	50	LEU	CB-CA-C	-5.53	101.28	110.68
1	B	183	VAL	CB-CA-C	-5.51	104.14	111.80
1	F	195	ARG	CG-CD-NE	-5.49	99.93	112.00
1	B	223	PHE	CA-C-O	-5.48	115.55	121.36
1	D	220	GLN	N-CA-C	5.48	119.22	112.54
1	F	220	GLN	N-CA-C	5.48	119.22	112.54
1	C	183	VAL	CB-CA-C	-5.47	104.19	111.80
1	A	172	LEU	CA-CB-CG	-5.45	97.24	116.30
1	B	65	ARG	N-CA-C	-5.45	105.50	111.82
1	A	220	GLN	N-CA-C	5.43	119.16	112.54
1	E	102	GLU	CA-C-N	-5.42	113.07	119.84
1	E	102	GLU	C-N-CA	-5.42	113.07	119.84
1	B	14	LEU	N-CA-C	5.41	117.72	108.90
1	B	222	SER	CB-CA-C	-5.39	101.75	109.84
1	F	256	ALA	N-CA-C	-5.39	107.36	114.31
1	A	162	ILE	CB-CA-C	-5.39	104.23	110.91
1	F	172	LEU	CA-CB-CG	-5.38	97.47	116.30
1	E	223	PHE	CA-C-O	-5.38	115.66	121.36
1	E	194	GLU	N-CA-C	-5.37	104.83	111.33
1	F	183	VAL	CB-CA-C	-5.37	104.33	111.80
1	A	315	VAL	CB-CA-C	-5.34	102.52	111.29
1	E	195	ARG	CG-CD-NE	-5.34	100.25	112.00
1	F	108	GLU	N-CA-C	-5.33	99.08	108.20
1	F	72	TYR	N-CA-C	-5.33	103.32	109.93
1	B	198	ASN	N-CA-C	5.32	117.83	111.71
1	C	50	LEU	CB-CA-C	-5.32	101.64	110.68
1	C	72	TYR	N-CA-C	-5.32	103.34	109.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	195	ARG	CG-CD-NE	-5.31	100.33	112.00
1	E	256	ALA	N-CA-C	-5.30	107.47	114.31
1	A	56	VAL	CB-CA-C	-5.30	103.27	110.90
1	C	272	PHE	N-CA-C	5.30	117.53	110.53
1	F	315	VAL	CB-CA-C	-5.30	102.60	111.29
1	B	252	ILE	N-CA-C	5.30	116.66	110.62
1	A	166	THR	CA-C-N	-5.29	115.69	123.00
1	A	166	THR	C-N-CA	-5.29	115.69	123.00
1	E	315	VAL	CB-CA-C	-5.29	102.62	111.29
1	E	14	LEU	N-CA-C	5.28	117.51	108.90
1	F	72	TYR	CA-C-N	-5.27	113.25	119.84
1	F	72	TYR	C-N-CA	-5.27	113.25	119.84
1	A	247	THR	N-CA-C	-5.27	105.45	111.14
1	C	268	LEU	CB-CA-C	-5.26	100.56	110.67
1	D	162	ILE	CB-CA-C	-5.26	104.59	110.96
1	A	195	ARG	CG-CD-NE	-5.26	100.43	112.00
1	C	148	GLY	N-CA-C	-5.26	106.42	112.73
1	B	257	LEU	CB-CA-C	-5.25	102.64	110.88
1	C	166	THR	CA-C-N	-5.25	115.76	123.00
1	C	166	THR	C-N-CA	-5.25	115.76	123.00
1	B	296	LEU	N-CA-C	-5.24	105.48	111.14
1	D	269	LEU	CB-CG-CD2	-5.23	95.01	110.70
1	B	315	VAL	CB-CA-C	-5.22	102.72	111.29
1	B	69	ASP	N-CA-C	-5.22	100.01	108.41
1	A	272	PHE	N-CA-C	5.21	117.41	110.53
1	C	315	VAL	CB-CA-C	-5.21	102.75	111.29
1	D	268	LEU	CB-CA-C	-5.20	100.68	110.67
1	E	257	LEU	CB-CA-C	-5.20	102.72	110.88
1	E	15	GLY	CA-C-O	5.20	125.28	120.81
1	F	247	THR	N-CA-C	-5.20	105.53	111.14
1	B	267	THR	N-CA-C	5.20	116.94	111.28
1	F	268	LEU	CB-CA-C	-5.20	100.69	110.67
1	F	269	LEU	CB-CG-CD2	-5.20	95.11	110.70
1	C	269	LEU	CB-CG-CD2	-5.19	95.14	110.70
1	A	269	LEU	CB-CG-CD2	-5.17	95.18	110.70
1	A	268	LEU	CB-CA-C	-5.17	100.75	110.67
1	D	89	VAL	N-CA-CB	5.17	116.25	110.62
1	C	16	VAL	N-CA-C	-5.17	98.56	107.24
1	D	166	THR	CA-C-N	-5.16	115.88	123.00
1	D	166	THR	C-N-CA	-5.16	115.88	123.00
1	F	166	THR	CA-C-N	-5.16	115.88	123.00
1	F	166	THR	C-N-CA	-5.16	115.88	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	222	SER	CA-C-N	-5.15	113.93	122.11
1	F	222	SER	C-N-CA	-5.15	113.93	122.11
1	C	214	ALA	N-CA-C	-5.14	105.75	111.36
1	F	50	LEU	CB-CA-C	-5.14	101.94	110.68
1	F	265	ILE	N-CA-C	5.12	115.27	110.30
1	D	315	VAL	CB-CA-C	-5.12	102.89	111.29
1	F	272	PHE	N-CA-C	5.12	117.29	110.53
1	A	256	ALA	N-CA-C	-5.12	107.71	114.31
1	A	50	LEU	CB-CA-C	-5.12	101.98	110.68
1	C	200	ILE	N-CA-C	-5.11	106.70	111.45
1	F	222	SER	CB-CA-C	-5.11	102.17	109.84
1	B	172	LEU	CA-CB-CG	-5.10	98.44	116.30
1	D	296	LEU	N-CA-C	-5.10	105.63	111.14
1	B	102	GLU	CA-C-N	-5.09	113.47	119.84
1	B	102	GLU	C-N-CA	-5.09	113.47	119.84
1	A	162	ILE	N-CA-CB	5.09	116.27	110.72
1	C	170	CYS	N-CA-CB	-5.09	102.47	110.77
1	A	281	LEU	N-CA-C	5.08	118.26	111.75
1	E	172	LEU	CA-CB-CG	-5.08	98.53	116.30
1	C	127	LEU	CA-CB-CG	-5.08	98.53	116.30
1	D	272	PHE	N-CA-C	5.07	117.22	110.53
1	D	281	LEU	N-CA-C	5.06	118.23	111.75
1	A	222	SER	CA-C-N	-5.06	114.07	122.11
1	A	222	SER	C-N-CA	-5.06	114.07	122.11
1	A	250	VAL	N-CA-C	5.05	115.77	110.62
1	A	200	ILE	N-CA-C	-5.05	106.15	110.74
1	E	198	ASN	N-CA-C	5.05	117.51	111.71
1	B	195	ARG	CG-CD-NE	-5.04	100.91	112.00
1	F	250	VAL	N-CA-C	5.04	115.76	110.62
1	A	267	THR	N-CA-C	5.03	116.76	111.28
1	E	258	MET	N-CA-C	5.03	120.92	109.81
1	E	275	GLU	N-CA-C	5.02	118.87	112.34
1	D	127	LEU	CA-CB-CG	-5.02	98.74	116.30
1	A	204	HIS	N-CA-C	-5.01	101.77	109.79
1	C	108	GLU	N-CA-C	-5.01	100.57	108.73
1	B	15	GLY	CA-C-O	5.00	125.11	120.81

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	A	177	PRO	Peptide
1	A	178	GLY	Peptide
1	A	333	LEU	Peptide
1	B	174	GLY	Peptide
1	B	177	PRO	Peptide
1	B	178	GLY	Peptide
1	B	209	MET	Peptide
1	C	174	GLY	Peptide
1	C	178	GLY	Peptide
1	C	209	MET	Peptide
1	C	31	LYS	Peptide
1	D	174	GLY	Peptide
1	D	178	GLY	Peptide
1	D	209	MET	Peptide
1	D	31	LYS	Peptide
1	E	174	GLY	Peptide
1	E	177	PRO	Peptide
1	E	209	MET	Peptide
1	F	174	GLY	Peptide
1	F	333	LEU	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	A	2472	0	2524	123	0
1	B	2472	0	2524	106	0
1	C	2472	0	2524	117	0
1	D	2472	0	2524	108	0
1	E	2472	0	2524	103	0
1	F	2472	0	2524	122	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	27	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	12	1	0
3	C	27	0	12	2	0
3	D	27	0	12	3	0
3	E	27	0	12	1	0
3	F	27	0	12	2	0
All	All	15000	0	15216	639	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 21.

