



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 04:46 PM UTC

PDB ID : 8PRW / pdb_00008prw
EMDB ID : EMD-17840
Title : Cryo-EM structure of the yeast fatty acid synthase at 1.9 angstrom resolution
Authors : Singh, K.; Bunzel, G.; Graf, B.; Yip, K.M.; Stark, H.; Chari, A.
Deposited on : 2023-07-12
Resolution : 1.90 Å(reported)

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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

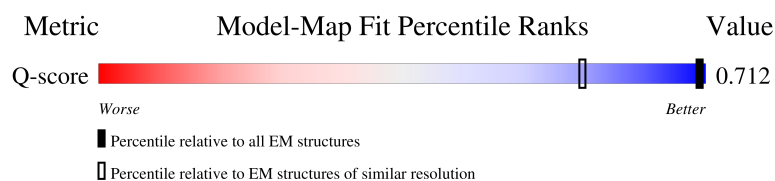
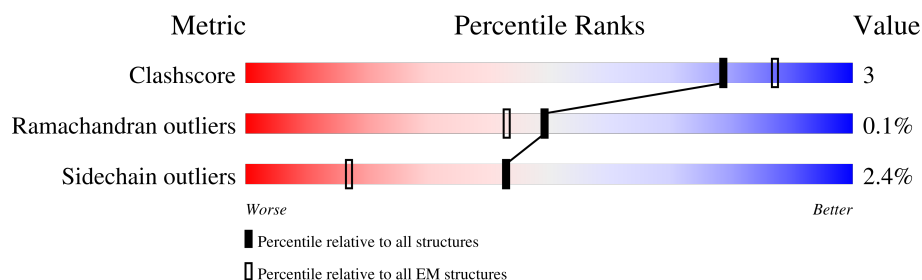
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1185 (1.40 - 2.40)

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	1887	
1	B	1887	
1	C	1887	
1	D	1887	

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Mol	Chain	Length	Quality of chain
1	E	1887	77%7%16%
1	F	1887	76%7%16%
2	G	2051	90%9%.
2	H	2051	90%9% .
2	I	2051	90%9% ..
2	J	2051	89%9% ..
2	K	2051	90%9% .
2	L	2051	90%9% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 179064 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.

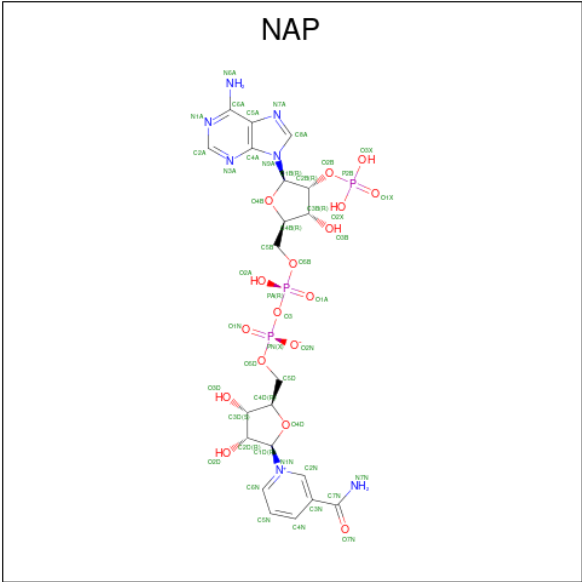
- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1584	Total	C	N	O	S	0	0
			12379	7837	2089	2405	48		
1	B	1584	Total	C	N	O	S	0	0
			12379	7837	2089	2405	48		
1	C	1584	Total	C	N	O	S	0	0
			12379	7837	2089	2405	48		
1	D	1584	Total	C	N	O	S	0	0
			12379	7837	2089	2405	48		
1	E	1584	Total	C	N	O	S	0	0
			12379	7837	2089	2405	48		
1	F	1584	Total	C	N	O	S	0	0
			12379	7837	2089	2405	48		

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

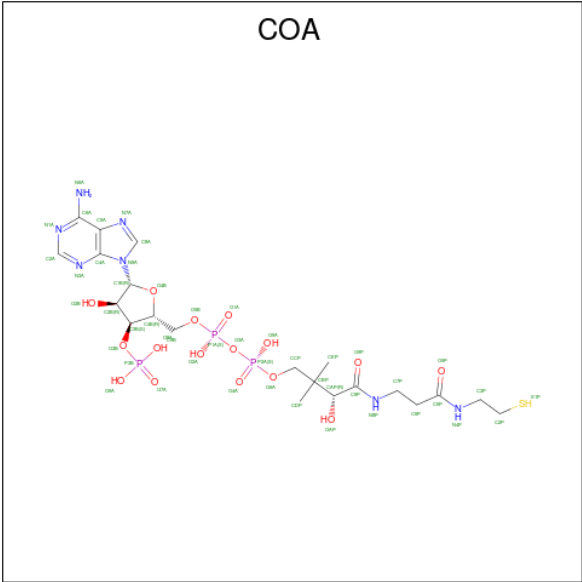
Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	2034	Total	C	N	O	S	0	0
			16010	10261	2661	3032	56		
2	J	2034	Total	C	N	O	S	0	0
			16010	10261	2661	3032	56		
2	I	2034	Total	C	N	O	S	0	0
			16010	10261	2661	3032	56		
2	H	2034	Total	C	N	O	S	0	0
			16010	10261	2661	3032	56		
2	K	2034	Total	C	N	O	S	0	0
			16010	10261	2661	3032	56		
2	L	2034	Total	C	N	O	S	0	0
			16010	10261	2661	3032	56		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



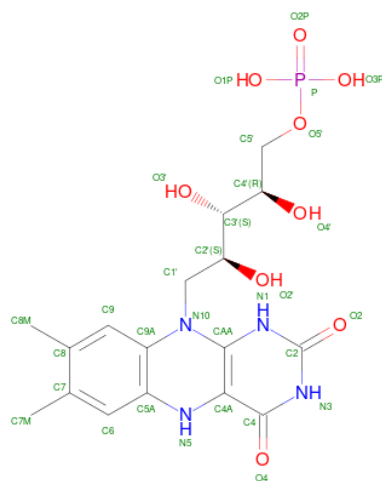
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	G	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	B	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	C	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	D	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	E	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	F	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	J	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	I	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	H	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	K	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	L	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 4 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
4	G	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	
4	J	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	
4	I	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	
4	H	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	
4	K	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	
4	L	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	

- Molecule 5 is 1-DEOXY-1-(7,8-DIMETHYL-2,4-DIOXO-3,4-DIHYDRO-2H-BENZO[G]PT ERIDIN-1-ID-10(5H)-YL)-5-O-PHOSPHONATO-D-RIBITOL (CCD ID: FNR) (formula: C₁₇H₂₃N₄O₉P) (labeled as "Ligand of Interest" by depositor).



- Molecule 6 is water.

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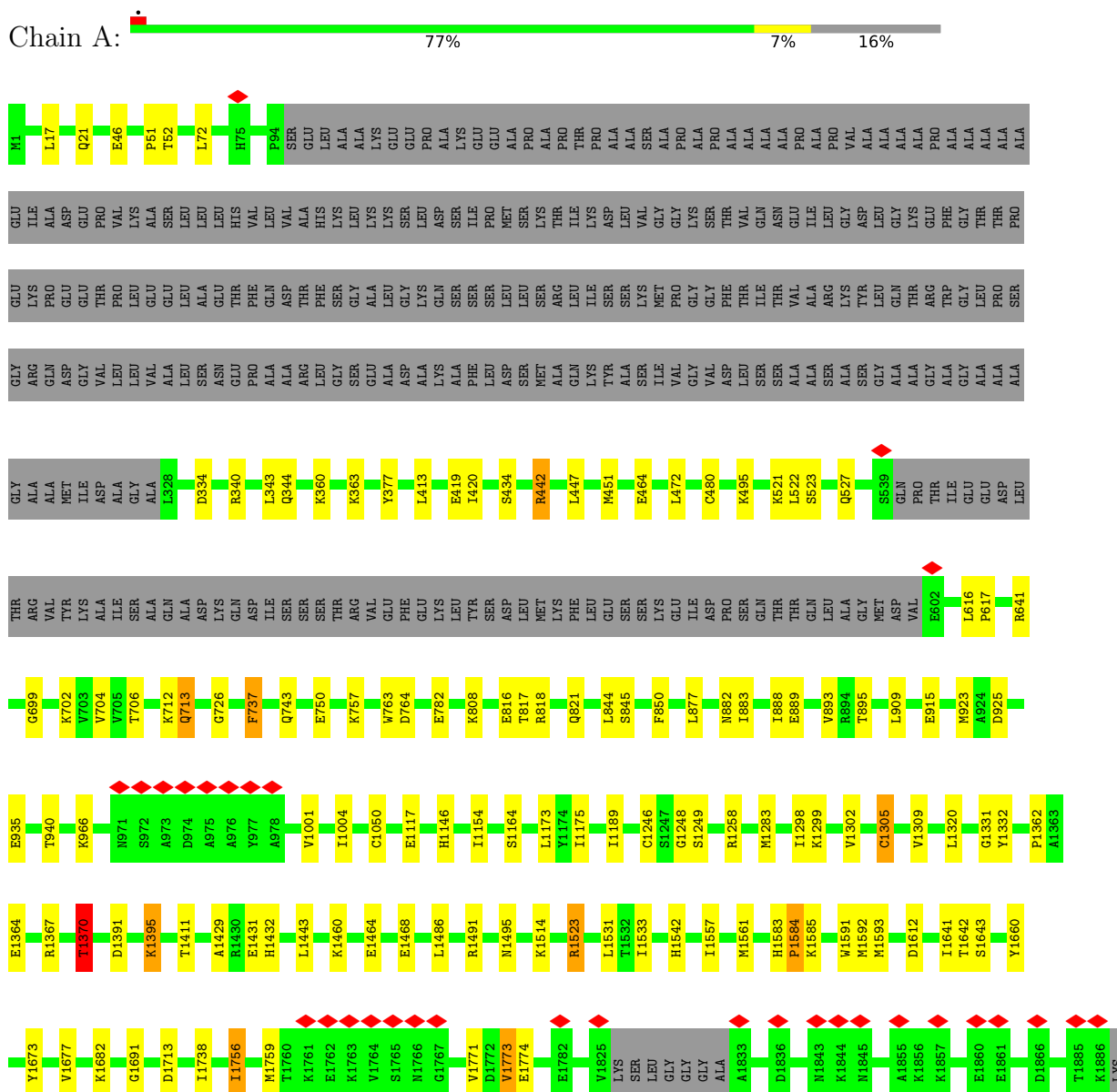
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Mol	Chain	Residues	Atoms		AltConf
6	F	901	Total 901	O 901	0
6	J	364	Total 364	O 364	0
6	I	367	Total 367	O 367	0
6	H	377	Total 377	O 377	0
6	K	389	Total 389	O 389	0
6	L	377	Total 377	O 377	0

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.

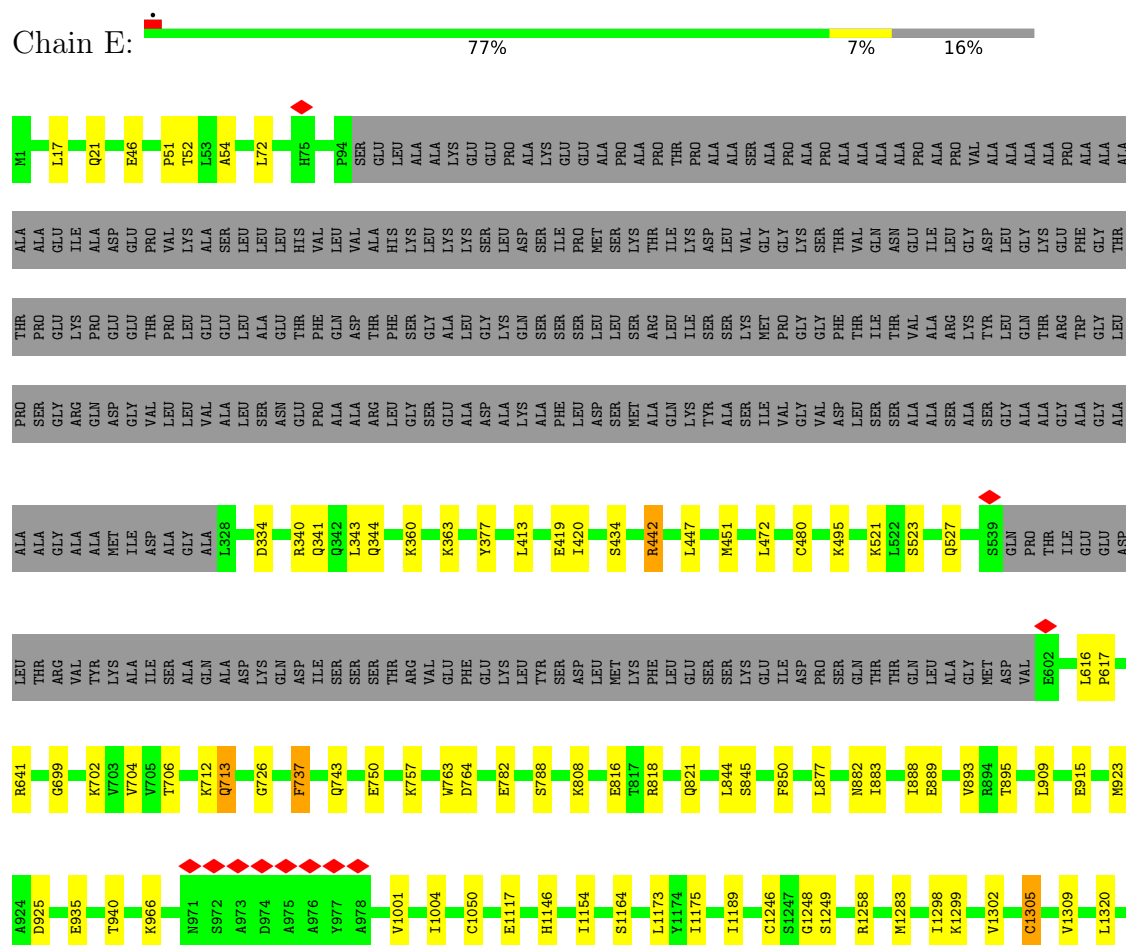
- Molecule 1: Fatty acid synthase subunit alpha

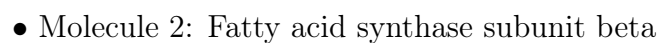


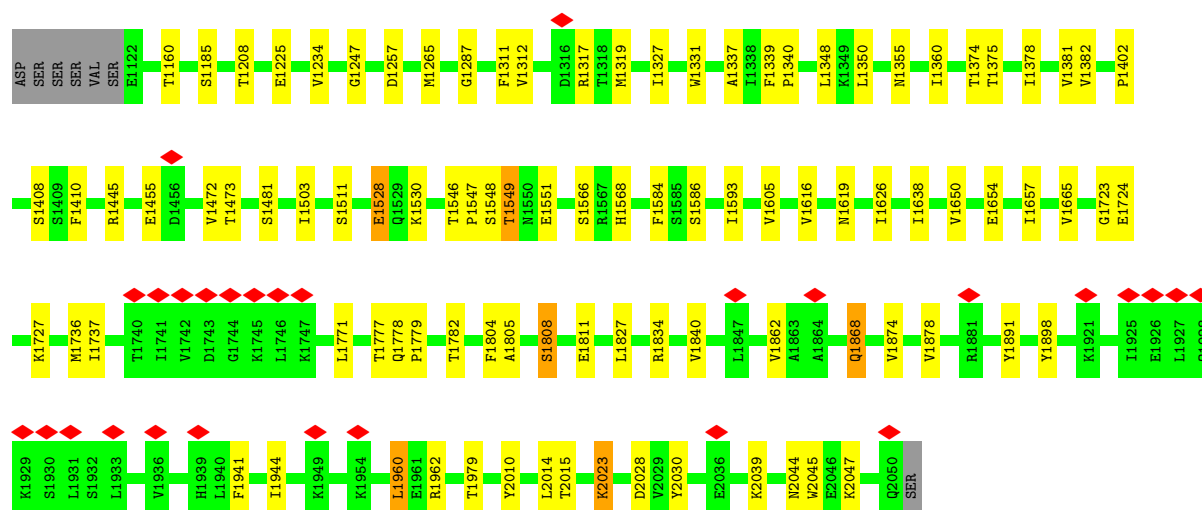
- Molecule 1: Fatty acid synthase subunit alpha



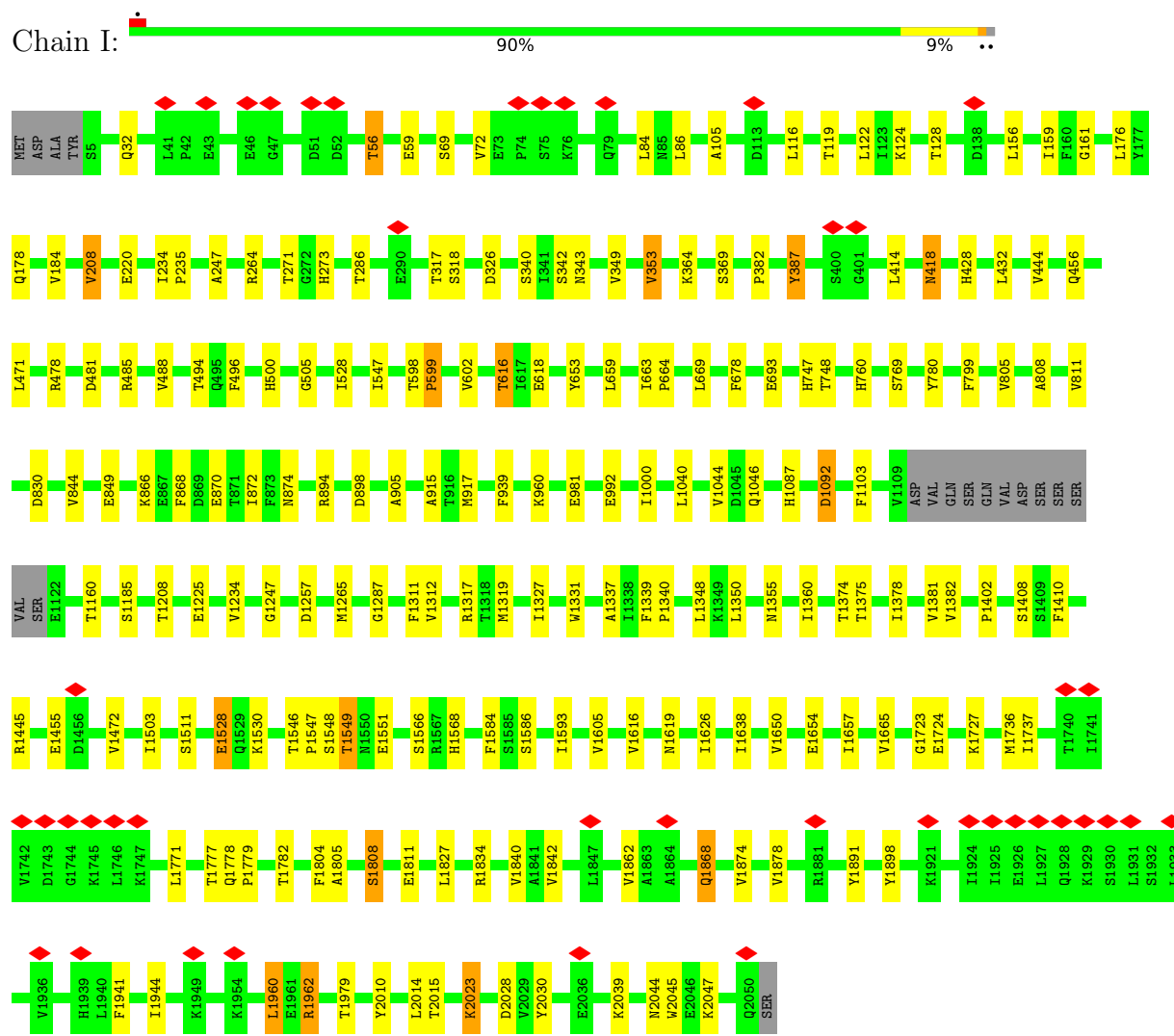
- Molecule 1: Fatty acid synthase subunit alpha



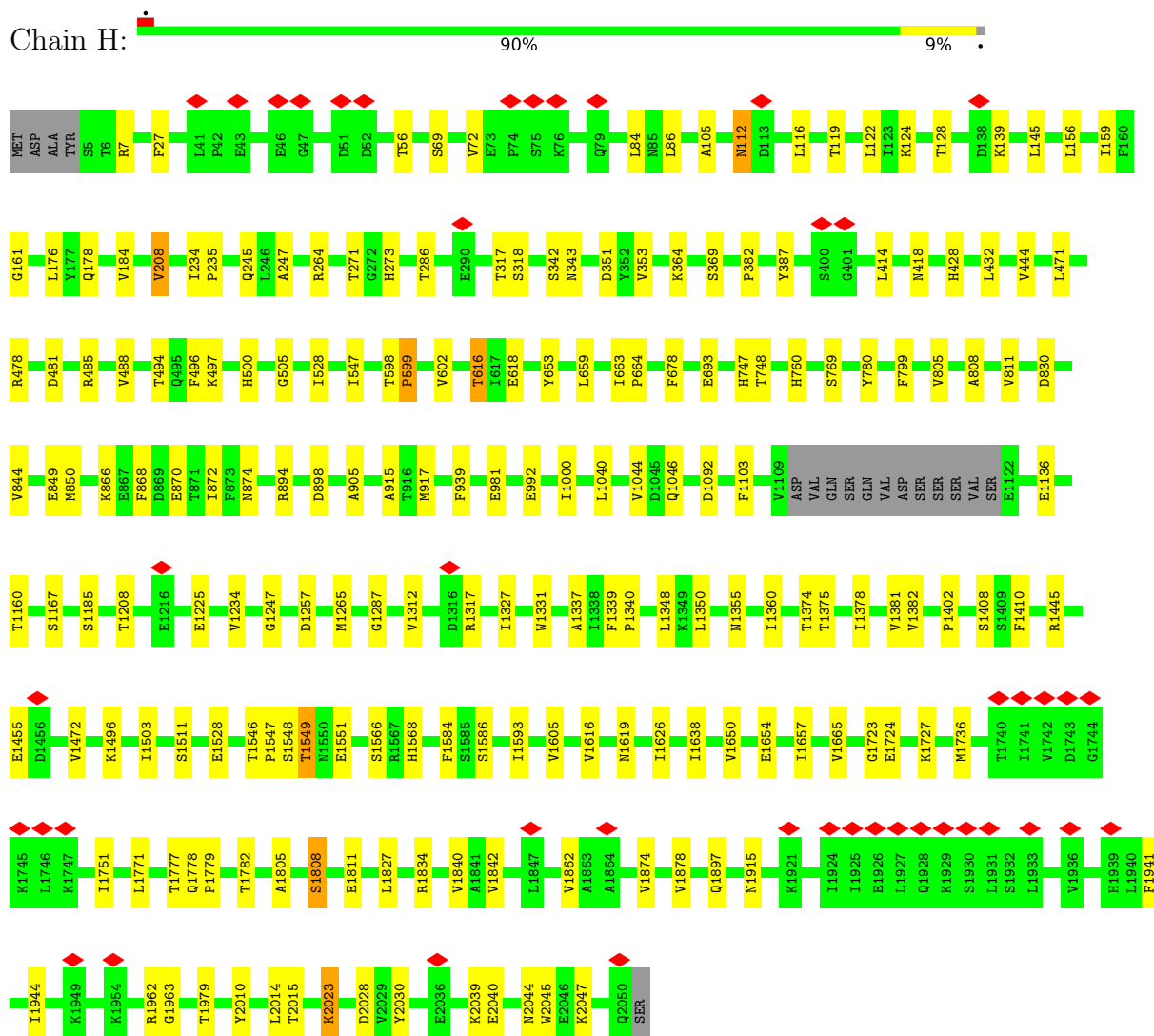




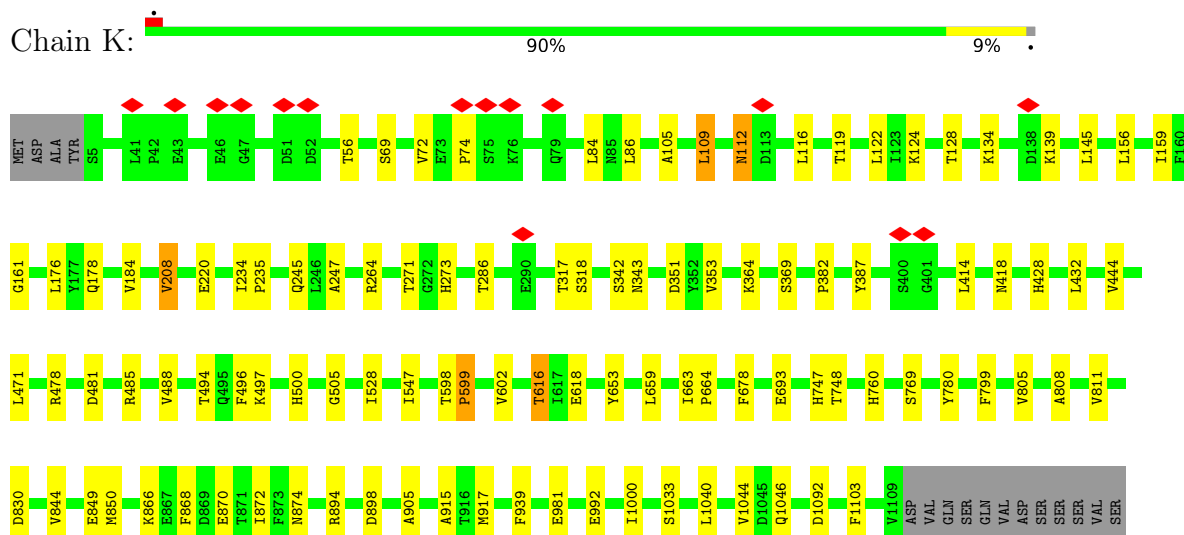
• Molecule 2: Fatty acid synthase subunit beta

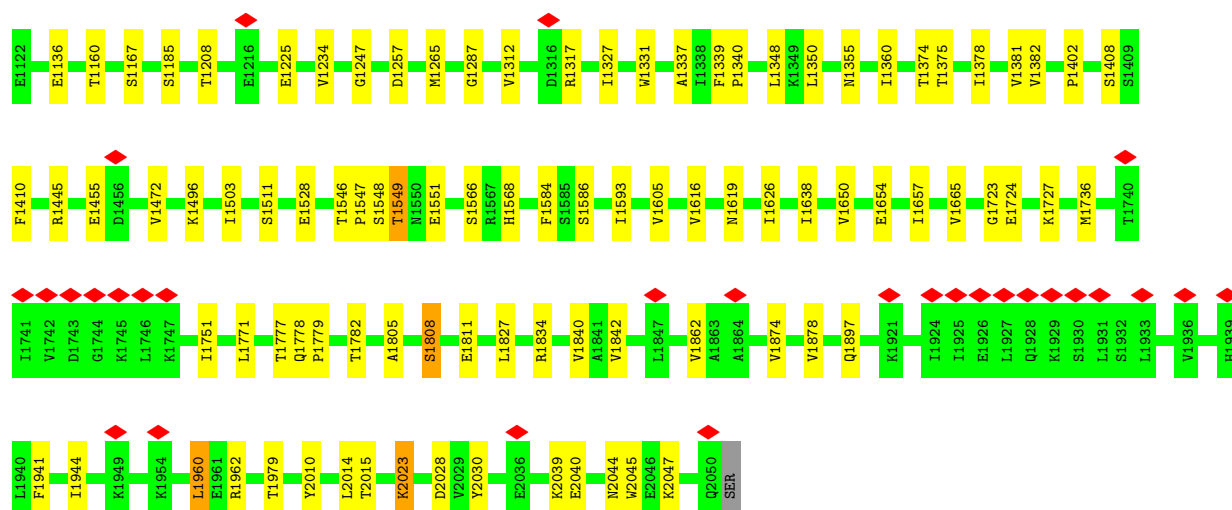


• Molecule 2: Fatty acid synthase subunit beta



• Molecule 2: Fatty acid synthase subunit beta





• Molecule 2: Fatty acid synthase subunit beta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	255481	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.109	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.01	Depositor
Map size ($\text{\AA}$)	344.4, 344.4, 344.4	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.615, 0.615, 0.615	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: J8W, FNR, NAP, COA

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	1.14	13/12613 (0.1%)	1.35	8/17048 (0.0%)
1	B	1.14	14/12613 (0.1%)	1.35	9/17048 (0.1%)
1	C	1.14	11/12613 (0.1%)	1.35	9/17048 (0.1%)
1	D	1.14	10/12613 (0.1%)	1.35	9/17048 (0.1%)
1	E	1.14	14/12613 (0.1%)	1.35	11/17048 (0.1%)
1	F	1.14	13/12613 (0.1%)	1.35	8/17048 (0.0%)
2	G	0.96	0/16362	1.40	8/22199 (0.0%)
2	H	0.96	1/16362 (0.0%)	1.40	8/22199 (0.0%)
2	I	0.96	1/16362 (0.0%)	1.40	10/22199 (0.0%)
2	J	0.96	0/16362	1.40	9/22199 (0.0%)
2	K	0.96	1/16362 (0.0%)	1.40	9/22199 (0.0%)
2	L	0.96	0/16362	1.40	8/22199 (0.0%)
All	All	1.04	78/173850 (0.0%)	1.38	106/235482 (0.0%)

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
2	G	0	1
2	H	0	1
2	I	0	1
2	J	0	1
2	K	0	1
2	L	0	1
All	All	0	6

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	699	GLY	C-O	-6.83	1.16	1.24
1	E	699	GLY	C-O	-6.83	1.16	1.24
1	B	699	GLY	C-O	-6.83	1.16	1.24
1	F	699	GLY	C-O	-6.83	1.16	1.24
1	D	699	GLY	C-O	-6.80	1.16	1.24
1	C	699	GLY	C-O	-6.74	1.16	1.24
1	F	1429	ALA	C-O	-6.71	1.15	1.24
1	B	1429	ALA	C-O	-6.67	1.15	1.24
1	A	1429	ALA	C-O	-6.63	1.15	1.24
1	E	1429	ALA	C-O	-6.63	1.15	1.24
1	C	1429	ALA	C-O	-6.62	1.15	1.24
1	D	1429	ALA	C-O	-6.58	1.15	1.24
1	D	1395	LYS	C-O	-6.41	1.16	1.24
1	E	1395	LYS	C-O	-6.34	1.16	1.24
1	B	1395	LYS	C-O	-6.33	1.16	1.24
1	F	1395	LYS	C-O	-6.33	1.16	1.24
1	C	1395	LYS	C-O	-6.32	1.16	1.24
1	F	737	PHE	C-O	-6.27	1.15	1.23
1	A	1395	LYS	C-O	-6.26	1.16	1.24
1	B	737	PHE	C-O	-6.24	1.15	1.23
1	C	737	PHE	C-O	-6.24	1.15	1.23
1	D	737	PHE	C-O	-6.24	1.15	1.23
1	E	737	PHE	C-O	-6.19	1.15	1.23
1	A	737	PHE	C-O	-6.17	1.15	1.23
1	C	1249	SER	CA-CB	-5.98	1.43	1.53
1	B	1249	SER	CA-CB	-5.98	1.43	1.53
1	F	1249	SER	CA-CB	-5.98	1.43	1.53
1	D	1249	SER	CA-CB	-5.95	1.43	1.53
1	A	1249	SER	CA-CB	-5.89	1.43	1.53
1	E	1249	SER	CA-CB	-5.89	1.43	1.53
1	C	1309	VAL	C-O	-5.72	1.17	1.24
1	D	1309	VAL	C-O	-5.72	1.17	1.24
1	B	1309	VAL	C-O	-5.66	1.17	1.24
1	F	1309	VAL	C-O	-5.66	1.17	1.24
1	A	1309	VAL	C-O	-5.61	1.17	1.24
1	E	1309	VAL	C-O	-5.60	1.17	1.24
1	A	1320	LEU	C-O	-5.33	1.17	1.24
1	B	1542	HIS	CE1-NE2	5.27	1.37	1.32
1	E	1320	LEU	C-O	-5.27	1.17	1.24
1	F	1320	LEU	C-O	-5.27	1.17	1.24
1	A	1542	HIS	CE1-NE2	5.26	1.37	1.32
1	B	1320	LEU	C-O	-5.24	1.17	1.24
1	C	1542	HIS	CE1-NE2	5.22	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	1542	HIS	CE1-NE2	5.20	1.37	1.32
1	D	442	ARG	C-O	-5.19	1.16	1.24
1	D	1542	HIS	CE1-NE2	5.18	1.37	1.32
1	E	1542	HIS	CE1-NE2	5.17	1.37	1.32
1	A	1593	MET	C-O	-5.14	1.18	1.24
1	F	442	ARG	C-O	-5.14	1.17	1.24
1	C	442	ARG	C-O	-5.13	1.17	1.24
1	A	442	ARG	C-O	-5.12	1.17	1.24
1	E	442	ARG	C-O	-5.12	1.17	1.24
1	E	1593	MET	C-O	-5.12	1.18	1.24
1	B	1585	LYS	C-O	-5.09	1.17	1.24
1	C	1585	LYS	C-O	-5.09	1.17	1.24
1	D	1585	LYS	C-O	-5.09	1.17	1.24
1	B	442	ARG	C-O	-5.08	1.17	1.24
1	B	789	GLU	C-O	-5.08	1.18	1.24
1	B	1593	MET	C-O	-5.08	1.18	1.24
1	F	1593	MET	C-O	-5.08	1.18	1.24
1	A	1585	LYS	C-O	-5.07	1.17	1.24
2	I	184	VAL	N-CA	5.07	1.50	1.46
1	F	788	SER	C-O	-5.05	1.18	1.24
1	E	788	SER	C-O	-5.05	1.18	1.24
1	A	1584	PRO	C-O	-5.04	1.17	1.24
1	B	788	SER	C-O	-5.04	1.18	1.24
1	E	1584	PRO	C-O	-5.04	1.17	1.24
1	C	1593	MET	C-O	-5.04	1.18	1.24
1	D	1593	MET	C-O	-5.04	1.18	1.24
1	C	1584	PRO	C-O	-5.03	1.17	1.24
1	A	1691	GLY	CA-C	-5.01	1.46	1.52
1	E	1691	GLY	CA-C	-5.01	1.46	1.52
2	H	184	VAL	N-CA	5.01	1.50	1.46
2	K	184	VAL	N-CA	5.01	1.50	1.46
1	E	1585	LYS	C-O	-5.01	1.17	1.24
1	F	1585	LYS	C-O	-5.01	1.17	1.24
1	B	1584	PRO	C-O	-5.01	1.17	1.24
1	F	1584	PRO	C-O	-5.01	1.17	1.24

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	432	LEU	CA-C-N	7.48	124.95	120.24
2	H	432	LEU	C-N-CA	7.48	124.95	120.24
2	G	432	LEU	CA-C-N	7.48	124.95	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	432	LEU	C-N-CA	7.48	124.95	120.24
2	L	432	LEU	CA-C-N	7.47	124.95	120.24
2	L	432	LEU	C-N-CA	7.47	124.95	120.24
2	K	432	LEU	CA-C-N	7.46	124.94	120.24
2	K	432	LEU	C-N-CA	7.46	124.94	120.24
2	I	432	LEU	CA-C-N	7.42	124.92	120.24
2	I	432	LEU	C-N-CA	7.42	124.92	120.24
2	J	432	LEU	CA-C-N	7.42	124.91	120.24
2	J	432	LEU	C-N-CA	7.42	124.91	120.24
1	C	1523	ARG	NE-CZ-NH2	-7.37	112.56	119.20
1	D	1523	ARG	NE-CZ-NH2	-7.35	112.59	119.20
1	F	1523	ARG	NE-CZ-NH2	-7.33	112.61	119.20
1	E	1523	ARG	NE-CZ-NH2	-7.26	112.67	119.20
1	A	1523	ARG	NE-CZ-NH2	-7.22	112.70	119.20
1	B	1523	ARG	NE-CZ-NH2	-7.22	112.70	119.20
1	F	1612	ASP	CA-CB-CG	6.50	119.10	112.60
1	B	1612	ASP	CA-CB-CG	6.48	119.08	112.60
1	D	1612	ASP	CA-CB-CG	6.46	119.06	112.60
1	A	1612	ASP	CA-CB-CG	6.46	119.06	112.60
1	C	1612	ASP	CA-CB-CG	6.43	119.03	112.60
1	E	1612	ASP	CA-CB-CG	6.43	119.03	112.60
1	F	1189	ILE	CB-CA-C	6.37	117.13	110.88
1	B	1189	ILE	CB-CA-C	6.37	117.12	110.88
1	A	1189	ILE	CB-CA-C	6.35	117.10	110.88
1	C	1189	ILE	CB-CA-C	6.33	117.09	110.88
1	D	1189	ILE	CB-CA-C	6.31	117.06	110.88
1	E	1189	ILE	CB-CA-C	6.29	117.05	110.88
1	C	1370	THR	OG1-CB-CG2	6.04	121.39	109.30
1	A	1370	THR	OG1-CB-CG2	6.04	121.38	109.30
1	E	1370	THR	OG1-CB-CG2	6.04	121.38	109.30
1	F	1370	THR	OG1-CB-CG2	6.03	121.36	109.30
1	D	1370	THR	OG1-CB-CG2	6.01	121.32	109.30
1	B	1370	THR	OG1-CB-CG2	5.96	121.22	109.30
2	H	387	TYR	CA-C-N	5.89	126.48	119.94
2	H	387	TYR	C-N-CA	5.89	126.48	119.94
2	K	387	TYR	CA-C-N	5.89	126.48	119.94
2	K	387	TYR	C-N-CA	5.89	126.48	119.94
2	G	387	TYR	CA-C-N	5.88	126.47	119.94
2	G	387	TYR	C-N-CA	5.88	126.47	119.94
2	I	387	TYR	CA-C-N	5.88	126.47	119.94
2	I	387	TYR	C-N-CA	5.88	126.47	119.94
2	L	387	TYR	CA-C-N	5.88	126.47	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	387	TYR	C-N-CA	5.88	126.47	119.94
2	J	387	TYR	CA-C-N	5.86	126.45	119.94
2	J	387	TYR	C-N-CA	5.86	126.45	119.94
1	C	1432	HIS	CA-CB-CG	-5.81	107.99	113.80
1	D	1432	HIS	CA-CB-CG	-5.81	107.99	113.80
1	A	1432	HIS	CA-CB-CG	-5.81	107.99	113.80
1	F	1432	HIS	CA-CB-CG	-5.79	108.00	113.80
1	B	1432	HIS	CA-CB-CG	-5.79	108.01	113.80
1	E	1432	HIS	CA-CB-CG	-5.77	108.03	113.80
1	D	1523	ARG	CG-CD-NE	-5.58	99.73	112.00
1	C	1523	ARG	CG-CD-NE	-5.57	99.75	112.00
1	F	1523	ARG	CG-CD-NE	-5.55	99.79	112.00
1	A	1523	ARG	CG-CD-NE	-5.54	99.81	112.00
1	E	1523	ARG	CG-CD-NE	-5.54	99.82	112.00
1	B	1523	ARG	CG-CD-NE	-5.53	99.84	112.00
1	C	1258	ARG	CA-C-N	5.38	126.07	119.99
1	C	1258	ARG	C-N-CA	5.38	126.07	119.99
1	E	1258	ARG	CA-C-N	5.37	126.06	119.99
1	E	1258	ARG	C-N-CA	5.37	126.06	119.99
1	D	1258	ARG	CA-C-N	5.35	126.04	119.99
1	D	1258	ARG	C-N-CA	5.35	126.04	119.99
1	F	1258	ARG	CA-C-N	5.34	126.03	119.99
1	F	1258	ARG	C-N-CA	5.34	126.03	119.99
1	B	1258	ARG	CA-C-N	5.34	126.03	119.99
1	B	1258	ARG	C-N-CA	5.34	126.03	119.99
1	A	1258	ARG	CA-C-N	5.32	126.00	119.99
1	A	1258	ARG	C-N-CA	5.32	126.00	119.99
2	J	1528	GLU	CB-CG-CD	5.31	121.62	112.60
2	I	1528	GLU	CB-CG-CD	5.29	121.60	112.60
2	G	939	PHE	CA-CB-CG	-5.17	108.63	113.80
2	J	939	PHE	CA-CB-CG	-5.16	108.64	113.80
2	K	939	PHE	CA-CB-CG	-5.15	108.65	113.80
2	I	939	PHE	CA-CB-CG	-5.14	108.66	113.80
2	L	939	PHE	CA-CB-CG	-5.14	108.66	113.80
2	H	939	PHE	CA-CB-CG	-5.14	108.66	113.80
2	G	799	PHE	CA-CB-CG	-5.10	108.70	113.80
2	L	799	PHE	CA-CB-CG	-5.10	108.70	113.80
2	L	418	ASN	CB-CA-C	5.09	117.68	110.24
2	J	418	ASN	CB-CA-C	5.09	117.67	110.24
2	J	760	HIS	CB-CA-C	5.09	115.52	110.33
2	I	760	HIS	CB-CA-C	5.09	115.52	110.33
2	H	760	HIS	CB-CA-C	5.08	115.51	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	418	ASN	CB-CA-C	5.08	117.66	110.24
2	I	799	PHE	CA-CB-CG	-5.07	108.73	113.80
2	G	418	ASN	CB-CA-C	5.07	117.64	110.24
2	I	418	ASN	CB-CA-C	5.07	117.64	110.24
2	G	760	HIS	CB-CA-C	5.07	115.50	110.33
2	H	799	PHE	CA-CB-CG	-5.07	108.73	113.80
2	H	418	ASN	CB-CA-C	5.06	117.63	110.24
2	I	220	GLU	CB-CG-CD	5.05	121.19	112.60
2	K	760	HIS	CB-CA-C	5.05	115.48	110.33
1	E	54	ALA	CA-C-N	5.04	125.68	120.03
1	E	54	ALA	C-N-CA	5.04	125.68	120.03
2	L	760	HIS	CB-CA-C	5.04	115.47	110.33
1	B	833	PHE	CA-CB-CG	-5.03	108.77	113.80
2	K	799	PHE	CA-CB-CG	-5.03	108.77	113.80
2	K	220	GLU	CB-CG-CD	5.03	121.15	112.60
1	D	1370	THR	N-CA-CB	-5.02	102.43	110.46
1	E	1370	THR	N-CA-CB	-5.01	102.45	110.46
2	J	799	PHE	CA-CB-CG	-5.00	108.80	113.80
1	C	833	PHE	CA-CB-CG	-5.00	108.80	113.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	1503	ILE	Peptide
2	H	1503	ILE	Peptide
2	I	1503	ILE	Peptide
2	J	1503	ILE	Peptide
2	K	1503	ILE	Peptide
2	L	1503	ILE	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	12379	0	12317	76	0
1	B	12379	0	12317	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	12379	0	12317	78	0
1	D	12379	0	12317	79	0
1	E	12379	0	12317	75	0
1	F	12379	0	12317	85	0
2	G	16010	0	15979	91	0
2	H	16010	0	15979	87	0
2	I	16010	0	15979	95	0
2	J	16010	0	15979	101	0
2	K	16010	0	15979	89	0
2	L	16010	0	15979	91	0
3	A	48	0	25	2	0
3	B	48	0	25	3	0
3	C	48	0	25	3	0
3	D	48	0	25	3	0
3	E	48	0	25	2	0
3	F	48	0	25	3	0
3	G	48	0	25	1	0
3	H	48	0	25	1	0
3	I	48	0	25	1	0
3	J	48	0	25	1	0
3	K	48	0	25	1	0
3	L	48	0	25	1	0
4	G	48	0	32	0	0
4	H	48	0	32	2	0
4	I	48	0	32	1	0
4	J	48	0	32	1	0
4	K	48	0	32	1	0
4	L	48	0	32	0	0
5	G	31	0	22	1	0
5	H	31	0	22	2	0
5	I	31	0	22	1	0
5	J	31	0	22	1	0
5	K	31	0	22	2	0
5	L	31	0	22	2	0
6	A	914	0	0	10	0
6	B	894	0	0	9	0
6	C	901	0	0	10	0
6	D	908	0	0	14	0
6	E	906	0	0	9	0
6	F	901	0	0	8	0
6	G	382	0	0	2	0
6	H	377	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	367	0	0	3	0
6	J	364	0	0	3	0
6	K	389	0	0	4	0
6	L	377	0	0	2	0
All	All	179064	0	170400	964	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 3.

