



Full wwPDB EM Validation Report ⓘ

Nov 11, 2024 – 09:36 PM JST

PDB ID : 7Y42
EMDB ID : EMD-33600
Title : Cryo-EM structure of the SARS-CoV-2 spike glycoprotein in complex with all-trans retinoic acid
Authors : Xiang, Y.; Wang, L.
Deposited on : 2022-06-13
Resolution : 3.45 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

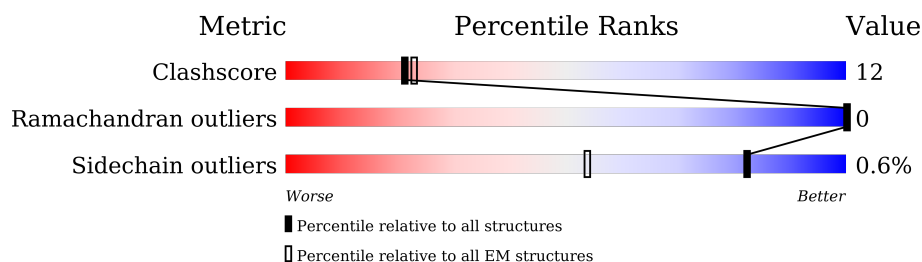
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.45 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1121	 64% 22% 14%
1	B	1121	 64% 22% 14%
1	D	1121	 64% 22% 14%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	REA	D	1310	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23058 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	968	Total	C	N	O	S	0	0
			7538	4811	1251	1446	30		
1	B	968	Total	C	N	O	S	0	0
			7538	4811	1251	1446	30		
1	D	968	Total	C	N	O	S	0	0
			7538	4811	1251	1446	30		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	PHE	CYS	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	166	PHE	CYS	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
D	166	PHE	CYS	engineered mutation	UNP P0DTC2
D	986	PRO	LYS	engineered mutation	UNP P0DTC2
D	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



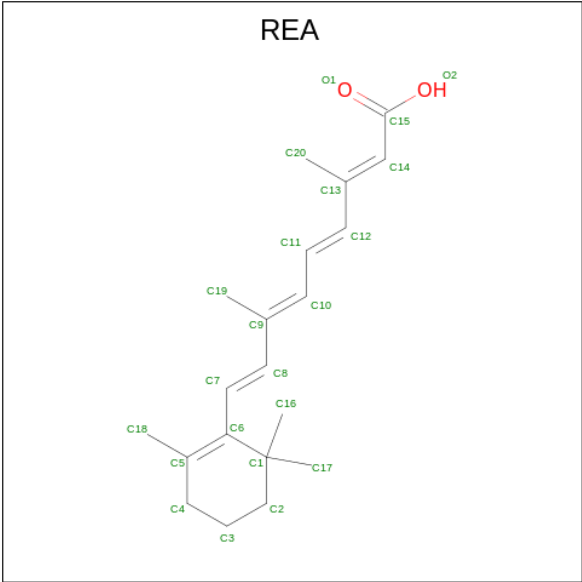
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	A	1	14	8	1	5	0
2	A	1	14	8	1	5	0
2	A	1	14	8	1	5	0
2	A	1	14	8	1	5	0
2	A	1	14	8	1	5	0
2	A	1	14	8	1	5	0
2	A	1	14	8	1	5	0
2	A	1	14	8	1	5	0
2	A	1	14	8	1	5	0
2	B	1	14	8	1	5	0
2	B	1	14	8	1	5	0
2	B	1	14	8	1	5	0
2	B	1	14	8	1	5	0
2	B	1	14	8	1	5	0

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Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 3 is RETINOIC ACID (three-letter code: REA) (formula: C₂₀H₂₈O₂) (labeled as "Ligand of Interest" by depositor).

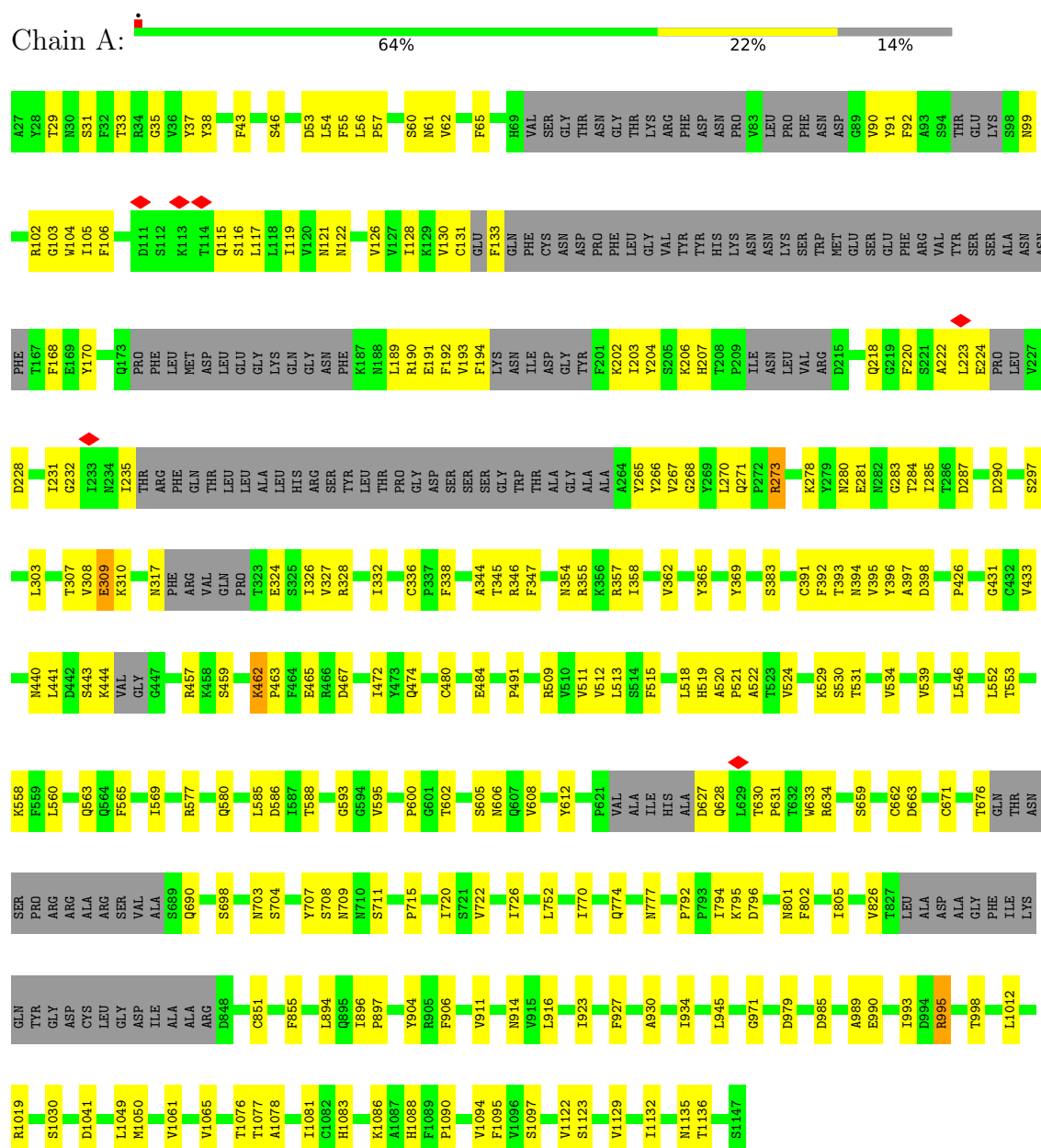


Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			22	20	2	
3	B	1	Total	C	O	0
			22	20	2	
3	D	1	Total	C	O	0
			22	20	2	

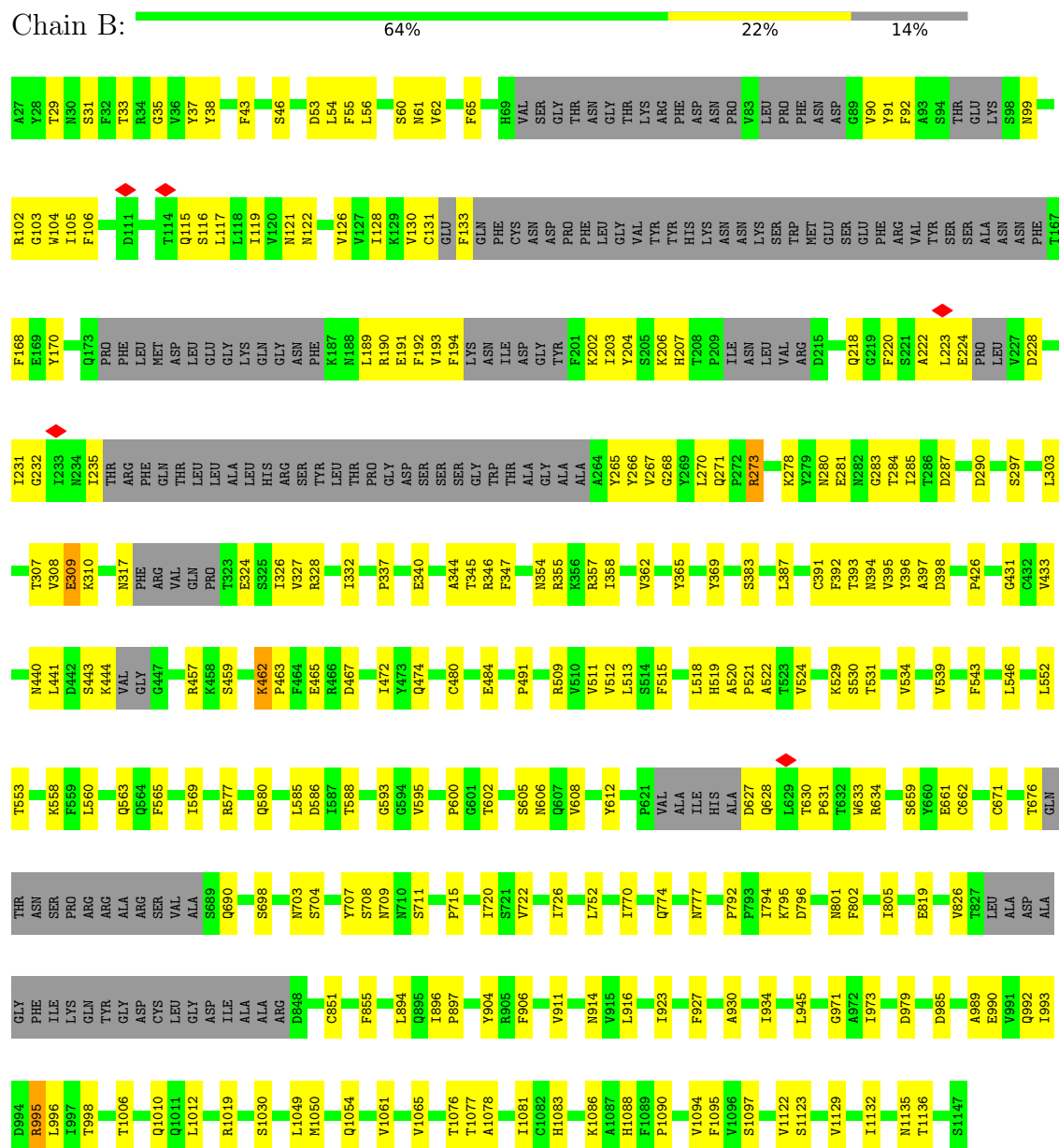
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

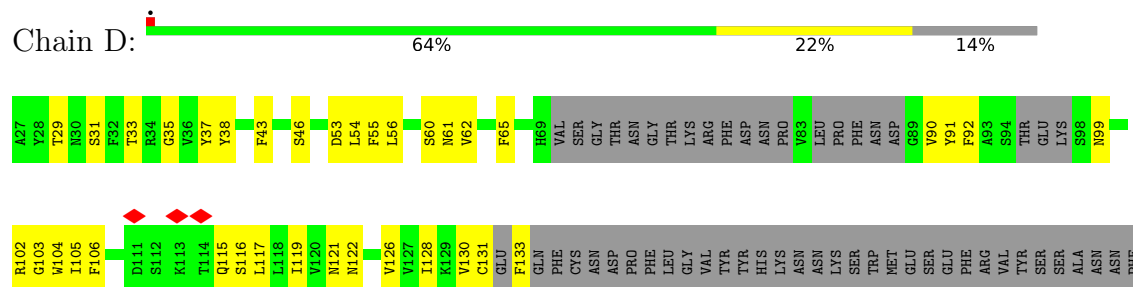
• Molecule 1: Spike glycoprotein



• Molecule 1: Spike glycoprotein



• Molecule 1: Spike glycoprotein



E990	T167	T169	T170	Q173	PRO	PHE	LEU	MET	ASP	LEU	GLU	GLY	LYS	GLN	GLY	ASN	PHE	K187	N188	L189	R190	E191	F192	V193	F194	LYS	ASN	ILE	ASP	GLY	TYR	F201	K202	I203	Y204	S205	K206	H207	T208	P209	ILE	ASN	LEU	VAL	ARG	D215	Q218	G219	T220	S221	A222	L223	E224	PRO	LEU	V227	D228
Y991	I231	G232	I233	N234	I235	THR	ARG	PHE	GLN	THR	LEU	LEU	ALA	LEU	HIS	ARG	SER	TYR	LEU	THR	PRO	GLY	ASP	SER	SER	SER	GLY	TRP	THR	ALA	GLY	ALA	A264	Y265	Y266	Y267	G268	Y269	L270	Q271	F272	R273	K278	Y279	N280	E281	N282	G283	T284	I285	T286	D287	D290	S297			
Y992	L303	T307	V308	E309	K310	N317	PHE	ARG	GLN	VAL	GLN	PRO	T323	E324	S325	I326	V327	R328	I332	P337	E340	A344	T345	R346	F347	N354	R355	K356	R357	I358	V362	A363	L368	F377	S383	C391	F392	T393	N394	V395	Y396	A397	D398	P426	G431	C432	V433										
Y993	N440	L441	D442	S443	K444	VAL	GLY	G447	R457	K458	S459	K462	P463	F464	E465	R466	D467	I472	Y473	Q474	C480	E484	P491	R509	V510	V511	V512	L513	S514	F515	L518	H519	A520	P521	A522	T523	V524	K529	S530	T531	V534	V539	F543	L546	L552												
Y994	T553	K558	F559	L560	Q563	Q564	F565	I569	R577	Q580	L585	D586	L587	T588	G593	G594	V595	P600	G601	T602	S605	N606	Q607	V608	Y612	Y621	VAL	ALA	ILE	HIS	ALA	D627	Q628	L629	T630	P631	T632	W633	R634	S659	Y660	E661	C662	C671	T676	GLN											
Y995	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
T996	GLY	PHE	ILE	LYS	PRO	GLN	TYR	GLY	ASP	CYS	GLY	ASP	ILE	ALA	ARG	D848	C851	F855	S884	T887	L894	Q895	I896	P897	Y904	R905	F906	V911	N914	V915	L916	I923	F927	A930	I934	L945	G971	A972	I973	D979	D985	A989															
L1012	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
R1019	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
D1041	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
L1049	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
M1050	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
Q1054	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
V1061	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
V1065	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
T1076	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
T1077	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
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T1081	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
C1082	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
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K1086	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
A1087	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
H1088	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
F1089	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
P1090	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
V1094	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
F1095	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
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S1097	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
V1122	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
S1123	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
V1129	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
I1132	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
N1135	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704	Y707	S708	N709	N710	S711	P715	I720	S721	V722	I726	L752	I770	Q774	N777	P792	P793	I794	K795	D796	N801	F802	I805	E819	V826	T827	LEU	ALA	ASP	ALA													
T1136	THR	ASN	SER	PRO	ARG	ARG	ALA	ARG	VAL	ALA	S689	Q690	S698	N703	L704																																										

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66436	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)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.723	Depositor
Minimum map value	-0.954	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.175	Depositor
Map size (Å)	310.40002, 310.40002, 310.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9700001, 0.9700001, 0.9700001	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.35	0/7698	0.49	0/10466
1	B	0.35	0/7698	0.49	0/10466
1	D	0.35	0/7698	0.49	0/10466
All	All	0.35	0/23094	0.49	0/31398

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	7538	0	7342	185	0
1	B	7538	0	7342	189	0
1	D	7538	0	7342	190	0
2	A	126	0	117	1	0
2	B	126	0	117	1	0
2	D	126	0	117	1	0
3	A	22	0	27	5	0
3	B	22	0	27	7	0
3	D	22	0	27	9	0
All	All	23058	0	22458	530	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 12.