All (639) 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:D:332:GLU:C	1:D:333:LEU:HD12	1.99	0.88
1:E:87:ILE:HG23	1:E:130:MET:HE1	1.55	0.88
1:A:49:LYS:NZ	1:C:149:TYR:OH	2.07	0.88
1:C:332:GLU:C	1:C:333:LEU:HD12	1.98	0.87
1:B:87:ILE:HG23	1:B:130:MET:HE1	1.56	0.87
1:D:149:TYR:OH	1:F:49:LYS:NZ	2.07	0.87
1:F:87:ILE:HG23	1:F:130:MET:HE1	1.58	0.85
1:A:87:ILE:HG23	1:A:130:MET:HE1	1.58	0.84
1:D:87:ILE:HG23	1:D:130:MET:HE1	1.60	0.84
1:A:149:TYR:OH	1:B:49:LYS:NZ	2.11	0.83
1:C:87:ILE:HG23	1:C:130:MET:HE1	1.60	0.83
1:F:332:GLU:C	1:F:333:LEU:HD12	2.04	0.83
1:A:332:GLU:C	1:A:333:LEU:HD12	2.04	0.81
1:E:49:LYS:NZ	1:F:149:TYR:OH	2.13	0.81
1:B:332:GLU:C	1:B:333:LEU:HD12	2.07	0.79
1:E:332:GLU:C	1:E:333:LEU:HD12	2.09	0.78
1:F:258:MET:SD	1:F:296:LEU:CD1	2.72	0.77
1:D:325:GLY:O	1:D:326:ALA:C	2.27	0.77
1:A:258:MET:SD	1:A:296:LEU:CD1	2.73	0.77
1:F:325:GLY:O	1:F:326:ALA:C	2.28	0.76
1:C:141:VAL:HG23	1:C:146:MET:HE3	1.68	0.76
1:C:325:GLY:O	1:C:326:ALA:C	2.28	0.76
1:C:82:ILE:HG22	1:C:82:ILE:O	1.86	0.76
1:D:141:VAL:HG23	1:D:146:MET:HE3	1.67	0.75
1:D:258:MET:SD	1:D:296:LEU:CD1	2.75	0.75
1:B:82:ILE:O	1:B:82:ILE:HG22	1.86	0.75
1:C:258:MET:SD	1:C:296:LEU:CD1	2.75	0.75
1:B:325:GLY:O	1:B:326:ALA:C	2.29	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258:MET:SD	1:E:296:LEU:CD1	2.75	0.74
1:A:325:GLY:O	1:A:326:ALA:C	2.30	0.74
1:D:82:ILE:HG22	1:D:82:ILE:O	1.86	0.74
1:B:258:MET:SD	1:B:296:LEU:CD1	2.75	0.73
1:F:141:VAL:HG23	1:F:146:MET:HE3	1.69	0.73
1:E:82:ILE:O	1:E:82:ILE:HG22	1.86	0.73
1:B:141:VAL:HG23	1:B:146:MET:HE3	1.72	0.72
1:C:332:GLU:O	1:C:333:LEU:HD12	1.89	0.72
1:A:141:VAL:HG23	1:A:146:MET:HE3	1.70	0.72
1:E:141:VAL:HG23	1:E:146:MET:HE3	1.71	0.72
1:A:82:ILE:HG22	1:A:82:ILE:O	1.88	0.72
1:F:82:ILE:HG22	1:F:82:ILE:O	1.88	0.72
1:C:159:ILE:HG22	1:C:160:VAL:N	2.05	0.72
1:F:112:VAL:HB	1:F:326:ALA:HB1	1.72	0.71
1:D:332:GLU:O	1:D:333:LEU:HD12	1.90	0.71
1:E:325:GLY:O	1:E:326:ALA:C	2.28	0.71
1:A:236:ARG:NH1	1:A:239:GLY:O	2.24	0.70
1:B:332:GLU:O	1:B:333:LEU:HD12	1.92	0.69
1:D:112:VAL:HB	1:D:326:ALA:HB1	1.74	0.69
1:E:224:VAL:HG12	1:E:255:GLU:HG3	1.73	0.69
1:F:332:GLU:O	1:F:333:LEU:HD12	1.92	0.69
1:A:332:GLU:O	1:A:333:LEU:HD12	1.91	0.69
1:B:236:ARG:NH1	1:B:239:GLY:O	2.26	0.69
1:F:236:ARG:NH1	1:F:239:GLY:O	2.25	0.69
1:E:332:GLU:O	1:E:333:LEU:HD12	1.92	0.68
1:F:224:VAL:HG12	1:F:255:GLU:HG3	1.75	0.68
1:D:224:VAL:HG12	1:D:255:GLU:HG3	1.75	0.68
1:D:159:ILE:HG22	1:D:160:VAL:N	2.06	0.68
1:A:112:VAL:HB	1:A:326:ALA:HB1	1.74	0.68
1:A:159:ILE:HG22	1:A:160:VAL:N	2.08	0.68
1:B:224:VAL:HG12	1:B:255:GLU:HG3	1.74	0.68
1:E:236:ARG:NH1	1:E:239:GLY:O	2.26	0.68
1:A:224:VAL:HG12	1:A:255:GLU:HG3	1.75	0.67
1:C:224:VAL:HG12	1:C:255:GLU:HG3	1.75	0.67
1:F:325:GLY:O	1:F:327:LEU:N	2.27	0.67
1:E:113:ILE:HD13	1:E:127:LEU:HD22	1.76	0.67
1:B:113:ILE:HD13	1:B:127:LEU:HD22	1.76	0.67
1:A:325:GLY:O	1:A:327:LEU:N	2.29	0.66
1:D:325:GLY:O	1:D:327:LEU:N	2.28	0.66
1:C:325:GLY:O	1:C:327:LEU:N	2.28	0.66
1:A:113:ILE:HD13	1:A:127:LEU:HD22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:VAL:HB	1:C:326:ALA:HB1	1.77	0.66
1:E:325:GLY:O	1:E:327:LEU:N	2.29	0.66
1:E:191:TYR:C	1:E:191:TYR:CD2	2.74	0.65
1:E:112:VAL:HB	1:E:326:ALA:HB1	1.78	0.65
1:F:113:ILE:HD13	1:F:127:LEU:HD22	1.77	0.65
1:F:159:ILE:HG22	1:F:160:VAL:N	2.10	0.65
1:D:18:LEU:HD12	1:D:23:THR:OG1	1.97	0.65
1:D:191:TYR:C	1:D:191:TYR:CD2	2.73	0.65
1:B:191:TYR:C	1:B:191:TYR:CD2	2.75	0.65
1:E:18:LEU:HD12	1:E:23:THR:OG1	1.97	0.64
1:F:18:LEU:HD12	1:F:23:THR:OG1	1.97	0.64
1:B:18:LEU:HD12	1:B:23:THR:OG1	1.98	0.64
1:B:325:GLY:O	1:B:327:LEU:N	2.30	0.64
1:F:223:PHE:HE1	1:F:251:LYS:HG3	1.62	0.64
1:A:223:PHE:HE1	1:A:251:LYS:HG3	1.63	0.64
1:C:191:TYR:C	1:C:191:TYR:CD2	2.74	0.64
1:A:18:LEU:HD12	1:A:23:THR:OG1	1.98	0.64
1:C:236:ARG:NH1	1:C:239:GLY:O	2.31	0.64
1:B:112:VAL:HB	1:B:326:ALA:HB1	1.79	0.63
1:C:223:PHE:HE1	1:C:251:LYS:HG3	1.64	0.63
1:C:18:LEU:HD12	1:C:23:THR:OG1	1.98	0.63
1:D:236:ARG:NH1	1:D:239:GLY:O	2.31	0.63
1:B:159:ILE:HG22	1:B:160:VAL:N	2.14	0.62
1:E:108:GLU:HG2	1:E:136:HIS:NE2	2.14	0.62
1:C:188:ALA:O	1:C:189:GLY:C	2.43	0.62
1:F:191:TYR:C	1:F:191:TYR:CD2	2.77	0.62
1:A:191:TYR:C	1:A:191:TYR:CD2	2.78	0.62
1:C:113:ILE:HD13	1:C:127:LEU:HD22	1.82	0.62
1:D:223:PHE:HE1	1:D:251:LYS:HG3	1.64	0.61
1:D:141:VAL:CG2	1:D:146:MET:HE3	2.31	0.61
1:D:113:ILE:HD13	1:D:127:LEU:HD22	1.82	0.61
1:C:216:ALA:O	1:C:217:VAL:C	2.40	0.61
1:D:188:ALA:O	1:D:189:GLY:C	2.42	0.61
1:E:159:ILE:HG22	1:E:160:VAL:N	2.14	0.60
1:F:108:GLU:HG2	1:F:136:HIS:NE2	2.16	0.60
1:A:300:VAL:O	1:A:301:LYS:C	2.44	0.60
1:B:108:GLU:HG2	1:B:136:HIS:NE2	2.14	0.60
1:C:141:VAL:CG2	1:C:146:MET:HE3	2.31	0.60
1:C:20:THR:O	1:C:20:THR:OG1	2.18	0.60
1:E:223:PHE:HE1	1:E:251:LYS:HG3	1.67	0.60
1:F:141:VAL:CG2	1:F:146:MET:HE3	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:THR:O	1:F:20:THR:OG1	2.19	0.60
1:F:188:ALA:O	1:F:189:GLY:C	2.45	0.60
1:C:323:CYS:O	1:C:324:ARG:C	2.45	0.60
1:B:223:PHE:HE1	1:B:251:LYS:HG3	1.67	0.59
1:A:108:GLU:HG2	1:A:136:HIS:NE2	2.16	0.59
1:A:188:ALA:O	1:A:189:GLY:C	2.44	0.59
1:D:108:GLU:HG2	1:D:136:HIS:NE2	2.17	0.59
1:A:53:ARG:HB2	1:A:54:PRO:HD2	1.84	0.59
1:A:141:VAL:CG2	1:A:146:MET:HE3	2.32	0.59
1:B:20:THR:O	1:B:20:THR:OG1	2.18	0.59
1:F:300:VAL:O	1:F:301:LYS:C	2.45	0.59
1:A:20:THR:O	1:A:20:THR:OG1	2.19	0.59
1:C:53:ARG:HB2	1:C:54:PRO:HD2	1.84	0.59
1:D:323:CYS:O	1:D:324:ARG:C	2.45	0.59
1:F:146:MET:HG3	1:F:326:ALA:H	1.68	0.59
1:B:188:ALA:O	1:B:189:GLY:C	2.46	0.58
1:D:82:ILE:O	1:D:82:ILE:CG2	2.51	0.58
1:C:108:GLU:HG2	1:C:136:HIS:NE2	2.17	0.58
1:D:53:ARG:HB2	1:D:54:PRO:HD2	1.84	0.58
1:B:82:ILE:O	1:B:82:ILE:CG2	2.52	0.58
1:E:141:VAL:CG2	1:E:146:MET:HE3	2.34	0.58
1:F:218:LYS:HE2	3:F:402:ADP:N3	2.18	0.57
1:A:218:LYS:HE2	3:A:402:ADP:N3	2.19	0.57
1:C:82:ILE:O	1:C:82:ILE:CG2	2.51	0.57
1:D:20:THR:HG21	1:D:165:GLY:HA3	1.87	0.57
1:B:53:ARG:HB2	1:B:54:PRO:HD2	1.86	0.57
1:B:214:ALA:O	1:B:215:CYS:C	2.46	0.57
1:F:53:ARG:HB2	1:F:54:PRO:HD2	1.85	0.57
1:A:146:MET:HG3	1:A:326:ALA:H	1.69	0.57
1:E:147:VAL:HG12	1:E:148:GLY:N	2.20	0.57
1:C:20:THR:HG21	1:C:165:GLY:HA3	1.86	0.57
1:F:82:ILE:O	1:F:82:ILE:CG2	2.53	0.56
1:B:141:VAL:CG2	1:B:146:MET:HE3	2.35	0.56
1:E:188:ALA:O	1:E:189:GLY:C	2.48	0.56
1:F:42:PRO:HA	1:F:68:LEU:HD23	1.86	0.56
1:A:218:LYS:O	1:A:219:GLU:C	2.47	0.56
1:E:82:ILE:O	1:E:82:ILE:CG2	2.52	0.56
1:A:323:CYS:O	1:A:324:ARG:C	2.48	0.56
1:B:157:THR:HB	1:B:172:LEU:HB2	1.88	0.56
1:E:265:ILE:O	1:E:266:GLU:C	2.48	0.56
1:A:82:ILE:O	1:A:82:ILE:CG2	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:ARG:HB2	1:E:54:PRO:HD2	1.87	0.56
1:E:214:ALA:O	1:E:215:CYS:C	2.46	0.56
1:A:42:PRO:HA	1:A:68:LEU:HD23	1.88	0.56
1:D:73:PRO:HD2	1:D:74:LEU:H	1.71	0.56
1:E:89:VAL:O	1:E:90:ALA:C	2.45	0.56
1:F:323:CYS:O	1:F:324:ARG:C	2.49	0.56
1:E:73:PRO:HD2	1:E:74:LEU:H	1.70	0.55
1:C:73:PRO:HD2	1:C:74:LEU:H	1.71	0.55
1:B:216:ALA:O	1:B:217:VAL:C	2.47	0.55
1:A:239:GLY:HA2	1:C:277:GLN:OE1	2.06	0.55
1:B:147:VAL:HG12	1:B:148:GLY:N	2.20	0.55
1:C:157:THR:HB	1:C:172:LEU:HB2	1.89	0.55
1:E:157:THR:HB	1:E:172:LEU:HB2	1.88	0.55
1:A:216:ALA:O	1:A:217:VAL:C	2.46	0.55
1:C:332:GLU:C	1:C:333:LEU:CD1	2.78	0.55
1:D:157:THR:HB	1:D:172:LEU:HB2	1.89	0.55
1:D:277:GLN:OE1	1:F:239:GLY:HA2	2.07	0.55
1:E:102:GLU:HG3	1:E:102:GLU:O	2.07	0.55
1:F:265:ILE:O	1:F:266:GLU:C	2.49	0.55
1:E:323:CYS:O	1:E:324:ARG:C	2.50	0.55
1:F:218:LYS:O	1:F:219:GLU:C	2.47	0.55
1:D:102:GLU:O	1:D:102:GLU:HG3	2.08	0.54
1:D:265:ILE:O	1:D:266:GLU:C	2.49	0.54
1:B:300:VAL:O	1:B:301:LYS:C	2.50	0.54
1:C:265:ILE:O	1:C:266:GLU:C	2.48	0.54
1:F:102:GLU:O	1:F:102:GLU:HG3	2.08	0.54
1:C:288:GLY:O	1:C:289:GLY:C	2.50	0.54
1:F:157:THR:HB	1:F:172:LEU:HB2	1.89	0.54
1:D:146:MET:HG3	1:D:326:ALA:H	1.73	0.54
1:A:265:ILE:O	1:A:266:GLU:C	2.49	0.54
1:B:73:PRO:HD2	1:B:74:LEU:H	1.72	0.54
1:B:218:LYS:O	1:B:219:GLU:C	2.50	0.54
1:C:300:VAL:O	1:C:301:LYS:C	2.50	0.54
1:A:157:THR:HB	1:A:172:LEU:HB2	1.90	0.54
1:E:49:LYS:HZ1	1:F:333:LEU:CD1	2.21	0.54
1:E:20:THR:O	1:E:20:THR:OG1	2.18	0.53
1:E:300:VAL:O	1:E:301:LYS:C	2.51	0.53
1:C:14:LEU:HD23	1:C:27:SER:HA	1.91	0.53
1:C:146:MET:HG3	1:C:326:ALA:H	1.73	0.53
1:E:42:PRO:HA	1:E:68:LEU:HD23	1.89	0.53
1:A:102:GLU:O	1:A:102:GLU:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:PRO:HA	1:B:68:LEU:HD23	1.91	0.53
1:B:102:GLU:HG3	1:B:102:GLU:O	2.07	0.53
1:B:323:CYS:O	1:B:324:ARG:C	2.50	0.53
1:F:223:PHE:CD1	1:F:223:PHE:C	2.87	0.53
1:A:14:LEU:HD23	1:A:27:SER:HA	1.91	0.53
1:D:20:THR:O	1:D:20:THR:OG1	2.18	0.53
1:D:300:VAL:O	1:D:301:LYS:C	2.51	0.53
1:C:102:GLU:O	1:C:102:GLU:HG3	2.07	0.53
1:D:288:GLY:O	1:D:289:GLY:C	2.50	0.53
1:B:14:LEU:HD23	1:B:27:SER:HA	1.91	0.53
1:F:31:LYS:HE3	1:F:102:GLU:HG2	1.91	0.52
1:B:265:ILE:O	1:B:266:GLU:C	2.49	0.52
1:F:89:VAL:O	1:F:90:ALA:C	2.50	0.52
1:D:31:LYS:HE3	1:D:102:GLU:HG2	1.92	0.52
1:E:218:LYS:O	1:E:219:GLU:C	2.50	0.52
1:A:277:GLN:OE1	1:B:239:GLY:HA2	2.09	0.52
1:D:14:LEU:HD23	1:D:27:SER:HA	1.92	0.52
1:B:218:LYS:HE2	3:B:402:ADP:N3	2.25	0.52
1:C:305:ARG:N	1:C:306:PRO:CD	2.73	0.52
1:E:189:GLY:O	1:E:190:ASN:C	2.51	0.52
1:B:89:VAL:O	1:B:90:ALA:C	2.47	0.51
1:B:326:ALA:O	1:B:329:LEU:HB3	2.10	0.51
1:C:182:GLN:O	1:C:183:VAL:HG23	2.09	0.51
1:D:216:ALA:O	1:D:217:VAL:C	2.42	0.51
1:A:300:VAL:O	1:A:303:LYS:N	2.43	0.51
1:E:288:GLY:O	1:E:289:GLY:C	2.52	0.51
1:B:22:HIS:HB3	1:B:34:LEU:HD11	1.92	0.51
1:E:73:PRO:CD	1:E:74:LEU:H	2.23	0.51
1:E:14:LEU:HD23	1:E:27:SER:HA	1.91	0.51
1:E:31:LYS:HE3	1:E:102:GLU:HG2	1.92	0.51
1:F:160:VAL:HG13	1:F:169:ILE:HG12	1.92	0.51
1:A:31:LYS:HE3	1:A:102:GLU:HG2	1.91	0.51
1:A:288:GLY:O	1:A:289:GLY:C	2.54	0.51
1:C:218:LYS:O	1:C:219:GLU:C	2.52	0.51
1:D:182:GLN:O	1:D:183:VAL:HG23	2.10	0.51
1:E:22:HIS:HB3	1:E:34:LEU:HD11	1.92	0.51
1:C:31:LYS:HE3	1:C:102:GLU:HG2	1.92	0.51
1:E:239:GLY:HA2	1:F:277:GLN:OE1	2.11	0.51
1:A:223:PHE:CD1	1:A:223:PHE:C	2.88	0.50
1:B:31:LYS:HE3	1:B:102:GLU:HG2	1.91	0.50
1:D:305:ARG:N	1:D:306:PRO:CD	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:LEU:HD23	1:F:27:SER:HA	1.92	0.50
1:E:188:ALA:HA	1:E:257:LEU:HD21	1.93	0.50
1:F:214:ALA:O	1:F:215:CYS:C	2.52	0.50
1:F:332:GLU:C	1:F:333:LEU:CD1	2.83	0.50
1:D:42:PRO:HA	1:D:68:LEU:HD23	1.93	0.50
1:D:332:GLU:C	1:D:333:LEU:CD1	2.78	0.50
1:E:218:LYS:HE2	3:E:402:ADP:N3	2.27	0.50
1:F:216:ALA:O	1:F:217:VAL:C	2.47	0.50
1:E:326:ALA:O	1:E:329:LEU:HB3	2.10	0.50
1:A:333:LEU:CD1	1:B:49:LYS:HZ1	2.24	0.50
1:B:15:GLY:O	1:B:25:VAL:HA	2.11	0.50
1:F:258:MET:SD	1:F:296:LEU:HD12	2.51	0.50
1:A:89:VAL:O	1:A:90:ALA:C	2.51	0.50
1:A:326:ALA:O	1:A:329:LEU:HB3	2.11	0.50
1:B:288:GLY:O	1:B:289:GLY:C	2.51	0.50
1:D:218:LYS:O	1:D:219:GLU:C	2.51	0.50
1:C:159:ILE:CG2	1:C:160:VAL:N	2.75	0.50
1:B:73:PRO:CD	1:B:74:LEU:H	2.25	0.50
1:B:300:VAL:O	1:B:303:LYS:N	2.45	0.50
1:C:22:HIS:HB3	1:C:34:LEU:HD11	1.93	0.50
1:F:326:ALA:O	1:F:329:LEU:HB3	2.11	0.50
1:B:188:ALA:HA	1:B:257:LEU:HD21	1.94	0.49
1:D:22:HIS:HB3	1:D:34:LEU:HD11	1.94	0.49
1:F:188:ALA:HA	1:F:257:LEU:HD21	1.94	0.49
1:B:108:GLU:HG2	1:B:136:HIS:CE1	2.47	0.49
1:F:300:VAL:O	1:F:303:LYS:N	2.45	0.49
1:E:108:GLU:HG2	1:E:136:HIS:CE1	2.47	0.49
1:E:160:VAL:HG13	1:E:169:ILE:HG12	1.95	0.49
1:F:20:THR:HG21	1:F:165:GLY:HA3	1.94	0.49
1:F:147:VAL:HG12	1:F:148:GLY:N	2.27	0.49
1:C:326:ALA:O	1:C:329:LEU:HB3	2.12	0.49
1:D:326:ALA:O	1:D:329:LEU:HB3	2.13	0.49
1:D:333:LEU:CD1	1:F:49:LYS:HZ1	2.26	0.49
1:E:20:THR:HG21	1:E:165:GLY:HA3	1.95	0.49
1:B:20:THR:HG21	1:B:165:GLY:HA3	1.95	0.49
1:A:20:THR:HG21	1:A:165:GLY:HA3	1.94	0.49
1:A:214:ALA:O	1:A:215:CYS:C	2.53	0.49
1:A:160:VAL:HG13	1:A:169:ILE:HG12	1.93	0.49
1:D:258:MET:SD	1:D:296:LEU:HD12	2.53	0.49
1:E:300:VAL:O	1:E:303:LYS:N	2.45	0.49
1:C:42:PRO:HA	1:C:68:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:GLN:CB	1:C:274:PRO:HG3	2.44	0.48
1:D:188:ALA:HA	1:D:257:LEU:HD21	1.95	0.48
1:F:182:GLN:O	1:F:183:VAL:HG23	2.13	0.48
1:F:189:GLY:O	1:F:190:ASN:C	2.55	0.48
1:E:146:MET:HG3	1:E:326:ALA:H	1.79	0.48
1:A:182:GLN:O	1:A:183:VAL:HG23	2.12	0.48
1:A:258:MET:SD	1:A:296:LEU:HD12	2.51	0.48
1:D:147:VAL:HG12	1:D:148:GLY:N	2.28	0.48
1:D:193:ASP:O	1:D:194:GLU:C	2.54	0.48
1:E:223:PHE:CD1	1:E:223:PHE:C	2.91	0.48
1:B:193:ASP:O	1:B:194:GLU:C	2.55	0.48
1:C:325:GLY:C	1:C:327:LEU:N	2.72	0.48
1:E:15:GLY:O	1:E:25:VAL:HA	2.13	0.48
1:F:288:GLY:O	1:F:289:GLY:C	2.55	0.48
1:B:13:PHE:HA	1:B:110:CYS:O	2.14	0.48
1:B:223:PHE:CD1	1:B:223:PHE:C	2.91	0.48
1:A:296:LEU:O	1:A:297:ALA:C	2.57	0.48
1:C:89:VAL:O	1:C:90:ALA:C	2.56	0.48
1:C:147:VAL:HG12	1:C:148:GLY:N	2.28	0.48
1:F:325:GLY:C	1:F:327:LEU:N	2.72	0.48
1:A:108:GLU:HG2	1:A:136:HIS:CE1	2.49	0.48
1:A:188:ALA:HA	1:A:257:LEU:HD21	1.96	0.48
1:D:89:VAL:O	1:D:90:ALA:C	2.55	0.48
1:A:147:VAL:HG12	1:A:148:GLY:N	2.28	0.48
1:F:144:PRO:HB2	1:F:170:CYS:HB3	1.96	0.48
1:A:15:GLY:O	1:A:25:VAL:HA	2.14	0.47
1:E:13:PHE:HA	1:E:110:CYS:O	2.14	0.47
1:B:146:MET:HG3	1:B:326:ALA:H	1.80	0.47
1:C:193:ASP:O	1:C:194:GLU:C	2.54	0.47
1:D:223:PHE:CD1	1:D:223:PHE:C	2.92	0.47
1:A:325:GLY:C	1:A:327:LEU:N	2.73	0.47
1:B:73:PRO:HB3	1:B:89:VAL:HG12	1.96	0.47
1:D:108:GLU:HG2	1:D:136:HIS:CE1	2.49	0.47
1:D:274:PRO:HG3	1:F:208:GLN:CB	2.43	0.47
1:A:159:ILE:CG2	1:A:160:VAL:N	2.77	0.47
1:A:332:GLU:C	1:A:333:LEU:CD1	2.83	0.47
1:C:15:GLY:O	1:C:25:VAL:HA	2.15	0.47
1:C:73:PRO:HB3	1:C:89:VAL:HG12	1.97	0.47
1:C:189:GLY:O	1:C:190:ASN:C	2.53	0.47
1:A:22:HIS:HB3	1:A:34:LEU:HD11	1.95	0.47
1:C:258:MET:SD	1:C:296:LEU:HD12	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLY:HA2	1:C:175:THR:HG21	1.97	0.47
1:B:262:ILE:HG22	1:B:263:GLU:N	2.29	0.47
1:E:325:GLY:C	1:E:327:LEU:N	2.72	0.47
1:C:143:GLU:O	1:C:144:PRO:C	2.57	0.47
1:C:188:ALA:HA	1:C:257:LEU:HD21	1.97	0.47
1:D:159:ILE:CG2	1:D:160:VAL:N	2.75	0.47
1:F:22:HIS:HB3	1:F:34:LEU:HD11	1.96	0.47
1:A:73:PRO:HB3	1:A:89:VAL:HG12	1.96	0.47
1:C:67:TYR:CD1	1:C:67:TYR:C	2.93	0.47
1:D:175:THR:HG21	1:F:47:GLY:HA2	1.96	0.47