All (964) 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:A:915:GLU:OE1	6:A:2001:HOH:O	1.69	1.10
1:E:915:GLU:OE1	6:E:2001:HOH:O	1.70	1.10
1:F:915:GLU:OE1	6:F:2001:HOH:O	1.70	1.08
1:B:915:GLU:OE1	6:B:2001:HOH:O	1.70	1.08
1:C:915:GLU:OE1	6:C:2001:HOH:O	1.69	1.06
1:D:915:GLU:OE1	6:D:2001:HOH:O	1.69	1.05
1:E:882:ASN:O	6:E:2002:HOH:O	1.84	0.93
1:A:882:ASN:O	6:A:2002:HOH:O	1.85	0.92
2:K:56:THR:HG21	2:K:112:ASN:HD22	1.33	0.91
2:H:56:THR:HG21	2:H:112:ASN:HD22	1.33	0.91
1:A:1302:VAL:HG21	1:E:1302:VAL:HG21	1.59	0.84
1:C:1302:VAL:HG21	1:F:1302:VAL:HG21	1.59	0.84
1:B:1302:VAL:HG21	1:D:1302:VAL:HG21	1.59	0.84
2:L:74:PRO:O	2:L:134:LYS:NZ	2.15	0.80
1:E:750:GLU:OE1	6:E:2003:HOH:O	2.00	0.79
1:B:750:GLU:OE1	6:B:2002:HOH:O	2.00	0.79
2:J:894:ARG:NH1	2:J:898:ASP:OD2	2.15	0.79
2:I:894:ARG:NH1	2:I:898:ASP:OD2	2.15	0.79
1:A:750:GLU:OE1	6:A:2003:HOH:O	2.00	0.79
2:G:894:ARG:NH1	2:G:898:ASP:OD2	2.15	0.79
2:L:894:ARG:NH1	2:L:898:ASP:OD2	2.15	0.79
2:K:894:ARG:NH1	2:K:898:ASP:OD2	2.15	0.78
2:H:894:ARG:NH1	2:H:898:ASP:OD2	2.16	0.78
2:G:808:ALA:O	2:G:811:VAL:HG22	1.83	0.78
1:F:750:GLU:OE1	6:F:2002:HOH:O	2.01	0.78
1:D:750:GLU:OE1	6:D:2002:HOH:O	2.02	0.77
1:A:816:GLU:OE1	6:A:2004:HOH:O	2.01	0.77
1:C:750:GLU:OE1	6:C:2002:HOH:O	2.02	0.77
1:E:816:GLU:OE2	6:E:2004:HOH:O	2.02	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:816:GLU:OE1	6:F:2003:HOH:O	2.03	0.76
1:B:816:GLU:OE1	6:B:2003:HOH:O	2.03	0.75
1:C:816:GLU:OE2	6:C:2003:HOH:O	2.02	0.75
1:D:816:GLU:OE2	6:D:2003:HOH:O	2.02	0.75
2:K:74:PRO:O	2:K:134:LYS:NZ	2.19	0.75
2:G:74:PRO:O	2:G:134:LYS:NZ	2.19	0.75
2:G:108:LEU:HB3	2:G:114:THR:HG21	1.70	0.72
2:L:108:LEU:HB3	2:L:114:THR:HG21	1.70	0.71
2:I:1811:GLU:OE2	2:I:2010:TYR:OH	2.08	0.71
2:J:1811:GLU:OE2	2:J:2010:TYR:OH	2.08	0.71
2:G:1811:GLU:OE2	2:G:2010:TYR:OH	2.08	0.70
2:H:1811:GLU:OE2	2:H:2010:TYR:OH	2.08	0.70
2:K:1811:GLU:OE2	2:K:2010:TYR:OH	2.08	0.70
2:L:1811:GLU:OE2	2:L:2010:TYR:OH	2.08	0.70
1:B:1486:LEU:HD22	1:B:1756:ILE:HD11	1.74	0.69
1:D:1486:LEU:HD22	1:D:1756:ILE:HD11	1.74	0.69
1:F:1486:LEU:HD22	1:F:1756:ILE:HD11	1.75	0.69
1:C:1486:LEU:HD22	1:C:1756:ILE:HD11	1.74	0.69
1:A:1486:LEU:HD22	1:A:1756:ILE:HD11	1.74	0.68
1:E:1486:LEU:HD22	1:E:1756:ILE:HD11	1.74	0.68
2:K:849:GLU:OE1	6:K:2401:HOH:O	2.13	0.67
2:H:849:GLU:OE1	6:H:2401:HOH:O	2.13	0.67
2:L:849:GLU:OE1	6:L:2401:HOH:O	2.13	0.67
1:B:1471:LYS:HD3	1:B:1759:MET:HE2	1.77	0.67
1:F:1471:LYS:HD3	1:F:1759:MET:HE2	1.77	0.67
2:J:616:THR:HG23	6:J:2462:HOH:O	1.94	0.66
2:I:849:GLU:OE1	6:I:2401:HOH:O	2.13	0.66
2:L:616:THR:HG23	6:L:2461:HOH:O	1.95	0.66
2:K:616:THR:HG23	6:K:2463:HOH:O	1.95	0.66
2:G:616:THR:HG23	6:G:2465:HOH:O	1.95	0.66
2:G:849:GLU:OE1	6:G:2401:HOH:O	2.13	0.66
2:H:616:THR:HG23	6:H:2462:HOH:O	1.95	0.66
2:I:616:THR:HG23	6:I:2459:HOH:O	1.95	0.66
2:L:326:ASP:OD2	2:L:387:TYR:OH	2.13	0.66
1:C:991:ASP:OD1	6:C:2004:HOH:O	2.13	0.66
2:J:849:GLU:OE1	6:J:2401:HOH:O	2.13	0.65
1:D:991:ASP:OD1	6:D:2004:HOH:O	2.13	0.65
1:E:1464:GLU:HG3	1:E:1773:VAL:HG13	1.78	0.65
1:A:1464:GLU:HG3	1:A:1773:VAL:HG13	1.78	0.65
1:F:1464:GLU:HG3	1:F:1773:VAL:HG13	1.78	0.65
1:B:1464:GLU:HG3	1:B:1773:VAL:HG13	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1370:THR:HG23	6:D:2102:HOH:O	1.98	0.64
1:C:1370:THR:HG23	6:C:2100:HOH:O	1.98	0.64
1:E:1468:GLU:OE1	1:E:1771:VAL:HG21	1.97	0.64
1:A:1468:GLU:OE1	1:A:1771:VAL:HG21	1.97	0.63
2:J:326:ASP:OD2	2:J:387:TYR:OH	2.13	0.63
2:L:1771:LEU:O	2:L:1777:THR:OG1	2.14	0.63
2:J:1771:LEU:O	2:J:1777:THR:OG1	2.14	0.63
2:G:1771:LEU:O	2:G:1777:THR:OG1	2.14	0.63
2:I:1771:LEU:O	2:I:1777:THR:OG1	2.14	0.63
1:B:706:THR:HB	1:B:737:PHE:HB3	1.81	0.63
1:F:1370:THR:HG23	6:F:2100:HOH:O	1.98	0.63
1:A:1370:THR:HG23	6:A:2105:HOH:O	1.98	0.63
1:F:706:THR:HB	1:F:737:PHE:HB3	1.81	0.63
1:B:1370:THR:HG23	6:B:2104:HOH:O	1.98	0.63
1:E:1370:THR:HG23	6:E:2112:HOH:O	1.98	0.62
2:H:1771:LEU:O	2:H:1777:THR:OG1	2.14	0.62
2:K:1771:LEU:O	2:K:1777:THR:OG1	2.14	0.62
1:B:1302:VAL:CG2	1:D:1302:VAL:HG21	2.29	0.62
1:C:1302:VAL:HG21	1:F:1302:VAL:CG2	2.29	0.62
1:A:1673:TYR:CZ	1:A:1677:VAL:HG21	2.35	0.62
1:B:1673:TYR:CZ	1:B:1677:VAL:HG21	2.35	0.62
1:E:1673:TYR:CZ	1:E:1677:VAL:HG21	2.35	0.62
1:F:1673:TYR:CZ	1:F:1677:VAL:HG21	2.35	0.62
1:D:706:THR:HB	1:D:737:PHE:HB3	1.81	0.62
1:C:706:THR:HB	1:C:737:PHE:HB3	1.81	0.62
1:A:706:THR:HB	1:A:737:PHE:HB3	1.81	0.62
1:E:706:THR:HB	1:E:737:PHE:HB3	1.81	0.61
2:K:72:VAL:HG11	2:K:84:LEU:HD22	1.81	0.61
1:A:1486:LEU:CD2	1:A:1756:ILE:HD11	2.30	0.61
1:C:1302:VAL:CG2	1:F:1302:VAL:HG21	2.29	0.61
1:E:1486:LEU:CD2	1:E:1756:ILE:HD11	2.30	0.61
2:I:72:VAL:HG11	2:I:84:LEU:HD22	1.81	0.61
2:H:72:VAL:HG11	2:H:84:LEU:HD22	1.81	0.61
1:B:1302:VAL:HG21	1:D:1302:VAL:CG2	2.29	0.61
1:B:889:GLU:OE2	1:B:895:THR:OG1	2.16	0.61
2:J:72:VAL:HG11	2:J:84:LEU:HD22	1.81	0.61
1:C:1673:TYR:CZ	1:C:1677:VAL:HG21	2.35	0.61
1:D:1673:TYR:CZ	1:D:1677:VAL:HG21	2.35	0.61
1:B:451:MET:HE1	1:B:480:CYS:SG	2.41	0.61
1:C:451:MET:HE1	1:C:480:CYS:SG	2.41	0.61
1:D:451:MET:HE1	1:D:480:CYS:SG	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:451:MET:HE1	1:F:480:CYS:SG	2.41	0.60
1:E:451:MET:HE1	1:E:480:CYS:SG	2.41	0.60
1:A:451:MET:HE1	1:A:480:CYS:SG	2.41	0.60
1:B:1486:LEU:CD2	1:B:1756:ILE:HD11	2.31	0.60
1:F:1486:LEU:CD2	1:F:1756:ILE:HD11	2.31	0.60
1:A:845:SER:OG	1:F:845:SER:OG	2.20	0.60
1:B:845:SER:OG	1:E:845:SER:OG	2.20	0.60
1:D:1486:LEU:CD2	1:D:1756:ILE:HD11	2.30	0.60
1:C:1486:LEU:CD2	1:C:1756:ILE:HD11	2.30	0.60
1:C:845:SER:OG	1:D:845:SER:OG	2.20	0.60
2:I:1311:PHE:O	2:I:1319:MET:HE3	2.02	0.60
2:J:1311:PHE:O	2:J:1319:MET:HE3	2.02	0.59
1:B:340:ARG:NH1	1:B:344:GLN:OE1	2.33	0.59
1:B:1173:LEU:CD2	1:D:1175:ILE:HG12	2.33	0.59
1:C:1175:ILE:HG12	1:F:1173:LEU:CD2	2.33	0.59
1:B:1175:ILE:HG12	1:D:1173:LEU:CD2	2.33	0.58
1:C:1173:LEU:CD2	1:F:1175:ILE:HG12	2.33	0.58
2:H:1548:SER:HB3	2:H:1619:ASN:HD21	1.68	0.58
1:A:1173:LEU:CD2	1:E:1175:ILE:HG12	2.33	0.58
1:A:877:LEU:HD12	3:A:1901:NAP:H2D	1.84	0.58
1:E:877:LEU:HD12	3:E:1901:NAP:H2D	1.84	0.58
2:K:1548:SER:HB3	2:K:1619:ASN:HD21	1.68	0.58
1:A:1175:ILE:HG12	1:E:1173:LEU:CD2	2.34	0.58
1:A:1302:VAL:HG21	1:E:1302:VAL:CG2	2.30	0.58
1:A:1302:VAL:CG2	1:E:1302:VAL:HG21	2.30	0.58
1:D:889:GLU:OE2	1:D:895:THR:OG1	2.16	0.58
1:C:889:GLU:OE2	1:C:895:THR:OG1	2.17	0.57
1:F:889:GLU:OE2	1:F:895:THR:OG1	2.16	0.57
2:J:1548:SER:HB3	2:J:1619:ASN:HD21	1.68	0.57
2:I:1548:SER:HB3	2:I:1619:ASN:HD21	1.69	0.57
1:F:641:ARG:NH2	1:F:925:ASP:OD2	2.37	0.57
2:K:156:LEU:HD12	2:K:500:HIS:HB2	1.86	0.57
1:B:641:ARG:NH2	1:B:925:ASP:OD2	2.37	0.57
1:A:641:ARG:NH2	1:A:925:ASP:OD2	2.37	0.57
1:E:641:ARG:NH2	1:E:925:ASP:OD2	2.37	0.57
2:I:156:LEU:HD12	2:I:500:HIS:HB2	1.87	0.57
2:H:156:LEU:HD12	2:H:500:HIS:HB2	1.87	0.57
2:J:156:LEU:HD12	2:J:500:HIS:HB2	1.87	0.57
2:H:1103:PHE:O	2:H:1247:GLY:HA3	2.05	0.57
2:K:1103:PHE:O	2:K:1247:GLY:HA3	2.05	0.57
2:G:1548:SER:HB3	2:G:1619:ASN:HD21	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1523:ARG:NH2	6:C:2011:HOH:O	2.30	0.57
2:I:1103:PHE:O	2:I:1247:GLY:HA3	2.05	0.57
2:L:1548:SER:HB3	2:L:1619:ASN:HD21	1.68	0.57
2:J:1103:PHE:O	2:J:1247:GLY:HA3	2.05	0.57
1:F:877:LEU:HD12	3:F:1901:NAP:H2D	1.86	0.57
1:D:1523:ARG:NH2	6:D:2014:HOH:O	2.30	0.56
1:D:877:LEU:HD12	3:D:1901:NAP:H2D	1.85	0.56
2:I:1962:ARG:NH2	4:I:2301:COA:O2B	2.37	0.56
1:B:877:LEU:HD12	3:B:1901:NAP:H2D	1.86	0.56
1:C:641:ARG:NH2	1:C:925:ASP:OD2	2.37	0.56
1:C:877:LEU:HD12	3:C:1901:NAP:H2D	1.85	0.56
1:D:641:ARG:NH2	1:D:925:ASP:OD2	2.37	0.56
2:I:56:THR:HG22	2:I:59:GLU:OE2	2.04	0.56
2:G:1103:PHE:O	2:G:1247:GLY:HA3	2.05	0.56
2:L:1103:PHE:O	2:L:1247:GLY:HA3	2.05	0.56
2:J:1808:J8W:C3	2:J:1834:ARG:HH12	2.18	0.56
2:I:1808:J8W:C3	2:I:1834:ARG:HH12	2.18	0.56
1:B:1302:VAL:CG2	1:D:1302:VAL:CG2	2.84	0.55
1:C:1302:VAL:CG2	1:F:1302:VAL:CG2	2.84	0.55
2:G:124:LYS:O	2:G:128:THR:OG1	2.24	0.55
1:A:1682:LYS:HE3	2:G:992:GLU:O	2.06	0.55
2:J:1782:THR:HG22	2:J:1827:LEU:HD21	1.89	0.55
2:I:1782:THR:HG22	2:I:1827:LEU:HD21	1.89	0.55
2:G:1808:J8W:C3	2:G:1834:ARG:HH12	2.18	0.55
1:D:1682:LYS:HE3	2:K:992:GLU:O	2.07	0.55
2:L:1782:THR:HG22	2:L:1827:LEU:HD21	1.89	0.55
1:A:1302:VAL:CG2	1:E:1302:VAL:CG2	2.85	0.55
2:G:1782:THR:HG22	2:G:1827:LEU:HD21	1.89	0.55
2:L:1808:J8W:C3	2:L:1834:ARG:HH12	2.18	0.55
1:F:1682:LYS:HE3	2:J:992:GLU:O	2.06	0.54
2:I:1528:GLU:HG3	2:I:1530:LYS:O	2.06	0.54
2:J:1962:ARG:NH2	4:J:2301:COA:O2B	2.40	0.54
1:C:1682:LYS:HE3	2:H:992:GLU:O	2.07	0.54
1:E:1682:LYS:HE3	2:L:992:GLU:O	2.07	0.54
2:J:1528:GLU:HG3	2:J:1530:LYS:O	2.06	0.54
2:K:1782:THR:HG22	2:K:1827:LEU:HD21	1.89	0.54
1:A:340:ARG:NH1	1:A:344:GLN:OE1	2.33	0.54
1:E:1491:ARG:NH1	1:E:1495:ASN:OD1	2.41	0.54
2:H:1782:THR:HG22	2:H:1827:LEU:HD21	1.89	0.54
2:K:1808:J8W:C3	2:K:1834:ARG:HH12	2.18	0.54
1:A:1491:ARG:NH1	1:A:1495:ASN:OD1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:ARG:NH1	1:E:344:GLN:OE1	2.34	0.54
1:F:1491:ARG:NH1	1:F:1495:ASN:OD1	2.41	0.54
2:H:1808:J8W:C3	2:H:1834:ARG:HH12	2.18	0.54
1:B:1491:ARG:NH1	1:B:1495:ASN:OD1	2.41	0.54
1:C:1491:ARG:NH1	1:C:1495:ASN:OD1	2.41	0.54
1:D:1491:ARG:NH1	1:D:1495:ASN:OD1	2.41	0.54
2:H:7:ARG:HD3	2:H:27:PHE:CE1	2.43	0.54
1:B:1682:LYS:HE3	2:I:992:GLU:O	2.07	0.53
2:G:68:VAL:O	2:G:72:VAL:HG23	2.08	0.53
1:E:1523:ARG:NH2	6:E:2011:HOH:O	2.28	0.53
1:A:889:GLU:OE2	1:A:895:THR:OG1	2.16	0.53
1:B:1367:ARG:HD2	1:B:1370:THR:HG21	1.90	0.53
1:E:889:GLU:OE2	1:E:895:THR:OG1	2.16	0.53
1:F:1367:ARG:HD2	1:F:1370:THR:HG21	1.90	0.53
2:K:2044:ASN:O	2:K:2047:LYS:HG2	2.08	0.53
1:D:1367:ARG:HD2	1:D:1370:THR:HG21	1.90	0.53
2:H:2044:ASN:O	2:H:2047:LYS:HG2	2.08	0.53
1:A:1523:ARG:NH2	6:A:2012:HOH:O	2.29	0.53
1:C:1367:ARG:HD2	1:C:1370:THR:HG21	1.90	0.53
2:H:161:GLY:H	2:H:505:GLY:HA3	1.74	0.53
2:K:105:ALA:HB1	2:K:119:THR:CG2	2.39	0.53
2:L:68:VAL:O	2:L:72:VAL:HG23	2.08	0.53
1:C:46:GLU:OE2	1:C:51:PRO:HA	2.09	0.53
1:D:46:GLU:OE2	1:D:51:PRO:HA	2.09	0.53
2:K:161:GLY:H	2:K:505:GLY:HA3	1.74	0.53
2:L:161:GLY:H	2:L:505:GLY:HA3	1.74	0.53
2:G:161:GLY:H	2:G:505:GLY:HA3	1.74	0.53
1:C:1592:MET:HE2	1:C:1641:ILE:HG23	1.91	0.53
2:H:105:ALA:HB1	2:H:119:THR:CG2	2.39	0.53
1:D:1592:MET:HE2	1:D:1641:ILE:HG23	1.91	0.52
2:I:161:GLY:H	2:I:505:GLY:HA3	1.74	0.52
1:A:1367:ARG:HD2	1:A:1370:THR:HG21	1.90	0.52
2:G:156:LEU:HD22	2:G:502:LEU:HG	1.92	0.52
1:F:1529:TYR:OH	6:F:2004:HOH:O	2.18	0.52
2:J:161:GLY:H	2:J:505:GLY:HA3	1.74	0.52
2:L:105:ALA:HB1	2:L:119:THR:CG2	2.39	0.52
2:G:105:ALA:HB1	2:G:119:THR:CG2	2.39	0.52
1:B:1523:ARG:NH2	6:B:2009:HOH:O	2.29	0.52
2:L:156:LEU:HD22	2:L:502:LEU:HG	1.92	0.52
1:B:46:GLU:OE1	1:B:51:PRO:HA	2.10	0.52
1:E:1367:ARG:HD2	1:E:1370:THR:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1523:ARG:NH2	6:F:2009:HOH:O	2.29	0.52
1:B:1529:TYR:OH	6:B:2004:HOH:O	2.18	0.52
1:F:46:GLU:OE1	1:F:51:PRO:HA	2.10	0.52
2:J:105:ALA:HB1	2:J:119:THR:CG2	2.39	0.52
2:I:105:ALA:HB1	2:I:119:THR:CG2	2.39	0.52
1:C:340:ARG:NH1	1:C:344:GLN:OE1	2.33	0.52
1:C:1309:VAL:HG23	6:C:2454:HOH:O	2.09	0.52
1:F:630:ILE:O	1:F:653:ARG:NH2	2.42	0.52
1:B:630:ILE:O	1:B:653:ARG:NH2	2.42	0.52
1:B:1592:MET:HE2	1:B:1641:ILE:HG23	1.91	0.52
1:F:1592:MET:HE2	1:F:1641:ILE:HG23	1.91	0.52
1:A:1592:MET:HE2	1:A:1641:ILE:HG23	1.91	0.51
1:D:1309:VAL:HG23	6:D:2462:HOH:O	2.09	0.51
5:H:2302:FNR:H4'	5:H:2302:FNR:H1	1.59	0.51
1:E:1592:MET:HE2	1:E:1641:ILE:HG23	1.91	0.51
1:A:46:GLU:OE1	1:A:51:PRO:HA	2.10	0.51
1:C:712:LYS:NZ	6:C:2068:HOH:O	2.44	0.51
1:E:46:GLU:OE1	1:E:51:PRO:HA	2.10	0.51
2:G:1874:VAL:O	2:G:1878:VAL:HG23	2.11	0.51
1:D:340:ARG:NH1	1:D:344:GLN:OE1	2.33	0.51
1:D:712:LYS:NZ	6:D:2071:HOH:O	2.44	0.51
2:L:1874:VAL:O	2:L:1878:VAL:HG23	2.11	0.51
1:D:764:ASP:OD2	1:D:818:ARG:HD3	2.11	0.51
2:J:1874:VAL:O	2:J:1878:VAL:HG23	2.11	0.51
1:C:764:ASP:OD2	1:C:818:ARG:HD3	2.11	0.51
2:I:1874:VAL:O	2:I:1878:VAL:HG23	2.11	0.51
2:G:1360:ILE:CD1	2:G:1402:PRO:HB2	2.41	0.51
2:H:69:SER:HA	2:H:72:VAL:HG12	1.93	0.51
2:L:1360:ILE:CD1	2:L:1402:PRO:HB2	2.41	0.51
2:J:1360:ILE:CD1	2:J:1402:PRO:HB2	2.41	0.50
2:K:69:SER:HA	2:K:72:VAL:HG12	1.93	0.50
1:B:808:LYS:HE3	1:E:782:GLU:O	2.11	0.50
2:H:1360:ILE:CD1	2:H:1402:PRO:HB2	2.41	0.50
2:K:1360:ILE:CD1	2:K:1402:PRO:HB2	2.41	0.50
2:I:1360:ILE:CD1	2:I:1402:PRO:HB2	2.41	0.50
1:A:782:GLU:O	1:F:808:LYS:HE3	2.12	0.50
1:C:447:LEU:HG	1:C:451:MET:HE2	1.94	0.50
1:C:782:GLU:O	1:D:808:LYS:HE3	2.12	0.50
1:D:447:LEU:HG	1:D:451:MET:HE2	1.94	0.50
1:E:764:ASP:OD2	1:E:818:ARG:HD3	2.11	0.50
1:A:764:ASP:OD2	1:A:818:ARG:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:808:LYS:HE3	1:D:782:GLU:O	2.12	0.50
1:E:712:LYS:NZ	6:E:2069:HOH:O	2.44	0.50
2:K:1874:VAL:O	2:K:1878:VAL:HG23	2.11	0.50
2:J:69:SER:HA	2:J:72:VAL:HG12	1.93	0.50
2:I:69:SER:HA	2:I:72:VAL:HG12	1.93	0.50
1:D:1367:ARG:O	1:D:1370:THR:HB	2.12	0.50
1:F:1471:LYS:HD3	1:F:1759:MET:CE	2.42	0.50
2:H:1874:VAL:O	2:H:1878:VAL:HG23	2.11	0.50
2:H:1878:VAL:HG22	2:H:1944:ILE:HG12	1.94	0.50
2:K:1878:VAL:HG22	2:K:1944:ILE:HG12	1.94	0.50
2:L:1350:LEU:HD11	2:L:1410:PHE:HB3	1.94	0.50
1:A:712:LYS:NZ	6:A:2069:HOH:O	2.44	0.50
1:A:808:LYS:HE3	1:F:782:GLU:O	2.12	0.50
1:B:764:ASP:OD2	1:B:818:ARG:HD3	2.11	0.50
1:B:782:GLU:O	1:E:808:LYS:HE3	2.12	0.50
1:C:1367:ARG:O	1:C:1370:THR:HB	2.12	0.50
1:F:764:ASP:OD2	1:F:818:ARG:HD3	2.11	0.50
2:K:805:VAL:O	2:K:811:VAL:HG21	2.12	0.50
2:L:805:VAL:O	2:L:811:VAL:HG21	2.12	0.50
2:G:1350:LEU:HD11	2:G:1410:PHE:HB3	1.94	0.49
1:B:1464:GLU:CG	1:B:1773:VAL:HG13	2.42	0.49
1:F:1464:GLU:CG	1:F:1773:VAL:HG13	2.42	0.49
2:H:805:VAL:O	2:H:811:VAL:HG21	2.12	0.49
2:G:915:ALA:HA	2:G:1000:ILE:HD11	1.95	0.49
2:I:1350:LEU:HD11	2:I:1410:PHE:HB3	1.95	0.49
1:D:817:THR:OG1	6:D:2006:HOH:O	2.20	0.49
2:J:1350:LEU:HD11	2:J:1410:PHE:HB3	1.95	0.49
2:J:1782:THR:CG2	2:J:1827:LEU:HD21	2.43	0.49
2:K:1782:THR:CG2	2:K:1827:LEU:HD21	2.43	0.49
2:L:915:ALA:HA	2:L:1000:ILE:HD11	1.95	0.49
2:L:1736:MET:HG2	2:L:1751:ILE:HD13	1.94	0.49
2:G:1736:MET:HG2	2:G:1751:ILE:HD13	1.94	0.49
2:G:1782:THR:CG2	2:G:1827:LEU:HD21	2.43	0.49
1:E:1367:ARG:O	1:E:1370:THR:HB	2.12	0.49
2:J:915:ALA:HA	2:J:1000:ILE:HD11	1.95	0.49
2:I:805:VAL:O	2:I:811:VAL:HG21	2.12	0.49
2:I:915:ALA:HA	2:I:1000:ILE:HD11	1.95	0.49
2:I:1782:THR:CG2	2:I:1827:LEU:HD21	2.43	0.49
2:K:159:ILE:HA	2:K:271:THR:O	2.13	0.49
2:L:1782:THR:CG2	2:L:1827:LEU:HD21	2.43	0.49
1:B:447:LEU:HG	1:B:451:MET:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:159:ILE:HA	2:H:271:THR:O	2.13	0.49
2:H:1782:THR:CG2	2:H:1827:LEU:HD21	2.43	0.49
1:A:1367:ARG:O	1:A:1370:THR:HB	2.12	0.49
1:A:1464:GLU:CG	1:A:1773:VAL:HG13	2.42	0.49
2:J:805:VAL:O	2:J:811:VAL:HG21	2.12	0.49
2:I:159:ILE:HA	2:I:271:THR:O	2.13	0.49
1:E:1464:GLU:CG	1:E:1773:VAL:HG13	2.42	0.49
1:F:447:LEU:HG	1:F:451:MET:HE2	1.94	0.49
1:E:447:LEU:HG	1:E:451:MET:HE2	1.94	0.49
2:J:159:ILE:HA	2:J:271:THR:O	2.13	0.49
1:A:447:LEU:HG	1:A:451:MET:HE2	1.94	0.49
2:G:1546:THR:HG21	2:G:1616:VAL:HG11	1.95	0.49
2:I:1878:VAL:HG22	2:I:1944:ILE:HG12	1.94	0.49
2:K:915:ALA:HA	2:K:1000:ILE:HD11	1.95	0.49
2:L:1546:THR:HG21	2:L:1616:VAL:HG11	1.95	0.49
2:G:149:VAL:HG21	2:G:156:LEU:HD12	1.94	0.49
2:I:32:GLN:HA	2:H:7:ARG:NH2	2.28	0.49
2:H:1350:LEU:HD11	2:H:1410:PHE:HB3	1.95	0.49
2:K:124:LYS:O	2:K:128:THR:OG1	2.24	0.49
2:J:1878:VAL:HG22	2:J:1944:ILE:HG12	1.94	0.48
2:H:1736:MET:HG2	2:H:1751:ILE:HD13	1.94	0.48
2:L:149:VAL:HG21	2:L:156:LEU:HD12	1.94	0.48
1:B:1533:ILE:HD11	1:B:1561:MET:HE1	1.95	0.48
2:J:1287:GLY:HA3	2:J:1374:THR:HG23	1.95	0.48
2:H:915:ALA:HA	2:H:1000:ILE:HD11	1.95	0.48
2:K:1350:LEU:HD11	2:K:1410:PHE:HB3	1.95	0.48
1:F:1533:ILE:HD11	1:F:1561:MET:HE1	1.95	0.48
2:I:1287:GLY:HA3	2:I:1374:THR:HG23	1.95	0.48
2:H:124:LYS:O	2:H:128:THR:OG1	2.24	0.48
2:K:1736:MET:HG2	2:K:1751:ILE:HD13	1.94	0.48
2:L:1878:VAL:HG22	2:L:1944:ILE:HG12	1.94	0.48
1:B:1367:ARG:O	1:B:1370:THR:HB	2.12	0.48
1:C:877:LEU:CD1	3:C:1901:NAP:H2D	2.44	0.48
1:F:1367:ARG:O	1:F:1370:THR:HB	2.12	0.48
2:K:2044:ASN:HB3	2:K:2047:LYS:HD3	1.95	0.48
2:G:1878:VAL:HG22	2:G:1944:ILE:HG12	1.94	0.48
2:G:1384:GLN:HE21	2:G:1389:ILE:CD1	2.27	0.48
1:D:877:LEU:CD1	3:D:1901:NAP:H2D	2.44	0.48
1:F:877:LEU:CD1	3:F:1901:NAP:H2D	2.44	0.48
2:J:1546:THR:HG21	2:J:1616:VAL:HG11	1.95	0.48
2:I:1546:THR:HG21	2:I:1616:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2044:ASN:HB3	2:H:2047:LYS:HD3	1.96	0.48
2:G:159:ILE:HA	2:G:271:THR:O	2.13	0.48
2:K:1593:ILE:HD13	2:K:1626:ILE:HD13	1.96	0.48
2:L:1384:GLN:HE21	2:L:1389:ILE:CD1	2.27	0.48
2:L:1593:ILE:HD13	2:L:1626:ILE:HD13	1.96	0.48
2:G:1593:ILE:HD13	2:G:1626:ILE:HD13	1.96	0.48
1:B:712:LYS:NZ	6:B:2071:HOH:O	2.46	0.48
2:H:1593:ILE:HD13	2:H:1626:ILE:HD13	1.96	0.48
2:L:159:ILE:HA	2:L:271:THR:O	2.13	0.48
1:B:877:LEU:CD1	3:B:1901:NAP:H2D	2.44	0.48
1:F:712:LYS:NZ	6:F:2072:HOH:O	2.46	0.48
2:I:1593:ILE:HD13	2:I:1626:ILE:HD13	1.96	0.48
1:A:1533:ILE:HD11	1:A:1561:MET:HE1	1.95	0.48
2:J:1593:ILE:HD13	2:J:1626:ILE:HD13	1.96	0.48
1:B:888:ILE:HD11	1:B:940:THR:HG22	1.97	0.47
1:E:1533:ILE:HD11	1:E:1561:MET:HE1	1.95	0.47
1:D:491:LYS:NZ	6:D:2057:HOH:O	2.42	0.47
1:F:888:ILE:HD11	1:F:940:THR:HG22	1.97	0.47
2:H:1355:ASN:ND2	2:H:1408:SER:OG	2.48	0.47
2:K:1355:ASN:ND2	2:K:1408:SER:OG	2.48	0.47
1:A:704:VAL:HG23	1:A:763:TRP:CZ3	2.50	0.47
2:J:48:PHE:HA	2:J:53:GLU:OE2	2.13	0.47
2:H:808:ALA:HB3	2:H:811:VAL:HG23	1.95	0.47
2:G:1778:GLN:HB2	2:G:1779:PRO:HD3	1.96	0.47
1:C:1201:SER:OG	1:C:1203:ASP:OD1	2.27	0.47
1:E:704:VAL:HG23	1:E:763:TRP:CZ3	2.50	0.47
1:F:1431:GLU:OE2	1:F:1523:ARG:HD2	2.15	0.47
2:J:45:THR:HG22	2:J:53:GLU:OE2	2.13	0.47
2:J:808:ALA:HB3	2:J:811:VAL:HG23	1.96	0.47
2:I:808:ALA:HB3	2:I:811:VAL:HG23	1.96	0.47
2:H:471:LEU:HD11	2:H:478:ARG:HG2	1.97	0.47
2:H:1287:GLY:HA3	2:H:1374:THR:HG23	1.95	0.47
2:K:109:LEU:HD12	2:K:119:THR:HG21	1.96	0.47
2:K:471:LEU:HD11	2:K:478:ARG:HG2	1.97	0.47
2:L:1778:GLN:HB2	2:L:1779:PRO:HD3	1.96	0.47
1:A:1431:GLU:OE2	1:A:1523:ARG:HD2	2.15	0.47
2:G:1234:VAL:HG12	2:G:1265:MET:HG3	1.97	0.47
1:B:1431:GLU:OE2	1:B:1523:ARG:HD2	2.15	0.47
1:B:1471:LYS:HD3	1:B:1759:MET:CE	2.42	0.47
1:C:704:VAL:HG23	1:C:763:TRP:CZ3	2.50	0.47
1:D:704:VAL:HG23	1:D:763:TRP:CZ3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1431:GLU:OE2	1:E:1523:ARG:HD2	2.15	0.47
2:H:868:PHE:CD1	2:H:872:ILE:HD12	2.50	0.47
2:H:870:GLU:O	2:H:874:ASN:ND2	2.48	0.47
2:H:1546:THR:HG21	2:H:1616:VAL:HG11	1.95	0.47
2:H:2030:TYR:CE1	2:H:2039:LYS:HB2	2.50	0.47
2:K:808:ALA:HB3	2:K:811:VAL:HG23	1.95	0.47
2:K:868:PHE:CD1	2:K:872:ILE:HD12	2.50	0.47
2:K:870:GLU:O	2:K:874:ASN:ND2	2.48	0.47
2:K:1287:GLY:HA3	2:K:1374:THR:HG23	1.95	0.47
2:K:1546:THR:HG21	2:K:1616:VAL:HG11	1.95	0.47
2:K:2030:TYR:CE1	2:K:2039:LYS:HB2	2.50	0.47
2:L:124:LYS:O	2:L:128:THR:OG1	2.24	0.47
2:L:1234:VAL:HG12	2:L:1265:MET:HG3	1.97	0.47
2:G:471:LEU:HD11	2:G:478:ARG:HG2	1.97	0.47
1:E:877:LEU:CD1	3:E:1901:NAP:H2D	2.43	0.47
2:I:414:LEU:HD12	2:I:414:LEU:O	2.15	0.47
2:L:471:LEU:HD11	2:L:478:ARG:HG2	1.97	0.47
1:A:877:LEU:CD1	3:A:1901:NAP:H2D	2.43	0.47
1:D:1533:ILE:HD11	1:D:1561:MET:HE1	1.95	0.47
2:J:414:LEU:O	2:J:414:LEU:HD12	2.15	0.47
2:J:870:GLU:O	2:J:874:ASN:ND2	2.48	0.47
2:I:870:GLU:O	2:I:874:ASN:ND2	2.48	0.47
1:C:1533:ILE:HD11	1:C:1561:MET:HE1	1.95	0.47
1:D:1529:TYR:OH	6:D:2005:HOH:O	2.18	0.47
2:I:326:ASP:OD1	2:I:387:TYR:OH	2.33	0.47
2:H:1234:VAL:HG12	2:H:1265:MET:HG3	1.97	0.47
2:J:1234:VAL:HG12	2:J:1265:MET:HG3	1.97	0.46
2:I:1355:ASN:ND2	2:I:1408:SER:OG	2.47	0.46
2:H:1778:GLN:HB2	2:H:1779:PRO:HD3	1.96	0.46
2:K:1234:VAL:HG12	2:K:1265:MET:HG3	1.97	0.46
2:K:1778:GLN:HB2	2:K:1779:PRO:HD3	1.96	0.46
2:G:870:GLU:O	2:G:874:ASN:ND2	2.48	0.46
2:J:1355:ASN:ND2	2:J:1408:SER:OG	2.47	0.46
2:K:2015:THR:HG23	2:K:2028:ASP:OD2	2.15	0.46
2:L:808:ALA:HB3	2:L:811:VAL:HG23	1.96	0.46
2:L:1355:ASN:ND2	2:L:1408:SER:OG	2.48	0.46
2:G:1355:ASN:ND2	2:G:1408:SER:OG	2.47	0.46
2:J:1374:THR:HG21	6:J:2666:HOH:O	2.16	0.46
2:I:1234:VAL:HG12	2:I:1265:MET:HG3	1.97	0.46
2:H:1584:PHE:CD2	2:H:1584:PHE:C	2.94	0.46
2:H:2015:THR:HG23	2:H:2028:ASP:OD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1584:PHE:CD2	2:K:1584:PHE:C	2.94	0.46
2:L:870:GLU:O	2:L:874:ASN:ND2	2.48	0.46
1:B:1673:TYR:CE1	1:B:1677:VAL:CG2	2.99	0.46
1:F:704:VAL:HG23	1:F:763:TRP:CZ3	2.50	0.46
1:F:1673:TYR:CE1	1:F:1677:VAL:CG2	2.99	0.46
2:J:2030:TYR:CE1	2:J:2039:LYS:HB2	2.50	0.46
2:L:868:PHE:CD1	2:L:872:ILE:HD12	2.50	0.46
2:L:2015:THR:HG23	2:L:2028:ASP:OD2	2.15	0.46
2:J:1665:VAL:HA	2:J:1805:ALA:O	2.16	0.46
2:G:868:PHE:CD1	2:G:872:ILE:HD12	2.50	0.46
2:G:2015:THR:HG23	2:G:2028:ASP:OD2	2.16	0.46
1:C:1431:GLU:OE2	1:C:1523:ARG:HD2	2.15	0.46
1:C:1529:TYR:OH	6:C:2005:HOH:O	2.18	0.46
2:J:868:PHE:CD1	2:J:872:ILE:HD12	2.50	0.46
2:I:1665:VAL:HA	2:I:1805:ALA:O	2.16	0.46
2:G:414:LEU:HD12	2:G:414:LEU:O	2.15	0.46
1:B:704:VAL:HG23	1:B:763:TRP:CZ3	2.50	0.46
1:D:1557:ILE:HD11	1:D:1642:THR:HG21	1.98	0.46
1:E:1246:CYS:HA	1:E:1299:LYS:O	2.16	0.46
2:J:2015:THR:HG23	2:J:2028:ASP:OD2	2.16	0.46
2:I:844:VAL:HG21	2:I:866:LYS:HD2	1.98	0.46
2:I:2030:TYR:CE1	2:I:2039:LYS:HB2	2.50	0.46
1:B:1557:ILE:HD11	1:B:1642:THR:HG21	1.97	0.46
1:C:420:ILE:CD1	1:C:472:LEU:HD23	2.46	0.46
1:C:1557:ILE:HD11	1:C:1642:THR:HG21	1.98	0.46
1:D:1431:GLU:OE2	1:D:1523:ARG:HD2	2.15	0.46
1:E:343:LEU:C	1:E:343:LEU:HD23	2.41	0.46
1:F:343:LEU:HD23	1:F:343:LEU:C	2.41	0.46
2:J:234:ILE:N	2:J:235:PRO:CD	2.79	0.46
2:J:844:VAL:HG21	2:J:866:LYS:HD2	1.98	0.46
2:I:868:PHE:CD1	2:I:872:ILE:HD12	2.50	0.46
2:I:1374:THR:HG21	6:I:2666:HOH:O	2.16	0.46
2:L:414:LEU:O	2:L:414:LEU:HD12	2.15	0.46
1:A:343:LEU:C	1:A:343:LEU:HD23	2.41	0.46
1:A:1246:CYS:HA	1:A:1299:LYS:O	2.16	0.46
2:G:1906:ALA:O	2:G:1909:THR:OG1	2.31	0.46
1:D:420:ILE:CD1	1:D:472:LEU:HD23	2.46	0.46
2:J:471:LEU:HD11	2:J:478:ARG:HG2	1.97	0.46
2:J:1778:GLN:HB2	2:J:1779:PRO:HD3	1.96	0.46
2:I:471:LEU:HD11	2:I:478:ARG:HG2	1.97	0.46
2:I:598:THR:HA	2:I:599:PRO:HA	1.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2015:THR:HG23	2:I:2028:ASP:OD2	2.16	0.46
2:H:234:ILE:N	2:H:235:PRO:CD	2.79	0.46
2:L:1473:THR:HG1	2:L:1481:SER:HG	1.63	0.46
1:A:1673:TYR:CE1	1:A:1677:VAL:CG2	2.99	0.46
1:B:343:LEU:C	1:B:343:LEU:HD23	2.41	0.46
2:I:234:ILE:N	2:I:235:PRO:CD	2.79	0.46
2:K:234:ILE:N	2:K:235:PRO:CD	2.79	0.46
