



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2021 – 02:12 PM JST

PDB ID : 7CZE
Title : Crystal structure of Epstein-Barr virus (EBV) gHgL and in complex with the ligand binding domain (LBD) of EphA2
Authors : Su, C.; Wu, L.L.; Song, H.; Chai, Y.; Qi, J.X.; Yan, J.H.; Gao, G.F.
Deposited on : 2020-09-08
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

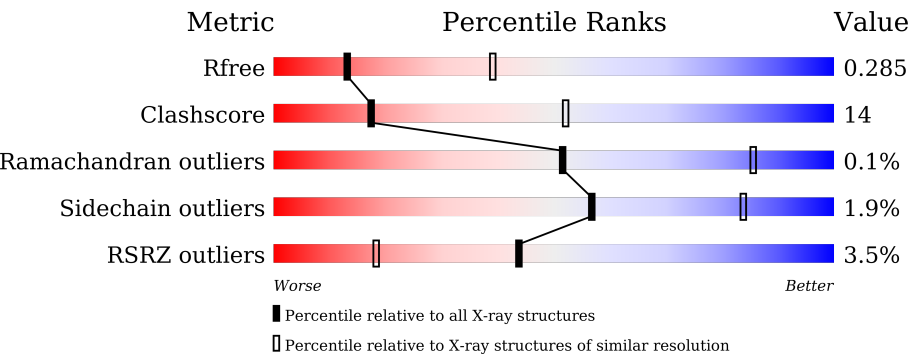
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	662	<div><div>3%</div><div><div></div><div>73%</div><div>25%</div><div>..</div></div></div>
1	C	662	<div><div>3%</div><div><div></div><div>74%</div><div>24%</div><div>..</div></div></div>
1	E	662	<div><div>4%</div><div><div></div><div>72%</div><div>26%</div><div>..</div></div></div>
1	G	662	<div><div>5%</div><div><div></div><div>72%</div><div>26%</div><div>..</div></div></div>
2	B	114	<div><div>3%</div><div><div></div><div>56%</div><div>36%</div><div>..</div></div></div>
2	D	114	<div><div>2%</div><div><div></div><div>62%</div><div>30%</div><div>.</div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	114	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>56%</div><div>35%</div><div>• • •</div></div></div>
2	H	114	<div><div><div></div><div></div><div></div></div><div><div>4%</div><div>60%</div><div>32%</div><div>• • •</div></div></div>
3	I	183	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>64%</div><div>25%</div><div>• 10%</div></div></div>
3	J	183	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>64%</div><div>25%</div><div>• 10%</div></div></div>
3	K	183	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>64%</div><div>25%</div><div>• 10%</div></div></div>
3	L	183	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>63%</div><div>26%</div><div>• 10%</div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29320 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Envelope glycoprotein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	655	Total	C	N	O	S	0	0	0
			5097	3268	842	956	31			
1	C	655	Total	C	N	O	S	0	0	0
			5097	3268	842	956	31			
1	E	655	Total	C	N	O	S	0	0	0
			5097	3268	842	956	31			
1	G	655	Total	C	N	O	S	0	0	0
			5097	3268	842	956	31			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	675	GLU	-	expression tag	UNP P03231
A	676	GLU	-	expression tag	UNP P03231
A	677	ARG	-	expression tag	UNP P03231
A	678	ALA	-	expression tag	UNP P03231
A	679	HIS	-	expression tag	UNP P03231
C	675	GLU	-	expression tag	UNP P03231
C	676	GLU	-	expression tag	UNP P03231
C	677	ARG	-	expression tag	UNP P03231
C	678	ALA	-	expression tag	UNP P03231
C	679	HIS	-	expression tag	UNP P03231
E	675	GLU	-	expression tag	UNP P03231
E	676	GLU	-	expression tag	UNP P03231
E	677	ARG	-	expression tag	UNP P03231
E	678	ALA	-	expression tag	UNP P03231
E	679	HIS	-	expression tag	UNP P03231
G	675	GLU	-	expression tag	UNP P03231
G	676	GLU	-	expression tag	UNP P03231
G	677	ARG	-	expression tag	UNP P03231
G	678	ALA	-	expression tag	UNP P03231
G	679	HIS	-	expression tag	UNP P03231

- Molecule 2 is a protein called Envelope glycoprotein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	109	Total	C	N	O	S	0	0	0
			842	532	146	160	4			
2	D	109	Total	C	N	O	S	0	0	0
			842	532	146	160	4			
2	F	109	Total	C	N	O	S	0	0	0
			842	532	146	160	4			
2	H	109	Total	C	N	O	S	0	0	0
			842	532	146	160	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	133	TRP	-	expression tag	UNP P03212
B	134	HIS	-	expression tag	UNP P03212
B	135	ARG	-	expression tag	UNP P03212
B	136	GLY	-	expression tag	UNP P03212
B	137	GLY	-	expression tag	UNP P03212
D	133	TRP	-	expression tag	UNP P03212
D	134	HIS	-	expression tag	UNP P03212
D	135	ARG	-	expression tag	UNP P03212
D	136	GLY	-	expression tag	UNP P03212
D	137	GLY	-	expression tag	UNP P03212
F	133	TRP	-	expression tag	UNP P03212
F	134	HIS	-	expression tag	UNP P03212
F	135	ARG	-	expression tag	UNP P03212
F	136	GLY	-	expression tag	UNP P03212
F	137	GLY	-	expression tag	UNP P03212
H	133	TRP	-	expression tag	UNP P03212
H	134	HIS	-	expression tag	UNP P03212
H	135	ARG	-	expression tag	UNP P03212
H	136	GLY	-	expression tag	UNP P03212
H	137	GLY	-	expression tag	UNP P03212

- Molecule 3 is a protein called Ephrin type-A receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	165	Total	C	N	O	S	0	1	0
			1335	862	216	248	9			
3	J	165	Total	C	N	O	S	0	1	0
			1335	862	216	248	9			
3	K	165	Total	C	N	O	S	0	1	0
			1335	862	216	248	9			

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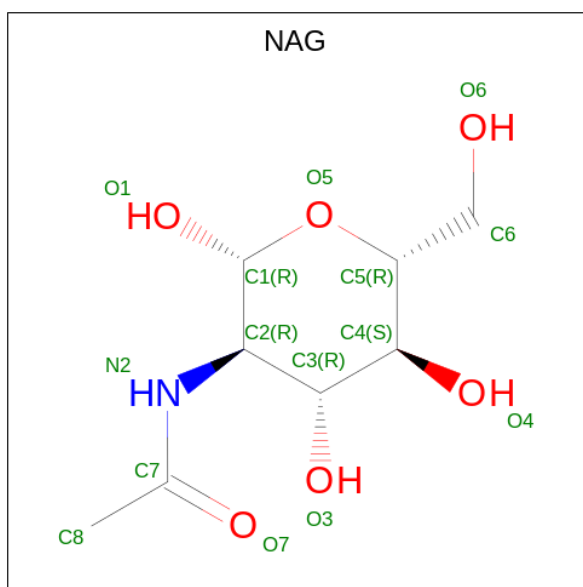
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	165	Total	C	N	O	S	0	1	0
			1335	862	216	248	9			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	201	HIS	-	expression tag	UNP P29317
I	202	HIS	-	expression tag	UNP P29317
I	203	HIS	-	expression tag	UNP P29317
I	204	HIS	-	expression tag	UNP P29317
I	205	HIS	-	expression tag	UNP P29317
I	206	HIS	-	expression tag	UNP P29317
I	207	HIS	-	expression tag	UNP P29317
I	208	HIS	-	expression tag	UNP P29317
J	201	HIS	-	expression tag	UNP P29317
J	202	HIS	-	expression tag	UNP P29317
J	203	HIS	-	expression tag	UNP P29317
J	204	HIS	-	expression tag	UNP P29317
J	205	HIS	-	expression tag	UNP P29317
J	206	HIS	-	expression tag	UNP P29317
J	207	HIS	-	expression tag	UNP P29317
J	208	HIS	-	expression tag	UNP P29317
K	201	HIS	-	expression tag	UNP P29317
K	202	HIS	-	expression tag	UNP P29317
K	203	HIS	-	expression tag	UNP P29317
K	204	HIS	-	expression tag	UNP P29317
K	205	HIS	-	expression tag	UNP P29317
K	206	HIS	-	expression tag	UNP P29317
K	207	HIS	-	expression tag	UNP P29317
K	208	HIS	-	expression tag	UNP P29317
L	201	HIS	-	expression tag	UNP P29317
L	202	HIS	-	expression tag	UNP P29317
L	203	HIS	-	expression tag	UNP P29317
L	204	HIS	-	expression tag	UNP P29317
L	205	HIS	-	expression tag	UNP P29317
L	206	HIS	-	expression tag	UNP P29317
L	207	HIS	-	expression tag	UNP P29317
L	208	HIS	-	expression tag	UNP P29317

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		

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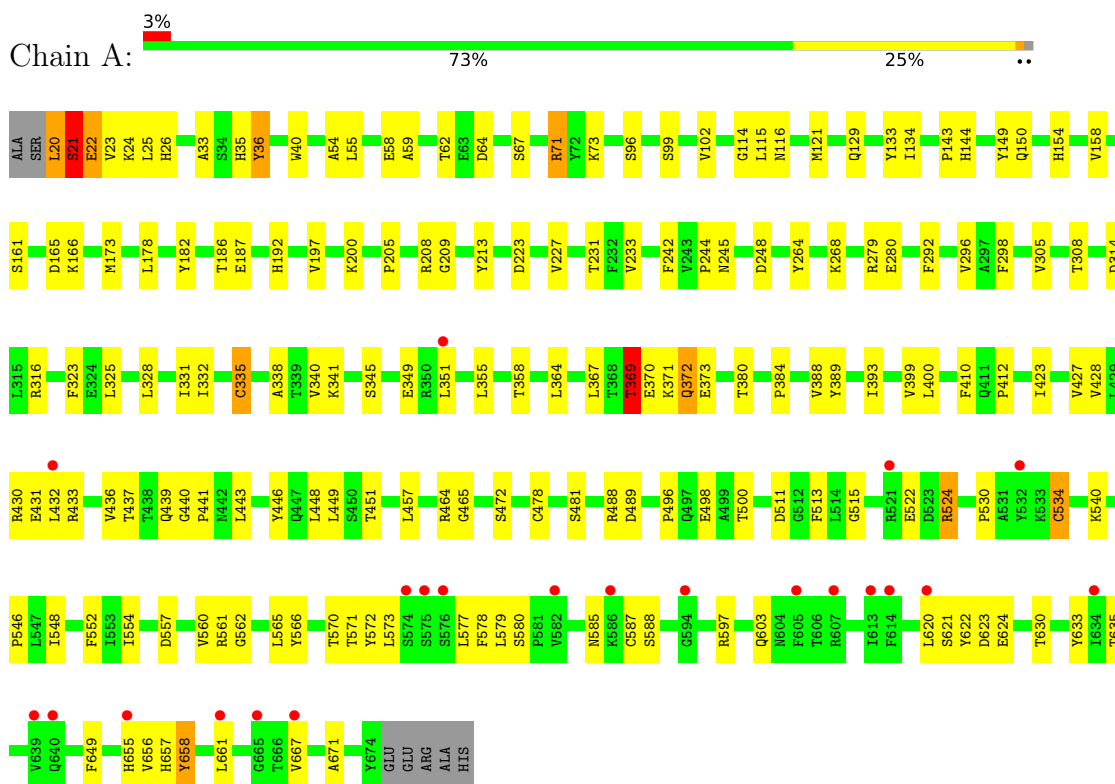
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots

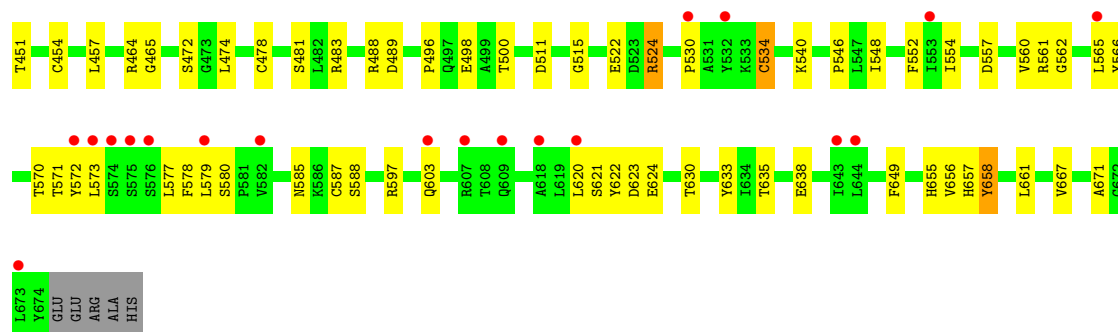
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Envelope glycoprotein H

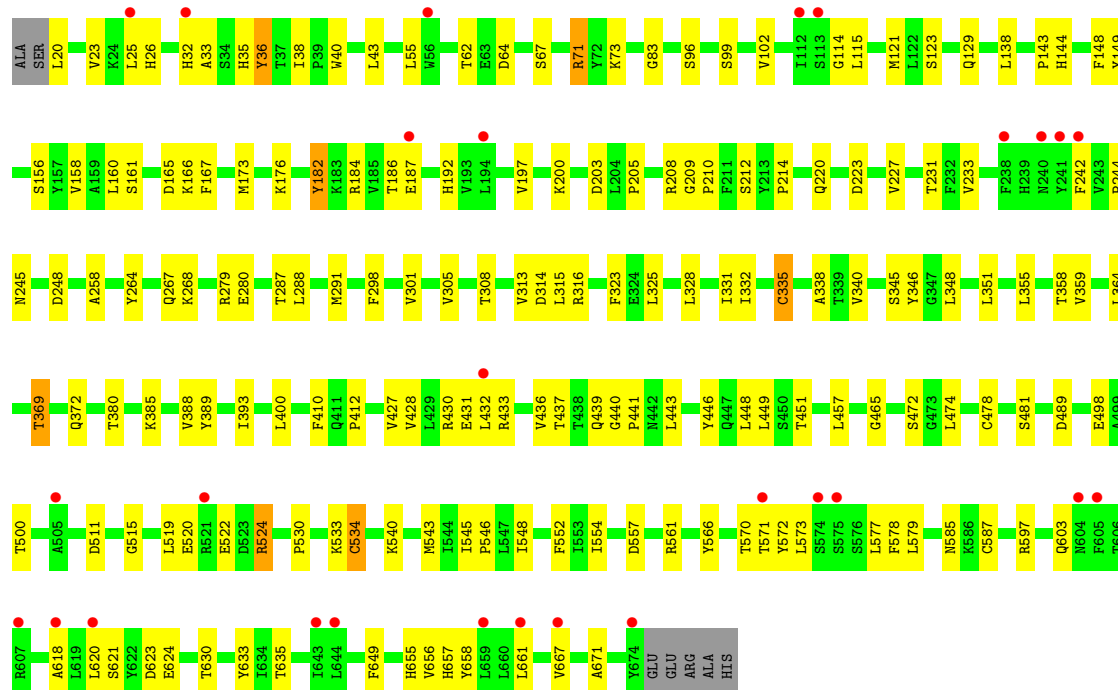


• Molecule 1: Envelope glycoprotein H

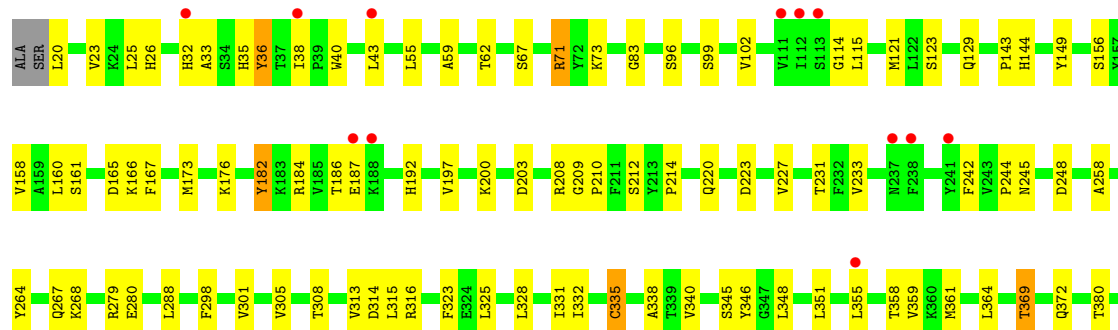
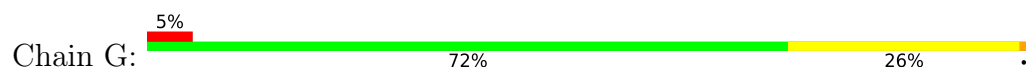


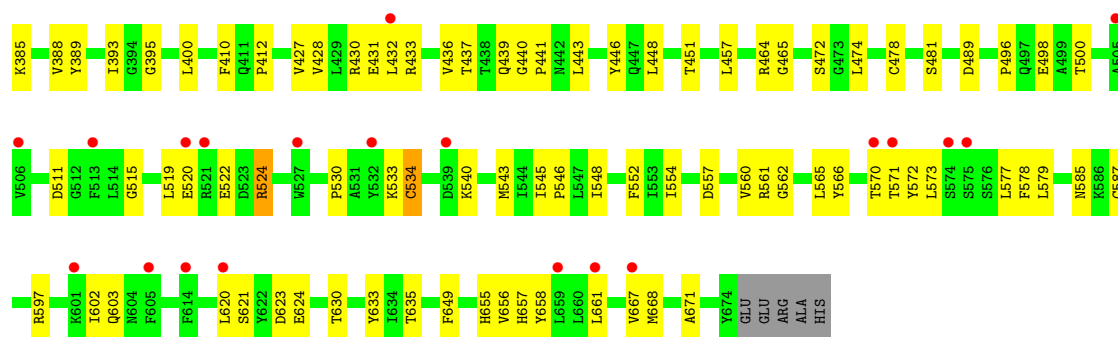


• Molecule 1: Envelope glycoprotein H



• Molecule 1: Envelope glycoprotein H





• Molecule 2: Envelope glycoprotein L



• Molecule 2: Envelope glycoprotein L

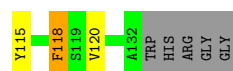


• Molecule 2: Envelope glycoprotein L



• Molecule 2: Envelope glycoprotein L





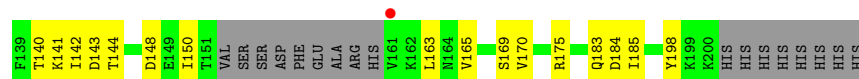
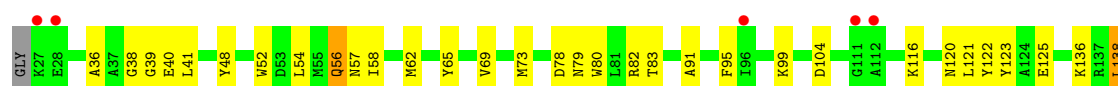
• Molecule 3: Ephrin type-A receptor 2



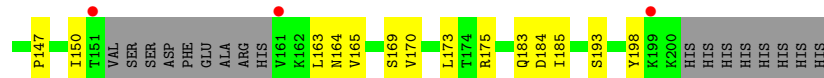
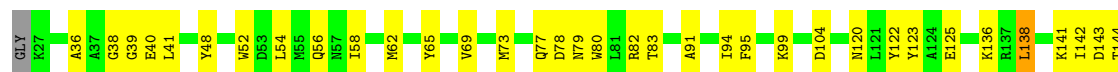
• Molecule 3: Ephrin type-A receptor 2



• Molecule 3: Ephrin type-A receptor 2



• Molecule 3: Ephrin type-A receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	94.46Å 113.81Å 119.65Å 90.03° 90.17° 89.89°	Depositor
Resolution (Å)	41.22 – 3.00 41.22 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (41.22-3.00) 97.9 (41.22-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.257 , 0.285 0.255 , 0.285	Depositor DCC
R_{free} test set	5133 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å ²)	83.4	Xtriage
Anisotropy	0.760	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.013 for h,-l,k 0.013 for h,l,-k 0.408 for h,-k,-l 0.145 for -h,k,-l 0.146 for -h,-k,l 0.017 for -h,-l,-k 0.018 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	29320	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.31	0/5206	0.57	0/7066
1	C	0.30	0/5206	0.57	0/7066
1	E	0.28	0/5206	0.56	0/7066
1	G	0.28	0/5206	0.56	0/7066
2	B	0.34	0/857	0.69	1/1164 (0.1%)
2	D	0.35	0/857	0.70	1/1164 (0.1%)
2	F	0.33	0/857	0.66	1/1164 (0.1%)
2	H	0.33	0/857	0.66	1/1164 (0.1%)
3	I	0.44	1/1370 (0.1%)	0.66	1/1853 (0.1%)
3	J	0.34	0/1370	0.65	1/1853 (0.1%)
3	K	0.38	1/1370 (0.1%)	0.67	1/1853 (0.1%)
3	L	0.33	0/1370	0.63	1/1853 (0.1%)
All	All	0.32	2/29732 (0.0%)	0.60	8/40332 (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
1	A	0	1
1	C	0	3
1	E	0	3
1	G	0	3
2	B	0	2
2	D	0	2
2	F	0	1
2	H	0	1
3	I	0	2
3	J	0	2
3	K	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	3
All	All	0	26

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	56	GLN	CD-NE2	10.36	1.58	1.32
3	K	56	GLN	CD-NE2	6.96	1.50	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	138	LEU	CA-CB-CG	6.57	130.40	115.30
2	B	40	LEU	CA-CB-CG	6.52	130.30	115.30
2	D	40	LEU	CA-CB-CG	6.48	130.20	115.30
3	I	138	LEU	CA-CB-CG	6.38	129.97	115.30
2	H	40	LEU	CA-CB-CG	6.25	129.69	115.30
2	F	40	LEU	CA-CB-CG	6.25	129.67	115.30
3	K	138	LEU	CA-CB-CG	5.97	129.03	115.30
3	L	138	LEU	CA-CB-CG	5.72	128.47	115.30

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	572	TYR	Peptide
2	B	35	ARG	Peptide
2	B	36	ALA	Peptide
1	C	20	LEU	Peptide
1	C	369	THR	Peptide
1	C	572	TYR	Peptide
2	D	35	ARG	Peptide
2	D	36	ALA	Peptide
1	E	20	LEU	Peptide
1	E	369	THR	Peptide
1	E	572	TYR	Peptide
2	F	35	ARG	Peptide
1	G	20	LEU	Peptide
1	G	369	THR	Peptide
1	G	572	TYR	Peptide
2	H	35	ARG	Peptide

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Mol	Chain	Res	Type	Group
3	I	36	ALA	Peptide
3	I	38	GLY	Peptide
3	J	36	ALA	Peptide
3	J	38	GLY	Peptide
3	K	36	ALA	Peptide
3	K	38	GLY	Peptide
3	K	39	GLY	Peptide
3	L	36	ALA	Peptide
3	L	38	GLY	Peptide
3	L	39	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5097	0	5113	154	0
1	C	5097	0	5113	129	0
1	E	5097	0	5113	140	0
1	G	5097	0	5113	136	0
2	B	842	0	828	34	0
2	D	842	0	828	35	0
2	F	842	0	828	40	0
2	H	842	0	828	40	0
3	I	1335	0	1293	36	0
3	J	1335	0	1293	39	0
3	K	1335	0	1293	38	0
3	L	1335	0	1293	33	0
4	A	28	0	26	2	0
4	B	28	0	26	1	0
4	C	28	0	26	2	0
4	D	28	0	26	2	0
4	E	28	0	26	2	0
4	F	28	0	26	0	0
4	G	28	0	26	2	0
4	H	28	0	26	1	0
All	All	29320	0	29144	807	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 14.