All (530) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:368:LEU:HD23	3:D:1310:REA:H12	1.58	0.85
1:B:104:TRP:HE1	1:B:106:PHE:HE1	1.26	0.82
1:A:104:TRP:HE1	1:A:106:PHE:HE1	1.26	0.81
1:D:104:TRP:HE1	1:D:106:PHE:HE1	1.26	0.81
1:D:99:ASN:O	1:D:102:ARG:NH1	2.15	0.80
1:B:99:ASN:O	1:B:102:ARG:NH1	2.15	0.78
1:A:99:ASN:O	1:A:102:ARG:NH1	2.15	0.77
1:A:354:ASN:OD1	1:A:355:ARG:N	2.18	0.76
1:A:365:TYR:HB2	3:A:1310:REA:H10	1.67	0.76
1:B:354:ASN:OD1	1:B:355:ARG:N	2.18	0.75
1:D:354:ASN:OD1	1:D:355:ARG:N	2.18	0.74
1:B:365:TYR:HB2	3:B:1310:REA:H10	1.70	0.73
1:A:273:ARG:NH1	1:A:290:ASP:OD2	2.23	0.72
1:D:280:ASN:OD1	1:D:284:THR:N	2.23	0.71
1:D:273:ARG:NH1	1:D:290:ASP:OD2	2.23	0.71
1:B:273:ARG:NH1	1:B:290:ASP:OD2	2.23	0.71
1:B:280:ASN:OD1	1:B:284:THR:N	2.23	0.70
1:A:280:ASN:OD1	1:A:284:THR:N	2.23	0.70
1:B:1135:ASN:OD1	1:B:1136:THR:N	2.19	0.70
1:D:1135:ASN:OD1	1:D:1136:THR:N	2.19	0.70
1:D:206:LYS:HD2	1:D:223:LEU:HA	1.74	0.69
1:B:206:LYS:HD2	1:B:223:LEU:HA	1.74	0.69
1:B:116:SER:OG	1:B:130:VAL:O	2.12	0.68
1:A:398:ASP:HB2	1:A:512:VAL:HG22	1.76	0.68
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.76	0.68
1:A:206:LYS:HD2	1:A:223:LEU:HA	1.74	0.68
1:D:116:SER:OG	1:D:130:VAL:O	2.12	0.67
1:D:128:ILE:HB	1:D:170:TYR:HB3	1.77	0.67
1:D:398:ASP:HB2	1:D:512:VAL:HG22	1.76	0.67
1:A:116:SER:OG	1:A:130:VAL:O	2.12	0.67
1:A:628:GLN:HA	1:A:634:ARG:HD2	1.75	0.67
1:D:722:VAL:HG22	1:D:1065:VAL:HG22	1.76	0.67
1:B:128:ILE:HB	1:B:170:TYR:HB3	1.77	0.67
1:D:628:GLN:HA	1:D:634:ARG:HD2	1.75	0.67
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.19	0.67
1:B:104:TRP:NE1	1:B:106:PHE:HE1	1.93	0.67
1:B:628:GLN:HA	1:B:634:ARG:HD2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.76	0.67
1:A:826:VAL:HG22	1:A:945:LEU:HD13	1.77	0.66
1:B:826:VAL:HG22	1:B:945:LEU:HD13	1.77	0.66
1:B:398:ASP:HB2	1:B:512:VAL:HG22	1.76	0.66
1:A:128:ILE:HB	1:A:170:TYR:HB3	1.77	0.66
1:A:309:GLU:OE1	1:A:309:GLU:HA	1.96	0.66
1:B:309:GLU:HA	1:B:309:GLU:OE1	1.96	0.66
1:D:206:LYS:NZ	1:D:222:ALA:O	2.22	0.65
1:D:1129:VAL:HB	1:D:1132:ILE:HD11	1.78	0.65
1:A:104:TRP:NE1	1:A:106:PHE:HE1	1.93	0.65
1:D:826:VAL:HG22	1:D:945:LEU:HD13	1.77	0.65
1:B:560:LEU:HB2	1:B:563:GLN:HB2	1.78	0.65
1:B:1129:VAL:HB	1:B:1132:ILE:HD11	1.78	0.65
1:D:309:GLU:OE1	1:D:309:GLU:HA	1.96	0.65
1:D:104:TRP:NE1	1:D:106:PHE:HE1	1.93	0.65
1:D:324:GLU:HG2	1:D:539:VAL:HG12	1.79	0.64
1:D:91:TYR:HB2	1:D:270:LEU:HG	1.80	0.64
1:A:91:TYR:HB2	1:A:270:LEU:HG	1.80	0.64
1:B:324:GLU:HG2	1:B:539:VAL:HG12	1.79	0.64
1:D:560:LEU:HB2	1:D:563:GLN:HB2	1.78	0.64
1:A:1129:VAL:HB	1:A:1132:ILE:HD11	1.78	0.64
1:A:324:GLU:HG2	1:A:539:VAL:HG12	1.79	0.64
1:A:202:LYS:NZ	1:A:228:ASP:OD2	2.31	0.63
1:A:560:LEU:HB2	1:A:563:GLN:HB2	1.78	0.63
1:B:91:TYR:HB2	1:B:270:LEU:HG	1.80	0.63
1:A:369:TYR:HD2	3:A:1310:REA:H14	1.62	0.63
1:A:513:LEU:HD12	3:A:1310:REA:H163	1.80	0.63
1:D:202:LYS:NZ	1:D:228:ASP:OD2	2.31	0.62
1:B:202:LYS:NZ	1:B:228:ASP:OD2	2.31	0.62
1:A:327:VAL:H	1:A:531:THR:HG22	1.65	0.61
1:D:327:VAL:H	1:D:531:THR:HG22	1.65	0.61
1:B:46:SER:N	1:B:280:ASN:O	2.33	0.61
1:A:1076:THR:OG1	1:A:1097:SER:OG	2.18	0.61
1:D:393:THR:HG21	1:D:519:HIS:HB3	1.82	0.61
1:A:393:THR:HG21	1:A:519:HIS:HB3	1.82	0.61
1:B:327:VAL:H	1:B:531:THR:HG22	1.65	0.61
1:A:31:SER:HB2	1:A:60:SER:H	1.65	0.61
1:B:31:SER:HB2	1:B:60:SER:H	1.64	0.60
1:D:31:SER:HB2	1:D:60:SER:H	1.65	0.60
1:B:365:TYR:CD1	3:B:1310:REA:H10	2.36	0.60
1:B:369:TYR:CD2	3:B:1310:REA:H14	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1076:THR:OG1	1:B:1097:SER:OG	2.18	0.60
1:D:1086:LYS:HD3	1:D:1122:VAL:HG11	1.84	0.60
1:A:369:TYR:CD2	3:A:1310:REA:H14	2.36	0.60
1:A:659:SER:HB3	1:A:698:SER:HB3	1.83	0.60
1:B:393:THR:HG21	1:B:519:HIS:HB3	1.82	0.60
1:D:46:SER:N	1:D:280:ASN:O	2.33	0.60
1:D:795:LYS:HZ2	1:D:801:ASN:HA	1.67	0.60
1:D:1076:THR:OG1	1:D:1097:SER:OG	2.18	0.60
1:D:659:SER:HB3	1:D:698:SER:HB3	1.83	0.60
1:B:369:TYR:HD2	3:B:1310:REA:H14	1.67	0.59
1:B:1086:LYS:HD3	1:B:1122:VAL:HG11	1.84	0.59
1:B:795:LYS:HZ2	1:B:801:ASN:HA	1.67	0.59
1:A:795:LYS:HZ2	1:A:801:ASN:HA	1.68	0.59
1:A:46:SER:N	1:A:280:ASN:O	2.33	0.59
1:B:168:PHE:CE2	1:B:170:TYR:HB2	2.38	0.59
1:B:659:SER:HB3	1:B:698:SER:HB3	1.83	0.59
1:A:168:PHE:CE2	1:A:170:TYR:HB2	2.38	0.59
1:D:168:PHE:CE2	1:D:170:TYR:HB2	2.37	0.59
1:A:1086:LYS:HD3	1:A:1122:VAL:HG11	1.84	0.58
1:A:317:ASN:HB3	1:A:593:GLY:HA2	1.85	0.58
1:B:317:ASN:HB3	1:B:593:GLY:HA2	1.85	0.58
1:D:303:LEU:HD12	1:D:308:VAL:HG12	1.86	0.58
1:A:303:LEU:HD12	1:A:308:VAL:HG12	1.86	0.58
1:A:630:THR:HG23	1:A:633:TRP:HB2	1.86	0.58
1:B:630:THR:HG23	1:B:633:TRP:HB2	1.86	0.58
1:D:53:ASP:OD1	1:D:54:LEU:N	2.34	0.58
1:A:676:THR:HA	1:A:690:GLN:HA	1.86	0.58
1:B:303:LEU:HD12	1:B:308:VAL:HG12	1.85	0.58
1:B:387:LEU:HD22	3:B:1310:REA:H171	1.86	0.58
1:A:280:ASN:OD1	1:A:283:GLY:N	2.37	0.58
1:A:563:GLN:O	1:A:577:ARG:NH1	2.37	0.58
1:B:563:GLN:O	1:B:577:ARG:NH1	2.37	0.57
1:D:630:THR:HG23	1:D:633:TRP:HB2	1.86	0.57
1:A:1081:ILE:HD11	1:A:1135:ASN:HB3	1.87	0.57
1:B:280:ASN:OD1	1:B:283:GLY:N	2.37	0.57
1:B:365:TYR:CB	3:B:1310:REA:H10	2.35	0.57
1:D:280:ASN:OD1	1:D:283:GLY:N	2.37	0.57
1:D:317:ASN:HB3	1:D:593:GLY:HA2	1.85	0.57
1:A:104:TRP:NE1	1:A:106:PHE:CE1	2.72	0.57
1:D:104:TRP:NE1	1:D:106:PHE:CE1	2.72	0.57
1:D:474:GLN:NE2	1:D:480:CYS:H	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:563:GLN:O	1:D:577:ARG:NH1	2.37	0.57
1:D:676:THR:HA	1:D:690:GLN:HA	1.86	0.57
1:A:474:GLN:NE2	1:A:480:CYS:H	2.03	0.56
1:D:332:ILE:HB	1:D:362:VAL:HG13	1.87	0.56
1:B:676:THR:HA	1:B:690:GLN:HA	1.86	0.56
1:A:326:ILE:HD11	1:A:534:VAL:HG22	1.88	0.56
1:D:363:ALA:CB	3:D:1310:REA:H183	2.35	0.56
1:A:431:GLY:HA2	1:A:515:PHE:CE1	2.40	0.56
1:B:53:ASP:OD1	1:B:54:LEU:N	2.34	0.56
1:B:431:GLY:HA2	1:B:515:PHE:CE1	2.40	0.56
1:D:752:LEU:HD11	1:D:990:GLU:HG3	1.88	0.56
1:B:271:GLN:N	1:B:271:GLN:OE1	2.39	0.56
1:B:474:GLN:NE2	1:B:480:CYS:H	2.03	0.56
1:D:431:GLY:HA2	1:D:515:PHE:CE1	2.40	0.56
1:A:332:ILE:HB	1:A:362:VAL:HG13	1.87	0.56
1:A:513:LEU:CD1	3:A:1310:REA:H163	2.36	0.56
1:D:795:LYS:NZ	1:D:801:ASN:HA	2.21	0.56
1:A:752:LEU:HD11	1:A:990:GLU:HG3	1.88	0.55
1:B:332:ILE:HB	1:B:362:VAL:HG13	1.87	0.55
1:B:752:LEU:HD11	1:B:990:GLU:HG3	1.88	0.55
1:D:271:GLN:OE1	1:D:271:GLN:N	2.39	0.55
1:B:206:LYS:NZ	1:B:222:ALA:O	2.22	0.55
1:B:795:LYS:NZ	1:B:801:ASN:HA	2.21	0.55
1:B:326:ILE:HD11	1:B:534:VAL:HG22	1.88	0.55
1:A:795:LYS:NZ	1:A:801:ASN:HA	2.21	0.55
1:A:271:GLN:OE1	1:A:271:GLN:N	2.39	0.55
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	1.89	0.55
1:B:38:TYR:OH	1:B:284:THR:HA	2.07	0.55
1:D:1081:ILE:HD11	1:D:1135:ASN:HB3	1.87	0.55
1:A:529:LYS:HG2	1:A:530:SER:H	1.72	0.55
1:B:104:TRP:NE1	1:B:106:PHE:CE1	2.72	0.55
1:B:1081:ILE:HD11	1:B:1135:ASN:HB3	1.87	0.55
1:D:38:TYR:OH	1:D:284:THR:HA	2.07	0.55
1:A:31:SER:N	1:A:60:SER:O	2.37	0.54
1:D:529:LYS:HG2	1:D:530:SER:H	1.72	0.54
1:A:707:TYR:HB3	1:B:792:PRO:HG3	1.89	0.54
1:D:326:ILE:HD11	1:D:534:VAL:HG22	1.88	0.54
1:A:395:VAL:HG12	1:A:515:PHE:HB3	1.89	0.54
1:D:328:ARG:NH1	1:D:580:GLN:HB2	2.23	0.54
1:D:395:VAL:HG12	1:D:515:PHE:HB3	1.89	0.54
1:A:328:ARG:NH1	1:A:580:GLN:HB2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:ILE:HD12	1:A:923:ILE:HG23	1.89	0.54
1:A:792:PRO:HG3	1:D:707:TYR:HB3	1.88	0.54
1:B:29:THR:O	1:B:61:ASN:HA	2.08	0.54
1:B:529:LYS:HG2	1:B:530:SER:H	1.72	0.54
1:B:131:CYS:O	1:B:133:PHE:N	2.41	0.54
1:D:33:THR:HG21	1:D:218:GLN:HA	1.90	0.54
1:A:38:TYR:OH	1:A:284:THR:HA	2.07	0.54
1:B:707:TYR:HB3	1:D:792:PRO:HG3	1.88	0.54
1:B:851:CYS:O	1:B:855:PHE:HD2	1.90	0.54
1:D:31:SER:N	1:D:60:SER:O	2.37	0.54
1:D:377:PHE:HE1	3:D:1310:REA:H192	1.73	0.54
1:D:770:ILE:HD11	1:D:1012:LEU:HD23	1.89	0.54
1:B:395:VAL:HG12	1:B:515:PHE:HB3	1.89	0.54
1:D:851:CYS:O	1:D:855:PHE:HD2	1.90	0.54
1:A:33:THR:HG21	1:A:218:GLN:HA	1.90	0.53
1:A:271:GLN:HG2	1:A:273:ARG:HD3	1.90	0.53
1:D:29:THR:O	1:D:61:ASN:HA	2.08	0.53
1:B:271:GLN:HG2	1:B:273:ARG:HD3	1.90	0.53
1:B:770:ILE:HD11	1:B:1012:LEU:HD23	1.89	0.53
1:A:131:CYS:O	1:A:133:PHE:N	2.41	0.53
1:A:552:LEU:HD13	1:A:585:LEU:HD23	1.91	0.53
1:B:31:SER:N	1:B:60:SER:O	2.38	0.53
1:B:720:ILE:HD12	1:B:923:ILE:HG23	1.89	0.53
1:D:271:GLN:HG2	1:D:273:ARG:HD3	1.90	0.53
1:B:92:PHE:HB3	1:B:192:PHE:O	2.08	0.53
1:A:92:PHE:HB3	1:A:192:PHE:O	2.08	0.53
1:D:131:CYS:O	1:D:133:PHE:N	2.41	0.53
1:A:851:CYS:O	1:A:855:PHE:HD2	1.90	0.53
1:B:33:THR:HG21	1:B:218:GLN:HA	1.90	0.53
1:D:552:LEU:HD13	1:D:585:LEU:HD23	1.91	0.53
1:A:29:THR:O	1:A:61:ASN:HA	2.08	0.53
1:D:720:ILE:HD12	1:D:923:ILE:HG23	1.89	0.53
1:B:328:ARG:NH1	1:B:580:GLN:HB2	2.23	0.52
1:A:281:GLU:OE1	1:A:281:GLU:N	2.38	0.52
1:A:206:LYS:NZ	1:A:222:ALA:O	2.22	0.52
1:D:38:TYR:N	1:D:223:LEU:O	2.30	0.52
1:D:92:PHE:HB3	1:D:192:PHE:O	2.08	0.52
1:D:462:LYS:HB2	1:D:465:GLU:HG3	1.92	0.52
1:A:53:ASP:OD1	1:A:54:LEU:N	2.34	0.52
1:A:231:ILE:HG13	1:A:232:GLY:N	2.25	0.52
1:B:191:GLU:HB3	1:B:193:VAL:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:LEU:HD13	1:B:585:LEU:HD23	1.91	0.52
1:D:191:GLU:HB3	1:D:193:VAL:HG23	1.91	0.52
1:B:231:ILE:HG13	1:B:232:GLY:N	2.25	0.52
1:A:191:GLU:HB3	1:A:193:VAL:HG23	1.91	0.51
1:B:462:LYS:HB2	1:B:465:GLU:HG3	1.92	0.51
1:B:457:ARG:HG2	1:B:459:SER:H	1.75	0.51
1:D:457:ARG:HG2	1:D:459:SER:H	1.75	0.51
1:D:802:PHE:HD1	1:D:805:ILE:HD11	1.76	0.51
1:B:802:PHE:HD1	1:B:805:ILE:HD11	1.76	0.51
1:D:90:VAL:O	1:D:194:PHE:HB2	2.11	0.51
1:D:231:ILE:HG13	1:D:232:GLY:N	2.25	0.51
1:B:906:PHE:HE1	1:B:1049:LEU:HD11	1.76	0.51
1:A:457:ARG:HG2	1:A:459:SER:H	1.75	0.51
1:A:802:PHE:HD1	1:A:805:ILE:HD11	1.76	0.51
1:D:484:GLU:N	1:D:484:GLU:OE1	2.44	0.51
1:A:520:ALA:HB3	1:A:521:PRO:HD3	1.92	0.51
1:B:281:GLU:OE1	1:B:281:GLU:N	2.38	0.51
1:A:90:VAL:O	1:A:194:PHE:HB2	2.11	0.51
1:A:307:THR:HA	1:A:602:THR:HG21	1.93	0.51
1:A:462:LYS:HB2	1:A:465:GLU:HG3	1.92	0.51
1:B:391:CYS:HB3	1:B:522:ALA:HB1	1.93	0.50
1:D:307:THR:HA	1:D:602:THR:HG21	1.93	0.50
1:D:520:ALA:HB3	1:D:521:PRO:HD3	1.92	0.50
1:B:90:VAL:O	1:B:194:PHE:HB2	2.11	0.50
1:B:563:GLN:HG2	1:D:43:PHE:HD1	1.76	0.50
1:A:38:TYR:N	1:A:223:LEU:O	2.30	0.50
1:A:906:PHE:HE1	1:A:1049:LEU:HD11	1.76	0.50
1:B:989:ALA:O	1:B:993:ILE:HG12	2.12	0.50
1:D:726:ILE:HD12	1:D:1061:VAL:HG22	1.93	0.50
1:B:307:THR:HA	1:B:602:THR:HG21	1.93	0.50
1:B:726:ILE:HD12	1:B:1061:VAL:HG22	1.93	0.50
1:D:457:ARG:NH2	1:D:467:ASP:OD2	2.38	0.50
1:A:588:THR:HG23	1:B:855:PHE:HE1	1.77	0.50
1:B:971:GLY:O	1:B:995:ARG:NH2	2.45	0.50
1:D:989:ALA:O	1:D:993:ILE:HG12	2.12	0.50
1:B:91:TYR:HB3	1:B:268:GLY:C	2.32	0.50
1:A:91:TYR:HB3	1:A:268:GLY:C	2.32	0.49
1:A:391:CYS:HB3	1:A:522:ALA:HB1	1.93	0.49
1:A:989:ALA:O	1:A:993:ILE:HG12	2.12	0.49
1:B:472:ILE:HA	1:B:491:PRO:HD3	1.94	0.49
1:B:484:GLU:OE1	1:B:484:GLU:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:906:PHE:HE1	1:D:1049:LEU:HD11	1.76	0.49
1:A:43:PHE:HD1	1:D:563:GLN:HG2	1.76	0.49
1:A:971:GLY:O	1:A:995:ARG:NH2	2.45	0.49
1:A:472:ILE:HA	1:A:491:PRO:HD3	1.94	0.49
1:A:484:GLU:N	1:A:484:GLU:OE1	2.43	0.49
1:B:121:ASN:HA	1:B:126:VAL:HG12	1.95	0.49
1:B:457:ARG:NH2	1:B:467:ASP:OD2	2.38	0.49
1:A:121:ASN:HA	1:A:126:VAL:HG12	1.95	0.49
1:A:563:GLN:HG2	1:B:43:PHE:HD1	1.76	0.49
1:D:91:TYR:HB3	1:D:268:GLY:C	2.32	0.49
1:D:391:CYS:HB3	1:D:522:ALA:HB1	1.93	0.49
1:A:726:ILE:HD12	1:A:1061:VAL:HG22	1.93	0.49
1:A:855:PHE:HE1	1:D:588:THR:HG23	1.77	0.49
1:B:520:ALA:HB3	1:B:521:PRO:HD3	1.92	0.49
1:B:770:ILE:O	1:B:774:GLN:HG2	2.13	0.49
1:D:971:GLY:O	1:D:995:ARG:NH2	2.45	0.49
1:A:189:LEU:HD11	1:A:266:TYR:HB2	1.95	0.49
1:B:441:LEU:HD22	1:B:509:ARG:NH2	2.28	0.49
1:B:558:LYS:NZ	2:D:1303:NAG:O5	2.46	0.49
1:D:441:LEU:HD22	1:D:509:ARG:NH2	2.28	0.49
1:A:441:LEU:HD22	1:A:509:ARG:NH2	2.28	0.48
1:B:588:THR:HG23	1:D:855:PHE:HE1	1.77	0.48
1:D:472:ILE:HA	1:D:491:PRO:HD3	1.94	0.48
1:B:193:VAL:O	1:B:204:TYR:N	2.31	0.48
1:D:121:ASN:HA	1:D:126:VAL:HG12	1.95	0.48
1:D:193:VAL:O	1:D:204:TYR:N	2.32	0.48
1:B:121:ASN:OD1	1:B:122:ASN:N	2.43	0.48
1:B:703:ASN:OD1	1:B:704:SER:N	2.47	0.48
1:B:715:PRO:HD3	1:D:894:LEU:HD13	1.95	0.48
1:D:189:LEU:HD11	1:D:266:TYR:HB2	1.95	0.48
1:D:770:ILE:O	1:D:774:GLN:HG2	2.13	0.48
1:A:715:PRO:HD3	1:B:894:LEU:HD13	1.95	0.48
1:A:770:ILE:O	1:A:774:GLN:HG2	2.13	0.48
2:A:1303:NAG:O5	1:D:558:LYS:NZ	2.46	0.48
1:B:189:LEU:HD11	1:B:266:TYR:HB2	1.95	0.48
1:A:563:GLN:NE2	1:B:43:PHE:HA	2.29	0.48
1:A:310:LYS:NZ	1:A:663:ASP:OD2	2.28	0.48
1:D:703:ASN:OD1	1:D:704:SER:N	2.47	0.48
1:D:794:ILE:HG13	1:D:796:ASP:H	1.79	0.48
1:A:115:GLN:OE1	1:A:115:GLN:N	2.46	0.47
1:A:894:LEU:HD13	1:D:715:PRO:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:GLN:NE2	1:D:43:PHE:HA	2.29	0.47
1:D:927:PHE:HE1	1:D:1065:VAL:HG21	1.79	0.47
1:A:43:PHE:HA	1:D:563:GLN:NE2	2.29	0.47
1:A:927:PHE:HE1	1:A:1065:VAL:HG21	1.79	0.47
1:B:927:PHE:HE1	1:B:1065:VAL:HG21	1.79	0.47
1:A:565:PHE:O	1:B:43:PHE:N	2.32	0.47
1:D:513:LEU:HD13	3:D:1310:REA:H31	1.96	0.47
1:A:344:ALA:HB3	1:A:347:PHE:HE1	1.80	0.47
1:A:703:ASN:OD1	1:A:704:SER:N	2.47	0.47
1:B:38:TYR:N	1:B:223:LEU:O	2.30	0.47
1:B:553:THR:HG23	1:B:586:ASP:HB2	1.97	0.47
1:B:662:CYS:HB2	1:B:671:CYS:HB3	1.60	0.47
1:D:90:VAL:HB	1:D:194:PHE:HD2	1.79	0.47
1:A:457:ARG:NH2	1:A:467:ASP:OD2	2.38	0.47
1:A:794:ILE:HG13	1:A:796:ASP:H	1.79	0.47
1:A:795:LYS:NZ	1:A:801:ASN:OD1	2.42	0.47
1:B:65:PHE:HB2	1:B:265:TYR:CD2	2.50	0.47
1:B:794:ILE:HG13	1:B:796:ASP:H	1.79	0.47
1:B:357:ARG:HH21	1:B:396:TYR:HE2	1.62	0.46
1:D:121:ASN:OD1	1:D:122:ASN:N	2.43	0.46
1:D:440:ASN:OD1	1:D:441:LEU:N	2.48	0.46
1:D:631:PRO:HA	1:D:634:ARG:HB2	1.97	0.46
1:B:90:VAL:HB	1:B:194:PHE:HD2	1.79	0.46
1:B:440:ASN:OD1	1:B:441:LEU:N	2.48	0.46
1:D:344:ALA:HB3	1:D:347:PHE:HE1	1.79	0.46
1:A:65:PHE:HB2	1:A:265:TYR:CD2	2.51	0.46
1:A:90:VAL:HB	1:A:194:PHE:HD2	1.79	0.46
1:A:440:ASN:OD1	1:A:441:LEU:N	2.48	0.46
1:A:777:ASN:OD1	1:A:1019:ARG:NH1	2.46	0.46
1:D:105:ILE:HG13	1:D:117:LEU:O	2.15	0.46
1:D:546:LEU:HD21	1:D:565:PHE:HE2	1.81	0.46
1:D:553:THR:HG23	1:D:586:ASP:HB2	1.97	0.46
1:A:631:PRO:HA	1:A:634:ARG:HB2	1.97	0.46
1:B:206:LYS:HB3	1:B:224:GLU:H	1.81	0.46
1:D:190:ARG:HA	1:D:207:HIS:HB2	1.98	0.46
1:B:631:PRO:HA	1:B:634:ARG:HB2	1.97	0.46
1:D:206:LYS:HB3	1:D:224:GLU:H	1.81	0.46
1:A:310:LYS:HG2	1:A:600:PRO:HA	1.98	0.46
1:A:546:LEU:HD21	1:A:565:PHE:HE2	1.81	0.46
1:B:546:LEU:HD21	1:B:565:PHE:HE2	1.81	0.46
1:B:534:VAL:HG21	1:B:539:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:PHE:HB2	1:D:265:TYR:CD2	2.50	0.46
1:A:105:ILE:HG13	1:A:117:LEU:O	2.15	0.46
1:A:392:PHE:HB2	1:A:524:VAL:HG13	1.98	0.46
1:A:534:VAL:HG21	1:A:539:VAL:HG11	1.98	0.46
1:A:558:LYS:NZ	2:B:1303:NAG:O5	2.46	0.46
1:B:344:ALA:HB3	1:B:347:PHE:HE1	1.80	0.46
1:B:569:ILE:HD12	1:B:569:ILE:H	1.81	0.46
1:D:569:ILE:HD12	1:D:569:ILE:H	1.81	0.46
1:A:553:THR:HG23	1:A:586:ASP:HB2	1.97	0.46
1:D:103:GLY:HA3	1:D:119:ILE:O	2.17	0.46
1:D:267:VAL:HG12	1:D:268:GLY:N	2.31	0.46
1:D:534:VAL:HG21	1:D:539:VAL:HG11	1.98	0.46
1:A:35:GLY:HA2	1:A:56:LEU:HB3	1.98	0.45
1:B:105:ILE:HG13	1:B:117:LEU:O	2.15	0.45
1:B:310:LYS:HG2	1:B:600:PRO:HA	1.98	0.45
1:B:392:PHE:HB2	1:B:524:VAL:HG13	1.98	0.45
1:A:345:THR:O	1:A:346:ARG:HD3	2.17	0.45
1:D:363:ALA:HB1	3:D:1310:REA:H183	1.97	0.45
1:D:595:VAL:HG12	1:D:612:TYR:CD1	2.52	0.45
1:A:569:ILE:HD12	1:A:569:ILE:H	1.81	0.45
1:B:802:PHE:CD1	1:B:805:ILE:HD11	2.52	0.45
1:D:363:ALA:HB3	3:D:1310:REA:H183	1.97	0.45
1:D:1077:THR:OG1	1:D:1078:ALA:N	2.49	0.45
1:B:190:ARG:HA	1:B:207:HIS:HB2	1.97	0.45
1:D:37:TYR:HA	1:D:223:LEU:H	1.82	0.45
1:D:310:LYS:HG2	1:D:600:PRO:HA	1.98	0.45
1:A:708:SER:HB3	1:A:711:SER:HB3	1.98	0.45
1:A:906:PHE:CD2	1:A:916:LEU:HB2	2.52	0.45
1:B:115:GLN:OE1	1:B:115:GLN:N	2.46	0.45
1:D:357:ARG:HH21	1:D:396:TYR:HE2	1.62	0.45
1:A:103:GLY:HA3	1:A:119:ILE:O	2.17	0.45
1:A:190:ARG:HA	1:A:207:HIS:HB2	1.98	0.45
1:B:267:VAL:HG12	1:B:268:GLY:N	2.31	0.45
1:B:1077:THR:OG1	1:B:1078:ALA:N	2.50	0.45
1:A:206:LYS:HB3	1:A:224:GLU:H	1.81	0.45
1:B:345:THR:O	1:B:346:ARG:HD3	2.17	0.45
1:B:777:ASN:OD1	1:B:1019:ARG:NH1	2.46	0.45
1:D:884:SER:HG	1:D:887:THR:HG1	1.63	0.45
1:D:906:PHE:CD2	1:D:916:LEU:HB2	2.52	0.45
1:A:595:VAL:HG12	1:A:612:TYR:CD1	2.52	0.45
1:A:802:PHE:CD1	1:A:805:ILE:HD11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:VAL:HG12	1:A:268:GLY:N	2.31	0.45
1:A:1090:PRO:HG3	1:A:1095:PHE:CE2	2.52	0.45
1:B:358:ILE:HB	1:B:395:VAL:HG23	1.99	0.45
1:B:595:VAL:HG12	1:B:612:TYR:CD1	2.52	0.45
1:D:35:GLY:HA2	1:D:56:LEU:HB3	1.98	0.45
1:B:393:THR:HG21	1:B:519:HIS:CB	2.48	0.44
1:B:433:VAL:HG13	1:B:512:VAL:HG12	1.99	0.44
1:B:906:PHE:CD2	1:B:916:LEU:HB2	2.52	0.44
1:D:392:PHE:HB2	1:D:524:VAL:HG13	1.98	0.44
1:A:37:TYR:HA	1:A:223:LEU:H	1.82	0.44
1:A:358:ILE:HB	1:A:395:VAL:HG23	2.00	0.44
1:B:35:GLY:HA2	1:B:56:LEU:HB3	1.98	0.44
1:B:1090:PRO:HG3	1:B:1095:PHE:CE2	2.52	0.44
1:D:433:VAL:HG13	1:D:512:VAL:HG12	2.00	0.44
1:D:802:PHE:CD1	1:D:805:ILE:HD11	2.52	0.44
1:B:708:SER:HB3	1:B:711:SER:HB3	1.99	0.44
1:B:103:GLY:HA3	1:B:119:ILE:O	2.17	0.44
1:D:930:ALA:O	1:D:934:ILE:HG12	2.17	0.44
1:A:357:ARG:HH21	1:A:396:TYR:HE2	1.62	0.44
1:D:345:THR:O	1:D:346:ARG:HD3	2.17	0.44
1:A:1077:THR:OG1	1:A:1078:ALA:N	2.49	0.44
1:A:37:TYR:OH	1:A:54:LEU:O	2.20	0.44
1:A:90:VAL:HB	1:A:194:PHE:CD2	2.53	0.44
1:A:904:TYR:OH	1:D:1094:VAL:HG12	2.18	0.44
1:B:394:ASN:O	1:B:515:PHE:HA	2.18	0.44
1:B:930:ALA:O	1:B:934:ILE:HG12	2.18	0.44
1:D:397:ALA:HA	1:D:513:LEU:HD23	2.00	0.44
1:D:90:VAL:HB	1:D:194:PHE:CD2	2.53	0.44
1:B:37:TYR:HA	1:B:223:LEU:H	1.82	0.44
1:D:394:ASN:O	1:D:515:PHE:HA	2.18	0.44
1:D:1090:PRO:HG3	1:D:1095:PHE:CE2	2.52	0.44
1:A:433:VAL:HG13	1:A:512:VAL:HG12	2.00	0.43
1:A:605:SER:OG	1:A:606:ASN:N	2.51	0.43
1:D:358:ILE:HB	1:D:395:VAL:HG23	2.00	0.43
1:D:398:ASP:O	1:D:511:VAL:HA	2.18	0.43
1:D:1083:HIS:HB3	1:D:1088:HIS:CE1	2.53	0.43
1:A:116:SER:O	1:A:130:VAL:HG13	2.18	0.43
1:A:1083:HIS:HB3	1:A:1088:HIS:CE1	2.53	0.43
1:D:708:SER:HB3	1:D:711:SER:HB3	1.99	0.43
1:B:116:SER:O	1:B:130:VAL:HG13	2.18	0.43
1:B:1083:HIS:HB3	1:B:1088:HIS:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:SER:O	1:D:130:VAL:HG13	2.18	0.43
1:A:206:LYS:HB2	1:A:224:GLU:HB2	2.01	0.43
1:B:206:LYS:HB2	1:B:224:GLU:HB2	2.01	0.43
1:B:290:ASP:O	1:B:297:SER:HB3	2.18	0.43
1:D:106:PHE:HB3	1:D:235:ILE:HG23	2.01	0.43
1:D:115:GLN:OE1	1:D:115:GLN:N	2.46	0.43
1:D:194:PHE:HA	1:D:203:ILE:HA	2.00	0.43
1:D:290:ASP:O	1:D:297:SER:HB3	2.18	0.43
1:D:795:LYS:NZ	1:D:801:ASN:OD1	2.42	0.43
1:A:398:ASP:O	1:A:511:VAL:HA	2.18	0.43
1:A:1094:VAL:HG12	1:B:904:TYR:OH	2.18	0.43
1:B:90:VAL:HB	1:B:194:PHE:CD2	2.53	0.43
1:B:595:VAL:HG12	1:B:612:TYR:HD1	1.84	0.43
1:D:91:TYR:HD2	1:D:268:GLY:HA3	1.84	0.43
1:D:474:GLN:HE22	1:D:480:CYS:H	1.66	0.43
1:A:62:VAL:HG23	1:A:267:VAL:O	2.19	0.43
1:A:290:ASP:O	1:A:297:SER:HB3	2.18	0.43
1:A:397:ALA:HA	1:A:513:LEU:HD23	2.00	0.43
1:B:398:ASP:O	1:B:511:VAL:HA	2.18	0.43
1:D:206:LYS:HB2	1:D:224:GLU:HB2	2.01	0.43
1:D:281:GLU:OE1	1:D:281:GLU:N	2.38	0.43
1:D:605:SER:OG	1:D:606:ASN:N	2.51	0.43
1:A:194:PHE:HA	1:A:203:ILE:HA	2.00	0.43
1:A:344:ALA:HB3	1:A:347:PHE:CE1	2.54	0.43
1:B:397:ALA:HA	1:B:513:LEU:HD23	2.00	0.43
1:B:426:PRO:HB3	1:B:463:PRO:HB3	2.01	0.43
1:D:777:ASN:OD1	1:D:1019:ARG:NH1	2.46	0.43
1:A:930:ALA:O	1:A:934:ILE:HG12	2.17	0.42
1:B:62:VAL:HG23	1:B:267:VAL:O	2.19	0.42
1:B:91:TYR:HD2	1:B:268:GLY:HA3	1.84	0.42
1:B:605:SER:OG	1:B:606:ASN:N	2.51	0.42
1:D:906:PHE:HB3	1:D:911:VAL:HG23	2.02	0.42
1:A:595:VAL:HG12	1:A:612:TYR:HD1	1.84	0.42
1:D:62:VAL:HG23	1:D:267:VAL:O	2.19	0.42
1:D:377:PHE:HE1	3:D:1310:REA:C19	2.32	0.42
1:B:344:ALA:HB3	1:B:347:PHE:CE1	2.54	0.42
1:B:795:LYS:NZ	1:B:801:ASN:OD1	2.42	0.42
1:A:53:ASP:HB3	1:A:55:PHE:CE2	2.55	0.42
1:B:474:GLN:HE22	1:B:480:CYS:H	1.67	0.42
1:A:995:ARG:HA	1:A:998:THR:HG22	2.02	0.42
1:B:906:PHE:HB3	1:B:911:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:THR:HG21	1:A:519:HIS:CB	2.48	0.42
1:D:795:LYS:HD2	1:D:795:LYS:O	2.19	0.42
1:A:91:TYR:HD2	1:A:268:GLY:HA3	1.84	0.42
1:A:336:CYS:O	1:A:338:PHE:N	2.49	0.42
1:A:394:ASN:O	1:A:515:PHE:HA	2.18	0.42
1:A:662:CYS:HB2	1:A:671:CYS:HB3	1.60	0.42
1:A:1123:SER:CB	1:B:914:ASN:HD22	2.33	0.42
1:B:194:PHE:HA	1:B:203:ILE:HA	2.00	0.42
1:A:906:PHE:HB3	1:A:911:VAL:HG23	2.02	0.42
1:D:1049:LEU:HD23	1:D:1049:LEU:HA	1.88	0.42
1:A:193:VAL:O	1:A:204:TYR:N	2.31	0.42
1:A:220:PHE:CE2	1:A:285:ILE:HG22	2.55	0.42
1:A:426:PRO:HB3	1:A:463:PRO:HB3	2.01	0.42
1:A:474:GLN:HE22	1:A:480:CYS:H	1.66	0.42
1:B:106:PHE:HB3	1:B:235:ILE:HG23	2.01	0.42
1:B:996:LEU:HD23	1:B:996:LEU:HA	1.87	0.42
1:D:595:VAL:HG12	1:D:612:TYR:HD1	1.84	0.42
1:A:278:LYS:HD3	1:A:287:ASP:HB2	2.02	0.42
1:A:795:LYS:HD2	1:A:795:LYS:O	2.19	0.42
1:B:53:ASP:HB3	1:B:55:PHE:CE2	2.55	0.42
1:B:220:PHE:CE2	1:B:285:ILE:HG22	2.55	0.42
1:B:278:LYS:HD3	1:B:287:ASP:HB2	2.02	0.42
1:B:383:SER:OG	1:D:985:ASP:OD2	2.29	0.42
1:B:795:LYS:HD2	1:B:795:LYS:O	2.19	0.42
1:A:106:PHE:HB3	1:A:235:ILE:HG23	2.01	0.41
1:A:383:SER:OG	1:B:985:ASP:OD2	2.29	0.41
1:A:985:ASP:OD2	1:D:383:SER:OG	2.29	0.41
1:D:53:ASP:HB3	1:D:55:PHE:CE2	2.55	0.41
1:A:518:LEU:HD12	1:B:979:ASP:OD1	2.21	0.41
1:A:220:PHE:HE2	1:A:285:ILE:HG22	1.85	0.41
1:A:443:SER:O	1:A:444:LYS:HE2	2.21	0.41
1:B:1094:VAL:HG12	1:D:904:TYR:OH	2.19	0.41
1:D:220:PHE:HE2	1:D:285:ILE:HG22	1.85	0.41
1:D:278:LYS:HD3	1:D:287:ASP:HB2	2.02	0.41
1:D:344:ALA:HB3	1:D:347:PHE:CE1	2.54	0.41
1:D:443:SER:O	1:D:444:LYS:HE2	2.21	0.41
1:D:819:GLU:HG3	1:D:1054:GLN:OE1	2.21	0.41
1:A:709:ASN:ND2	1:B:796:ASP:OD2	2.54	0.41
1:B:220:PHE:HE2	1:B:285:ILE:HG22	1.85	0.41
1:B:627:ASP:O	1:B:634:ARG:NH2	2.54	0.41
1:D:426:PRO:HB3	1:D:463:PRO:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:543:PHE:HE2	1:D:552:LEU:HD11	1.86	0.41
1:D:606:ASN:O	1:D:608:VAL:HG13	2.21	0.41
1:D:995:ARG:HA	1:D:998:THR:HG22	2.02	0.41
1:B:365:TYR:CG	3:B:1310:REA:H10	2.56	0.41
1:B:709:ASN:ND2	1:D:796:ASP:OD2	2.54	0.41
1:D:973:ILE:HG12	1:D:992:GLN:OE1	2.21	0.41
1:A:606:ASN:O	1:A:608:VAL:HG13	2.20	0.41
1:A:796:ASP:OD2	1:D:709:ASN:ND2	2.53	0.41
1:A:1030:SER:OG	1:D:1041:ASP:HB3	2.21	0.41
1:D:337:PRO:HB3	1:D:340:GLU:HB3	2.03	0.41
1:D:393:THR:HG21	1:D:519:HIS:CB	2.48	0.41
1:D:896:ILE:HG13	1:D:897:PRO:HD2	2.03	0.41
1:A:896:ILE:HG13	1:A:897:PRO:HD2	2.03	0.41
1:A:979:ASP:OD1	1:D:518:LEU:HD12	2.21	0.41
1:B:37:TYR:OH	1:B:54:LEU:O	2.20	0.41
1:B:326:ILE:HD12	1:B:539:VAL:HG21	2.03	0.41
1:B:896:ILE:HG13	1:B:897:PRO:HD2	2.03	0.41
1:B:973:ILE:HG12	1:B:992:GLN:OE1	2.21	0.41
1:B:1123:SER:CB	1:D:914:ASN:HD22	2.33	0.41
1:D:363:ALA:HB1	3:D:1310:REA:C18	2.51	0.41
1:D:627:ASP:O	1:D:634:ARG:NH2	2.54	0.41
1:A:1041:ASP:HB3	1:B:1030:SER:OG	2.22	0.41
1:B:543:PHE:HE2	1:B:552:LEU:HD11	1.86	0.41
1:B:819:GLU:HG3	1:B:1054:GLN:OE1	2.21	0.41
1:D:220:PHE:CE2	1:D:285:ILE:HG22	2.55	0.41
1:A:121:ASN:OD1	1:A:122:ASN:N	2.43	0.40
1:A:326:ILE:HD12	1:A:539:VAL:HG21	2.03	0.40
1:A:627:ASP:O	1:A:634:ARG:NH2	2.54	0.40
1:A:914:ASN:HD22	1:D:1123:SER:CB	2.33	0.40
1:B:606:ASN:O	1:B:608:VAL:HG13	2.20	0.40
1:B:337:PRO:HB3	1:B:340:GLU:HB3	2.03	0.40
1:B:518:LEU:HD12	1:D:979:ASP:OD1	2.21	0.40
1:B:995:ARG:HA	1:B:998:THR:HG22	2.02	0.40
1:D:392:PHE:CZ	3:D:1310:REA:H173	2.56	0.40
1:D:326:ILE:HD12	1:D:539:VAL:HG21	2.03	0.40
1:D:662:CYS:HB2	1:D:671:CYS:HB3	1.60	0.40
1:A:57:PRO:HB2	1:A:60:SER:HB3	2.04	0.40
1:B:443:SER:O	1:B:444:LYS:HE2	2.21	0.40
1:B:1006:THR:O	1:B:1010:GLN:HG2	2.22	0.40
1:D:661:GLU:HG2	1:D:661:GLU:O	2.22	0.40
1:A:43:PHE:N	1:D:565:PHE:O	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:661:GLU:HG2	1:B:661:GLU:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	938/1121 (84%)	849 (90%)	89 (10%)	0	100	100
1	B	938/1121 (84%)	849 (90%)	89 (10%)	0	100	100
1	D	938/1121 (84%)	848 (90%)	90 (10%)	0	100	100
All	All	2814/3363 (84%)	2546 (90%)	268 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	841/972 (86%)	836 (99%)	5 (1%)	84	91
1	B	841/972 (86%)	836 (99%)	5 (1%)	84	91
1	D	841/972 (86%)	836 (99%)	5 (1%)	84	91
All	All	2523/2916 (86%)	2508 (99%)	15 (1%)	82	91