2:L:1906:ALA:O	2:L:1909:THR:OG1	2.31	0.46
1:F:1557:ILE:HD11	1:F:1642:THR:HG21	1.98	0.45
2:I:1778:GLN:HB2	2:I:1779:PRO:HD3	1.96	0.45
2:I:1868:GLN:HG3	2:I:1898:TYR:CE2	2.51	0.45
2:H:1665:VAL:HA	2:H:1805:ALA:O	2.16	0.45
2:K:1665:VAL:HA	2:K:1805:ALA:O	2.16	0.45
2:L:844:VAL:HG21	2:L:866:LYS:HD2	1.99	0.45
1:A:1298:ILE:HB	1:E:1411:THR:HG23	1.98	0.45
1:A:1411:THR:HG23	1:E:1298:ILE:HB	1.98	0.45
2:G:326:ASP:OD1	2:G:387:TYR:OH	2.33	0.45
2:G:844:VAL:HG21	2:G:866:LYS:HD2	1.99	0.45
2:G:1384:GLN:HE21	2:G:1389:ILE:HD12	1.81	0.45
1:E:1673:TYR:CE1	1:E:1677:VAL:CG2	2.99	0.45
2:I:1584:PHE:CD2	2:I:1584:PHE:C	2.93	0.45
2:H:414:LEU:HD12	2:H:414:LEU:O	2.15	0.45
2:L:1384:GLN:HE21	2:L:1389:ILE:HD12	1.81	0.45
2:G:1473:THR:HG1	2:G:1481:SER:HG	1.64	0.45
1:C:343:LEU:C	1:C:343:LEU:HD23	2.41	0.45
1:C:1246:CYS:HA	1:C:1299:LYS:O	2.16	0.45
1:D:1246:CYS:HA	1:D:1299:LYS:O	2.16	0.45
2:J:1868:GLN:HG3	2:J:1898:TYR:CE2	2.51	0.45
2:K:414:LEU:HD12	2:K:414:LEU:O	2.15	0.45
2:L:1665:VAL:HA	2:L:1805:ALA:O	2.16	0.45
5:L:2302:FNR:H1	5:L:2302:FNR:H4'	1.65	0.45
1:A:420:ILE:CD1	1:A:472:LEU:HD23	2.47	0.45
2:G:1665:VAL:HA	2:G:1805:ALA:O	2.16	0.45
1:C:1673:TYR:CE1	1:C:1677:VAL:CG2	2.99	0.45
1:D:343:LEU:HD23	1:D:343:LEU:C	2.41	0.45
1:D:1673:TYR:CE1	1:D:1677:VAL:CG2	2.99	0.45
1:E:420:ILE:CD1	1:E:472:LEU:HD23	2.47	0.45
2:J:1584:PHE:CD2	2:J:1584:PHE:C	2.94	0.45
2:L:1605:VAL:HG22	2:L:1657:ILE:HD12	1.99	0.45
2:G:1605:VAL:HG22	2:G:1657:ILE:HD12	1.99	0.45
1:C:1248:GLY:O	1:C:1331:GLY:HA2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1248:GLY:O	1:D:1331:GLY:HA2	2.17	0.45
2:J:598:THR:HA	2:J:599:PRO:HA	1.82	0.45
2:I:124:LYS:O	2:I:128:THR:OG1	2.24	0.45
2:H:844:VAL:HG21	2:H:866:LYS:HD2	1.98	0.45
2:K:844:VAL:HG21	2:K:866:LYS:HD2	1.98	0.45
2:G:234:ILE:N	2:G:235:PRO:CD	2.79	0.45
2:G:1584:PHE:C	2:G:1584:PHE:CD2	2.94	0.45
1:B:420:ILE:CD1	1:B:472:LEU:HD23	2.46	0.45
1:B:1246:CYS:HA	1:B:1299:LYS:O	2.16	0.45
1:F:1246:CYS:HA	1:F:1299:LYS:O	2.16	0.45
1:A:1557:ILE:HD11	1:A:1642:THR:HG21	1.97	0.45
1:E:1557:ILE:HD11	1:E:1642:THR:HG21	1.97	0.45
1:F:420:ILE:CD1	1:F:472:LEU:HD23	2.46	0.45
2:H:1374:THR:HG21	6:H:2682:HOH:O	2.16	0.45
2:L:234:ILE:N	2:L:235:PRO:CD	2.79	0.45
2:L:1584:PHE:C	2:L:1584:PHE:CD2	2.94	0.45
1:B:1248:GLY:O	1:B:1331:GLY:HA2	2.17	0.45
2:J:1547:PRO:HD3	2:J:1584:PHE:CZ	2.52	0.45
2:I:1547:PRO:HD3	2:I:1584:PHE:CZ	2.52	0.45
2:H:1605:VAL:HG22	2:H:1657:ILE:HD12	1.99	0.45
2:G:1547:PRO:HD3	2:G:1584:PHE:CZ	2.52	0.45
2:H:1782:THR:HG21	2:H:1827:LEU:HD11	1.99	0.45
2:K:663:ILE:HB	2:K:664:PRO:HD3	1.99	0.45
2:K:1605:VAL:HG22	2:K:1657:ILE:HD12	1.99	0.45
2:K:1782:THR:HG21	2:K:1827:LEU:HD11	1.99	0.45
2:L:369:SER:HB2	2:L:428:HIS:HB2	1.99	0.45
2:L:1547:PRO:HD3	2:L:1584:PHE:CZ	2.52	0.45
2:G:369:SER:HB2	2:G:428:HIS:HB2	1.99	0.45
1:F:1248:GLY:O	1:F:1331:GLY:HA2	2.17	0.45
2:H:663:ILE:HB	2:H:664:PRO:HD3	1.99	0.45
2:K:1374:THR:HG21	6:K:2691:HOH:O	2.16	0.45
1:B:1713:ASP:HB3	1:B:1738:ILE:HG21	1.99	0.44
1:F:1713:ASP:HB3	1:F:1738:ILE:HG21	1.99	0.44
2:J:960:LYS:HA	2:J:960:LYS:HE2	1.99	0.44
2:I:264:ARG:NH1	2:I:286:THR:O	2.51	0.44
2:I:663:ILE:HB	2:I:664:PRO:HD3	1.99	0.44
2:I:960:LYS:HE2	2:I:960:LYS:HA	1.99	0.44
1:A:616:LEU:N	1:A:617:PRO:CD	2.81	0.44
2:G:2044:ASN:HB3	2:G:2047:LYS:HD3	2.00	0.44
1:B:1298:ILE:HB	1:D:1411:THR:HG23	1.98	0.44
1:C:702:LYS:HD3	1:C:702:LYS:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1411:THR:HG23	1:F:1298:ILE:HB	1.98	0.44
1:E:616:LEU:N	1:E:617:PRO:CD	2.81	0.44
2:J:264:ARG:NH1	2:J:286:THR:O	2.51	0.44
2:J:663:ILE:HB	2:J:664:PRO:HD3	1.99	0.44
2:L:2044:ASN:HB3	2:L:2047:LYS:HD3	2.00	0.44
1:D:702:LYS:HD3	1:D:702:LYS:N	2.33	0.44
1:B:743:GLN:NE2	1:E:377:TYR:CE1	2.85	0.44
2:J:1960:LEU:HD12	2:J:1960:LEU:HA	1.91	0.44
1:A:377:TYR:CE1	1:F:743:GLN:NE2	2.85	0.44
2:H:1547:PRO:HD3	2:H:1584:PHE:CZ	2.52	0.44
2:L:1782:THR:HG21	2:L:1827:LEU:HD11	1.99	0.44
2:G:1782:THR:HG21	2:G:1827:LEU:HD11	1.99	0.44
1:C:1298:ILE:HB	1:F:1411:THR:HG23	1.98	0.44
1:F:702:LYS:N	1:F:702:LYS:HD3	2.33	0.44
2:J:1605:VAL:HG22	2:J:1657:ILE:HD12	1.99	0.44
2:I:1605:VAL:HG22	2:I:1657:ILE:HD12	1.99	0.44
2:K:1547:PRO:HD3	2:K:1584:PHE:CZ	2.52	0.44
1:B:702:LYS:HD3	1:B:702:LYS:N	2.33	0.44
1:B:1411:THR:HG23	1:D:1298:ILE:HB	1.98	0.44
1:C:442:ARG:HD3	1:C:726:GLY:O	2.18	0.44
1:D:442:ARG:HD3	1:D:726:GLY:O	2.18	0.44
2:L:1040:LEU:O	2:L:1046:GLN:HA	2.18	0.44
1:A:442:ARG:HD3	1:A:726:GLY:O	2.18	0.44
1:C:616:LEU:N	1:C:617:PRO:CD	2.81	0.44
1:E:442:ARG:HD3	1:E:726:GLY:O	2.18	0.44
2:H:264:ARG:NH1	2:H:286:THR:O	2.50	0.44
2:K:264:ARG:NH1	2:K:286:THR:O	2.50	0.44
2:K:1225:GLU:OE1	2:K:1566:SER:OG	2.35	0.44
2:G:1040:LEU:O	2:G:1046:GLN:HA	2.18	0.44
1:D:616:LEU:N	1:D:617:PRO:CD	2.81	0.44
2:H:1040:LEU:O	2:H:1046:GLN:HA	2.18	0.44
2:H:1225:GLU:OE1	2:H:1566:SER:OG	2.35	0.44
2:G:264:ARG:NH1	2:G:286:THR:O	2.51	0.43
1:C:377:TYR:CE1	1:D:743:GLN:NE2	2.86	0.43
1:C:743:GLN:NE2	1:D:377:TYR:CE1	2.86	0.43
1:F:616:LEU:N	1:F:617:PRO:CD	2.81	0.43
2:J:618:GLU:HG2	2:J:678:PHE:CE2	2.53	0.43
2:I:528:ILE:HG21	2:I:547:ILE:HG13	2.00	0.43
2:K:1040:LEU:O	2:K:1046:GLN:HA	2.18	0.43
2:L:264:ARG:NH1	2:L:286:THR:O	2.51	0.43
1:B:616:LEU:N	1:B:617:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:850:PHE:CE2	1:D:923:MET:HE2	2.53	0.43
1:E:1248:GLY:O	1:E:1331:GLY:HA2	2.17	0.43
2:J:528:ILE:HG21	2:J:547:ILE:HG13	2.00	0.43
2:J:1808:J8W:O9	2:J:1834:ARG:NH1	2.38	0.43
2:I:618:GLU:HG2	2:I:678:PHE:CE2	2.53	0.43
2:I:1549:THR:OG1	2:I:1551:GLU:OE1	2.34	0.43
2:I:1782:THR:HG21	2:I:1827:LEU:HD11	1.99	0.43
2:H:369:SER:HB2	2:H:428:HIS:HB2	1.99	0.43
2:H:1339:PHE:N	2:H:1340:PRO:CD	2.81	0.43
2:K:1339:PHE:N	2:K:1340:PRO:CD	2.81	0.43
1:B:442:ARG:HD3	1:B:726:GLY:O	2.18	0.43
2:J:369:SER:HB2	2:J:428:HIS:HB2	1.99	0.43
2:J:1040:LEU:O	2:J:1046:GLN:HA	2.18	0.43
2:J:1339:PHE:N	2:J:1340:PRO:CD	2.81	0.43
2:J:1549:THR:OG1	2:J:1551:GLU:OE1	2.34	0.43
2:I:369:SER:HB2	2:I:428:HIS:HB2	1.99	0.43
2:K:369:SER:HB2	2:K:428:HIS:HB2	1.99	0.43
1:A:1248:GLY:O	1:A:1331:GLY:HA2	2.17	0.43
2:G:618:GLU:HG2	2:G:678:PHE:CE2	2.53	0.43
2:G:1339:PHE:N	2:G:1340:PRO:CD	2.81	0.43
1:C:59:ARG:NH2	4:H:2301:COA:O1A	2.50	0.43
1:C:850:PHE:CE2	1:C:923:MET:HE2	2.53	0.43
1:F:442:ARG:HD3	1:F:726:GLY:O	2.18	0.43
1:F:1107:GLU:OE1	1:F:1191:THR:OG1	2.36	0.43
1:F:1154:ILE:HA	1:F:1164:SER:O	2.19	0.43
1:F:1460:LYS:HE2	1:F:1774:GLU:OE2	2.18	0.43
2:J:317:THR:HG22	2:K:1312:VAL:HG21	2.00	0.43
2:J:1782:THR:HG21	2:J:1827:LEU:HD11	1.99	0.43
2:I:317:THR:HG22	2:H:1312:VAL:HG21	2.00	0.43
2:I:1040:LEU:O	2:I:1046:GLN:HA	2.18	0.43
2:L:618:GLU:HG2	2:L:678:PHE:CE2	2.53	0.43
1:A:1713:ASP:HB3	1:A:1738:ILE:HG21	1.99	0.43
2:G:663:ILE:HB	2:G:664:PRO:HD3	1.99	0.43
2:G:1312:VAL:HG21	2:H:317:THR:HG22	2.00	0.43
1:B:1154:ILE:HA	1:B:1164:SER:O	2.19	0.43
1:B:1460:LYS:HE2	1:B:1774:GLU:OE2	2.18	0.43
1:F:413:LEU:HG	1:F:451:MET:HG2	2.01	0.43
2:I:1339:PHE:N	2:I:1340:PRO:CD	2.81	0.43
2:K:317:THR:HG22	2:L:1312:VAL:HG21	2.00	0.43
2:L:663:ILE:HB	2:L:664:PRO:HD3	1.99	0.43
2:L:1339:PHE:N	2:L:1340:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:LYS:HD3	1:A:702:LYS:N	2.33	0.43
1:B:413:LEU:HG	1:B:451:MET:HG2	2.01	0.43
1:E:702:LYS:HD3	1:E:702:LYS:N	2.33	0.43
1:E:1154:ILE:HA	1:E:1164:SER:O	2.19	0.43
2:H:1723:GLY:O	2:H:1727:LYS:HG2	2.19	0.43
2:K:1723:GLY:O	2:K:1727:LYS:HG2	2.19	0.43
1:A:1154:ILE:HA	1:A:1164:SER:O	2.19	0.43
2:G:1327:ILE:O	2:G:1331:TRP:HB2	2.19	0.43
1:E:850:PHE:CE2	1:E:923:MET:HE2	2.53	0.43
2:J:1723:GLY:O	2:J:1727:LYS:HG2	2.19	0.43
2:J:2044:ASN:HB3	2:J:2047:LYS:HD3	2.00	0.43
2:I:1723:GLY:O	2:I:1727:LYS:HG2	2.19	0.43
2:I:2044:ASN:HB3	2:I:2047:LYS:HD3	2.00	0.43
2:L:1327:ILE:O	2:L:1331:TRP:HB2	2.19	0.43
2:L:1723:GLY:O	2:L:1727:LYS:HG2	2.19	0.43
1:A:850:PHE:CE2	1:A:923:MET:HE2	2.53	0.43
1:D:1713:ASP:HB3	1:D:1738:ILE:HG21	1.99	0.43
2:H:618:GLU:HG2	2:H:678:PHE:CE2	2.54	0.43
1:A:1443:LEU:HD23	1:A:1443:LEU:HA	1.89	0.43
2:G:1723:GLY:O	2:G:1727:LYS:HG2	2.19	0.43
1:B:377:TYR:CE1	1:E:743:GLN:NE2	2.85	0.43
1:E:1713:ASP:HB3	1:E:1738:ILE:HG21	1.99	0.43
2:J:264:ARG:NH1	2:J:456:GLN:HG3	2.34	0.43
2:J:1327:ILE:O	2:J:1331:TRP:HB2	2.19	0.43
2:I:1327:ILE:O	2:I:1331:TRP:HB2	2.19	0.43
2:K:618:GLU:HG2	2:K:678:PHE:CE2	2.54	0.43
1:C:1713:ASP:HB3	1:C:1738:ILE:HG21	1.99	0.43
2:J:2023:LYS:HG3	2:J:2045:TRP:CD2	2.54	0.43
2:I:264:ARG:NH1	2:I:456:GLN:HG3	2.34	0.43
2:I:2023:LYS:HG3	2:I:2045:TRP:CD2	2.54	0.43
2:K:1960:LEU:HD12	2:K:1960:LEU:HA	1.90	0.43
2:L:56:THR:CG2	2:L:112:ASN:HD22	2.32	0.43
2:G:56:THR:CG2	2:G:112:ASN:HD22	2.32	0.42
2:G:264:ARG:NH1	2:G:456:GLN:HG3	2.34	0.42
2:G:528:ILE:HG21	2:G:547:ILE:HG13	2.00	0.42
1:B:878:MET:HG3	3:B:1901:NAP:N7N	2.34	0.42
1:E:1443:LEU:HD23	1:E:1443:LEU:HA	1.89	0.42
1:F:878:MET:HG3	3:F:1901:NAP:N7N	2.34	0.42
2:H:176:LEU:HD13	2:H:247:ALA:HB3	2.01	0.42
2:H:481:ASP:OD2	2:H:485:ARG:NH1	2.52	0.42
2:K:481:ASP:OD2	2:K:485:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:481:ASP:OD2	2:L:485:ARG:NH1	2.52	0.42
2:G:481:ASP:OD2	2:G:485:ARG:NH1	2.52	0.42
1:B:1117:GLU:O	1:D:1146:HIS:HE1	2.02	0.42
1:C:878:MET:HG3	3:C:1901:NAP:N7N	2.35	0.42
1:C:1154:ILE:HA	1:C:1164:SER:O	2.19	0.42
1:D:1154:ILE:HA	1:D:1164:SER:O	2.19	0.42
1:F:378:LEU:HD23	1:F:378:LEU:HA	1.89	0.42
1:F:419:GLU:HG3	6:F:2108:HOH:O	2.18	0.42
2:J:1445:ARG:NH2	2:J:1455:GLU:O	2.52	0.42
2:I:1445:ARG:NH2	2:I:1455:GLU:O	2.53	0.42
2:H:1360:ILE:HD13	2:H:1402:PRO:HB2	2.01	0.42
2:K:176:LEU:HD13	2:K:247:ALA:HB3	2.02	0.42
2:L:264:ARG:NH1	2:L:456:GLN:HG3	2.34	0.42
2:L:528:ILE:HG21	2:L:547:ILE:HG13	2.01	0.42
1:A:413:LEU:HG	1:A:451:MET:HG2	2.01	0.42
1:A:1117:GLU:O	1:E:1146:HIS:HE1	2.02	0.42
1:A:1305:CYS:HB3	1:A:1583:HIS:CE1	2.54	0.42
2:G:1337:ALA:HB1	2:G:1378:ILE:HG12	2.02	0.42
1:B:419:GLU:HG3	6:B:2107:HOH:O	2.18	0.42
1:C:1146:HIS:HE1	1:F:1117:GLU:O	2.02	0.42
1:E:1305:CYS:HB3	1:E:1583:HIS:CE1	2.54	0.42
2:J:2023:LYS:HG3	2:J:2045:TRP:CG	2.55	0.42
2:H:1445:ARG:NH2	2:H:1455:GLU:O	2.53	0.42
2:K:1445:ARG:NH2	2:K:1455:GLU:O	2.53	0.42
1:A:1673:TYR:O	1:A:1677:VAL:HG23	2.20	0.42
2:G:747:HIS:HE1	2:G:780:TYR:OH	2.03	0.42
1:D:878:MET:HG3	3:D:1901:NAP:N7N	2.35	0.42
1:E:413:LEU:HG	1:E:451:MET:HG2	2.01	0.42
1:E:1460:LYS:HE2	1:E:1774:GLU:OE2	2.18	0.42
1:E:1673:TYR:O	1:E:1677:VAL:HG23	2.20	0.42
1:F:1274:ILE:HD12	1:F:1274:ILE:HA	1.90	0.42
2:H:1337:ALA:HB1	2:H:1378:ILE:HG12	2.02	0.42
2:K:1337:ALA:HB1	2:K:1378:ILE:HG12	2.02	0.42
2:L:747:HIS:HE1	2:L:780:TYR:OH	2.02	0.42
2:L:1337:ALA:HB1	2:L:1378:ILE:HG12	2.02	0.42
2:L:2023:LYS:HG3	2:L:2045:TRP:CD2	2.54	0.42
1:A:743:GLN:NE2	1:F:377:TYR:CE1	2.85	0.42
1:A:817:THR:OG1	6:A:2006:HOH:O	2.22	0.42
1:B:1673:TYR:O	1:B:1677:VAL:HG23	2.20	0.42
1:C:413:LEU:HG	1:C:451:MET:HG2	2.01	0.42
1:C:1443:LEU:HD23	1:C:1443:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1337:ALA:HB1	2:J:1378:ILE:HG12	2.02	0.42
2:I:1337:ALA:HB1	2:I:1378:ILE:HG12	2.02	0.42
2:I:2023:LYS:HG3	2:I:2045:TRP:CG	2.55	0.42
2:K:2023:LYS:HG3	2:K:2045:TRP:CD2	2.54	0.42
2:L:1905:ARG:O	2:L:1909:THR:HG23	2.19	0.42
1:A:1146:HIS:HE1	1:E:1117:GLU:O	2.02	0.42
1:A:1302:VAL:HG23	1:E:1302:VAL:HG23	2.02	0.42
1:A:1460:LYS:HE2	1:A:1774:GLU:OE2	2.18	0.42
2:G:1445:ARG:NH2	2:G:1455:GLU:O	2.53	0.42
2:G:2023:LYS:HG3	2:G:2045:TRP:CD2	2.54	0.42
1:B:850:PHE:CE2	1:B:923:MET:HE2	2.53	0.42
1:F:1673:TYR:O	1:F:1677:VAL:HG23	2.20	0.42
2:H:1915:ASN:HD21	2:H:1963:GLY:CA	2.33	0.42
2:H:2023:LYS:HG3	2:H:2045:TRP:CD2	2.54	0.42
2:L:1445:ARG:NH2	2:L:1455:GLU:O	2.53	0.42
5:G:2302:FNR:N5	3:G:2303:NAP:C4N	2.83	0.42
1:B:378:LEU:HD23	1:B:378:LEU:HA	1.89	0.42
1:B:1274:ILE:HD12	1:B:1274:ILE:HA	1.90	0.42
1:D:413:LEU:HG	1:D:451:MET:HG2	2.01	0.42
1:F:415:SER:OG	1:F:1629:LYS:NZ	2.53	0.42
1:F:850:PHE:CE2	1:F:923:MET:HE2	2.53	0.42
2:J:481:ASP:OD2	2:J:485:ARG:NH1	2.52	0.42
2:I:747:HIS:HE1	2:I:780:TYR:OH	2.02	0.42
2:H:598:THR:HA	2:H:599:PRO:HA	1.82	0.42
2:K:1033:SER:OG	6:K:2402:HOH:O	2.21	0.42
2:G:1905:ARG:O	2:G:1909:THR:HG23	2.19	0.42
1:B:415:SER:OG	1:B:1629:LYS:NZ	2.53	0.42
1:F:1443:LEU:HD23	1:F:1443:LEU:HA	1.89	0.42
2:J:72:VAL:HG11	2:J:84:LEU:CD2	2.49	0.42
2:J:747:HIS:HE1	2:J:780:TYR:OH	2.02	0.42
2:J:1360:ILE:HD13	2:J:1402:PRO:HB2	2.01	0.42
2:I:72:VAL:HG11	2:I:84:LEU:CD2	2.49	0.42
2:I:1360:ILE:HD13	2:I:1402:PRO:HB2	2.02	0.42
2:H:273:HIS:CD2	2:H:488:VAL:HG11	2.55	0.42
1:B:1146:HIS:HE1	1:D:1117:GLU:O	2.02	0.42
1:D:1443:LEU:HD23	1:D:1443:LEU:HA	1.89	0.42
1:F:1305:CYS:HB3	1:F:1583:HIS:CE1	2.54	0.42
2:J:56:THR:HG22	2:J:112:ASN:HD22	1.85	0.42
2:I:481:ASP:OD2	2:I:485:ARG:NH1	2.52	0.42
2:K:273:HIS:CD2	2:K:488:VAL:HG11	2.55	0.42
2:K:528:ILE:HG21	2:K:547:ILE:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1360:ILE:HD13	2:K:1402:PRO:HB2	2.01	0.42
2:L:2023:LYS:HG3	2:L:2045:TRP:CG	2.55	0.42
5:L:2302:FNR:N5	3:L:2303:NAP:C4N	2.83	0.42
1:A:419:GLU:HG3	6:A:2104:HOH:O	2.19	0.42
1:A:713:GLN:NE2	6:A:2137:HOH:O	2.53	0.42
2:G:2023:LYS:HG3	2:G:2045:TRP:CG	2.55	0.42
1:B:1305:CYS:HB3	1:B:1583:HIS:CE1	2.54	0.42
1:E:419:GLU:HG3	6:E:2109:HOH:O	2.19	0.42
1:E:713:GLN:NE2	6:E:2143:HOH:O	2.53	0.42
1:E:888:ILE:HD11	1:E:940:THR:HG22	2.02	0.42
5:J:2302:FNR:N5	3:J:2303:NAP:C4N	2.83	0.42
2:H:528:ILE:HG21	2:H:547:ILE:HG13	2.00	0.42
2:L:176:LEU:HD13	2:L:247:ALA:HB3	2.01	0.42
1:A:888:ILE:HD11	1:A:940:THR:HG22	2.02	0.41
2:G:176:LEU:HD13	2:G:247:ALA:HB3	2.01	0.41
2:G:208:VAL:HG13	2:G:235:PRO:HG2	2.02	0.41
1:C:415:SER:OG	1:C:1629:LYS:NZ	2.53	0.41
1:D:415:SER:OG	1:D:1629:LYS:NZ	2.53	0.41
5:I:2302:FNR:N5	3:I:2303:NAP:C4N	2.83	0.41
2:H:72:VAL:HG11	2:H:84:LEU:CD2	2.49	0.41
2:K:1897:GLN:NE2	4:K:2301:COA:H143	2.35	0.41
2:L:960:LYS:HA	2:L:960:LYS:HE2	2.02	0.41
2:L:1360:ILE:HD13	2:L:1402:PRO:HB2	2.02	0.41
1:A:1584:PRO:HG3	1:A:1591:TRP:CE3	2.55	0.41
2:G:960:LYS:HA	2:G:960:LYS:HE2	2.02	0.41
1:C:1117:GLU:O	1:F:1146:HIS:HE1	2.02	0.41
1:D:821:GLN:OE1	1:D:909:LEU:HD23	2.21	0.41
1:E:1584:PRO:HG3	1:E:1591:TRP:CE3	2.55	0.41
2:I:176:LEU:HD13	2:I:247:ALA:HB3	2.01	0.41
2:H:1327:ILE:O	2:H:1331:TRP:HB2	2.19	0.41
2:L:208:VAL:HG13	2:L:235:PRO:HG2	2.02	0.41
1:C:821:GLN:OE1	1:C:909:LEU:HD23	2.21	0.41
1:E:21:GLN:NE2	2:L:1808:J8W:O	2.47	0.41
1:F:17:LEU:HD23	2:J:2014:LEU:HD23	2.02	0.41
2:J:273:HIS:CD2	2:J:488:VAL:HG11	2.55	0.41
2:J:364:LYS:HA	2:J:382:PRO:HG2	2.03	0.41
2:I:273:HIS:CD2	2:I:488:VAL:HG11	2.55	0.41
2:I:364:LYS:HA	2:I:382:PRO:HG2	2.03	0.41
2:H:1208:THR:HB	2:H:1568:HIS:CE1	2.56	0.41
2:K:598:THR:HA	2:K:599:PRO:HA	1.82	0.41
2:K:1208:THR:HB	2:K:1568:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:2302:FNR:H1	5:K:2302:FNR:H4'	1.65	0.41
1:A:21:GLN:NE2	2:G:1808:J8W:O	2.48	0.41
2:G:1360:ILE:HD13	2:G:1402:PRO:HB2	2.02	0.41
1:D:1305:CYS:HB3	1:D:1583:HIS:CE1	2.54	0.41
2:J:56:THR:CG2	2:J:112:ASN:HD22	2.32	0.41
2:J:124:LYS:O	2:J:128:THR:OG1	2.24	0.41
2:J:176:LEU:HD13	2:J:247:ALA:HB3	2.01	0.41
2:J:1087:HIS:HA	2:J:1092:ASP:OD2	2.21	0.41
2:J:1473:THR:HG1	2:J:1481:SER:HG	1.65	0.41
2:H:2023:LYS:HG3	2:H:2045:TRP:CG	2.55	0.41
2:K:72:VAL:HG11	2:K:84:LEU:CD2	2.49	0.41
2:K:1327:ILE:O	2:K:1331:TRP:HB2	2.19	0.41
2:K:2023:LYS:HG3	2:K:2045:TRP:CG	2.55	0.41
1:B:821:GLN:OE1	1:B:909:LEU:HD23	2.21	0.41
1:B:1568:GLU:O	6:B:2005:HOH:O	2.21	0.41
1:C:378:LEU:HD23	1:C:378:LEU:HA	1.89	0.41
1:C:1305:CYS:HB3	1:C:1583:HIS:CE1	2.54	0.41
1:C:1425:ILE:HD12	1:C:1425:ILE:HA	1.96	0.41
1:D:1425:ILE:HD12	1:D:1425:ILE:HA	1.96	0.41
2:I:1087:HIS:HA	2:I:1092:ASP:OD2	2.21	0.41
2:H:747:HIS:HE1	2:H:780:TYR:OH	2.03	0.41
2:H:1549:THR:OG1	2:H:1551:GLU:OE2	2.36	0.41
5:H:2302:FNR:N5	3:H:2303:NAP:C4N	2.84	0.41
1:B:523:SER:O	1:B:527:GLN:HG3	2.21	0.41
1:D:419:GLU:HG3	6:D:2101:HOH:O	2.19	0.41
1:D:1673:TYR:O	1:D:1677:VAL:HG23	2.20	0.41
1:F:523:SER:O	1:F:527:GLN:HG3	2.21	0.41
1:F:821:GLN:OE1	1:F:909:LEU:HD23	2.21	0.41
2:K:747:HIS:HE1	2:K:780:TYR:OH	2.02	0.41
2:K:1549:THR:OG1	2:K:1551:GLU:OE2	2.36	0.41
2:L:245:GLN:HG2	2:L:505:GLY:HA2	2.02	0.41
2:G:56:THR:HG22	2:G:112:ASN:HD22	1.85	0.41
2:G:245:GLN:HG2	2:G:505:GLY:HA2	2.03	0.41
2:G:273:HIS:CD2	2:G:488:VAL:HG11	2.55	0.41
2:G:1593:ILE:HD13	2:G:1626:ILE:CD1	2.51	0.41
1:D:378:LEU:HD23	1:D:378:LEU:HA	1.89	0.41
1:F:431:GLU:HA	1:F:434:SER:OG	2.21	0.41
2:L:273:HIS:CD2	2:L:488:VAL:HG11	2.55	0.41
2:L:1593:ILE:HD13	2:L:1626:ILE:CD1	2.51	0.41
2:G:364:LYS:HA	2:G:382:PRO:HG2	2.03	0.41
2:G:1087:HIS:HA	2:G:1092:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1673:TYR:O	1:C:1677:VAL:HG23	2.20	0.41
5:K:2302:FNR:N5	3:K:2303:NAP:C4N	2.84	0.41
2:L:56:THR:HG22	2:L:112:ASN:HD22	1.85	0.41
2:G:317:THR:HG22	2:I:1312:VAL:HG21	2.02	0.41
2:G:905:ALA:HA	2:G:917:MET:SD	2.60	0.41
2:G:1327:ILE:HD12	2:G:1327:ILE:HA	1.99	0.41
1:B:17:LEU:HD23	2:I:2014:LEU:HD23	2.03	0.41
1:B:431:GLU:HA	1:B:434:SER:OG	2.21	0.41
1:B:1531:LEU:HD21	1:B:1660:TYR:CZ	2.56	0.41
1:C:823:ILE:HD13	1:C:865:CYS:HB3	2.03	0.41
1:F:21:GLN:NE2	2:J:1808:J8W:O	2.47	0.41
1:F:1531:LEU:HD21	1:F:1660:TYR:CZ	2.56	0.41
2:H:208:VAL:HG13	2:H:235:PRO:HG2	2.02	0.41
2:H:1897:GLN:NE2	4:H:2301:COA:H143	2.36	0.41
2:K:145:LEU:HD11	2:K:156:LEU:HD11	2.02	0.41
2:K:208:VAL:HG13	2:K:235:PRO:HG2	2.02	0.41
2:K:1638:ILE:O	2:K:1654:GLU:HA	2.21	0.41
2:L:364:LYS:HA	2:L:382:PRO:HG2	2.03	0.41
2:L:905:ALA:HA	2:L:917:MET:SD	2.60	0.41
2:L:1087:HIS:HA	2:L:1092:ASP:OD2	2.21	0.41
1:B:1432:HIS:NE2	1:B:1434:SER:OG	2.54	0.41
1:C:419:GLU:HG3	6:C:2104:HOH:O	2.20	0.41
1:D:823:ILE:HD13	1:D:865:CYS:HB3	2.03	0.41
1:F:1584:PRO:HG3	1:F:1591:TRP:CE3	2.55	0.41
2:H:145:LEU:HD11	2:H:156:LEU:HD11	2.02	0.41
2:L:494:THR:HA	2:L:496:PHE:CE2	2.56	0.41
2:G:494:THR:HA	2:G:496:PHE:CE2	2.56	0.40
2:G:1549:THR:OG1	2:G:1551:GLU:OE1	2.34	0.40
1:B:1302:VAL:HG23	1:D:1302:VAL:HG23	2.02	0.40
1:B:1584:PRO:HG3	1:B:1591:TRP:CE3	2.55	0.40
1:C:523:SER:O	1:C:527:GLN:HG3	2.21	0.40
1:D:17:LEU:HD23	2:K:2014:LEU:HD23	2.03	0.40
1:E:1531:LEU:HD21	1:E:1660:TYR:CZ	2.56	0.40
1:F:1432:HIS:NE2	1:F:1434:SER:OG	2.54	0.40
2:J:340:SER:O	2:J:418:ASN:HA	2.21	0.40
2:H:364:LYS:HA	2:H:382:PRO:HG2	2.03	0.40
2:H:1638:ILE:O	2:H:1654:GLU:HA	2.21	0.40
2:K:364:LYS:HA	2:K:382:PRO:HG2	2.03	0.40
1:A:17:LEU:HD23	2:G:2014:LEU:HD23	2.03	0.40
1:A:1531:LEU:HD21	1:A:1660:TYR:CZ	2.56	0.40
1:C:1302:VAL:HG23	1:F:1302:VAL:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:431:GLU:HA	1:D:434:SER:OG	2.21	0.40
1:D:713:GLN:NE2	6:D:2161:HOH:O	2.54	0.40
1:D:1017:ARG:NH1	6:D:2060:HOH:O	2.43	0.40
1:E:523:SER:O	1:E:527:GLN:HG3	2.21	0.40
2:J:905:ALA:HA	2:J:917:MET:SD	2.60	0.40
2:J:1225:GLU:OE1	2:J:1566:SER:OG	2.35	0.40
2:J:1638:ILE:O	2:J:1654:GLU:HA	2.21	0.40
2:I:653:TYR:CD1	2:I:659:LEU:HD11	2.56	0.40
2:I:905:ALA:HA	2:I:917:MET:SD	2.60	0.40
2:I:1638:ILE:O	2:I:1654:GLU:HA	2.21	0.40
2:H:245:GLN:HG2	2:H:505:GLY:HA2	2.02	0.40
2:H:494:THR:HA	2:H:496:PHE:CE2	2.56	0.40
2:H:653:TYR:CD1	2:H:659:LEU:HD11	2.56	0.40
2:K:653:TYR:CD1	2:K:659:LEU:HD11	2.56	0.40
1:A:523:SER:O	1:A:527:GLN:HG3	2.21	0.40
1:A:821:GLN:OE1	1:A:909:LEU:HD23	2.21	0.40
2:G:1208:THR:HB	2:G:1568:HIS:CE1	2.56	0.40
1:B:21:GLN:NE2	2:I:1808:J8W:O	2.47	0.40
1:B:29:ILE:HG12	2:I:1891:TYR:HB3	2.04	0.40
1:C:17:LEU:HD23	2:H:2014:LEU:HD23	2.03	0.40
1:C:348:ARG:HD2	1:E:341:GLN:HE22	1.85	0.40
1:C:1584:PRO:HG3	1:C:1591:TRP:CE3	2.55	0.40
1:D:523:SER:O	1:D:527:GLN:HG3	2.21	0.40
1:D:888:ILE:HD11	1:D:940:THR:HG22	2.03	0.40
1:D:1584:PRO:HG3	1:D:1591:TRP:CE3	2.55	0.40
1:F:29:ILE:HG12	2:J:1891:TYR:HB3	2.04	0.40
1:F:337:VAL:CG1	1:F:341:GLN:NE2	2.85	0.40
2:J:208:VAL:HG13	2:J:235:PRO:HG2	2.02	0.40
2:J:494:THR:HA	2:J:496:PHE:CE2	2.56	0.40
2:J:653:TYR:CD1	2:J:659:LEU:HD11	2.56	0.40
2:J:1312:VAL:HG21	2:L:317:THR:HG22	2.02	0.40
2:I:340:SER:O	2:I:418:ASN:HA	2.22	0.40
2:I:1593:ILE:HD13	2:I:1626:ILE:CD1	2.51	0.40
2:H:905:ALA:HA	2:H:917:MET:SD	2.60	0.40
2:K:245:GLN:HG2	2:K:505:GLY:HA2	2.02	0.40
2:L:1208:THR:HB	2:L:1568:HIS:CE1	2.56	0.40
2:L:1327:ILE:HD12	2:L:1327:ILE:HA	1.99	0.40
1:A:522:LEU:HD23	1:A:522:LEU:HA	2.00	0.40
2:G:1804:PHE:CZ	2:G:2010:TYR:HB2	2.57	0.40
2:G:2036:GLU:N	2:G:2037:PRO:CD	2.84	0.40
1:B:1491:ARG:NE	1:B:1744:TYR:O	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:888:ILE:HD11	1:C:940:THR:HG22	2.03	0.40
1:E:17:LEU:HD23	2:L:2014:LEU:HD23	2.03	0.40
1:E:821:GLN:OE1	1:E:909:LEU:HD23	2.21	0.40
2:J:245:GLN:HG2	2:J:505:GLY:HA2	2.03	0.40
2:J:349:VAL:O	2:J:353:VAL:HG13	2.22	0.40
2:J:355:LYS:O	2:J:358:SER:OG	2.38	0.40
2:J:1208:THR:HB	2:J:1568:HIS:CE1	2.56	0.40
2:J:1593:ILE:HD13	2:J:1626:ILE:CD1	2.51	0.40
2:J:1804:PHE:CZ	2:J:2010:TYR:HB2	2.57	0.40
2:I:208:VAL:HG13	2:I:235:PRO:HG2	2.02	0.40
2:I:494:THR:HA	2:I:496:PHE:CE2	2.56	0.40
2:I:1208:THR:HB	2:I:1568:HIS:CE1	2.56	0.40
2:I:1225:GLU:OE1	2:I:1566:SER:OG	2.35	0.40
2:I:1804:PHE:CZ	2:I:2010:TYR:HB2	2.57	0.40
2:K:494:THR:HA	2:K:496:PHE:CE2	2.56	0.40
2:K:905:ALA:HA	2:K:917:MET:SD	2.61	0.40
2:L:1549:THR:OG1	2:L:1551:GLU:OE1	2.34	0.40
2:L:1804:PHE:CZ	2:L:2010:TYR:HB2	2.57	0.40
2:L:2036:GLU:N	2:L:2037:PRO:CD	2.84	0.40
1:A:844:LEU:HG	1:F:844:LEU:HG	2.03	0.40
2:G:653:TYR:CD1	2:G:659:LEU:HD11	2.56	0.40
2:G:1638:ILE:O	2:G:1654:GLU:HA	2.21	0.40
1:B:823:ILE:HD13	1:B:865:CYS:HB3	2.03	0.40
1:B:844:LEU:HG	1:E:844:LEU:HG	2.03	0.40
1:C:1462:TRP:CH2	1:C:1466:GLU:HG3	2.57	0.40
1:C:1491:ARG:NE	1:C:1744:TYR:O	2.51	0.40
1:D:1462:TRP:CH2	1:D:1466:GLU:HG3	2.57	0.40
1:F:823:ILE:HD13	1:F:865:CYS:HB3	2.03	0.40
1:F:1657:HIS:CG	1:F:1658:PRO:HD2	2.57	0.40
2:I:349:VAL:O	2:I:353:VAL:HG13	2.22	0.40
2:I:1960:LEU:HD12	2:I:1960:LEU:HA	1.91	0.40
2:K:1593:ILE:HD13	2:K:1626:ILE:CD1	2.51	0.40
2:L:653:TYR:CD1	2:L:659:LEU:HD11	2.56	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	1576/1887 (84%)	1527 (97%)	49 (3%)	0	100	100
1	B	1576/1887 (84%)	1527 (97%)	49 (3%)	0	100	100
1	C	1576/1887 (84%)	1526 (97%)	50 (3%)	0	100	100
1	D	1576/1887 (84%)	1528 (97%)	48 (3%)	0	100	100
1	E	1576/1887 (84%)	1527 (97%)	49 (3%)	0	100	100
1	F	1576/1887 (84%)	1527 (97%)	49 (3%)	0	100	100
2	G	2029/2051 (99%)	1966 (97%)	60 (3%)	3 (0%)	48	40
2	H	2029/2051 (99%)	1966 (97%)	60 (3%)	3 (0%)	48	40
2	I	2029/2051 (99%)	1966 (97%)	60 (3%)	3 (0%)	48	40
2	J	2029/2051 (99%)	1966 (97%)	60 (3%)	3 (0%)	48	40
2	K	2029/2051 (99%)	1966 (97%)	60 (3%)	3 (0%)	48	40
2	L	2029/2051 (99%)	1966 (97%)	60 (3%)	3 (0%)	48	40
All	All	21630/23628 (92%)	20958 (97%)	654 (3%)	18 (0%)	49	40