All (807) 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:20:LEU:CD1	1:A:40:TRP:CB	2.14	1.26
1:A:20:LEU:CD1	1:A:40:TRP:HB3	1.68	1.20
3:K:40:GLU:HG3	3:K:41:LEU:H	1.10	1.15
3:L:40:GLU:HG3	3:L:41:LEU:H	1.11	1.13
1:A:20:LEU:HD12	1:A:40:TRP:HB3	1.17	1.12
3:I:40:GLU:HG3	3:I:41:LEU:H	1.14	1.06
3:J:40:GLU:HG3	3:J:41:LEU:H	1.16	1.04
1:A:20:LEU:CD1	1:A:40:TRP:CG	2.42	1.03
1:A:20:LEU:HD13	1:A:40:TRP:CB	1.91	1.01
1:A:20:LEU:HD12	1:A:40:TRP:CB	1.89	0.91
1:A:20:LEU:HD13	1:A:40:TRP:CG	2.03	0.91
1:A:373:GLU:HG2	1:A:423:ILE:CD1	2.04	0.88
1:C:571:THR:HG23	1:C:573:LEU:H	1.35	0.88
1:A:571:THR:HG23	1:A:573:LEU:H	1.35	0.88
1:E:571:THR:HG23	1:E:573:LEU:H	1.37	0.87
1:G:571:THR:HG23	1:G:573:LEU:H	1.37	0.87
1:A:367:LEU:O	1:A:372:GLN:NE2	2.08	0.86
3:I:40:GLU:HG3	3:I:41:LEU:N	1.90	0.86
3:J:40:GLU:HG3	3:J:41:LEU:N	1.92	0.84
1:C:114:GLY:HA2	1:C:358:THR:HG21	1.60	0.84
1:C:649:PHE:HA	1:C:658:TYR:HE2	1.41	0.83
1:G:649:PHE:HA	1:G:658:TYR:HE2	1.43	0.83
1:E:114:GLY:HA2	1:E:358:THR:HG21	1.61	0.82
1:A:649:PHE:HA	1:A:658:TYR:HE2	1.44	0.81
3:K:40:GLU:HG3	3:K:41:LEU:N	1.86	0.81
1:A:20:LEU:HD11	1:A:40:TRP:CG	2.15	0.81
1:A:114:GLY:HA2	1:A:358:THR:HG21	1.63	0.81
2:B:34:LEU:HD12	2:B:38:HIS:HB3	1.63	0.81
3:L:40:GLU:HG3	3:L:41:LEU:N	1.86	0.80
2:D:34:LEU:HD12	2:D:38:HIS:HB3	1.65	0.79
1:G:114:GLY:HA2	1:G:358:THR:HG21	1.65	0.78
1:E:400:LEU:HD22	1:E:446:TYR:CD1	2.17	0.78
3:K:123:TYR:HE2	3:K:125:GLU:HG3	1.47	0.78
2:H:34:LEU:HD12	2:H:38:HIS:HB3	1.66	0.77
1:G:400:LEU:HD22	1:G:446:TYR:CD1	2.18	0.77
3:L:123:TYR:HE2	3:L:125:GLU:HG3	1.49	0.77
2:F:34:LEU:HD12	2:F:38:HIS:HB3	1.64	0.77
1:E:649:PHE:HA	1:E:658:TYR:HE2	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:123:TYR:HE2	3:J:125:GLU:HG3	1.49	0.77
1:A:20:LEU:HD13	1:A:40:TRP:HB2	1.66	0.76
3:I:123:TYR:HE2	3:I:125:GLU:HG3	1.51	0.75
2:F:69:ASN:HD22	2:F:70:GLY:N	1.84	0.74
2:H:24:TRP:HA	2:H:24:TRP:CE3	2.22	0.74
2:D:69:ASN:HD22	2:D:70:GLY:N	1.86	0.74
1:A:373:GLU:HG2	1:A:423:ILE:HD12	1.68	0.74
2:H:69:ASN:HD22	2:H:70:GLY:N	1.83	0.73
2:B:69:ASN:HD22	2:B:70:GLY:N	1.86	0.72
3:L:79:ASN:HB2	3:L:184:ASP:HB3	1.72	0.72
1:A:116:ASN:HD22	1:A:371:LYS:HE3	1.54	0.71
2:H:24:TRP:HA	2:H:24:TRP:HE3	1.56	0.70
1:A:20:LEU:CD1	1:A:40:TRP:HB2	2.16	0.70
1:A:20:LEU:HD13	1:A:40:TRP:CD1	2.27	0.69
1:A:373:GLU:HG2	1:A:423:ILE:HD13	1.75	0.69
1:E:102:VAL:HG11	1:E:351:LEU:HD12	1.75	0.69
1:E:428:VAL:HG21	1:E:446:TYR:CD2	2.27	0.69
1:E:428:VAL:HG21	1:E:446:TYR:CE2	2.28	0.69
1:G:102:VAL:HG11	1:G:351:LEU:HD12	1.75	0.69
1:G:428:VAL:HG21	1:G:446:TYR:CE2	2.29	0.68
3:K:79:ASN:HB2	3:K:184:ASP:HB3	1.75	0.68
1:G:428:VAL:HG21	1:G:446:TYR:CD2	2.27	0.68
1:C:436:VAL:HG12	1:C:437:THR:H	1.59	0.68
1:A:400:LEU:HD22	1:A:446:TYR:CD1	2.28	0.67
1:C:400:LEU:HD22	1:C:446:TYR:CD1	2.29	0.67
1:A:436:VAL:HG12	1:A:437:THR:H	1.59	0.67
1:A:323:PHE:HD1	1:A:380:THR:HG1	1.43	0.67
2:H:100:LEU:HD12	2:H:105:ARG:HB3	1.76	0.67
2:B:100:LEU:HD12	2:B:105:ARG:HB3	1.77	0.67
1:E:400:LEU:HD22	1:E:446:TYR:HD1	1.56	0.67
3:J:120:ASN:HB2	3:J:183:GLN:HB3	1.76	0.66
2:D:100:LEU:HD12	2:D:105:ARG:HB3	1.78	0.66
1:E:55:LEU:HD11	2:F:95:ARG:HH12	1.59	0.66
1:E:436:VAL:HG12	1:E:437:THR:H	1.58	0.66
1:E:187:GLU:HB3	3:J:63:PRO:HD2	1.77	0.66
1:G:436:VAL:HG12	1:G:437:THR:H	1.58	0.66
1:G:649:PHE:HA	1:G:658:TYR:CE2	2.29	0.66
1:G:25:LEU:HD12	2:H:107:LEU:HD21	1.77	0.66
1:C:102:VAL:HG11	1:C:351:LEU:HD12	1.78	0.65
1:E:25:LEU:HD12	2:F:107:LEU:HD21	1.77	0.65
3:I:99:LYS:HG2	3:I:165:VAL:HG22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:79:ASN:HB2	3:J:184:ASP:HB3	1.78	0.65
3:L:123:TYR:CE2	3:L:125:GLU:HG3	2.31	0.65
1:G:400:LEU:HD22	1:G:446:TYR:HD1	1.58	0.65
1:E:649:PHE:HA	1:E:658:TYR:CE2	2.30	0.64
1:E:433:ARG:NH2	1:E:524:ARG:HH11	1.95	0.64
2:F:70:GLY:O	2:F:73:GLN:NE2	2.31	0.64
1:G:245:ASN:ND2	1:G:248:ASP:OD2	2.30	0.64
1:A:33:ALA:HB1	1:A:35:HIS:CE1	2.33	0.64
1:G:433:ARG:NH2	1:G:524:ARG:HH11	1.96	0.64
1:A:102:VAL:HG11	1:A:351:LEU:HD12	1.80	0.64
1:C:657:HIS:C	1:C:658:TYR:HD1	2.01	0.64
1:C:428:VAL:HG21	1:C:446:TYR:CE2	2.32	0.64
1:A:428:VAL:HG21	1:A:446:TYR:CE2	2.33	0.63
1:C:323:PHE:HD1	1:C:380:THR:HG1	1.46	0.63
1:E:566:TYR:CE1	1:E:597:ARG:HD3	2.33	0.63
1:G:55:LEU:HD11	2:H:95:ARG:HH12	1.64	0.63
2:H:70:GLY:O	2:H:73:GLN:NE2	2.32	0.63
1:C:245:ASN:ND2	1:C:248:ASP:OD2	2.32	0.63
3:I:79:ASN:HB2	3:I:184:ASP:HB3	1.80	0.63
1:A:511:ASP:O	1:A:515:GLY:N	2.31	0.62
1:G:566:TYR:CE1	1:G:597:ARG:HD3	2.34	0.62
2:H:67:PRO:O	2:H:68:LYS:HG3	2.00	0.62
1:E:323:PHE:HD1	1:E:380:THR:HG1	1.45	0.62
1:A:231:THR:HG22	1:A:233:VAL:H	1.64	0.62
1:A:657:HIS:C	1:A:658:TYR:HD1	2.03	0.62
2:F:67:PRO:O	2:F:68:LYS:HG3	2.00	0.62
1:A:393:ILE:HD13	1:A:439:GLN:HG3	1.82	0.62
1:E:548:ILE:HG21	4:E:702:NAG:H82	1.81	0.62
2:H:34:LEU:HD11	2:H:78:ARG:HG2	1.82	0.62
1:C:25:LEU:HD23	2:D:48:ILE:HB	1.80	0.62
1:C:393:ILE:HD13	1:C:439:GLN:HG3	1.82	0.62
2:H:78:ARG:HH22	3:K:56:GLN:HE21	1.47	0.62
1:E:161:SER:OG	1:E:165:ASP:HA	2.00	0.61
2:F:100:LEU:HD12	2:F:105:ARG:HB3	1.82	0.61
2:B:67:PRO:O	2:B:68:LYS:HG3	1.99	0.61
1:G:323:PHE:HD1	1:G:380:THR:HG1	1.46	0.61
1:A:305:VAL:O	1:A:308:THR:HG22	1.99	0.61
1:C:465:GLY:HA3	1:C:472:SER:HB2	1.83	0.61
1:E:245:ASN:ND2	1:E:248:ASP:OD2	2.33	0.61
1:C:231:THR:HG22	1:C:233:VAL:H	1.65	0.61
2:H:60:SER:HB2	2:H:118:PHE:CD2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LEU:HD23	2:B:48:ILE:HB	1.82	0.60
2:D:67:PRO:O	2:D:68:LYS:HG3	2.00	0.60
1:C:133:TYR:HD2	1:C:134:ILE:N	1.99	0.60
1:C:511:ASP:O	1:C:515:GLY:N	2.33	0.60
2:F:62:ALA:HB3	2:F:80:ALA:HB3	1.83	0.60
1:C:400:LEU:HD22	1:C:446:TYR:CE1	2.36	0.60
1:C:433:ARG:NH2	1:C:524:ARG:HH11	2.00	0.60
1:E:657:HIS:C	1:E:658:TYR:HD1	2.04	0.60
1:A:373:GLU:CG	1:A:423:ILE:HD12	2.31	0.60
1:E:305:VAL:O	1:E:308:THR:HG22	2.02	0.60
1:G:393:ILE:HD13	1:G:439:GLN:HG3	1.84	0.60
1:C:548:ILE:HG21	4:C:702:NAG:H82	1.84	0.60
1:G:540:LYS:HB2	1:G:557:ASP:HB2	1.83	0.60
3:K:99:LYS:HB3	3:K:163:LEU:HD11	1.82	0.60
1:C:328:LEU:HG	1:C:332:ILE:HD11	1.84	0.60
2:H:62:ALA:HB3	2:H:80:ALA:HB3	1.84	0.60
1:C:305:VAL:O	1:C:308:THR:HG22	2.00	0.59
1:E:231:THR:HG22	1:E:233:VAL:H	1.67	0.59
1:C:649:PHE:HA	1:C:658:TYR:CE2	2.30	0.59
1:A:400:LEU:HD22	1:A:446:TYR:CE1	2.37	0.59
1:A:488:ARG:NH1	1:A:511:ASP:OD1	2.36	0.59
1:C:279:ARG:HG3	1:C:280:GLU:HG2	1.83	0.59
2:F:60:SER:HB2	2:F:118:PHE:CD2	2.37	0.59
1:A:540:LYS:HB2	1:A:557:ASP:HB2	1.83	0.59
1:E:62:THR:HG21	2:F:34:LEU:HD23	1.83	0.59
3:J:99:LYS:HG2	3:J:165:VAL:HG22	1.84	0.59
1:G:161:SER:OG	1:G:165:ASP:HA	2.01	0.59
2:B:60:SER:HB2	2:B:118:PHE:CD2	2.38	0.59
2:B:62:ALA:HB3	2:B:80:ALA:HB3	1.84	0.59
3:J:80:TRP:HH2	3:J:122:TYR:CE2	2.21	0.59
3:K:123:TYR:CE2	3:K:125:GLU:HG3	2.33	0.59
1:G:305:VAL:O	1:G:308:THR:HG22	2.03	0.59
3:K:99:LYS:HG2	3:K:165:VAL:HG22	1.84	0.59
1:A:433:ARG:NH2	1:A:524:ARG:HH11	2.00	0.59
1:C:385:LYS:NZ	3:K:148:ASP:OD2	2.29	0.59
1:C:488:ARG:NH1	1:C:511:ASP:OD1	2.36	0.59
3:I:78:ASP:OD1	3:I:183:GLN:NE2	2.36	0.59
1:A:428:VAL:HG21	1:A:446:TYR:CD2	2.38	0.58
1:G:657:HIS:C	1:G:658:TYR:HD1	2.06	0.58
1:C:261:TYR:HD2	1:C:300:LYS:HD3	1.67	0.58
1:C:540:LYS:HB2	1:C:557:ASP:HB2	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:ASN:HD22	2:D:69:ASN:C	2.06	0.58
1:A:530:PRO:HD2	1:A:585:ASN:HD21	1.68	0.58
1:C:242:PHE:CZ	1:C:244:PRO:HG3	2.39	0.58
2:D:86:VAL:HG11	2:D:115:TYR:HB2	1.85	0.58
1:A:279:ARG:HG3	1:A:280:GLU:HG2	1.84	0.58
1:E:332:ILE:HG22	1:E:338:ALA:HB3	1.86	0.58
1:G:62:THR:HG21	2:H:34:LEU:HD23	1.85	0.58
3:J:52:TRP:HA	3:J:69:VAL:HB	1.86	0.58
2:D:60:SER:HB2	2:D:118:PHE:CD2	2.39	0.58
1:G:332:ILE:HG22	1:G:338:ALA:HB3	1.86	0.58
1:A:393:ILE:HD12	1:A:393:ILE:H	1.69	0.58
1:E:328:LEU:HG	1:E:332:ILE:HD11	1.85	0.58
1:G:231:THR:HG22	1:G:233:VAL:H	1.69	0.58
3:I:52:TRP:HA	3:I:69:VAL:HB	1.86	0.57
1:A:369:THR:O	1:A:369:THR:OG1	2.21	0.57
1:A:649:PHE:HA	1:A:658:TYR:CE2	2.32	0.57
3:J:123:TYR:CE2	3:J:125:GLU:HG3	2.36	0.57
1:C:530:PRO:HD2	1:C:585:ASN:HD21	1.69	0.57
1:A:489:ASP:OD1	1:A:489:ASP:N	2.35	0.57
1:E:393:ILE:HD13	1:E:439:GLN:HG3	1.86	0.57
1:A:372:GLN:HG2	1:A:399:VAL:HG22	1.87	0.57
1:E:33:ALA:HB1	1:E:35:HIS:CE1	2.40	0.57
1:E:298:PHE:CD1	1:E:325:LEU:HD22	2.39	0.57
1:C:393:ILE:HD12	1:C:393:ILE:H	1.70	0.57
1:G:242:PHE:CZ	1:G:244:PRO:HG3	2.40	0.57
1:A:245:ASN:ND2	1:A:248:ASP:OD2	2.37	0.57
2:F:34:LEU:HD11	2:F:78:ARG:HG2	1.87	0.57
1:A:465:GLY:HA3	1:A:472:SER:HB2	1.87	0.56
3:L:99:LYS:HG2	3:L:165:VAL:HG22	1.87	0.56
1:G:298:PHE:CD1	1:G:325:LEU:HD22	2.39	0.56
1:A:328:LEU:HG	1:A:332:ILE:HD11	1.87	0.56
1:E:160:LEU:HB3	1:E:338:ALA:HB2	1.86	0.56
1:E:197:VAL:HB	1:E:227:VAL:HB	1.88	0.56
1:A:158:VAL:HG22	1:A:340:VAL:HG22	1.88	0.56
2:B:69:ASN:HD22	2:B:69:ASN:C	2.09	0.56
1:A:62:THR:HG21	2:B:34:LEU:HD23	1.86	0.56
1:A:432:LEU:HD21	1:A:443:LEU:HD11	1.89	0.55
1:G:530:PRO:HD2	1:G:585:ASN:HD21	1.71	0.55
1:C:623:ASP:OD1	1:C:624:GLU:N	2.38	0.55
1:E:530:PRO:HD2	1:E:585:ASN:HD21	1.71	0.55
2:D:24:TRP:N	2:D:24:TRP:CD1	2.73	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:540:LYS:HB2	1:E:557:ASP:HB2	1.88	0.55
1:A:566:TYR:CD2	1:A:667:VAL:HB	2.41	0.55
3:I:120:ASN:HB2	3:I:183:GLN:HB3	1.88	0.55
3:I:123:TYR:CE2	3:I:125:GLU:HG3	2.38	0.55
3:I:143:ASP:OD1	3:I:144:THR:N	2.37	0.55
1:C:489:ASP:OD1	1:C:489:ASP:N	2.38	0.55
3:L:99:LYS:HB3	3:L:163:LEU:HD11	1.87	0.55
1:A:242:PHE:CZ	1:A:244:PRO:HG3	2.42	0.55
1:G:393:ILE:HD12	1:G:393:ILE:H	1.70	0.55
1:A:623:ASP:OD1	1:A:624:GLU:N	2.39	0.55
1:C:566:TYR:CD2	1:C:667:VAL:HB	2.41	0.55
2:F:24:TRP:CD1	2:F:24:TRP:N	2.72	0.55
1:G:115:LEU:HD23	1:G:355:LEU:HD23	1.87	0.55
1:G:160:LEU:HB3	1:G:338:ALA:HB2	1.89	0.55
2:H:69:ASN:HD22	2:H:69:ASN:C	2.10	0.55
1:A:22:GLU:OE2	1:A:24:LYS:NZ	2.39	0.55
1:C:55:LEU:HD11	2:D:95:ARG:HH12	1.71	0.55
1:C:620:LEU:HD13	1:C:661:LEU:HD13	1.88	0.54
1:E:393:ILE:H	1:E:393:ILE:HD12	1.70	0.54
2:F:64:LEU:O	2:F:77:SER:HA	2.07	0.54
1:G:412:PRO:HD3	1:G:457:LEU:HB3	1.89	0.54
3:L:80:TRP:HH2	3:L:122:TYR:CE2	2.25	0.54
1:C:62:THR:HG21	2:D:34:LEU:HD23	1.88	0.54
2:D:62:ALA:HB3	2:D:80:ALA:HB3	1.88	0.54
2:D:70:GLY:O	2:D:73:GLN:NE2	2.39	0.54
1:G:33:ALA:HB1	1:G:35:HIS:CE1	2.42	0.54
1:E:96:SER:HB2	1:E:99:SER:OG	2.07	0.54
1:E:566:TYR:CD2	1:E:667:VAL:HB	2.41	0.54
1:A:121:MET:HE2	1:A:351:LEU:HD13	1.90	0.54
1:C:298:PHE:CD1	1:C:325:LEU:HD22	2.42	0.54
3:L:143:ASP:OD1	3:L:144:THR:N	2.40	0.54
3:J:58:ILE:HA	3:J:62:MET:O	2.08	0.54
1:G:96:SER:HB2	1:G:99:SER:OG	2.09	0.53
1:A:298:PHE:CD1	1:A:325:LEU:HD22	2.43	0.53
1:C:23:VAL:HG23	1:C:40:TRP:HE1	1.73	0.53
1:C:331:ILE:O	1:C:335:CYS:HB2	2.08	0.53
2:H:64:LEU:O	2:H:77:SER:HA	2.09	0.53
3:J:143:ASP:OD1	3:J:144:THR:N	2.38	0.53
1:E:43:LEU:HD21	2:F:104:LEU:HD21	1.91	0.53
3:I:80:TRP:HH2	3:I:122:TYR:CE2	2.26	0.53
2:B:70:GLY:O	2:B:73:GLN:NE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:123:TYR:CE1	3:K:170:VAL:HG21	2.44	0.53
1:A:149:TYR:CE2	1:A:208:ARG:HA	2.43	0.53
3:L:123:TYR:CE1	3:L:170:VAL:HG21	2.43	0.53
1:A:115:LEU:HD23	1:A:355:LEU:HD23	1.90	0.53
1:A:205:PRO:O	1:A:213:TYR:OH	2.15	0.53
1:G:158:VAL:HG22	1:G:340:VAL:HG22	1.91	0.53
1:G:328:LEU:HG	1:G:332:ILE:HD11	1.90	0.53
1:G:566:TYR:CD2	1:G:667:VAL:HB	2.43	0.52
1:E:242:PHE:CZ	1:E:244:PRO:HG3	2.45	0.52
1:A:36:TYR:CD2	2:B:107:LEU:HB2	2.45	0.52
1:A:548:ILE:HG21	4:A:702:NAG:H82	1.92	0.52
1:C:149:TYR:CZ	1:C:208:ARG:HG3	2.45	0.52
1:C:432:LEU:HD21	1:C:443:LEU:HD11	1.92	0.52
1:G:489:ASP:N	1:G:489:ASP:OD1	2.42	0.52
1:A:26:HIS:HD1	1:A:35:HIS:CG	2.28	0.52
1:A:451:THR:HA	1:A:481:SER:HB2	1.92	0.52
1:A:149:TYR:CZ	1:A:208:ARG:HG3	2.45	0.52
2:B:86:VAL:HG11	2:B:115:TYR:HB2	1.91	0.52
1:C:36:TYR:CD2	2:D:107:LEU:HB2	2.45	0.52
1:G:436:VAL:HG12	1:G:437:THR:N	2.25	0.52
1:C:621:SER:HB3	1:C:630:THR:OG1	2.10	0.52
3:K:40:GLU:OE1	3:K:54:LEU:HD11	2.10	0.52
3:K:80:TRP:HH2	3:K:122:TYR:CE2	2.27	0.52
3:K:143:ASP:OD1	3:K:144:THR:N	2.42	0.52
1:A:331:ILE:O	1:A:335:CYS:HB2	2.09	0.52
1:E:436:VAL:HG12	1:E:437:THR:N	2.25	0.52
1:G:623:ASP:OD1	1:G:624:GLU:N	2.43	0.52
3:J:95:PHE:CD1	3:J:169:SER:HB3	2.45	0.52
3:L:40:GLU:OE1	3:L:54:LEU:HD11	2.10	0.52
1:C:431:GLU:OE1	1:C:443:LEU:HD13	2.10	0.52
1:G:656:VAL:HG12	1:G:658:TYR:HE1	1.74	0.52
1:C:566:TYR:CE2	1:C:667:VAL:HB	2.44	0.51
1:E:412:PRO:HD3	1:E:457:LEU:HB3	1.92	0.51
1:A:620:LEU:HD13	1:A:661:LEU:HD13	1.91	0.51
1:C:267:GLN:HG2	1:C:474:LEU:HD13	1.92	0.51
1:E:511:ASP:O	1:E:515:GLY:N	2.40	0.51
3:J:77:GLN:O	3:J:185:ILE:HA	2.10	0.51
1:A:566:TYR:CE2	1:A:667:VAL:HB	2.45	0.51
1:C:428:VAL:HG21	1:C:446:TYR:CD2	2.45	0.51
2:H:60:SER:HB2	2:H:118:PHE:HD2	1.76	0.51
1:A:565:LEU:C	1:A:566:TYR:HD1	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:TYR:HE2	1:C:296:VAL:CG1	2.23	0.51
2:D:96:SER:O	2:D:100:LEU:HD23	2.10	0.51
1:A:431:GLU:OE1	1:A:443:LEU:HD13	2.11	0.51
1:C:205:PRO:O	1:C:213:TYR:OH	2.16	0.51
1:C:412:PRO:HD3	1:C:457:LEU:HB3	1.93	0.51
2:F:69:ASN:HD22	2:F:69:ASN:C	2.12	0.51
2:F:86:VAL:HG11	2:F:115:TYR:HB2	1.92	0.51
3:I:95:PHE:CD1	3:I:169:SER:HB3	2.45	0.51
1:C:133:TYR:CD1	1:C:341:LYS:HG2	2.46	0.51
1:G:23:VAL:HG23	1:G:40:TRP:HE1	1.76	0.51
1:C:565:LEU:C	1:C:566:TYR:HD1	2.13	0.51
1:C:566:TYR:CE1	1:C:597:ARG:HD3	2.45	0.51
1:G:548:ILE:HD12	1:G:548:ILE:H	1.76	0.51
1:C:121:MET:HE2	1:C:351:LEU:HD13	1.93	0.50
1:E:115:LEU:HD23	1:E:355:LEU:HD23	1.93	0.50
1:G:279:ARG:HG3	1:G:280:GLU:HG2	1.93	0.50
1:A:566:TYR:CE1	1:A:597:ARG:HD3	2.45	0.50
2:D:46:SER:HB3	2:D:67:PRO:HG3	1.93	0.50
1:E:620:LEU:HD13	1:E:661:LEU:HD13	1.92	0.50
1:E:623:ASP:OD1	1:E:624:GLU:N	2.44	0.50
3:I:163:LEU:HD21	3:I:192:LEU:HD12	1.92	0.50
1:A:149:TYR:CE1	1:A:208:ARG:HG3	2.46	0.50
1:A:410:PHE:CE1	1:A:630:THR:HB	2.46	0.50
1:A:621:SER:HB3	1:A:630:THR:OG1	2.11	0.50
1:E:32:HIS:NE2	3:L:73:MET:HG3	2.27	0.50
3:K:40:GLU:CD	3:K:65:TYR:HD2	2.14	0.50
1:C:161:SER:OG	1:C:165:ASP:HA	2.11	0.50
1:E:314:ASP:OD2	1:E:316:ARG:HB2	2.12	0.50
2:B:96:SER:O	2:B:100:LEU:HD23	2.11	0.50
1:C:328:LEU:O	1:C:332:ILE:HG13	2.11	0.50
1:G:548:ILE:HG21	4:G:702:NAG:H82	1.93	0.50
1:A:197:VAL:HB	1:A:227:VAL:HB	1.92	0.50
1:E:522:GLU:OE2	1:E:524:ARG:NH2	2.43	0.50
2:B:46:SER:HB3	2:B:67:PRO:HG3	1.94	0.50
1:E:158:VAL:HG22	1:E:340:VAL:HG22	1.94	0.50
1:G:121:MET:HE2	1:G:351:LEU:HD13	1.93	0.50
1:G:620:LEU:HD13	1:G:661:LEU:HD13	1.92	0.50
3:J:40:GLU:CG	3:J:41:LEU:H	2.06	0.50
1:E:71:ARG:NH1	1:E:208:ARG:HH22	2.10	0.50
1:E:431:GLU:OE1	1:E:443:LEU:HD13	2.12	0.50
1:E:656:VAL:HG12	1:E:658:TYR:HE1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:511:ASP:O	1:G:515:GLY:N	2.43	0.50
1:C:548:ILE:H	1:C:548:ILE:HD12	1.77	0.49
1:E:621:SER:HB3	1:E:630:THR:OG1	2.12	0.49
1:G:267:GLN:HG2	1:G:474:LEU:HD13	1.94	0.49
1:C:166:LYS:HE2	1:C:187:GLU:OE2	2.12	0.49
1:C:436:VAL:HG12	1:C:437:THR:N	2.26	0.49
1:E:489:ASP:OD1	1:E:489:ASP:N	2.44	0.49
2:F:118:PHE:HD1	2:F:118:PHE:N	2.10	0.49
1:G:621:SER:HB3	1:G:630:THR:OG1	2.13	0.49
2:H:118:PHE:HD1	2:H:118:PHE:N	2.10	0.49
3:I:40:GLU:CG	3:I:41:LEU:N	2.70	0.49
1:A:23:VAL:HG23	1:A:40:TRP:HE1	1.77	0.49
1:G:298:PHE:HE2	1:G:340:VAL:HG21	1.77	0.49
3:L:78:ASP:OD1	3:L:183:GLN:NE2	2.46	0.49
1:A:129:GLN:OE1	1:A:345:SER:HB2	2.13	0.49
1:A:436:VAL:HG12	1:A:437:THR:N	2.26	0.49
1:C:451:THR:HA	1:C:481:SER:HB2	1.94	0.49
1:E:83:GLY:HA2	1:E:220:GLN:O	2.13	0.49
1:E:465:GLY:HA3	1:E:472:SER:HB2	1.95	0.49
2:F:81:ASN:ND2	2:F:84:ASN:OD1	2.46	0.49
3:J:40:GLU:OE1	3:J:54:LEU:HD11	2.13	0.49
1:A:623:ASP:OD1	1:A:655:HIS:HB3	2.11	0.49
1:E:279:ARG:HG3	1:E:280:GLU:HG2	1.94	0.49
1:G:43:LEU:HD21	2:H:104:LEU:HD21	1.94	0.49
1:G:400:LEU:HD22	1:G:446:TYR:CE1	2.47	0.49
2:H:46:SER:HB3	2:H:67:PRO:HG3	1.95	0.49
3:I:58:ILE:HA	3:I:62:MET:O	2.12	0.49
3:K:120:ASN:HB2	3:K:183:GLN:HB3	1.95	0.49
1:A:332:ILE:HG22	1:A:338:ALA:HB3	1.94	0.49
1:A:448:LEU:HD22	1:A:546:PRO:O	2.13	0.49
2:H:118:PHE:N	2:H:118:PHE:CD1	2.81	0.49
1:A:633:TYR:CE2	1:A:635:THR:HG22	2.48	0.49
1:C:149:TYR:CE1	1:C:208:ARG:HG3	2.47	0.49
1:C:197:VAL:HB	1:C:227:VAL:HB	1.93	0.49
1:C:623:ASP:OD1	1:C:655:HIS:HB3	2.12	0.49
1:E:428:VAL:HG21	1:E:446:TYR:HD2	1.76	0.49
2:F:46:SER:HB3	2:F:67:PRO:HG3	1.93	0.49
3:I:40:GLU:CG	3:I:41:LEU:H	2.05	0.49
1:A:548:ILE:HD12	1:A:548:ILE:H	1.78	0.49
2:B:34:LEU:HD11	2:B:78:ARG:HG2	1.94	0.49
1:E:35:HIS:C	1:E:36:TYR:HD1	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:118:PHE:N	2:F:118:PHE:CD1	2.81	0.49
1:G:25:LEU:HD23	2:H:48:ILE:HB	1.95	0.49
1:G:432:LEU:HD21	1:G:443:LEU:HD11	1.95	0.49
1:G:522:GLU:OE2	1:G:524:ARG:NE	2.43	0.49
1:G:633:TYR:CE2	1:G:635:THR:HG22	2.48	0.49
3:I:83:THR:HG21	3:I:180:LEU:HB2	1.95	0.49
1:A:161:SER:OG	1:A:165:ASP:HA	2.13	0.49
1:E:315:LEU:HD22	1:E:351:LEU:HD21	1.95	0.49
1:G:186:THR:HG21	1:G:192:HIS:HE2	1.78	0.49
1:E:23:VAL:HG23	1:E:40:TRP:HE1	1.78	0.48
3:J:122:TYR:CD1	3:J:141:LYS:HA	2.48	0.48
1:C:380:THR:HG22	1:C:430:ARG:NH2	2.28	0.48
1:C:633:TYR:CE2	1:C:635:THR:HG22	2.48	0.48
1:E:633:TYR:CD2	1:E:635:THR:HG22	2.47	0.48
1:A:369:THR:HA	1:A:372:GLN:HB2	1.95	0.48
1:A:380:THR:HG22	1:A:430:ARG:NH2	2.29	0.48
1:A:522:GLU:HG3	1:A:524:ARG:HE	1.79	0.48
1:C:389:TYR:OH	3:K:140:THR:HG21	2.13	0.48
1:E:427:VAL:HG22	1:E:430:ARG:HH21	1.77	0.48
3:L:147:PRO:O	3:L:164:ASN:ND2	2.47	0.48
1:E:267:GLN:HG2	1:E:474:LEU:HD13	1.96	0.48
1:E:346:TYR:HB2	1:E:385:LYS:NZ	2.28	0.48
1:E:633:TYR:CE2	1:E:635:THR:HG22	2.49	0.48
1:G:346:TYR:HB2	1:G:385:LYS:NZ	2.29	0.48
1:G:566:TYR:CE2	1:G:667:VAL:HB	2.49	0.48
3:L:125:GLU:HB3	3:L:175:ARG:HG3	1.95	0.48
1:A:400:LEU:HD22	1:A:446:TYR:HD1	1.73	0.48
2:B:118:PHE:N	2:B:118:PHE:HD1	2.12	0.48
1:E:328:LEU:O	1:E:332:ILE:HG13	2.14	0.48
1:E:534:CYS:HB3	1:E:587:CYS:HB3	1.68	0.48
3:L:40:GLU:CD	3:L:65:TYR:HD2	2.17	0.48
1:C:570:THR:OG1	1:C:571:THR:N	2.47	0.48
1:E:298:PHE:HE2	1:E:340:VAL:HG21	1.78	0.48
1:E:566:TYR:CE2	1:E:667:VAL:HB	2.49	0.48
3:I:40:GLU:CD	3:I:65:TYR:HD2	2.16	0.48
1:C:26:HIS:HB2	2:D:49:TYR:CD1	2.49	0.48
1:C:133:TYR:CE1	1:C:341:LYS:HG2	2.48	0.48
1:C:410:PHE:CE1	1:C:630:THR:HB	2.49	0.48
2:D:118:PHE:N	2:D:118:PHE:HD1	2.12	0.48
2:F:96:SER:O	2:F:100:LEU:HD23	2.14	0.48
1:G:410:PHE:CE1	1:G:630:THR:HB	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:465:GLY:HA3	1:G:472:SER:HB2	1.95	0.48
1:A:133:TYR:CD1	1:A:341:LYS:HG2	2.48	0.48