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	273	ARG
1	A	309	GLU
1	A	462	LYS
1	A	995	ARG
1	A	1050	MET
1	B	273	ARG
1	B	309	GLU
1	B	462	LYS
1	B	995	ARG
1	B	1050	MET
1	D	273	ARG
1	D	309	GLU
1	D	462	LYS
1	D	995	ARG
1	D	1050	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	474	GLN
1	B	474	GLN
1	D	474	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

30 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
2	NAG	D	1309	1	14,14,15	0.25	0	17,19,21	0.39	0
2	NAG	B	1305	1	14,14,15	0.18	0	17,19,21	0.44	0
3	REA	A	1310	-	22,22,22	2.66	5 (22%)	30,30,30	2.07	11 (36%)
2	NAG	B	1303	1	14,14,15	0.23	0	17,19,21	0.57	0
2	NAG	A	1309	1	14,14,15	0.25	0	17,19,21	0.39	0
2	NAG	B	1304	1	14,14,15	0.16	0	17,19,21	0.45	0
2	NAG	A	1307	1	14,14,15	0.29	0	17,19,21	0.47	0
2	NAG	B	1302	1	14,14,15	0.20	0	17,19,21	0.38	0
2	NAG	A	1305	1	14,14,15	0.18	0	17,19,21	0.45	0
2	NAG	A	1301	1	14,14,15	0.26	0	17,19,21	0.56	0
2	NAG	D	1303	1	14,14,15	0.23	0	17,19,21	0.56	0
2	NAG	D	1301	1	14,14,15	0.26	0	17,19,21	0.56	0
2	NAG	D	1306	1	14,14,15	0.20	0	17,19,21	0.47	0
2	NAG	A	1303	1	14,14,15	0.24	0	17,19,21	0.56	0
3	REA	D	1310	-	22,22,22	2.66	5 (22%)	30,30,30	2.07	11 (36%)
2	NAG	B	1306	1	14,14,15	0.21	0	17,19,21	0.46	0
2	NAG	A	1306	1	14,14,15	0.21	0	17,19,21	0.47	0
2	NAG	D	1308	1	14,14,15	0.24	0	17,19,21	0.44	0
3	REA	B	1310	-	22,22,22	2.67	5 (22%)	30,30,30	2.07	11 (36%)
2	NAG	B	1308	1	14,14,15	0.22	0	17,19,21	0.44	0
2	NAG	B	1309	1	14,14,15	0.25	0	17,19,21	0.39	0
2	NAG	B	1301	1	14,14,15	0.27	0	17,19,21	0.56	0
2	NAG	D	1302	1	14,14,15	0.19	0	17,19,21	0.37	0
2	NAG	D	1307	1	14,14,15	0.28	0	17,19,21	0.48	0
2	NAG	A	1302	1	14,14,15	0.20	0	17,19,21	0.38	0
2	NAG	B	1307	1	14,14,15	0.28	0	17,19,21	0.48	0
2	NAG	A	1304	1	14,14,15	0.16	0	17,19,21	0.45	0
2	NAG	D	1304	1	14,14,15	0.15	0	17,19,21	0.44	0
2	NAG	D	1305	1	14,14,15	0.17	0	17,19,21	0.45	0
2	NAG	A	1308	1	14,14,15	0.22	0	17,19,21	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1309	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
3	REA	A	1310	-	-	11/15/32/32	0/1/1/1
2	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1302	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
2	NAG	D	1303	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1301	1	-	1/6/23/26	0/1/1/1
2	NAG	D	1306	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
3	REA	D	1310	-	-	11/15/32/32	0/1/1/1
2	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
2	NAG	D	1308	1	-	2/6/23/26	0/1/1/1
3	REA	B	1310	-	-	11/15/32/32	0/1/1/1
2	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1309	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
2	NAG	D	1302	1	-	4/6/23/26	0/1/1/1
2	NAG	D	1307	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
2	NAG	D	1304	1	-	2/6/23/26	0/1/1/1
2	NAG	D	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1308	1	-	2/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1310	REA	C10-C9	8.37	1.46	1.35
3	A	1310	REA	C10-C9	8.35	1.46	1.35
3	D	1310	REA	C10-C9	8.35	1.46	1.35
3	D	1310	REA	C11-C12	5.08	1.47	1.34
3	A	1310	REA	C11-C12	5.08	1.47	1.34
3	B	1310	REA	C11-C12	5.07	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1310	REA	C8-C7	4.71	1.47	1.33
3	D	1310	REA	C8-C7	4.70	1.47	1.33
3	A	1310	REA	C8-C7	4.68	1.47	1.33
3	A	1310	REA	C14-C13	4.45	1.41	1.35
3	B	1310	REA	C14-C13	4.45	1.41	1.35
3	D	1310	REA	C14-C13	4.42	1.41	1.35
3	D	1310	REA	C5-C6	2.53	1.38	1.34
3	A	1310	REA	C5-C6	2.48	1.38	1.34
3	B	1310	REA	C5-C6	2.47	1.38	1.34

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1310	REA	C7-C8-C9	-4.06	120.11	126.23
3	A	1310	REA	C7-C8-C9	-4.03	120.14	126.23
3	D	1310	REA	C7-C8-C9	-4.02	120.16	126.23
3	D	1310	REA	C1-C6-C5	-3.92	117.10	122.61
3	B	1310	REA	C1-C6-C5	-3.91	117.10	122.61
3	A	1310	REA	C1-C6-C5	-3.91	117.11	122.61
3	B	1310	REA	C18-C5-C4	3.69	120.71	113.62
3	A	1310	REA	C18-C5-C4	3.69	120.70	113.62
3	D	1310	REA	C18-C5-C4	3.69	120.70	113.62
3	A	1310	REA	C18-C5-C6	-3.64	120.44	124.53
3	D	1310	REA	C18-C5-C6	-3.64	120.44	124.53
3	B	1310	REA	C18-C5-C6	-3.61	120.47	124.53
3	A	1310	REA	C3-C4-C5	-3.25	108.28	114.08
3	D	1310	REA	C3-C4-C5	-3.25	108.28	114.08
3	B	1310	REA	C3-C4-C5	-3.24	108.29	114.08
3	B	1310	REA	O2-C15-C14	3.18	123.36	113.50
3	D	1310	REA	O2-C15-C14	3.17	123.35	113.50
3	A	1310	REA	O2-C15-C14	3.17	123.33	113.50
3	B	1310	REA	C4-C5-C6	-2.71	118.80	122.73
3	B	1310	REA	C11-C10-C9	-2.69	123.47	127.31
3	A	1310	REA	C4-C5-C6	-2.68	118.84	122.73
3	D	1310	REA	C4-C5-C6	-2.68	118.84	122.73
3	A	1310	REA	C11-C10-C9	-2.68	123.49	127.31
3	D	1310	REA	C11-C10-C9	-2.68	123.49	127.31
3	A	1310	REA	C17-C1-C6	-2.59	106.09	110.30
3	D	1310	REA	C17-C1-C6	-2.58	106.11	110.30
3	B	1310	REA	C17-C1-C6	-2.57	106.13	110.30
3	B	1310	REA	O2-C15-O1	-2.49	117.49	122.67
3	D	1310	REA	O2-C15-O1	-2.49	117.49	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1310	REA	O2-C15-O1	-2.47	117.53	122.67
3	B	1310	REA	C8-C7-C6	-2.17	121.09	127.20
3	A	1310	REA	C8-C7-C6	-2.16	121.14	127.20
3	D	1310	REA	C8-C7-C6	-2.15	121.17	127.20

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1310	REA	C6-C7-C8-C9
3	A	1310	REA	C11-C10-C9-C8
3	A	1310	REA	C11-C10-C9-C19
3	A	1310	REA	C12-C13-C14-C15
3	A	1310	REA	C20-C13-C14-C15
3	B	1310	REA	C6-C7-C8-C9
3	B	1310	REA	C11-C10-C9-C8
3	B	1310	REA	C11-C10-C9-C19
3	B	1310	REA	C12-C13-C14-C15
3	B	1310	REA	C20-C13-C14-C15
3	D	1310	REA	C6-C7-C8-C9
3	D	1310	REA	C11-C10-C9-C8
3	D	1310	REA	C11-C10-C9-C19
3	D	1310	REA	C12-C13-C14-C15
3	D	1310	REA	C20-C13-C14-C15
2	A	1306	NAG	O5-C5-C6-O6
2	B	1306	NAG	O5-C5-C6-O6
2	D	1306	NAG	O5-C5-C6-O6
2	A	1308	NAG	C4-C5-C6-O6
2	B	1308	NAG	C4-C5-C6-O6
2	D	1308	NAG	C4-C5-C6-O6
2	A	1306	NAG	C4-C5-C6-O6
2	B	1306	NAG	C4-C5-C6-O6
2	D	1306	NAG	C4-C5-C6-O6
2	A	1302	NAG	C8-C7-N2-C2
2	A	1302	NAG	O7-C7-N2-C2
2	B	1302	NAG	C8-C7-N2-C2
2	B	1302	NAG	O7-C7-N2-C2
2	D	1302	NAG	C8-C7-N2-C2
2	D	1302	NAG	O7-C7-N2-C2
2	A	1302	NAG	O5-C5-C6-O6
2	B	1302	NAG	O5-C5-C6-O6
2	D	1302	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	1310	REA	C7-C8-C9-C19
3	B	1310	REA	C7-C8-C9-C19
3	D	1310	REA	C7-C8-C9-C19
3	A	1310	REA	C7-C8-C9-C10
3	B	1310	REA	C7-C8-C9-C10
3	D	1310	REA	C7-C8-C9-C10
3	A	1310	REA	C13-C14-C15-O2
3	B	1310	REA	C13-C14-C15-O2
3	D	1310	REA	C13-C14-C15-O2
2	A	1302	NAG	C4-C5-C6-O6
2	B	1302	NAG	C4-C5-C6-O6
2	D	1302	NAG	C4-C5-C6-O6
2	B	1308	NAG	O5-C5-C6-O6
2	D	1308	NAG	O5-C5-C6-O6
2	A	1308	NAG	O5-C5-C6-O6
2	A	1309	NAG	O5-C5-C6-O6
2	B	1309	NAG	O5-C5-C6-O6
2	D	1309	NAG	O5-C5-C6-O6
3	A	1310	REA	C11-C12-C13-C20
3	B	1310	REA	C11-C12-C13-C20
3	D	1310	REA	C11-C12-C13-C20
3	A	1310	REA	C13-C14-C15-O1
3	B	1310	REA	C13-C14-C15-O1
3	D	1310	REA	C13-C14-C15-O1
2	A	1304	NAG	C4-C5-C6-O6
2	B	1304	NAG	C4-C5-C6-O6
2	D	1304	NAG	C4-C5-C6-O6
2	B	1304	NAG	O5-C5-C6-O6
2	A	1304	NAG	O5-C5-C6-O6
2	D	1304	NAG	O5-C5-C6-O6
3	A	1310	REA	C11-C12-C13-C14
3	B	1310	REA	C11-C12-C13-C14
3	D	1310	REA	C11-C12-C13-C14
2	A	1301	NAG	C3-C2-N2-C7
2	B	1301	NAG	C3-C2-N2-C7
2	D	1301	NAG	C3-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 24 short contacts:

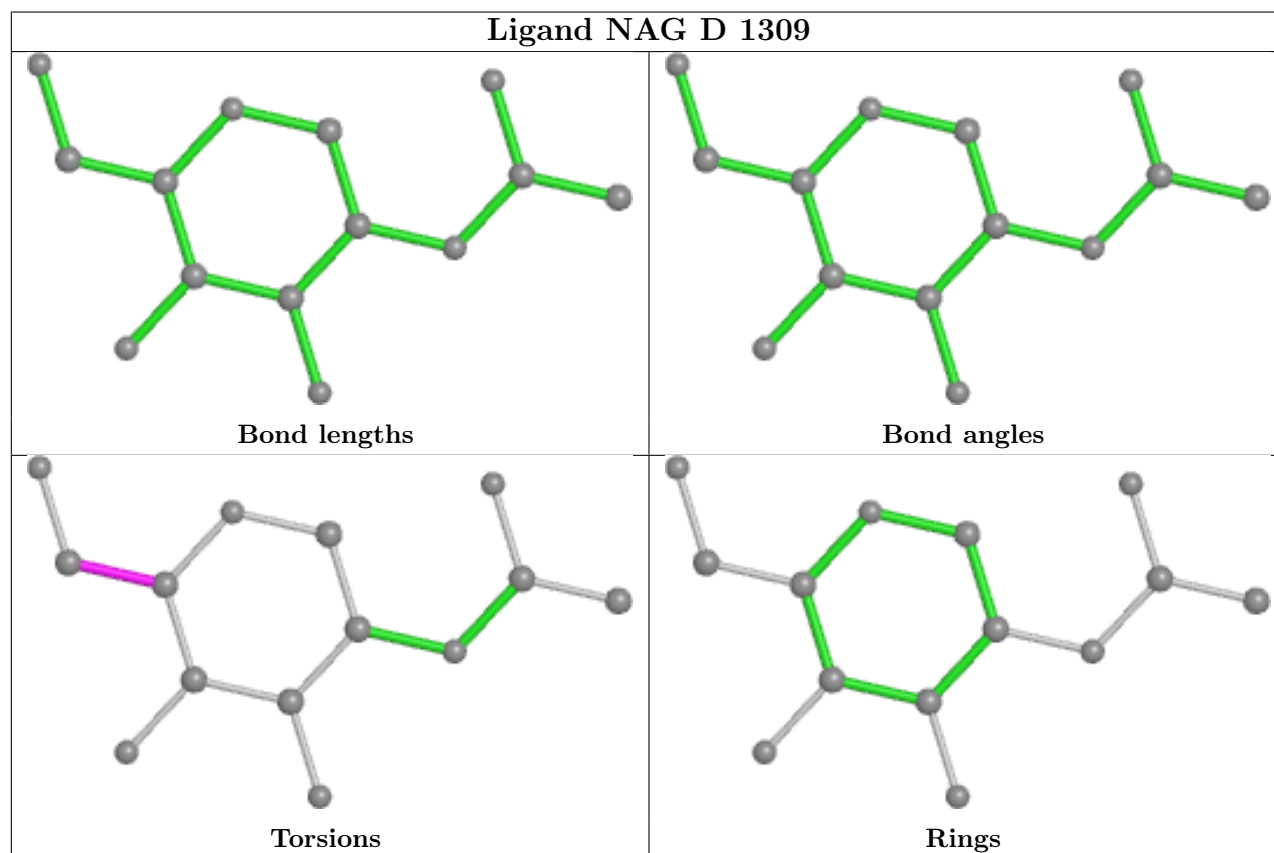
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1310	REA	5	0

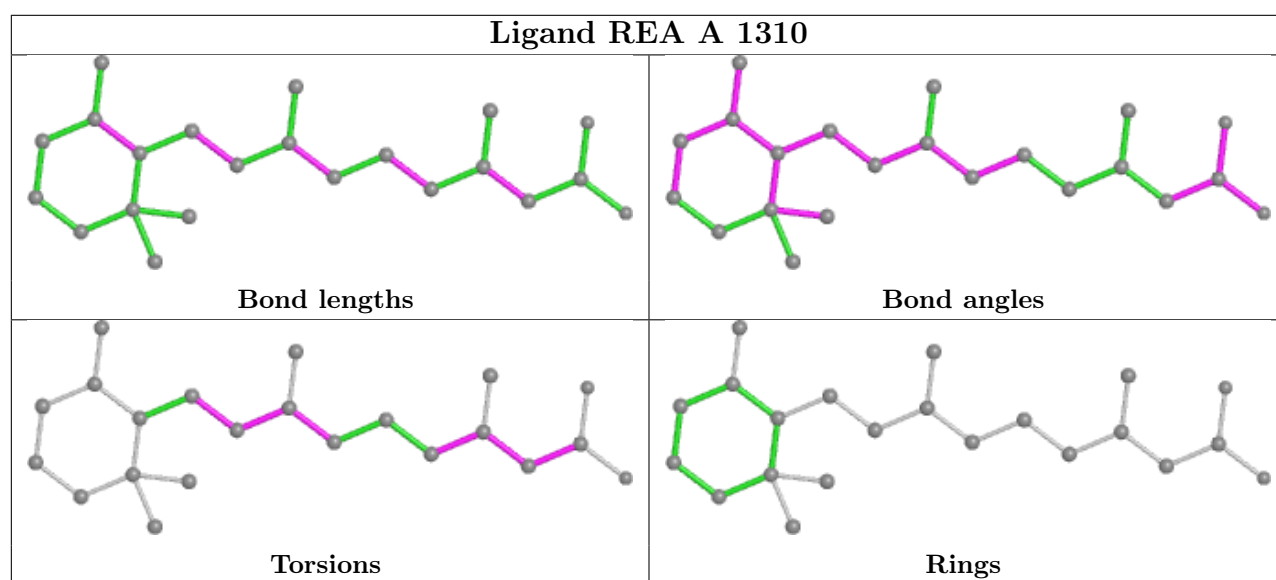
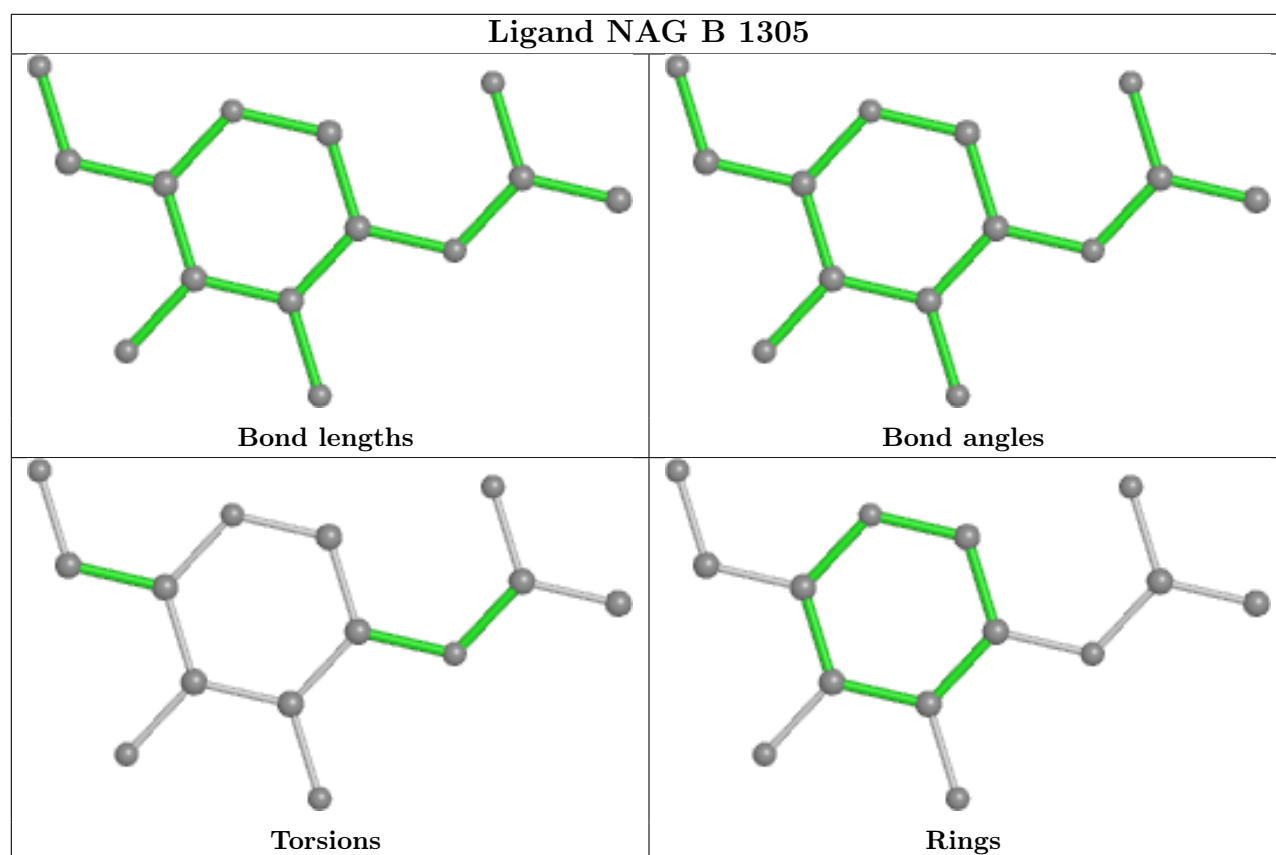
Continued on next page...