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	343	ASN
2	J	343	ASN
2	I	343	ASN
2	H	343	ASN
2	K	343	ASN
2	L	343	ASN
2	G	769	SER
2	J	769	SER
2	I	769	SER
2	H	769	SER
2	K	769	SER
2	L	769	SER

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Mol	Chain	Res	Type
2	G	1044	VAL
2	J	1044	VAL
2	I	1044	VAL
2	H	1044	VAL
2	K	1044	VAL
2	L	1044	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	1340/1566 (86%)	1309 (98%)	31 (2%)	44	40
1	B	1340/1566 (86%)	1312 (98%)	28 (2%)	47	44
1	C	1340/1566 (86%)	1311 (98%)	29 (2%)	45	42
1	D	1340/1566 (86%)	1312 (98%)	28 (2%)	47	44
1	E	1340/1566 (86%)	1310 (98%)	30 (2%)	45	42
1	F	1340/1566 (86%)	1310 (98%)	30 (2%)	45	42
2	G	1772/1788 (99%)	1730 (98%)	42 (2%)	43	38
2	H	1772/1788 (99%)	1724 (97%)	48 (3%)	39	34
2	I	1772/1788 (99%)	1728 (98%)	44 (2%)	42	37
2	J	1772/1788 (99%)	1730 (98%)	42 (2%)	43	38
2	K	1772/1788 (99%)	1722 (97%)	50 (3%)	38	32
2	L	1772/1788 (99%)	1732 (98%)	40 (2%)	44	40
All	All	18672/20124 (93%)	18230 (98%)	442 (2%)	43	38

All (442) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	THR
1	A	72	LEU
1	A	334	ASP
1	A	360	LYS

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Mol	Chain	Res	Type
1	A	363	LYS
1	A	434	SER
1	A	464	GLU
1	A	495	LYS
1	A	521	LYS
1	A	713	GLN
1	A	757	LYS
1	A	883	ILE
1	A	893	VAL
1	A	935	GLU
1	A	966	LYS
1	A	1001	VAL
1	A	1004	ILE
1	A	1050	CYS
1	A	1283	MET
1	A	1305	CYS
1	A	1332	TYR
1	A	1362	PRO
1	A	1364	GLU
1	A	1370	THR
1	A	1391	ASP
1	A	1395	LYS
1	A	1514	LYS
1	A	1643	SER
1	A	1756	ILE
1	A	1759	MET
1	A	1773	VAL
2	G	86	LEU
2	G	116	LEU
2	G	122	LEU
2	G	208	VAL
2	G	318	SER
2	G	342	SER
2	G	353	VAL
2	G	415	LYS
2	G	444	VAL
2	G	599	PRO
2	G	602	VAL
2	G	616	THR
2	G	693	GLU
2	G	748	THR
2	G	830	ASP

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Mol	Chain	Res	Type
2	G	877	LYS
2	G	981	GLU
2	G	1092	ASP
2	G	1160	THR
2	G	1185	SER
2	G	1257	ASP
2	G	1288	LYS
2	G	1317	ARG
2	G	1348	LEU
2	G	1375	THR
2	G	1381	VAL
2	G	1382	VAL
2	G	1472	VAL
2	G	1511	SER
2	G	1528	GLU
2	G	1549	THR
2	G	1586	SER
2	G	1650	VAL
2	G	1682	LYS
2	G	1724	GLU
2	G	1840	VAL
2	G	1862	VAL
2	G	1941	PHE
2	G	1960	LEU
2	G	1979	THR
2	G	2023	LYS
2	G	2040	GLU
1	B	52	THR
1	B	72	LEU
1	B	360	LYS
1	B	363	LYS
1	B	434	SER
1	B	495	LYS
1	B	521	LYS
1	B	713	GLN
1	B	883	ILE
1	B	893	VAL
1	B	935	GLU
1	B	945	LYS
1	B	966	LYS
1	B	999	LYS
1	B	1001	VAL

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Mol	Chain	Res	Type
1	B	1004	ILE
1	B	1050	CYS
1	B	1283	MET
1	B	1305	CYS
1	B	1332	TYR
1	B	1362	PRO
1	B	1364	GLU
1	B	1370	THR
1	B	1391	ASP
1	B	1395	LYS
1	B	1643	SER
1	B	1756	ILE
1	B	1773	VAL
1	C	52	THR
1	C	62	LYS
1	C	72	LEU
1	C	360	LYS
1	C	363	LYS
1	C	434	SER
1	C	521	LYS
1	C	713	GLN
1	C	883	ILE
1	C	893	VAL
1	C	935	GLU
1	C	945	LYS
1	C	966	LYS
1	C	999	LYS
1	C	1001	VAL
1	C	1004	ILE
1	C	1050	CYS
1	C	1283	MET
1	C	1305	CYS
1	C	1332	TYR
1	C	1362	PRO
1	C	1364	GLU
1	C	1370	THR
1	C	1391	ASP
1	C	1395	LYS
1	C	1514	LYS
1	C	1643	SER
1	C	1756	ILE
1	C	1759	MET

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Mol	Chain	Res	Type
1	D	52	THR
1	D	62	LYS
1	D	72	LEU
1	D	360	LYS
1	D	363	LYS
1	D	434	SER
1	D	521	LYS
1	D	713	GLN
1	D	883	ILE
1	D	893	VAL
1	D	945	LYS
1	D	966	LYS
1	D	999	LYS
1	D	1001	VAL
1	D	1004	ILE
1	D	1050	CYS
1	D	1283	MET
1	D	1305	CYS
1	D	1332	TYR
1	D	1362	PRO
1	D	1364	GLU
1	D	1370	THR
1	D	1391	ASP
1	D	1395	LYS
1	D	1514	LYS
1	D	1643	SER
1	D	1756	ILE
1	D	1759	MET
1	E	52	THR
1	E	72	LEU
1	E	334	ASP
1	E	360	LYS
1	E	363	LYS
1	E	434	SER
1	E	495	LYS
1	E	521	LYS
1	E	713	GLN
1	E	757	LYS
1	E	883	ILE
1	E	893	VAL
1	E	935	GLU
1	E	966	LYS

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Mol	Chain	Res	Type
1	E	1001	VAL
1	E	1004	ILE
1	E	1050	CYS
1	E	1283	MET
1	E	1305	CYS
1	E	1332	TYR
1	E	1362	PRO
1	E	1364	GLU
1	E	1370	THR
1	E	1391	ASP
1	E	1395	LYS
1	E	1514	LYS
1	E	1643	SER
1	E	1756	ILE
1	E	1759	MET
1	E	1773	VAL
1	F	52	THR
1	F	72	LEU
1	F	340	ARG
1	F	360	LYS
1	F	363	LYS
1	F	434	SER
1	F	495	LYS
1	F	521	LYS
1	F	713	GLN
1	F	883	ILE
1	F	893	VAL
1	F	935	GLU
1	F	945	LYS
1	F	966	LYS
1	F	999	LYS
1	F	1001	VAL
1	F	1004	ILE
1	F	1050	CYS
1	F	1283	MET
1	F	1305	CYS
1	F	1332	TYR
1	F	1362	PRO
1	F	1364	GLU
1	F	1370	THR
1	F	1391	ASP
1	F	1395	LYS

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Mol	Chain	Res	Type
1	F	1514	LYS
1	F	1643	SER
1	F	1756	ILE
1	F	1773	VAL
2	J	86	LEU
2	J	116	LEU
2	J	122	LEU
2	J	178	GLN
2	J	208	VAL
2	J	318	SER
2	J	342	SER
2	J	353	VAL
2	J	444	VAL
2	J	599	PRO
2	J	602	VAL
2	J	616	THR
2	J	669	LEU
2	J	693	GLU
2	J	715	GLN
2	J	748	THR
2	J	830	ASP
2	J	981	GLU
2	J	1092	ASP
2	J	1160	THR
2	J	1185	SER
2	J	1257	ASP
2	J	1317	ARG
2	J	1348	LEU
2	J	1375	THR
2	J	1381	VAL
2	J	1382	VAL
2	J	1472	VAL
2	J	1511	SER
2	J	1549	THR
2	J	1586	SER
2	J	1650	VAL
2	J	1724	GLU
2	J	1736	MET
2	J	1737	ILE
2	J	1840	VAL
2	J	1862	VAL
2	J	1868	GLN

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Mol	Chain	Res	Type
2	J	1941	PHE
2	J	1960	LEU
2	J	1979	THR
2	J	2023	LYS
2	I	56	THR
2	I	86	LEU
2	I	116	LEU
2	I	122	LEU
2	I	178	GLN
2	I	208	VAL
2	I	318	SER
2	I	342	SER
2	I	353	VAL
2	I	444	VAL
2	I	599	PRO
2	I	602	VAL
2	I	616	THR
2	I	669	LEU
2	I	693	GLU
2	I	748	THR
2	I	830	ASP
2	I	981	GLU
2	I	1092	ASP
2	I	1160	THR
2	I	1185	SER
2	I	1257	ASP
2	I	1317	ARG
2	I	1348	LEU
2	I	1375	THR
2	I	1381	VAL
2	I	1382	VAL
2	I	1472	VAL
2	I	1511	SER
2	I	1549	THR
2	I	1586	SER
2	I	1650	VAL
2	I	1724	GLU
2	I	1736	MET
2	I	1737	ILE
2	I	1840	VAL
2	I	1842	VAL
2	I	1862	VAL

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Mol	Chain	Res	Type
2	I	1868	GLN
2	I	1941	PHE
2	I	1960	LEU
2	I	1962	ARG
2	I	1979	THR
2	I	2023	LYS
2	H	86	LEU
2	H	112	ASN
2	H	116	LEU
2	H	122	LEU
2	H	139	LYS
2	H	178	GLN
2	H	208	VAL
2	H	318	SER
2	H	342	SER
2	H	351	ASP
2	H	353	VAL
2	H	444	VAL
2	H	497	LYS
2	H	599	PRO
2	H	602	VAL
2	H	616	THR
2	H	693	GLU
2	H	748	THR
2	H	830	ASP
2	H	850	MET
2	H	981	GLU
2	H	1092	ASP
2	H	1136	GLU
2	H	1160	THR
2	H	1167	SER
2	H	1185	SER
2	H	1257	ASP
2	H	1317	ARG
2	H	1348	LEU
2	H	1375	THR
2	H	1381	VAL
2	H	1382	VAL
2	H	1472	VAL
2	H	1496	LYS
2	H	1511	SER
2	H	1528	GLU

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Mol	Chain	Res	Type
2	H	1549	THR
2	H	1586	SER
2	H	1650	VAL
2	H	1724	GLU
2	H	1840	VAL
2	H	1842	VAL
2	H	1862	VAL
2	H	1941	PHE
2	H	1962	ARG
2	H	1979	THR
2	H	2023	LYS
2	H	2040	GLU
2	K	86	LEU
2	K	109	LEU
2	K	112	ASN
2	K	116	LEU
2	K	122	LEU
2	K	139	LYS
2	K	178	GLN
2	K	208	VAL
2	K	318	SER
2	K	342	SER
2	K	351	ASP
2	K	353	VAL
2	K	444	VAL
2	K	497	LYS
2	K	599	PRO
2	K	602	VAL
2	K	616	THR
2	K	693	GLU
2	K	748	THR
2	K	830	ASP
2	K	850	MET
2	K	981	GLU
2	K	1092	ASP
2	K	1136	GLU
2	K	1160	THR
2	K	1167	SER
2	K	1185	SER
2	K	1257	ASP
2	K	1317	ARG
2	K	1348	LEU

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Mol	Chain	Res	Type
2	K	1375	THR
2	K	1381	VAL
2	K	1382	VAL
2	K	1472	VAL
2	K	1496	LYS
2	K	1511	SER
2	K	1528	GLU
2	K	1549	THR
2	K	1586	SER
2	K	1650	VAL
2	K	1724	GLU
2	K	1840	VAL
2	K	1842	VAL
2	K	1862	VAL
2	K	1941	PHE
2	K	1960	LEU
2	K	1962	ARG
2	K	1979	THR
2	K	2023	LYS
2	K	2040	GLU
2	L	86	LEU
2	L	116	LEU
2	L	122	LEU
2	L	208	VAL
2	L	318	SER
2	L	342	SER
2	L	353	VAL
2	L	415	LYS
2	L	444	VAL
2	L	599	PRO
2	L	602	VAL
2	L	616	THR
2	L	693	GLU
2	L	748	THR
2	L	830	ASP
2	L	877	LYS
2	L	981	GLU
2	L	1092	ASP
2	L	1160	THR
2	L	1185	SER
2	L	1257	ASP
2	L	1317	ARG

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Mol	Chain	Res	Type
2	L	1348	LEU
2	L	1375	THR
2	L	1381	VAL
2	L	1382	VAL
2	L	1472	VAL
2	L	1511	SER
2	L	1528	GLU
2	L	1549	THR
2	L	1586	SER
2	L	1650	VAL
2	L	1682	LYS
2	L	1724	GLU
2	L	1840	VAL
2	L	1862	VAL
2	L	1941	PHE
2	L	1960	LEU
2	L	1979	THR
2	L	2023	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (268) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	618	ASN
1	A	669	ASN
1	A	739	GLN
1	A	758	ASN
1	A	979	GLN
1	A	1112	ASN
1	A	1123	GLN
1	A	1272	ASN
1	A	1507	GLN
1	A	1552	ASN
1	A	1695	ASN
1	A	1845	ASN
2	G	79	GLN
2	G	102	HIS
2	G	224	ASN
2	G	245	GLN
2	G	376	ASN
2	G	440	ASN
2	G	451	ASN

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Mol	Chain	Res	Type
2	G	456	GLN
2	G	718	ASN
2	G	747	HIS
2	G	760	HIS
2	G	1008	GLN
2	G	1012	GLN
2	G	1046	GLN
2	G	1202	GLN
2	G	1341	ASN
2	G	1355	ASN
2	G	1384	GLN
2	G	1434	HIS
2	G	1529	GLN
2	G	1595	ASN
2	G	1619	ASN
2	G	1633	ASN
2	G	1851	ASN
2	G	1912	ASN
2	G	1928	GLN
2	G	1995	ASN
2	G	2020	GLN
2	G	2027	GLN
1	B	40	ASN
1	B	341	GLN
1	B	618	ASN
1	B	669	ASN
1	B	739	GLN
1	B	758	ASN
1	B	854	HIS
1	B	979	GLN
1	B	1112	ASN
1	B	1123	GLN
1	B	1272	ASN
1	B	1507	GLN
1	B	1695	ASN
1	B	1802	GLN
1	B	1845	ASN
1	B	1873	HIS
1	C	40	ASN
1	C	63	ASN
1	C	618	ASN
1	C	669	ASN

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Mol	Chain	Res	Type
1	C	739	GLN
1	C	758	ASN
1	C	979	GLN
1	C	1112	ASN
1	C	1123	GLN
1	C	1272	ASN
1	C	1507	GLN
1	C	1695	ASN
1	C	1845	ASN
1	C	1877	GLN
1	D	40	ASN
1	D	618	ASN
1	D	669	ASN
1	D	739	GLN
1	D	758	ASN
1	D	979	GLN
1	D	1112	ASN
1	D	1123	GLN
1	D	1272	ASN
1	D	1507	GLN
1	D	1695	ASN
1	D	1845	ASN
1	D	1877	GLN
1	E	40	ASN
1	E	341	GLN
1	E	618	ASN
1	E	669	ASN
1	E	739	GLN
1	E	758	ASN
1	E	979	GLN
1	E	1112	ASN
1	E	1123	GLN
1	E	1272	ASN
1	E	1507	GLN
1	E	1695	ASN
1	E	1845	ASN
1	F	40	ASN
1	F	344	GLN
1	F	618	ASN
1	F	669	ASN
1	F	739	GLN
1	F	758	ASN

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Mol	Chain	Res	Type
1	F	854	HIS
1	F	979	GLN
1	F	1112	ASN
1	F	1123	GLN
1	F	1272	ASN
1	F	1507	GLN
1	F	1552	ASN
1	F	1695	ASN
1	F	1845	ASN
1	F	1873	HIS
2	J	79	GLN
2	J	102	HIS
2	J	224	ASN
2	J	245	GLN
2	J	376	ASN
2	J	390	ASN
2	J	440	ASN
2	J	456	GLN
2	J	718	ASN
2	J	723	HIS
2	J	725	ASN
2	J	747	HIS
2	J	760	HIS
2	J	1008	GLN
2	J	1012	GLN
2	J	1202	GLN
2	J	1341	ASN
2	J	1355	ASN
2	J	1384	GLN
2	J	1529	GLN
2	J	1595	ASN
2	J	1619	ASN
2	J	1633	ASN
2	J	1851	ASN
2	J	1872	GLN
2	J	1890	ASN
2	J	1912	ASN
2	J	1928	GLN
2	J	1995	ASN
2	J	2020	GLN
2	I	79	GLN
2	I	102	HIS

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Mol	Chain	Res	Type
2	I	224	ASN
2	I	245	GLN
2	I	376	ASN
2	I	390	ASN
2	I	440	ASN
2	I	456	GLN
2	I	718	ASN
2	I	723	HIS
2	I	725	ASN
2	I	747	HIS
2	I	760	HIS
2	I	1008	GLN
2	I	1012	GLN
2	I	1202	GLN
2	I	1341	ASN
2	I	1355	ASN
2	I	1384	GLN
2	I	1434	HIS
2	I	1529	GLN
2	I	1595	ASN
2	I	1619	ASN
2	I	1627	GLN
2	I	1633	ASN
2	I	1851	ASN
2	I	1872	GLN
2	I	1890	ASN
2	I	1912	ASN
2	I	1928	GLN
2	I	1995	ASN
2	I	2020	GLN
2	H	79	GLN
2	H	102	HIS
2	H	112	ASN
2	H	224	ASN
2	H	245	GLN
2	H	376	ASN
2	H	440	ASN
2	H	456	GLN
2	H	553	ASN
2	H	718	ASN
2	H	723	HIS
2	H	725	ASN

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Mol	Chain	Res	Type
2	H	747	HIS
2	H	760	HIS
2	H	1008	GLN
2	H	1012	GLN
2	H	1341	ASN
2	H	1355	ASN
2	H	1384	GLN
2	H	1529	GLN
2	H	1595	ASN
2	H	1619	ASN
2	H	1633	ASN
2	H	1697	HIS
2	H	1851	ASN
2	H	1872	GLN
2	H	1896	GLN
2	H	1912	ASN
2	H	1915	ASN
2	H	1983	ASN
2	H	1995	ASN
2	H	2020	GLN
2	K	79	GLN
2	K	102	HIS
2	K	112	ASN
2	K	224	ASN
2	K	245	GLN
2	K	376	ASN
2	K	440	ASN
2	K	456	GLN
2	K	718	ASN
2	K	723	HIS
2	K	725	ASN
2	K	747	HIS
2	K	760	HIS
2	K	1008	GLN
2	K	1012	GLN
2	K	1341	ASN
2	K	1355	ASN
2	K	1384	GLN
2	K	1529	GLN
2	K	1595	ASN
2	K	1619	ASN
2	K	1633	ASN

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Mol	Chain	Res	Type
2	K	1697	HIS
2	K	1851	ASN
2	K	1912	ASN
2	K	1928	GLN
2	K	1983	ASN
2	K	1995	ASN
2	K	2020	GLN
2	K	2027	GLN
2	L	79	GLN
2	L	102	HIS
2	L	155	GLN
2	L	224	ASN
2	L	245	GLN
2	L	376	ASN
2	L	384	GLN
2	L	440	ASN
2	L	451	ASN
2	L	456	GLN
2	L	718	ASN
2	L	747	HIS
2	L	760	HIS
2	L	1008	GLN
2	L	1012	GLN
2	L	1202	GLN
2	L	1341	ASN
2	L	1355	ASN
2	L	1384	GLN
2	L	1434	HIS
2	L	1529	GLN
2	L	1595	ASN
2	L	1619	ASN
2	L	1633	ASN
2	L	1851	ASN
2	L	1912	ASN
2	L	1928	GLN
2	L	1995	ASN
2	L	2020	GLN
2	L	2027	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	J8W	K	1808	2	10,11,12	1.78	1 (10%)	8,13,15	1.65	2 (25%)
2	J8W	L	1808	2	10,11,12	1.77	1 (10%)	8,13,15	1.65	2 (25%)
2	J8W	H	1808	2	10,11,12	1.77	1 (10%)	8,13,15	1.59	2 (25%)
2	J8W	J	1808	2	10,11,12	1.76	1 (10%)	8,13,15	1.65	2 (25%)
2	J8W	I	1808	2	10,11,12	1.76	1 (10%)	8,13,15	1.59	2 (25%)
2	J8W	G	1808	2	10,11,12	1.77	1 (10%)	8,13,15	1.60	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	J8W	K	1808	2	-	2/9/11/13	-
2	J8W	L	1808	2	-	2/9/11/13	-
2	J8W	H	1808	2	-	2/9/11/13	-
2	J8W	J	1808	2	-	2/9/11/13	-
2	J8W	I	1808	2	-	2/9/11/13	-
2	J8W	G	1808	2	-	2/9/11/13	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1808	J8W	OG-C2	4.75	1.47	1.33
2	K	1808	J8W	OG-C2	4.75	1.47	1.33
2	L	1808	J8W	OG-C2	4.74	1.47	1.33
2	J	1808	J8W	OG-C2	4.74	1.47	1.33
2	G	1808	J8W	OG-C2	4.73	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1808	J8W	OG-C2	4.73	1.47	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1808	J8W	C3-C1-C2	-3.18	101.75	113.18
2	J	1808	J8W	C3-C1-C2	-3.18	101.77	113.18
2	K	1808	J8W	C3-C1-C2	-3.18	101.77	113.18
2	H	1808	J8W	C3-C1-C2	-3.18	101.77	113.18
2	L	1808	J8W	C3-C1-C2	-3.17	101.78	113.18
2	I	1808	J8W	C3-C1-C2	-3.17	101.80	113.18
2	G	1808	J8W	CB-OG-C2	2.28	125.45	117.12
2	L	1808	J8W	CB-OG-C2	2.28	125.45	117.12
2	H	1808	J8W	CB-OG-C2	2.27	125.41	117.12
2	K	1808	J8W	CB-OG-C2	2.26	125.40	117.12
2	J	1808	J8W	CB-OG-C2	2.26	125.37	117.12
2	I	1808	J8W	CB-OG-C2	2.25	125.36	117.12

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1808	J8W	C-CA-CB-OG
2	J	1808	J8W	C-CA-CB-OG
2	I	1808	J8W	C-CA-CB-OG
2	H	1808	J8W	C-CA-CB-OG
2	K	1808	J8W	C-CA-CB-OG
2	L	1808	J8W	C-CA-CB-OG
2	G	1808	J8W	O7-C2-OG-CB
2	J	1808	J8W	O7-C2-OG-CB
2	I	1808	J8W	O7-C2-OG-CB
2	H	1808	J8W	O7-C2-OG-CB
2	K	1808	J8W	O7-C2-OG-CB
2	L	1808	J8W	O7-C2-OG-CB

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1808	J8W	1	0
2	L	1808	J8W	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1808	J8W	1	0
2	J	1808	J8W	3	0
2	I	1808	J8W	2	0
2	G	1808	J8W	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	B	1901	-	50,52,52	1.47	8 (16%)	71,80,80	1.85	19 (26%)
3	NAP	K	2303	-	50,52,52	1.42	6 (12%)	71,80,80	1.68	15 (21%)
4	COA	G	2301	-	47,50,50	0.54	1 (2%)	69,75,75	0.72	1 (1%)
3	NAP	E	1901	-	50,52,52	1.47	7 (14%)	71,80,80	1.85	18 (25%)
3	NAP	G	2303	-	50,52,52	1.43	6 (12%)	71,80,80	1.65	15 (21%)
5	FNR	L	2302	-	32,33,33	0.87	2 (6%)	41,50,50	0.93	2 (4%)
5	FNR	J	2302	-	32,33,33	0.86	2 (6%)	41,50,50	0.93	2 (4%)
5	FNR	H	2302	-	32,33,33	0.86	2 (6%)	41,50,50	0.92	2 (4%)
5	FNR	I	2302	-	32,33,33	0.89	2 (6%)	41,50,50	0.93	2 (4%)
5	FNR	G	2302	-	32,33,33	0.87	2 (6%)	41,50,50	0.93	2 (4%)
3	NAP	A	1901	-	50,52,52	1.47	7 (14%)	71,80,80	1.84	18 (25%)
4	COA	L	2301	-	47,50,50	0.55	0	69,75,75	0.72	1 (1%)
3	NAP	D	1901	-	50,52,52	1.48	8 (16%)	71,80,80	1.89	20 (28%)
3	NAP	J	2303	-	50,52,52	1.42	6 (12%)	71,80,80	1.66	15 (21%)
3	NAP	C	1901	-	50,52,52	1.48	7 (14%)	71,80,80	1.89	19 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	H	2303	-	50,52,52	1.42	6 (12%)	71,80,80	1.68	15 (21%)
4	COA	I	2301	-	47,50,50	0.54	1 (2%)	69,75,75	0.72	1 (1%)
3	NAP	F	1901	-	50,52,52	1.47	8 (16%)	71,80,80	1.85	19 (26%)
4	COA	H	2301	-	47,50,50	0.55	1 (2%)	69,75,75	0.74	2 (2%)
3	NAP	L	2303	-	50,52,52	1.43	6 (12%)	71,80,80	1.64	15 (21%)
3	NAP	I	2303	-	50,52,52	1.42	6 (12%)	71,80,80	1.66	15 (21%)
5	FNR	K	2302	-	32,33,33	0.86	2 (6%)	41,50,50	0.93	2 (4%)
4	COA	J	2301	-	47,50,50	0.54	1 (2%)	69,75,75	0.73	1 (1%)
4	COA	K	2301	-	47,50,50	0.56	1 (2%)	69,75,75	0.74	2 (2%)

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	NAP	B	1901	-	-	4/35/67/67	0/5/5/5
3	NAP	K	2303	-	-	5/35/67/67	0/5/5/5
4	COA	G	2301	-	-	15/48/64/64	0/3/3/3
3	NAP	E	1901	-	-	4/35/67/67	0/5/5/5
3	NAP	G	2303	-	-	5/35/67/67	0/5/5/5
5	FNR	L	2302	-	-	1/18/18/18	0/3/3/3
5	FNR	J	2302	-	-	1/18/18/18	0/3/3/3
5	FNR	H	2302	-	-	1/18/18/18	0/3/3/3
5	FNR	I	2302	-	-	1/18/18/18	0/3/3/3
5	FNR	G	2302	-	-	1/18/18/18	0/3/3/3
3	NAP	A	1901	-	-	4/35/67/67	0/5/5/5
4	COA	L	2301	-	-	15/48/64/64	0/3/3/3
3	NAP	D	1901	-	-	4/35/67/67	0/5/5/5
3	NAP	J	2303	-	-	6/35/67/67	0/5/5/5
3	NAP	C	1901	-	-	4/35/67/67	0/5/5/5
3	NAP	H	2303	-	-	5/35/67/67	0/5/5/5
4	COA	I	2301	-	-	13/48/64/64	0/3/3/3
3	NAP	F	1901	-	-	4/35/67/67	0/5/5/5
4	COA	H	2301	-	-	14/48/64/64	0/3/3/3
3	NAP	L	2303	-	-	5/35/67/67	0/5/5/5
3	NAP	I	2303	-	-	5/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FNR	K	2302	-	-	1/18/18/18	0/3/3/3
4	COA	J	2301	-	-	14/48/64/64	0/3/3/3
4	COA	K	2301	-	-	14/48/64/64	0/3/3/3