1:A:173:MET:HB3	1:A:178:LEU:HD13	1.96	0.48
1:A:570:THR:OG1	1:A:571:THR:N	2.47	0.48
1:E:548:ILE:H	1:E:548:ILE:HD12	1.78	0.48
1:G:314:ASP:OD2	1:G:316:ARG:HB2	2.14	0.48
1:G:428:VAL:HG21	1:G:446:TYR:HD2	1.77	0.48
1:G:431:GLU:OE1	1:G:443:LEU:HD13	2.14	0.48
1:C:149:TYR:CE2	1:C:208:ARG:HA	2.48	0.48
1:E:121:MET:HE2	1:E:351:LEU:HD13	1.96	0.48
1:G:197:VAL:HB	1:G:227:VAL:HB	1.95	0.48
2:H:40:LEU:HD12	2:H:45:ILE:HG12	1.96	0.48
3:I:77:GLN:O	3:I:185:ILE:HA	2.14	0.48
1:G:315:LEU:HD22	1:G:351:LEU:HD21	1.96	0.48
1:G:623:ASP:OD1	1:G:655:HIS:HB3	2.13	0.48
3:K:125:GLU:HB3	3:K:175:ARG:HG3	1.95	0.48
1:A:166:LYS:HE2	1:A:187:GLU:OE2	2.14	0.47
1:E:187:GLU:CB	3:J:63:PRO:HD2	2.44	0.47
1:G:32:HIS:NE2	3:K:73:MET:HG3	2.29	0.47
1:G:534:CYS:HB3	1:G:587:CYS:HB3	1.67	0.47
1:A:36:TYR:N	1:A:36:TYR:CD1	2.83	0.47
1:C:314:ASP:OD2	1:C:316:ARG:HB2	2.13	0.47
1:E:301:VAL:HG21	1:E:325:LEU:HD11	1.96	0.47
2:F:24:TRP:N	2:F:24:TRP:HD1	2.12	0.47
1:G:67:SER:OG	4:G:701:NAG:H61	2.14	0.47
3:L:122:TYR:CD1	3:L:141:LYS:HA	2.48	0.47
1:G:380:THR:HG22	1:G:430:ARG:NH2	2.29	0.47
3:I:40:GLU:OE1	3:I:54:LEU:HD11	2.14	0.47
1:A:54:ALA:O	1:A:58:GLU:HG3	2.14	0.47
2:D:118:PHE:N	2:D:118:PHE:CD1	2.83	0.47
1:G:264:TYR:CZ	1:G:268:LYS:HD2	2.49	0.47
1:A:36:TYR:N	1:A:36:TYR:HD1	2.13	0.47
2:B:93:LEU:HB2	2:B:108:LEU:HD13	1.96	0.47
3:J:123:TYR:CE1	3:J:170:VAL:HG21	2.49	0.47
3:J:163:LEU:HD21	3:J:192:LEU:HD12	1.95	0.47
3:L:95:PHE:CD1	3:L:169:SER:HB3	2.50	0.47
3:L:123:TYR:HD1	3:L:142:ILE:HD11	1.78	0.47
1:A:656:VAL:HG12	1:A:658:TYR:HE1	1.79	0.47
2:B:118:PHE:N	2:B:118:PHE:CD1	2.83	0.47
1:C:129:GLN:OE1	1:C:345:SER:HB2	2.15	0.47
1:C:534:CYS:HB3	1:C:587:CYS:HB3	1.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:24:TRP:N	2:D:24:TRP:HD1	2.12	0.47
2:D:34:LEU:HD11	2:D:78:ARG:HG2	1.96	0.47
1:E:166:LYS:HE2	1:E:187:GLU:CD	2.35	0.47
1:E:182:TYR:HE2	1:E:288:LEU:HB3	1.78	0.47
1:G:35:HIS:C	1:G:36:TYR:HD1	2.17	0.47
1:G:633:TYR:CD2	1:G:635:THR:HG22	2.49	0.47
2:H:86:VAL:HG11	2:H:115:TYR:HB2	1.96	0.47
2:H:96:SER:O	2:H:100:LEU:HD23	2.15	0.47
3:K:95:PHE:CD1	3:K:169:SER:HB3	2.50	0.47
1:A:55:LEU:HD11	2:B:95:ARG:HH12	1.80	0.47
1:C:36:TYR:HD1	1:C:36:TYR:N	2.13	0.47
1:C:36:TYR:N	1:C:36:TYR:CD1	2.83	0.47
2:D:93:LEU:HB2	2:D:108:LEU:HD13	1.97	0.47
1:E:38:ILE:HD11	2:F:107:LEU:HD23	1.96	0.47
1:G:182:TYR:CD1	1:G:182:TYR:N	2.83	0.47
1:C:400:LEU:HD22	1:C:446:TYR:HD1	1.75	0.47
1:C:427:VAL:HG22	1:C:430:ARG:HH21	1.79	0.47
1:C:656:VAL:HG12	1:C:658:TYR:HE1	1.79	0.47
1:E:36:TYR:HD1	1:E:36:TYR:N	2.13	0.47
1:E:149:TYR:CE1	1:E:208:ARG:HG3	2.50	0.47
1:E:432:LEU:HD21	1:E:443:LEU:HD11	1.97	0.47
1:G:26:HIS:HB2	2:H:49:TYR:CD1	2.49	0.47
3:L:120:ASN:HB2	3:L:183:GLN:HB3	1.97	0.47
1:C:54:ALA:O	1:C:58:GLU:HG3	2.15	0.46
1:E:186:THR:HG21	1:E:192:HIS:HE2	1.79	0.46
1:G:182:TYR:N	1:G:182:TYR:HD1	2.13	0.46
1:G:448:LEU:HD11	1:G:545:ILE:HG23	1.97	0.46
2:H:77:SER:OG	3:K:57:ASN:HB3	2.13	0.46
1:C:133:TYR:CD2	1:C:134:ILE:N	2.82	0.46
1:G:36:TYR:HD1	1:G:36:TYR:N	2.13	0.46
2:B:83:LEU:HD22	2:B:115:TYR:CE1	2.51	0.46
1:E:570:THR:OG1	1:E:571:THR:N	2.47	0.46
2:F:30:HIS:HD1	2:F:32:THR:HG23	1.81	0.46
3:K:123:TYR:HD1	3:K:142:ILE:HD11	1.80	0.46
1:A:314:ASP:OD2	1:A:316:ARG:HB2	2.15	0.46
1:A:498:GLU:HB2	1:A:500:THR:HG22	1.97	0.46
1:C:64:ASP:OD1	1:C:64:ASP:N	2.48	0.46
1:C:560:VAL:HG22	1:C:562:GLY:H	1.81	0.46
1:C:448:LEU:HD22	1:C:546:PRO:O	2.16	0.46
1:E:359:VAL:HG11	1:E:364:LEU:HD13	1.97	0.46
1:G:533:LYS:O	1:G:561:ARG:NH1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:522:GLU:HG3	1:C:524:ARG:HE	1.81	0.46
1:E:149:TYR:CZ	1:E:208:ARG:HG3	2.50	0.46
1:G:166:LYS:HE2	1:G:187:GLU:CD	2.35	0.46
1:G:328:LEU:O	1:G:332:ILE:HG13	2.16	0.46
1:G:522:GLU:OE2	1:G:524:ARG:NH2	2.47	0.46
3:I:123:TYR:CE1	3:I:170:VAL:HG21	2.50	0.46
1:C:570:THR:HG21	1:C:577:LEU:N	2.31	0.46
1:E:522:GLU:OE2	1:E:524:ARG:NE	2.46	0.46
2:H:93:LEU:HB2	2:H:108:LEU:HD13	1.97	0.46
3:J:104:ASP:HB3	3:J:150:ILE:HG22	1.98	0.46
1:A:570:THR:HG21	1:A:577:LEU:N	2.31	0.46
1:E:623:ASP:OD1	1:E:655:HIS:HB3	2.15	0.46
1:E:331:ILE:O	1:E:335:CYS:HB2	2.16	0.46
3:I:58:ILE:HG22	3:I:63:PRO:HD3	1.97	0.46
1:A:26:HIS:HB2	2:B:49:TYR:CD1	2.51	0.46
1:C:389:TYR:CD2	3:K:123:TYR:HE1	2.34	0.46
1:E:26:HIS:HB2	2:F:49:TYR:CD1	2.50	0.46
1:E:36:TYR:N	1:E:36:TYR:CD1	2.84	0.46
1:E:579:LEU:HD22	1:E:667:VAL:HG11	1.97	0.46
1:A:67:SER:OG	4:A:701:NAG:H61	2.15	0.45
1:A:427:VAL:HG22	1:A:430:ARG:HH21	1.80	0.45
1:E:71:ARG:HH21	1:E:209:GLY:HA3	1.81	0.45
1:E:410:PHE:CE1	1:E:630:THR:HB	2.51	0.45
1:E:533:LYS:O	1:E:561:ARG:NH1	2.49	0.45
1:G:36:TYR:N	1:G:36:TYR:CD1	2.84	0.45
1:G:71:ARG:NH1	1:G:208:ARG:HH22	2.14	0.45
1:G:83:GLY:HA2	1:G:220:GLN:O	2.16	0.45
1:G:121:MET:HE3	1:G:348:LEU:HD13	1.97	0.45
1:G:570:THR:OG1	1:G:571:THR:N	2.48	0.45
1:A:264:TYR:CZ	1:A:268:LYS:HD2	2.51	0.45
1:C:148:PHE:CE1	1:C:205:PRO:HG2	2.51	0.45
1:C:633:TYR:CD2	1:C:635:THR:HG22	2.52	0.45
1:E:149:TYR:CE2	1:E:208:ARG:HA	2.52	0.45
1:E:156:SER:O	1:E:173:MET:HG2	2.17	0.45
1:E:388:VAL:O	1:E:389:TYR:HD1	1.99	0.45
2:F:93:LEU:HB2	2:F:108:LEU:HD13	1.98	0.45
3:I:104:ASP:HB3	3:I:150:ILE:HG22	1.99	0.45
3:L:56:GLN:HG3	3:L:65:TYR:CE1	2.52	0.45
1:A:560:VAL:HG22	1:A:562:GLY:H	1.82	0.45
1:C:388:VAL:O	1:C:389:TYR:HD1	1.98	0.45
2:D:75:VAL:HG23	3:J:55:MET:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:LYS:O	1:E:73:LYS:HG2	2.16	0.45
2:F:49:TYR:HB2	2:F:63:SER:OG	2.17	0.45
1:G:149:TYR:CE1	1:G:208:ARG:HG3	2.50	0.45
3:L:94:ILE:HG12	3:L:173:LEU:HD11	1.98	0.45
1:A:570:THR:HG22	1:A:577:LEU:HB3	1.98	0.45
1:E:121:MET:HE3	1:E:348:LEU:HD13	1.97	0.45
1:E:427:VAL:HA	1:E:430:ARG:HH21	1.81	0.45
1:G:427:VAL:HG22	1:G:430:ARG:HH21	1.81	0.45
3:I:122:TYR:CD1	3:I:141:LYS:HA	2.52	0.45
1:C:67:SER:OG	4:C:701:NAG:H61	2.17	0.45
1:E:264:TYR:CZ	1:E:268:LYS:HD2	2.51	0.45
1:G:176:LYS:HB3	1:G:203:ASP:HB3	1.98	0.45
1:G:359:VAL:HG11	1:G:364:LEU:HD13	1.99	0.45
2:H:30:HIS:HD1	2:H:32:THR:HG23	1.81	0.45
3:I:138:LEU:HD13	3:I:138:LEU:O	2.17	0.45
1:E:498:GLU:HB2	1:E:500:THR:HG22	1.99	0.45
1:E:570:THR:HG21	1:E:577:LEU:N	2.30	0.45
1:G:73:LYS:O	1:G:73:LYS:HG2	2.16	0.45
1:G:149:TYR:CE2	1:G:208:ARG:HA	2.52	0.45
1:G:388:VAL:O	1:G:389:TYR:HD1	1.99	0.45
3:J:78:ASP:OD1	3:J:183:GLN:NE2	2.45	0.45
1:A:412:PRO:HD3	1:A:457:LEU:HB3	1.99	0.45
1:E:25:LEU:HD23	2:F:48:ILE:HB	1.99	0.45
1:E:380:THR:HG22	1:E:430:ARG:NH2	2.32	0.45
1:A:21:SER:HB3	1:A:22:GLU:H	1.53	0.45
1:A:323:PHE:HD1	1:A:380:THR:OG1	2.00	0.45
2:B:56:CYS:SG	2:B:131:TYR:OH	2.72	0.45
2:D:83:LEU:HD22	2:D:115:TYR:CE1	2.52	0.45
1:E:522:GLU:HG3	1:E:524:ARG:HE	1.82	0.45
1:G:258:ALA:HB1	1:G:301:VAL:HG22	1.97	0.45
1:G:464:ARG:NH2	1:G:496:PRO:HB3	2.32	0.45
3:K:58:ILE:HA	3:K:62:MET:O	2.16	0.45
1:A:64:ASP:OD1	1:A:64:ASP:N	2.50	0.45
2:B:38:HIS:CE1	2:B:78:ARG:NH2	2.85	0.45
1:E:176:LYS:HB3	1:E:203:ASP:HB3	1.99	0.45
1:G:210:PRO:HB2	2:H:120:VAL:HG21	1.98	0.45
3:J:40:GLU:CD	3:J:65:TYR:HD2	2.18	0.45
3:K:78:ASP:OD1	3:K:183:GLN:NE2	2.50	0.44
1:C:26:HIS:O	2:D:49:TYR:HA	2.17	0.44
1:C:133:TYR:HD2	1:C:134:ILE:C	2.21	0.44
1:C:570:THR:HG22	1:C:577:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:74:LEU:HB3	3:J:54:LEU:HD23	1.98	0.44
1:A:20:LEU:HD23	1:A:20:LEU:HA	1.77	0.44
1:A:292:PHE:O	1:A:296:VAL:HG23	2.18	0.44
1:C:59:ALA:HA	1:C:208:ARG:HH11	1.81	0.44
1:E:258:ALA:HB1	1:E:301:VAL:HG22	1.99	0.44
1:E:400:LEU:HD22	1:E:446:TYR:CE1	2.50	0.44
1:G:38:ILE:HD11	2:H:107:LEU:HD23	1.98	0.44
1:G:369:THR:HG22	1:G:372:GLN:OE1	2.17	0.44
1:A:182:TYR:N	1:A:182:TYR:CD1	2.84	0.44
1:A:522:GLU:OE2	1:A:524:ARG:NH2	2.46	0.44
1:E:200:LYS:HA	1:E:223:ASP:O	2.16	0.44
3:I:125:GLU:HB3	3:I:175:ARG:HG3	1.98	0.44
3:L:99:LYS:HB2	3:L:193:SER:HB3	1.98	0.44
2:B:101:THR:O	2:B:104:LEU:N	2.51	0.44
1:C:561:ARG:HB3	1:C:588:SER:H	1.82	0.44
1:E:138:LEU:HD13	1:E:148:PHE:HB3	2.00	0.44
1:A:561:ARG:HB3	1:A:588:SER:H	1.82	0.44
1:A:656:VAL:HG12	1:A:658:TYR:CE1	2.53	0.44
1:C:115:LEU:HD23	1:C:355:LEU:HD23	2.00	0.44
1:C:182:TYR:N	1:C:182:TYR:CD1	2.86	0.44
2:D:70:GLY:HA2	4:D:202:NAG:HN2	1.82	0.44
1:G:182:TYR:HE2	1:G:288:LEU:HB3	1.83	0.44
1:G:184:ARG:NH1	1:G:186:THR:HG22	2.32	0.44
1:G:200:LYS:HA	1:G:223:ASP:O	2.18	0.44
1:G:427:VAL:HA	1:G:430:ARG:HH21	1.81	0.44
1:G:428:VAL:HA	1:G:431:GLU:OE2	2.18	0.44
3:I:41:LEU:HD23	3:I:41:LEU:HA	1.75	0.44
1:C:440:GLY:N	1:C:441:PRO:HD2	2.33	0.44
1:C:554:ILE:HG13	1:C:579:LEU:HG	1.99	0.44
2:D:51:VAL:HG22	2:D:61:LEU:O	2.18	0.44
3:I:91:ALA:HB2	3:I:198:TYR:CD1	2.53	0.44
3:J:163:LEU:CD2	3:J:192:LEU:HD12	2.48	0.44
1:A:579:LEU:HD22	1:A:667:VAL:HG11	1.99	0.43
2:B:64:LEU:O	2:B:77:SER:HA	2.18	0.43
1:C:292:PHE:O	1:C:296:VAL:HG23	2.18	0.43
1:G:579:LEU:HD22	1:G:667:VAL:HG11	1.99	0.43
3:J:83:THR:HG21	3:J:180:LEU:HB2	2.00	0.43
1:A:26:HIS:O	2:B:49:TYR:HA	2.18	0.43
1:A:400:LEU:HD23	1:A:449:LEU:HB2	2.00	0.43
1:A:513:PHE:CD2	1:A:513:PHE:O	2.70	0.43
1:A:534:CYS:HB3	1:A:587:CYS:HB3	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:HIS:HD1	2:B:32:THR:HG23	1.84	0.43
2:F:60:SER:HA	2:F:118:PHE:HE2	1.82	0.43
2:F:65:ASN:HA	2:F:76:ILE:O	2.17	0.43
1:G:440:GLY:N	1:G:441:PRO:HD2	2.34	0.43
1:A:603:GLN:NE2	1:A:671:ALA:HB3	2.33	0.43
2:B:51:VAL:HG22	2:B:61:LEU:O	2.18	0.43
1:C:323:PHE:HD1	1:C:380:THR:OG1	2.01	0.43
1:C:554:ILE:HA	1:C:578:PHE:O	2.18	0.43
2:H:70:GLY:HA2	4:H:202:NAG:HN2	1.83	0.43
3:K:120:ASN:HB3	3:K:122:TYR:HE1	1.83	0.43
1:A:440:GLY:N	1:A:441:PRO:HD2	2.34	0.43
2:B:70:GLY:HA2	4:B:202:NAG:HN2	1.83	0.43
1:C:400:LEU:HD23	1:C:449:LEU:HB2	2.00	0.43
1:E:440:GLY:N	1:E:441:PRO:HD2	2.34	0.43
3:K:116:LYS:HG3	3:K:185:ILE:HG13	2.00	0.43
3:L:52:TRP:HA	3:L:69:VAL:HB	2.00	0.43
1:A:59:ALA:HA	1:A:208:ARG:HH11	1.84	0.43
1:E:603:GLN:NE2	1:E:671:ALA:HB3	2.33	0.43
1:A:71:ARG:NH1	1:A:208:ARG:HH22	2.17	0.43
1:C:25:LEU:HD12	2:D:107:LEU:HD21	2.00	0.43
1:C:427:VAL:HA	1:C:430:ARG:HH21	1.84	0.43
1:E:182:TYR:CD1	1:E:182:TYR:N	2.87	0.43
1:E:369:THR:HG22	1:E:372:GLN:OE1	2.19	0.43
1:E:554:ILE:HG13	1:E:579:LEU:HG	2.00	0.43
2:F:60:SER:HB2	2:F:118:PHE:HD2	1.80	0.43
1:G:71:ARG:HH21	1:G:209:GLY:HA3	1.83	0.43
1:G:570:THR:HG21	1:G:577:LEU:N	2.32	0.43
3:J:58:ILE:HG22	3:J:63:PRO:HD3	1.99	0.43
3:K:65:TYR:N	3:K:65:TYR:CD1	2.86	0.43
3:K:122:TYR:CD1	3:K:141:LYS:HA	2.53	0.43
1:C:26:HIS:ND1	1:C:35:HIS:CD2	2.87	0.43
1:E:210:PRO:HB2	2:F:120:VAL:HG21	2.00	0.43
2:H:38:HIS:CD2	2:H:78:ARG:NH2	2.86	0.43
1:A:388:VAL:O	1:A:389:TYR:HD1	2.01	0.43
1:A:427:VAL:HA	1:A:430:ARG:HH21	1.84	0.43
1:C:498:GLU:HB2	1:C:500:THR:HG22	2.01	0.43
1:C:560:VAL:HG11	1:C:580:SER:OG	2.19	0.43
1:C:603:GLN:NE2	1:C:671:ALA:HB3	2.34	0.43
2:D:78:ARG:HH22	3:J:56:GLN:HE21	1.66	0.43
1:G:448:LEU:HD22	1:G:546:PRO:O	2.19	0.43
1:A:328:LEU:O	1:A:332:ILE:HG13	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:GLU:OE2	1:A:384:PRO:HG2	2.19	0.43
1:E:451:THR:HA	1:E:481:SER:HB2	1.99	0.43
2:F:51:VAL:HG22	2:F:61:LEU:O	2.18	0.43
2:F:60:SER:HB3	2:F:83:LEU:HG	1.99	0.43
3:J:123:TYR:HD1	3:J:142:ILE:HD11	1.84	0.43
3:L:77:GLN:O	3:L:185:ILE:HA	2.18	0.43
1:A:200:LYS:HA	1:A:223:ASP:O	2.18	0.43
1:A:560:VAL:HG11	1:A:580:SER:OG	2.19	0.43
1:C:182:TYR:HE2	1:C:242:PHE:CZ	2.36	0.43
1:C:301:VAL:HG21	1:C:325:LEU:HD11	2.00	0.43
1:C:332:ILE:HG22	1:C:338:ALA:HB3	2.01	0.43
1:C:464:ARG:NH2	1:C:496:PRO:HB3	2.34	0.43
1:E:212:SER:HB3	1:E:214:PRO:HD2	2.00	0.43
1:E:519:LEU:HD12	1:E:520:GLU:N	2.34	0.43
3:K:104:ASP:HB3	3:K:150:ILE:HG22	2.01	0.43
3:L:78:ASP:OD2	3:L:136:LYS:HE3	2.19	0.43
3:L:104:ASP:HB3	3:L:150:ILE:HG22	2.01	0.43
1:A:133:TYR:O	1:A:154:HIS:HA	2.19	0.42
1:A:513:PHE:CD2	1:A:513:PHE:C	2.92	0.42
1:E:182:TYR:N	1:E:182:TYR:HD1	2.17	0.42
1:E:448:LEU:HD11	1:E:545:ILE:HG23	2.02	0.42
1:G:543:MET:SD	1:G:545:ILE:HD11	2.59	0.42
2:H:60:SER:HA	2:H:118:PHE:HE2	1.83	0.42
1:G:603:GLN:NE2	1:G:671:ALA:HB3	2.35	0.42
2:F:93:LEU:HD13	2:F:108:LEU:HB2	2.01	0.42
3:J:83:THR:CG2	3:J:180:LEU:HB2	2.50	0.42
3:J:138:LEU:HD13	3:J:138:LEU:O	2.19	0.42
1:E:187:GLU:O	3:J:63:PRO:HD2	2.20	0.42
1:G:59:ALA:HA	1:G:208:ARG:HH11	1.84	0.42
1:G:602:ILE:HD11	1:G:668:MET:SD	2.60	0.42
1:A:133:TYR:CE1	1:A:341:LYS:HG2	2.55	0.42
1:A:554:ILE:HA	1:A:578:PHE:O	2.20	0.42
1:C:579:LEU:HD22	1:C:667:VAL:HG11	2.00	0.42
2:D:77:SER:OG	3:J:57:ASN:HB3	2.19	0.42
1:G:410:PHE:HE1	1:G:630:THR:HB	1.85	0.42
1:G:451:THR:HA	1:G:481:SER:HB2	2.00	0.42
1:G:554:ILE:HG13	1:G:579:LEU:HG	2.01	0.42
2:H:51:VAL:HG22	2:H:61:LEU:O	2.19	0.42
3:I:163:LEU:CD2	3:I:192:LEU:HD12	2.49	0.42
2:F:38:HIS:CE1	2:F:78:ARG:NH2	2.88	0.42
3:J:72:VAL:HG11	3:J:188:CYS:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:78:ASP:OD2	3:K:136:LYS:HE3	2.19	0.42
1:A:133:TYR:HD2	1:A:134:ILE:C	2.22	0.42
1:A:133:TYR:HD2	1:A:134:ILE:N	2.18	0.42
1:A:298:PHE:HE2	1:A:340:VAL:HG11	1.84	0.42
1:A:364:LEU:HD12	1:A:367:LEU:HD12	2.01	0.42
2:D:30:HIS:HD1	2:D:32:THR:HG23	1.85	0.42
2:D:100:LEU:HD12	2:D:105:ARG:CB	2.48	0.42
1:E:184:ARG:NH1	1:E:186:THR:HG22	2.34	0.42
1:G:554:ILE:HA	1:G:578:PHE:O	2.19	0.42
1:A:73:LYS:O	1:A:73:LYS:HG2	2.20	0.42
2:H:49:TYR:HB2	2:H:63:SER:OG	2.20	0.42
2:H:65:ASN:HA	2:H:76:ILE:O	2.19	0.42
3:L:138:LEU:HD13	3:L:138:LEU:O	2.20	0.42
1:A:464:ARG:NH2	1:A:496:PRO:HB3	2.34	0.42
2:B:100:LEU:HD12	2:B:105:ARG:CB	2.46	0.42
1:G:212:SER:HB3	1:G:214:PRO:HD2	2.01	0.42
3:K:138:LEU:HD13	3:K:138:LEU:O	2.20	0.42
1:A:186:THR:HG21	1:A:192:HIS:NE2	2.35	0.42
1:A:428:VAL:HA	1:A:431:GLU:OE2	2.20	0.42
2:B:65:ASN:HA	2:B:76:ILE:O	2.20	0.42
1:C:33:ALA:HB1	1:C:35:HIS:NE2	2.35	0.42
1:C:656:VAL:HG12	1:C:658:TYR:CE1	2.54	0.42
1:E:427:VAL:HG22	1:E:430:ARG:NH2	2.35	0.42
1:E:428:VAL:HA	1:E:431:GLU:OE2	2.20	0.42
1:G:167:PHE:HE1	1:G:182:TYR:HB3	1.85	0.42
1:G:560:VAL:HG22	1:G:562:GLY:H	1.85	0.42
3:J:41:LEU:HD23	3:J:41:LEU:HA	1.77	0.42
1:G:361:MET:HE3	1:G:395:GLY:HA3	2.02	0.41
3:J:40:GLU:CG	3:J:41:LEU:N	2.71	0.41
2:B:88:PHE:O	2:B:92:ILE:HG12	2.20	0.41
1:C:35:HIS:C	1:C:36:TYR:HD1	2.23	0.41
1:C:264:TYR:CZ	1:C:268:LYS:HD2	2.55	0.41
1:E:121:MET:CE	1:E:351:LEU:HD13	2.50	0.41
1:E:448:LEU:HD22	1:E:546:PRO:O	2.20	0.41
3:K:82:ARG:HD2	3:K:83:THR:O	2.20	0.41
3:L:82:ARG:HD2	3:L:83:THR:O	2.20	0.41
1:A:96:SER:HB2	1:A:99:SER:OG	2.20	0.41
1:A:633:TYR:CD2	1:A:635:THR:HG22	2.56	0.41
1:C:143:PRO:HG2	1:C:144:HIS:CE1	2.56	0.41
2:D:101:THR:O	2:D:104:LEU:N	2.54	0.41
1:E:570:THR:HG22	1:E:577:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:121:MET:CE	1:G:351:LEU:HD13	2.50	0.41
1:G:519:LEU:HD12	1:G:520:GLU:N	2.35	0.41
3:I:58:ILE:HG13	3:I:58:ILE:O	2.21	0.41
3:K:52:TRP:HA	3:K:69:VAL:HB	2.02	0.41
3:K:95:PHE:CE1	3:K:169:SER:HB3	2.55	0.41
1:A:428:VAL:HG11	1:A:446:TYR:CD2	2.54	0.41
1:C:73:LYS:O	1:C:73:LYS:HG2	2.21	0.41
1:G:331:ILE:O	1:G:335:CYS:HB2	2.20	0.41
3:L:95:PHE:CE1	3:L:169:SER:HB3	2.55	0.41
1:A:133:TYR:CD2	1:A:134:ILE:N	2.89	0.41
1:A:182:TYR:N	1:A:182:TYR:HD1	2.18	0.41
1:C:451:THR:HG23	1:C:483:ARG:HG3	2.02	0.41
2:F:88:PHE:O	2:F:92:ILE:HG12	2.19	0.41
3:I:34:PHE:CE1	3:I:40:GLU:HB3	2.54	0.41
1:C:71:ARG:HH21	1:C:209:GLY:HA3	1.86	0.41
1:E:428:VAL:HG21	1:E:446:TYR:HE2	1.81	0.41
1:G:129:GLN:OE1	1:G:345:SER:HB2	2.20	0.41
2:H:78:ARG:NH2	3:K:56:GLN:HE21	2.16	0.41
2:H:81:ASN:ND2	2:H:84:ASN:OD1	2.53	0.41
3:I:56:GLN:HG3	3:I:65:TYR:CE1	2.55	0.41
3:I:83:THR:CG2	3:I:180:LEU:HB2	2.51	0.41
1:E:400:LEU:HD23	1:E:449:LEU:HB2	2.03	0.41
1:G:123:SER:HB3	1:G:313:VAL:HG23	2.01	0.41
1:G:143:PRO:HG2	1:G:144:HIS:CE1	2.56	0.41
1:A:71:ARG:HH21	1:A:209:GLY:HA3	1.86	0.41
1:A:143:PRO:HG2	1:A:144:HIS:CE1	2.56	0.41
1:C:200:LYS:HA	1:C:223:ASP:O	2.20	0.41
1:C:638:GLU:OE1	1:C:638:GLU:N	2.53	0.41
1:G:498:GLU:HB2	1:G:500:THR:HG22	2.03	0.41
1:A:410:PHE:HE1	1:A:630:THR:HB	1.85	0.41
1:A:622:TYR:CE1	1:A:657:HIS:HB2	2.56	0.41
1:E:129:GLN:OE1	1:E:345:SER:HB2	2.21	0.41
1:E:167:PHE:HE1	1:E:182:TYR:HB3	1.86	0.41
1:G:186:THR:HG21	1:G:192:HIS:NE2	2.35	0.41
1:G:570:THR:H	1:G:570:THR:HG23	1.67	0.41
3:K:91:ALA:HB2	3:K:198:TYR:CD1	2.55	0.41
1:C:96:SER:HB2	1:C:99:SER:OG	2.21	0.41
1:E:545:ILE:HG21	1:E:618:ALA:HB2	2.02	0.41
2:F:34:LEU:HD13	3:L:58:ILE:HD13	2.03	0.41
1:G:565:LEU:C	1:G:566:TYR:HD1	2.24	0.41
3:I:121:LEU:C	3:I:122:TYR:HD1	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:91:ALA:HB2	3:L:198:TYR:CD1	2.55	0.41
1:A:22:GLU:HG2	1:A:23:VAL:N	2.36	0.40
1:E:67:SER:OG	4:E:701:NAG:H61	2.21	0.40
1:E:554:ILE:HA	1:E:578:PHE:O	2.21	0.40
2:F:82:GLY:O	2:F:86:VAL:HG23	2.21	0.40
1:G:570:THR:HG22	1:G:577:LEU:HB3	2.02	0.40
2:H:100:LEU:HD12	2:H:105:ARG:CB	2.48	0.40
3:J:125:GLU:HB3	3:J:175:ARG:HG3	2.01	0.40
1:A:35:HIS:C	1:A:36:TYR:HD1	2.25	0.40
1:C:389:TYR:CB	3:K:170:VAL:HG23	2.50	0.40
1:E:160:LEU:HB3	1:E:338:ALA:CB	2.50	0.40
1:E:543:MET:SD	1:E:545:ILE:HD11	2.61	0.40
2:F:40:LEU:HD12	2:F:45:ILE:HG12	2.03	0.40
1:G:149:TYR:CZ	1:G:208:ARG:HG3	2.55	0.40
3:J:85:TRP:HD1	3:J:179:TYR:CZ	2.40	0.40
3:K:121:LEU:C	3:K:122:TYR:HD1	2.25	0.40
1:A:20:LEU:HB3	1:A:21:SER:H	1.64	0.40
2:B:40:LEU:HD12	2:B:45:ILE:HG12	2.03	0.40
1:C:624:GLU:HG3	1:C:655:HIS:O	2.22	0.40
1:G:156:SER:O	1:G:173:MET:HG2	2.21	0.40
3:I:85:TRP:HD1	3:I:179:TYR:CZ	2.40	0.40
2:B:75:VAL:HG23	3:I:55:MET:HG2	2.03	0.40
1:C:622:TYR:CE1	1:C:657:HIS:HB2	2.57	0.40
1:E:143:PRO:HG2	1:E:144:HIS:CE1	2.57	0.40
1:E:148:PHE:CE1	1:E:205:PRO:HG2	2.56	0.40
1:E:287:THR:O	1:E:291:MET:HG3	2.20	0.40
1:G:160:LEU:HB3	1:G:338:ALA:CB	2.50	0.40
2:D:70:GLY:CA	4:D:202:NAG:HN2	2.34	0.40
1:E:64:ASP:OD1	1:E:64:ASP:N	2.54	0.40
1:E:123:SER:HB3	1:E:313:VAL:HG23	2.02	0.40
3:L:58:ILE:HA	3:L:62:MET:O	2.21	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	653/662 (99%)	648 (99%)	3 (0%)	2 (0%)	41	76
1	C	653/662 (99%)	651 (100%)	2 (0%)	0	100	100
1	E	653/662 (99%)	651 (100%)	2 (0%)	0	100	100
1	G	653/662 (99%)	651 (100%)	2 (0%)	0	100	100
2	B	107/114 (94%)	105 (98%)	2 (2%)	0	100	100
2	D	107/114 (94%)	104 (97%)	3 (3%)	0	100	100
2	F	107/114 (94%)	105 (98%)	2 (2%)	0	100	100
2	H	107/114 (94%)	104 (97%)	3 (3%)	0	100	100
3	I	162/183 (88%)	162 (100%)	0	0	100	100
3	J	162/183 (88%)	161 (99%)	1 (1%)	0	100	100
3	K	162/183 (88%)	162 (100%)	0	0	100	100
3	L	162/183 (88%)	162 (100%)	0	0	100	100
All	All	3688/3836 (96%)	3666 (99%)	20 (0%)	2 (0%)	51	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	369	THR