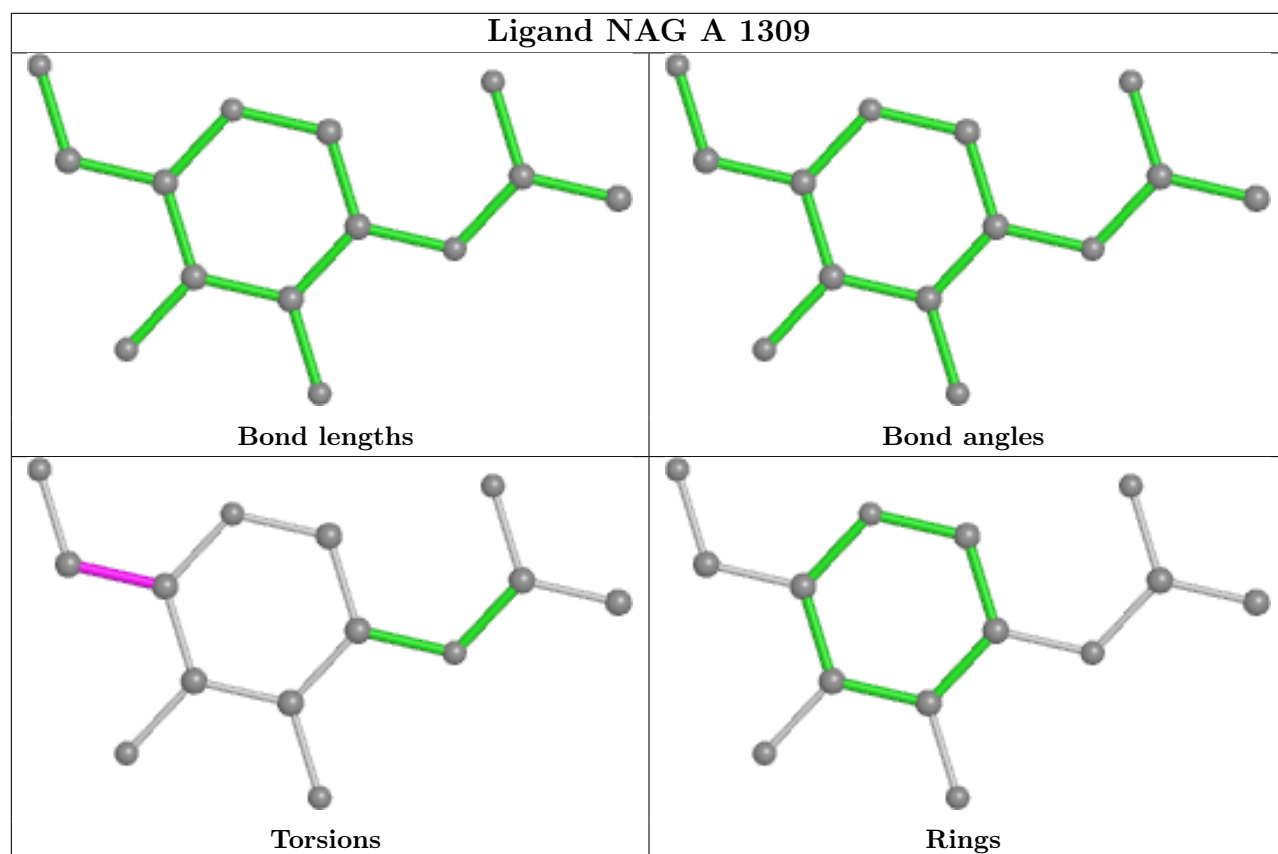
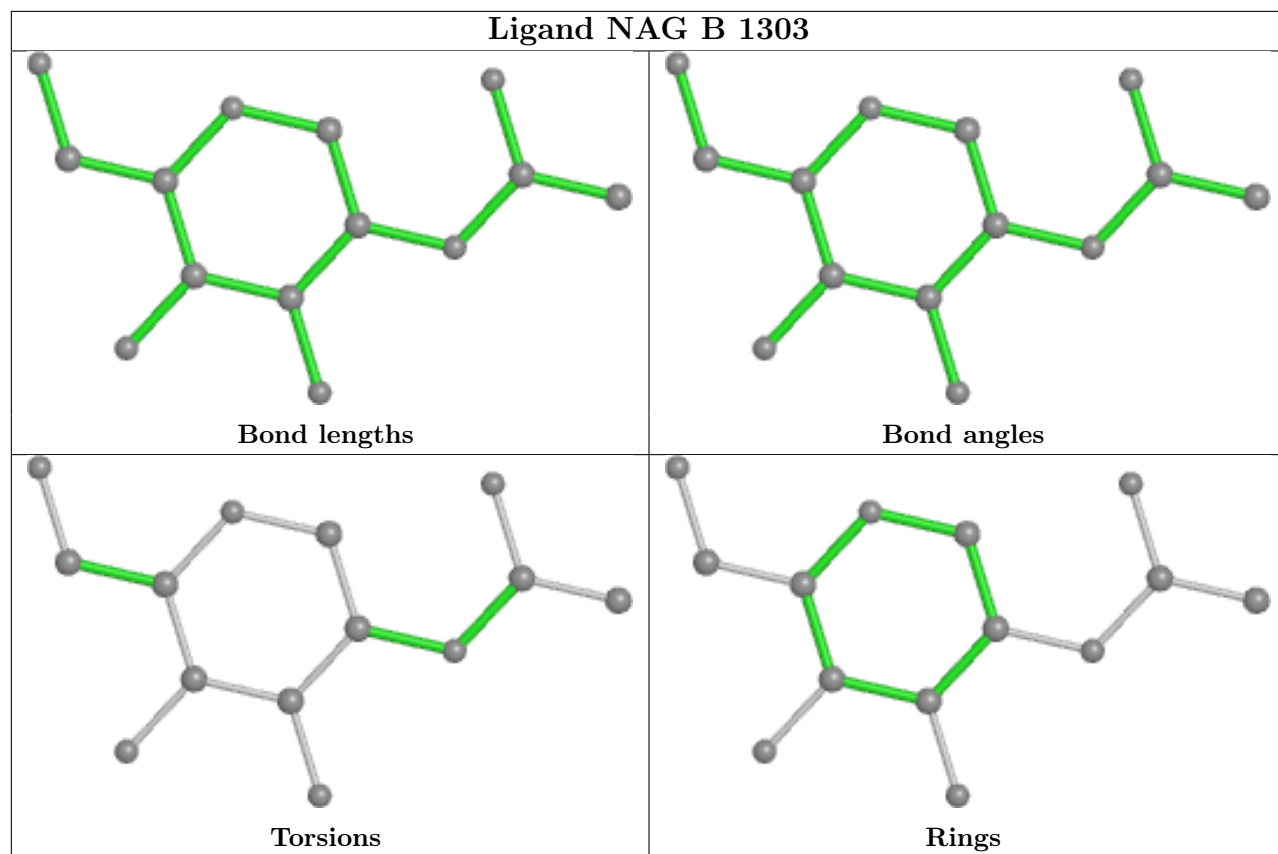
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1303	NAG	1	0
2	D	1303	NAG	1	0
2	A	1303	NAG	1	0
3	D	1310	REA	9	0
3	B	1310	REA	7	0

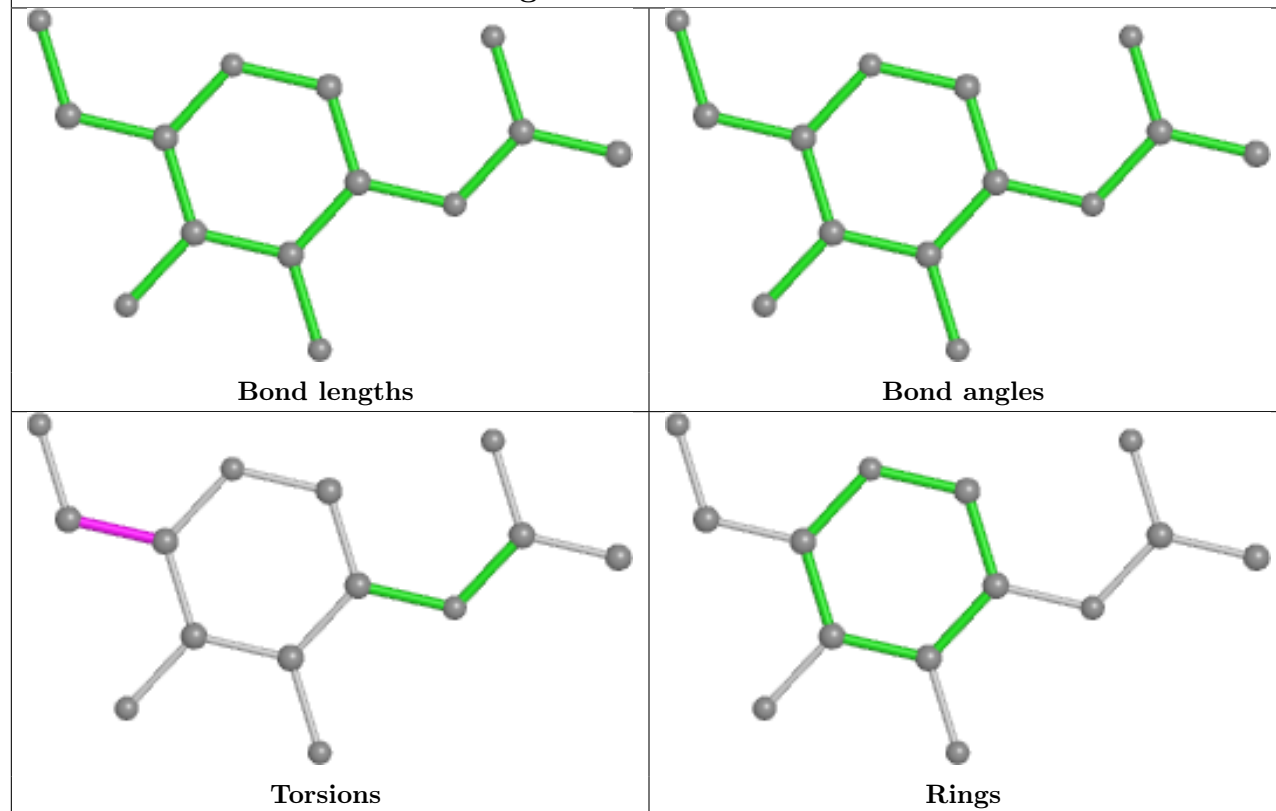
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