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	2303	NAP	C5A-C4A	4.76	1.47	1.39
3	K	2303	NAP	C5A-C4A	4.76	1.47	1.39
3	G	2303	NAP	C5A-C4A	4.75	1.47	1.39
3	H	2303	NAP	C5A-C4A	4.75	1.47	1.39
3	J	2303	NAP	C5A-C4A	4.74	1.47	1.39
3	I	2303	NAP	C5A-C4A	4.72	1.47	1.39
3	G	2303	NAP	PN-O3	4.36	1.64	1.59
3	H	2303	NAP	PN-O3	4.30	1.64	1.59
3	C	1901	NAP	C4A-N9A	-4.29	1.28	1.37
3	J	2303	NAP	PN-O3	4.28	1.64	1.59
3	A	1901	NAP	C4A-N9A	-4.28	1.28	1.37
3	E	1901	NAP	C4A-N9A	-4.26	1.28	1.37
3	D	1901	NAP	C4A-N9A	-4.26	1.28	1.37
3	F	1901	NAP	C4A-N9A	-4.26	1.28	1.37
3	B	1901	NAP	C4A-N9A	-4.25	1.28	1.37
3	I	2303	NAP	PN-O3	4.23	1.64	1.59
3	K	2303	NAP	PN-O3	4.22	1.64	1.59
3	L	2303	NAP	PN-O3	4.17	1.64	1.59
3	K	2303	NAP	PA-O3	3.51	1.63	1.59
3	L	2303	NAP	PA-O3	3.50	1.63	1.59
3	I	2303	NAP	PA-O3	3.48	1.63	1.59
3	G	2303	NAP	PA-O3	3.46	1.63	1.59
3	J	2303	NAP	PA-O3	3.43	1.63	1.59
3	H	2303	NAP	PA-O3	3.34	1.63	1.59
3	D	1901	NAP	PN-O3	-3.24	1.56	1.59
3	B	1901	NAP	PN-O3	-3.20	1.56	1.59
3	C	1901	NAP	PN-O3	-3.11	1.56	1.59
3	F	1901	NAP	PN-O3	-3.10	1.56	1.59
3	L	2303	NAP	C8A-N7A	3.09	1.37	1.31
3	A	1901	NAP	C4A-N3A	-3.09	1.28	1.34
3	E	1901	NAP	PN-O3	-3.07	1.56	1.59
3	E	1901	NAP	C4A-N3A	-3.05	1.28	1.34
3	I	2303	NAP	C8A-N7A	3.03	1.37	1.31
3	G	2303	NAP	C8A-N7A	3.03	1.37	1.31
3	H	2303	NAP	C8A-N7A	3.03	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	2303	NAP	C8A-N7A	3.02	1.37	1.31
3	A	1901	NAP	PN-O3	-3.00	1.56	1.59
3	J	2303	NAP	C8A-N7A	2.99	1.37	1.31
3	C	1901	NAP	C5A-N7A	-2.96	1.33	1.39
3	A	1901	NAP	C5A-N7A	-2.92	1.33	1.39
3	C	1901	NAP	C4A-N3A	-2.92	1.29	1.34
3	F	1901	NAP	C5A-N7A	-2.91	1.33	1.39
3	B	1901	NAP	C4A-N3A	-2.91	1.29	1.34
3	D	1901	NAP	C5A-N7A	-2.91	1.33	1.39
3	B	1901	NAP	C5A-N7A	-2.90	1.33	1.39
3	D	1901	NAP	C4A-N3A	-2.90	1.29	1.34
3	E	1901	NAP	C5A-N7A	-2.86	1.33	1.39
3	F	1901	NAP	C4A-N3A	-2.85	1.29	1.34
3	B	1901	NAP	C8A-N9A	-2.65	1.33	1.37
3	G	2303	NAP	O4D-C1D	2.62	1.44	1.40
3	A	1901	NAP	C8A-N9A	-2.61	1.33	1.37
3	F	1901	NAP	C8A-N9A	-2.60	1.33	1.37
3	C	1901	NAP	C8A-N9A	-2.58	1.33	1.37
3	E	1901	NAP	C8A-N9A	-2.57	1.33	1.37
3	A	1901	NAP	C2N-N1N	-2.55	1.32	1.35
3	C	1901	NAP	C2N-N1N	-2.55	1.32	1.35
3	D	1901	NAP	C2N-N1N	-2.55	1.32	1.35
3	L	2303	NAP	O4D-C1D	2.54	1.44	1.40
3	I	2303	NAP	O4D-C1D	2.53	1.44	1.40
3	K	2303	NAP	O4D-C1D	2.51	1.44	1.40
3	F	1901	NAP	C2N-N1N	-2.50	1.32	1.35
3	D	1901	NAP	C8A-N9A	-2.50	1.33	1.37
3	E	1901	NAP	C2N-N1N	-2.49	1.32	1.35
3	J	2303	NAP	O4D-C1D	2.48	1.44	1.40
3	H	2303	NAP	O4D-C1D	2.47	1.44	1.40
3	B	1901	NAP	C2N-N1N	-2.40	1.32	1.35
3	C	1901	NAP	C6N-N1N	2.37	1.40	1.35
3	D	1901	NAP	C6N-N1N	2.36	1.40	1.35
3	B	1901	NAP	C6N-N1N	2.33	1.40	1.35
3	F	1901	NAP	C6N-N1N	2.31	1.40	1.35
3	A	1901	NAP	C6N-N1N	2.26	1.40	1.35
3	E	1901	NAP	C6N-N1N	2.26	1.40	1.35
3	L	2303	NAP	C5A-C6A	2.25	1.47	1.41
3	H	2303	NAP	C5A-C6A	2.22	1.47	1.41
3	K	2303	NAP	C5A-C6A	2.21	1.47	1.41
3	I	2303	NAP	C5A-C6A	2.21	1.47	1.41
3	G	2303	NAP	C5A-C6A	2.21	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	2303	NAP	C5A-C6A	2.21	1.47	1.41
5	I	2302	FNR	C6-C7	-2.20	1.36	1.39
5	G	2302	FNR	C9-C8	-2.20	1.36	1.39
5	K	2302	FNR	C9-C8	-2.20	1.36	1.39
5	J	2302	FNR	C9-C8	-2.19	1.36	1.39
5	I	2302	FNR	C9-C8	-2.19	1.36	1.39
5	H	2302	FNR	C9-C8	-2.19	1.36	1.39
4	K	2301	COA	P3B-O3B	2.18	1.63	1.59
5	L	2302	FNR	C9-C8	-2.18	1.36	1.39
3	F	1901	NAP	O4D-C4D	-2.14	1.40	1.45
5	G	2302	FNR	C6-C7	-2.12	1.36	1.39
5	L	2302	FNR	C6-C7	-2.12	1.36	1.39
3	B	1901	NAP	O4D-C4D	-2.12	1.40	1.45
5	J	2302	FNR	C6-C7	-2.11	1.36	1.39
4	H	2301	COA	P3B-O3B	2.10	1.63	1.59
5	H	2302	FNR	C6-C7	-2.09	1.36	1.39
5	K	2302	FNR	C6-C7	-2.09	1.36	1.39
4	J	2301	COA	P3B-O3B	2.07	1.63	1.59
3	D	1901	NAP	P2B-O2B	2.02	1.63	1.59
4	I	2301	COA	P3B-O3B	2.00	1.63	1.59
4	G	2301	COA	P3B-O3B	2.00	1.63	1.59

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1901	NAP	C6N-N1N-C2N	5.71	126.73	121.88
3	C	1901	NAP	C6N-N1N-C2N	5.67	126.70	121.88
3	E	1901	NAP	C6N-N1N-C2N	5.67	126.70	121.88
3	A	1901	NAP	C6N-N1N-C2N	5.57	126.61	121.88
3	F	1901	NAP	C6N-N1N-C2N	5.53	126.58	121.88
3	B	1901	NAP	C6N-N1N-C2N	5.50	126.56	121.88
3	D	1901	NAP	O7N-C7N-C3N	5.31	126.09	119.60
3	C	1901	NAP	O7N-C7N-C3N	5.28	126.06	119.60
3	B	1901	NAP	O7N-C7N-C3N	5.12	125.86	119.60
3	F	1901	NAP	O7N-C7N-C3N	5.11	125.84	119.60
3	A	1901	NAP	O7N-C7N-C3N	5.09	125.82	119.60
3	E	1901	NAP	O7N-C7N-C3N	5.07	125.79	119.60
3	C	1901	NAP	C4D-O4D-C1D	-5.00	105.35	109.92
3	L	2303	NAP	C5A-C4A-N3A	-4.88	119.99	126.72
3	D	1901	NAP	C4D-O4D-C1D	-4.87	105.47	109.92
3	K	2303	NAP	C5A-C4A-N3A	-4.84	120.05	126.72
3	G	2303	NAP	C5A-C4A-N3A	-4.84	120.06	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2303	NAP	C5A-C4A-N3A	-4.79	120.12	126.72
3	E	1901	NAP	C4D-O4D-C1D	-4.76	105.56	109.92
3	J	2303	NAP	C5A-C4A-N3A	-4.76	120.17	126.72
3	A	1901	NAP	C4D-O4D-C1D	-4.74	105.58	109.92
3	F	1901	NAP	C4D-O4D-C1D	-4.67	105.65	109.92
3	I	2303	NAP	C5A-C4A-N3A	-4.64	120.32	126.72
3	B	1901	NAP	C4D-O4D-C1D	-4.64	105.67	109.92
3	K	2303	NAP	N3A-C4A-N9A	4.44	134.73	127.17
3	J	2303	NAP	N3A-C4A-N9A	4.43	134.71	127.17
3	H	2303	NAP	N3A-C4A-N9A	4.36	134.59	127.17
3	G	2303	NAP	N3A-C4A-N9A	4.36	134.58	127.17
3	L	2303	NAP	N3A-C4A-N9A	4.34	134.54	127.17
3	I	2303	NAP	N3A-C4A-N9A	4.33	134.54	127.17
3	I	2303	NAP	N3A-C2A-N1A	-4.00	122.53	128.58
3	H	2303	NAP	N3A-C2A-N1A	-3.98	122.56	128.58
3	J	2303	NAP	N3A-C2A-N1A	-3.94	122.62	128.58
3	G	2303	NAP	N3A-C2A-N1A	-3.93	122.63	128.58
3	K	2303	NAP	N3A-C2A-N1A	-3.91	122.66	128.58
3	L	2303	NAP	N3A-C2A-N1A	-3.86	122.73	128.58
3	D	1901	NAP	O2A-PA-O1A	3.67	129.50	112.44
3	C	1901	NAP	O2A-PA-O1A	3.65	129.40	112.44
3	E	1901	NAP	O2A-PA-O1A	3.60	129.18	112.44
3	A	1901	NAP	O2A-PA-O1A	3.56	129.02	112.44
3	B	1901	NAP	O2A-PA-O1A	3.54	128.91	112.44
3	F	1901	NAP	O2A-PA-O1A	3.51	128.77	112.44
3	J	2303	NAP	C4A-N9A-C8A	3.49	109.40	105.74
3	I	2303	NAP	C4A-N9A-C8A	3.49	109.40	105.74
4	L	2301	COA	P3B-O3B-C3B	-3.45	114.22	123.43
4	G	2301	COA	P3B-O3B-C3B	-3.42	114.30	123.43
3	F	1901	NAP	C5A-C4A-N3A	-3.39	122.05	126.72
3	K	2303	NAP	C4A-N9A-C8A	3.38	109.29	105.74
3	H	2303	NAP	C2A-N3A-C4A	3.38	120.09	111.83
3	B	1901	NAP	C5A-C4A-N3A	-3.38	122.06	126.72
3	K	2303	NAP	C2A-N3A-C4A	3.38	120.09	111.83
3	G	2303	NAP	C2A-N3A-C4A	3.37	120.07	111.83
3	L	2303	NAP	C2A-N3A-C4A	3.36	120.04	111.83
3	J	2303	NAP	C2A-N3A-C4A	3.35	120.02	111.83
3	H	2303	NAP	C4A-N9A-C8A	3.34	109.25	105.74
3	I	2303	NAP	C2A-N3A-C4A	3.33	119.97	111.83
3	I	2303	NAP	C2B-C1B-N9A	3.33	119.23	113.75
3	C	1901	NAP	O4D-C4D-C3D	3.32	111.75	105.15
3	G	2303	NAP	C4A-N9A-C8A	3.31	109.22	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1901	NAP	O4D-C4D-C3D	3.29	111.69	105.15
3	C	1901	NAP	C5A-C4A-N3A	-3.29	122.19	126.72
3	E	1901	NAP	O4D-C4D-C3D	3.27	111.64	105.15
3	A	1901	NAP	O4D-C4D-C3D	3.27	111.64	105.15
3	D	1901	NAP	C5A-C4A-N3A	-3.26	122.22	126.72
3	L	2303	NAP	C4A-N9A-C8A	3.25	109.15	105.74
3	E	1901	NAP	C5A-C4A-N3A	-3.23	122.26	126.72
3	A	1901	NAP	C5A-C4A-N3A	-3.22	122.28	126.72
3	F	1901	NAP	O4D-C4D-C3D	3.22	111.53	105.15
3	B	1901	NAP	O4D-C4D-C3D	3.20	111.51	105.15
4	H	2301	COA	P3B-O3B-C3B	-3.20	114.89	123.43
4	K	2301	COA	P3B-O3B-C3B	-3.16	115.00	123.43
3	K	2303	NAP	C3N-C7N-N7N	3.16	121.63	117.74
3	H	2303	NAP	C3N-C7N-N7N	3.15	121.62	117.74
3	H	2303	NAP	C2B-C1B-N9A	3.14	118.91	113.75
3	J	2303	NAP	C3N-C7N-N7N	3.11	121.57	117.74
3	K	2303	NAP	C2B-C1B-N9A	3.06	118.78	113.75
3	G	2303	NAP	C3N-C7N-N7N	3.04	121.49	117.74
3	L	2303	NAP	C3N-C7N-N7N	3.01	121.45	117.74
4	J	2301	COA	P3B-O3B-C3B	-2.98	115.46	123.43
3	H	2303	NAP	O2N-PN-O3	2.94	115.22	107.27
3	K	2303	NAP	O2N-PN-O3	2.91	115.15	107.27
3	C	1901	NAP	C4A-N9A-C8A	2.91	108.79	105.74
4	I	2301	COA	P3B-O3B-C3B	-2.89	115.72	123.43
3	L	2303	NAP	O2N-PN-O3	2.86	115.00	107.27
3	J	2303	NAP	O2N-PN-O3	2.85	114.98	107.27
3	G	2303	NAP	C2B-C1B-N9A	2.84	118.42	113.75
3	D	1901	NAP	C4A-N9A-C8A	2.83	108.71	105.74
3	G	2303	NAP	O2N-PN-O3	2.82	114.91	107.27
3	I	2303	NAP	O2N-PN-O3	2.82	114.89	107.27
3	E	1901	NAP	C4A-N9A-C8A	2.82	108.69	105.74
3	I	2303	NAP	C3N-C7N-N7N	2.81	121.20	117.74
3	D	1901	NAP	O7N-C7N-N7N	-2.76	118.62	122.62
3	A	1901	NAP	C4A-N9A-C8A	2.75	108.63	105.74
3	C	1901	NAP	O7N-C7N-N7N	-2.74	118.66	122.62
3	F	1901	NAP	C4A-N9A-C8A	2.70	108.57	105.74
3	J	2303	NAP	C2B-C1B-N9A	2.69	118.19	113.75
3	E	1901	NAP	C5N-C6N-N1N	-2.69	116.71	120.38
3	B	1901	NAP	C4A-N9A-C8A	2.69	108.56	105.74
3	A	1901	NAP	C4A-C5A-N7A	-2.68	107.52	110.58
3	D	1901	NAP	C4A-C5A-N7A	-2.68	107.52	110.58
3	C	1901	NAP	C4A-C5A-N7A	-2.68	107.52	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1901	NAP	O7N-C7N-N7N	-2.67	118.76	122.62
3	B	1901	NAP	C4A-C5A-N7A	-2.67	107.53	110.58
3	E	1901	NAP	C4A-C5A-N7A	-2.66	107.54	110.58
3	A	1901	NAP	C5N-C6N-N1N	-2.66	116.75	120.38
3	F	1901	NAP	C4A-C5A-N7A	-2.66	107.54	110.58
3	A	1901	NAP	O7N-C7N-N7N	-2.65	118.78	122.62
3	B	1901	NAP	O7N-C7N-N7N	-2.65	118.79	122.62
3	F	1901	NAP	O7N-C7N-N7N	-2.63	118.81	122.62
3	C	1901	NAP	C5N-C4N-C3N	2.60	122.92	120.36
3	C	1901	NAP	C5N-C6N-N1N	-2.59	116.86	120.38
3	D	1901	NAP	C5N-C6N-N1N	-2.57	116.87	120.38
3	D	1901	NAP	C5N-C4N-C3N	2.57	122.89	120.36
3	C	1901	NAP	O2N-PN-O3	2.56	114.20	107.27
3	F	1901	NAP	O2B-P2B-O1X	-2.55	100.24	109.33
5	I	2302	FNR	O3P-P-O5'	2.55	113.31	106.67
5	J	2302	FNR	O3P-P-O5'	2.55	113.31	106.67
3	D	1901	NAP	O2N-PN-O3	2.54	114.13	107.27
3	F	1901	NAP	O2N-PN-O3	2.53	114.11	107.27
3	B	1901	NAP	O2B-P2B-O1X	-2.52	100.35	109.33
3	F	1901	NAP	C5N-C6N-N1N	-2.52	116.94	120.38
3	H	2303	NAP	O3-PA-O1A	-2.51	103.15	110.70
3	B	1901	NAP	C5N-C6N-N1N	-2.51	116.97	120.38
3	B	1901	NAP	O2N-PN-O3	2.51	114.04	107.27
3	C	1901	NAP	N3A-C4A-N9A	2.50	131.42	127.17
3	L	2303	NAP	C2B-C1B-N9A	2.50	117.87	113.75
5	L	2302	FNR	O3P-P-O5'	2.49	113.16	106.67
5	K	2302	FNR	O3P-P-O5'	2.49	113.15	106.67
3	E	1901	NAP	O2B-P2B-O1X	-2.48	100.48	109.33
3	F	1901	NAP	N3A-C4A-N9A	2.48	131.38	127.17
5	H	2302	FNR	O3P-P-O5'	2.47	113.11	106.67
5	G	2302	FNR	O3P-P-O5'	2.47	113.10	106.67
3	K	2303	NAP	O3-PA-O1A	-2.47	103.28	110.70
3	B	1901	NAP	N3A-C4A-N9A	2.47	131.36	127.17
3	E	1901	NAP	O2N-PN-O3	2.46	113.92	107.27
3	A	1901	NAP	O2B-P2B-O1X	-2.45	100.59	109.33
3	D	1901	NAP	N3A-C4A-N9A	2.45	131.34	127.17
3	D	1901	NAP	O2B-P2B-O1X	-2.45	100.60	109.33
3	B	1901	NAP	N3A-C2A-N1A	-2.44	124.88	128.58
3	A	1901	NAP	O2N-PN-O3	2.44	113.88	107.27
3	C	1901	NAP	O2B-P2B-O1X	-2.43	100.69	109.33
3	F	1901	NAP	N3A-C2A-N1A	-2.43	124.91	128.58
3	E	1901	NAP	C5N-C4N-C3N	2.40	122.73	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	2303	NAP	O3-PA-O1A	-2.40	103.49	110.70
4	H	2301	COA	C2B-C3B-C4B	-2.34	99.14	103.24
3	E	1901	NAP	N3A-C4A-N9A	2.34	131.15	127.17
3	A	1901	NAP	N3A-C4A-N9A	2.34	131.15	127.17
3	A	1901	NAP	C5N-C4N-C3N	2.34	122.66	120.36
3	J	2303	NAP	O3-PA-O1A	-2.33	103.69	110.70
3	B	1901	NAP	C5N-C4N-C3N	2.32	122.64	120.36
3	J	2303	NAP	N9A-C8A-N7A	-2.32	110.65	113.94
3	I	2303	NAP	N9A-C8A-N7A	-2.31	110.66	113.94
3	B	1901	NAP	O4D-C4D-C5D	-2.30	101.97	109.33
3	I	2303	NAP	O3-PA-O1A	-2.29	103.81	110.70
3	C	1901	NAP	N3A-C2A-N1A	-2.29	125.12	128.58
3	F	1901	NAP	C5N-C4N-C3N	2.27	122.60	120.36
3	G	2303	NAP	O3-PA-O1A	-2.27	103.88	110.70
3	K	2303	NAP	N9A-C8A-N7A	-2.27	110.72	113.94
3	B	1901	NAP	C2A-N3A-C4A	2.27	117.37	111.83
3	F	1901	NAP	O4D-C4D-C5D	-2.26	102.08	109.33
3	F	1901	NAP	C2A-N3A-C4A	2.26	117.36	111.83
3	D	1901	NAP	N3A-C2A-N1A	-2.26	125.16	128.58
3	C	1901	NAP	O4D-C4D-C5D	-2.26	102.09	109.33
3	H	2303	NAP	N9A-C8A-N7A	-2.26	110.73	113.94
3	G	2303	NAP	N9A-C8A-N7A	-2.25	110.74	113.94
3	A	1901	NAP	O4D-C4D-C5D	-2.25	102.14	109.33
3	E	1901	NAP	O4D-C4D-C5D	-2.24	102.17	109.33
3	I	2303	NAP	C2A-N1A-C6A	2.24	122.40	118.73
3	D	1901	NAP	O4D-C4D-C5D	-2.22	102.22	109.33
3	H	2303	NAP	O3-PN-O1N	-2.21	104.05	110.70
3	L	2303	NAP	N9A-C8A-N7A	-2.21	110.80	113.94
3	I	2303	NAP	C4A-N9A-C1B	-2.21	121.47	126.63
3	H	2303	NAP	C2A-N1A-C6A	2.19	122.33	118.73
3	L	2303	NAP	O3-PN-O1N	-2.17	104.17	110.70
3	J	2303	NAP	C2A-N1A-C6A	2.17	122.29	118.73
3	F	1901	NAP	O2N-PN-O1N	2.15	122.44	112.44
3	I	2303	NAP	O3-PN-O1N	-2.15	104.24	110.70
3	C	1901	NAP	C2A-N3A-C4A	2.14	117.06	111.83
3	K	2303	NAP	C2A-N1A-C6A	2.14	122.24	118.73
3	G	2303	NAP	C2A-N1A-C6A	2.14	122.24	118.73
3	A	1901	NAP	O2N-PN-O1N	2.14	122.39	112.44
3	B	1901	NAP	O2N-PN-O1N	2.14	122.38	112.44
3	E	1901	NAP	O2N-PN-O1N	2.14	122.38	112.44
3	H	2303	NAP	C4A-N9A-C1B	-2.13	121.65	126.63
3	J	2303	NAP	C4A-N9A-C1B	-2.13	121.66	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	2303	NAP	O3-PN-O1N	-2.12	104.32	110.70
3	D	1901	NAP	C2A-N3A-C4A	2.12	117.02	111.83
3	A	1901	NAP	N3A-C2A-N1A	-2.12	125.38	128.58
4	K	2301	COA	C2B-C3B-C4B	-2.11	99.54	103.24
3	D	1901	NAP	O2N-PN-O1N	2.11	122.25	112.44
3	K	2303	NAP	C4A-N9A-C1B	-2.11	121.71	126.63
3	C	1901	NAP	O2N-PN-O1N	2.10	122.21	112.44
3	E	1901	NAP	N3A-C2A-N1A	-2.10	125.41	128.58
3	L	2303	NAP	C4A-C5A-N7A	-2.10	108.19	110.58
3	L	2303	NAP	C2A-N1A-C6A	2.09	122.17	118.73
3	K	2303	NAP	N6A-C6A-N1A	2.09	123.04	118.38
3	I	2303	NAP	N6A-C6A-N1A	2.09	123.02	118.38
3	J	2303	NAP	N6A-C6A-N1A	2.08	123.02	118.38
3	B	1901	NAP	C6N-N1N-C1D	-2.08	115.65	119.73
5	K	2302	FNR	C4-C4A-N5	2.06	121.64	116.37
3	A	1901	NAP	C2A-N3A-C4A	2.06	116.86	111.83
5	G	2302	FNR	C4-C4A-N5	2.06	121.63	116.37
3	J	2303	NAP	C5A-C6A-N6A	-2.05	118.20	123.29
3	G	2303	NAP	O3-PN-O1N	-2.05	104.52	110.70
3	J	2303	NAP	O3-PN-O1N	-2.05	104.53	110.70
3	G	2303	NAP	C4A-N9A-C1B	-2.05	121.84	126.63
5	H	2302	FNR	C4-C4A-N5	2.05	121.61	116.37
3	L	2303	NAP	C4A-N9A-C1B	-2.05	121.84	126.63
3	E	1901	NAP	C2A-N3A-C4A	2.05	116.83	111.83
3	F	1901	NAP	C6N-N1N-C1D	-2.05	115.71	119.73
3	H	2303	NAP	N6A-C6A-N1A	2.04	122.93	118.38
5	L	2302	FNR	C4-C4A-N5	2.04	121.59	116.37
3	G	2303	NAP	C4A-C5A-N7A	-2.04	108.25	110.58
3	K	2303	NAP	C5A-C6A-N6A	-2.03	118.26	123.29
5	J	2302	FNR	C4-C4A-N5	2.03	121.55	116.37
3	I	2303	NAP	C5A-C6A-N6A	-2.02	118.28	123.29
5	I	2302	FNR	C4-C4A-N5	2.02	121.54	116.37
3	G	2303	NAP	N6A-C6A-N1A	2.02	122.87	118.38
3	D	1901	NAP	O2A-PA-O3	-2.01	101.83	107.27
3	H	2303	NAP	O2A-PA-O1A	2.01	121.80	112.44
3	C	1901	NAP	C3N-C7N-N7N	-2.01	115.26	117.74
3	D	1901	NAP	C3N-C7N-N7N	-2.01	115.26	117.74
3	L	2303	NAP	N6A-C6A-N1A	2.01	122.85	118.38

There are no chirality outliers.

All (146) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2303	NAP	C5B-O5B-PA-O2A
3	G	2303	NAP	C5B-O5B-PA-O3
3	J	2303	NAP	C5B-O5B-PA-O2A
3	J	2303	NAP	C5B-O5B-PA-O3
3	I	2303	NAP	C5B-O5B-PA-O2A
3	I	2303	NAP	C5B-O5B-PA-O3
3	H	2303	NAP	C5B-O5B-PA-O2A
3	H	2303	NAP	C5B-O5B-PA-O3
3	K	2303	NAP	C5B-O5B-PA-O2A
3	K	2303	NAP	C5B-O5B-PA-O3
3	L	2303	NAP	C5B-O5B-PA-O2A
3	L	2303	NAP	C5B-O5B-PA-O3
4	G	2301	COA	C5B-O5B-P1A-O1A
4	G	2301	COA	C5B-O5B-P1A-O2A
4	J	2301	COA	C5B-O5B-P1A-O3A
4	H	2301	COA	C5B-O5B-P1A-O1A
4	H	2301	COA	C5B-O5B-P1A-O2A
4	K	2301	COA	C5B-O5B-P1A-O3A
4	L	2301	COA	C5B-O5B-P1A-O1A
4	L	2301	COA	C5B-O5B-P1A-O2A
4	L	2301	COA	C3B-C4B-C5B-O5B
4	K	2301	COA	O5P-C5P-N4P-C3P
4	H	2301	COA	O5P-C5P-N4P-C3P
4	G	2301	COA	O5P-C5P-N4P-C3P
4	L	2301	COA	O5P-C5P-N4P-C3P
4	G	2301	COA	C6P-C5P-N4P-C3P
4	J	2301	COA	C6P-C5P-N4P-C3P
4	I	2301	COA	C6P-C5P-N4P-C3P
4	H	2301	COA	C6P-C5P-N4P-C3P
4	K	2301	COA	C6P-C5P-N4P-C3P
4	L	2301	COA	C6P-C5P-N4P-C3P
4	G	2301	COA	C3B-C4B-C5B-O5B
4	L	2301	COA	O4B-C4B-C5B-O5B
4	J	2301	COA	O5P-C5P-N4P-C3P
4	I	2301	COA	O5P-C5P-N4P-C3P
4	G	2301	COA	O4B-C4B-C5B-O5B
4	J	2301	COA	O4B-C4B-C5B-O5B
4	H	2301	COA	O4B-C4B-C5B-O5B
4	J	2301	COA	C3B-C4B-C5B-O5B
4	G	2301	COA	P1A-O3A-P2A-O4A
4	J	2301	COA	P1A-O3A-P2A-O4A
4	I	2301	COA	P1A-O3A-P2A-O4A
4	K	2301	COA	P1A-O3A-P2A-O4A

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Mol	Chain	Res	Type	Atoms
4	L	2301	COA	P1A-O3A-P2A-O4A
4	H	2301	COA	C3B-C4B-C5B-O5B
4	K	2301	COA	C3B-C4B-C5B-O5B
3	A	1901	NAP	PN-O3-PA-O1A
3	B	1901	NAP	PN-O3-PA-O1A
3	C	1901	NAP	PN-O3-PA-O1A
3	D	1901	NAP	PN-O3-PA-O1A
3	E	1901	NAP	PN-O3-PA-O1A
3	F	1901	NAP	PN-O3-PA-O1A
4	G	2301	COA	CDP-CBP-CCP-O6A
4	J	2301	COA	CDP-CBP-CCP-O6A
4	I	2301	COA	CDP-CBP-CCP-O6A
4	H	2301	COA	CDP-CBP-CCP-O6A
4	K	2301	COA	CDP-CBP-CCP-O6A
4	L	2301	COA	CDP-CBP-CCP-O6A
4	I	2301	COA	C3B-C4B-C5B-O5B
3	J	2303	NAP	C4B-C5B-O5B-PA
3	I	2303	NAP	C4B-C5B-O5B-PA
3	K	2303	NAP	C4B-C5B-O5B-PA
3	L	2303	NAP	C4B-C5B-O5B-PA
4	G	2301	COA	S1P-C2P-C3P-N4P
4	J	2301	COA	S1P-C2P-C3P-N4P
4	I	2301	COA	S1P-C2P-C3P-N4P
4	H	2301	COA	CAP-CBP-CCP-O6A
4	H	2301	COA	S1P-C2P-C3P-N4P
4	K	2301	COA	S1P-C2P-C3P-N4P
4	L	2301	COA	S1P-C2P-C3P-N4P
3	J	2303	NAP	O4B-C4B-C5B-O5B
4	I	2301	COA	O4B-C4B-C5B-O5B
4	K	2301	COA	O4B-C4B-C5B-O5B
4	G	2301	COA	C5B-O5B-P1A-O3A
4	G	2301	COA	CCP-O6A-P2A-O4A
4	J	2301	COA	C5B-O5B-P1A-O1A
4	J	2301	COA	CCP-O6A-P2A-O4A
4	I	2301	COA	CCP-O6A-P2A-O4A
4	H	2301	COA	C5B-O5B-P1A-O3A
4	K	2301	COA	CCP-O6A-P2A-O4A
4	L	2301	COA	C5B-O5B-P1A-O3A
4	L	2301	COA	CCP-O6A-P2A-O4A
3	H	2303	NAP	C4B-C5B-O5B-PA
5	G	2302	FNR	C4'-C5'-O5'-P
5	J	2302	FNR	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
5	I	2302	FNR	C4'-C5'-O5'-P
5	H	2302	FNR	C4'-C5'-O5'-P
5	K	2302	FNR	C4'-C5'-O5'-P
5	L	2302	FNR	C4'-C5'-O5'-P
3	G	2303	NAP	O4B-C4B-C5B-O5B
3	I	2303	NAP	O4B-C4B-C5B-O5B
3	G	2303	NAP	C4B-C5B-O5B-PA
4	G	2301	COA	P2A-O3A-P1A-O2A
4	G	2301	COA	P1A-O3A-P2A-O5A
4	J	2301	COA	P1A-O3A-P2A-O5A
4	I	2301	COA	P1A-O3A-P2A-O5A
4	K	2301	COA	P1A-O3A-P2A-O5A
4	L	2301	COA	P2A-O3A-P1A-O2A
4	L	2301	COA	P1A-O3A-P2A-O5A
3	L	2303	NAP	O4B-C4B-C5B-O5B
3	H	2303	NAP	O4B-C4B-C5B-O5B
3	K	2303	NAP	O4B-C4B-C5B-O5B
3	A	1901	NAP	O4D-C1D-N1N-C6N
3	B	1901	NAP	O4D-C1D-N1N-C6N
3	C	1901	NAP	O4D-C1D-N1N-C6N
3	D	1901	NAP	O4D-C1D-N1N-C6N
3	E	1901	NAP	O4D-C1D-N1N-C6N
3	F	1901	NAP	O4D-C1D-N1N-C6N
4	K	2301	COA	P2A-O3A-P1A-O2A
3	C	1901	NAP	O4B-C4B-C5B-O5B
3	D	1901	NAP	O4B-C4B-C5B-O5B
3	H	2303	NAP	PA-O3-PN-O1N
3	K	2303	NAP	PA-O3-PN-O1N
3	L	2303	NAP	PA-O3-PN-O1N
4	J	2301	COA	P2A-O3A-P1A-O2A
4	I	2301	COA	P2A-O3A-P1A-O1A
4	I	2301	COA	P2A-O3A-P1A-O2A
4	K	2301	COA	P2A-O3A-P1A-O1A
3	A	1901	NAP	O4B-C4B-C5B-O5B
3	B	1901	NAP	O4B-C4B-C5B-O5B
3	E	1901	NAP	O4B-C4B-C5B-O5B
3	F	1901	NAP	O4B-C4B-C5B-O5B
4	G	2301	COA	C3B-O3B-P3B-O8A
4	J	2301	COA	C3B-O3B-P3B-O8A
4	I	2301	COA	C3B-O3B-P3B-O8A
4	H	2301	COA	C3B-O3B-P3B-O8A
4	K	2301	COA	C3B-O3B-P3B-O8A

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Mol	Chain	Res	Type	Atoms
4	L	2301	COA	C3B-O3B-P3B-O8A
4	H	2301	COA	CBP-CCP-O6A-P2A
4	G	2301	COA	CEP-CBP-CCP-O6A
4	I	2301	COA	CEP-CBP-CCP-O6A
4	H	2301	COA	CEP-CBP-CCP-O6A
4	K	2301	COA	CEP-CBP-CCP-O6A
4	L	2301	COA	CEP-CBP-CCP-O6A
4	H	2301	COA	O9P-C9P-N8P-C7P
3	A	1901	NAP	PN-O3-PA-O2A
3	G	2303	NAP	PA-O3-PN-O1N
3	B	1901	NAP	PN-O3-PA-O2A
3	C	1901	NAP	PN-O3-PA-O2A
3	D	1901	NAP	PN-O3-PA-O2A
3	E	1901	NAP	PN-O3-PA-O2A
3	F	1901	NAP	PN-O3-PA-O2A
3	J	2303	NAP	PA-O3-PN-O1N
3	I	2303	NAP	PA-O3-PN-O1N
4	J	2301	COA	P2A-O3A-P1A-O1A
3	J	2303	NAP	C3B-C4B-C5B-O5B

There are no ring outliers.