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	561/566 (99%)	546 (97%)	15 (3%)	44	77
1	C	561/566 (99%)	552 (98%)	9 (2%)	62	86
1	E	561/566 (99%)	553 (99%)	8 (1%)	67	88
1	G	561/566 (99%)	553 (99%)	8 (1%)	67	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	95/98 (97%)	90 (95%)	5 (5%)	22	58
2	D	95/98 (97%)	91 (96%)	4 (4%)	30	66
2	F	95/98 (97%)	90 (95%)	5 (5%)	22	58
2	H	95/98 (97%)	91 (96%)	4 (4%)	30	66
3	I	142/158 (90%)	140 (99%)	2 (1%)	67	88
3	J	142/158 (90%)	140 (99%)	2 (1%)	67	88
3	K	142/158 (90%)	140 (99%)	2 (1%)	67	88
3	L	142/158 (90%)	140 (99%)	2 (1%)	67	88
All	All	3192/3288 (97%)	3126 (98%)	66 (2%)	57	82

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	21	SER
1	A	22	GLU
1	A	36	TYR
1	A	71	ARG
1	A	150	GLN
1	A	335	CYS
1	A	369	THR
1	A	370	GLU
1	A	372	GLN
1	A	478	CYS
1	A	524	ARG
1	A	534	CYS
1	A	552	PHE
1	A	658	TYR
2	B	24	TRP
2	B	40	LEU
2	B	56	CYS
2	B	69	ASN
2	B	118	PHE
1	C	36	TYR
1	C	71	ARG
1	C	335	CYS
1	C	454	CYS
1	C	478	CYS
1	C	524	ARG