1:E:73:PRO:HB3	1:E:89:VAL:HG12	1.96	0.47
1:A:13:PHE:HA	1:A:110:CYS:O	2.15	0.47
1:A:76:ASP:O	1:A:78:VAL:N	2.48	0.47
1:A:193:ASP:O	1:A:194:GLU:C	2.58	0.47
1:E:258:MET:SD	1:E:296:LEU:HD12	2.54	0.47
1:F:108:GLU:HG2	1:F:136:HIS:CE1	2.49	0.47
1:C:108:GLU:HG2	1:C:136:HIS:CE1	2.50	0.47
1:B:160:VAL:HG13	1:B:169:ILE:HG12	1.97	0.46
1:B:325:GLY:C	1:B:327:LEU:N	2.73	0.46
1:F:15:GLY:O	1:F:25:VAL:HA	2.15	0.46
1:D:15:GLY:O	1:D:25:VAL:HA	2.15	0.46
1:A:193:ASP:OD1	1:A:218:LYS:CD	2.63	0.46
1:D:189:GLY:O	1:D:190:ASN:C	2.52	0.46
1:E:216:ALA:O	1:E:217:VAL:C	2.46	0.46
1:F:13:PHE:HA	1:F:110:CYS:O	2.16	0.46
1:E:182:GLN:O	1:E:183:VAL:HG23	2.16	0.46
1:F:296:LEU:O	1:F:297:ALA:C	2.57	0.46
1:B:182:GLN:O	1:B:183:VAL:HG23	2.15	0.46
1:C:300:VAL:O	1:C:303:LYS:N	2.48	0.46
1:D:73:PRO:HB3	1:D:89:VAL:HG12	1.97	0.46
1:D:218:LYS:HE2	3:D:402:ADP:N3	2.30	0.46
1:F:193:ASP:OD1	1:F:218:LYS:CD	2.64	0.46
1:F:73:PRO:HB3	1:F:89:VAL:HG12	1.96	0.46
1:A:144:PRO:HB2	1:A:170:CYS:HB3	1.98	0.46
1:B:257:LEU:HD23	1:B:257:LEU:HA	1.76	0.46
1:C:223:PHE:CD1	1:C:223:PHE:C	2.94	0.46
1:A:236:ARG:HH21	1:C:278:ALA:N	2.14	0.45
1:A:305:ARG:N	1:A:306:PRO:CD	2.79	0.45
1:B:73:PRO:CD	1:B:74:LEU:N	2.79	0.45
1:D:214:ALA:O	1:D:215:CYS:C	2.56	0.45
1:F:281:LEU:HD23	1:F:281:LEU:HA	1.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:289:GLY:HA3	3:F:402:ADP:O5'	2.14	0.45
1:A:36:LYS:HB3	1:A:38:VAL:CG1	2.46	0.45
1:B:305:ARG:N	1:B:306:PRO:CD	2.79	0.45
1:C:281:LEU:HA	1:C:281:LEU:HD23	1.60	0.45
1:D:73:PRO:CD	1:D:74:LEU:H	2.26	0.45
1:F:209:MET:HB2	1:F:209:MET:HE3	1.85	0.45
1:F:305:ARG:N	1:F:306:PRO:CD	2.79	0.45
1:C:92:HIS:O	1:C:93:LEU:C	2.58	0.45
1:D:73:PRO:CD	1:D:74:LEU:N	2.79	0.45
1:E:37:SER:C	1:E:38:VAL:HG12	2.40	0.45
1:F:67:TYR:CD1	1:F:67:TYR:C	2.94	0.45
1:B:143:GLU:N	1:B:144:PRO:HD2	2.31	0.45
1:D:300:VAL:O	1:D:303:LYS:N	2.49	0.45
1:E:332:GLU:C	1:E:333:LEU:CD1	2.86	0.45
1:C:193:ASP:OD1	1:C:218:LYS:CD	2.65	0.45
1:E:144:PRO:HB2	1:E:170:CYS:HB3	1.98	0.45
1:F:76:ASP:O	1:F:78:VAL:N	2.48	0.45
1:A:220:GLN:HG2	1:A:221:PHE:CE2	2.52	0.45
1:B:207:LEU:HD22	1:B:235:PHE:HB3	1.98	0.45
1:D:153:LYS:C	1:D:154:LEU:HG	2.42	0.45
1:E:46:ILE:HB	1:F:175:THR:HB	1.98	0.45
1:E:73:PRO:CD	1:E:74:LEU:N	2.77	0.45
1:E:110:CYS:HA	1:E:137:THR:O	2.17	0.45
1:E:143:GLU:N	1:E:144:PRO:HD2	2.32	0.45
1:E:172:LEU:O	1:E:174:GLY:N	2.49	0.45
1:E:193:ASP:O	1:E:194:GLU:C	2.53	0.45
1:F:143:GLU:N	1:F:144:PRO:HD2	2.31	0.45
1:A:49:LYS:NZ	1:C:149:TYR:HH	2.10	0.45
1:C:214:ALA:O	1:C:215:CYS:C	2.58	0.45
1:D:67:TYR:CD1	1:D:67:TYR:C	2.94	0.45
1:D:149:TYR:HH	1:F:49:LYS:NZ	2.13	0.45
1:D:193:ASP:OD1	1:D:218:LYS:CD	2.65	0.45
1:A:67:TYR:CD1	1:A:67:TYR:C	2.95	0.44
1:A:110:CYS:HA	1:A:137:THR:O	2.17	0.44
1:A:175:THR:HB	1:B:46:ILE:HB	1.99	0.44
1:A:289:GLY:HA3	3:A:402:ADP:O5'	2.16	0.44
1:F:36:LYS:HB3	1:F:38:VAL:CG1	2.46	0.44
1:F:110:CYS:HA	1:F:137:THR:O	2.17	0.44
1:A:257:LEU:HD23	1:A:257:LEU:HA	1.83	0.44
1:A:274:PRO:HG3	1:B:208:GLN:CB	2.48	0.44
1:C:153:LYS:C	1:C:154:LEU:HG	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:LYS:HE2	3:C:402:ADP:N3	2.31	0.44
1:E:207:LEU:HD22	1:E:235:PHE:HB3	1.98	0.44
1:A:201:LEU:CD2	1:A:209:MET:HE3	2.48	0.44
1:A:211:VAL:HG23	1:A:212:ASN:N	2.32	0.44
1:B:172:LEU:O	1:B:174:GLY:N	2.50	0.44
1:B:110:CYS:HA	1:B:137:THR:O	2.17	0.44
1:C:76:ASP:O	1:C:78:VAL:N	2.50	0.44
1:C:207:LEU:HD22	1:C:235:PHE:HB3	1.99	0.44
1:D:325:GLY:C	1:D:327:LEU:N	2.72	0.44
1:F:172:LEU:HD23	1:F:172:LEU:HA	1.93	0.44
1:F:201:LEU:CD2	1:F:209:MET:HE3	2.48	0.44
1:B:14:LEU:HD23	1:B:14:LEU:HA	1.81	0.44
1:B:258:MET:SD	1:B:296:LEU:HD12	2.54	0.44
1:D:278:ALA:N	1:F:236:ARG:HH21	2.14	0.44
1:A:49:LYS:HZ1	1:C:332:GLU:HB3	1.81	0.44
1:B:144:PRO:HB2	1:B:170:CYS:HB3	1.99	0.44
1:B:220:GLN:HG2	1:B:221:PHE:CE2	2.53	0.44
1:B:281:LEU:HD23	1:B:281:LEU:HA	1.59	0.44
1:C:172:LEU:HD23	1:C:172:LEU:HA	1.89	0.44
1:D:160:VAL:HG13	1:D:169:ILE:HG12	1.99	0.44
1:E:262:ILE:HG22	1:E:263:GLU:N	2.30	0.44
1:E:286:PHE:HB3	1:E:291:SER:HB2	2.00	0.44
1:F:193:ASP:O	1:F:194:GLU:C	2.56	0.44
1:F:220:GLN:HG2	1:F:221:PHE:CE2	2.52	0.44
1:A:220:GLN:O	1:A:294:ARG:NH2	2.51	0.44
1:C:13:PHE:HA	1:C:110:CYS:O	2.18	0.44
1:C:73:PRO:CD	1:C:74:LEU:N	2.80	0.44
1:C:269:LEU:HD12	1:C:269:LEU:HA	1.80	0.44
1:D:13:PHE:HA	1:D:110:CYS:O	2.18	0.44
1:D:300:VAL:HG12	1:D:312:VAL:HG21	1.99	0.44
1:A:143:GLU:N	1:A:144:PRO:HD2	2.33	0.44
1:B:220:GLN:O	1:B:294:ARG:NH2	2.51	0.44
1:D:144:PRO:HB2	1:D:170:CYS:HB3	2.00	0.44
1:E:220:GLN:O	1:E:294:ARG:NH2	2.50	0.44
1:E:305:ARG:N	1:E:306:PRO:CD	2.80	0.44
1:C:73:PRO:HG2	1:C:74:LEU:HG	2.00	0.44
1:C:262:ILE:HG22	1:C:263:GLU:N	2.33	0.44
1:B:36:LYS:HB3	1:B:38:VAL:CG1	2.48	0.43
1:D:193:ASP:OD1	1:D:218:LYS:HD3	2.18	0.43
1:A:31:LYS:CE	1:A:102:GLU:HG2	2.48	0.43
1:C:160:VAL:HG13	1:C:169:ILE:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:GLN:O	1:C:294:ARG:NH2	2.50	0.43
1:D:207:LEU:HD22	1:D:235:PHE:HB3	1.99	0.43
1:D:257:LEU:HD23	1:D:257:LEU:HA	1.80	0.43
1:D:258:MET:SD	1:D:296:LEU:HD11	2.58	0.43
1:E:76:ASP:O	1:E:78:VAL:N	2.49	0.43
1:F:268:LEU:HD23	1:F:268:LEU:HA	1.75	0.43
1:A:92:HIS:O	1:A:93:LEU:C	2.59	0.43
1:C:300:VAL:HG12	1:C:312:VAL:HG21	1.99	0.43
1:E:204:HIS:N	1:E:205:PRO:CD	2.81	0.43
1:E:281:LEU:HD23	1:E:281:LEU:HA	1.59	0.43
1:F:220:GLN:O	1:F:294:ARG:NH2	2.51	0.43
1:A:175:THR:HG21	1:B:47:GLY:HA2	2.01	0.43
1:D:73:PRO:HG3	1:D:93:LEU:HD22	2.00	0.43
1:D:268:LEU:HD23	1:D:268:LEU:HA	1.71	0.43
1:E:208:GLN:CB	1:F:274:PRO:HG3	2.48	0.43
1:E:220:GLN:HG2	1:E:221:PHE:CE2	2.53	0.43
1:B:193:ASP:OD1	1:B:218:LYS:CD	2.66	0.43
1:C:296:LEU:O	1:C:297:ALA:C	2.61	0.43
1:D:220:GLN:O	1:D:294:ARG:NH2	2.50	0.43
1:A:46:ILE:HB	1:C:175:THR:HB	2.01	0.43
1:B:189:GLY:O	1:B:190:ASN:C	2.54	0.43
1:C:193:ASP:OD1	1:C:218:LYS:HD3	2.18	0.43
1:E:36:LYS:HB3	1:E:38:VAL:CG1	2.48	0.43
1:E:209:MET:HG2	1:E:213:VAL:CG1	2.49	0.43
1:E:268:LEU:HA	1:E:268:LEU:HD23	1.70	0.43
1:F:51:LEU:HD12	1:F:51:LEU:HA	1.83	0.43
1:A:128:LEU:HD12	1:A:128:LEU:HA	1.84	0.43
1:A:193:ASP:OD1	1:A:218:LYS:HD3	2.18	0.43
1:A:286:PHE:HB3	1:A:291:SER:HB2	2.01	0.43
1:B:204:HIS:N	1:B:205:PRO:CD	2.81	0.43
1:C:73:PRO:CD	1:C:74:LEU:H	2.27	0.43
1:C:110:CYS:HA	1:C:137:THR:O	2.19	0.43
1:D:73:PRO:HG2	1:D:74:LEU:HG	2.00	0.43
1:E:73:PRO:HG2	1:E:74:LEU:HG	2.00	0.43
1:E:114:GLY:N	1:E:146:MET:HE1	2.34	0.43
1:C:36:LYS:HB3	1:C:38:VAL:CG1	2.49	0.43
1:E:201:LEU:CD2	1:E:209:MET:HE3	2.49	0.43
1:B:98:VAL:O	1:B:101:ALA:HB3	2.19	0.43
1:C:142:SER:OG	1:C:144:PRO:HG2	2.18	0.43
1:C:209:MET:HG2	1:C:213:VAL:CG1	2.49	0.43
1:D:110:CYS:HA	1:D:137:THR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:209:MET:HG2	1:F:213:VAL:CG1	2.49	0.43
1:A:209:MET:HG2	1:A:213:VAL:CG1	2.49	0.43
1:B:31:LYS:CE	1:B:102:GLU:HG2	2.49	0.43
1:C:31:LYS:CE	1:C:102:GLU:HG2	2.49	0.43
1:D:76:ASP:O	1:D:78:VAL:N	2.50	0.43
1:D:289:GLY:HA3	3:D:402:ADP:O5'	2.19	0.43
1:E:12:LEU:HD23	1:E:109:ILE:HG23	1.99	0.43
1:E:31:LYS:CE	1:E:102:GLU:HG2	2.49	0.43
1:F:73:PRO:HG3	1:F:93:LEU:HD22	2.01	0.43
1:A:258:MET:SD	1:A:296:LEU:HD11	2.57	0.42
1:B:12:LEU:HD23	1:B:109:ILE:HG23	1.99	0.42
1:B:201:LEU:CD2	1:B:209:MET:HE3	2.49	0.42
1:D:130:MET:HE3	1:D:130:MET:HB2	1.97	0.42
1:E:193:ASP:OD1	1:E:218:LYS:CD	2.67	0.42
1:F:31:LYS:CE	1:F:102:GLU:HG2	2.48	0.42
1:A:73:PRO:HG2	1:A:74:LEU:HG	2.01	0.42
1:A:195:ARG:O	1:A:196:LEU:C	2.59	0.42
1:B:76:ASP:O	1:B:78:VAL:N	2.49	0.42
1:B:209:MET:HG2	1:B:213:VAL:CG1	2.48	0.42
1:D:12:LEU:HD23	1:D:109:ILE:HG23	2.01	0.42
1:A:281:LEU:HD23	1:A:281:LEU:HA	1.67	0.42
1:C:144:PRO:HB2	1:C:170:CYS:HB3	2.01	0.42
1:D:169:ILE:HG21	1:D:169:ILE:HD13	1.70	0.42
1:D:209:MET:HG2	1:D:213:VAL:CG1	2.50	0.42
1:E:258:MET:SD	1:E:296:LEU:HD11	2.57	0.42
1:F:73:PRO:CD	1:F:74:LEU:H	2.33	0.42
1:F:211:VAL:HG23	1:F:212:ASN:N	2.34	0.42
1:A:143:GLU:O	1:A:144:PRO:C	2.61	0.42
1:A:172:LEU:O	1:A:174:GLY:N	2.53	0.42
1:A:189:GLY:O	1:A:190:ASN:C	2.58	0.42
1:A:200:ILE:HB	1:A:209:MET:HE1	2.01	0.42
1:B:286:PHE:HB3	1:B:291:SER:HB2	2.00	0.42
1:C:98:VAL:O	1:C:101:ALA:HB3	2.20	0.42
1:C:258:MET:SD	1:C:296:LEU:HD11	2.59	0.42
1:D:143:GLU:O	1:D:144:PRO:C	2.59	0.42
1:E:49:LYS:HZ1	1:F:333:LEU:HD11	1.83	0.42
1:E:98:VAL:O	1:E:101:ALA:HB3	2.19	0.42
1:A:146:MET:HE2	1:A:326:ALA:HB2	2.01	0.42
1:C:70:ILE:O	1:C:70:ILE:HG13	2.20	0.42
1:C:257:LEU:HD23	1:C:257:LEU:HA	1.80	0.42
1:F:172:LEU:O	1:F:174:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:286:PHE:HB3	1:F:291:SER:HB2	2.00	0.42
1:B:153:LYS:C	1:B:154:LEU:HG	2.45	0.42
1:B:209:MET:HE3	1:B:209:MET:HB2	1.85	0.42
1:C:73:PRO:HG3	1:C:93:LEU:HD22	2.00	0.42
1:C:200:ILE:HB	1:C:209:MET:HE1	2.02	0.42
1:D:262:ILE:HG22	1:D:263:GLU:N	2.33	0.42
1:F:12:LEU:HD23	1:F:109:ILE:HG23	2.01	0.42
1:F:193:ASP:OD1	1:F:218:LYS:HD3	2.19	0.42
1:B:102:GLU:N	1:B:103:PRO:HD3	2.35	0.42
1:E:47:GLY:HA2	1:F:175:THR:HG21	2.01	0.42
1:F:146:MET:HE2	1:F:326:ALA:HB2	2.02	0.42
1:F:262:ILE:HG22	1:F:263:GLU:N	2.35	0.42
1:A:207:LEU:HD22	1:A:235:PHE:HB3	2.02	0.42
1:D:209:MET:HE3	1:D:209:MET:HB2	1.81	0.42
1:E:89:VAL:O	1:E:92:HIS:N	2.53	0.42
1:F:284:ILE:HG22	1:F:312:VAL:HG13	2.01	0.42
1:D:70:ILE:O	1:D:70:ILE:HG13	2.20	0.42
1:D:117:ALA:O	1:D:184:THR:OG1	2.36	0.42
1:E:14:LEU:HD23	1:E:14:LEU:HA	1.80	0.42
1:F:98:VAL:O	1:F:101:ALA:HB3	2.20	0.42
1:A:73:PRO:HG3	1:A:93:LEU:HD22	2.02	0.42
1:B:73:PRO:HG2	1:B:74:LEU:HG	2.01	0.42
1:D:98:VAL:O	1:D:101:ALA:HB3	2.20	0.42
1:A:49:LYS:HZ1	1:C:332:GLU:CB	2.32	0.41
1:B:258:MET:SD	1:B:296:LEU:HD11	2.58	0.41
1:D:142:SER:OG	1:D:144:PRO:HG2	2.20	0.41
1:E:102:GLU:N	1:E:103:PRO:HD3	2.35	0.41
1:B:193:ASP:OD1	1:B:218:LYS:HD3	2.20	0.41
1:C:268:LEU:HD23	1:C:268:LEU:HA	1.71	0.41
1:D:296:LEU:O	1:D:297:ALA:C	2.61	0.41
1:A:14:LEU:HD23	1:A:14:LEU:HA	1.85	0.41
1:A:98:VAL:O	1:A:101:ALA:HB3	2.20	0.41
1:A:102:GLU:N	1:A:103:PRO:HD3	2.35	0.41
1:B:89:VAL:O	1:B:92:HIS:N	2.53	0.41
1:D:31:LYS:CE	1:D:102:GLU:HG2	2.49	0.41
1:D:274:PRO:HG3	1:F:208:GLN:HB2	2.02	0.41
1:E:92:HIS:O	1:E:93:LEU:C	2.62	0.41
1:E:169:ILE:HG21	1:E:169:ILE:HD13	1.70	0.41
1:F:51:LEU:HD22	1:F:68:LEU:HD22	2.02	0.41
1:F:73:PRO:HG2	1:F:74:LEU:HG	2.01	0.41
1:F:195:ARG:O	1:F:196:LEU:C	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ALA:N	1:B:236:ARG:HH21	2.19	0.41
1:B:169:ILE:HD13	1:B:169:ILE:HG21	1.69	0.41
1:B:195:ARG:O	1:B:196:LEU:C	2.61	0.41
1:C:211:VAL:HG23	1:C:212:ASN:N	2.35	0.41
1:C:289:GLY:HA3	3:C:402:ADP:O5'	2.20	0.41
1:D:175:THR:HB	1:F:46:ILE:HB	2.01	0.41
1:E:149:TYR:HA	1:E:154:LEU:HD11	2.02	0.41
1:A:12:LEU:HD23	1:A:109:ILE:HG23	2.01	0.41
1:A:254:CYS:C	1:A:256:ALA:H	2.28	0.41
1:F:159:ILE:CG2	1:F:160:VAL:N	2.77	0.41
1:A:262:ILE:HG22	1:A:263:GLU:N	2.35	0.41
1:B:37:SER:C	1:B:38:VAL:HG12	2.44	0.41
1:B:143:GLU:O	1:B:144:PRO:C	2.64	0.41
1:B:332:GLU:C	1:B:333:LEU:CD1	2.85	0.41
1:C:281:LEU:HD11	1:C:307:PHE:CB	2.50	0.41
1:D:333:LEU:HD11	1:F:49:LYS:HZ1	1.85	0.41
1:E:153:LYS:C	1:E:154:LEU:HG	2.45	0.41
1:A:142:SER:OG	1:A:144:PRO:HG2	2.20	0.41
1:A:284:ILE:HG22	1:A:312:VAL:HG13	2.02	0.41
1:B:172:LEU:HD23	1:B:172:LEU:HA	1.98	0.41
1:D:21:SER:N	3:D:402:ADP:O3B	2.50	0.41
1:D:36:LYS:HB3	1:D:38:VAL:CG1	2.50	0.41
1:D:274:PRO:HG3	1:F:208:GLN:HB3	2.03	0.41
1:F:300:VAL:HG12	1:F:312:VAL:HG21	2.01	0.41
1:A:208:GLN:HB2	1:C:274:PRO:HG3	2.02	0.41
1:B:39:VAL:HG22	1:B:57:VAL:HG13	2.03	0.41
1:C:254:CYS:C	1:C:256:ALA:H	2.29	0.41
1:D:157:THR:HA	1:D:283:ASN:HB3	2.03	0.41
1:F:117:ALA:O	1:F:184:THR:OG1	2.36	0.41
1:F:171:ALA:HB2	1:F:268:LEU:HD13	2.03	0.41
1:A:208:GLN:HB3	1:C:274:PRO:HG3	2.03	0.41
1:A:252:ILE:HG22	1:A:253:ALA:N	2.34	0.41
1:B:142:SER:OG	1:B:144:PRO:HG2	2.21	0.41
1:B:159:ILE:CG2	1:B:160:VAL:N	2.82	0.41
1:B:211:VAL:HG23	1:B:212:ASN:N	2.36	0.41
1:C:12:LEU:HD23	1:C:109:ILE:HG23	2.02	0.41
1:C:271:SER:OG	1:C:272:PHE:N	2.54	0.41
1:D:172:LEU:O	1:D:174:GLY:N	2.54	0.41
1:D:300:VAL:CG1	1:D:312:VAL:HG21	2.51	0.41
1:E:300:VAL:HG12	1:E:312:VAL:HG21	2.02	0.41
1:A:39:VAL:HG22	1:A:57:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ALA:HB2	1:A:268:LEU:HD13	2.02	0.41
1:A:268:LEU:HD23	1:A:268:LEU:HA	1.76	0.41
1:A:275:GLU:OE2	1:B:212:ASN:C	2.65	0.41
1:C:252:ILE:HG22	1:C:253:ALA:N	2.35	0.41
1:F:39:VAL:HG22	1:F:57:VAL:HG13	2.02	0.41
1:F:102:GLU:N	1:F:103:PRO:HD3	2.35	0.41
1:A:300:VAL:HG12	1:A:312:VAL:HG21	2.02	0.40
1:B:300:VAL:HG12	1:B:312:VAL:HG21	2.02	0.40
1:C:102:GLU:N	1:C:103:PRO:HD3	2.36	0.40
1:D:102:GLU:N	1:D:103:PRO:HD3	2.36	0.40
1:D:211:VAL:HG23	1:D:212:ASN:N	2.36	0.40
1:E:300:VAL:CG1	1:E:312:VAL:HG21	2.51	0.40
1:F:36:LYS:HB3	1:F:38:VAL:HG12	2.03	0.40
1:F:252:ILE:HG22	1:F:253:ALA:N	2.36	0.40
1:A:212:ASN:C	1:C:275:GLU:OE2	2.64	0.40
1:A:281:LEU:HD11	1:A:307:PHE:CB	2.51	0.40
1:E:39:VAL:HG22	1:E:57:VAL:HG13	2.02	0.40
1:E:128:LEU:HD12	1:E:128:LEU:HA	1.84	0.40
1:F:207:LEU:HD22	1:F:235:PHE:HB3	2.02	0.40
1:A:49:LYS:HZ3	1:C:149:TYR:HH	1.62	0.40
1:A:269:LEU:CD1	1:A:280:VAL:HG11	2.51	0.40
1:B:252:ILE:HG22	1:B:253:ALA:N	2.34	0.40
1:C:51:LEU:HA	1:C:51:LEU:HD12	1.84	0.40
1:C:128:LEU:HD12	1:C:128:LEU:HA	1.83	0.40
1:C:201:LEU:CD2	1:C:209:MET:HE3	2.52	0.40
1:C:300:VAL:CG1	1:C:312:VAL:HG21	2.50	0.40
1:F:143:GLU:O	1:F:144:PRO:C	2.63	0.40
1:F:169:ILE:HG21	1:F:169:ILE:HD13	1.73	0.40
1:F:269:LEU:CD1	1:F:280:VAL:HG11	2.51	0.40
1:C:162:ILE:HD11	1:C:261:ILE:HD13	2.04	0.40
1:C:172:LEU:O	1:C:174:GLY:N	2.55	0.40
1:D:252:ILE:HG22	1:D:253:ALA:N	2.36	0.40
1:E:23:THR:HB	1:E:35:LEU:HD12	2.04	0.40
1:F:142:SER:OG	1:F:144:PRO:HG2	2.22	0.40
1:F:258:MET:SD	1:F:296:LEU:HD11	2.57	0.40
1:C:146:MET:HE2	1:C:326:ALA:HB2	2.04	0.40
1:E:49:LYS:NZ	1:F:149:TYR:HH	2.18	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	A	323/347 (93%)	290 (90%)	23 (7%)	10 (3%)	3	21
1	B	323/347 (93%)	289 (90%)	26 (8%)	8 (2%)	4	24
1	C	323/347 (93%)	291 (90%)	22 (7%)	10 (3%)	3	21
1	D	323/347 (93%)	291 (90%)	22 (7%)	10 (3%)	3	21
1	E	323/347 (93%)	289 (90%)	26 (8%)	8 (2%)	4	24
1	F	323/347 (93%)	289 (90%)	24 (7%)	10 (3%)	3	21
All	All	1938/2082 (93%)	1739 (90%)	143 (7%)	56 (3%)	5	22