22 monomers are involved in 30 short contacts:

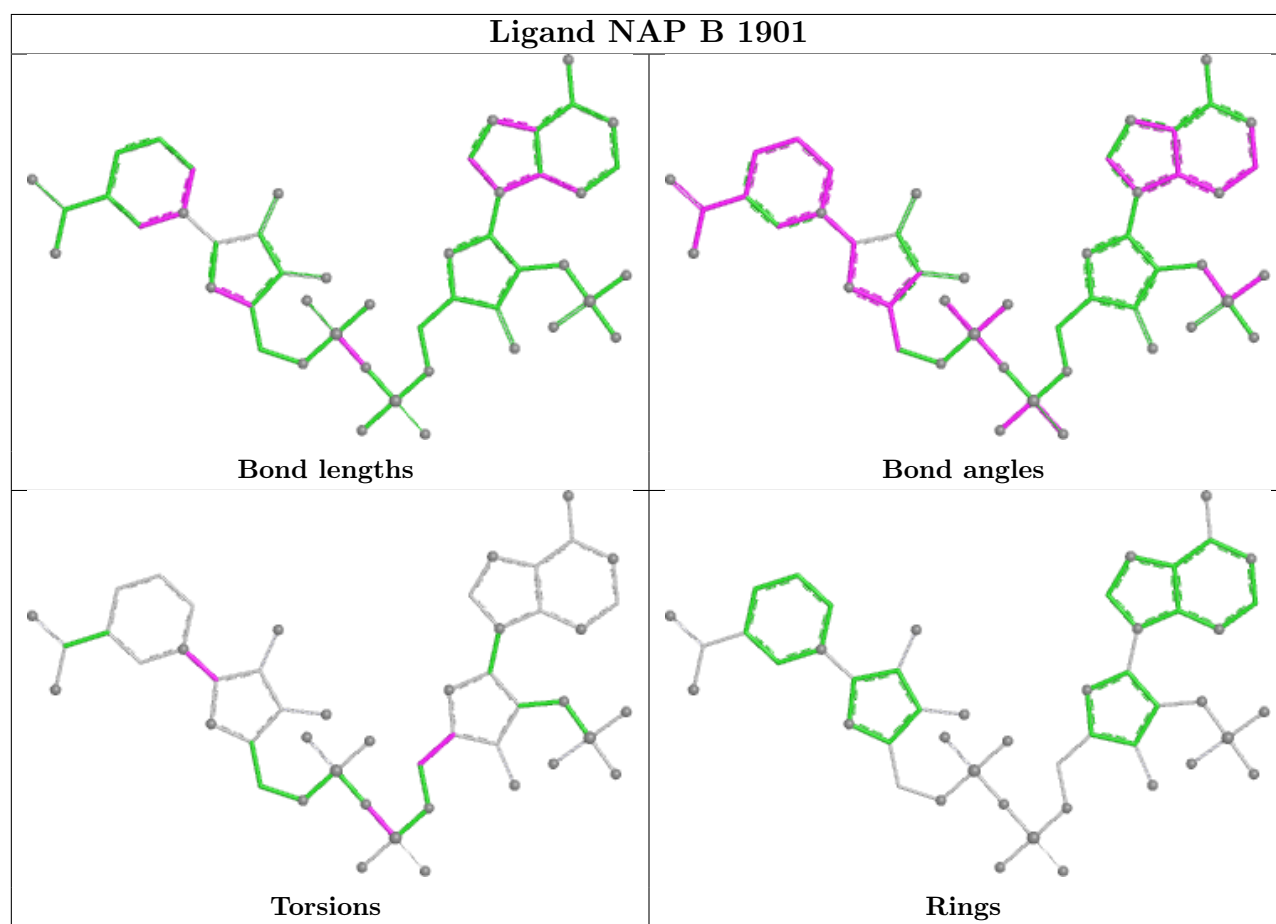
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1901	NAP	3	0
3	K	2303	NAP	1	0
3	E	1901	NAP	2	0
3	G	2303	NAP	1	0
5	L	2302	FNR	2	0
5	J	2302	FNR	1	0
5	H	2302	FNR	2	0
5	I	2302	FNR	1	0
5	G	2302	FNR	1	0
3	A	1901	NAP	2	0
3	D	1901	NAP	3	0
3	J	2303	NAP	1	0
3	C	1901	NAP	3	0
3	H	2303	NAP	1	0
4	I	2301	COA	1	0
3	F	1901	NAP	3	0
4	H	2301	COA	2	0
3	L	2303	NAP	1	0

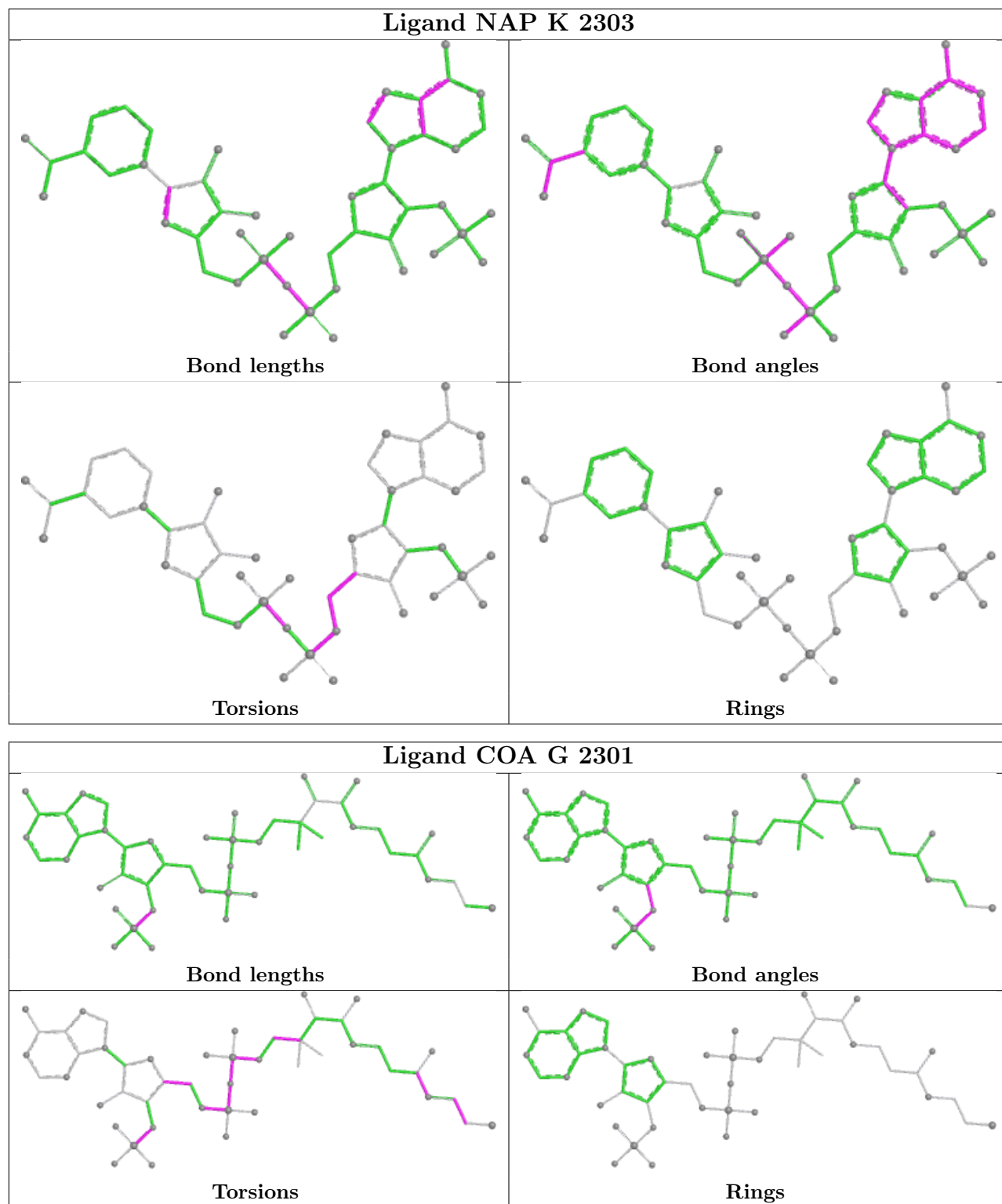
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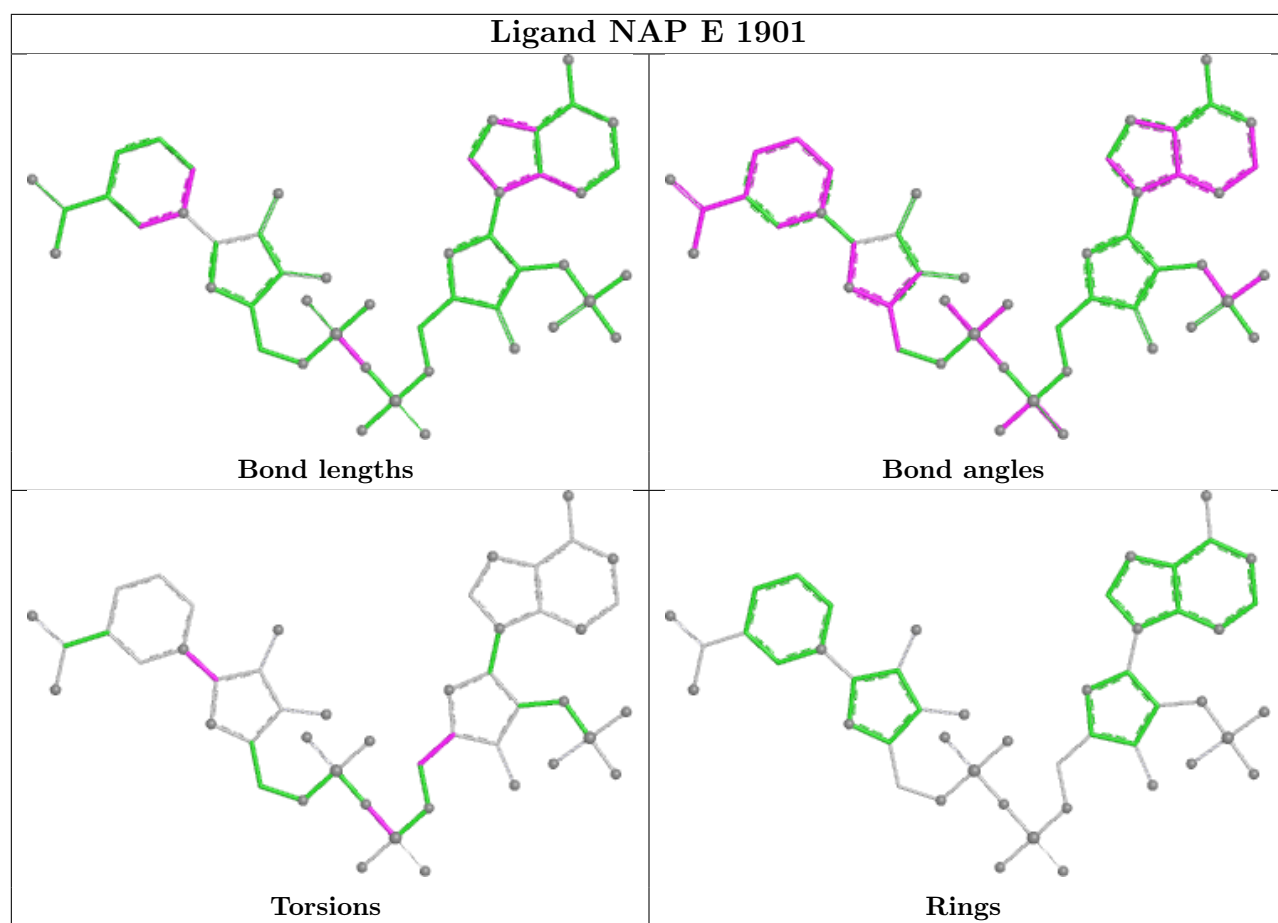
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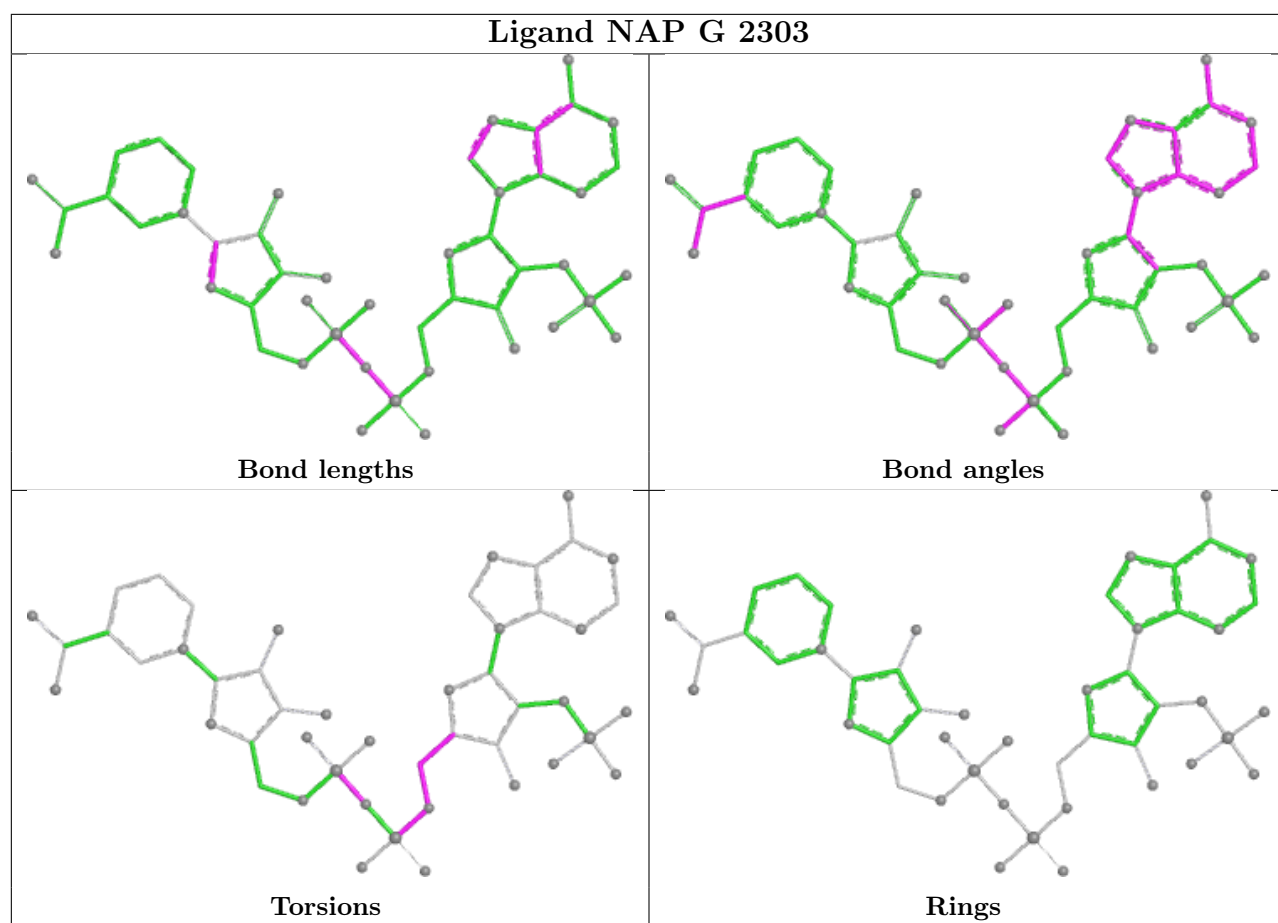
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	2303	NAP	1	0
5	K	2302	FNR	2	0
4	J	2301	COA	1	0
4	K	2301	COA	1	0

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.