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Mol	Chain	Res	Type
1	C	534	CYS
1	C	552	PHE
1	C	658	TYR
2	D	24	TRP
2	D	40	LEU
2	D	69	ASN
2	D	118	PHE
1	E	36	TYR
1	E	71	ARG
1	E	182	TYR
1	E	335	CYS
1	E	478	CYS
1	E	524	ARG
1	E	534	CYS
1	E	552	PHE
2	F	24	TRP
2	F	38	HIS
2	F	40	LEU
2	F	69	ASN
2	F	118	PHE
1	G	36	TYR
1	G	71	ARG
1	G	182	TYR
1	G	335	CYS
1	G	478	CYS
1	G	524	ARG
1	G	534	CYS
1	G	552	PHE
2	H	24	TRP
2	H	40	LEU
2	H	69	ASN
2	H	118	PHE
3	I	48[A]	TYR
3	I	48[B]	TYR
3	J	48[A]	TYR
3	J	48[B]	TYR
3	K	48[A]	TYR
3	K	48[B]	TYR
3	L	48[A]	TYR
3	L	48[B]	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	237	ASN
1	A	372	GLN
2	B	38	HIS
1	C	35	HIS
1	C	237	ASN
1	E	234	HIS
1	E	237	ASN
1	G	237	ASN
3	J	56	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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	$\# Z > 2$
4	NAG	A	702	1	14,14,15	0.51	0	17,19,21	0.81	1 (5%)
4	NAG	E	701	1	14,14,15	0.60	0	17,19,21	0.52	0
4	NAG	G	702	1	14,14,15	0.54	0	17,19,21	0.88	1 (5%)
4	NAG	B	202	2	14,14,15	0.28	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	F	201	2	14,14,15	0.44	0	17,19,21	0.64	1 (5%)
4	NAG	H	202	2	14,14,15	0.38	0	17,19,21	0.41	0
4	NAG	G	701	1	14,14,15	0.63	0	17,19,21	0.52	0
4	NAG	H	201	2	14,14,15	0.40	0	17,19,21	0.66	1 (5%)
4	NAG	C	701	1	14,14,15	0.42	0	17,19,21	0.50	0
4	NAG	E	702	1	14,14,15	0.48	0	17,19,21	0.84	1 (5%)
4	NAG	D	201	2	14,14,15	0.34	0	17,19,21	0.60	0
4	NAG	C	702	1	14,14,15	0.51	0	17,19,21	0.79	1 (5%)
4	NAG	D	202	2	14,14,15	0.36	0	17,19,21	0.48	0
4	NAG	F	202	2	14,14,15	0.31	0	17,19,21	0.40	0
4	NAG	A	701	1	14,14,15	0.36	0	17,19,21	0.47	0
4	NAG	B	201	2	14,14,15	0.33	0	17,19,21	0.79	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	702	1	-	2/6/23/26	0/1/1/1
4	NAG	E	701	1	-	0/6/23/26	0/1/1/1
4	NAG	G	702	1	-	2/6/23/26	0/1/1/1
4	NAG	B	202	2	-	2/6/23/26	0/1/1/1
4	NAG	F	201	2	-	1/6/23/26	0/1/1/1
4	NAG	H	202	2	-	2/6/23/26	0/1/1/1
4	NAG	G	701	1	-	0/6/23/26	0/1/1/1
4	NAG	H	201	2	-	0/6/23/26	0/1/1/1
4	NAG	C	701	1	-	0/6/23/26	0/1/1/1
4	NAG	E	702	1	-	2/6/23/26	0/1/1/1
4	NAG	D	201	2	-	0/6/23/26	0/1/1/1
4	NAG	C	702	1	-	2/6/23/26	0/1/1/1
4	NAG	D	202	2	-	2/6/23/26	0/1/1/1
4	NAG	F	202	2	-	2/6/23/26	0/1/1/1
4	NAG	A	701	1	-	0/6/23/26	0/1/1/1
4	NAG	B	201	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	702	NAG	C1-O5-C5	3.24	116.59	112.19
4	E	702	NAG	C1-O5-C5	2.96	116.20	112.19
4	B	201	NAG	C1-O5-C5	2.91	116.14	112.19
4	A	702	NAG	C1-O5-C5	2.88	116.10	112.19
4	C	702	NAG	C1-O5-C5	2.69	115.84	112.19
4	H	201	NAG	C1-O5-C5	2.20	115.17	112.19
4	F	201	NAG	C1-O5-C5	2.02	114.92	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	702	NAG	O5-C5-C6-O6
4	E	702	NAG	O5-C5-C6-O6
4	A	702	NAG	O5-C5-C6-O6
4	C	702	NAG	O5-C5-C6-O6
4	A	702	NAG	C4-C5-C6-O6
4	E	702	NAG	C4-C5-C6-O6
4	G	702	NAG	C4-C5-C6-O6
4	C	702	NAG	C4-C5-C6-O6
4	B	202	NAG	C8-C7-N2-C2
4	B	202	NAG	O7-C7-N2-C2
4	D	202	NAG	C8-C7-N2-C2
4	D	202	NAG	O7-C7-N2-C2
4	F	202	NAG	C8-C7-N2-C2
4	F	202	NAG	O7-C7-N2-C2
4	H	202	NAG	C8-C7-N2-C2
4	H	202	NAG	O7-C7-N2-C2
4	B	201	NAG	O5-C5-C6-O6
4	F	201	NAG	O5-C5-C6-O6

There are no ring outliers.

11 monomers are involved in 12 short contacts:

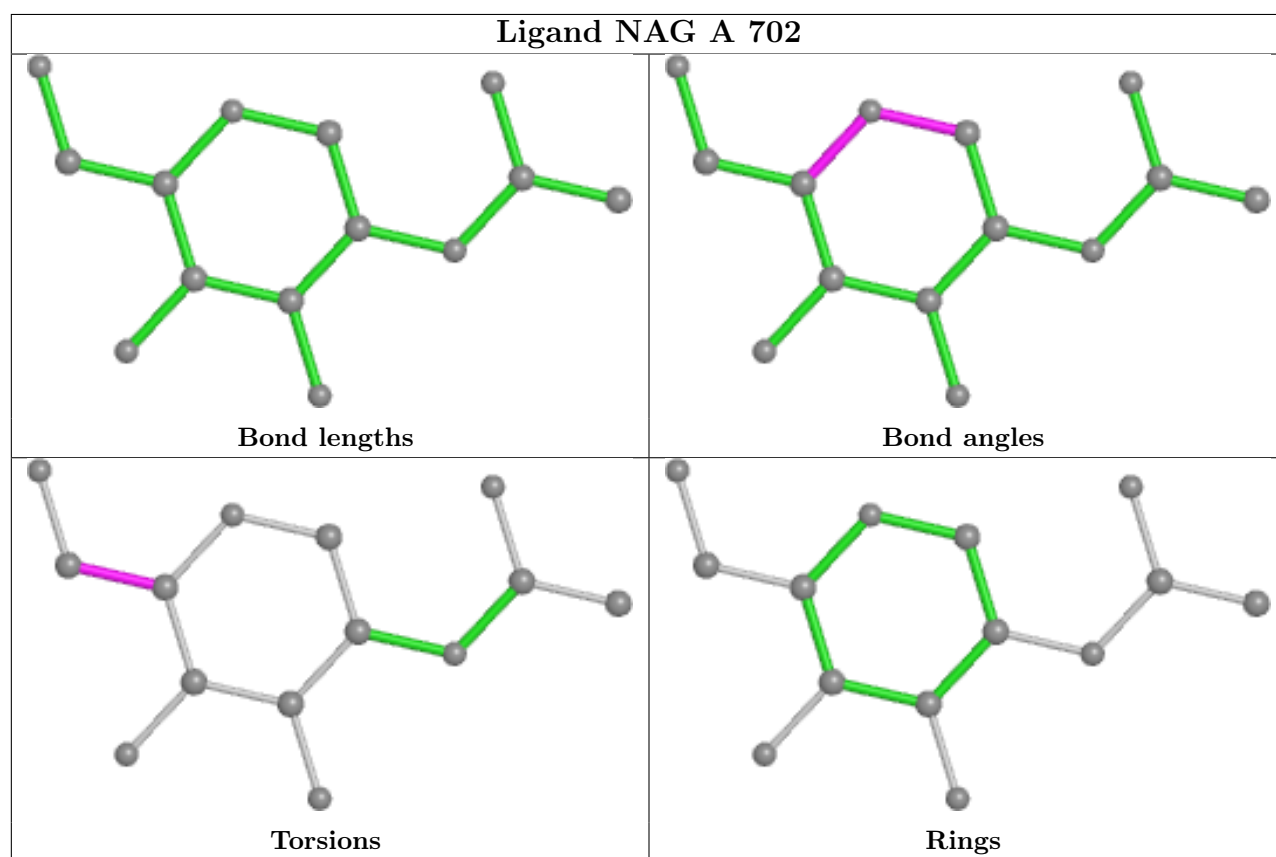
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	702	NAG	1	0
4	E	701	NAG	1	0
4	G	702	NAG	1	0
4	B	202	NAG	1	0
4	H	202	NAG	1	0
4	G	701	NAG	1	0
4	C	701	NAG	1	0

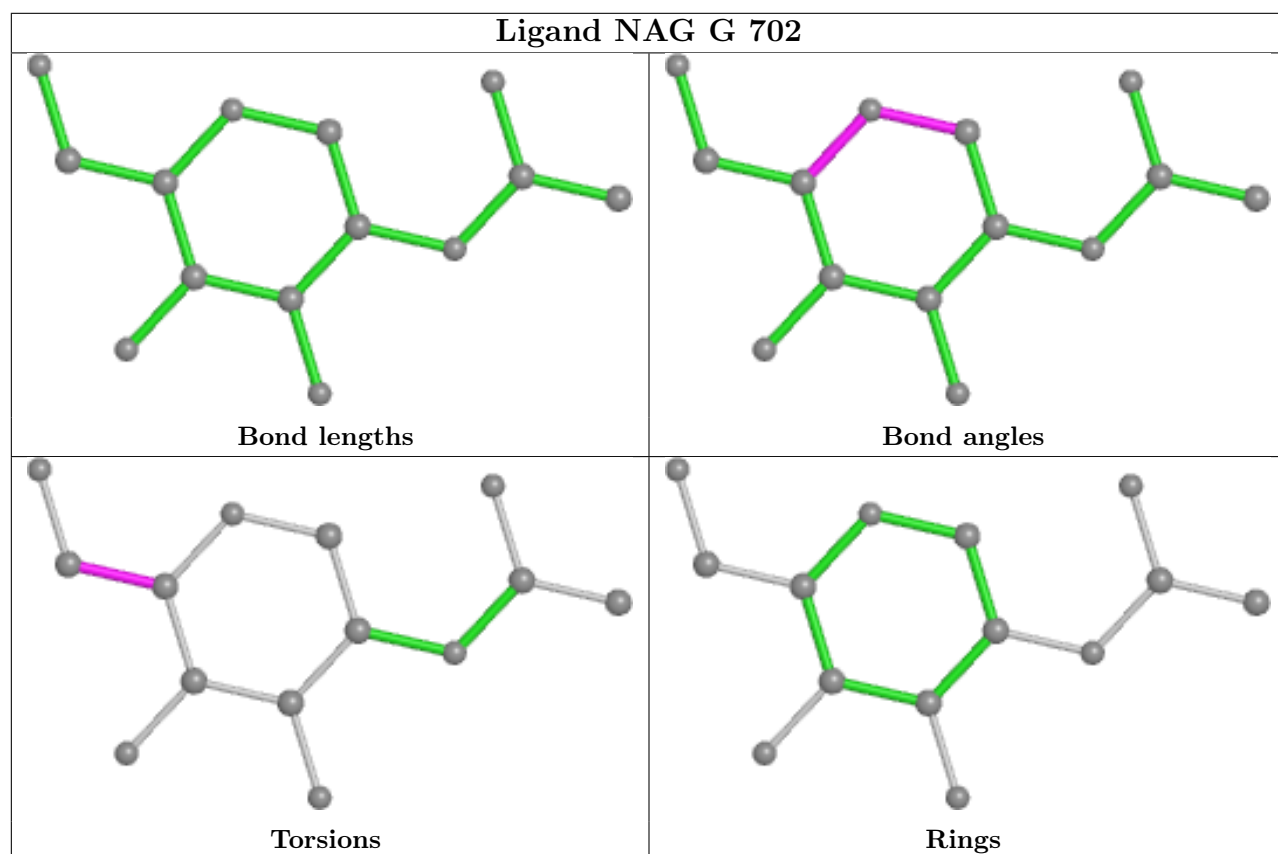
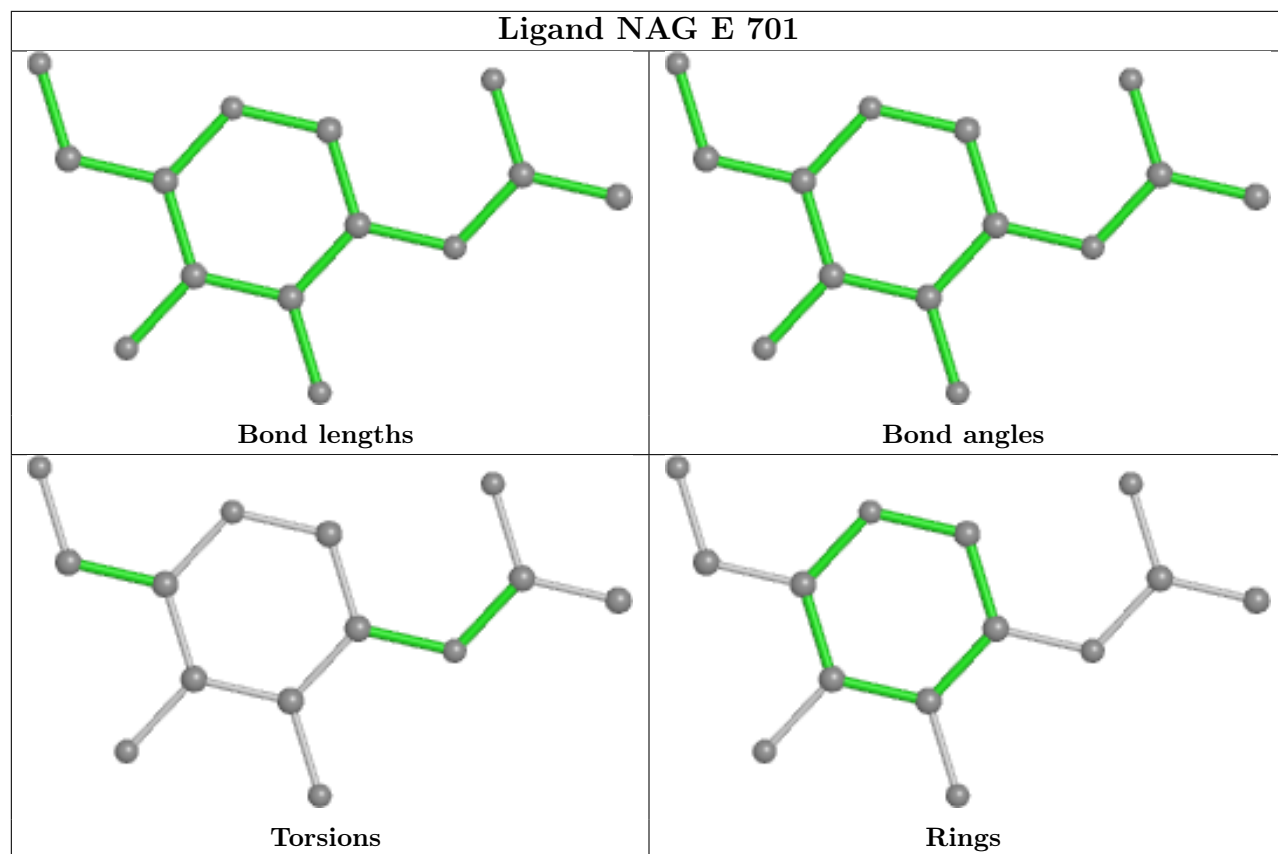
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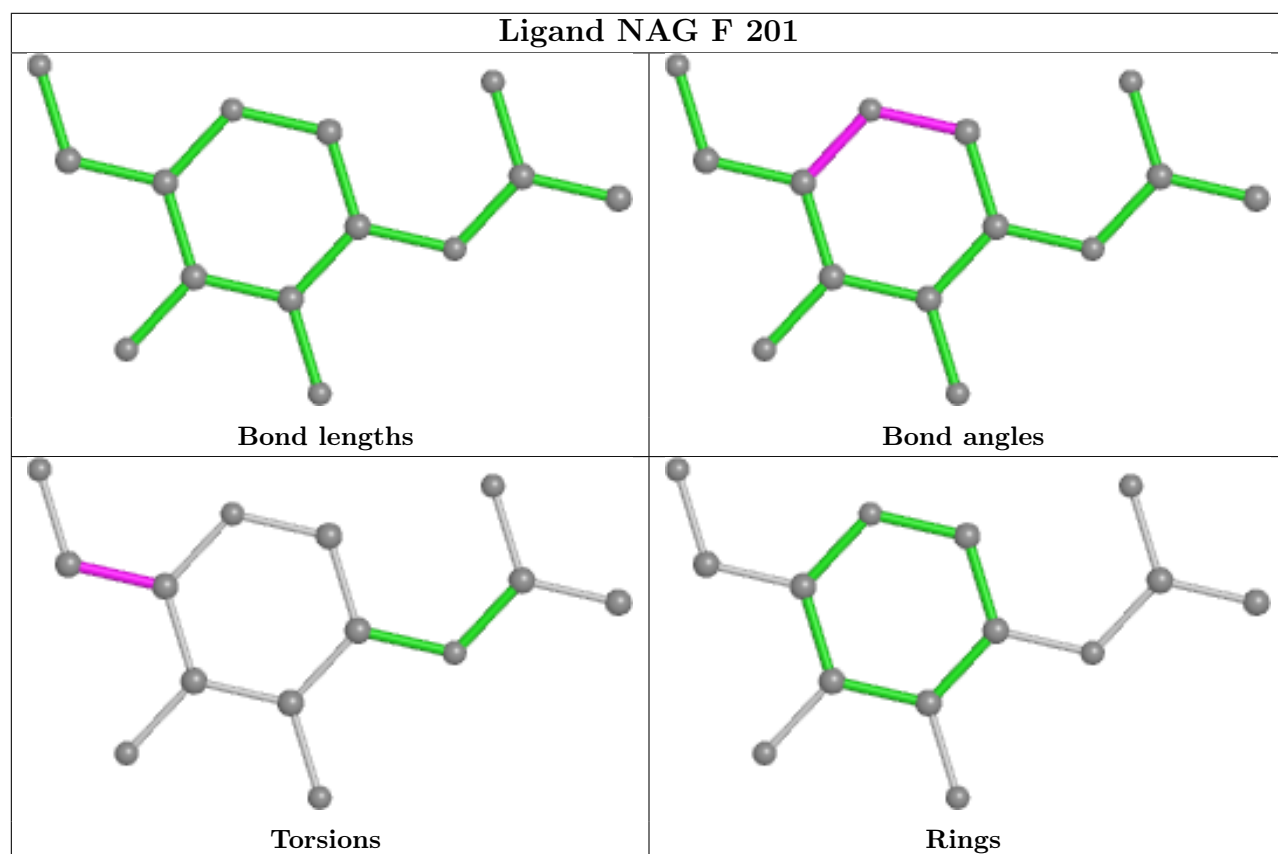
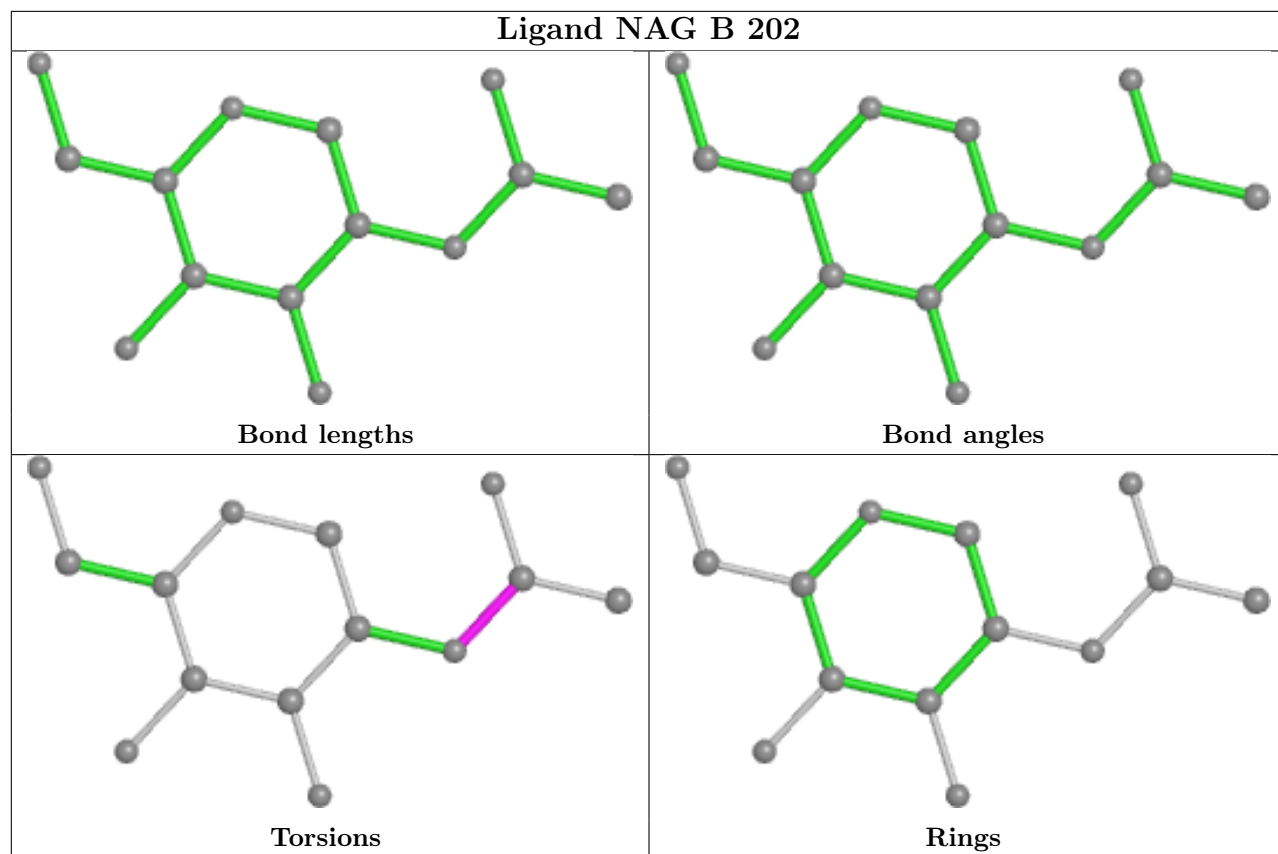
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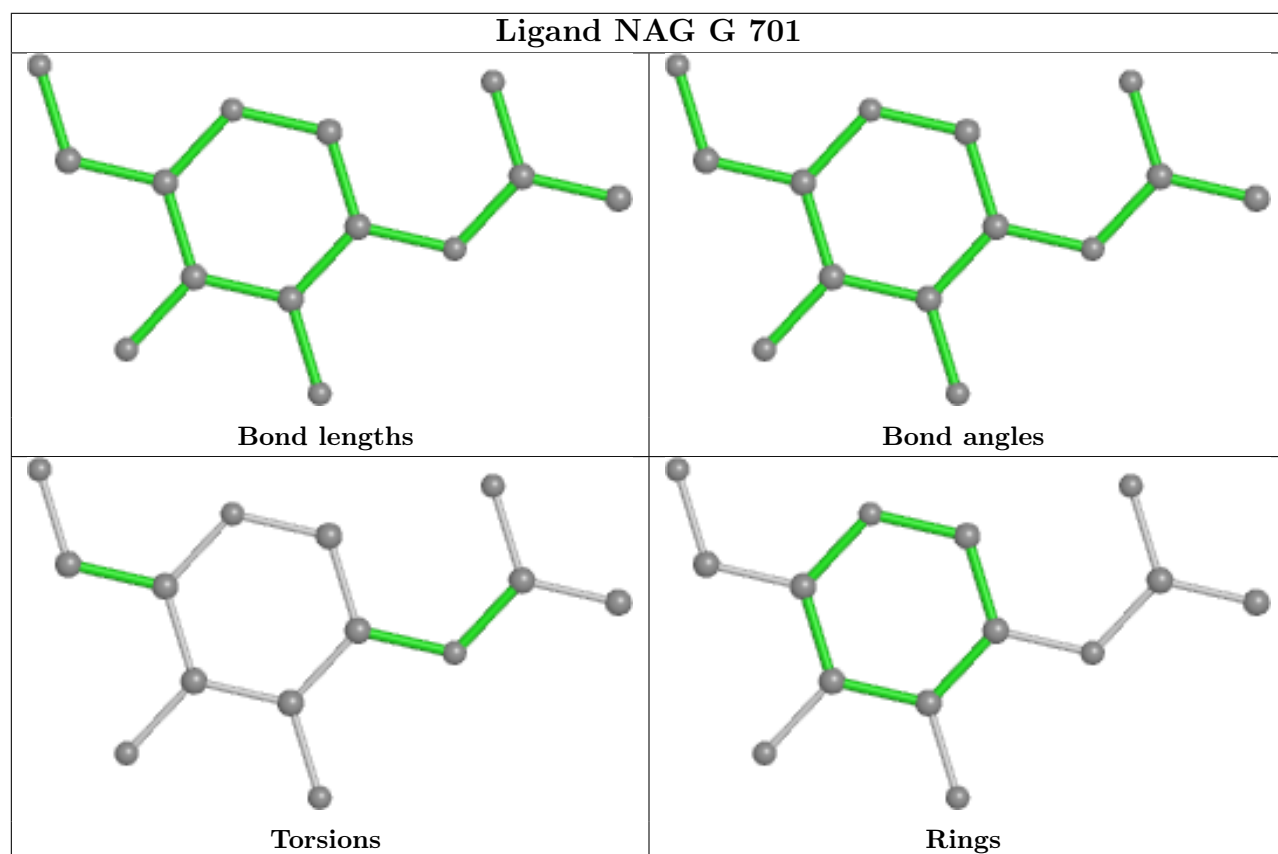
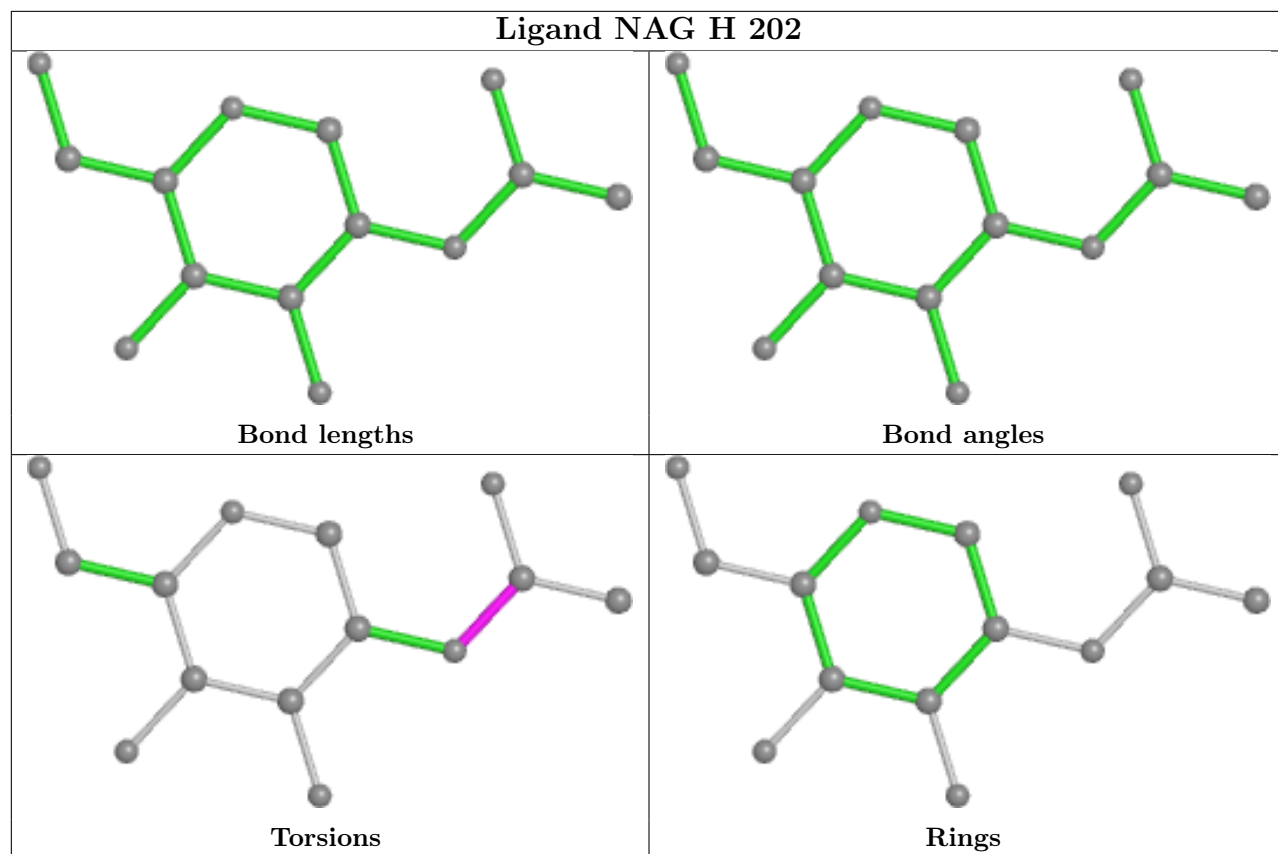
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	702	NAG	1	0
4	C	702	NAG	1	0
4	D	202	NAG	2	0
4	A	701	NAG	1	0