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	PRO
1	A	179	PRO
1	B	103	PRO
1	B	179	PRO
1	C	103	PRO
1	C	179	PRO
1	D	103	PRO
1	D	179	PRO
1	E	103	PRO
1	E	179	PRO
1	F	103	PRO
1	F	179	PRO
1	A	77	GLY
1	A	333	LEU
1	C	77	GLY
1	D	77	GLY
1	D	333	LEU
1	F	77	GLY
1	F	333	LEU
1	A	326	ALA

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Mol	Chain	Res	Type
1	B	333	LEU
1	C	326	ALA
1	C	333	LEU
1	D	326	ALA
1	E	333	LEU
1	F	326	ALA
1	A	187	LYS
1	B	326	ALA
1	E	326	ALA
1	F	187	LYS
1	B	77	GLY
1	C	187	LYS
1	E	77	GLY
1	A	189	GLY
1	A	322	GLY
1	C	78	VAL
1	D	78	VAL
1	D	187	LYS
1	A	78	VAL
1	C	189	GLY
1	D	189	GLY
1	F	78	VAL
1	F	189	GLY
1	F	322	GLY
1	A	315	VAL
1	B	189	GLY
1	C	322	GLY
1	D	322	GLY
1	E	189	GLY
1	F	315	VAL
1	B	322	GLY
1	E	78	VAL
1	E	322	GLY
1	B	78	VAL
1	D	315	VAL
1	C	315	VAL

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

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	268/285 (94%)	237 (88%)	31 (12%)	5	22
1	B	268/285 (94%)	237 (88%)	31 (12%)	5	22
1	C	268/285 (94%)	235 (88%)	33 (12%)	4	20
1	D	268/285 (94%)	235 (88%)	33 (12%)	4	20
1	E	268/285 (94%)	237 (88%)	31 (12%)	5	22
1	F	268/285 (94%)	237 (88%)	31 (12%)	5	22
All	All	1608/1710 (94%)	1418 (88%)	190 (12%)	7	21

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	13	PHE
1	A	20	THR
1	A	38	VAL
1	A	59	ASP
1	A	63	GLU
1	A	74	LEU
1	A	78	VAL
1	A	94	LEU
1	A	100	SER
1	A	109	ILE
1	A	110	CYS
1	A	112	VAL
1	A	118	ARG
1	A	126	LEU
1	A	127	LEU
1	A	130	MET
1	A	142	SER
1	A	146	MET
1	A	155	ILE
1	A	158	ILE
1	A	166	THR
1	A	176	VAL
1	A	185	LEU
1	A	195	ARG
1	A	252	ILE
1	A	258	MET

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Mol	Chain	Res	Type
1	A	259	PRO
1	A	262	ILE
1	A	267	THR
1	A	283	ASN
1	B	12	LEU
1	B	13	PHE
1	B	20	THR
1	B	38	VAL
1	B	48	LEU
1	B	59	ASP
1	B	63	GLU
1	B	74	LEU
1	B	78	VAL
1	B	94	LEU
1	B	100	SER
1	B	109	ILE
1	B	110	CYS
1	B	118	ARG
1	B	126	LEU
1	B	127	LEU
1	B	130	MET
1	B	142	SER
1	B	146	MET
1	B	155	ILE
1	B	158	ILE
1	B	166	THR
1	B	176	VAL
1	B	185	LEU
1	B	195	ARG
1	B	252	ILE
1	B	258	MET
1	B	259	PRO
1	B	262	ILE
1	B	267	THR
1	B	283	ASN
1	C	12	LEU
1	C	13	PHE
1	C	20	THR
1	C	38	VAL
1	C	48	LEU
1	C	59	ASP
1	C	63	GLU