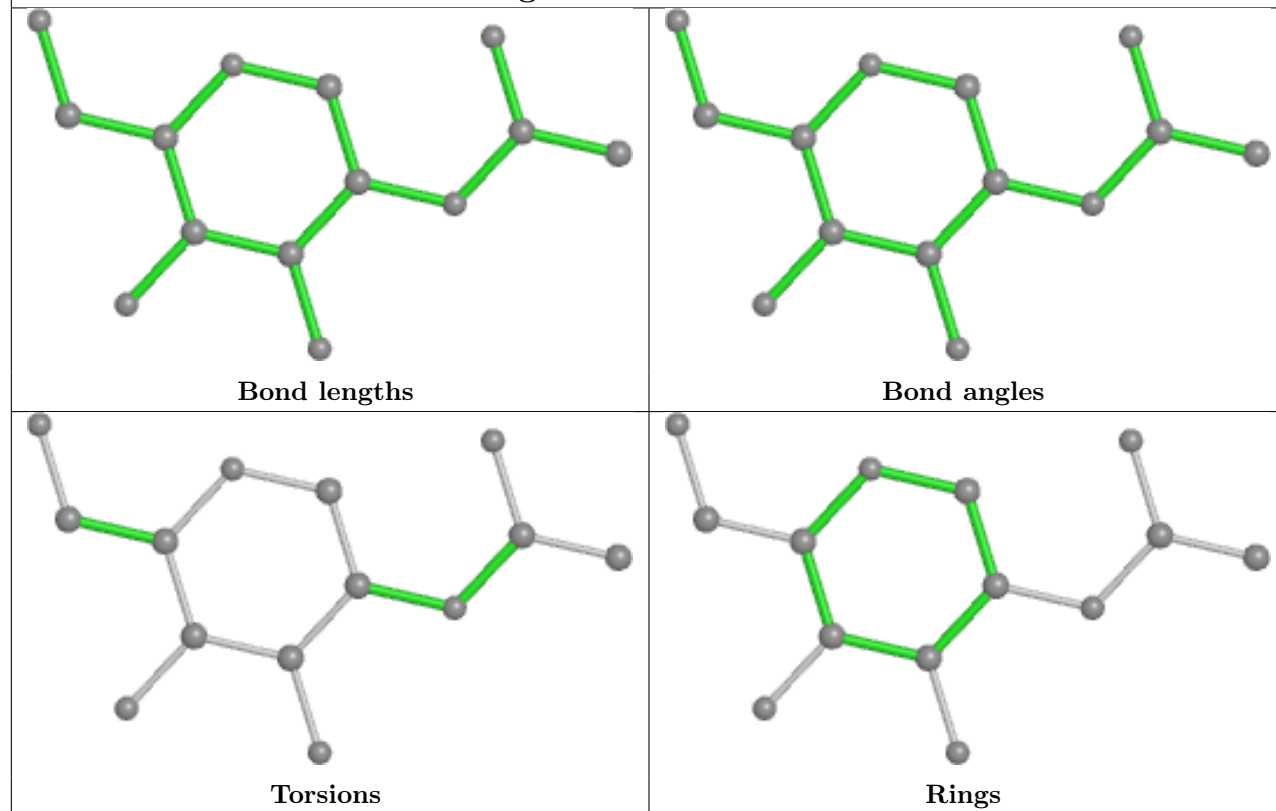




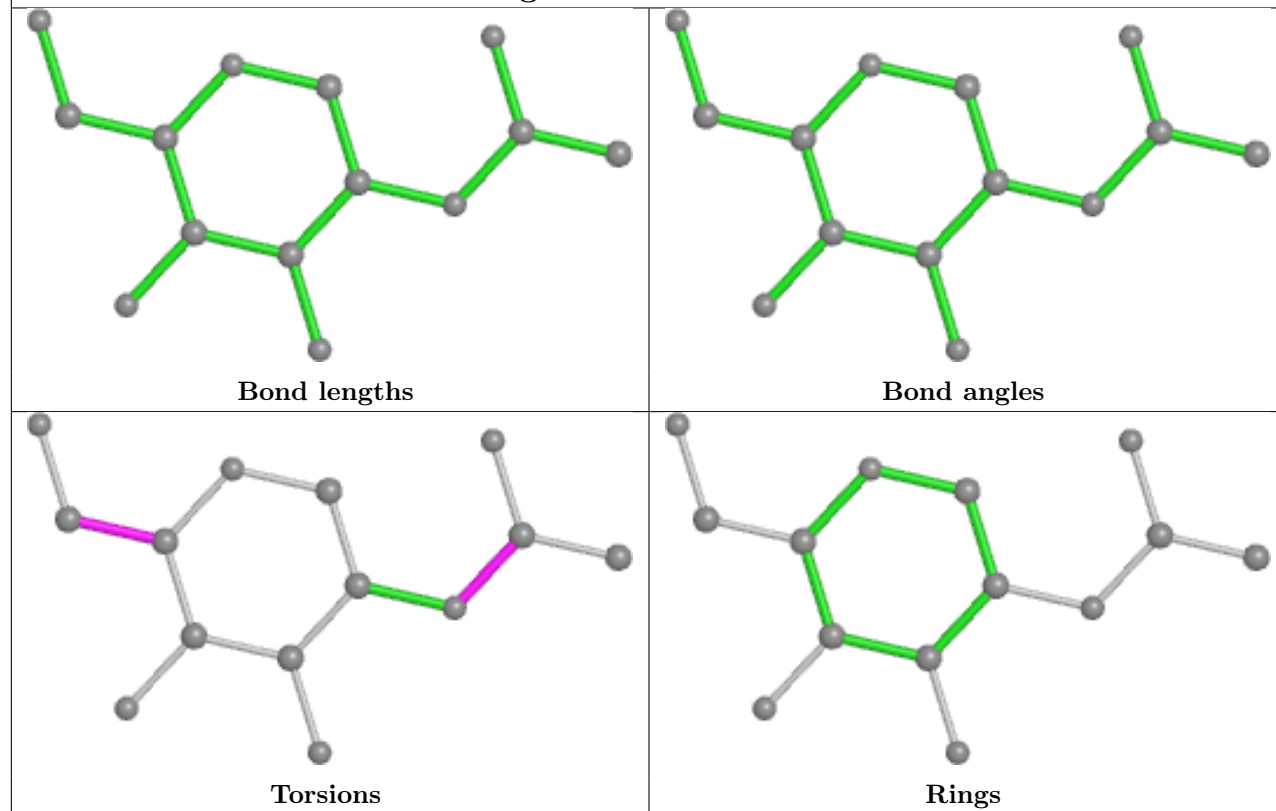
Ligand NAG B 1304



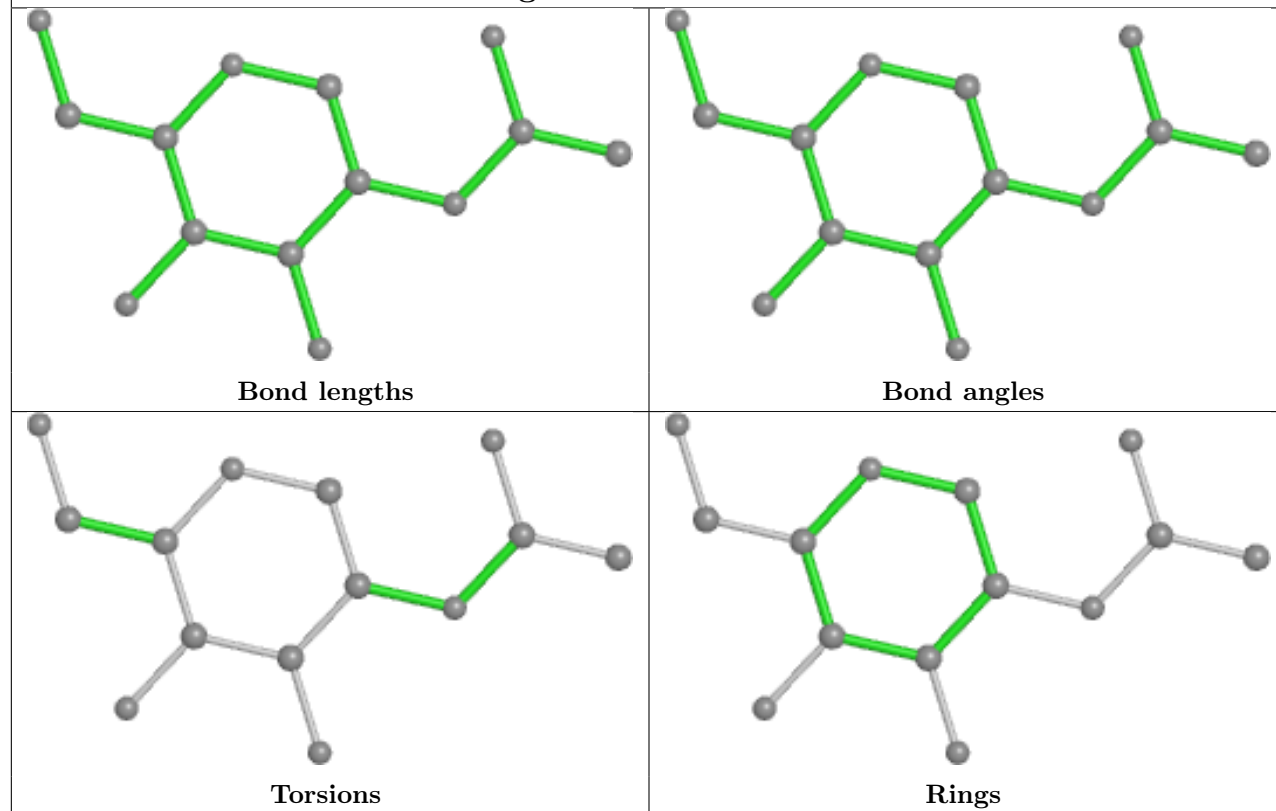
Ligand NAG A 1307



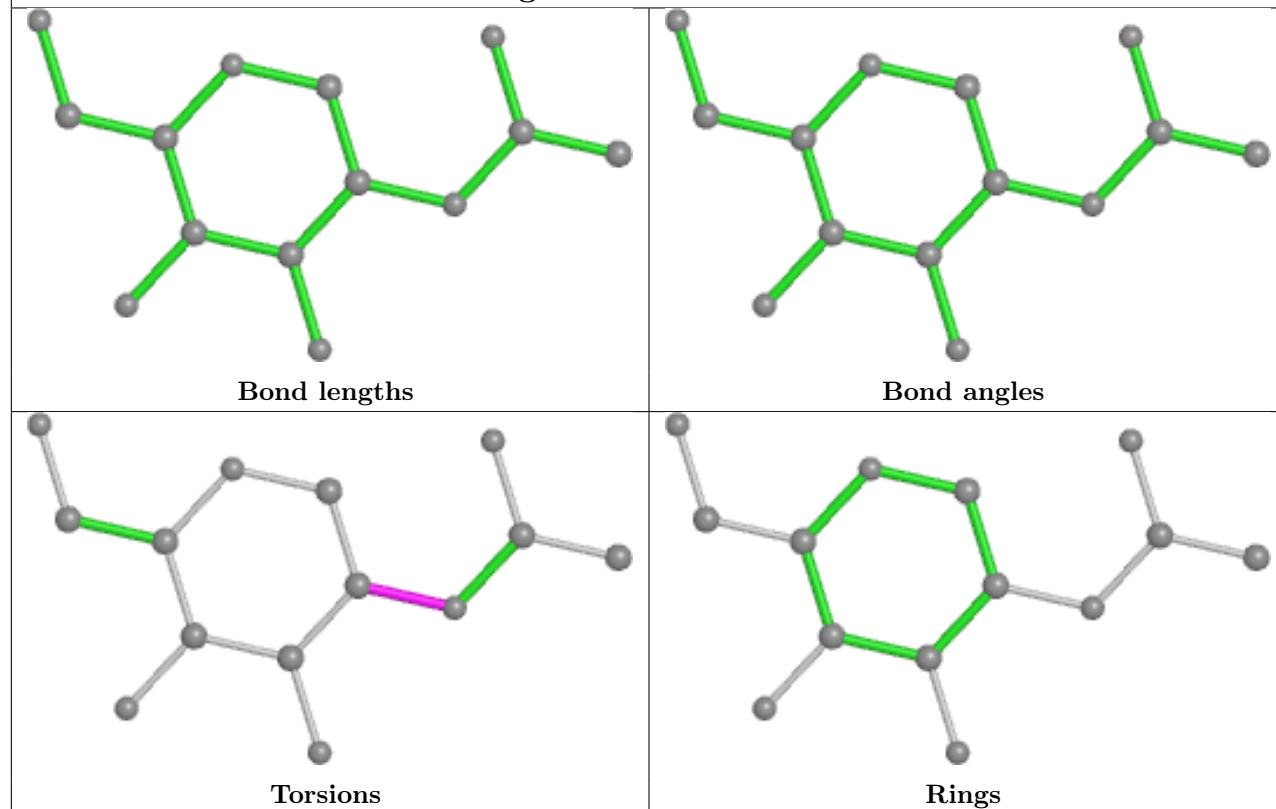
Ligand NAG B 1302



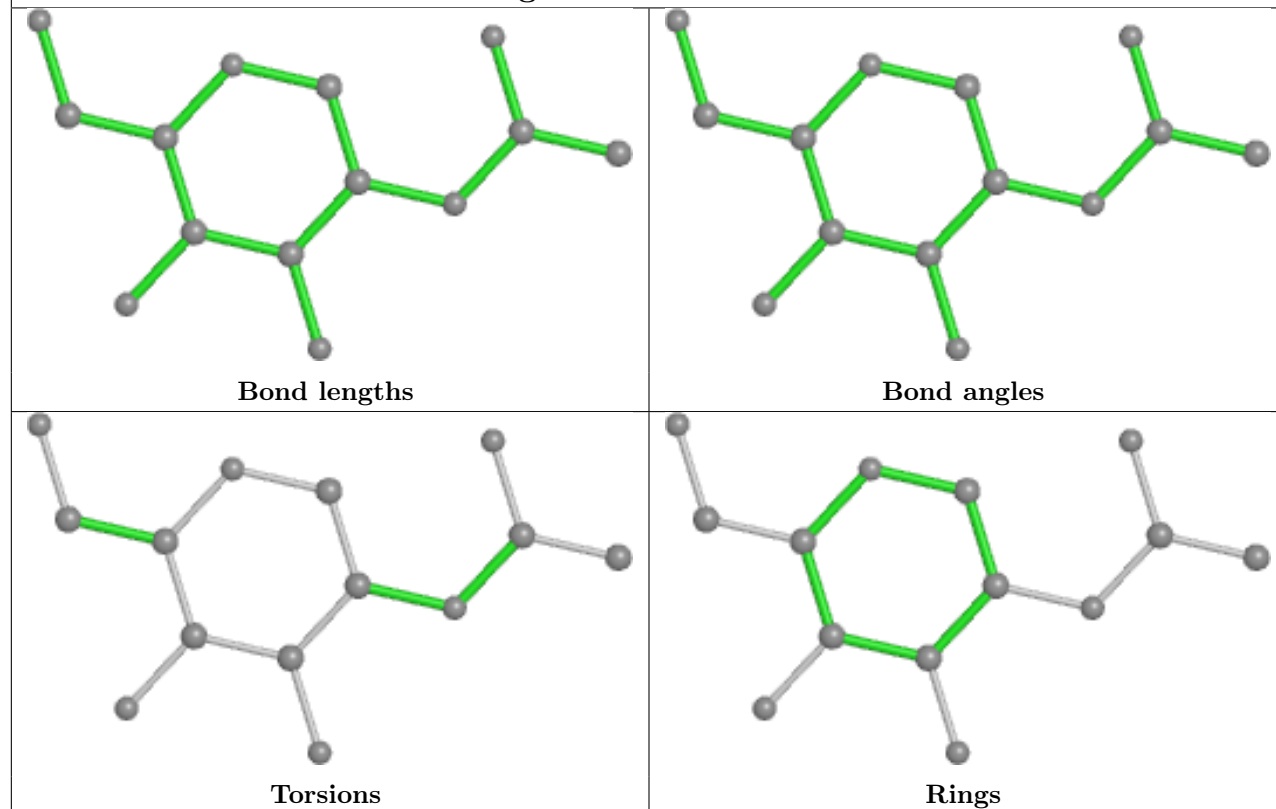
Ligand NAG A 1305



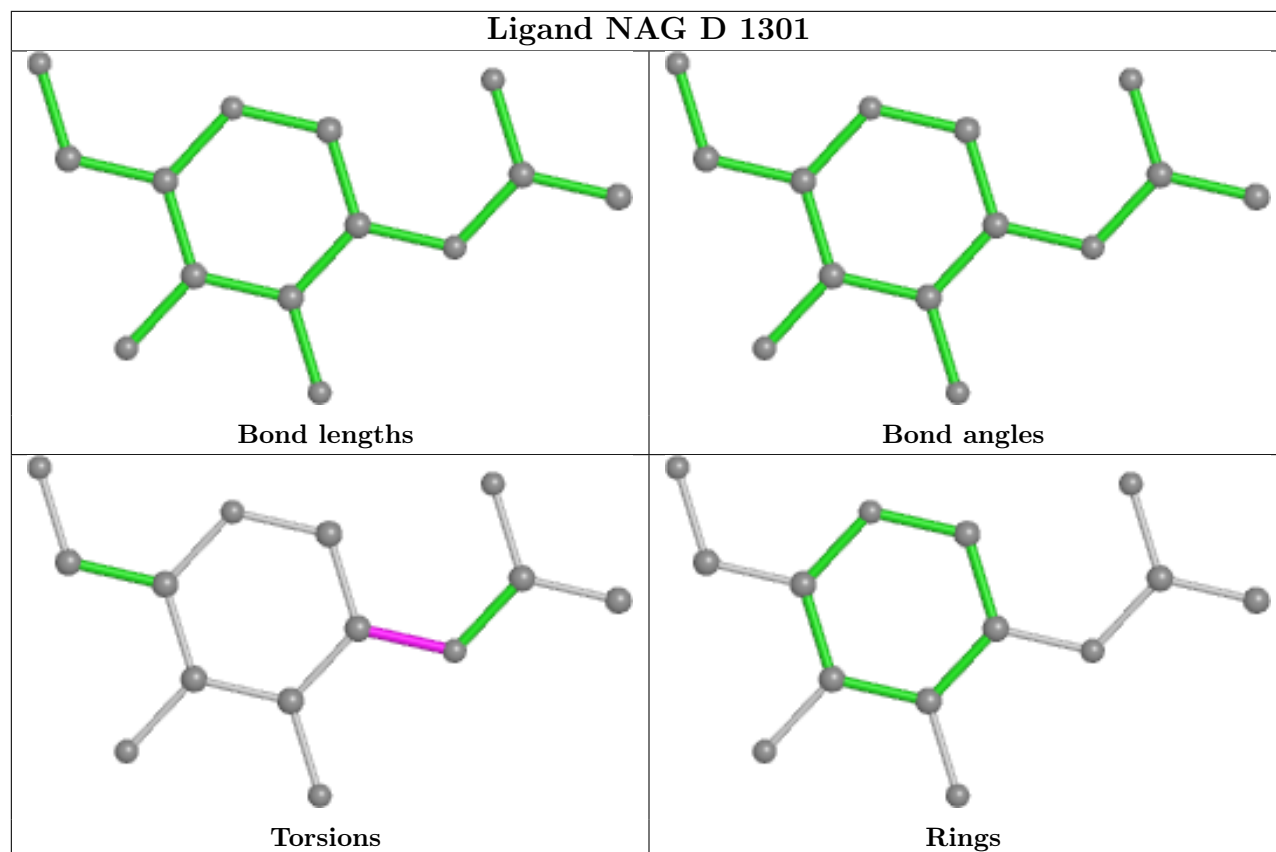
Ligand NAG A 1301



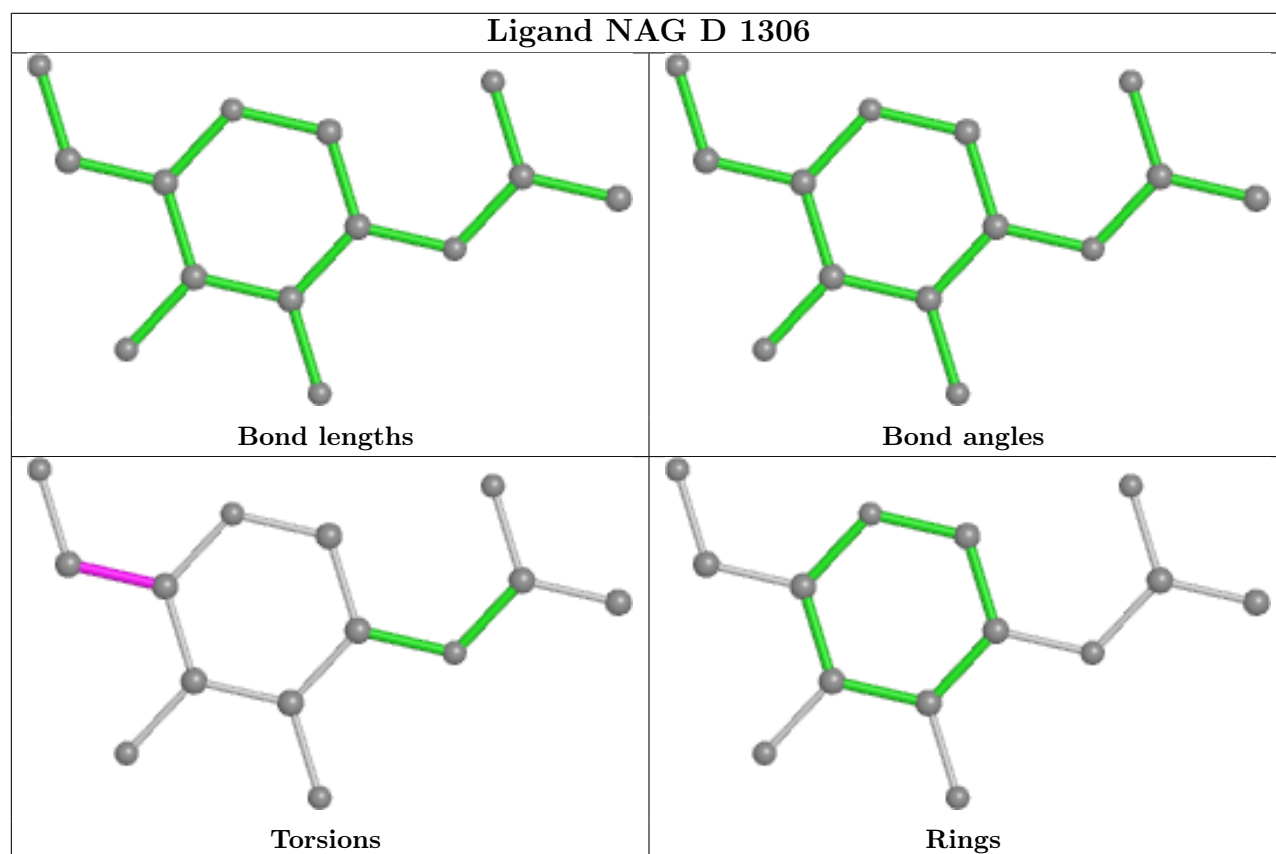
Ligand NAG D 1303

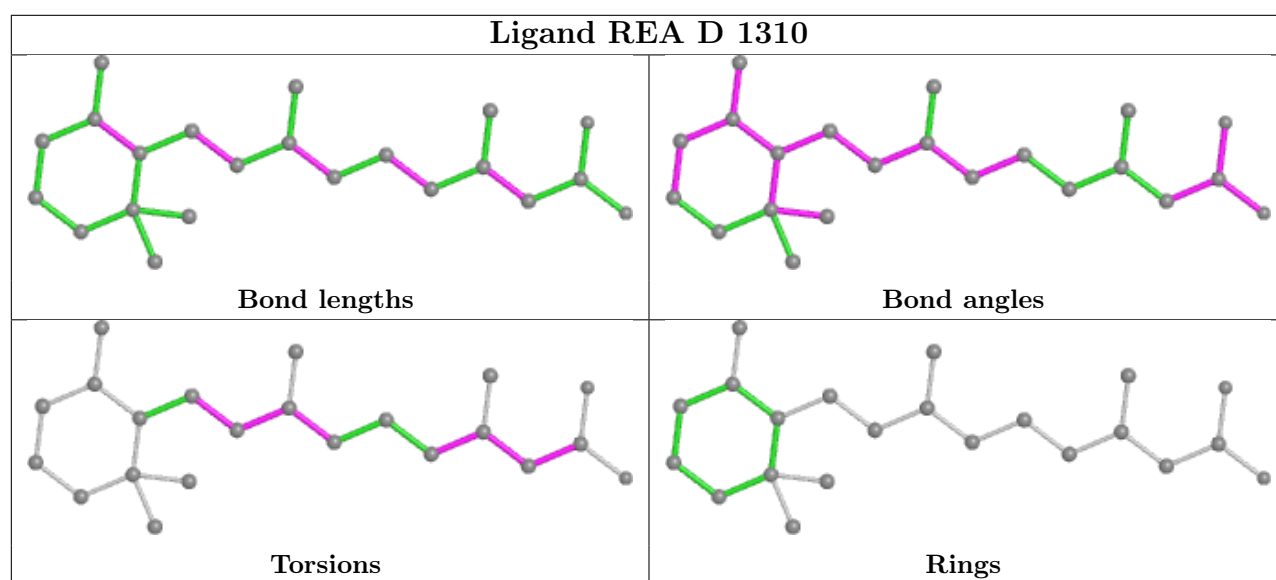
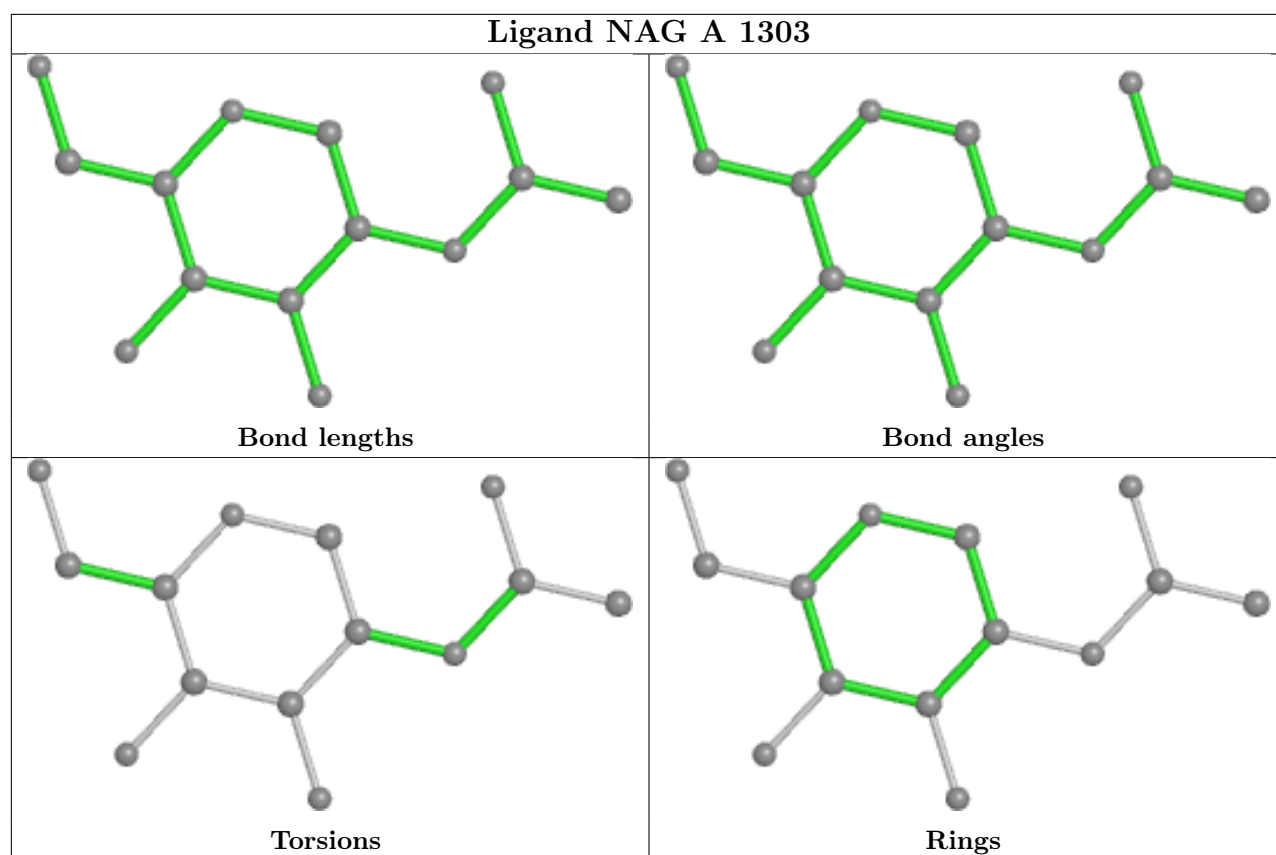


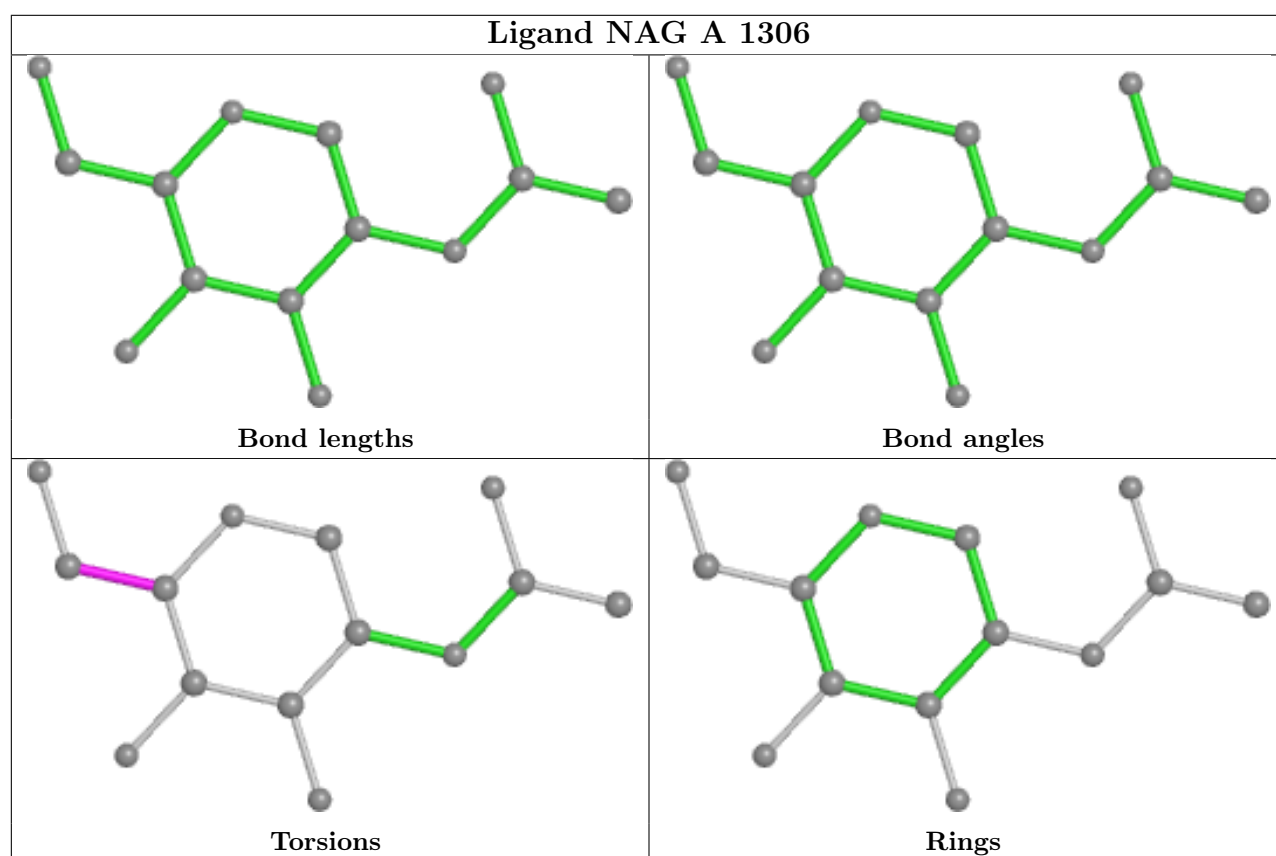
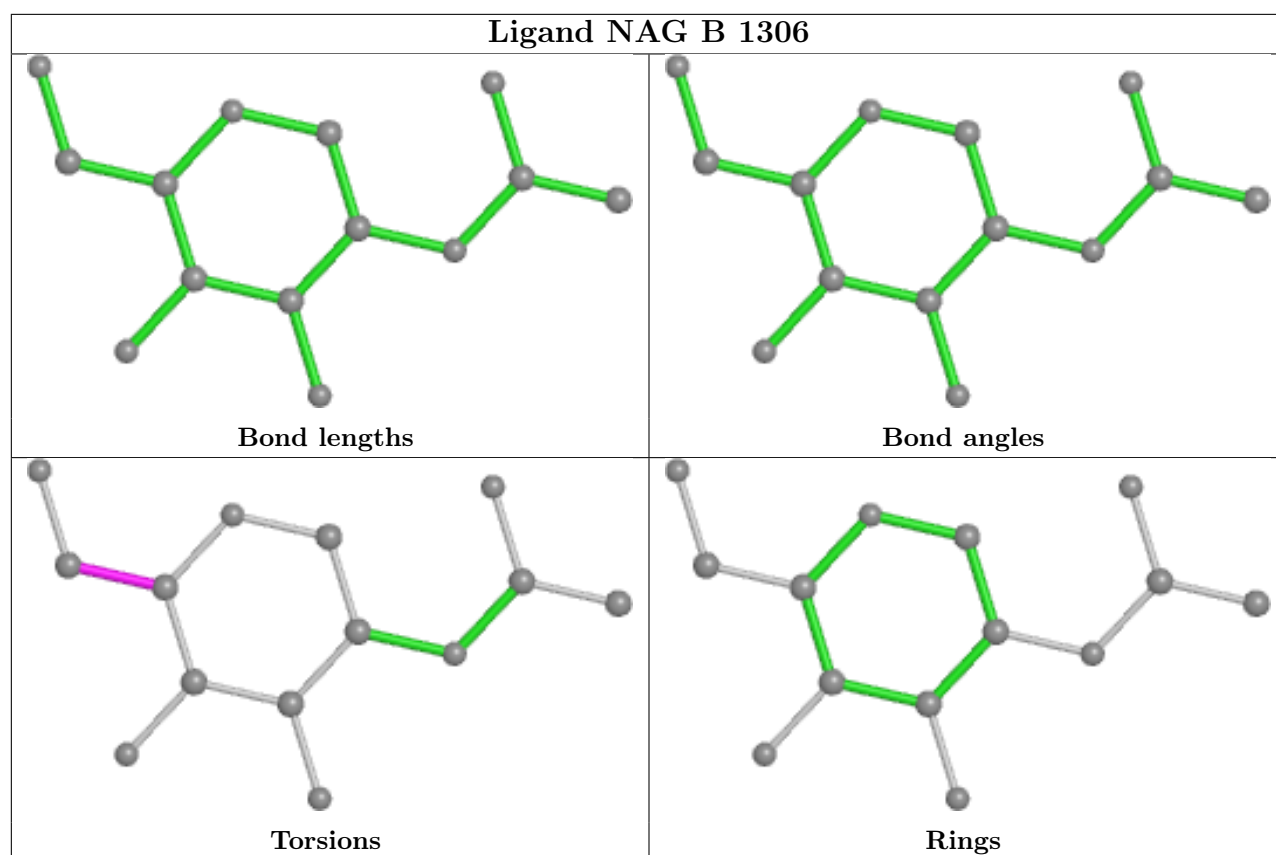
Ligand NAG D 1301

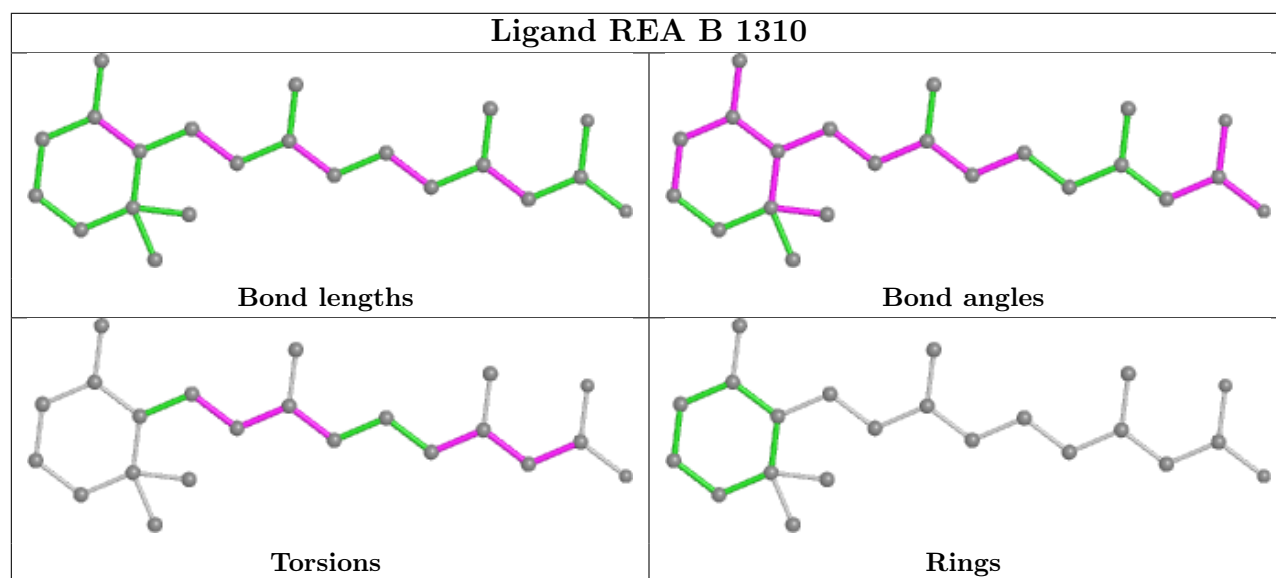
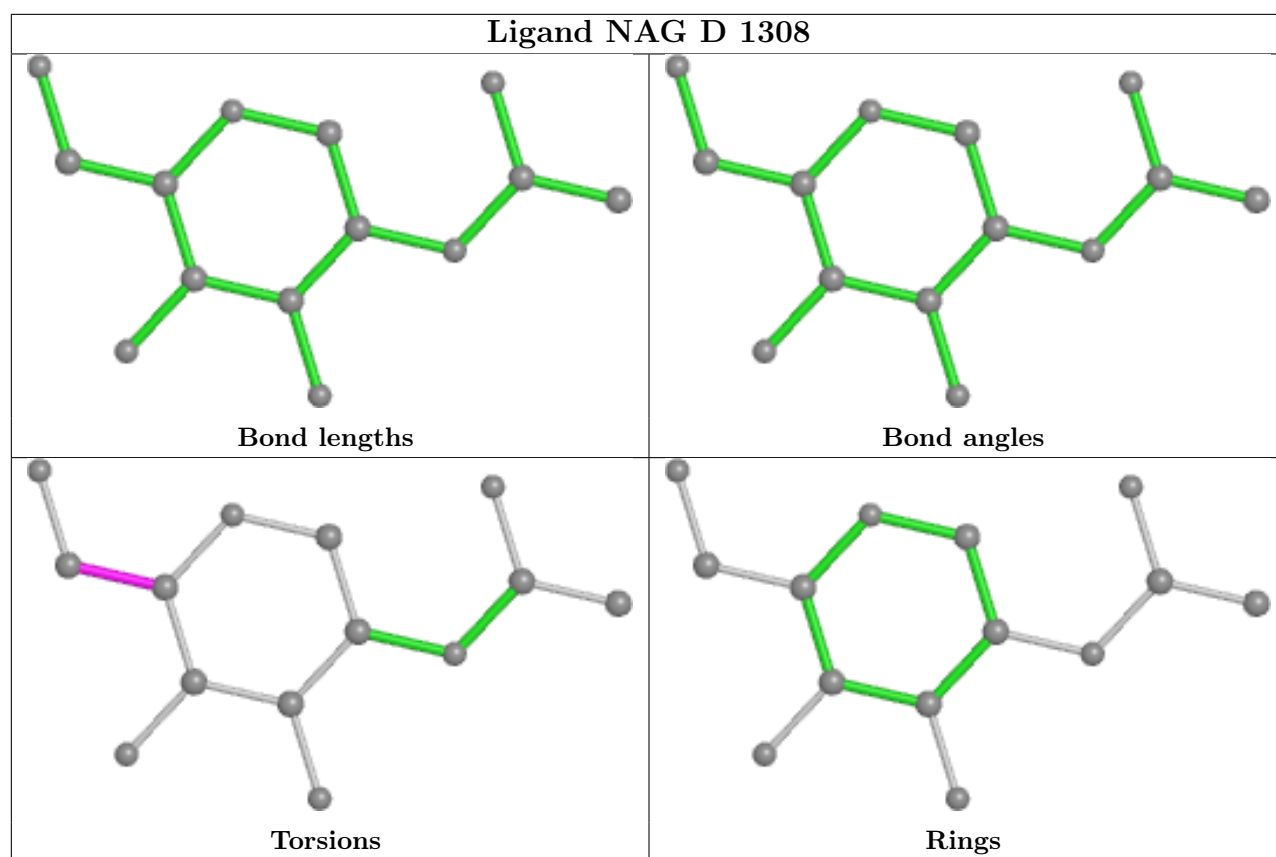