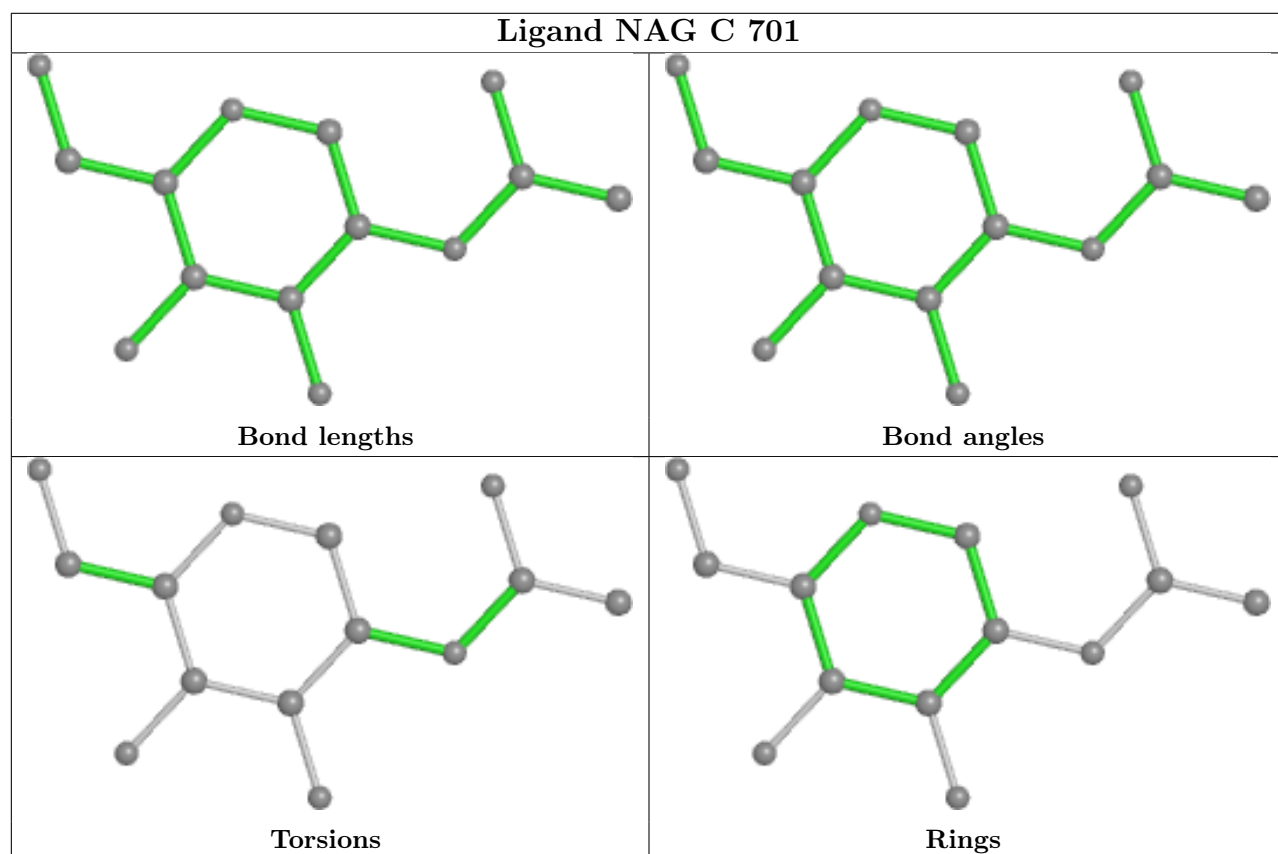
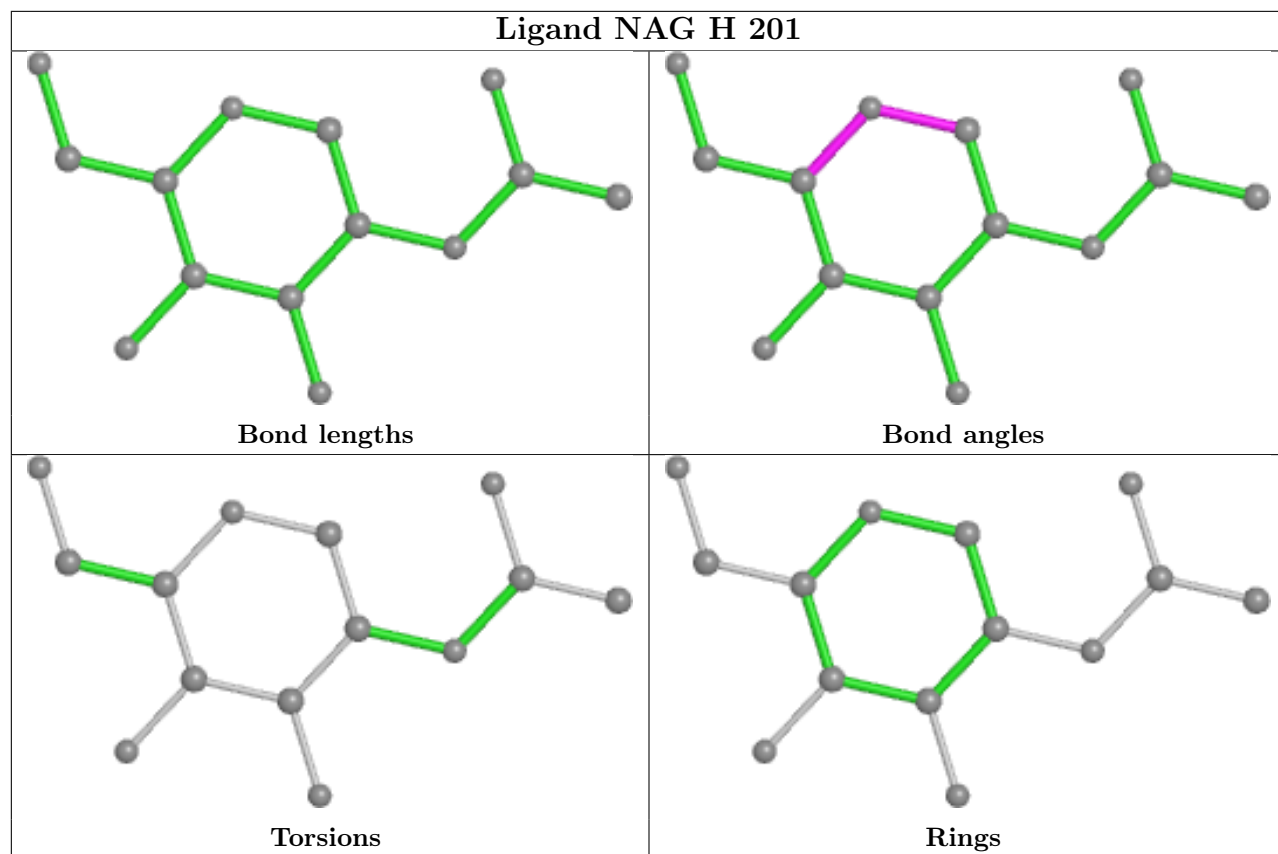
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

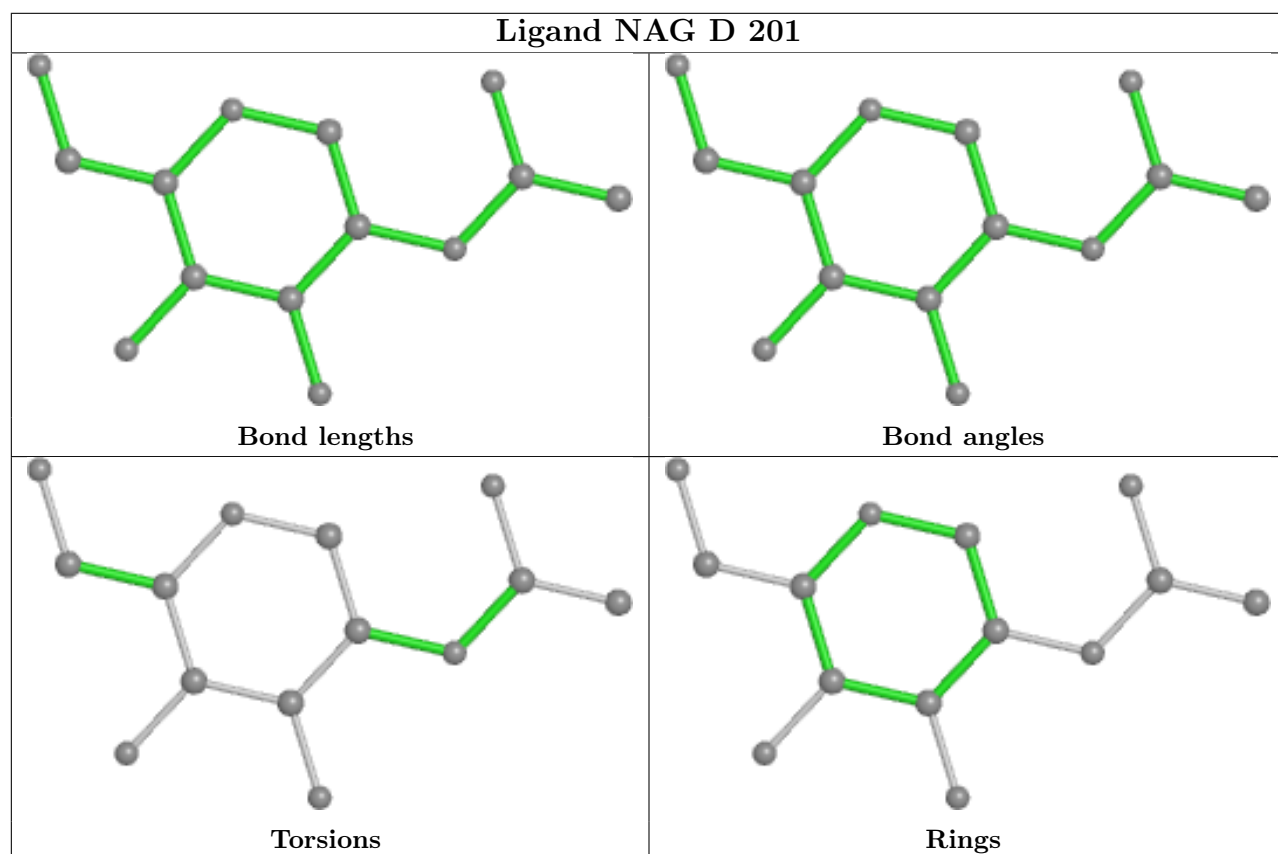
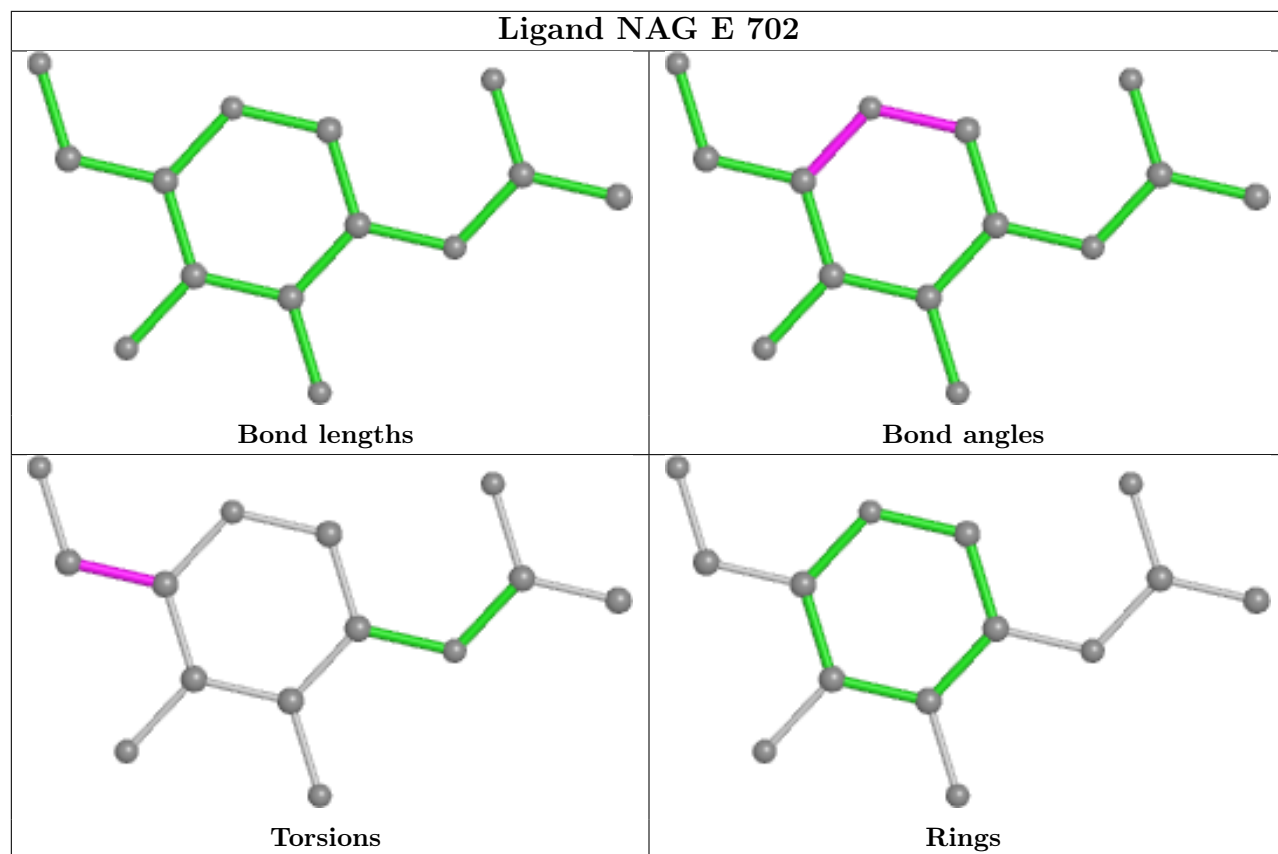


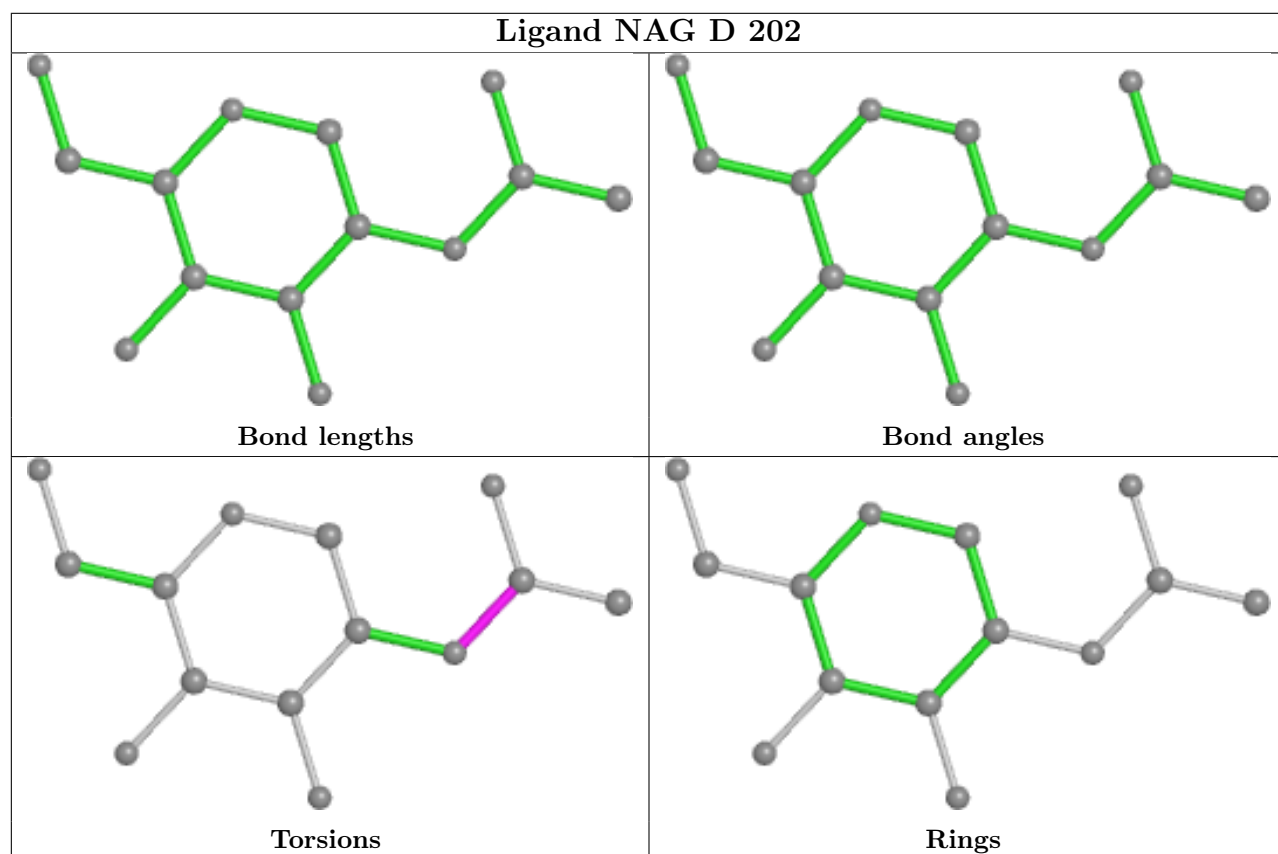
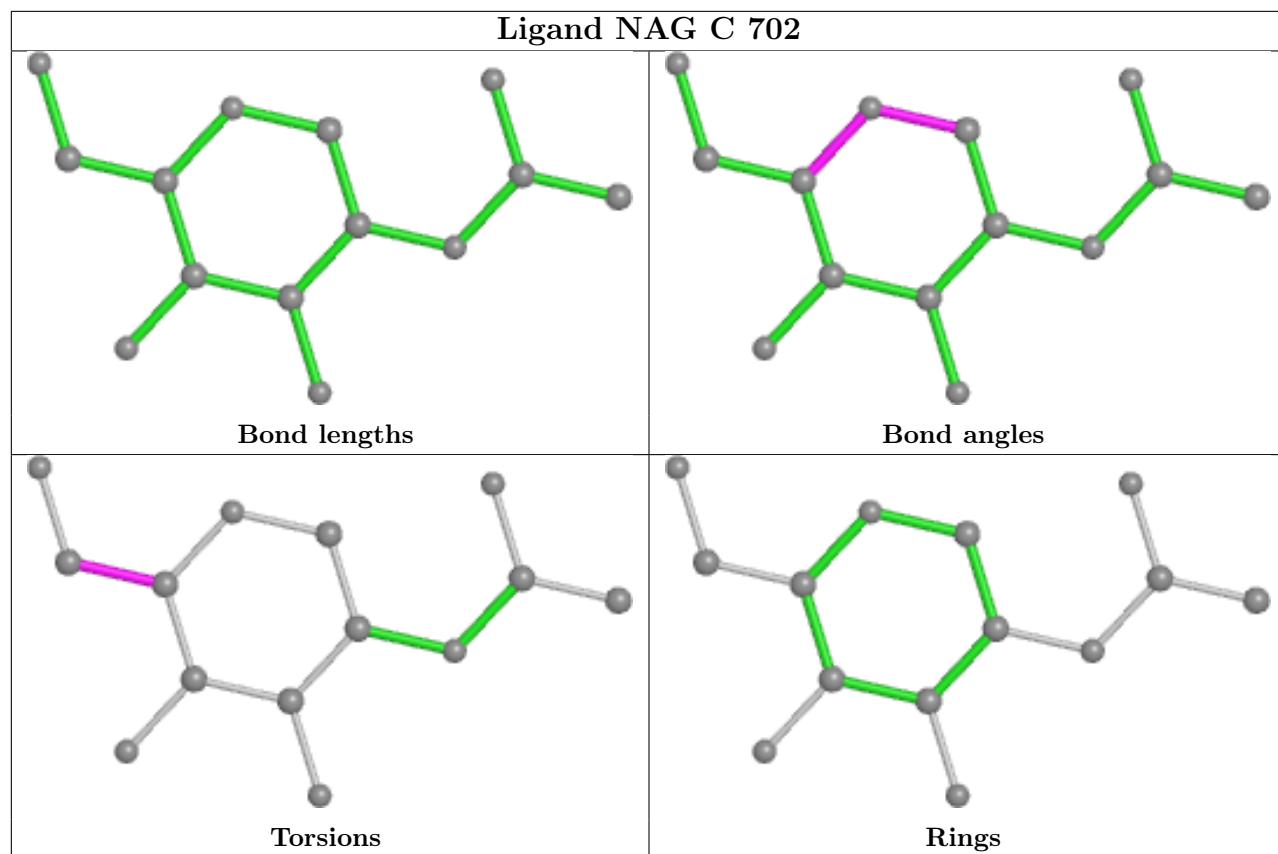