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Mol	Chain	Res	Type
1	C	74	LEU
1	C	78	VAL
1	C	94	LEU
1	C	100	SER
1	C	108	GLU
1	C	109	ILE
1	C	110	CYS
1	C	112	VAL
1	C	118	ARG
1	C	126	LEU
1	C	127	LEU
1	C	130	MET
1	C	142	SER
1	C	146	MET
1	C	155	ILE
1	C	166	THR
1	C	176	VAL
1	C	185	LEU
1	C	195	ARG
1	C	252	ILE
1	C	258	MET
1	C	259	PRO
1	C	262	ILE
1	C	267	THR
1	C	283	ASN
1	C	306	PRO
1	D	12	LEU
1	D	13	PHE
1	D	20	THR
1	D	38	VAL
1	D	48	LEU
1	D	59	ASP
1	D	63	GLU
1	D	74	LEU
1	D	78	VAL
1	D	94	LEU
1	D	100	SER
1	D	108	GLU
1	D	109	ILE
1	D	110	CYS
1	D	112	VAL
1	D	118	ARG

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Mol	Chain	Res	Type
1	D	126	LEU
1	D	127	LEU
1	D	130	MET
1	D	142	SER
1	D	146	MET
1	D	155	ILE
1	D	166	THR
1	D	176	VAL
1	D	185	LEU
1	D	195	ARG
1	D	252	ILE
1	D	258	MET
1	D	259	PRO
1	D	262	ILE
1	D	267	THR
1	D	283	ASN
1	D	306	PRO
1	E	12	LEU
1	E	13	PHE
1	E	20	THR
1	E	38	VAL
1	E	48	LEU
1	E	59	ASP
1	E	63	GLU
1	E	74	LEU
1	E	78	VAL
1	E	94	LEU
1	E	100	SER
1	E	109	ILE
1	E	110	CYS
1	E	112	VAL
1	E	118	ARG
1	E	126	LEU
1	E	127	LEU
1	E	130	MET
1	E	142	SER
1	E	146	MET
1	E	155	ILE
1	E	166	THR
1	E	176	VAL
1	E	185	LEU
1	E	195	ARG

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Mol	Chain	Res	Type
1	E	252	ILE
1	E	258	MET
1	E	259	PRO
1	E	262	ILE
1	E	267	THR
1	E	283	ASN
1	F	12	LEU
1	F	13	PHE
1	F	20	THR
1	F	38	VAL
1	F	59	ASP
1	F	63	GLU
1	F	74	LEU
1	F	78	VAL
1	F	94	LEU
1	F	100	SER
1	F	109	ILE
1	F	110	CYS
1	F	112	VAL
1	F	118	ARG
1	F	126	LEU
1	F	127	LEU
1	F	130	MET
1	F	142	SER
1	F	146	MET
1	F	155	ILE
1	F	158	ILE
1	F	166	THR
1	F	176	VAL
1	F	185	LEU
1	F	195	ARG
1	F	252	ILE
1	F	258	MET
1	F	259	PRO
1	F	262	ILE
1	F	267	THR
1	F	283	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN

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Mol	Chain	Res	Type
1	A	123	ASN
1	B	75	GLN
1	B	92	HIS
1	B	123	ASN
1	C	75	GLN
1	C	123	ASN
1	C	208	GLN
1	D	123	ASN
1	D	208	GLN
1	E	75	GLN
1	E	123	ASN
1	F	123	ASN

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](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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$
3	ADP	E	402	2	28,29,29	1.81	7 (25%)	43,45,45	2.85	19 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	C	402	2	28,29,29	1.95	6 (21%)	43,45,45	2.08	15 (34%)
3	ADP	B	402	2	28,29,29	1.77	8 (28%)	43,45,45	2.73	19 (44%)
3	ADP	A	402	2	28,29,29	1.70	5 (17%)	43,45,45	2.55	15 (34%)
3	ADP	D	402	2	28,29,29	1.94	8 (28%)	43,45,45	2.10	17 (39%)
3	ADP	F	402	2	28,29,29	1.75	6 (21%)	43,45,45	2.64	18 (41%)

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
3	ADP	E	402	2	-	1/16/32/32	0/3/3/3
3	ADP	C	402	2	-	2/16/32/32	0/3/3/3
3	ADP	B	402	2	-	1/16/32/32	0/3/3/3
3	ADP	A	402	2	-	2/16/32/32	0/3/3/3
3	ADP	D	402	2	-	2/16/32/32	0/3/3/3
3	ADP	F	402	2	-	2/16/32/32	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	ADP	C4-N9	-5.64	1.26	1.37
3	C	402	ADP	C4-N9	-5.56	1.26	1.37
3	C	402	ADP	C5-C4	4.82	1.47	1.39
3	F	402	ADP	C5-C4	4.70	1.47	1.39
3	D	402	ADP	C5-C4	4.65	1.47	1.39
3	A	402	ADP	C5-C4	4.53	1.47	1.39
3	B	402	ADP	C4-N9	-4.36	1.28	1.37
3	B	402	ADP	C5-C4	4.25	1.46	1.39
3	E	402	ADP	C4-N9	-4.21	1.28	1.37
3	E	402	ADP	C5-C4	4.16	1.46	1.39
3	A	402	ADP	C4-N9	-3.67	1.30	1.37
3	F	402	ADP	C4-N9	-3.56	1.30	1.37
3	F	402	ADP	C8-N7	3.17	1.37	1.31
3	A	402	ADP	C8-N7	2.96	1.37	1.31
3	D	402	ADP	PB-O1B	2.95	1.59	1.50
3	A	402	ADP	PA-O3A	2.87	1.62	1.59
3	E	402	ADP	C5-N7	-2.85	1.33	1.39
3	D	402	ADP	C5-N7	-2.84	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	ADP	C5-N7	-2.82	1.33	1.39
3	C	402	ADP	C5-N7	-2.76	1.34	1.39
3	C	402	ADP	PB-O1B	2.76	1.59	1.50
3	F	402	ADP	PA-O3A	2.68	1.62	1.59
3	F	402	ADP	PB-O1B	2.66	1.58	1.50
3	E	402	ADP	PB-O1B	2.62	1.58	1.50
3	E	402	ADP	O4'-C4'	-2.60	1.39	1.45
3	E	402	ADP	C8-N7	2.59	1.36	1.31
3	A	402	ADP	PB-O1B	2.45	1.58	1.50
3	B	402	ADP	O4'-C4'	-2.38	1.39	1.45
3	C	402	ADP	C2'-C3'	-2.37	1.47	1.53
3	B	402	ADP	C8-N7	2.35	1.36	1.31
3	B	402	ADP	PB-O1B	2.32	1.57	1.50
3	E	402	ADP	O2'-C2'	2.31	1.48	1.43
3	D	402	ADP	C2'-C3'	-2.31	1.47	1.53
3	D	402	ADP	O4'-C4'	-2.28	1.39	1.45
3	C	402	ADP	C6-N6	2.28	1.40	1.34
3	F	402	ADP	C3'-C4'	2.22	1.58	1.53
3	B	402	ADP	C2-N1	2.17	1.37	1.33
3	B	402	ADP	O2'-C2'	2.17	1.48	1.43
3	D	402	ADP	C8-N7	2.16	1.35	1.31
3	D	402	ADP	C6-N6	2.15	1.39	1.34

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	402	ADP	C4-N9-C8	8.89	115.07	105.74
3	A	402	ADP	C4-N9-C8	8.77	114.94	105.74
3	E	402	ADP	C4-N9-C8	7.31	113.42	105.74
3	B	402	ADP	C4-N9-C8	7.12	113.21	105.74
3	E	402	ADP	N6-C6-N1	5.56	130.75	118.38
3	F	402	ADP	C4-N9-C1'	-5.48	113.81	126.63
3	A	402	ADP	C4-N9-C1'	-5.48	113.81	126.63
3	B	402	ADP	N6-C6-N1	5.41	130.43	118.38
3	E	402	ADP	N3-C2-N1	-5.36	120.46	128.58
3	E	402	ADP	O4'-C1'-C2'	4.92	117.14	106.62
3	B	402	ADP	N3-C2-N1	-4.91	121.15	128.58
3	B	402	ADP	C5-C4-N9	-4.83	100.54	105.81
3	E	402	ADP	C5-C4-N9	-4.75	100.63	105.81
3	D	402	ADP	C2'-C1'-N9	-4.61	101.86	113.30
3	C	402	ADP	C2'-C1'-N9	-4.51	102.09	113.30
3	B	402	ADP	C4-N9-C1'	-4.50	116.11	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	402	ADP	C5-C6-N6	-4.49	112.17	123.29
3	E	402	ADP	C4-N9-C1'	-4.47	116.19	126.63
3	E	402	ADP	C2'-C1'-N9	-4.45	102.24	113.30
3	B	402	ADP	O4'-C1'-C2'	4.34	115.90	106.62
3	E	402	ADP	C2-N1-C6	4.30	125.80	118.73
3	F	402	ADP	N9-C8-N7	-4.28	107.86	113.94
3	A	402	ADP	C5-C4-N9	-4.27	101.15	105.81
3	B	402	ADP	C2'-C1'-N9	-4.25	102.74	113.30
3	D	402	ADP	N6-C6-N1	4.25	127.84	118.38
3	C	402	ADP	C4-N9-C1'	-4.23	116.74	126.63
3	F	402	ADP	C5-C4-N9	-4.22	101.21	105.81
3	F	402	ADP	N6-C6-N1	4.18	127.70	118.38
3	B	402	ADP	C2-N1-C6	4.18	125.60	118.73
3	B	402	ADP	C5-C6-N6	-4.17	112.95	123.29
3	F	402	ADP	C2'-C1'-N9	-4.17	102.95	113.30
3	A	402	ADP	N9-C8-N7	-4.16	108.03	113.94
3	C	402	ADP	N6-C6-N1	4.15	127.61	118.38
3	F	402	ADP	O4'-C1'-C2'	4.13	115.46	106.62
3	D	402	ADP	C4-N9-C1'	-4.11	117.03	126.63
3	C	402	ADP	C4-N9-C8	4.10	110.05	105.74
3	A	402	ADP	N6-C6-N1	4.08	127.47	118.38
3	D	402	ADP	C4-N9-C8	3.98	109.92	105.74
3	A	402	ADP	C2'-C1'-N9	-3.86	103.70	113.30
3	F	402	ADP	N3-C4-N9	3.77	133.57	127.17
3	C	402	ADP	N3-C2-N1	-3.73	122.94	128.58
3	E	402	ADP	O3A-PA-O1A	3.71	121.85	110.70
3	A	402	ADP	O4'-C1'-C2'	3.64	114.41	106.62
3	A	402	ADP	N3-C4-N9	3.58	133.26	127.17
3	F	402	ADP	C5-C6-N6	-3.51	114.58	123.29
3	B	402	ADP	O3A-PA-O1A	3.47	121.15	110.70
3	D	402	ADP	N3-C2-N1	-3.44	123.37	128.58
3	E	402	ADP	C3'-C2'-C1'	-3.39	95.05	101.46
3	A	402	ADP	C5-C6-N6	-3.38	114.91	123.29
3	F	402	ADP	O3A-PA-O1A	3.30	120.63	110.70
3	A	402	ADP	O3A-PA-O1A	3.27	120.55	110.70
3	F	402	ADP	C3'-C2'-C1'	-3.26	95.29	101.46
3	D	402	ADP	O4'-C1'-C2'	3.20	113.47	106.62
3	E	402	ADP	N3-C4-N9	3.18	132.58	127.17
3	E	402	ADP	N9-C8-N7	-3.13	109.49	113.94
3	E	402	ADP	C2'-C3'-C4'	2.99	108.39	102.61
3	D	402	ADP	C5-C6-N6	-2.97	115.93	123.29
3	B	402	ADP	N3-C4-N9	2.90	132.09	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	ADP	C4-C5-N7	2.89	113.89	110.58
3	C	402	ADP	C2-N1-C6	2.87	123.45	118.73
3	B	402	ADP	N9-C8-N7	-2.84	109.90	113.94
3	B	402	ADP	C2'-C3'-C4'	2.83	108.08	102.61
3	C	402	ADP	C5-C6-N6	-2.81	116.32	123.29
3	C	402	ADP	O4'-C1'-C2'	2.77	112.55	106.62
3	B	402	ADP	C3'-C2'-C1'	-2.75	96.26	101.46
3	C	402	ADP	C1'-N9-C8	2.70	133.09	127.09
3	D	402	ADP	C3'-C2'-C1'	-2.70	96.35	101.46
3	E	402	ADP	C4-C5-N7	2.70	113.67	110.58
3	D	402	ADP	C2-N1-C6	2.65	123.08	118.73
3	D	402	ADP	C1'-N9-C8	2.64	132.96	127.09
3	A	402	ADP	C3'-C2'-C1'	-2.54	96.67	101.46
3	D	402	ADP	N3-C4-N9	2.51	131.43	127.17
3	E	402	ADP	O5'-PA-O1A	2.49	118.81	108.94
3	C	402	ADP	N3-C4-N9	2.49	131.40	127.17
3	B	402	ADP	O5'-PA-O1A	2.45	118.64	108.94
3	C	402	ADP	O3'-C3'-C2'	-2.44	104.01	111.82
3	C	402	ADP	O5'-PA-O1A	2.42	118.51	108.94
3	D	402	ADP	O3'-C3'-C2'	-2.41	104.08	111.82
3	D	402	ADP	C2'-C3'-C4'	2.41	107.26	102.61
3	B	402	ADP	O3'-C3'-C2'	-2.35	104.27	111.82
3	F	402	ADP	O2'-C2'-C3'	2.34	119.33	111.82
3	E	402	ADP	C6-C5-C4	-2.29	114.05	117.18
3	C	402	ADP	C5-C4-N9	-2.27	103.33	105.81
3	C	402	ADP	O3A-PA-O1A	2.25	117.48	110.70
3	E	402	ADP	O2'-C2'-C3'	2.24	119.01	111.82
3	B	402	ADP	O3B-PB-O2B	2.24	116.19	107.80
3	D	402	ADP	O5'-PA-O1A	2.22	117.73	108.94
3	B	402	ADP	C6-C5-C4	-2.21	114.16	117.18
3	E	402	ADP	O3B-PB-O2B	2.21	116.07	107.80
3	F	402	ADP	C2-N1-C6	2.17	122.30	118.73
3	F	402	ADP	N3-C2-N1	-2.16	125.31	128.58
3	A	402	ADP	O2B-PB-O1B	2.14	119.17	110.83
3	C	402	ADP	C2-N3-C4	2.13	117.03	111.83
3	A	402	ADP	C6-C5-C4	-2.12	114.29	117.18
3	D	402	ADP	O3A-PA-O1A	2.11	117.06	110.70
3	D	402	ADP	C2-N3-C4	2.10	116.95	111.83
3	A	402	ADP	C4'-O4'-C1'	-2.08	104.87	109.47
3	F	402	ADP	C4'-O4'-C1'	-2.07	104.90	109.47
3	A	402	ADP	C2-N1-C6	2.04	122.07	118.73
3	D	402	ADP	C5-C4-N9	-2.03	103.60	105.81

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	402	ADP	C6-C5-C4	-2.03	114.41	117.18
3	F	402	ADP	O2B-PB-O1B	2.03	118.73	110.83
3	F	402	ADP	O3'-C3'-C4'	2.02	116.89	111.08

There are no chirality outliers.