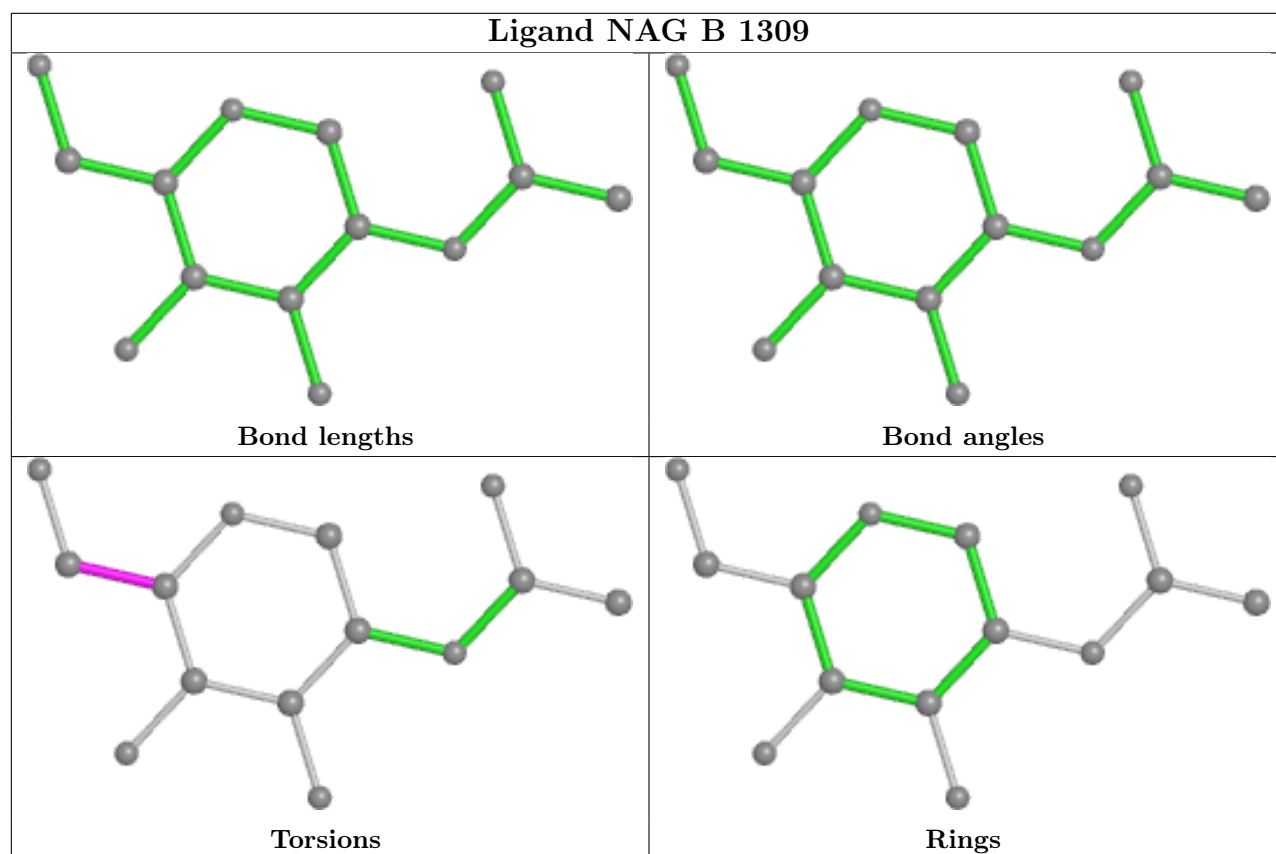
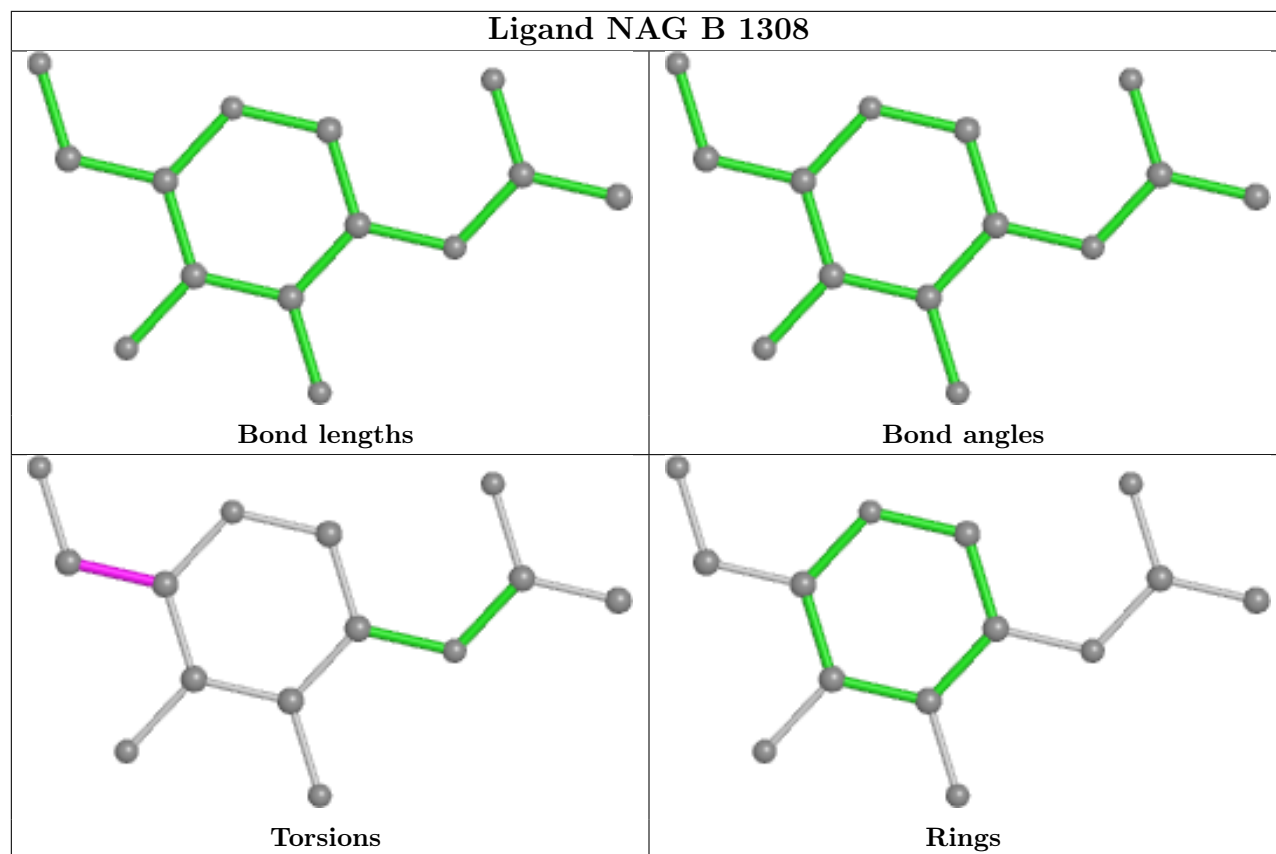
Ligand NAG D 1306



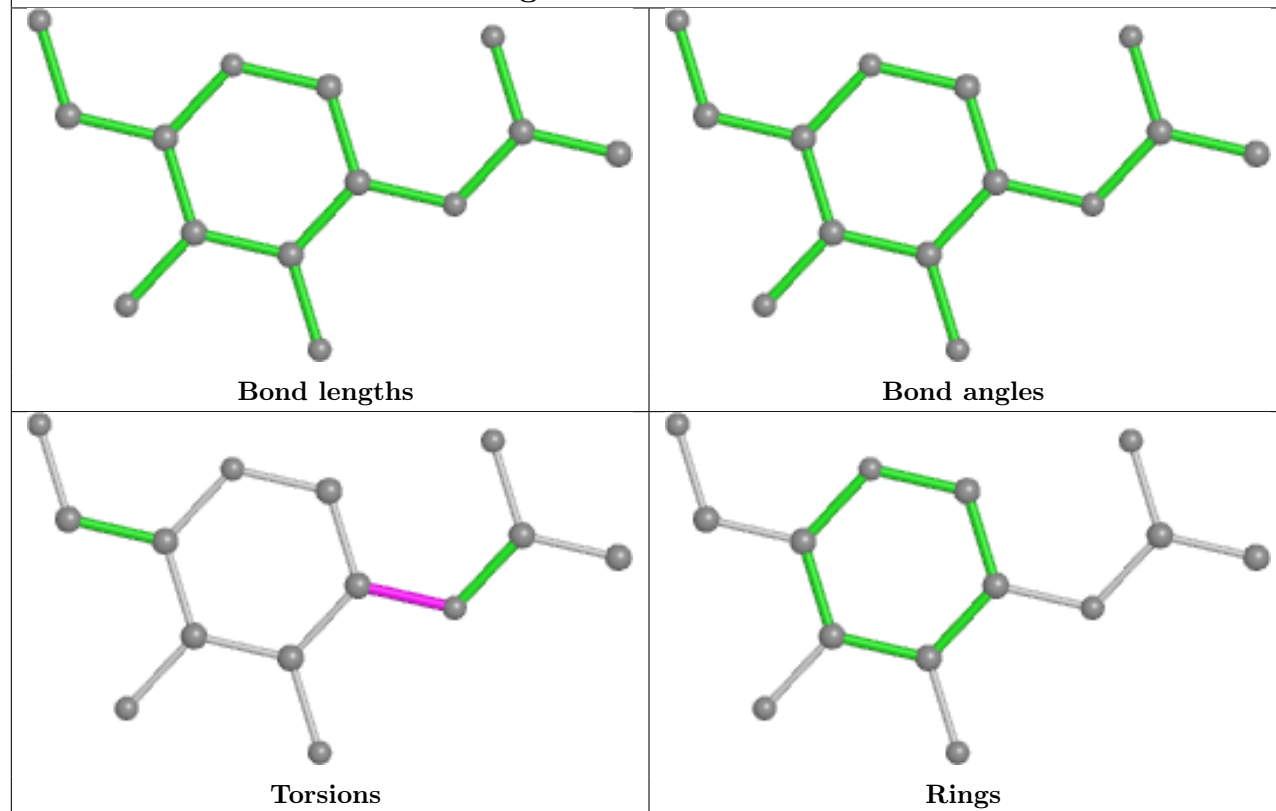




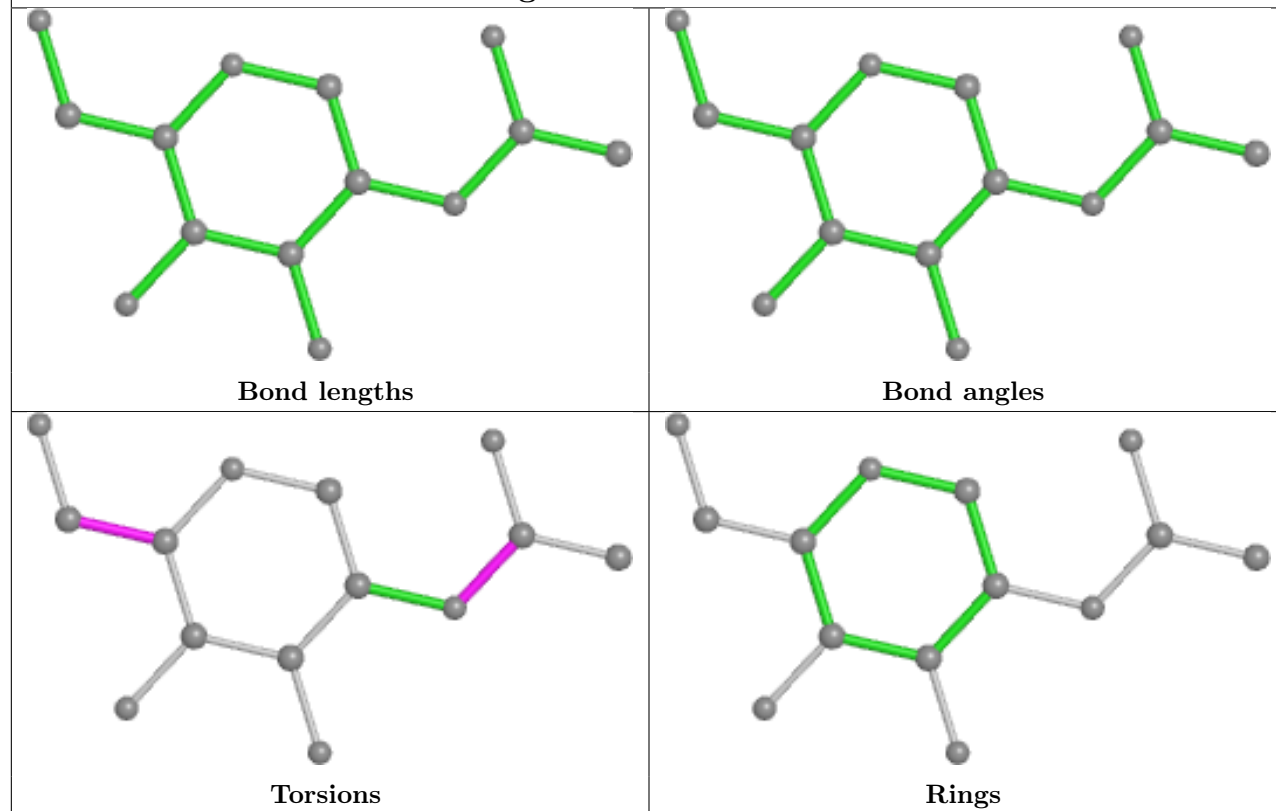


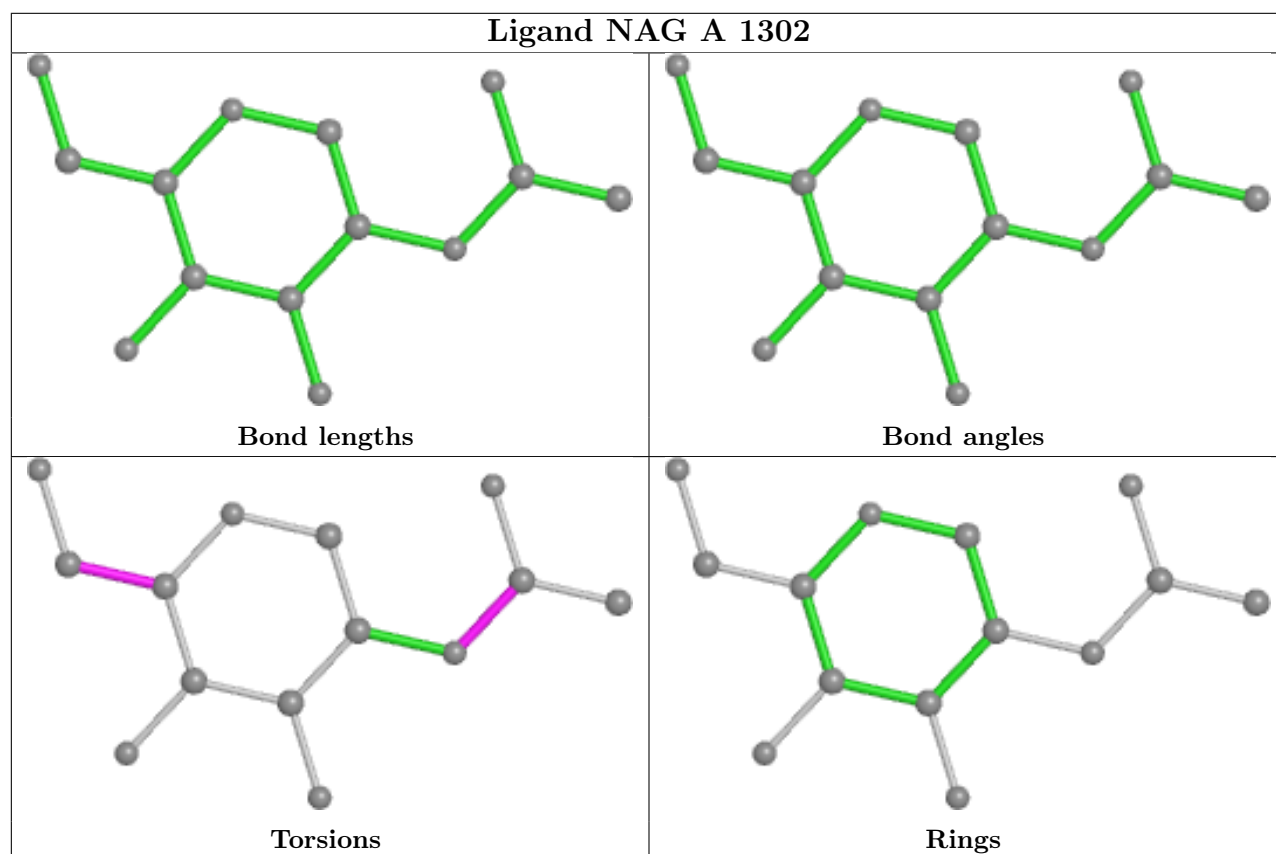
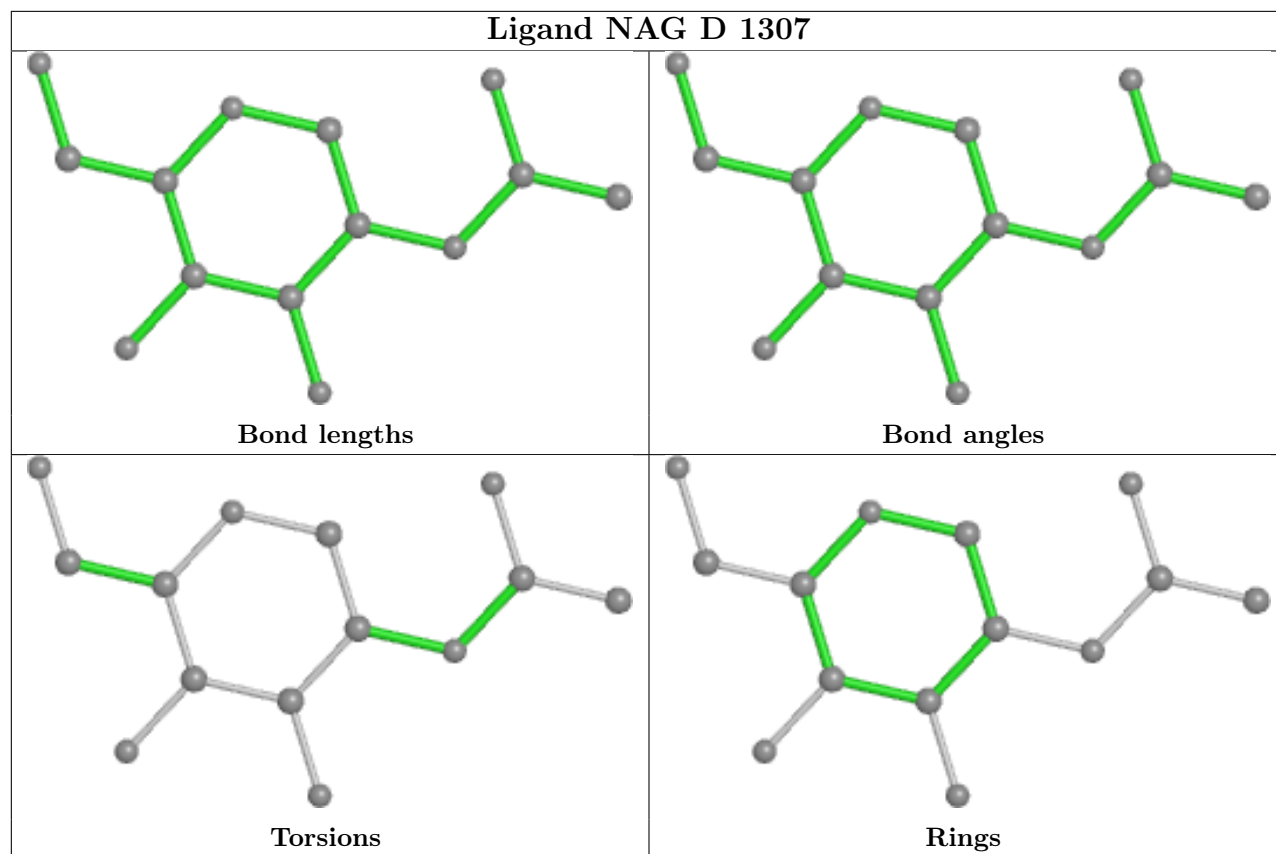


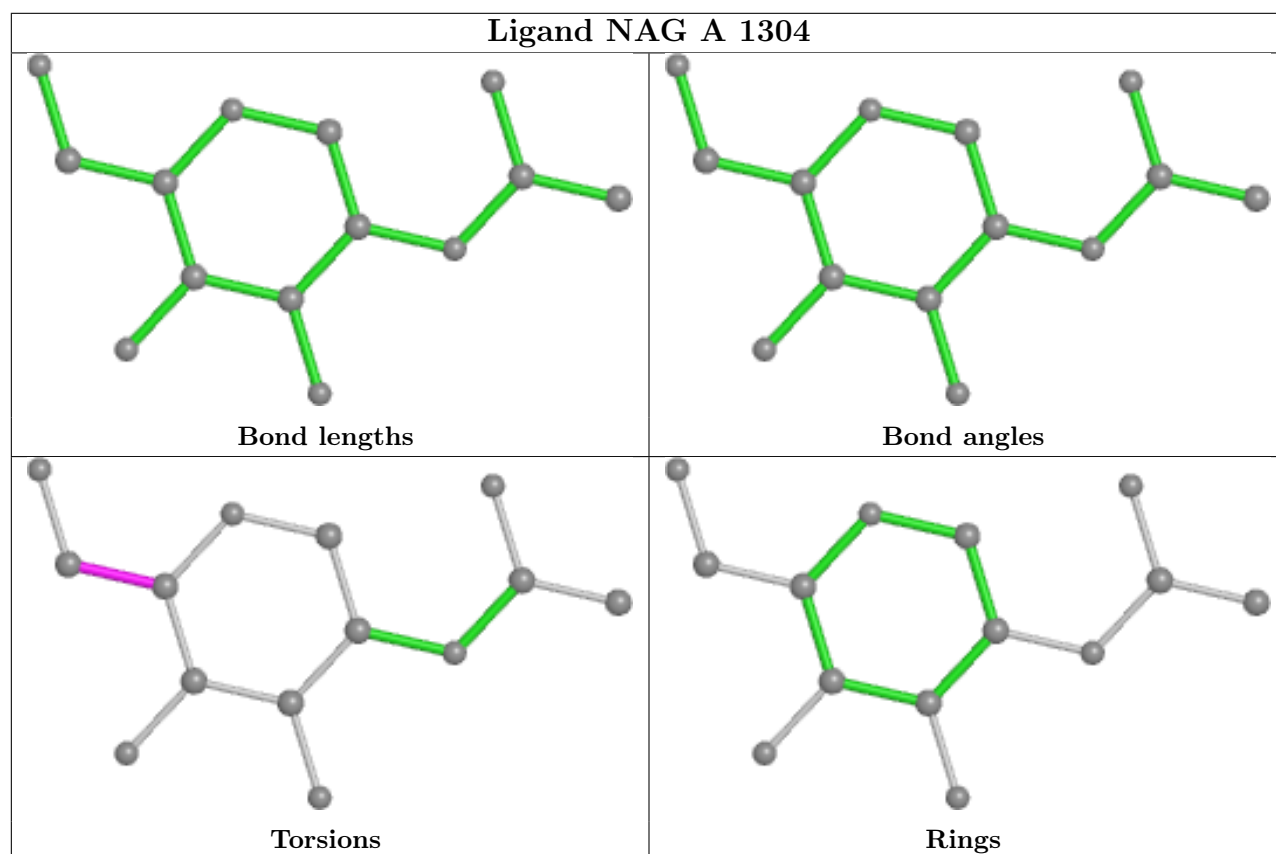
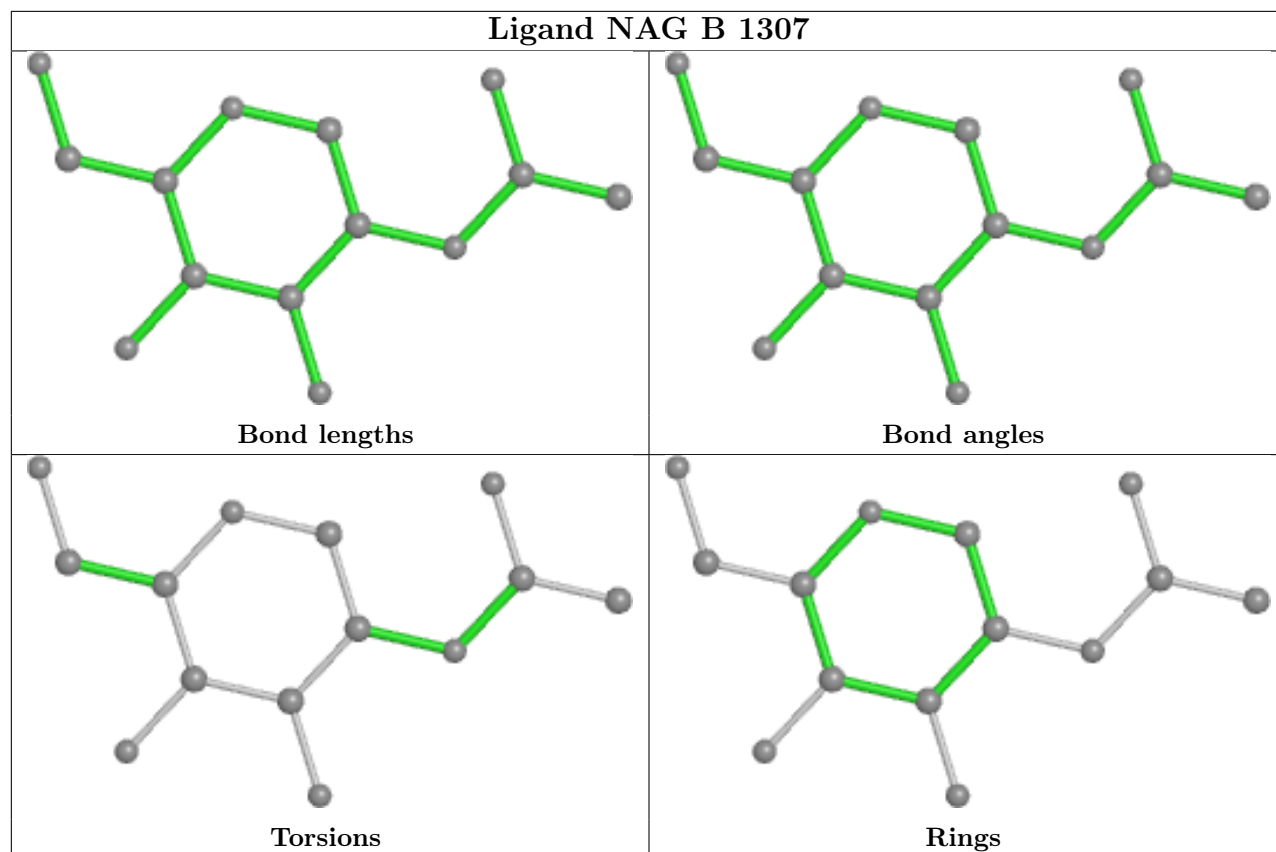
Ligand NAG B 1301