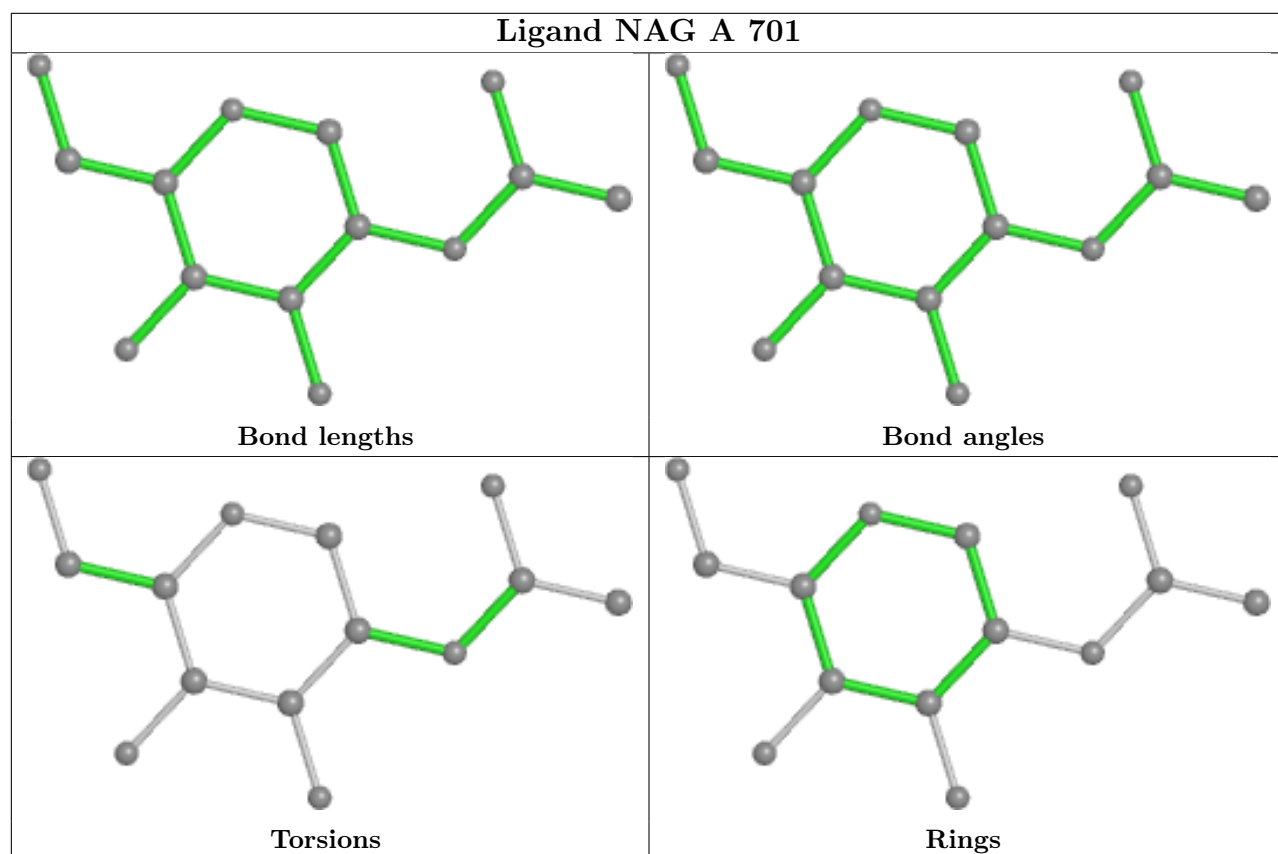
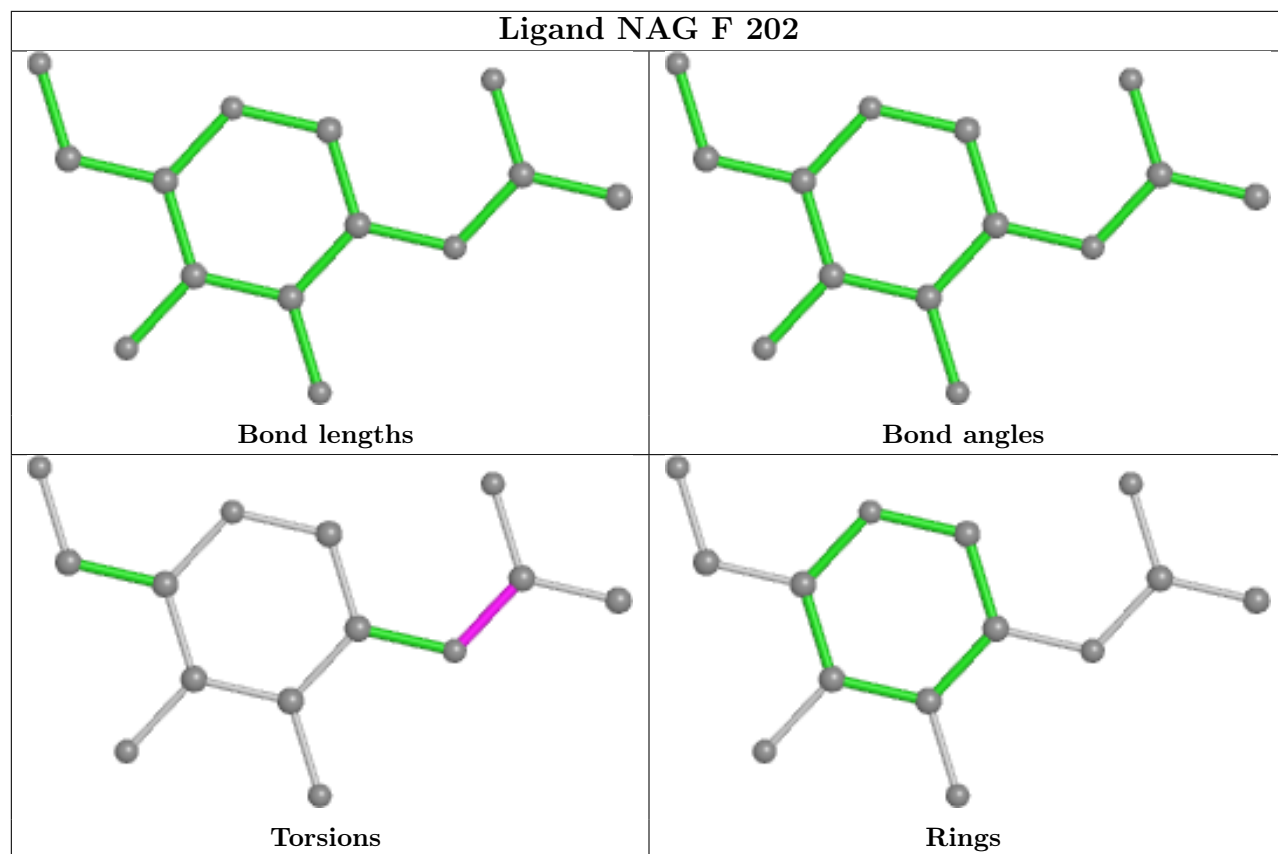


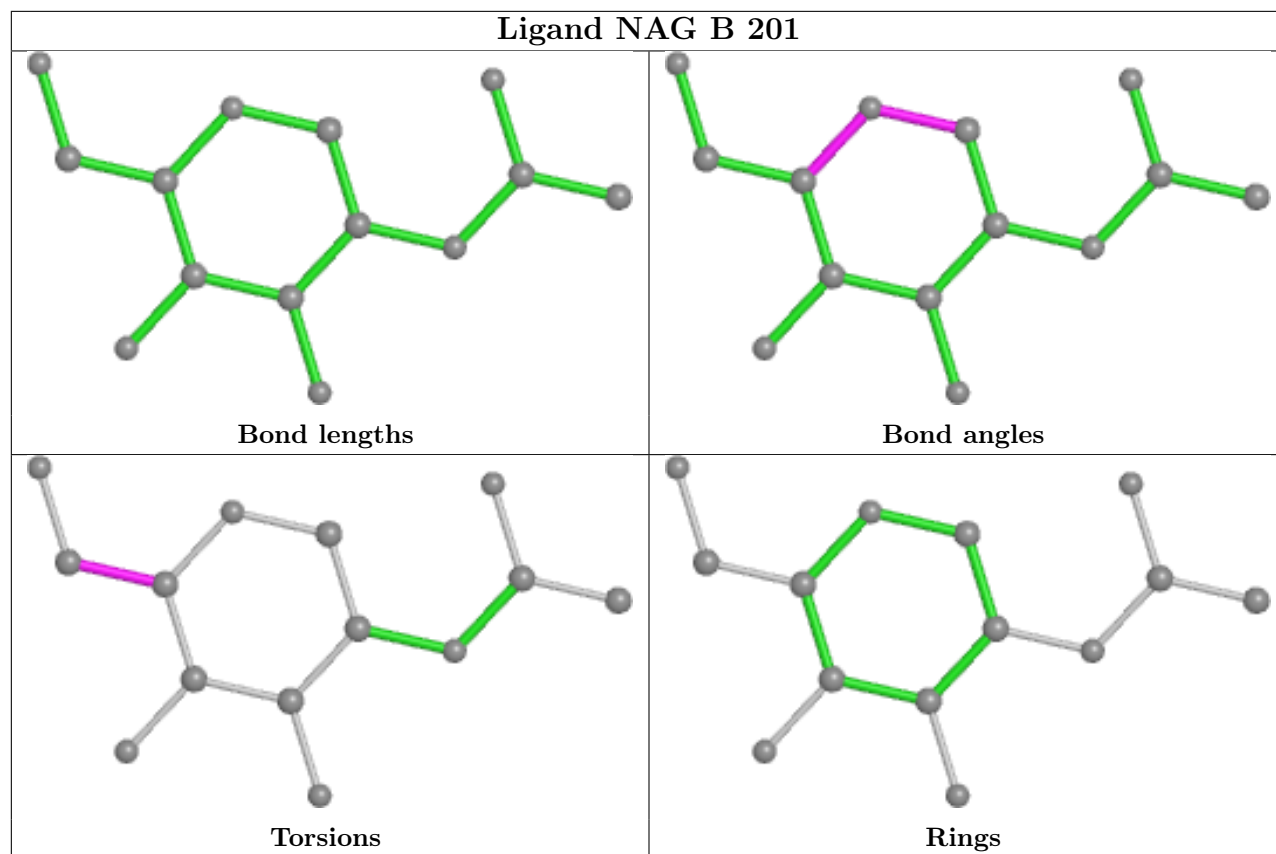












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	655/662 (98%)	-0.03	22 (3%)	45	19	61, 108, 208, 295	0
1	C	655/662 (98%)	-0.04	23 (3%)	44	18	62, 105, 207, 293	0
1	E	655/662 (98%)	0.09	28 (4%)	35	13	66, 115, 214, 305	0
1	G	655/662 (98%)	0.10	32 (4%)	29	11	70, 117, 213, 307	0
2	B	109/114 (95%)	-0.03	3 (2%)	53	25	70, 112, 173, 235	0
2	D	109/114 (95%)	-0.13	2 (1%)	68	40	75, 107, 137, 157	0
2	F	109/114 (95%)	-0.09	2 (1%)	68	40	86, 121, 178, 224	0
2	H	109/114 (95%)	0.14	4 (3%)	41	17	90, 125, 185, 262	0
3	I	165/183 (90%)	-0.15	2 (1%)	79	54	70, 105, 173, 230	0
3	J	165/183 (90%)	-0.12	4 (2%)	59	30	68, 103, 168, 232	0
3	K	165/183 (90%)	-0.14	6 (3%)	42	17	72, 108, 187, 252	0
3	L	165/183 (90%)	-0.02	3 (1%)	68	40	66, 104, 180, 238	0
All	All	3716/3836 (96%)	-0.00	131 (3%)	44	18	61, 111, 203, 307	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	575	SER	22.9
1	A	575	SER	20.4
1	G	521	ARG	13.8
1	E	575	SER	8.9
1	C	574	SER	8.2
1	A	607	ARG	6.3
2	H	35	ARG	6.2
1	C	618	ALA	6.1
1	E	521	ARG	6.0
1	A	574	SER	5.9
1	G	187	GLU	5.8

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Mol	Chain	Res	Type	RSRZ
1	C	607	ARG	5.7
3	K	161	VAL	5.6
3	L	161	VAL	5.3
1	E	667	VAL	5.3
1	E	659	LEU	5.3
1	A	576	SER	5.0
1	G	667	VAL	5.0
1	E	605	PHE	5.0
1	E	618	ALA	4.6
1	C	673	LEU	4.5
1	C	620	LEU	4.5
1	G	112	ILE	4.4
1	G	113	SER	4.4
1	G	661	LEU	4.3
1	C	609	GLN	4.3
3	L	199	LYS	4.3
1	E	574	SER	4.2
3	L	151	THR	4.2
1	E	604	ASN	4.1
1	E	238	PHE	4.0
1	G	605	PHE	4.0
1	C	32	HIS	4.0
1	G	520	GLU	4.0
1	A	614	PHE	3.9
1	E	240	ASN	3.9
1	C	579	LEU	3.8
2	B	37	GLN	3.8
1	G	614	PHE	3.8
1	A	667	VAL	3.7
1	E	571	THR	3.7
1	A	594	GLY	3.6
1	E	661	LEU	3.6
2	H	37	GLN	3.6
2	D	37	GLN	3.6
1	E	620	LEU	3.6
1	A	582	VAL	3.6
1	G	575	SER	3.6
1	G	574	SER	3.5
1	E	432	LEU	3.5
2	D	75	VAL	3.5
1	C	576	SER	3.4
1	C	33	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	505	ALA	3.4
1	E	505	ALA	3.3
1	C	532	TYR	3.3
1	C	31	GLY	3.2
1	G	188	LYS	3.2
1	E	113	SER	3.2
1	A	661	LEU	3.2
1	C	643	ILE	3.1
1	G	43	LEU	3.1
1	A	665	GLY	3.1
1	G	620	LEU	3.1
1	A	639	VAL	3.0
2	F	42	LEU	3.0
3	K	111	GLY	3.0
1	A	634	ILE	2.9
1	C	644	LEU	2.9
1	G	506	VAL	2.9
1	G	570	THR	2.9
1	E	187	GLU	2.9
1	A	613	ILE	2.8
1	E	607	ARG	2.8
1	E	644	LEU	2.8
1	C	573	LEU	2.8
1	C	603	GLN	2.7
1	C	572	TYR	2.7
3	J	27	LYS	2.7
1	G	111	VAL	2.7
1	G	532	TYR	2.6
1	E	674	TYR	2.6
3	K	112	ALA	2.6
1	A	532	TYR	2.6
1	C	530	PRO	2.5
1	A	432	LEU	2.5
1	A	521	ARG	2.5
1	A	586	LYS	2.5
1	G	432	LEU	2.5
1	E	241	TYR	2.5
1	A	605	PHE	2.4
1	G	241	TYR	2.4
1	G	571	THR	2.4
1	E	32	HIS	2.4
1	G	355	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	194	LEU	2.3
1	G	32	HIS	2.3
2	B	64	LEU	2.3
3	I	161	VAL	2.3
1	E	56	TRP	2.3
1	C	553	ILE	2.3
2	B	40	LEU	2.3
1	G	601	LYS	2.3
1	G	38	ILE	2.3
1	G	527	TRP	2.3
3	J	150	ILE	2.2
1	C	432	LEU	2.2
2	H	80	ALA	2.2
2	F	64	LEU	2.2
3	J	199	LYS	2.2
1	E	242	PHE	2.2
1	A	640	GLN	2.2
3	K	27	LYS	2.2
1	C	565	LEU	2.2
1	E	112	ILE	2.2
1	E	25	LEU	2.2
3	J	151	THR	2.1
1	G	659	LEU	2.1
1	A	620	LEU	2.1
2	H	85	VAL	2.1
1	E	643	ILE	2.1
1	G	238	PHE	2.1
1	A	351	LEU	2.1
1	G	539	ASP	2.0
3	I	66	MET	2.0
1	C	582	VAL	2.0
1	G	237	ASN	2.0
3	K	28	GLU	2.0
1	A	655	HIS	2.0
3	K	96	ILE	2.0
1	G	513	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

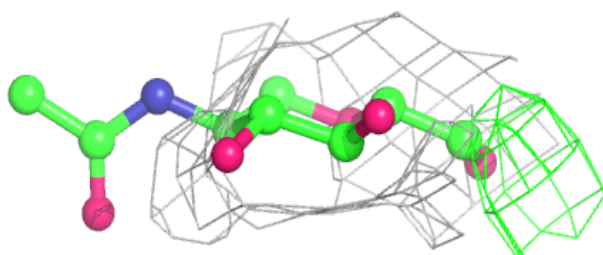
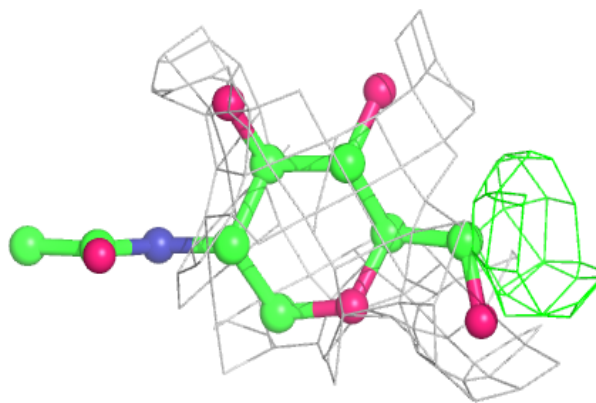
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	C	702	14/15	0.35	0.40	185,192,196,197	0
4	NAG	A	702	14/15	0.62	0.28	173,179,183,184	0
4	NAG	A	701	14/15	0.67	0.26	148,152,155,156	0
4	NAG	G	702	14/15	0.73	0.27	198,202,205,208	0
4	NAG	E	702	14/15	0.74	0.28	196,202,207,208	0
4	NAG	H	202	14/15	0.76	0.23	114,115,117,117	0
4	NAG	B	202	14/15	0.79	0.18	129,131,135,136	0
4	NAG	C	701	14/15	0.79	0.24	137,140,144,144	0
4	NAG	H	201	14/15	0.81	0.24	149,153,155,155	0
4	NAG	G	701	14/15	0.81	0.22	130,136,141,142	0
4	NAG	E	701	14/15	0.82	0.23	124,132,137,137	0
4	NAG	F	201	14/15	0.84	0.29	140,142,142,143	0
4	NAG	D	201	14/15	0.85	0.15	75,75,75,75	0
4	NAG	B	201	14/15	0.88	0.22	131,134,135,136	0
4	NAG	F	202	14/15	0.89	0.16	117,118,119,119	0
4	NAG	D	202	14/15	0.91	0.10	75,75,75,75	0

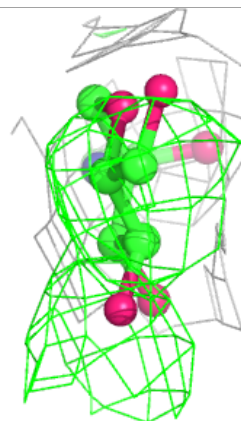
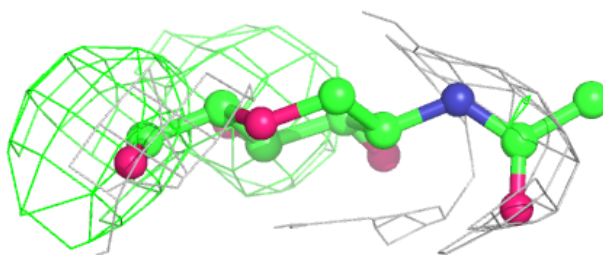
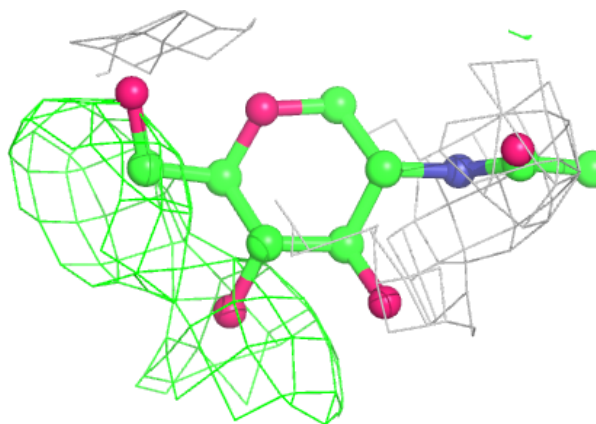
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAG C 702:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

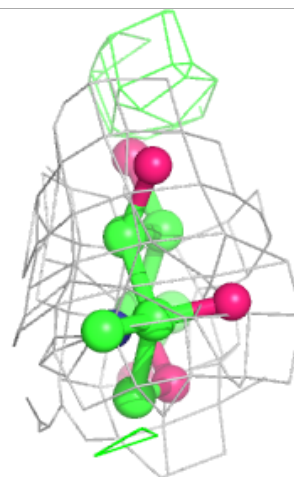
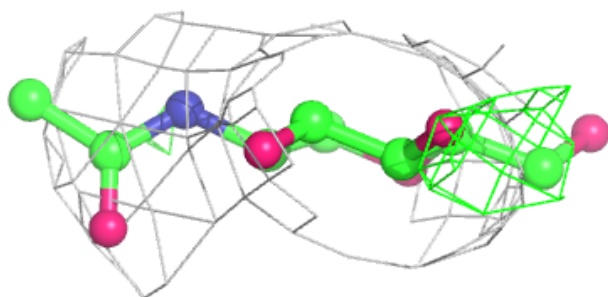
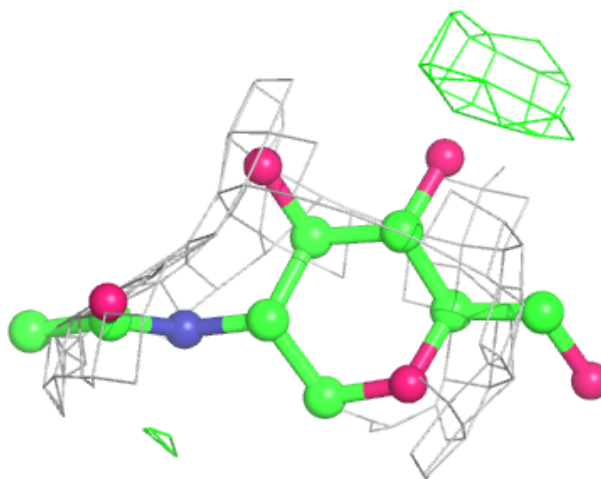
**Electron density around NAG A 702:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