All (10) torsion outliers are listed below:

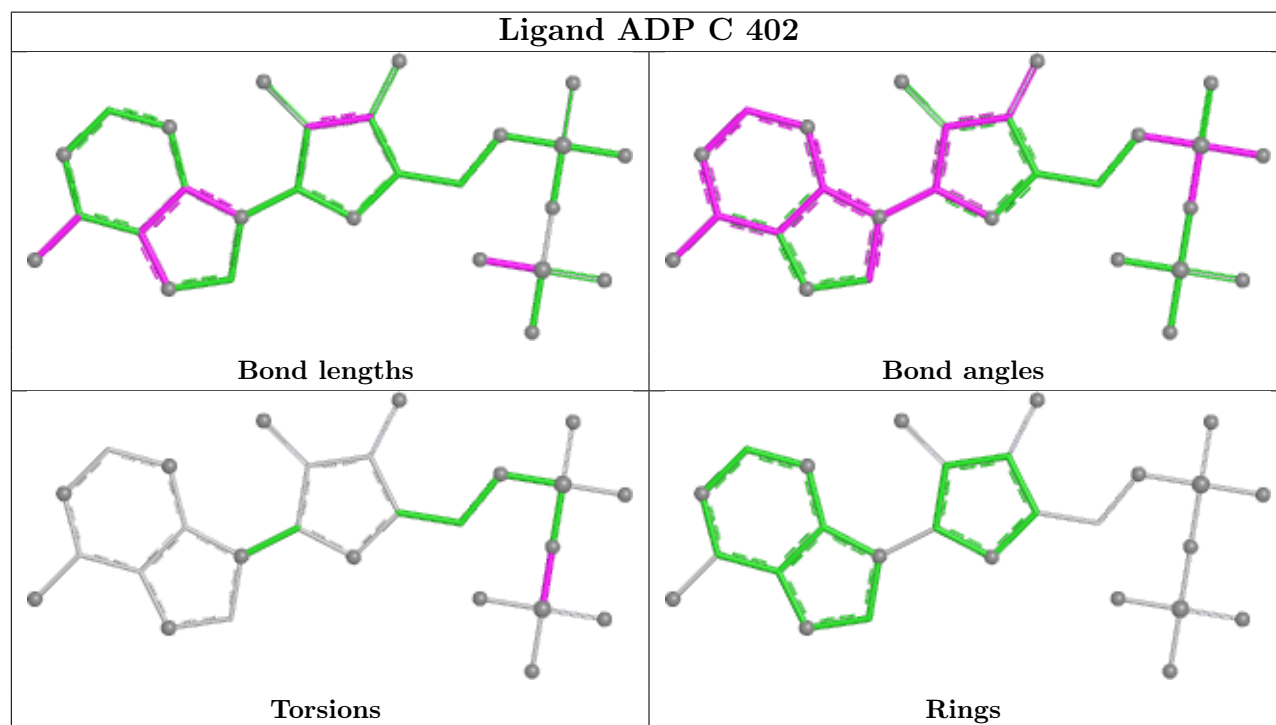
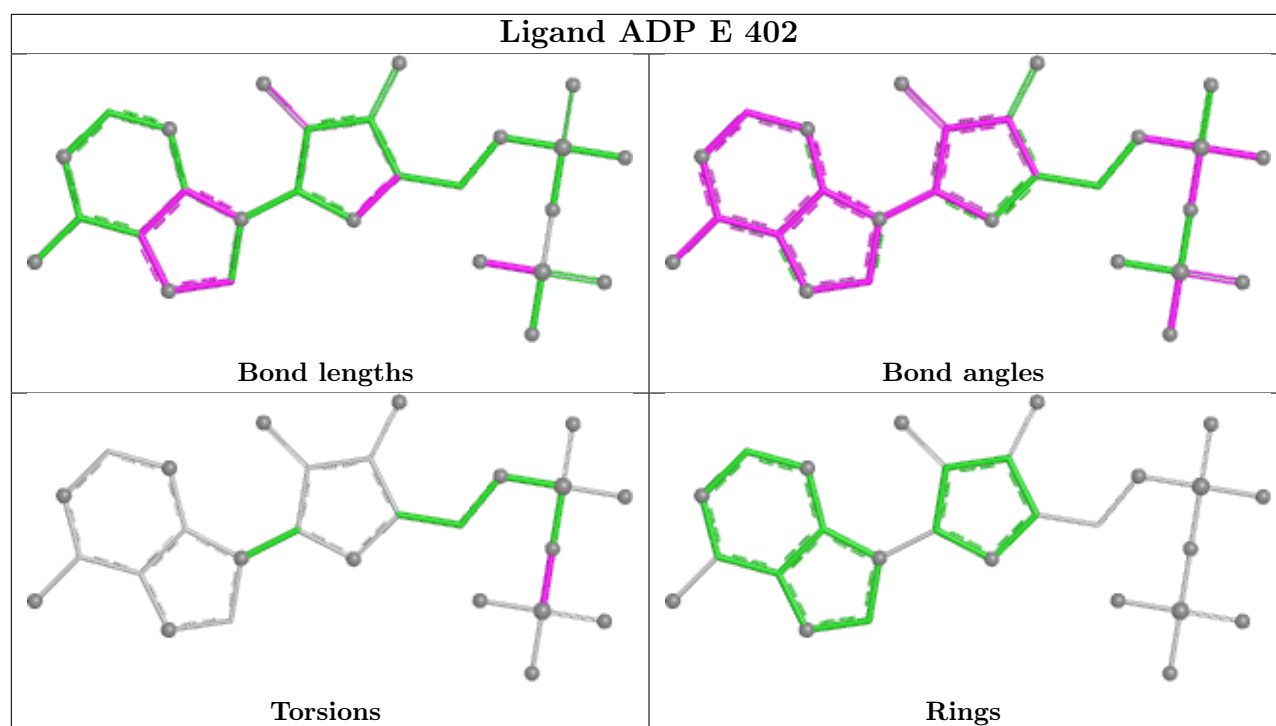
Mol	Chain	Res	Type	Atoms
3	A	402	ADP	PA-O3A-PB-O2B
3	B	402	ADP	PA-O3A-PB-O2B
3	C	402	ADP	PA-O3A-PB-O2B
3	D	402	ADP	PA-O3A-PB-O2B
3	E	402	ADP	PA-O3A-PB-O2B
3	F	402	ADP	PA-O3A-PB-O2B
3	A	402	ADP	PA-O3A-PB-O1B
3	C	402	ADP	PA-O3A-PB-O1B
3	D	402	ADP	PA-O3A-PB-O1B
3	F	402	ADP	PA-O3A-PB-O1B

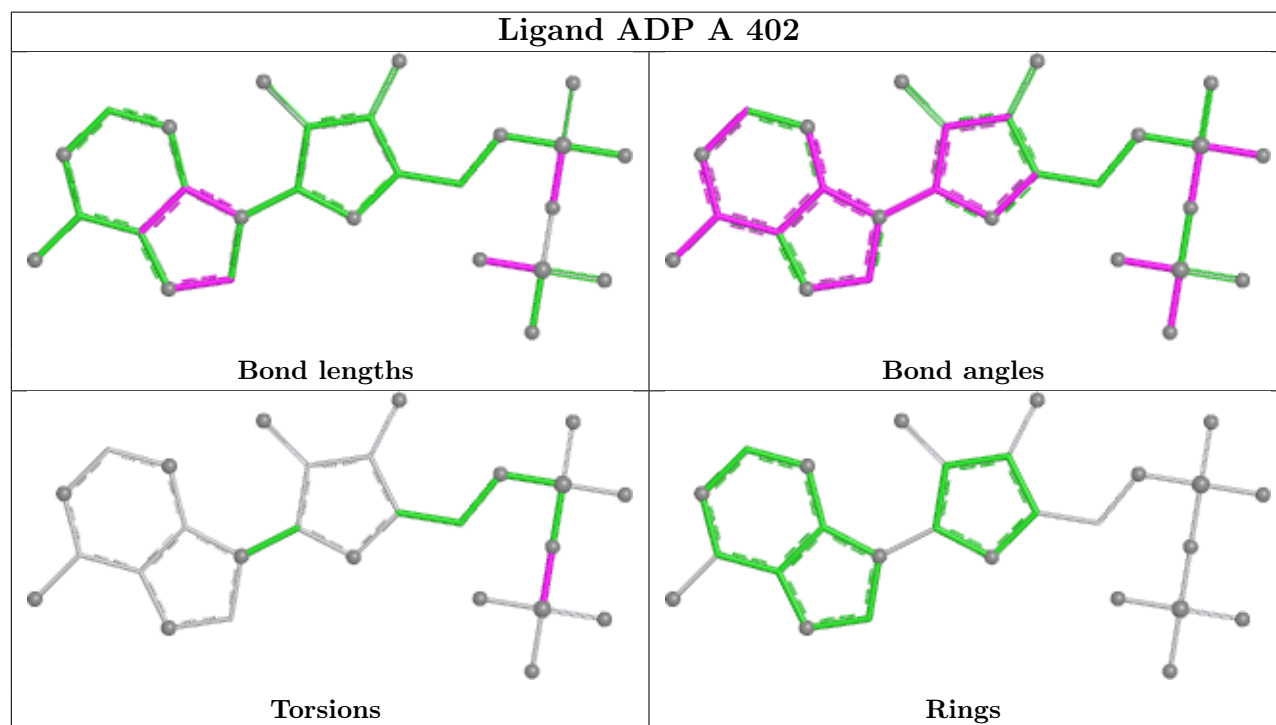
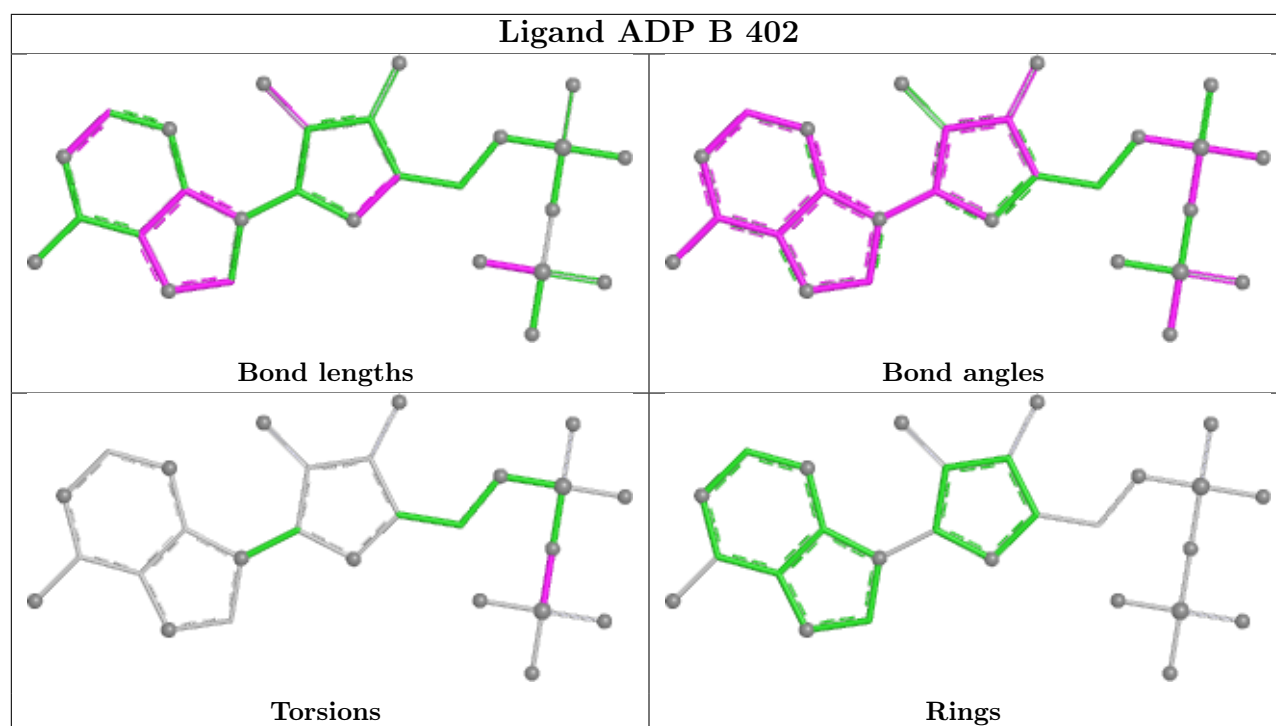
There are no ring outliers.

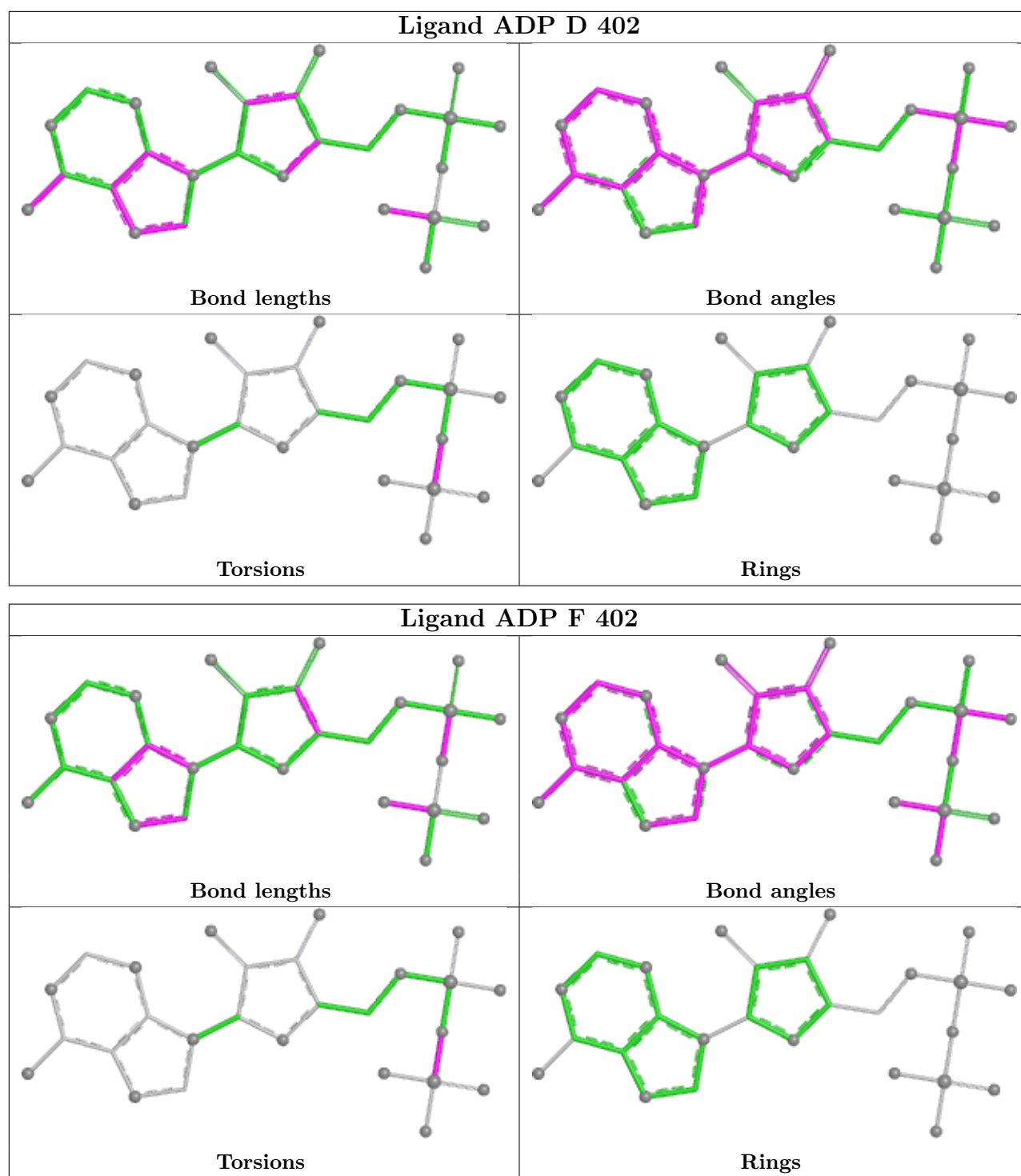
6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	402	ADP	1	0
3	C	402	ADP	2	0
3	B	402	ADP	1	0
3	A	402	ADP	2	0
3	D	402	ADP	3	0
3	F	402	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

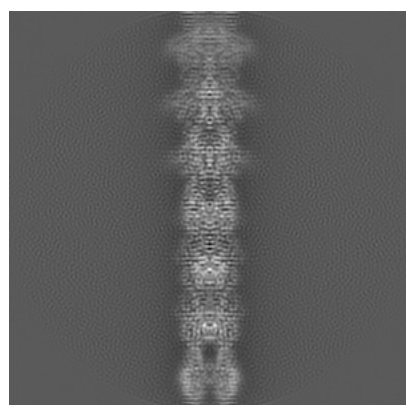
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4062. These allow visual inspection of the internal detail of the map and identification of artifacts.