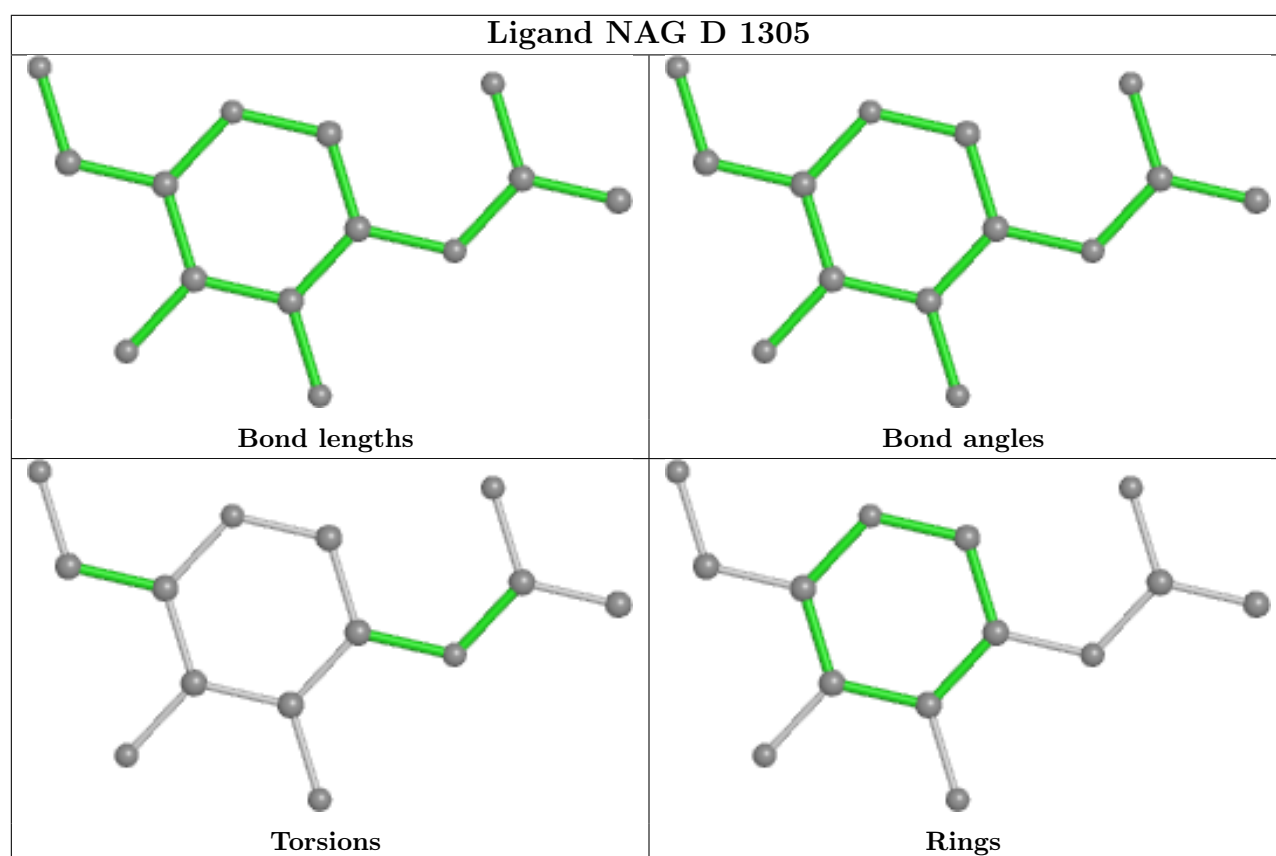
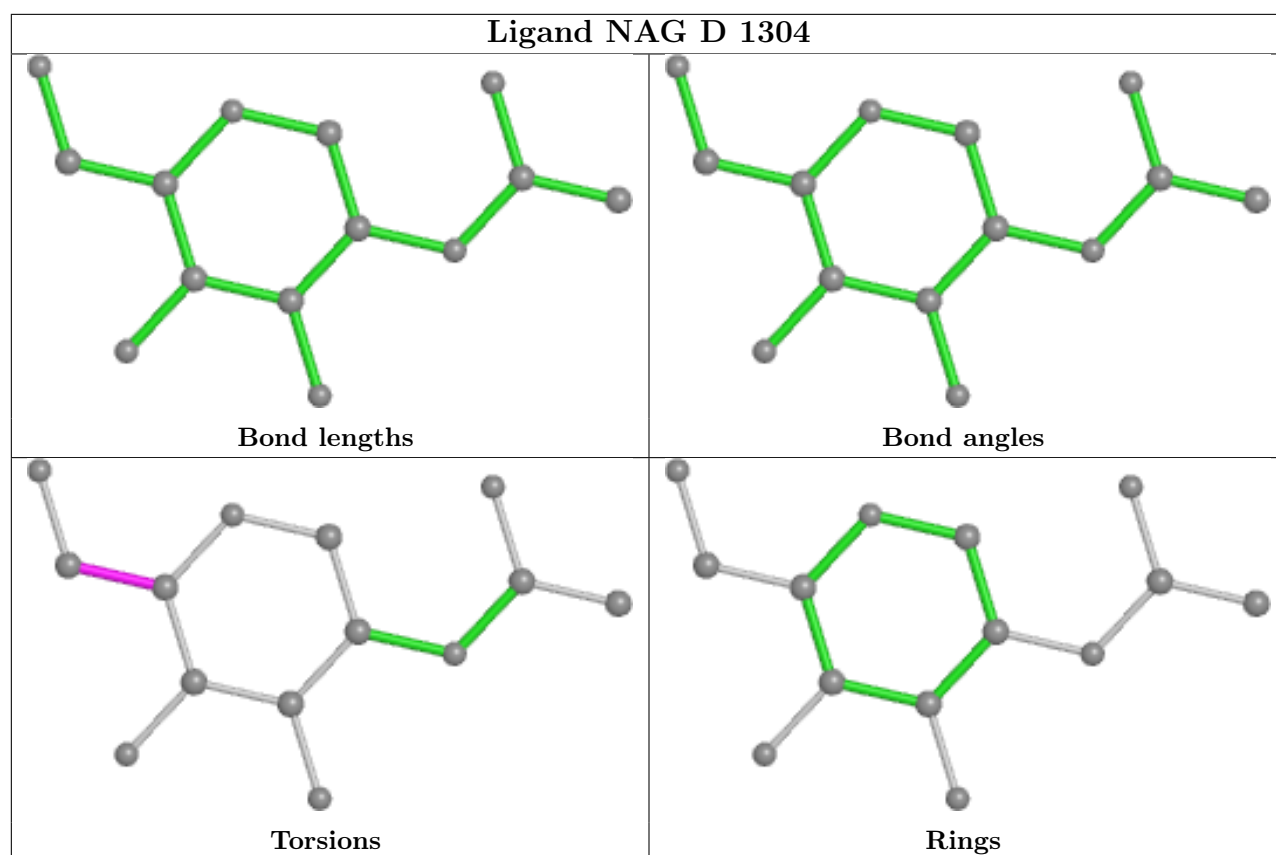


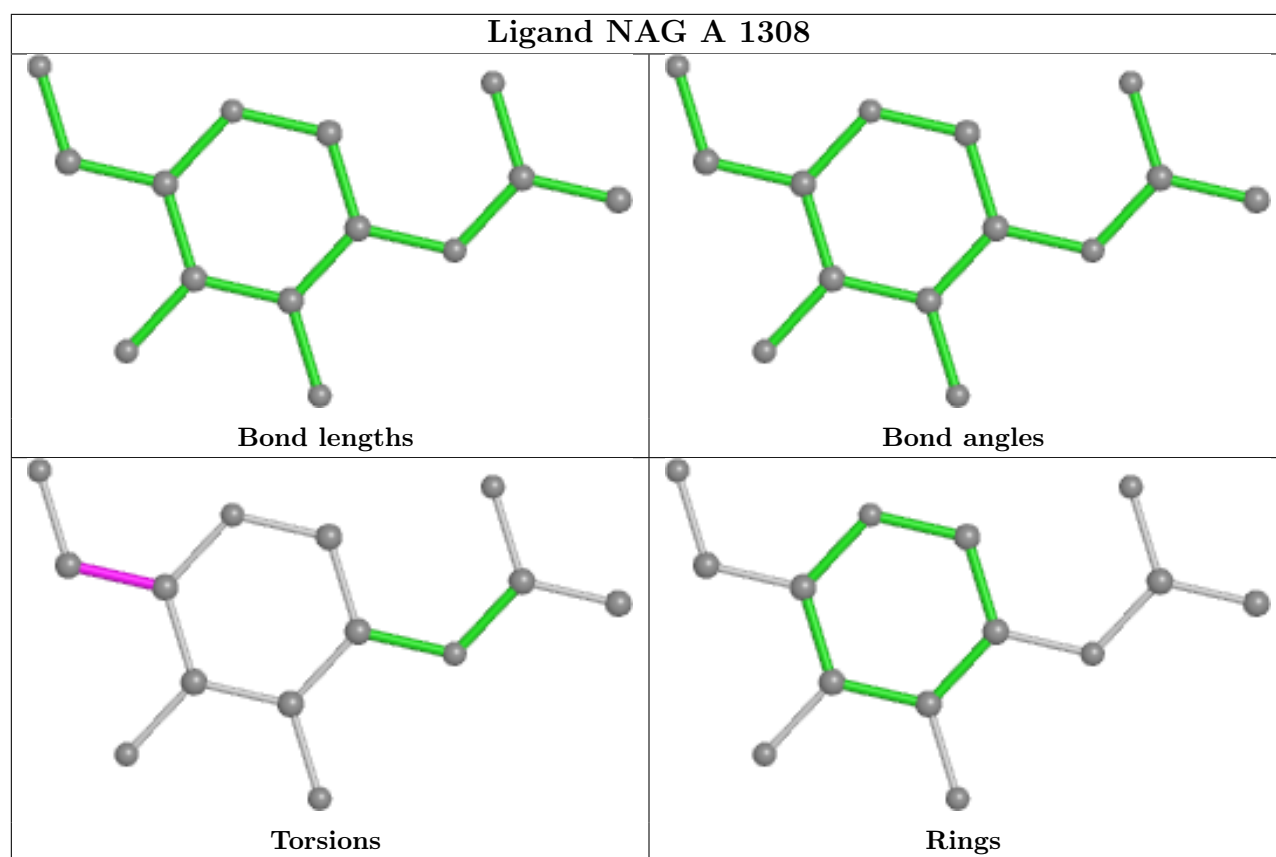
Ligand NAG D 1302











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.

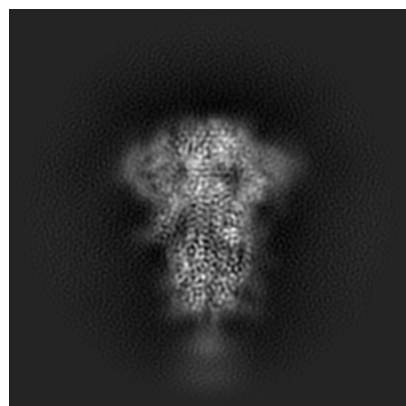
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33600. These allow visual inspection of the internal detail of the map and identification of artifacts.

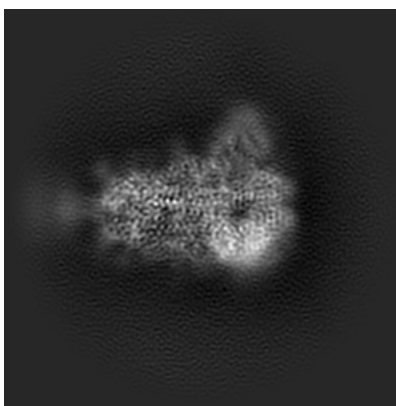
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

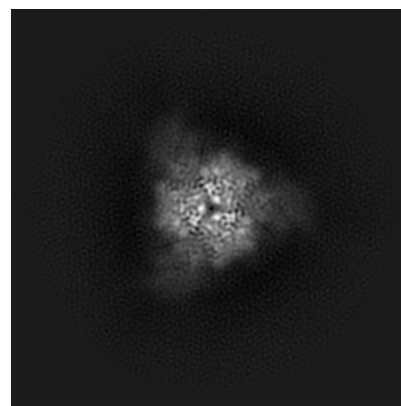
6.1.1 Primary map



X

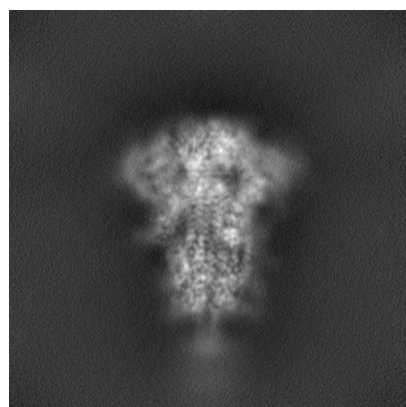


Y

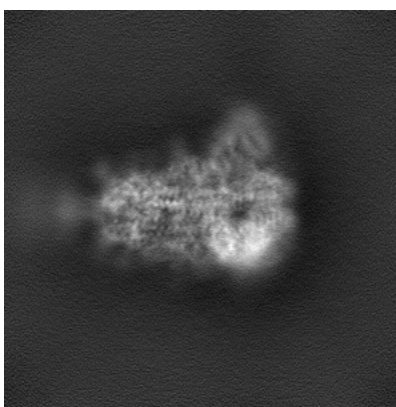


Z

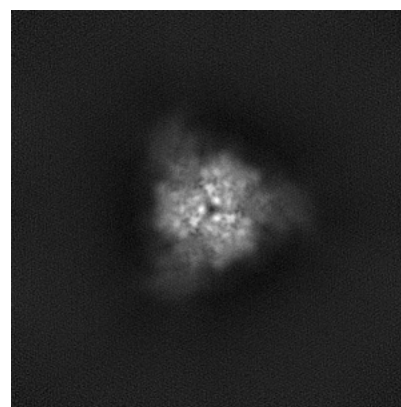
6.1.2 Raw map



X



Y

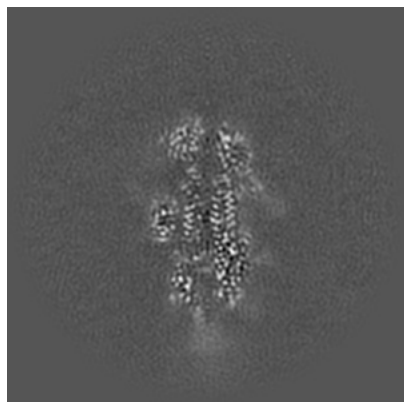


Z

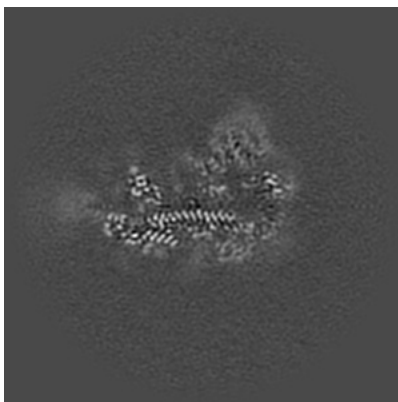
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

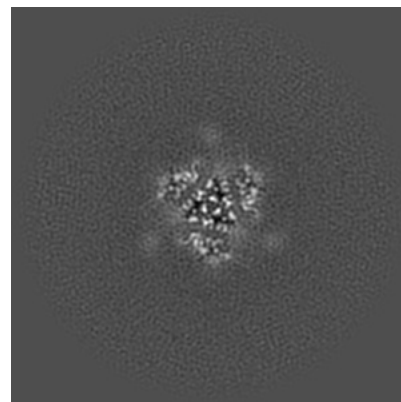
6.2.1 Primary map



X Index: 160

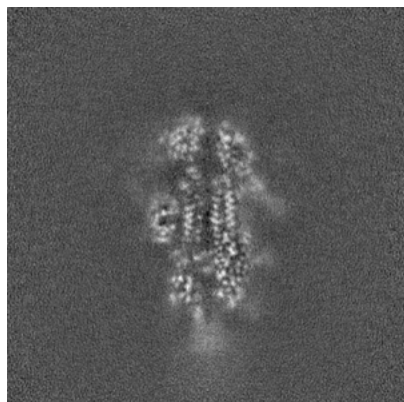


Y Index: 160

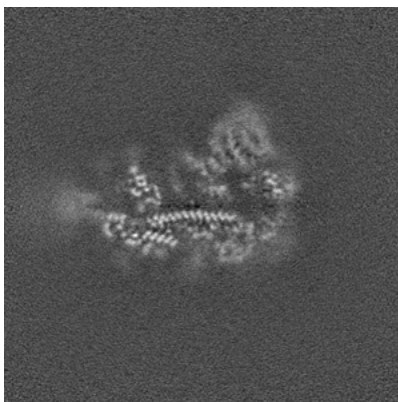


Z Index: 160

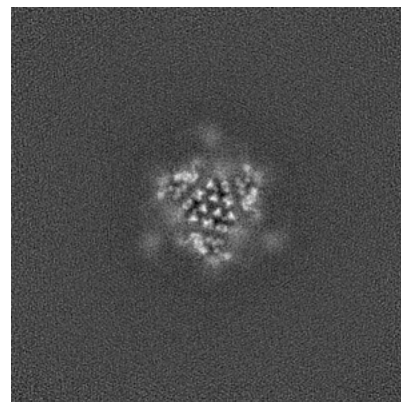
6.2.2 Raw map



X Index: 160



Y Index: 160

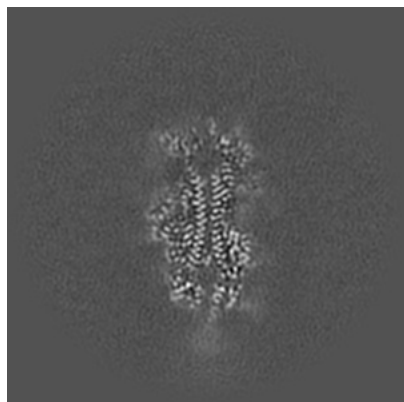


Z Index: 160

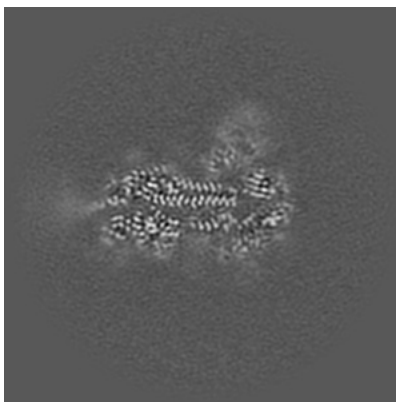
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

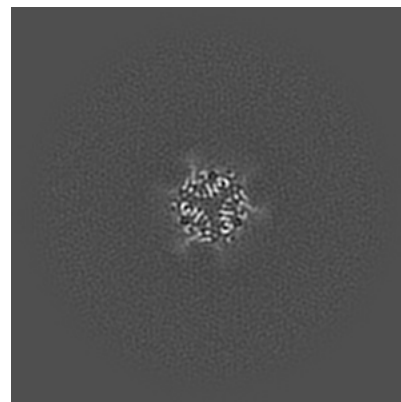
6.3.1 Primary map



X Index: 165

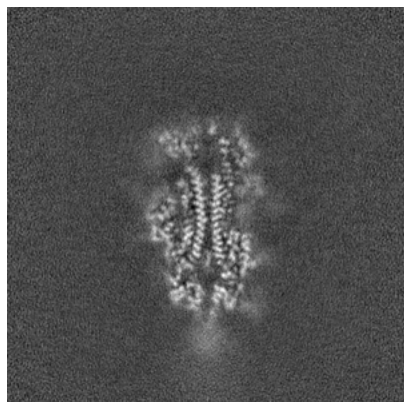


Y Index: 153

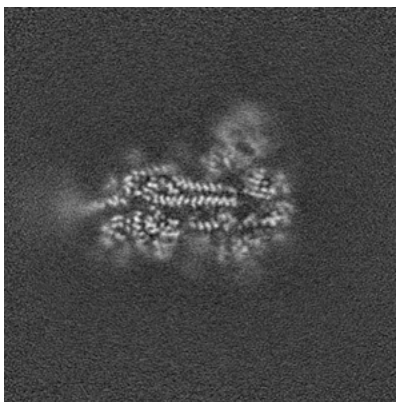


Z Index: 105

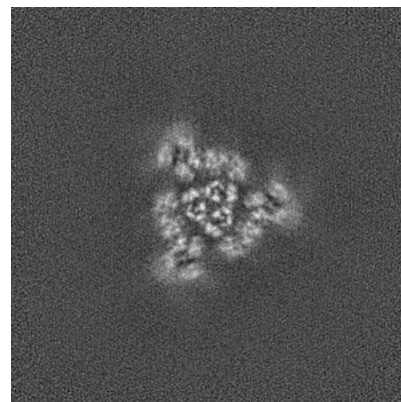
6.3.2 Raw map



X Index: 164



Y Index: 153

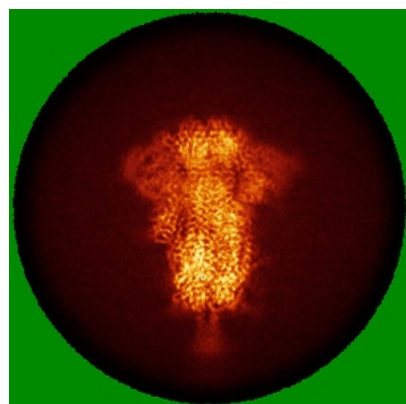


Z Index: 177

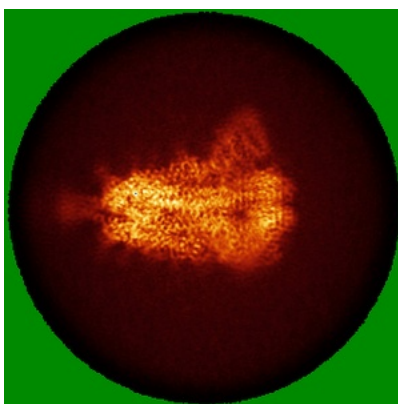
The images above show the largest variance slices of the map in three orthogonal directions.