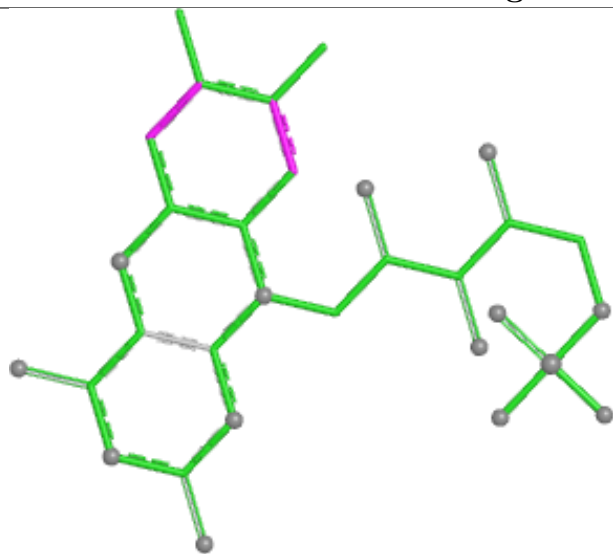




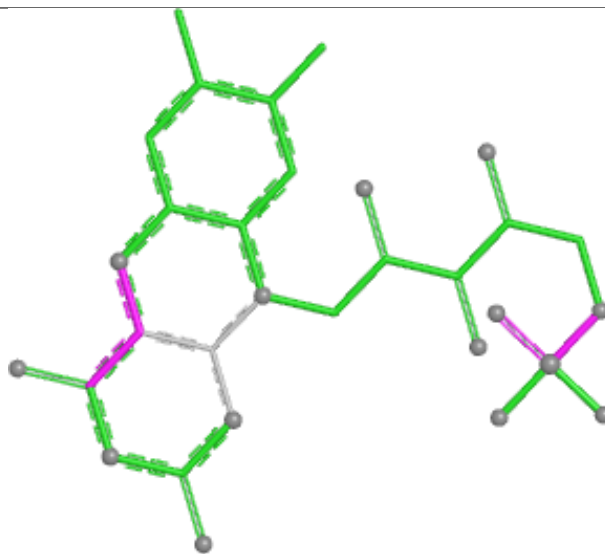




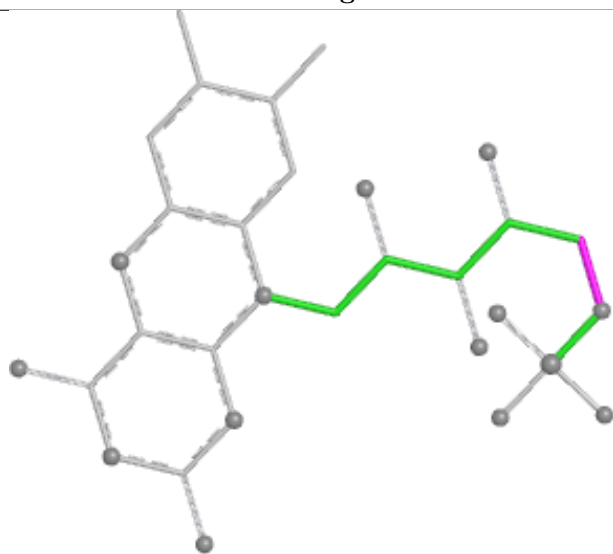
Ligand FNR L 2302



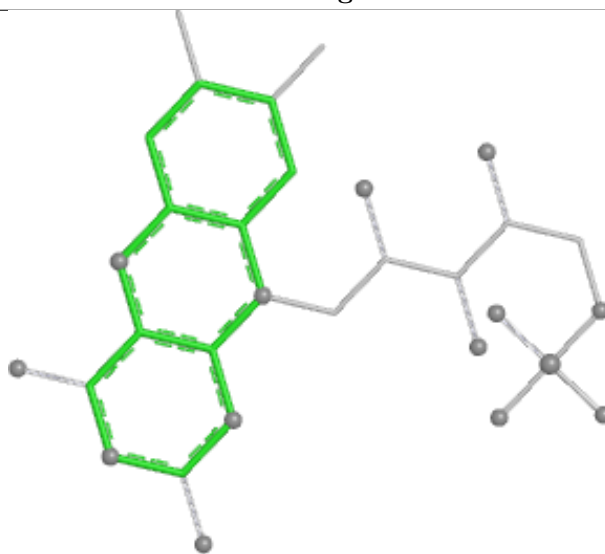
Bond lengths



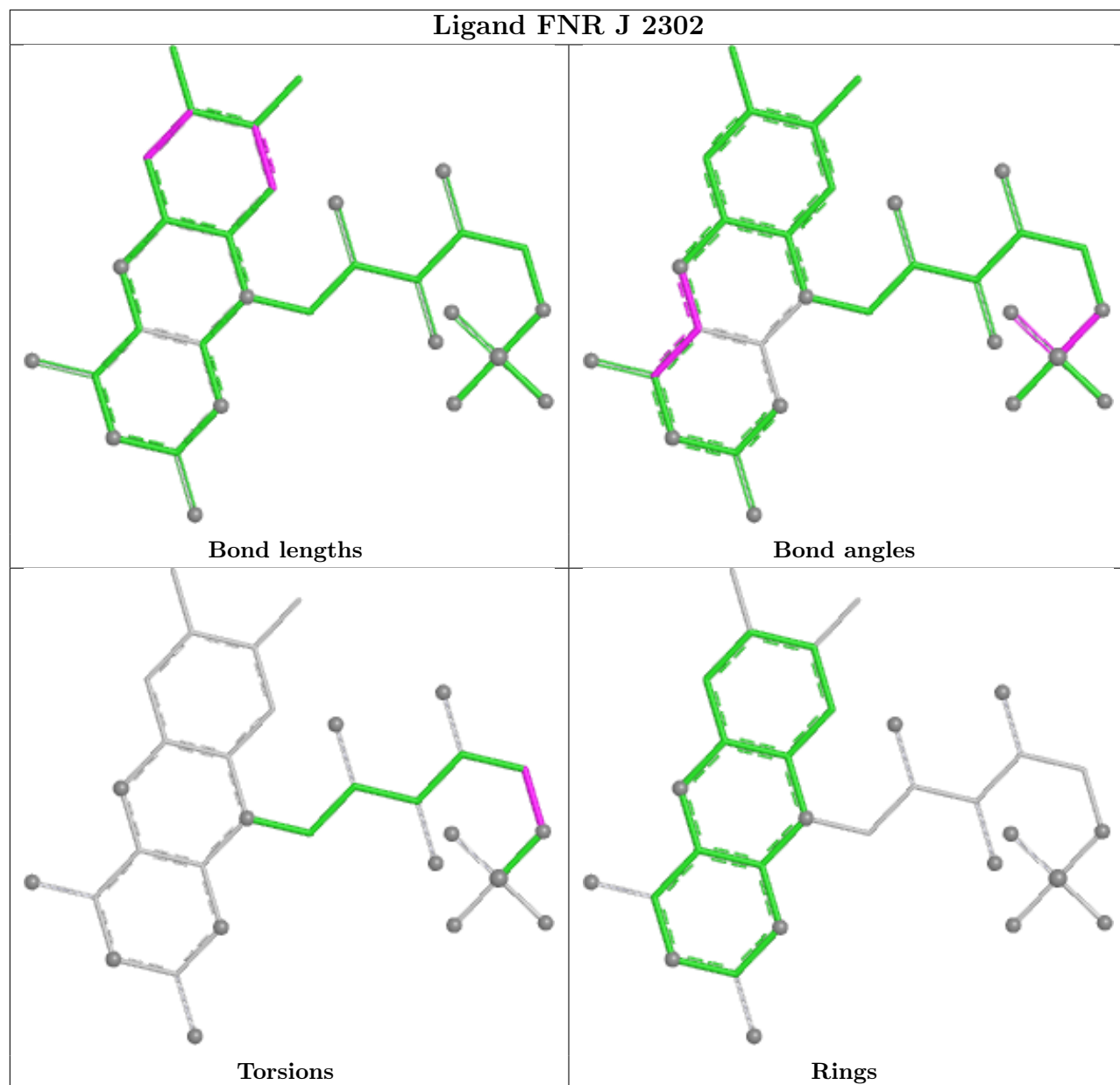
Bond angles



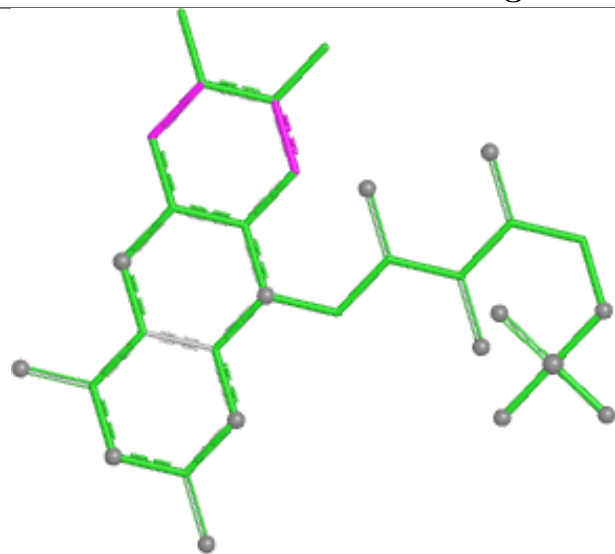
Torsions



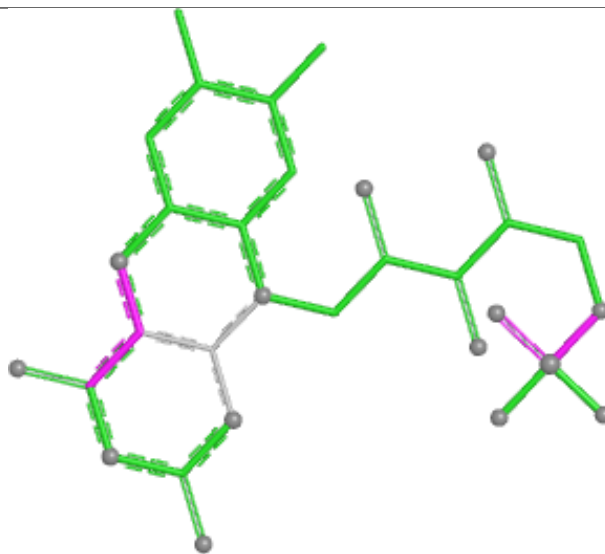
Rings



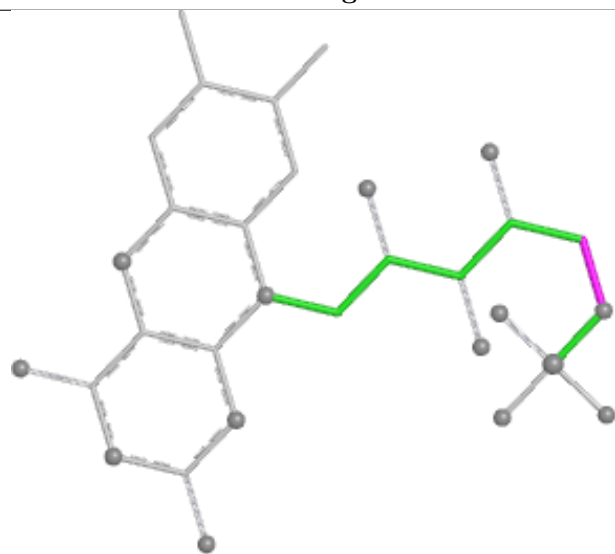
Ligand FNR H 2302



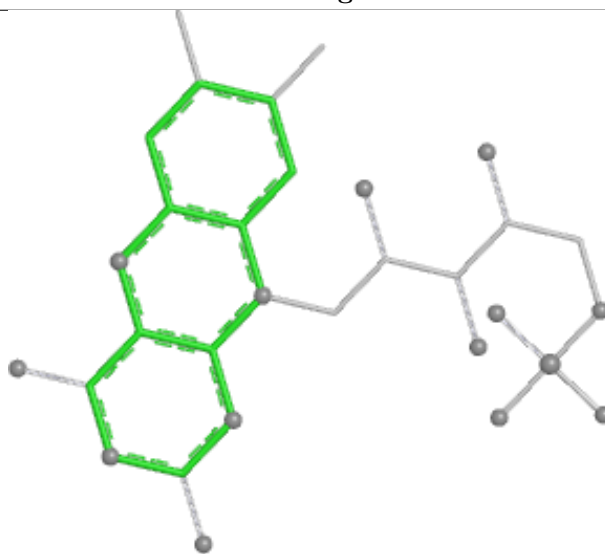
Bond lengths



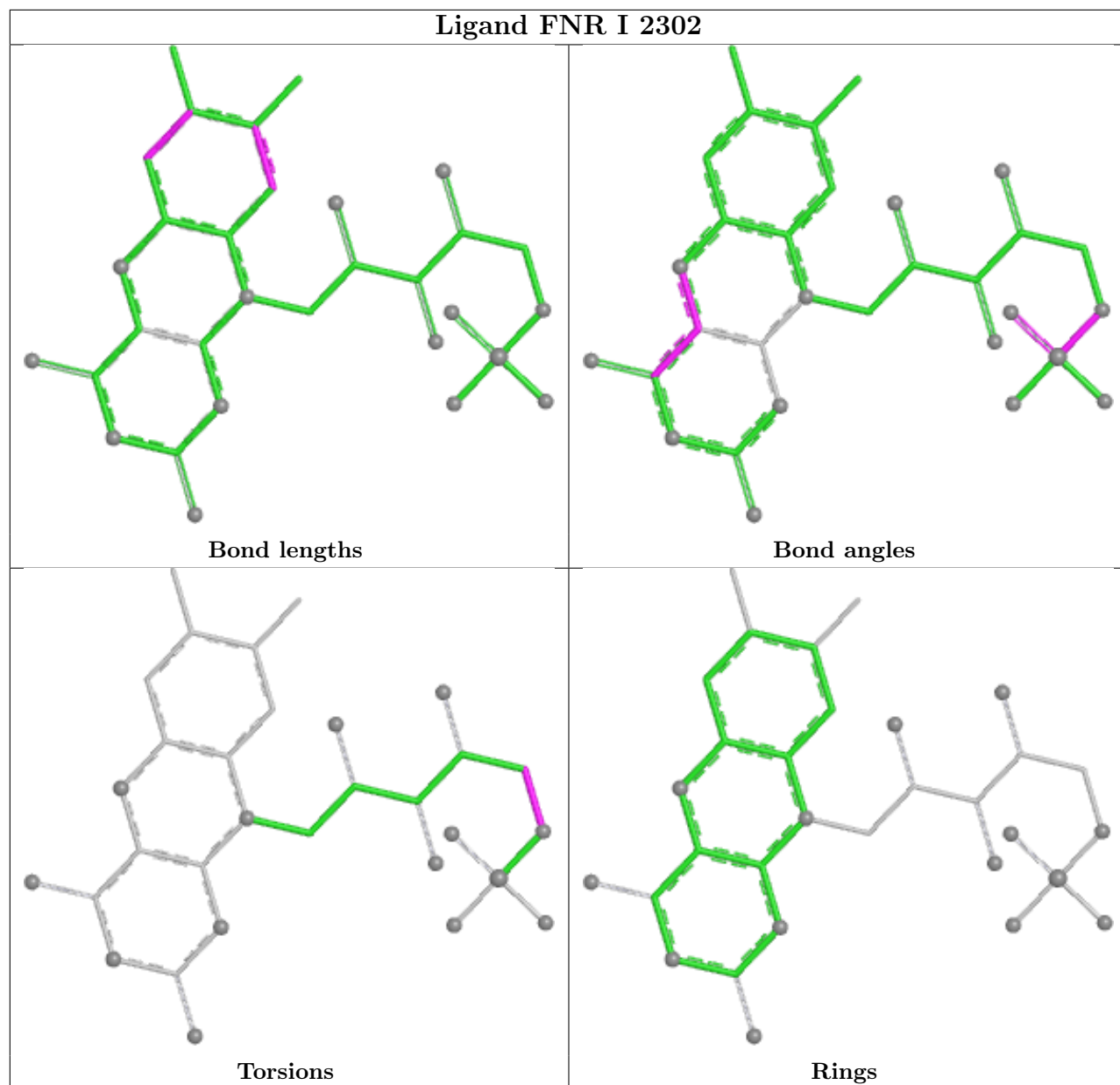
Bond angles



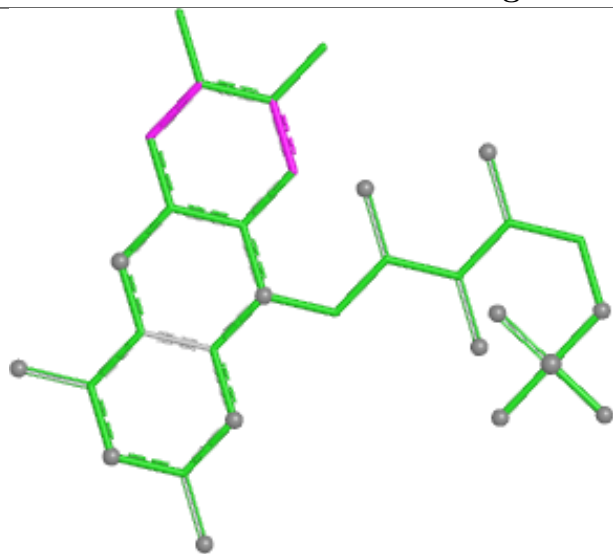
Torsions



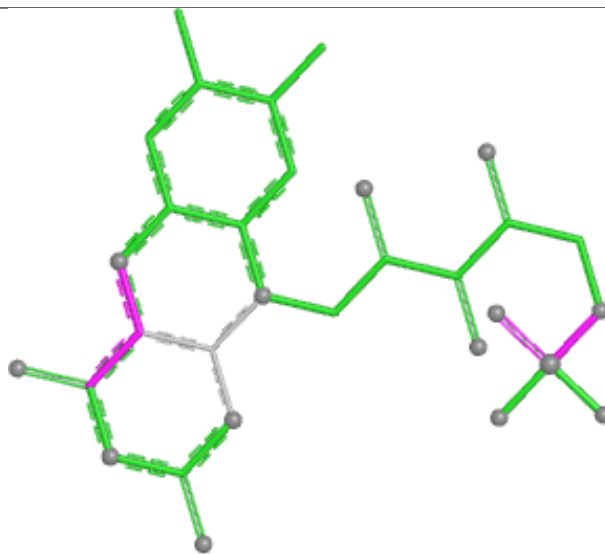
Rings



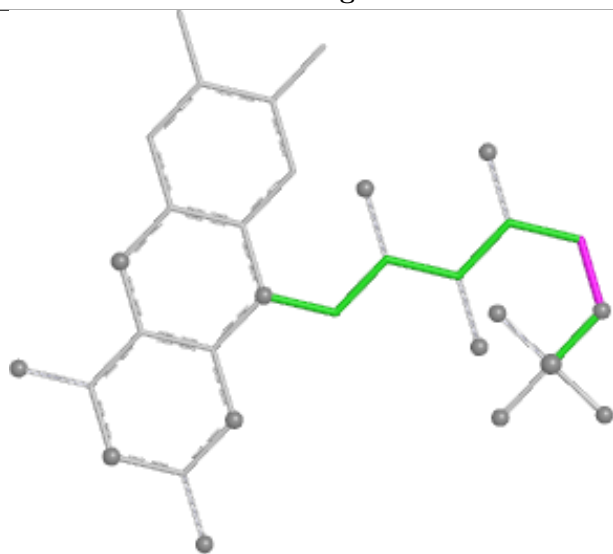
Ligand FNR G 2302



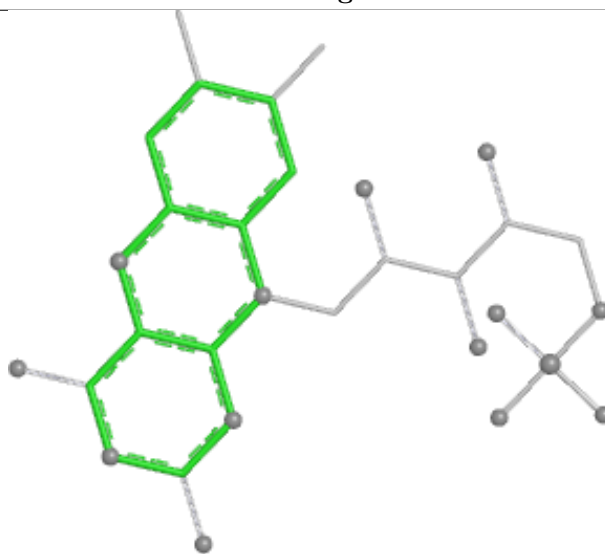
Bond lengths



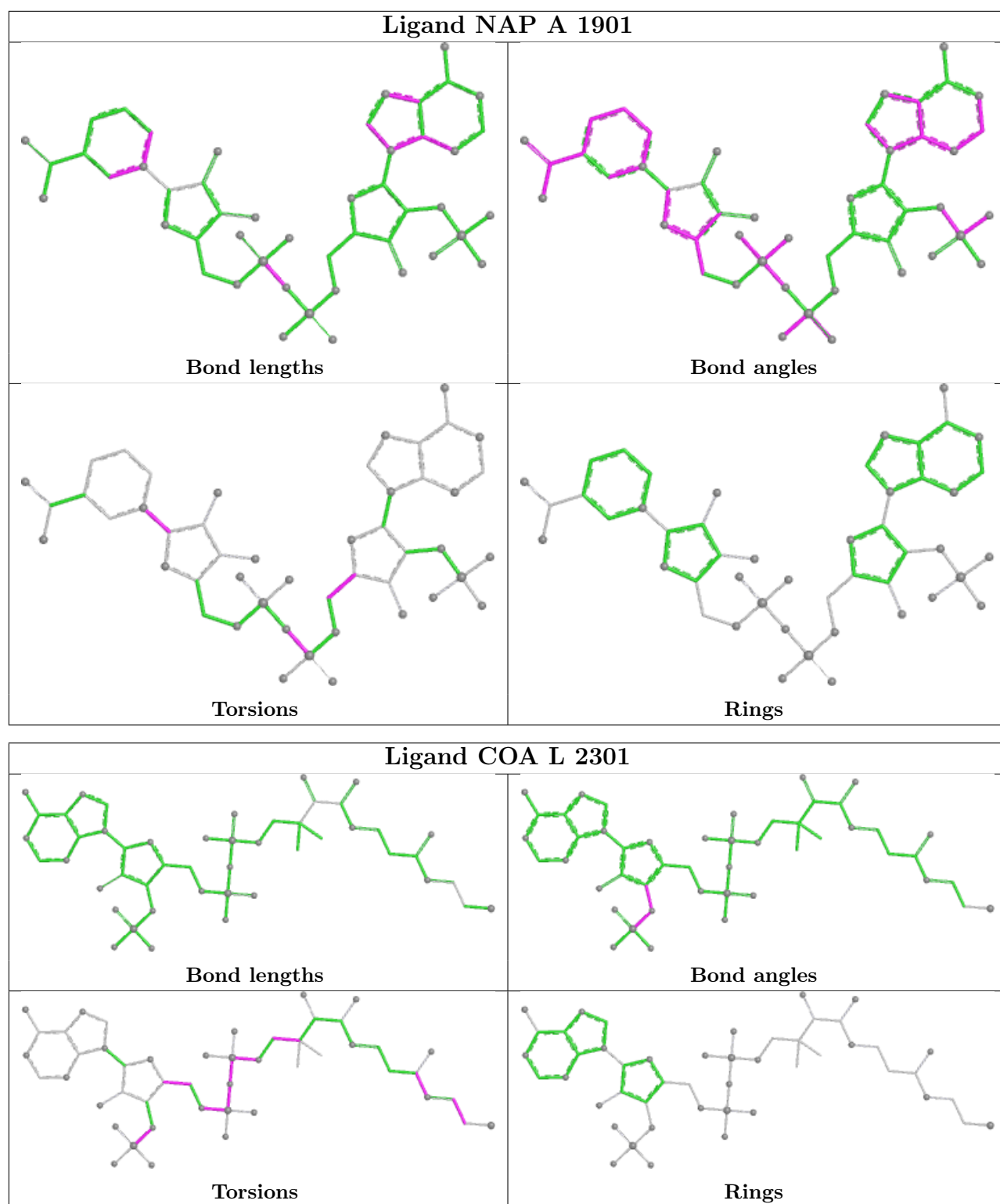
Bond angles

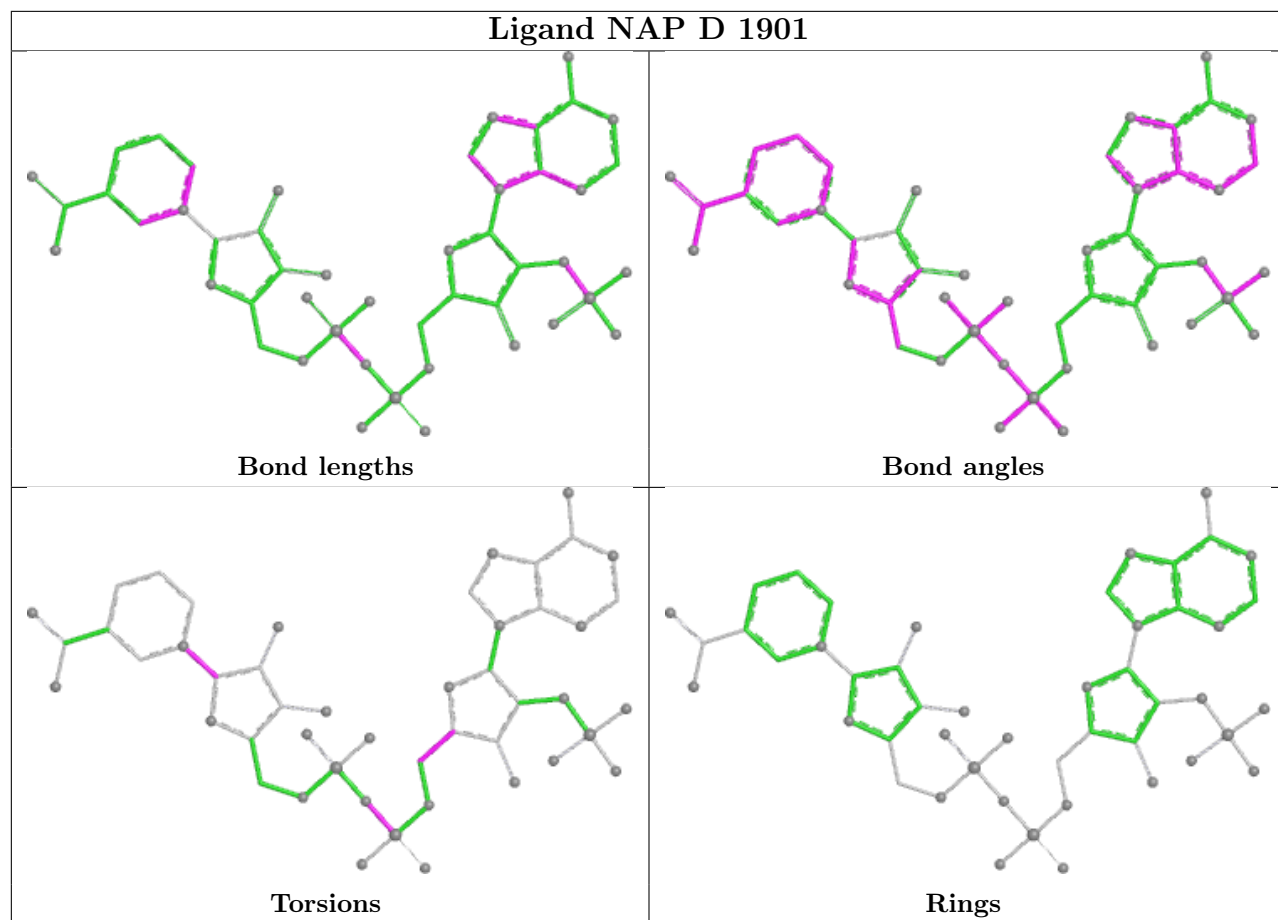


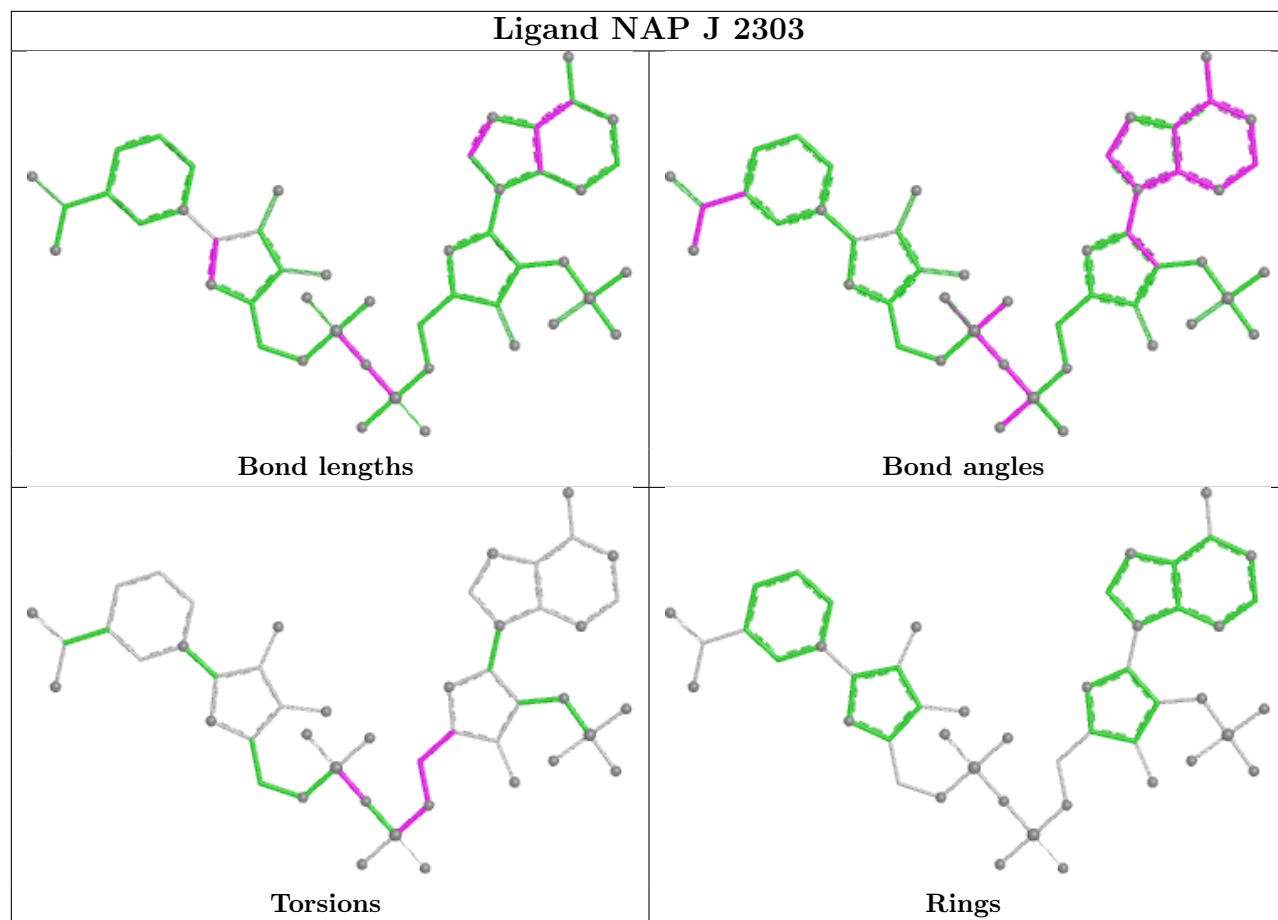
Torsions

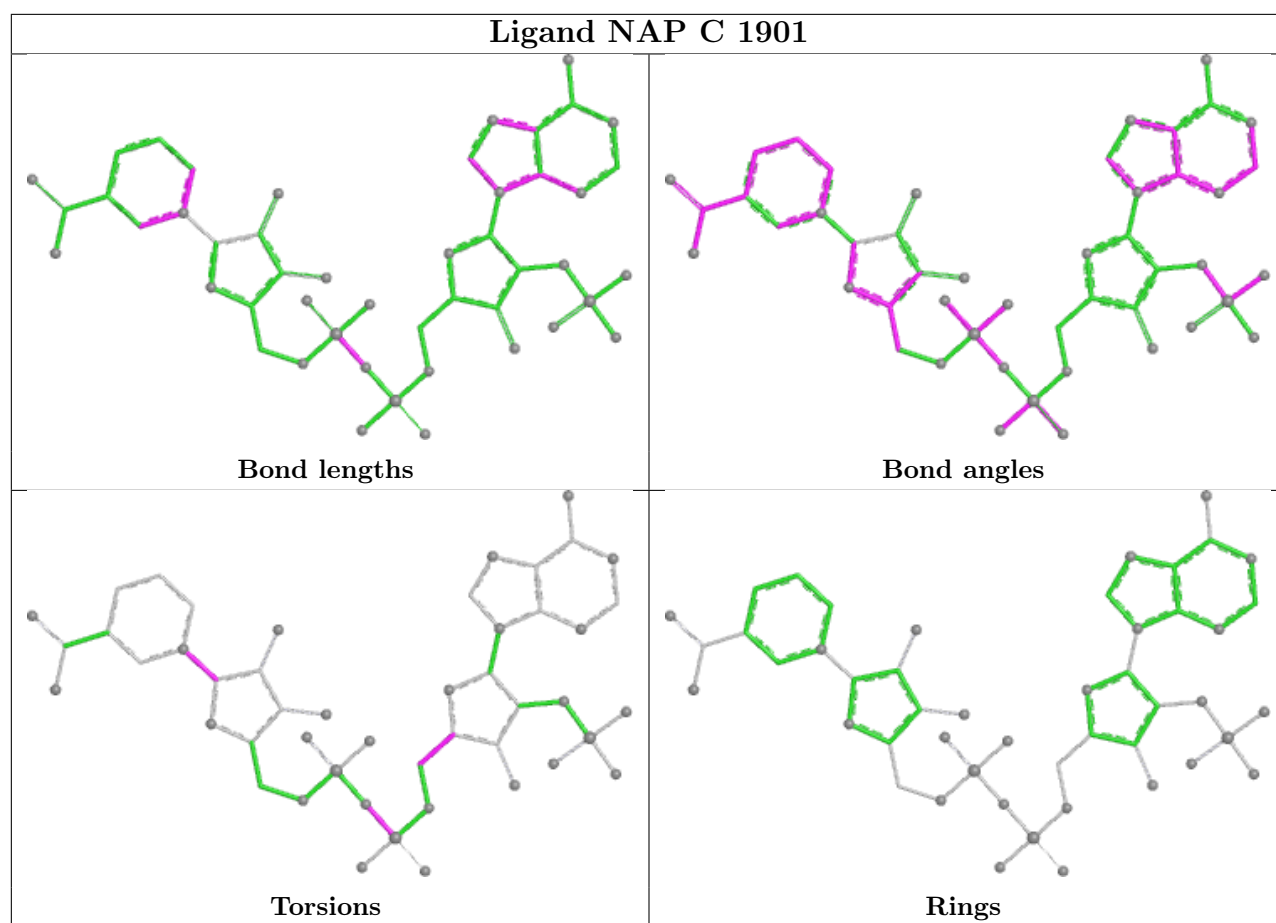


Rings

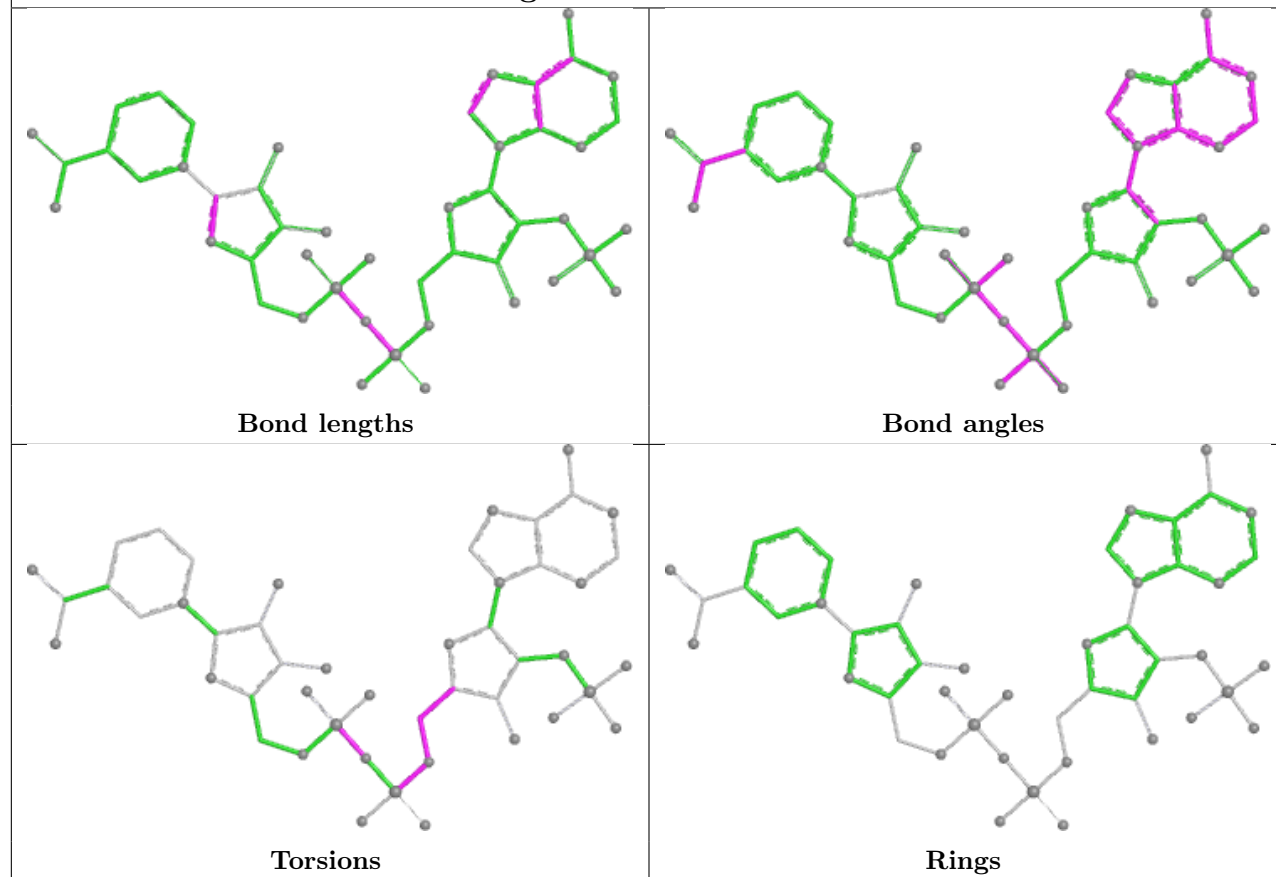




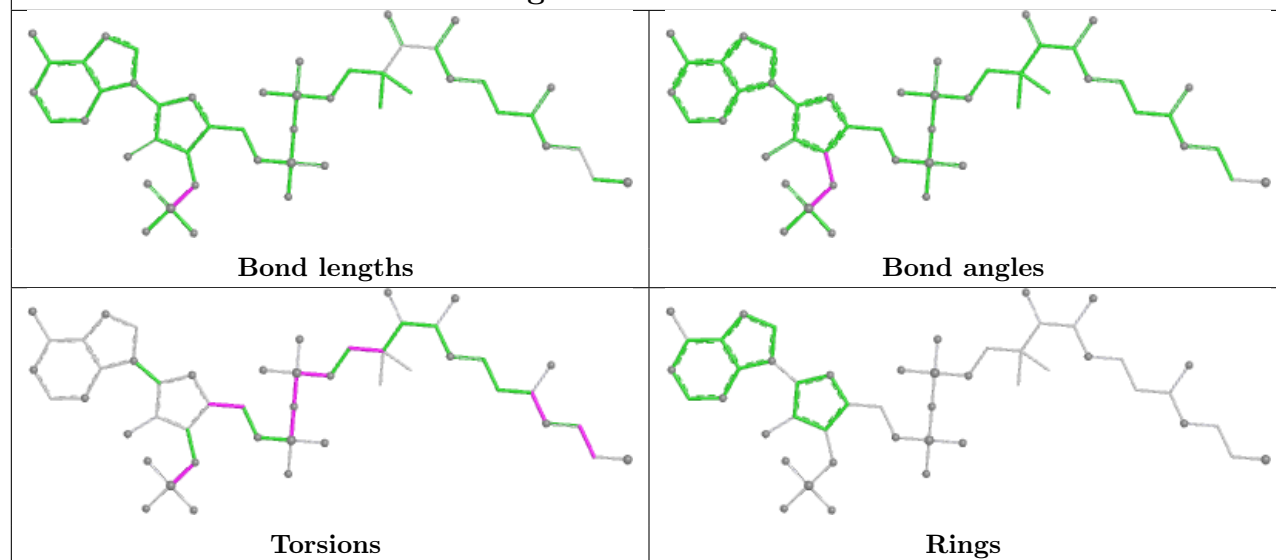


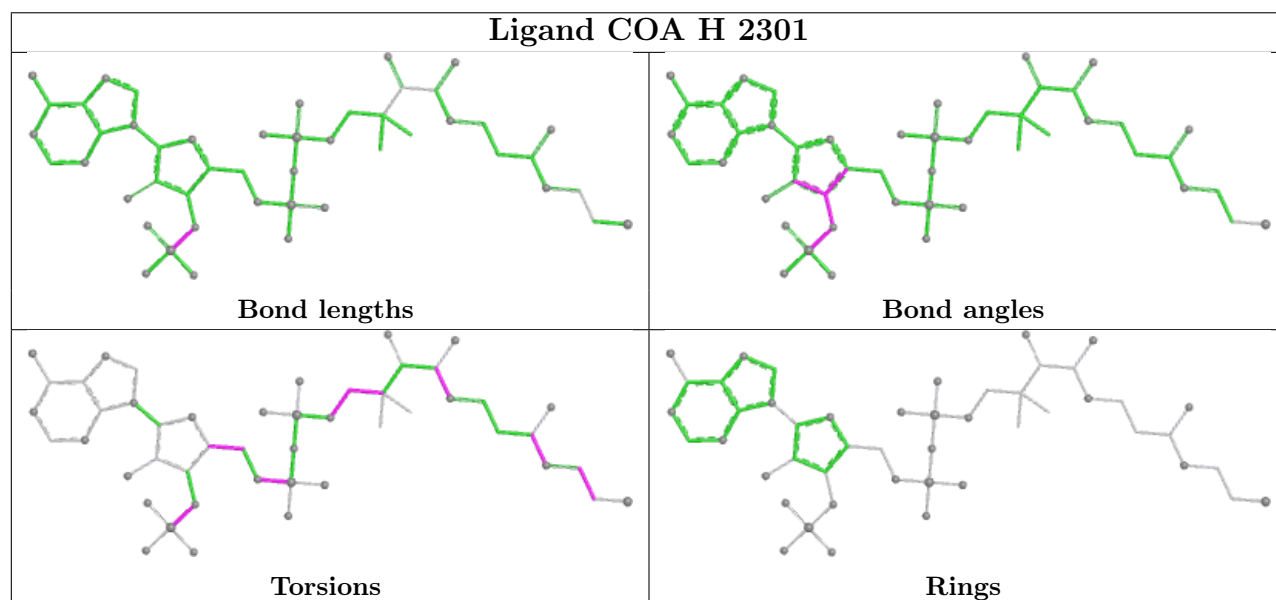
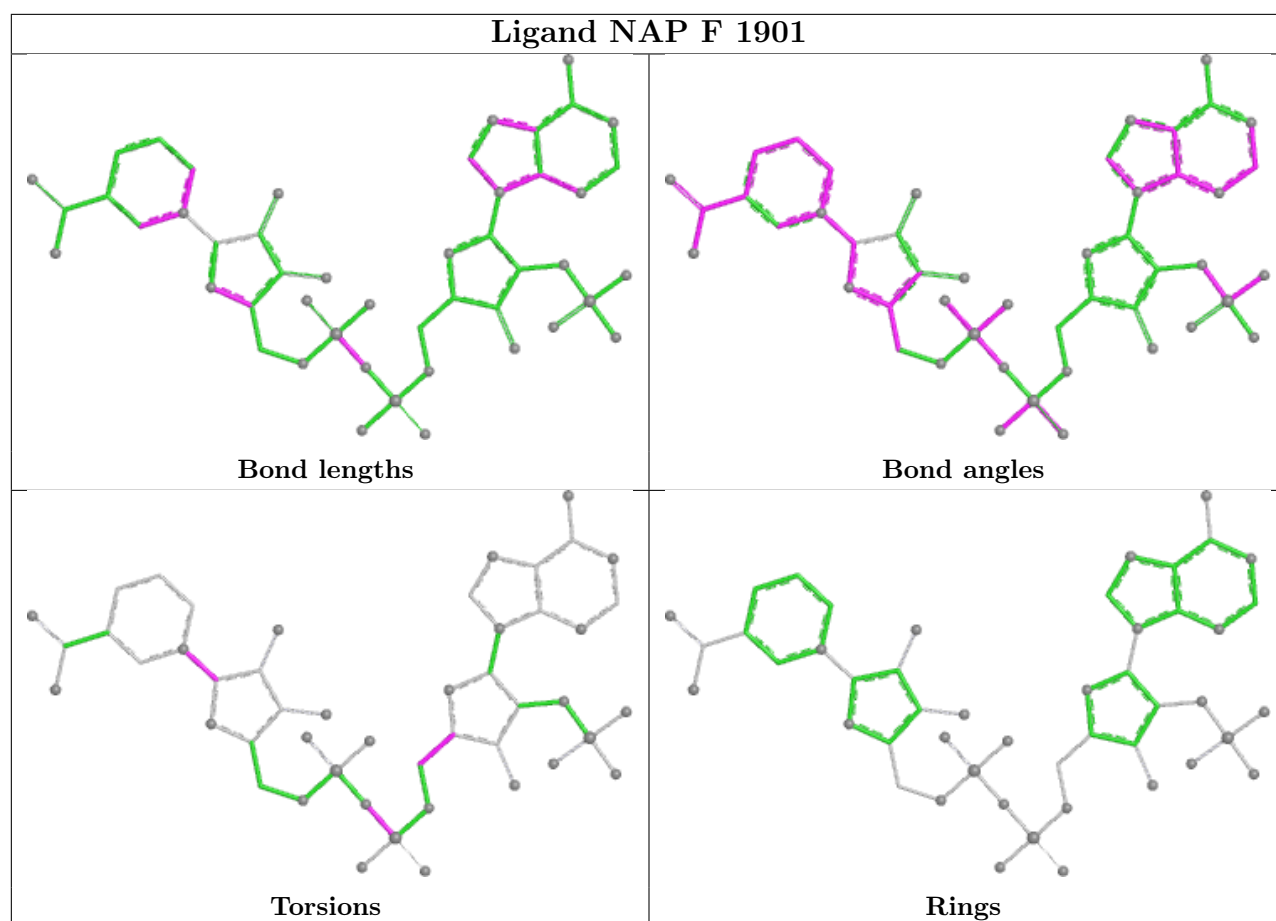


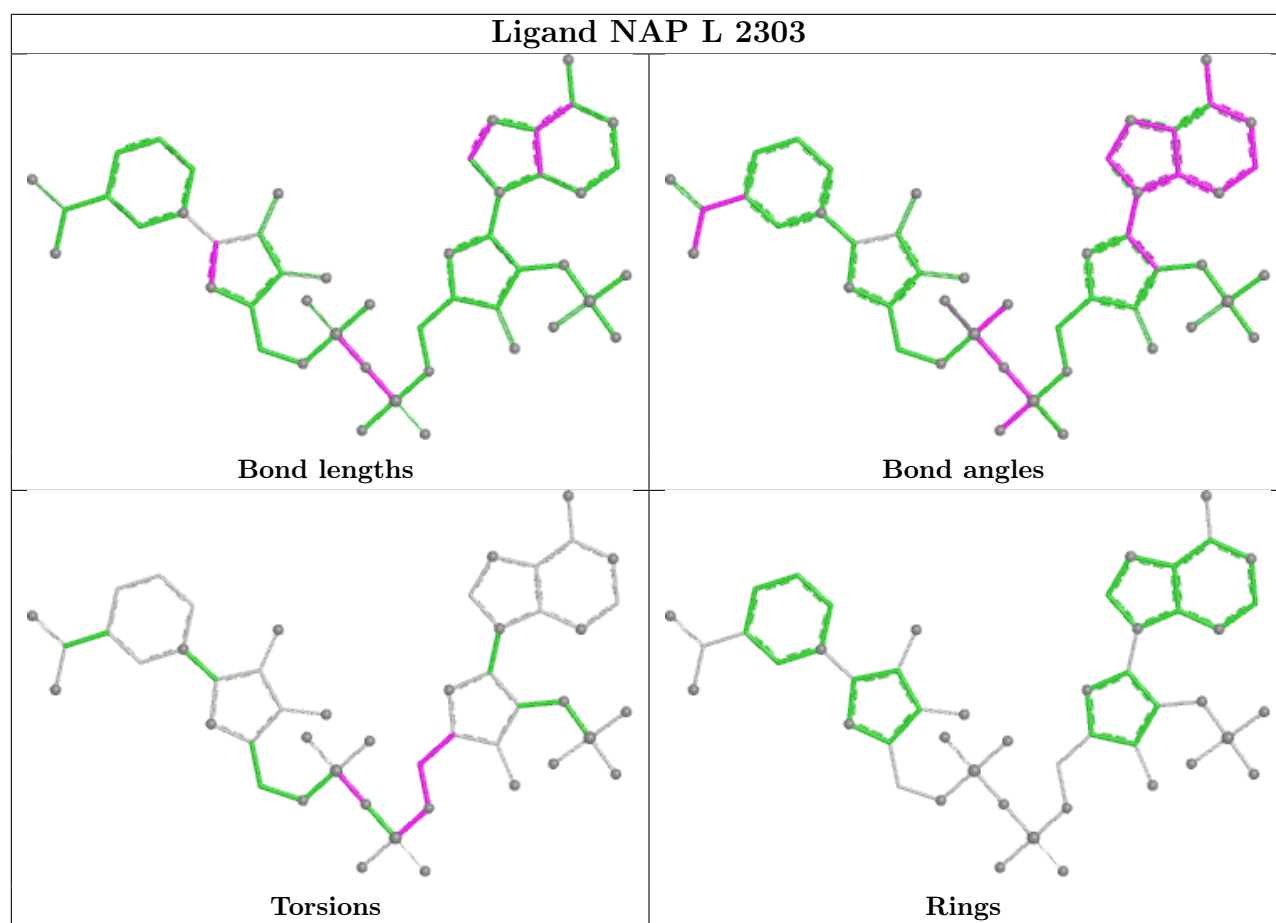
Ligand NAP H 2303

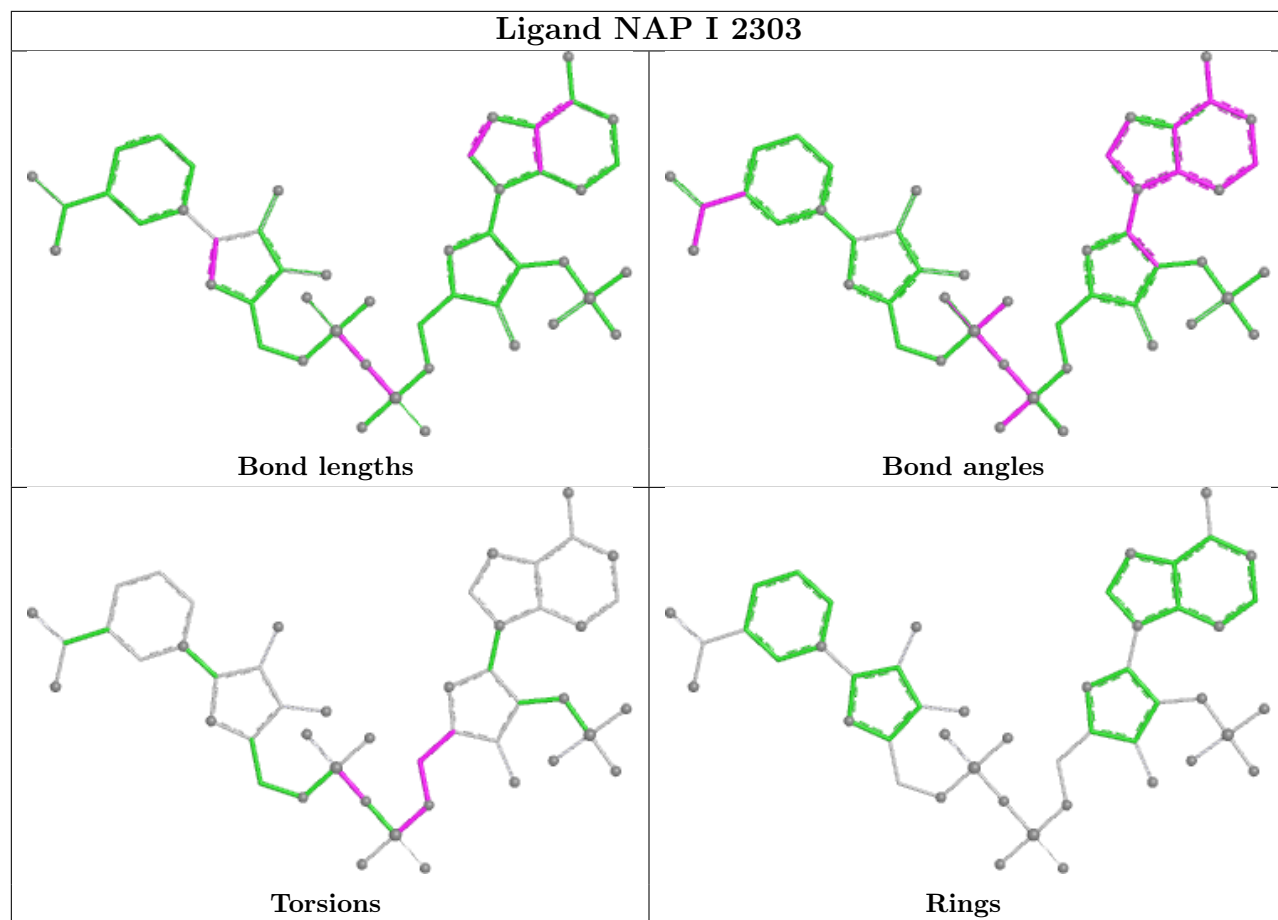


Ligand COA I 2301

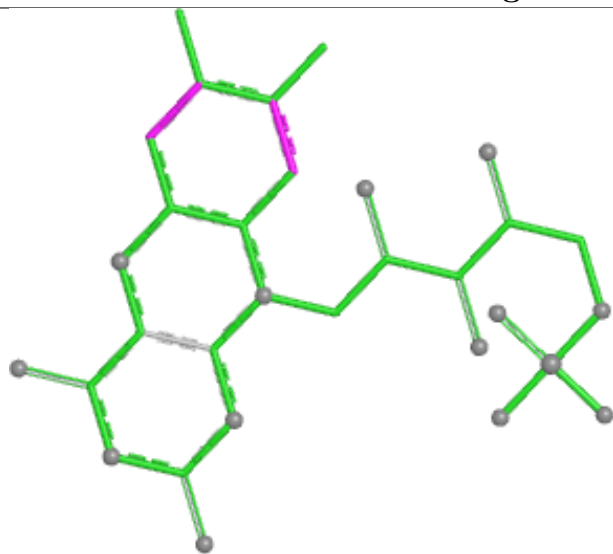




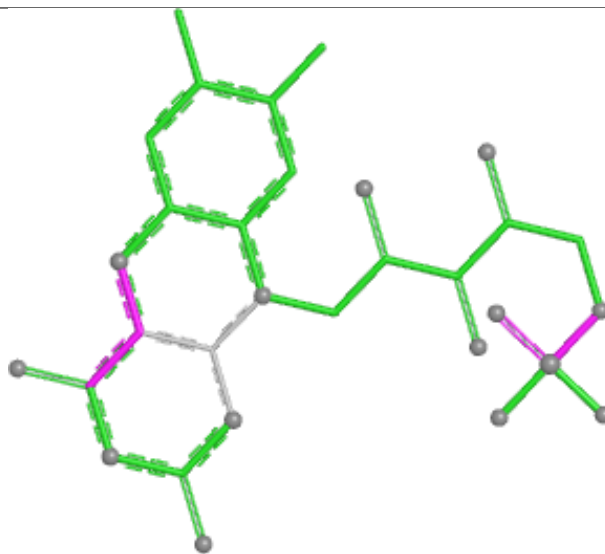




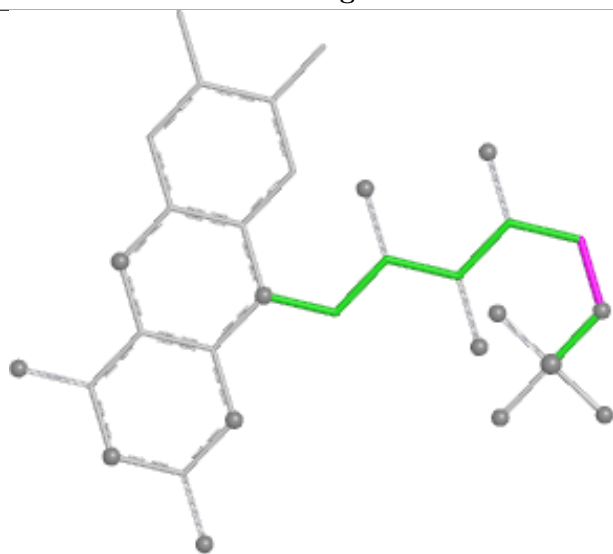
Ligand FNR K 2302



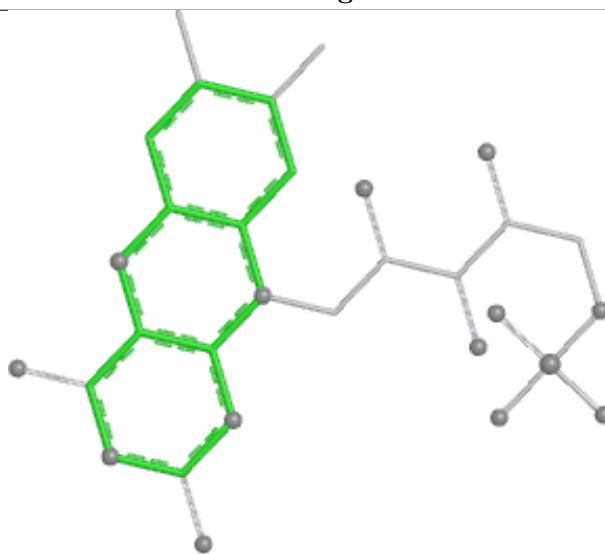
Bond lengths



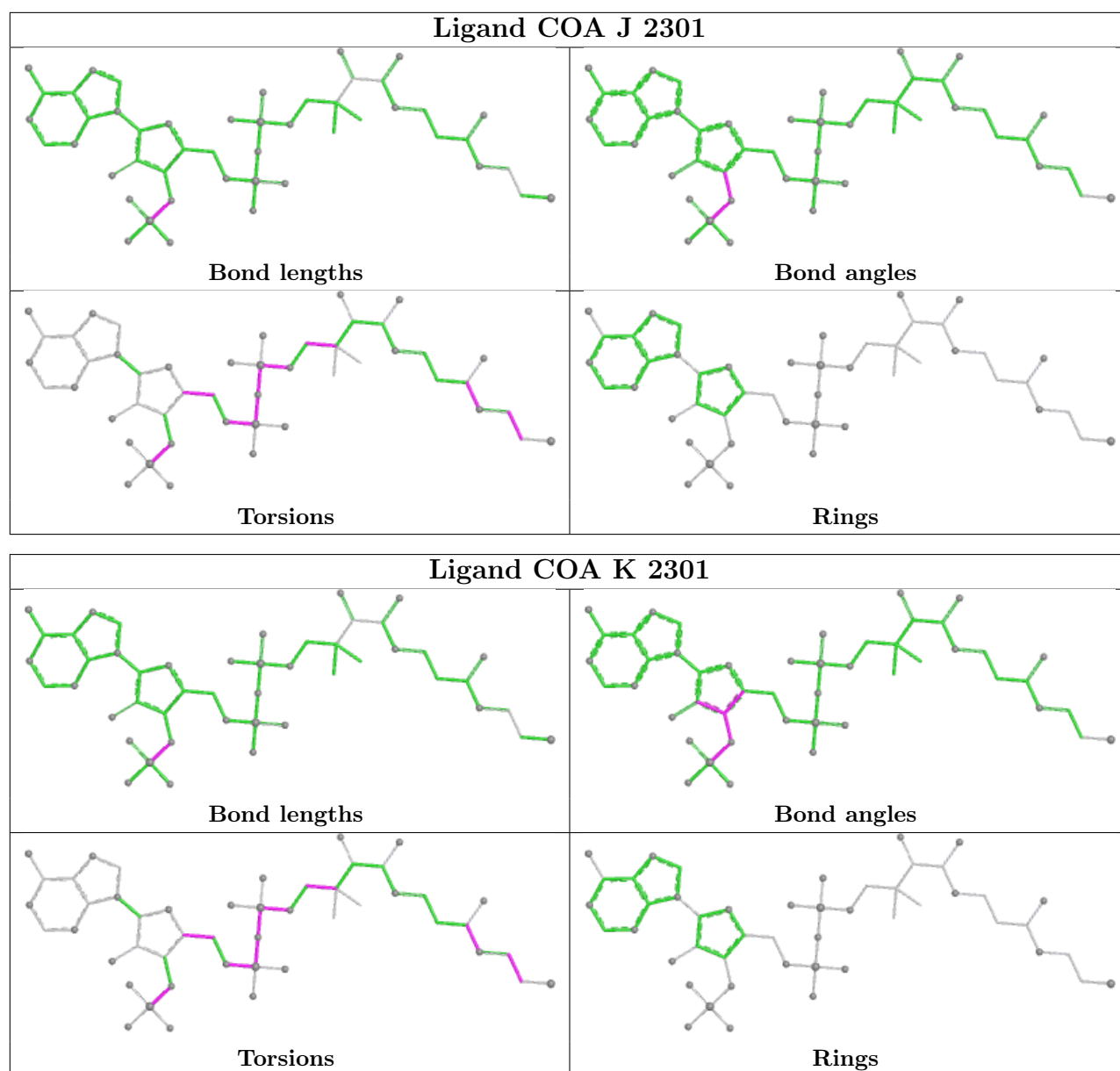
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

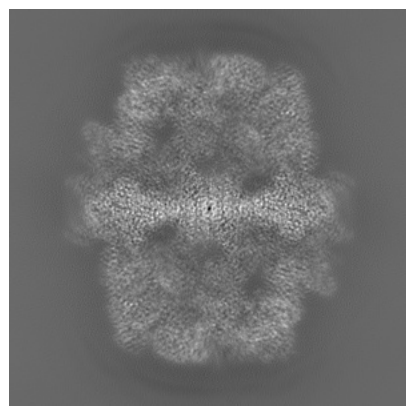
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17840. These allow visual inspection of the internal detail of the map and identification of artifacts.