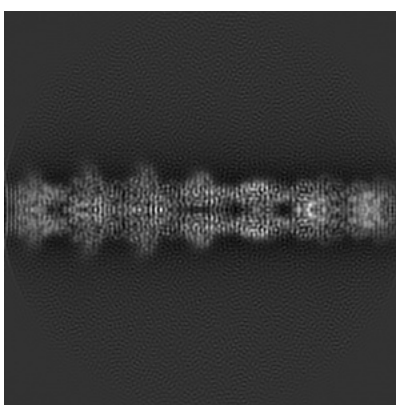
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

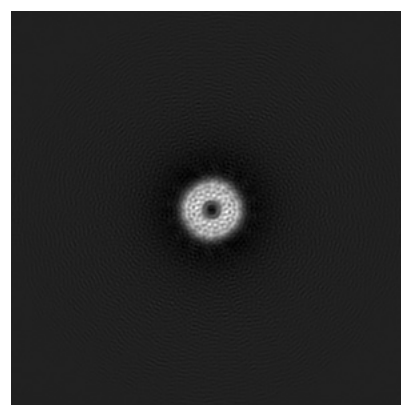
6.1.1 Primary map



X



Y

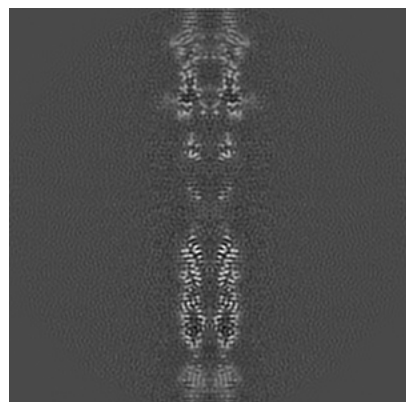


Z

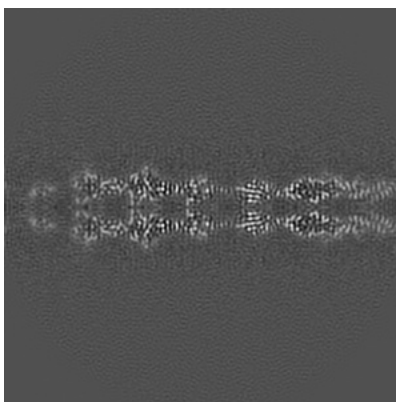
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

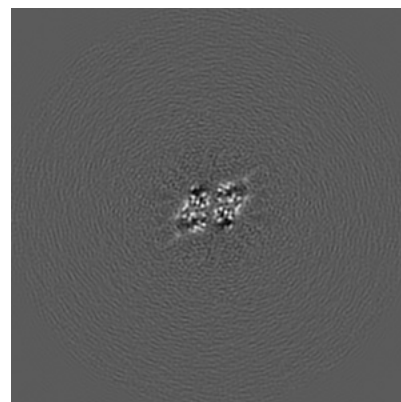
6.2.1 Primary map



X Index: 140



Y Index: 140

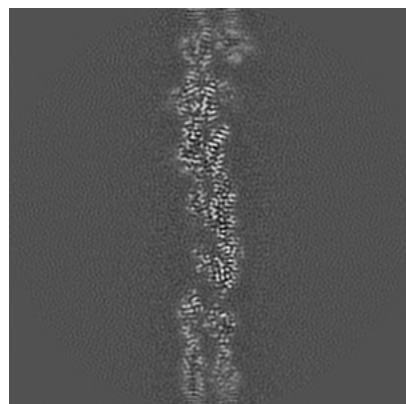


Z Index: 140

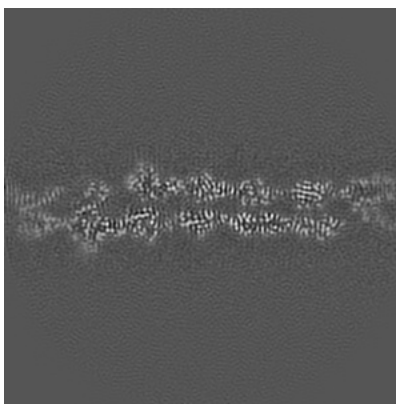
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

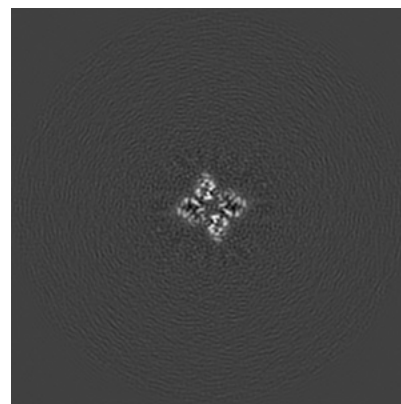
6.3.1 Primary map



X Index: 133



Y Index: 145

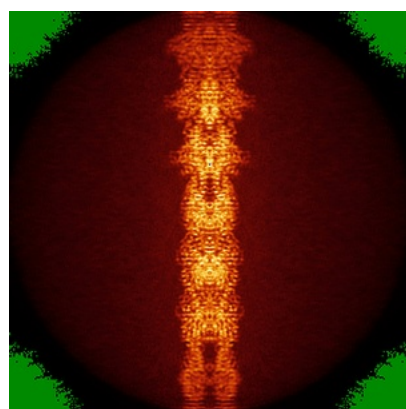


Z Index: 106

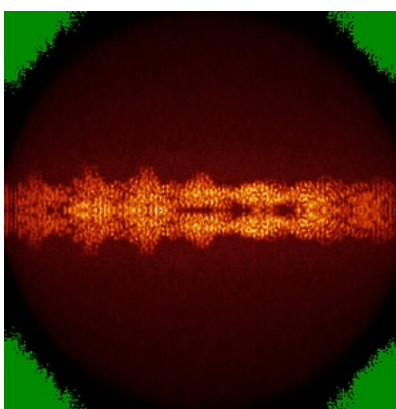
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

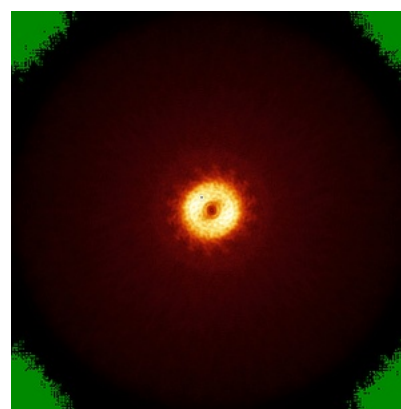
6.4.1 Primary map



X



Y

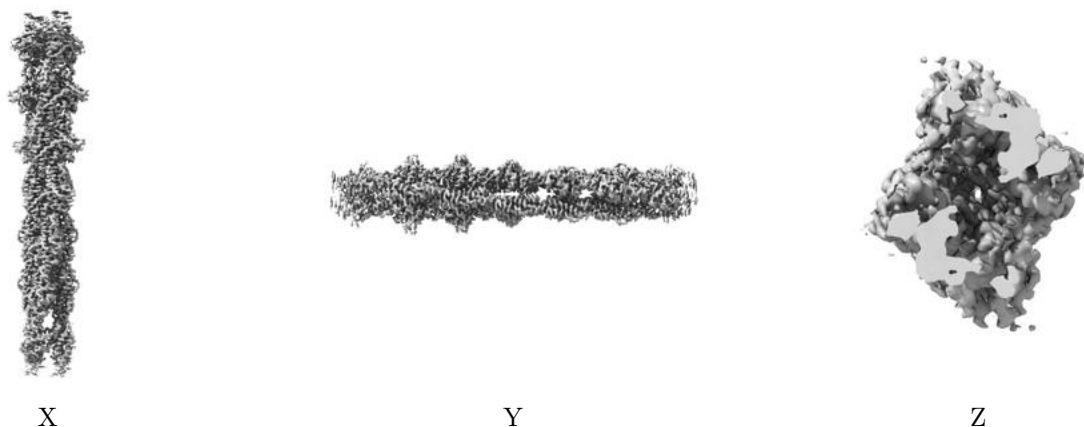


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.155. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

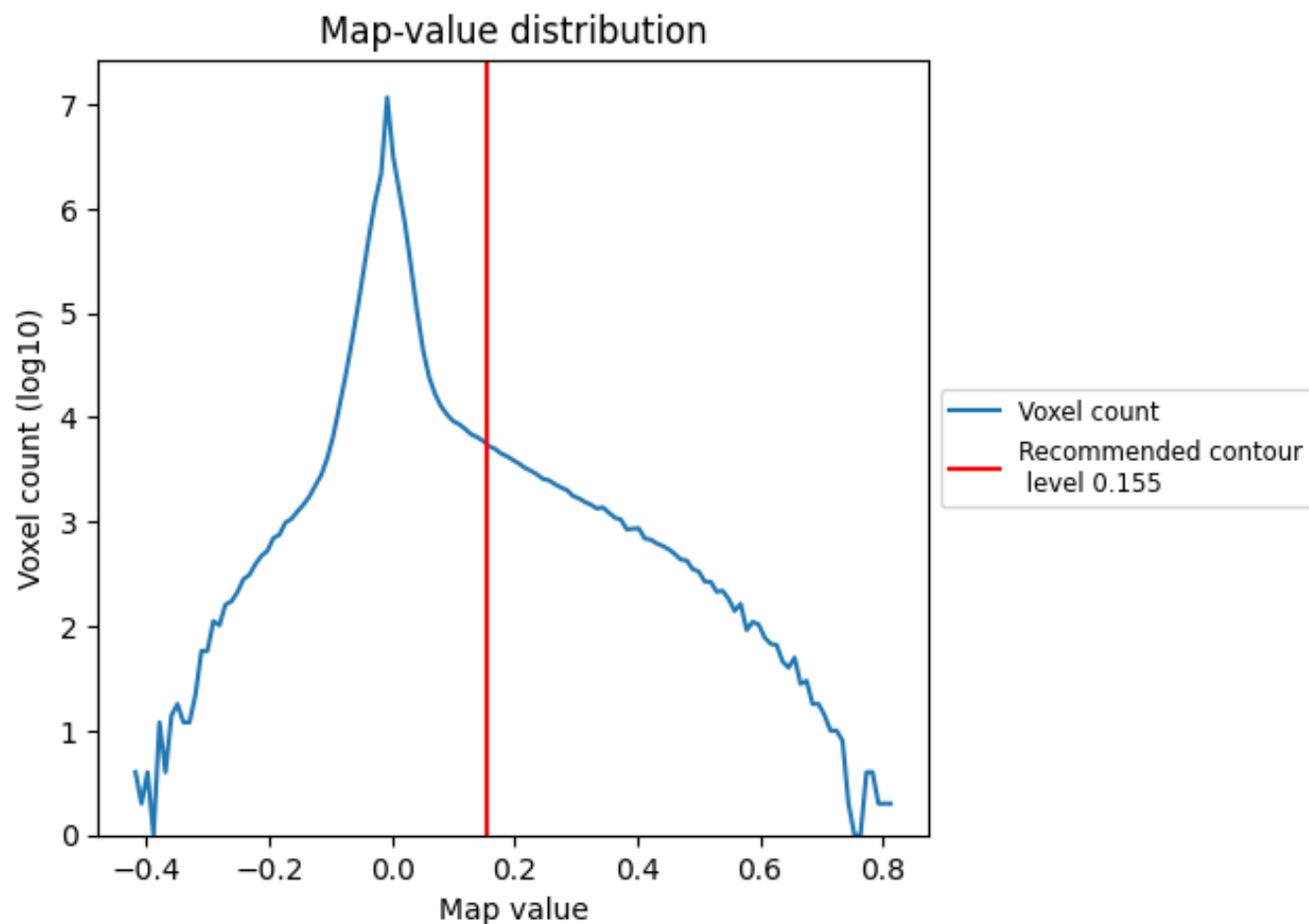
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

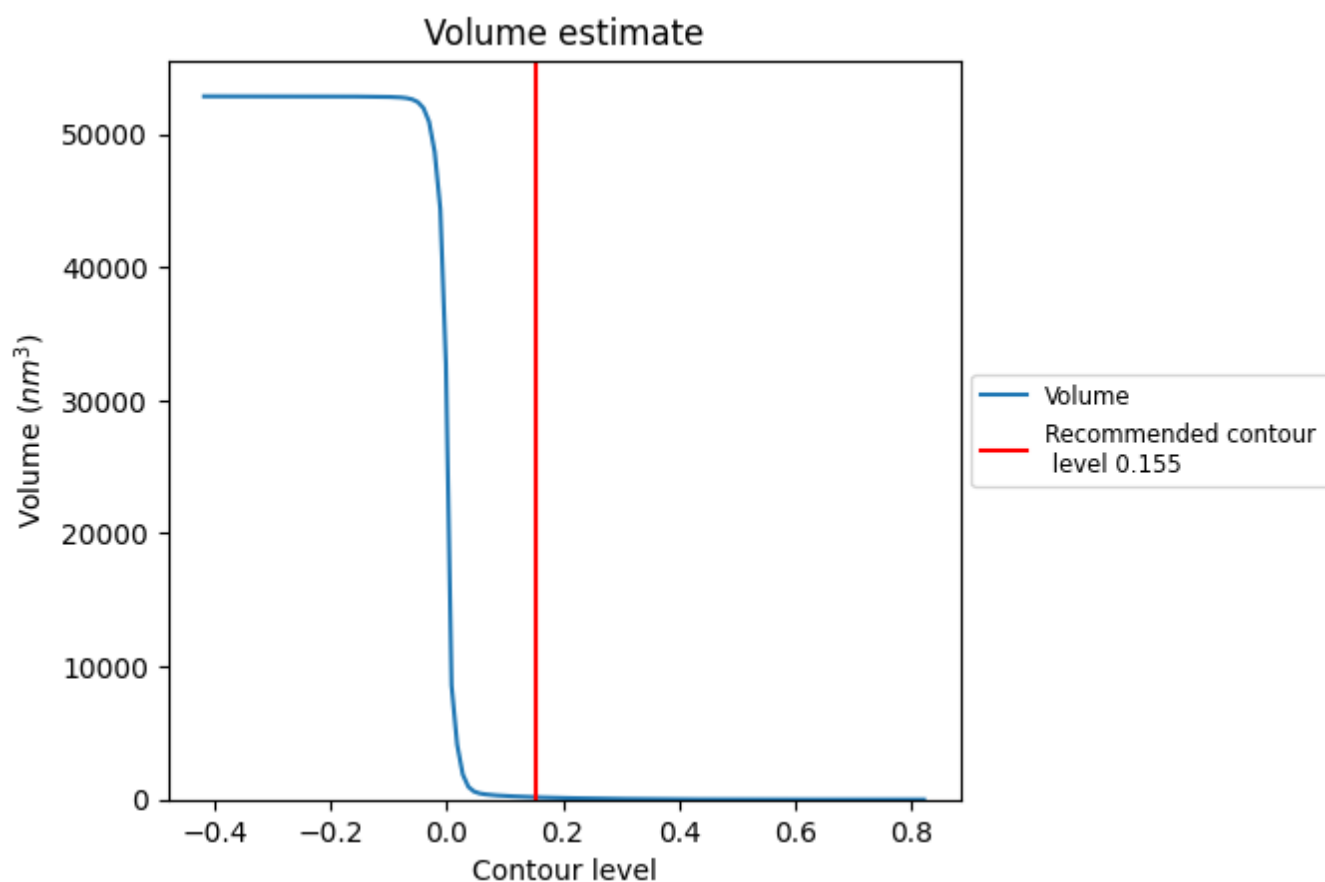
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