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

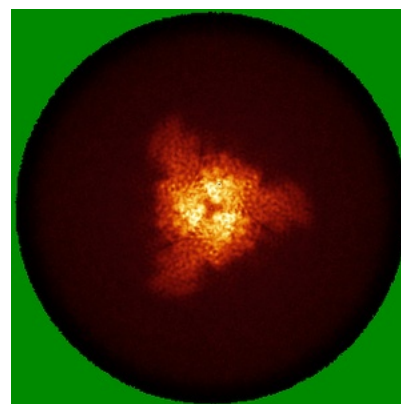
6.4.1 Primary map



X

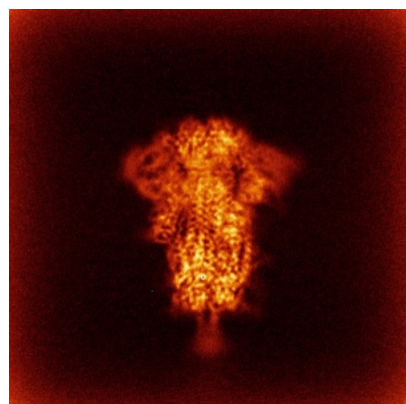


Y

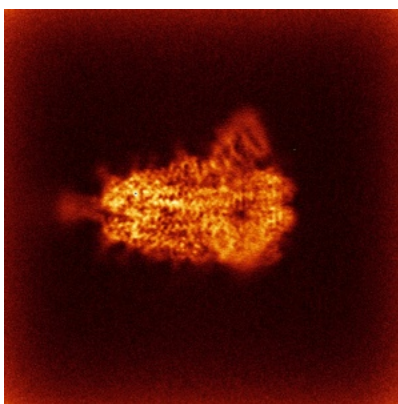


Z

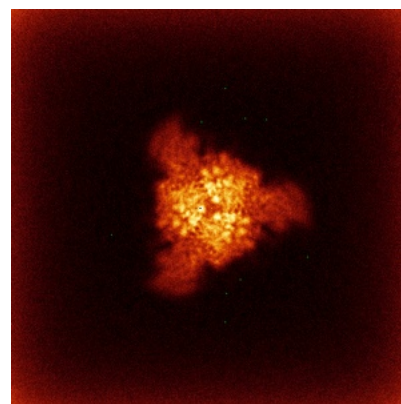
6.4.2 Raw map



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](#)

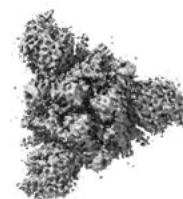
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.175. 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.

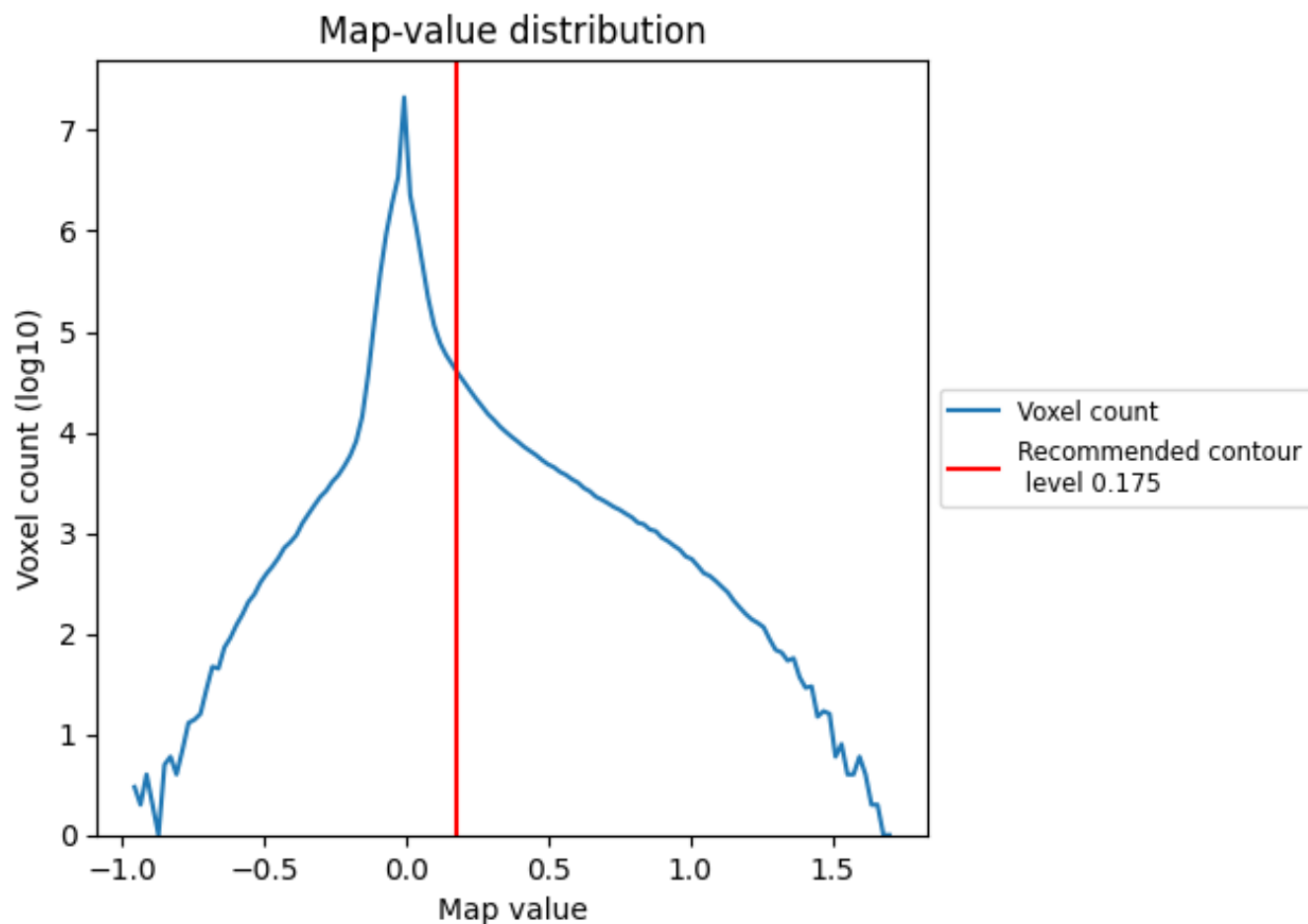
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

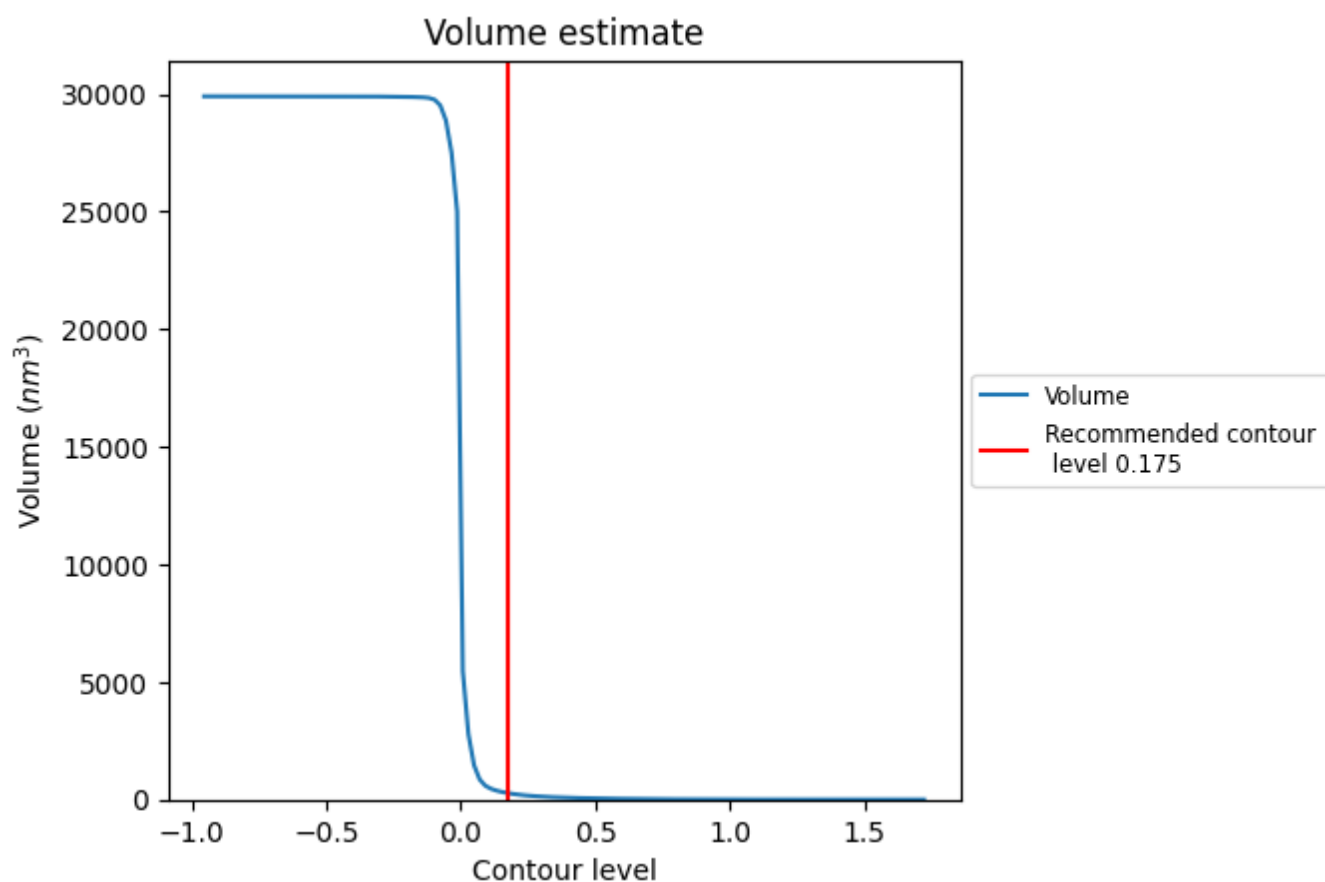
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

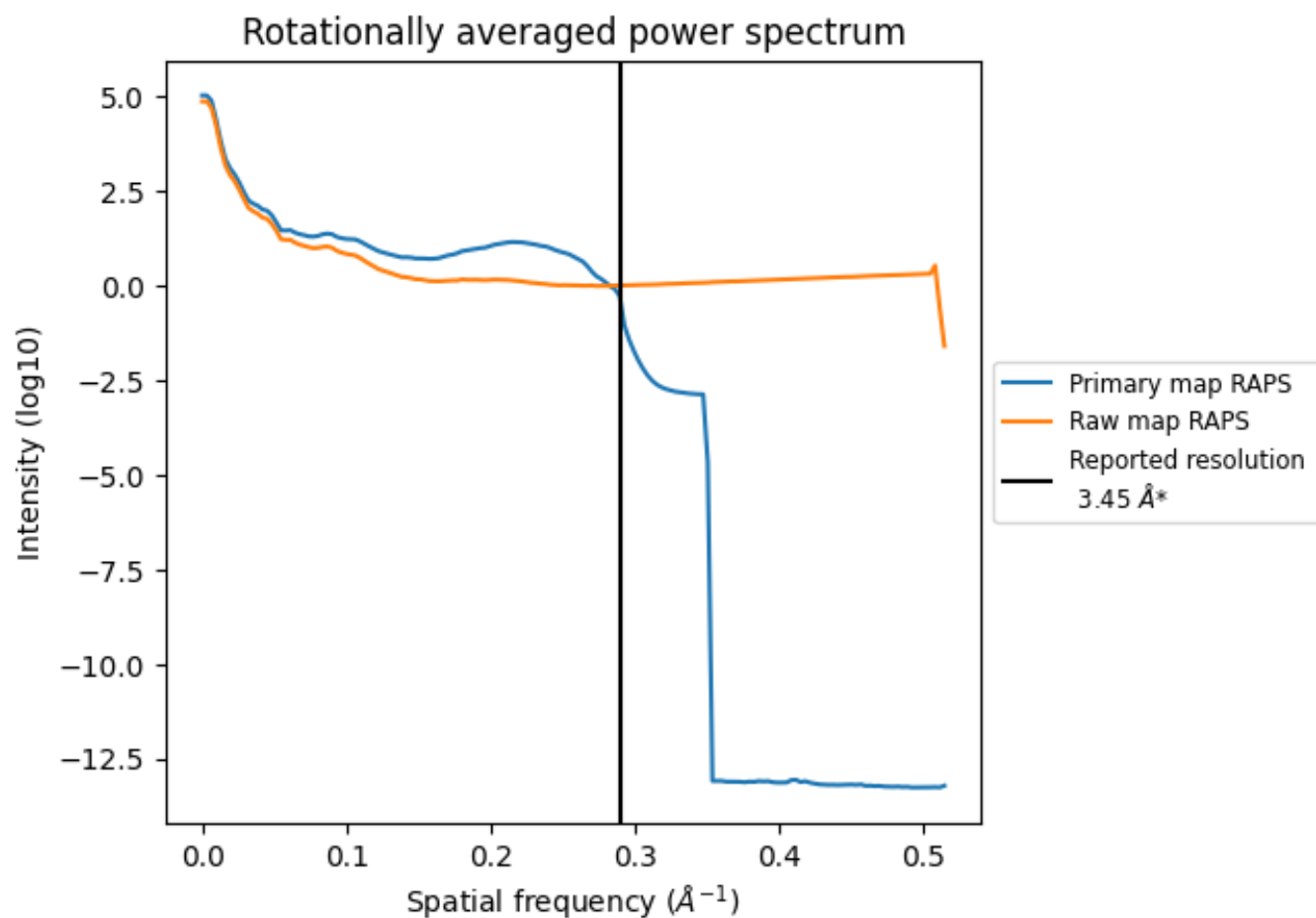
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 275 nm³; this corresponds to an approximate mass of 248 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 ⓘ

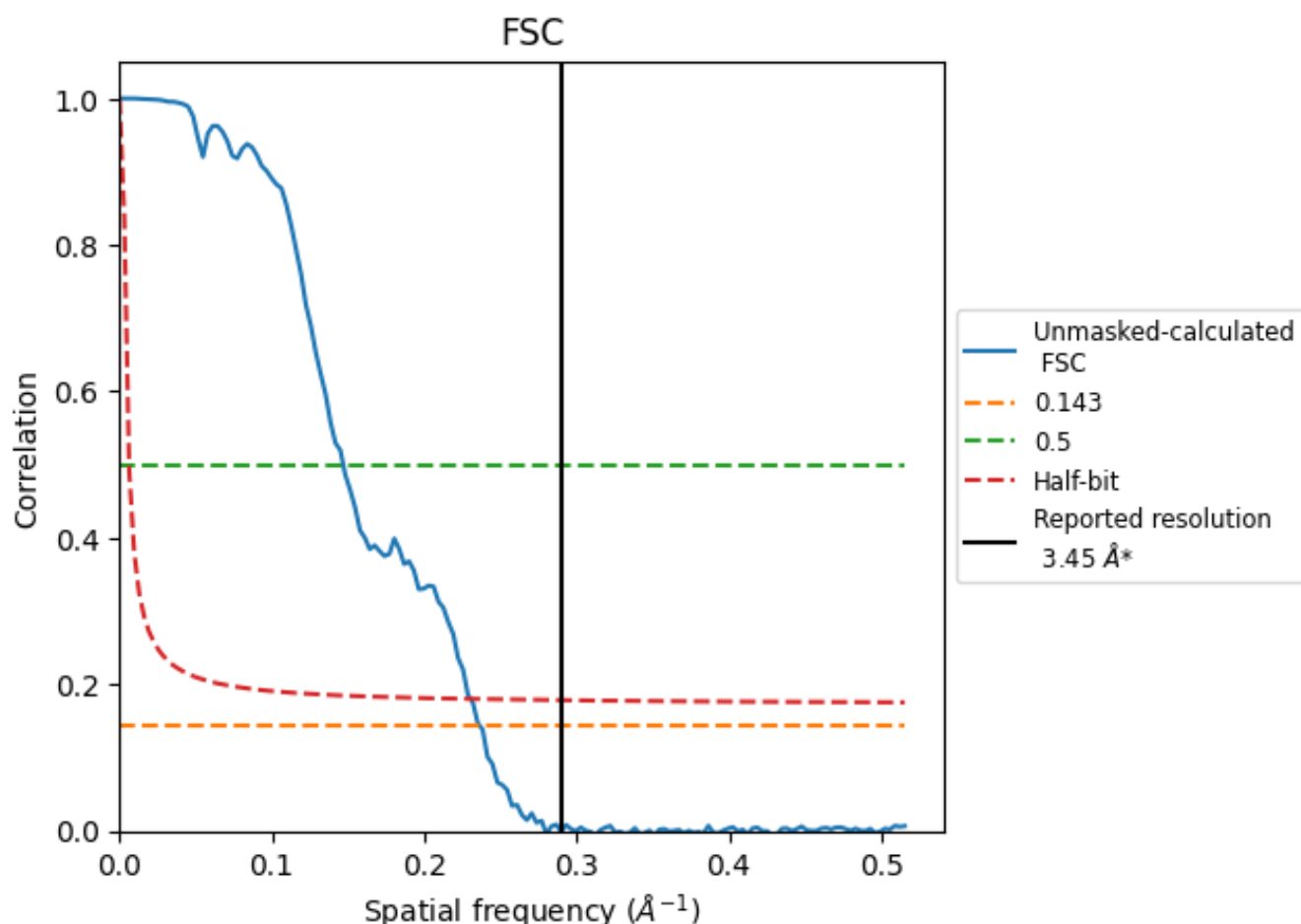


*Reported resolution corresponds to spatial frequency of 0.290 Å⁻¹

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 0.290 \AA^{-1}

8.2 Resolution estimates [i](#)

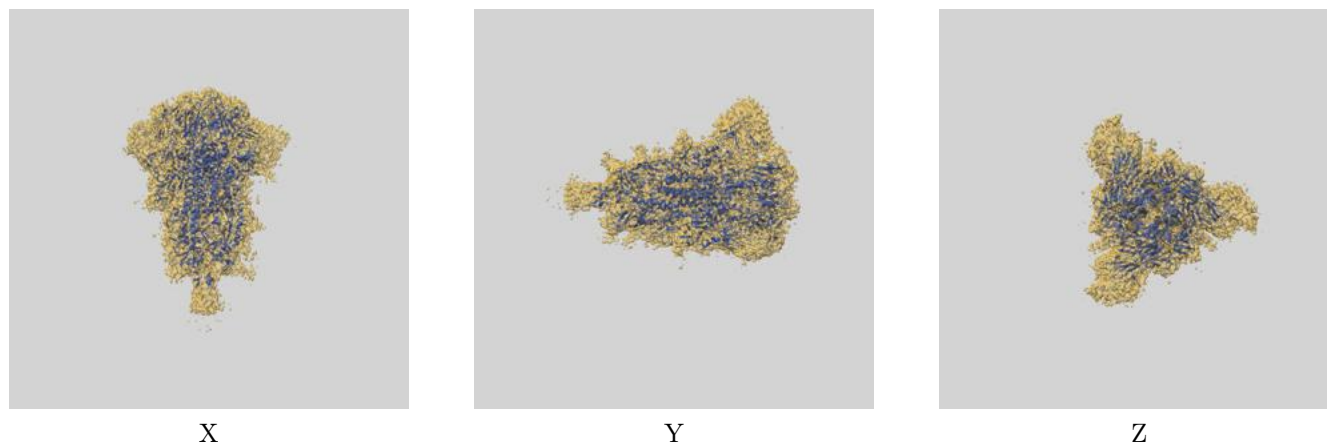
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.45	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.23	6.81	4.34

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.23 differs from the reported value 3.45 by more than 10 %

9 Map-model fit [i](#)

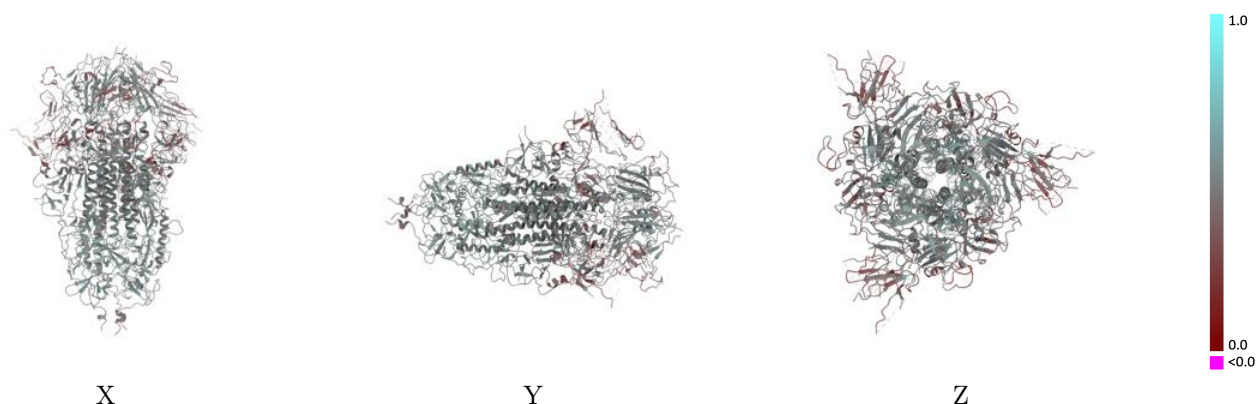
This section contains information regarding the fit between EMDB map EMD-33600 and PDB model 7Y42. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



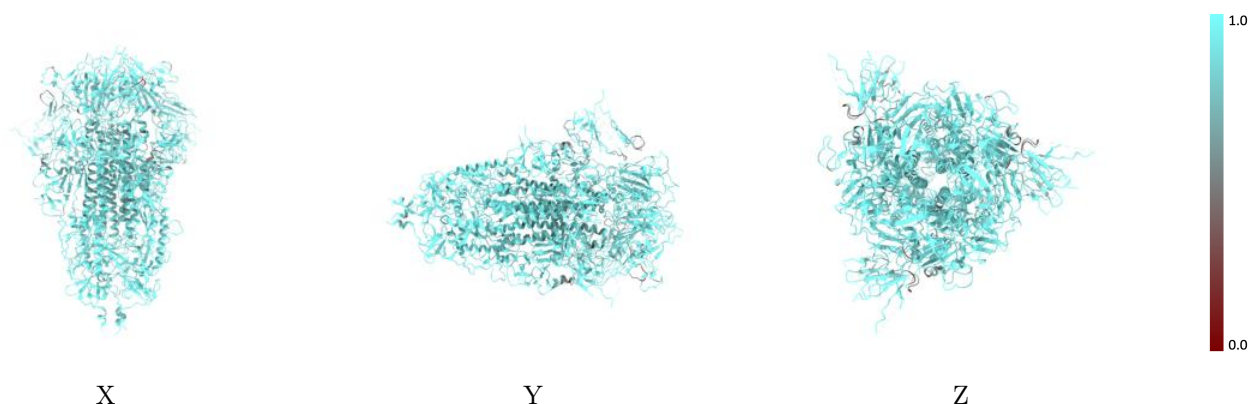
The images above show the 3D surface view of the map at the recommended contour level 0.175 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



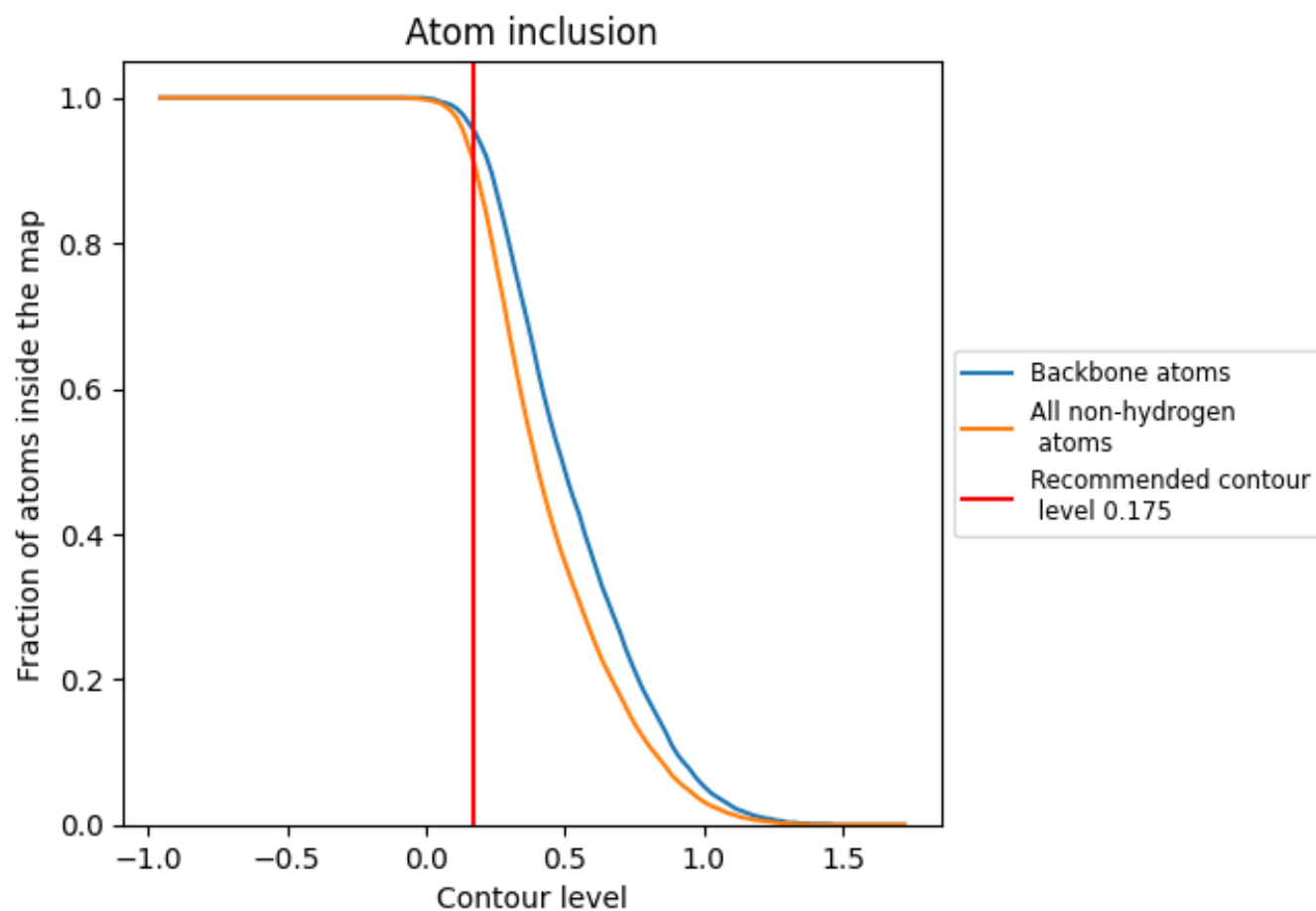
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.175).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% 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 (0.175) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9090	<div><div></div></div> 0.4730
A	<div><div></div></div> 0.9100	<div><div></div></div> 0.4730
B	<div><div></div></div> 0.9090	<div><div></div></div> 0.4730
D	<div><div></div></div> 0.9080	<div><div></div></div> 0.4720