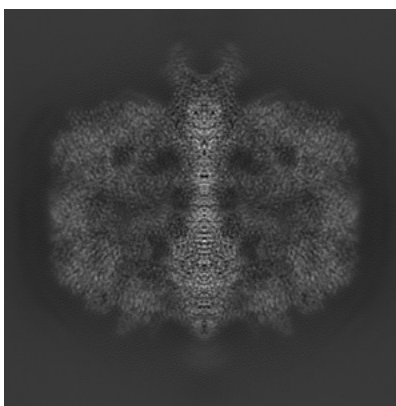
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

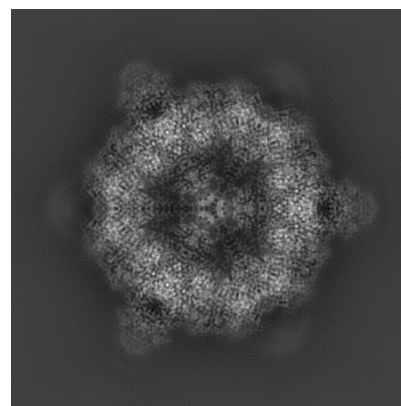
6.1.1 Primary map



X

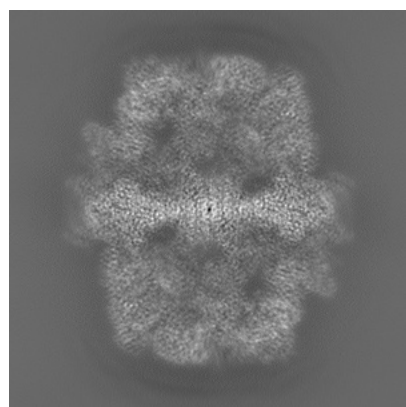


Y

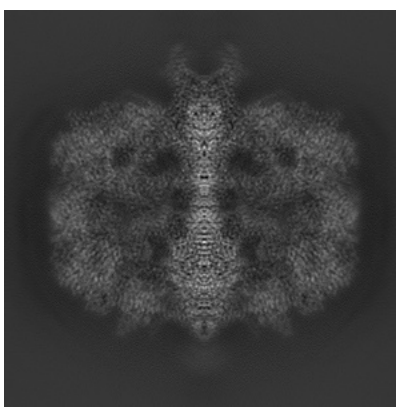


Z

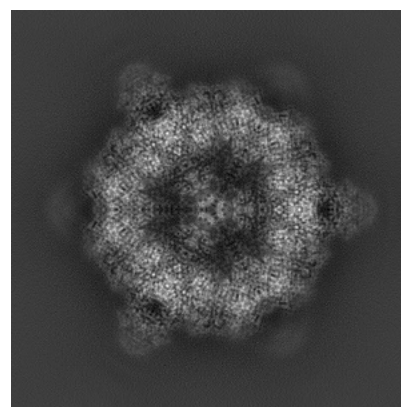
6.1.2 Raw map



X



Y

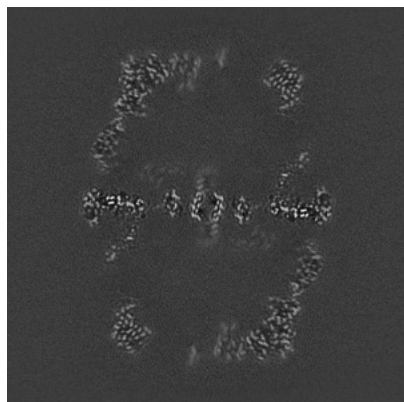


Z

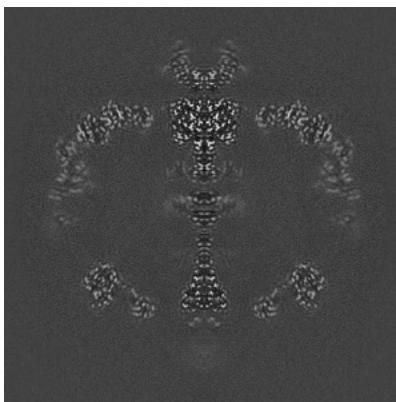
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

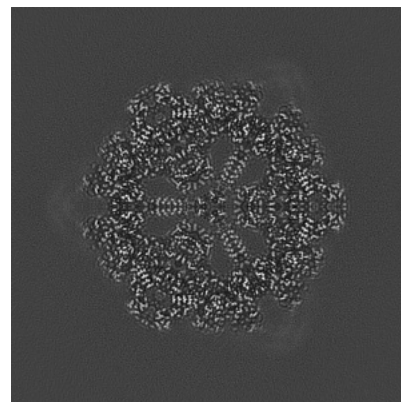
6.2.1 Primary map



X Index: 280

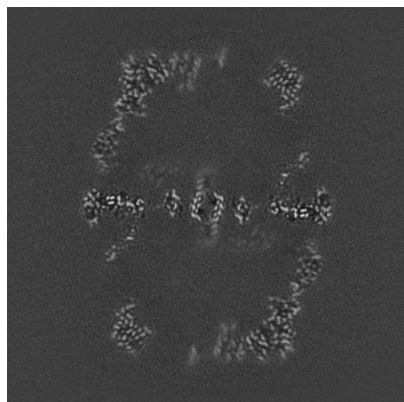


Y Index: 280

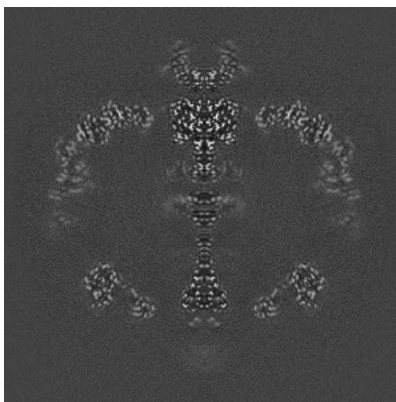


Z Index: 280

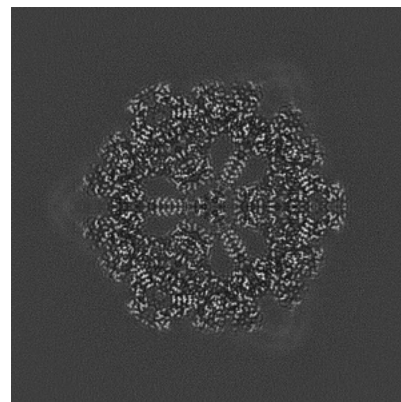
6.2.2 Raw map



X Index: 280



Y Index: 280

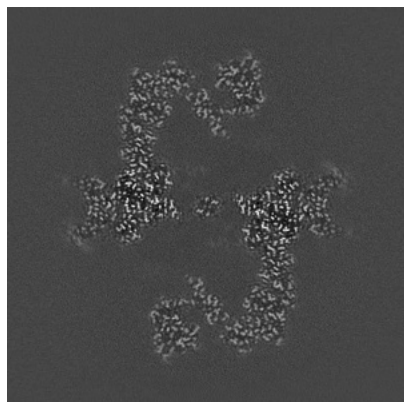


Z Index: 280

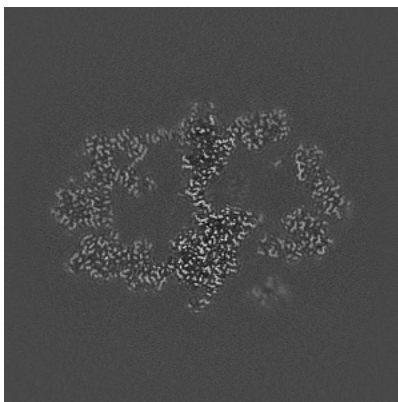
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

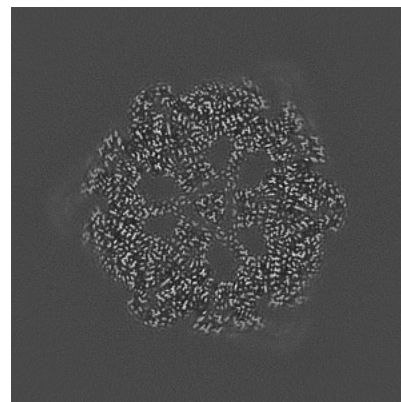
6.3.1 Primary map



X Index: 190

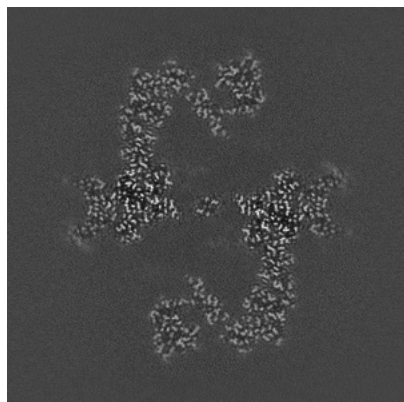


Y Index: 382

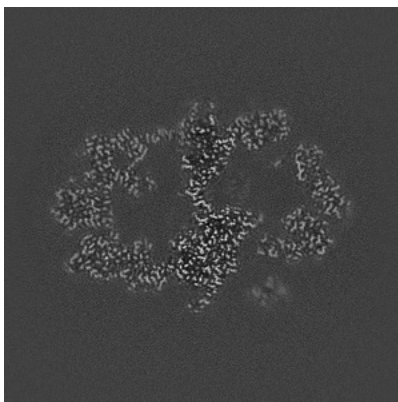


Z Index: 274

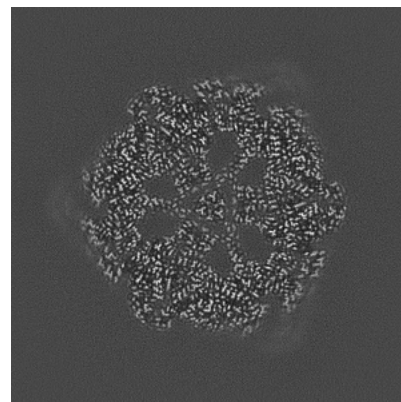
6.3.2 Raw map



X Index: 190



Y Index: 382

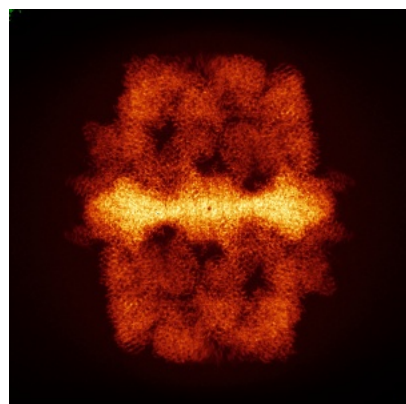


Z Index: 286

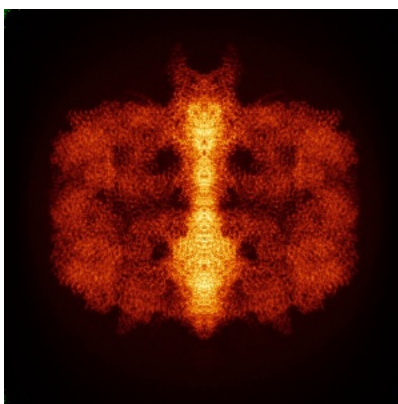
The images above show the largest variance slices of the map in three orthogonal directions.

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

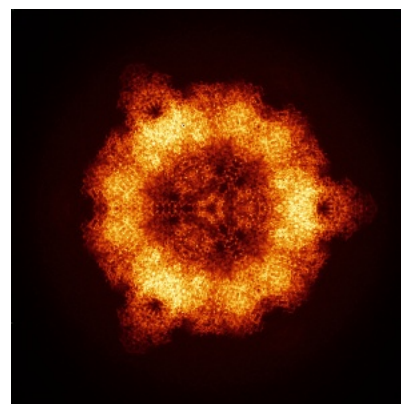
6.4.1 Primary map



X

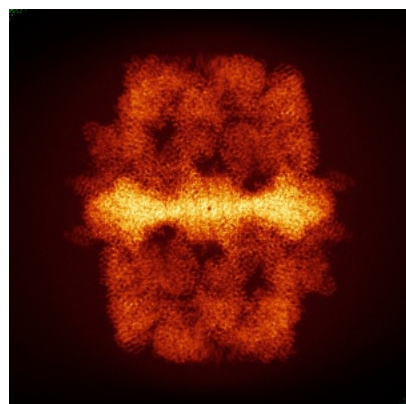


Y

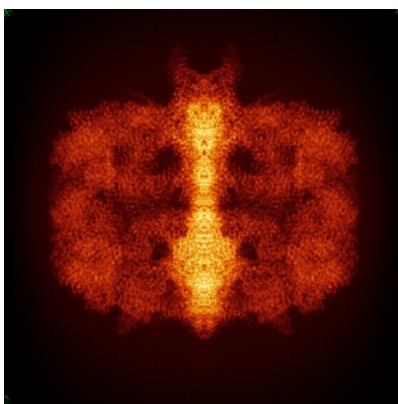


Z

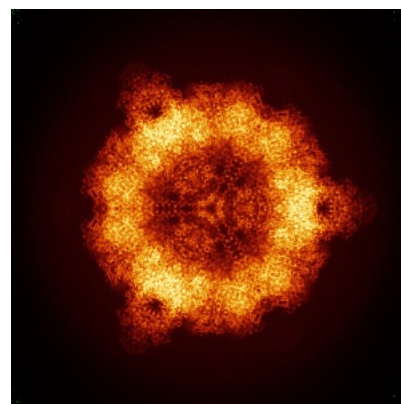
6.4.2 Raw map



X



Y

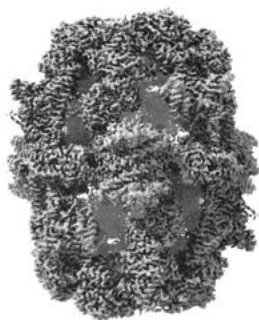


Z

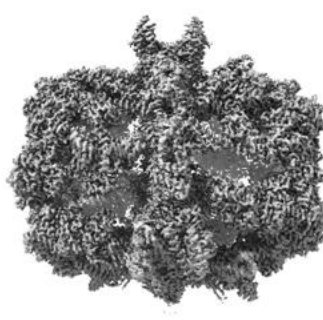
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

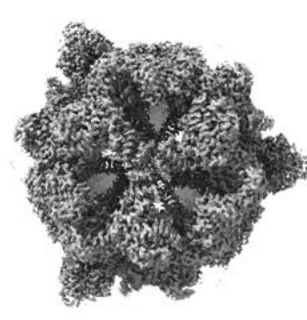
6.5.1 Primary map



X



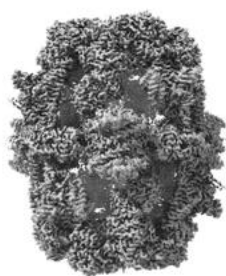
Y



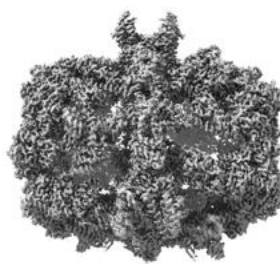
Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

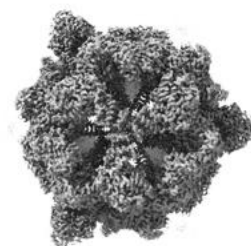
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

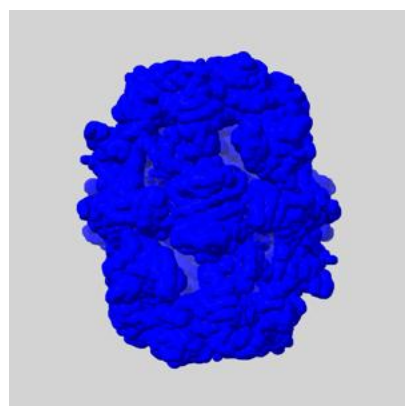
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

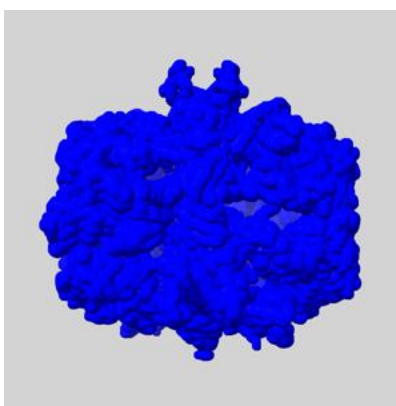
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

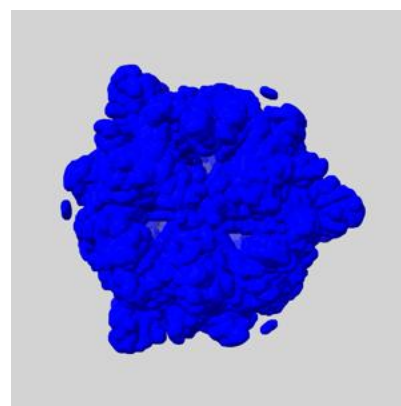
6.6.1 emd_17840_msk_1.map [i](#)



X



Y

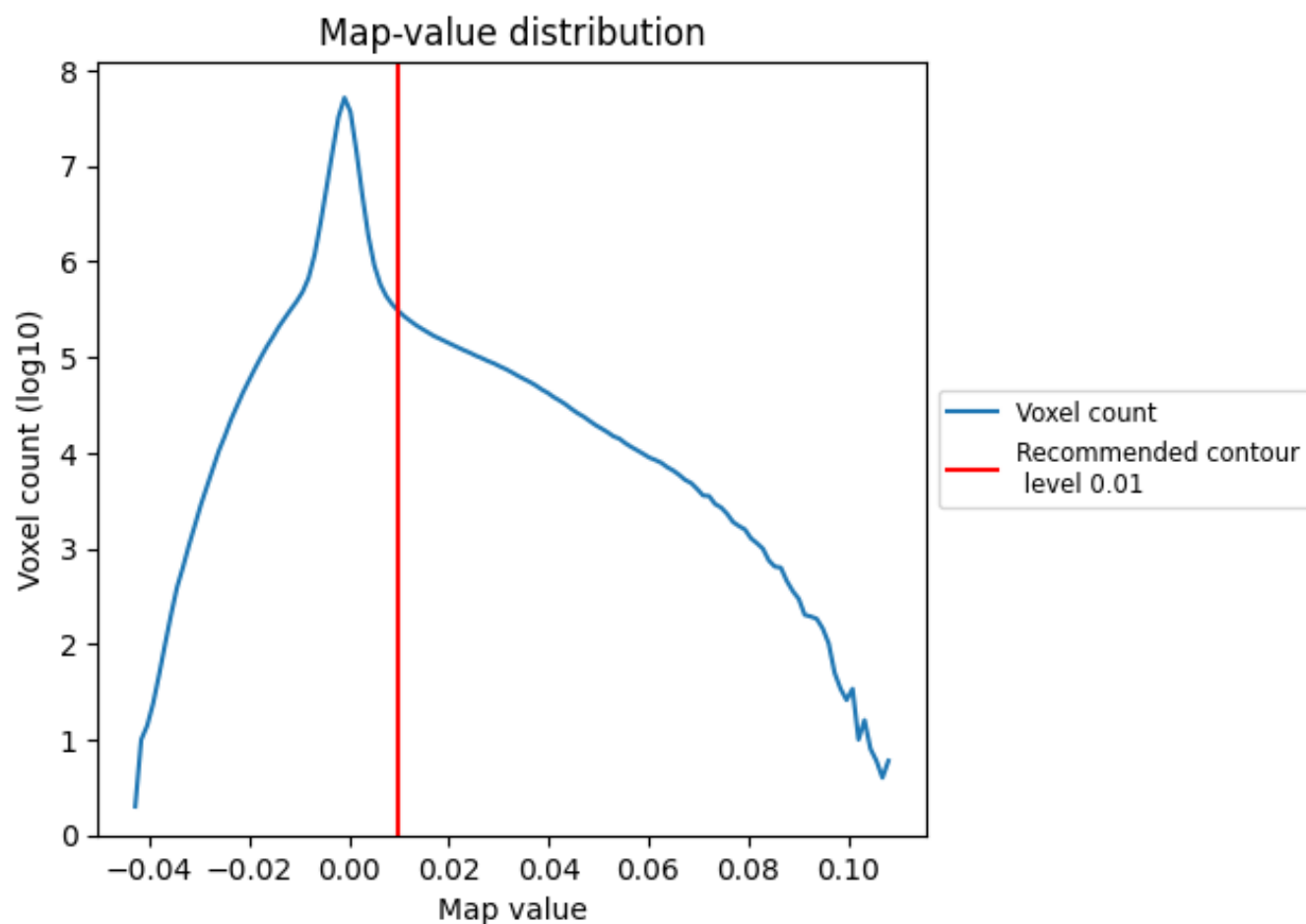


Z

7 Map analysis [i](#)

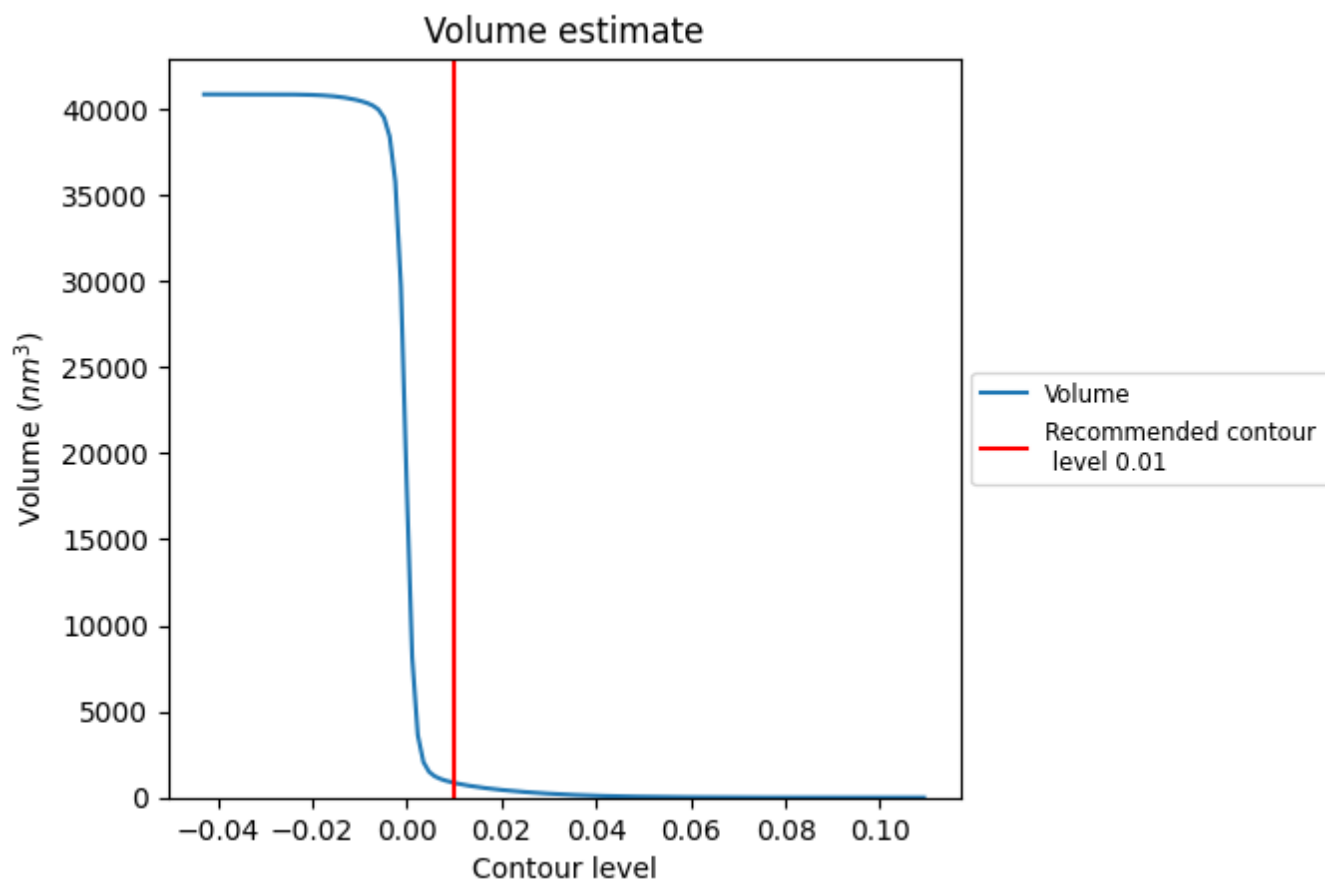
This section contains the results of statistical analysis of the map.

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.

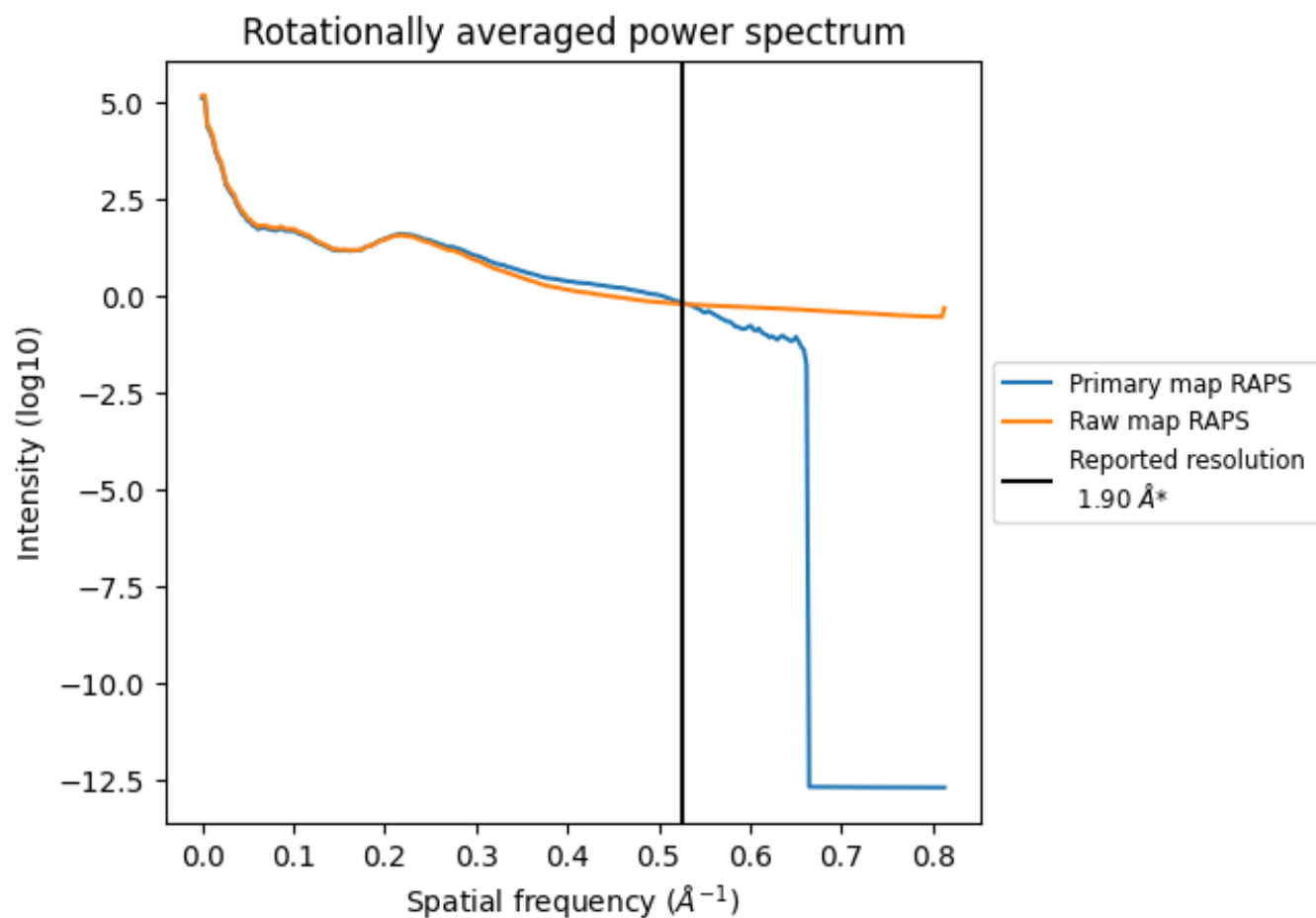
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 856 nm^3 ; this corresponds to an approximate mass of 773 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 ⓘ

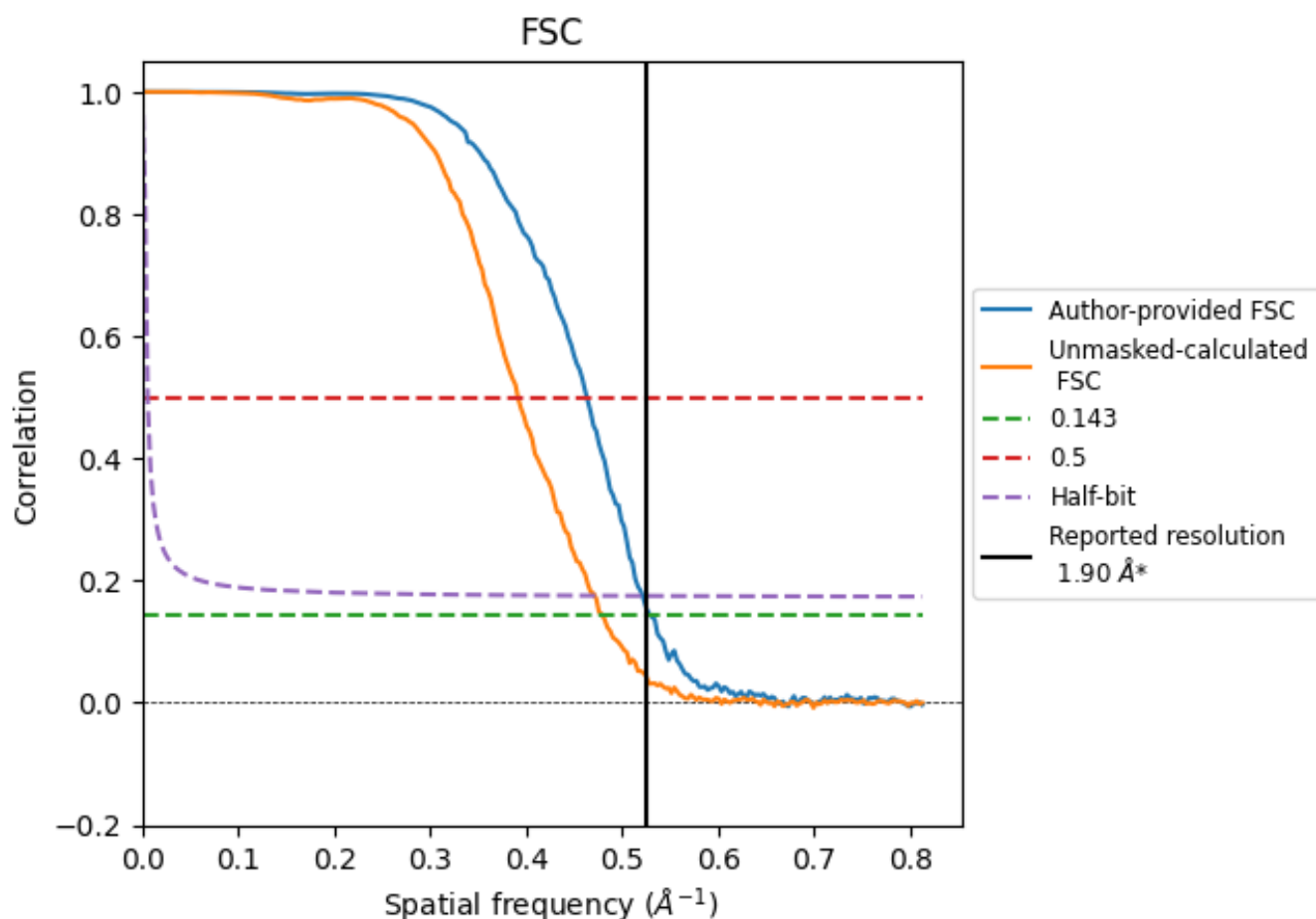


*Reported resolution corresponds to spatial frequency of 0.526 $\text{\AA}^{-1}$

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 0.526 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

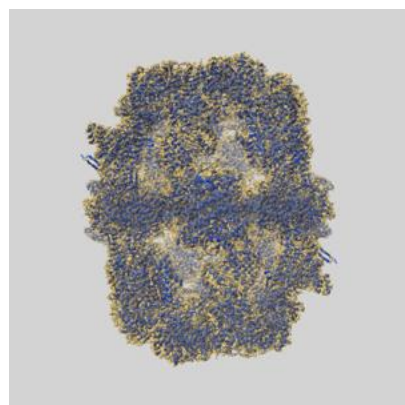
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.90	-	-
Author-provided FSC curve	1.89	2.16	1.92
Unmasked-calculated*	2.08	2.55	2.12

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

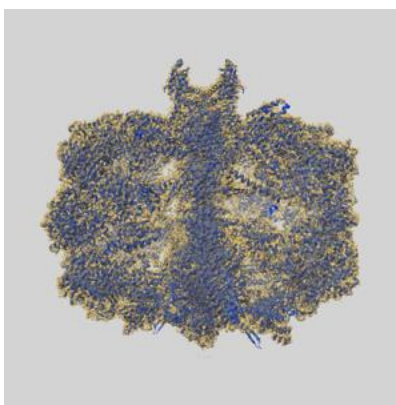
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17840 and PDB model 8PRW. Per-residue inclusion information can be found in section [3](#) on page [9](#).

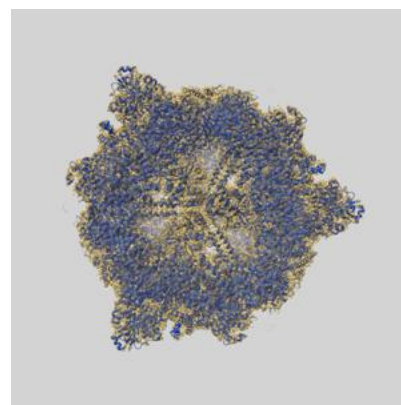
9.1 Map-model overlay [i](#)



X



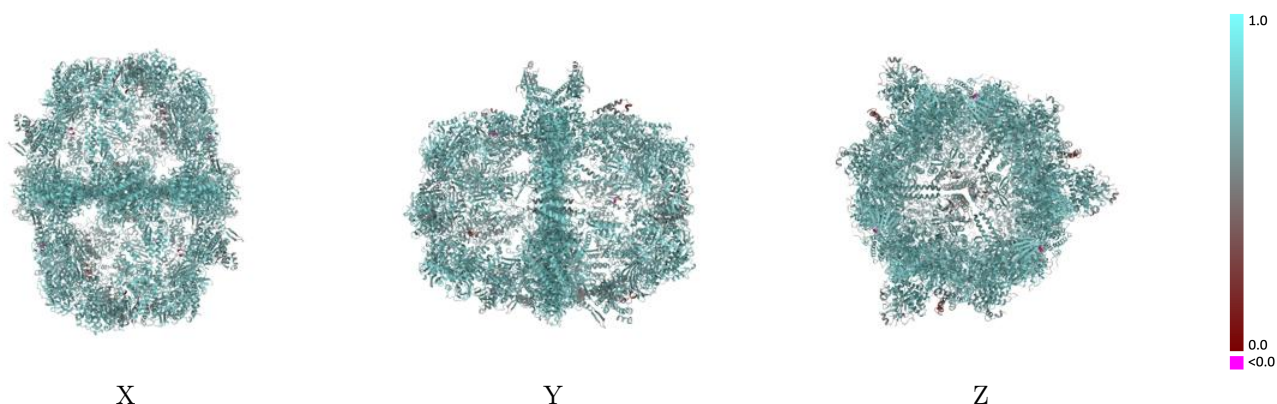
Y



Z

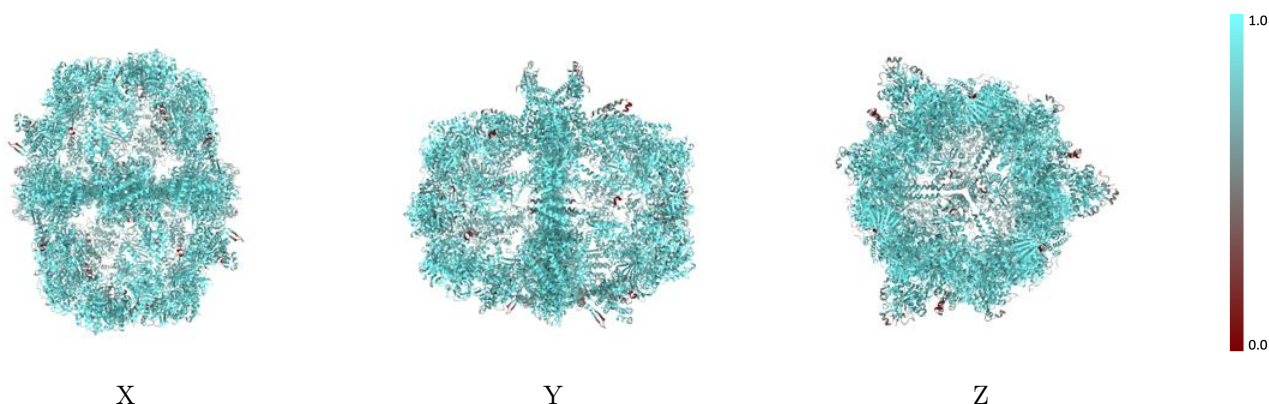
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



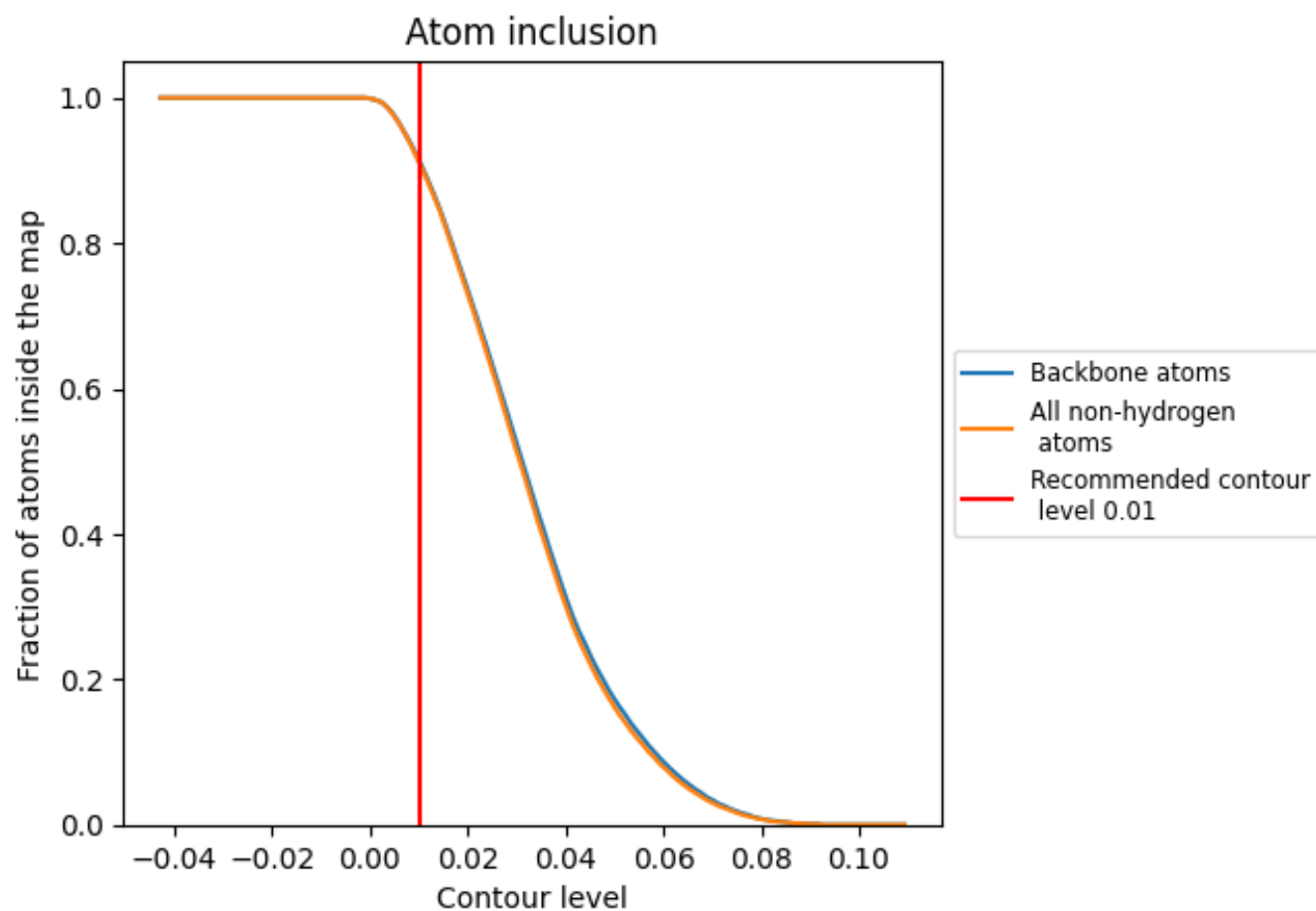
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 91% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9110	0.7120
A	0.9280	0.7410
B	0.9270	0.7400
C	0.9270	0.7400
D	0.9270	0.7400
E	0.9280	0.7410
F	0.9270	0.7410
G	0.9010	0.6900
H	0.9010	0.6890
I	0.9010	0.6890
J	0.9010	0.6900
K	0.9010	0.6900
L	0.9010	0.6890

1.0

0.0

<0.0