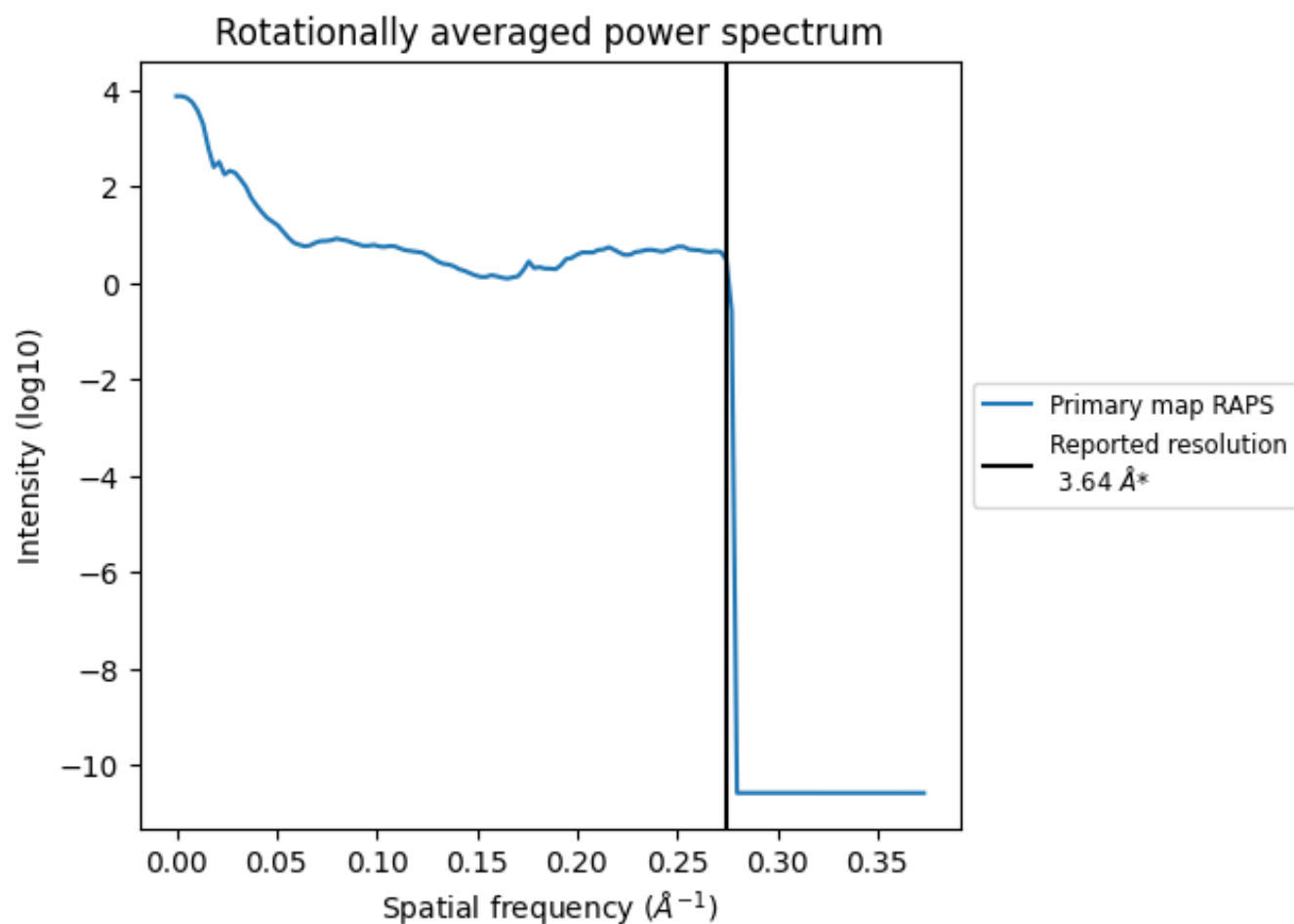
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 173 nm³; this corresponds to an approximate mass of 156 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

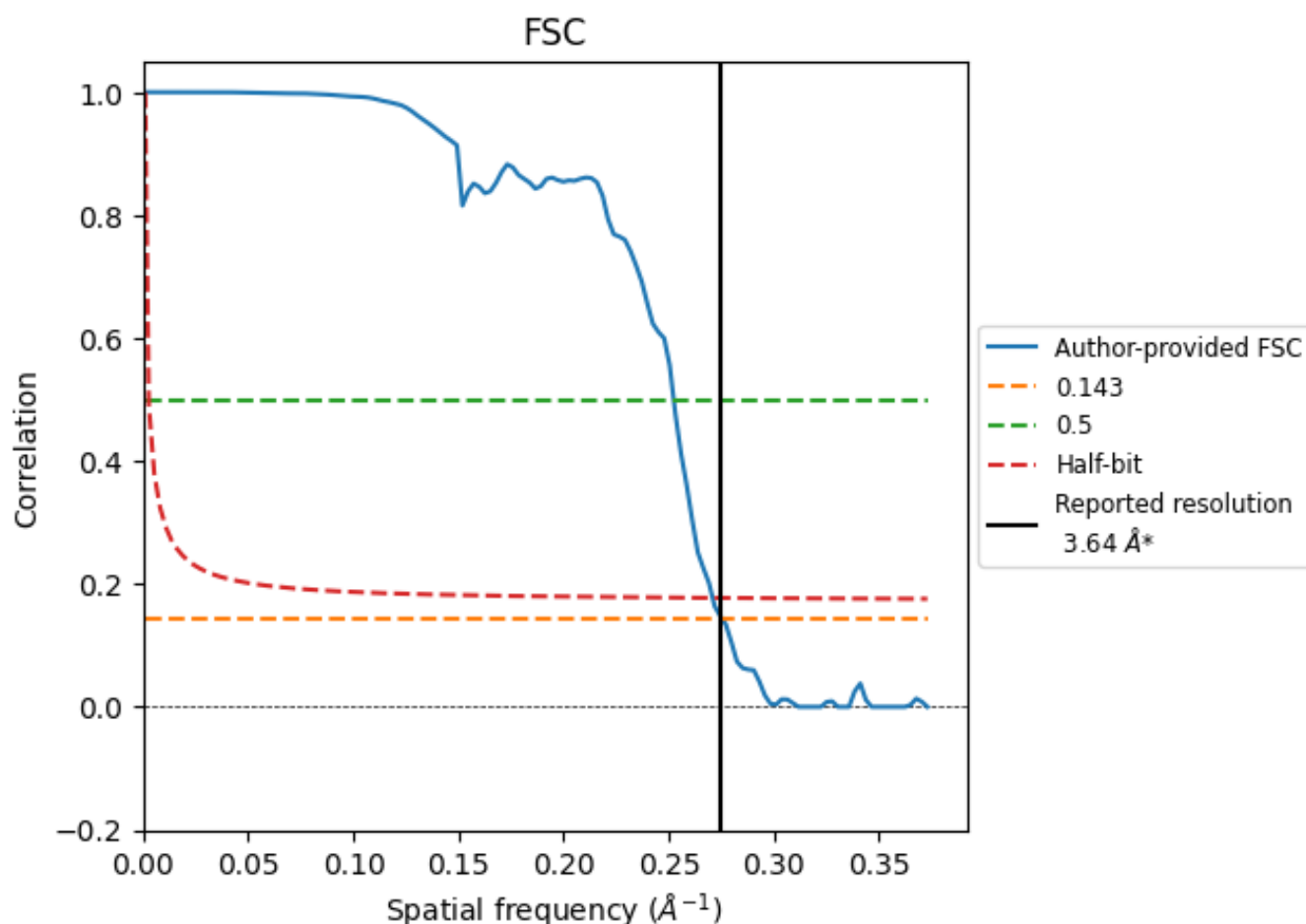


*Reported resolution corresponds to spatial frequency of 0.275 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.275 Å⁻¹

8.2 Resolution estimates [i](#)

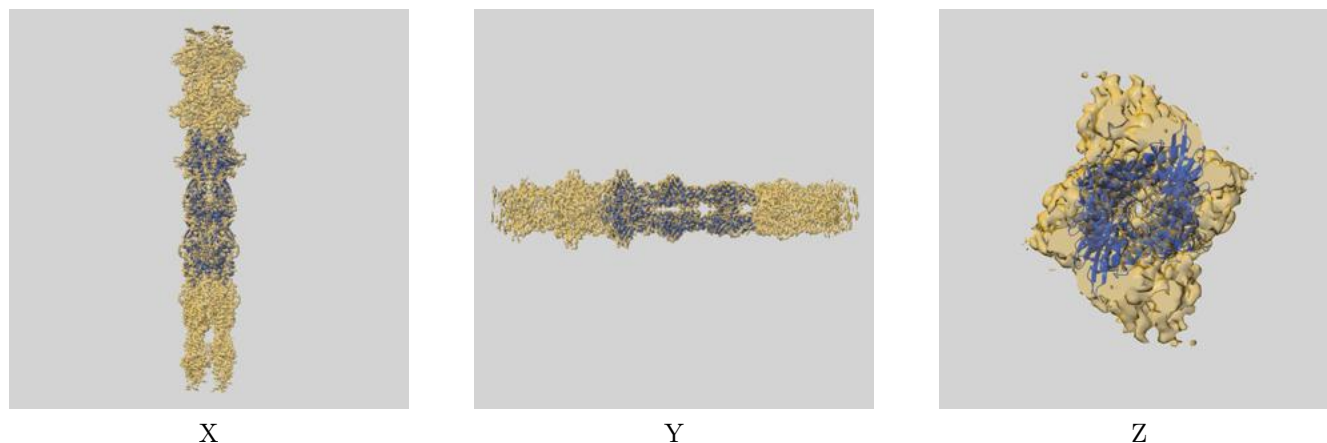
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.64	-	-
Author-provided FSC curve	3.63	3.96	3.69
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

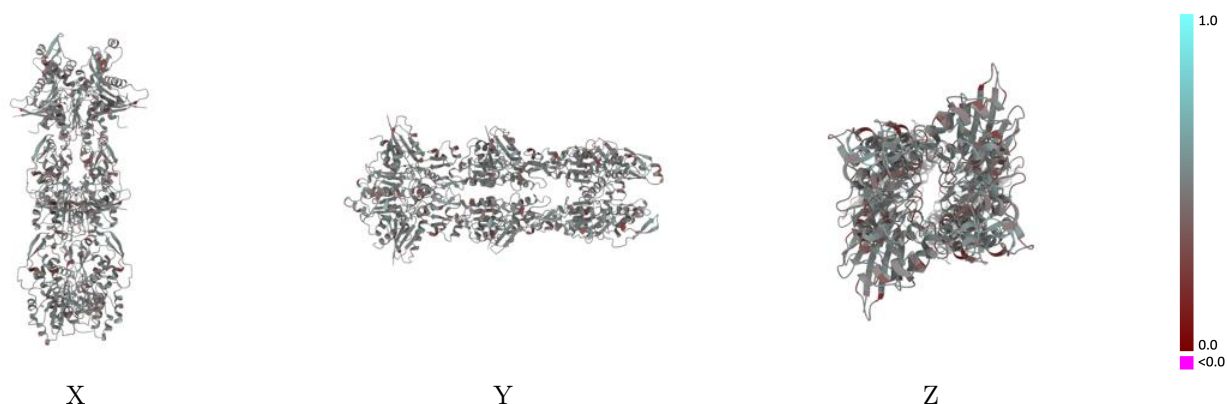
This section contains information regarding the fit between EMDB map EMD-4062 and PDB model 5LJV. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



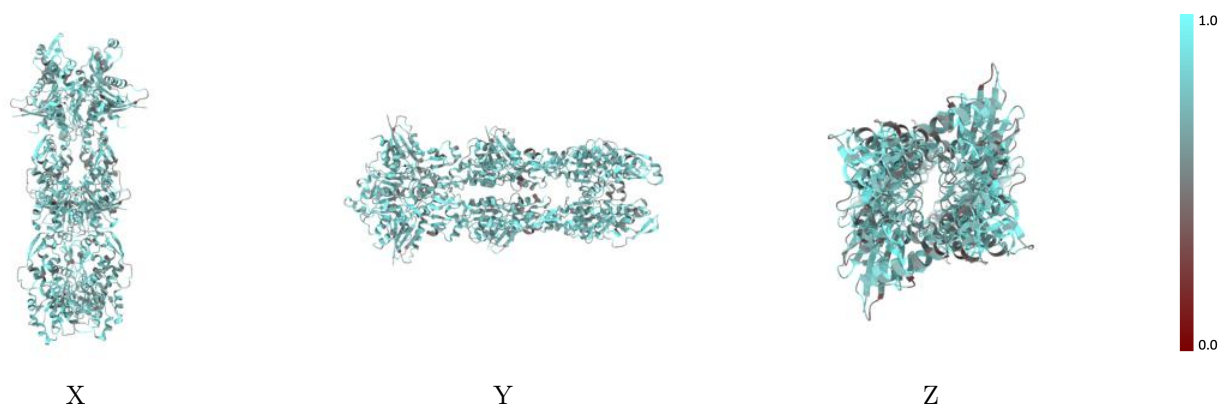
The images above show the 3D surface view of the map at the recommended contour level 0.155 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



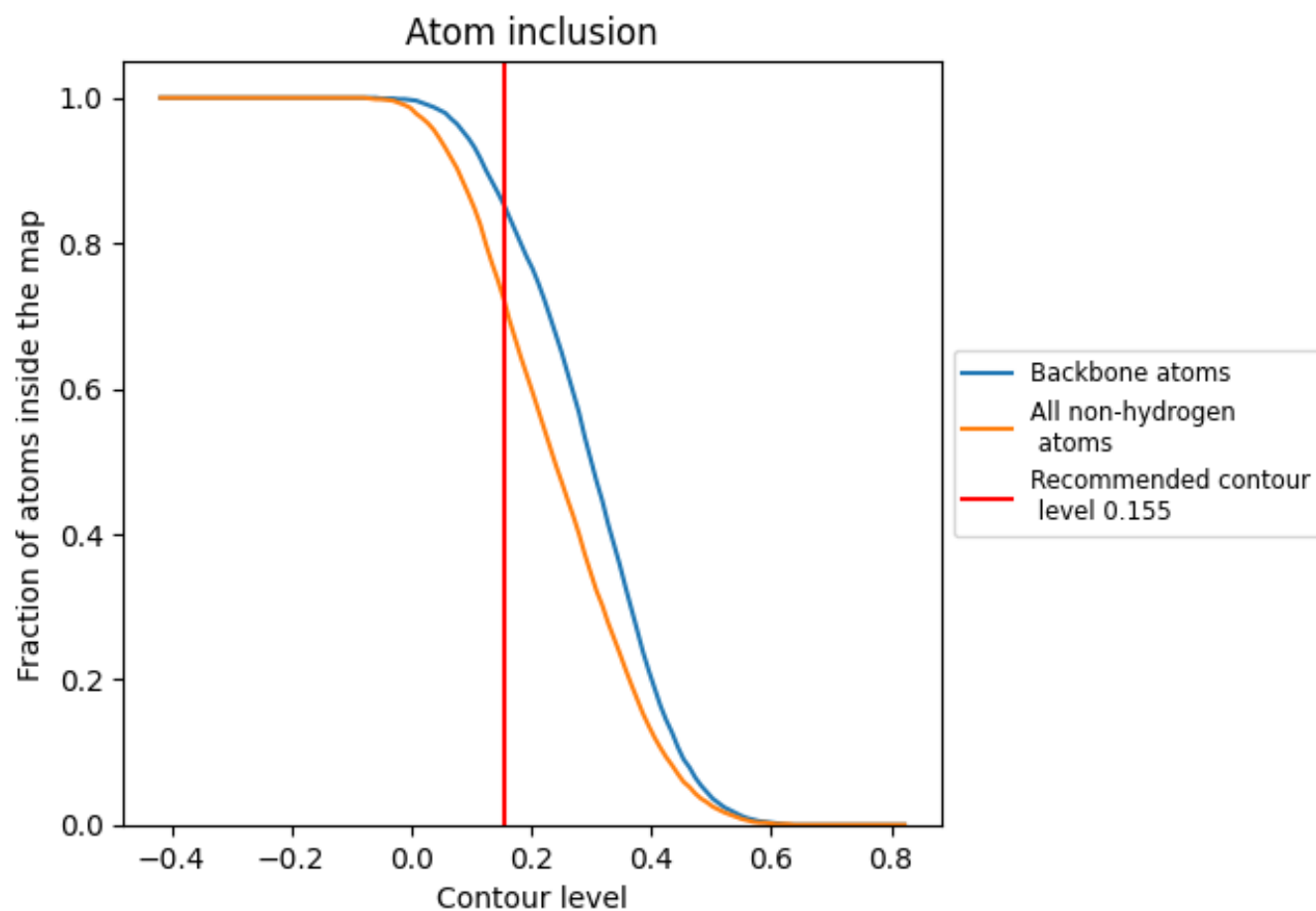
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.155).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.155) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7210	0.4670
A	0.7150	0.4640
B	0.7260	0.4690
C	0.7210	0.4680
D	0.7240	0.4690
E	0.7260	0.4690
F	0.7120	0.4630

1.0

0.0

<0.0