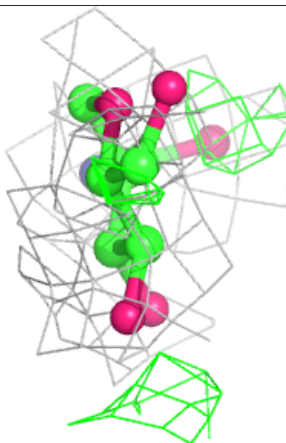
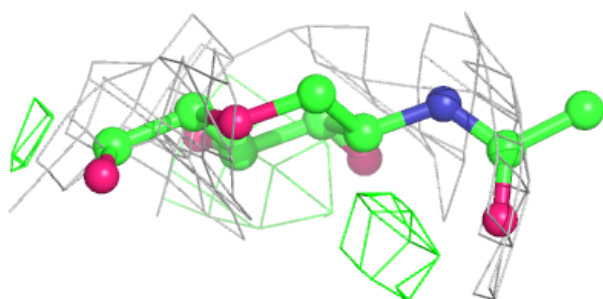
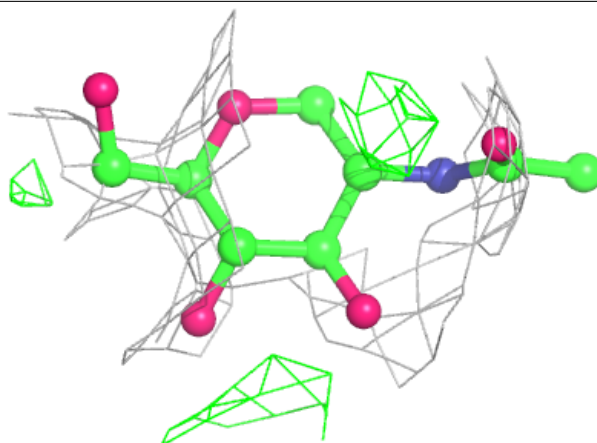
Electron density around NAG A 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

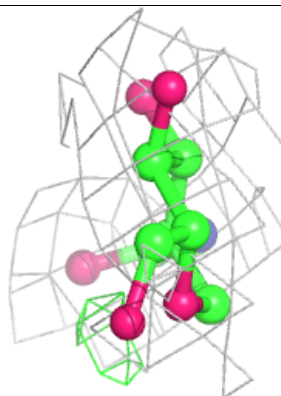
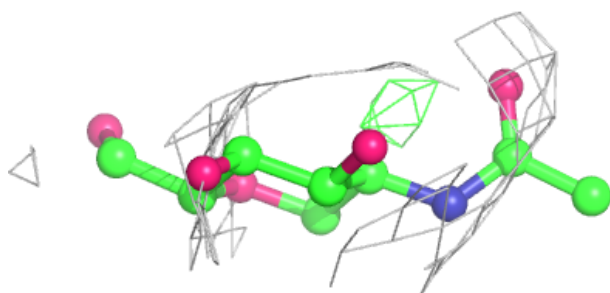
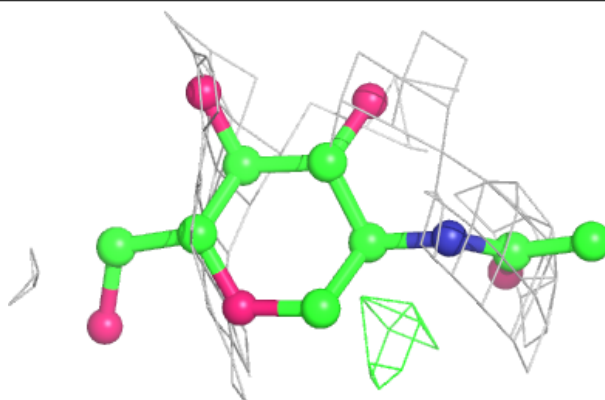


Electron density around NAG G 702:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

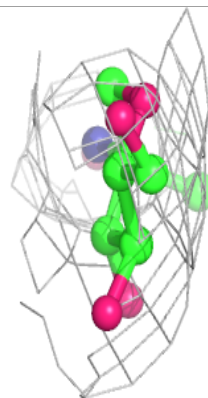
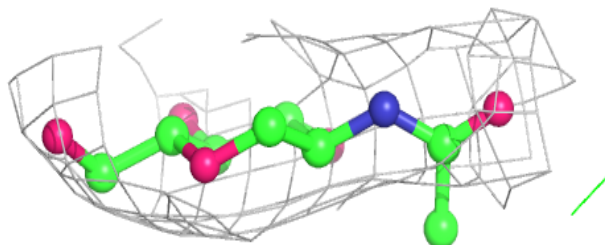
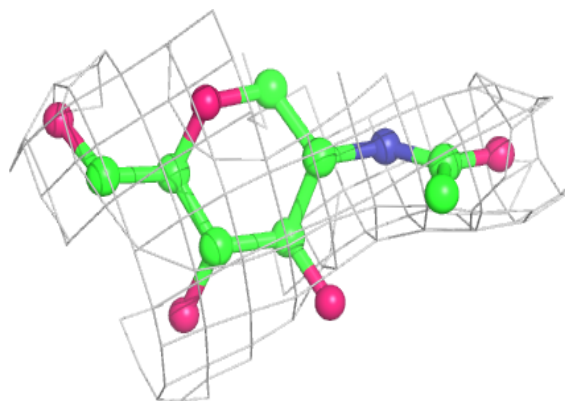
**Electron density around NAG E 702:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

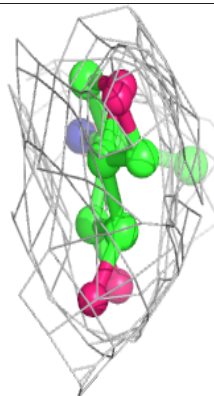
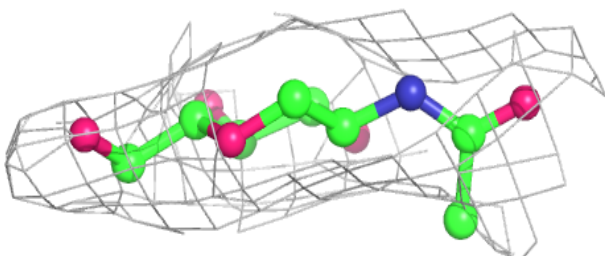
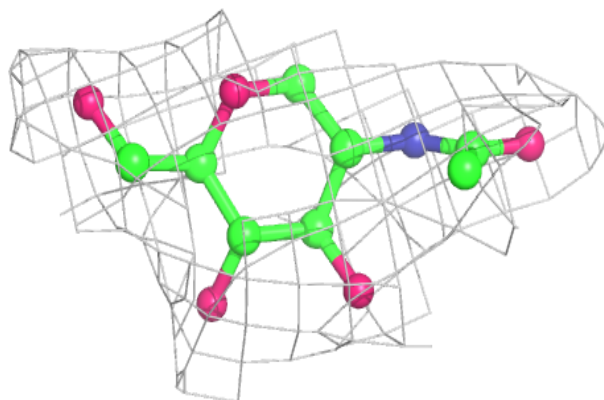


Electron density around NAG H 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

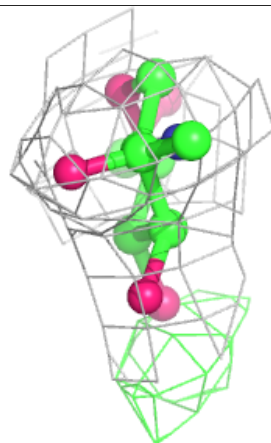
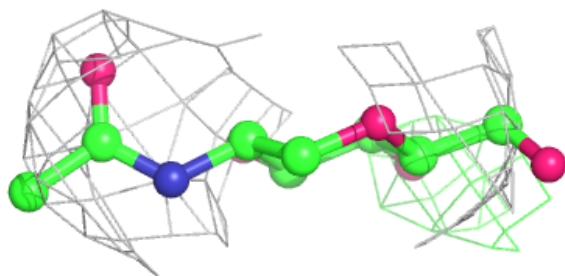
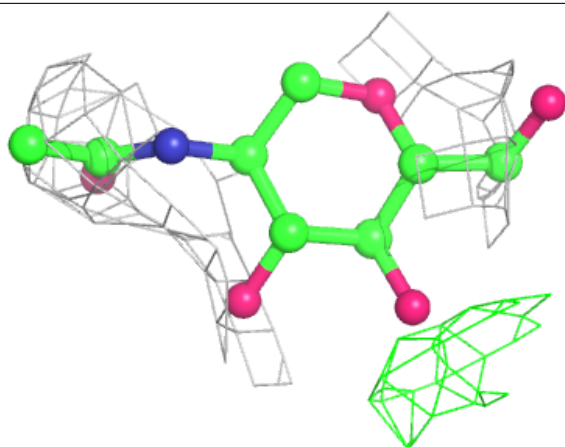
**Electron density around NAG B 202:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

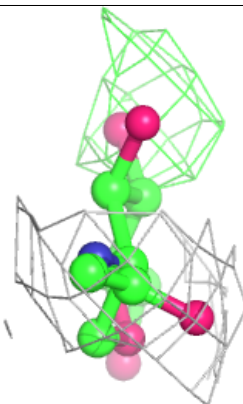
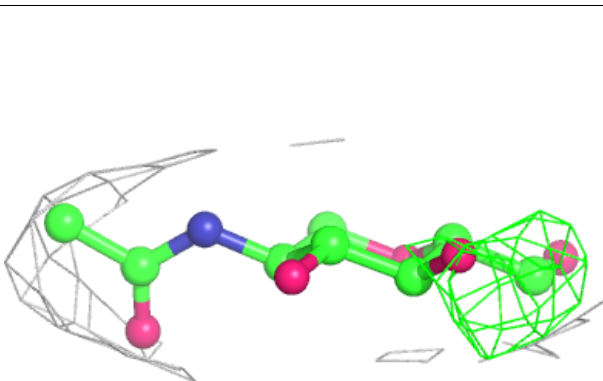
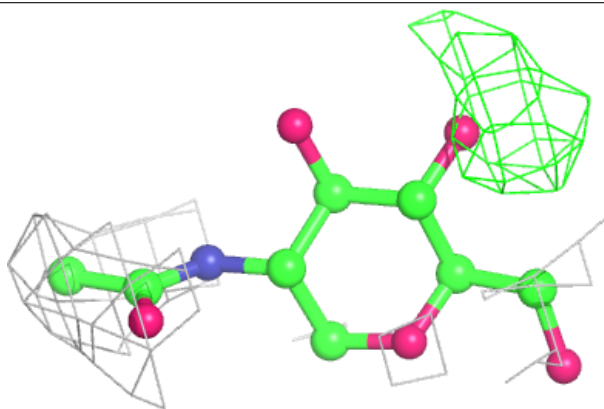


Electron density around NAG C 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

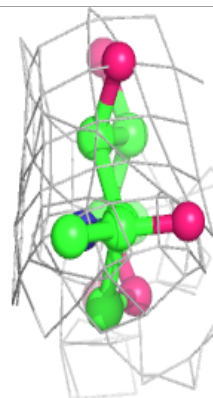
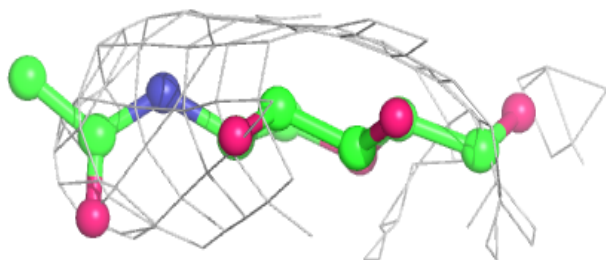
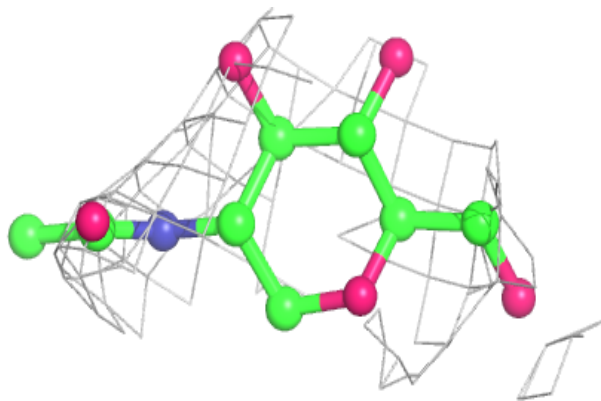
**Electron density around NAG H 201:**

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and green (positive)

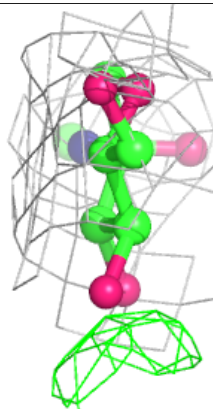
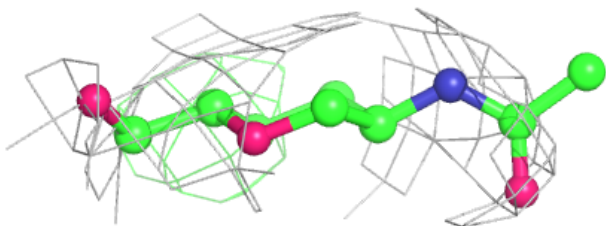
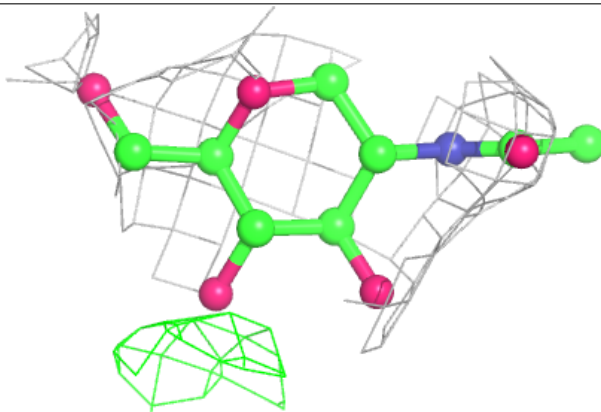


Electron density around NAG G 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

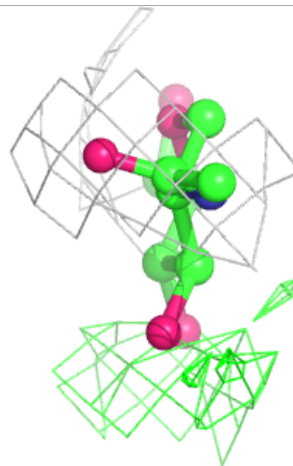
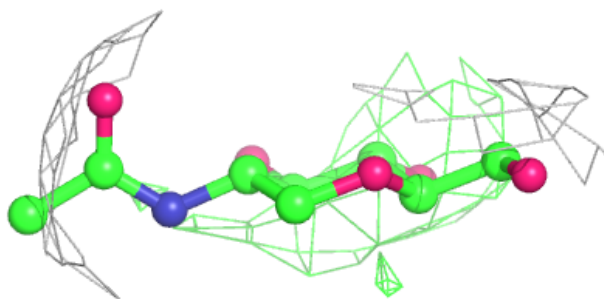
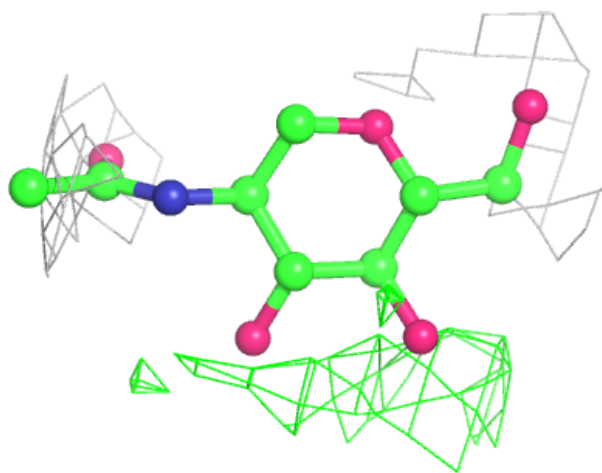
**Electron density around NAG E 701:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



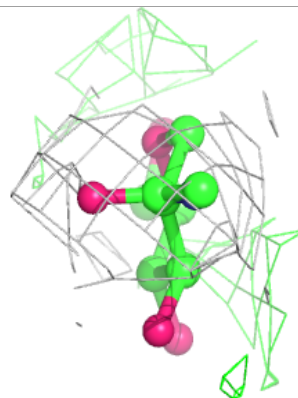
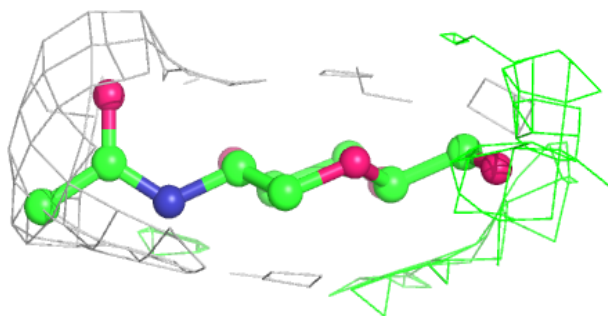
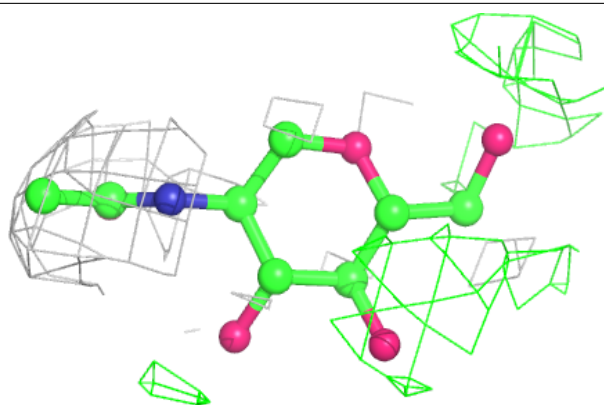
Electron density around NAG F 201:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

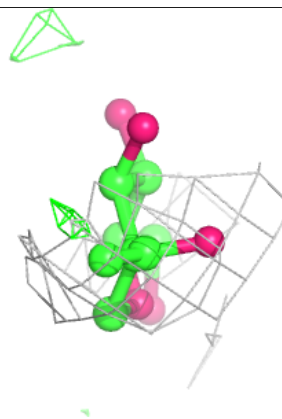
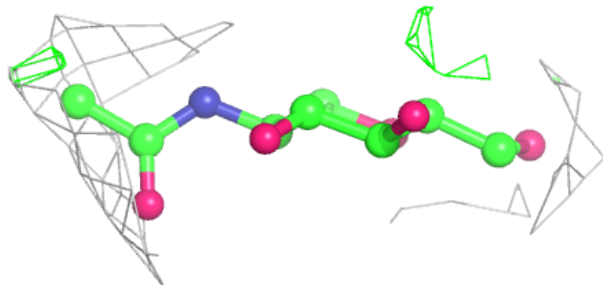
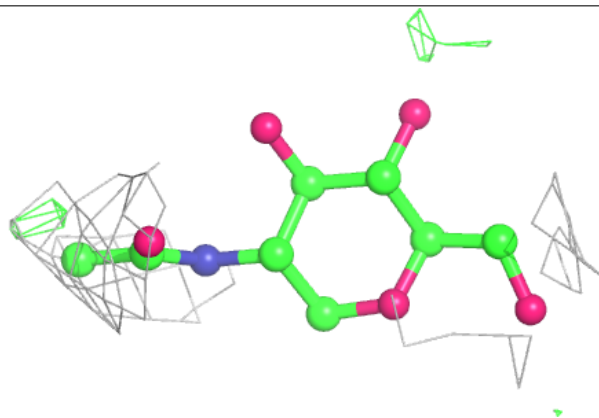


Electron density around NAG D 201:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

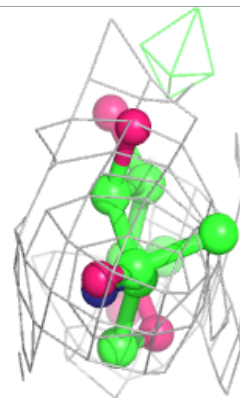
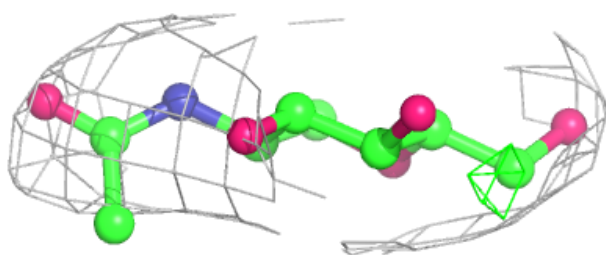
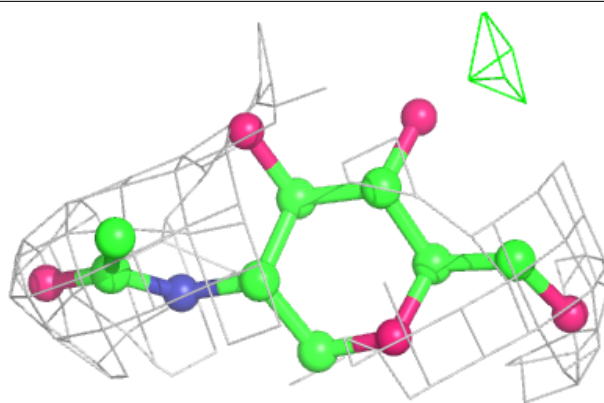
**Electron density around NAG B 201:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

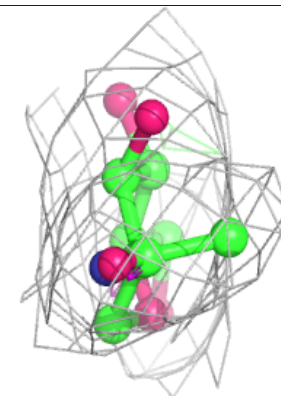
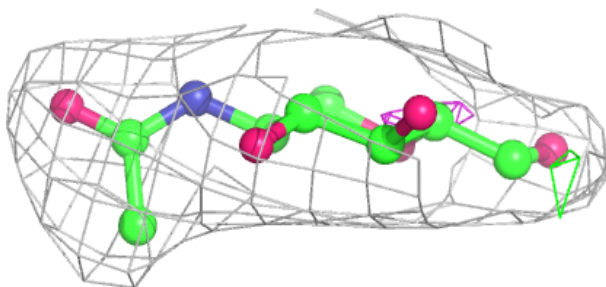
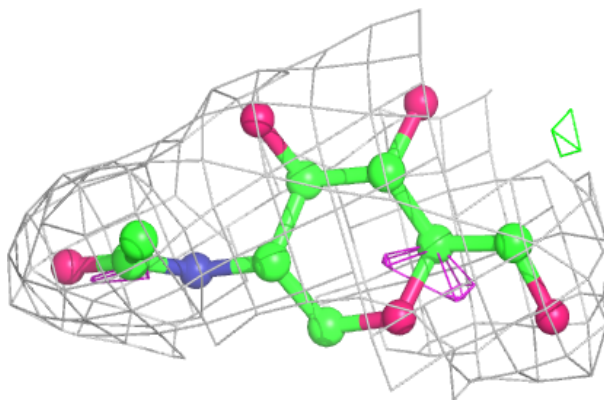


Electron density around NAG F 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NAG D 202:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.