Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 02:02 AM EST

PDB ID	:	7SFV
EMDB ID	:	EMD-25103
Title	:	CryoEM structure of Venezuelan Equine Encephalitis virus (VEEV) TC-83 strain VLP in complex with Fab hVEEV-63
Authors	:	Binshtein, E.; Crowe, J.E.
Deposited on	:	2021-10-04
Resolution	:	4.00 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:

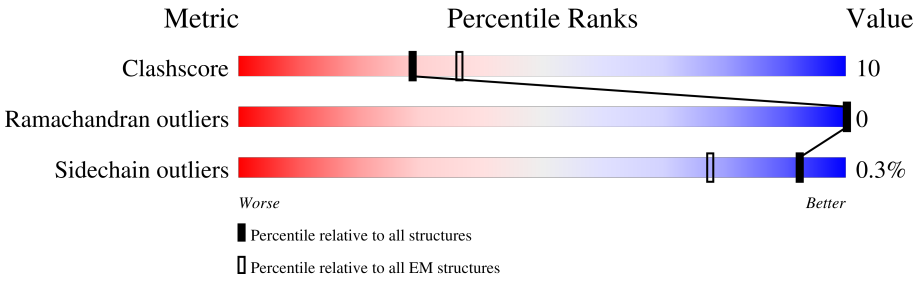
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	440	82% 18%
1	D	440	78% 22%
1	G	440	80% 20%
1	J	440	83% 17%
2	B	418	73% 27%
2	E	418	77% 23%
2	H	418	75% 24%
2	K	418	78% 22%
3	C	159	77% 23%

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Mol	Chain	Length	Quality of chain
3	F	159	65% 35%
3	I	159	70% 30%
3	L	159	70% 30%
4	M	218	78% 22%
4	O	218	73% 27%
4	Q	218	78% 22%
4	S	218	77% 23%
5	N	209	80% 20%
5	P	209	78% 22%
5	R	209	85% 15%
5	T	209	79% 21%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 42538 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 E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	440	Total	C	N	O	S	0	0
			3351	2136	550	644	21		
1	D	440	Total	C	N	O	S	0	0
			3351	2136	550	644	21		
1	G	440	Total	C	N	O	S	0	0
			3351	2136	550	644	21		
1	J	440	Total	C	N	O	S	0	0
			3351	2136	550	644	21		

- Molecule 2 is a protein called Spike glycoprotein E2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	418	Total	C	N	O	S	0	0
			3264	2064	575	600	25		
2	E	418	Total	C	N	O	S	0	0
			3264	2064	575	600	25		
2	H	418	Total	C	N	O	S	0	0
			3264	2064	575	600	25		
2	K	418	Total	C	N	O	S	0	0
			3264	2064	575	600	25		

- Molecule 3 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	159	Total	C	N	O	S	0	0
			1248	790	219	231	8		
3	F	159	Total	C	N	O	S	0	0
			1248	790	219	231	8		
3	I	159	Total	C	N	O	S	0	0
			1248	790	219	231	8		
3	L	159	Total	C	N	O	S	0	0
			1248	790	219	231	8		

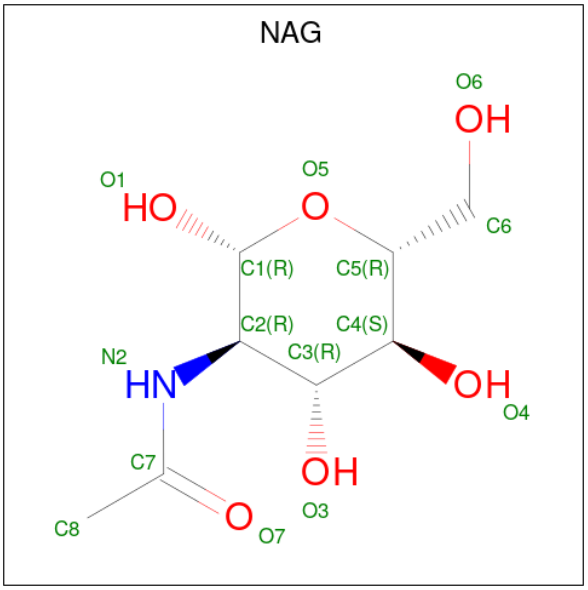
- Molecule 4 is a protein called hVEEV-63 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	218	Total	C	N	O	S	0	0
			1415	872	257	281	5		
4	O	218	Total	C	N	O	S	0	0
			1413	870	257	281	5		
4	Q	218	Total	C	N	O	S	0	0
			1415	872	257	281	5		
4	S	218	Total	C	N	O	S	0	0
			1413	870	257	281	5		

- Molecule 5 is a protein called hVEEV-63 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	209	Total	C	N	O	S	0	0
			1315	809	232	272	2		
5	P	209	Total	C	N	O	S	0	0
			1315	809	232	272	2		
5	R	209	Total	C	N	O	S	0	0
			1315	809	232	272	2		
5	T	209	Total	C	N	O	S	0	0
			1317	811	232	272	2		

- Molecule 6 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				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	

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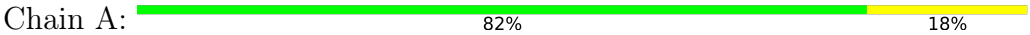
Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			28	16	2	10	
6	B	1	Total	C	N	O	0
			28	16	2	10	
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	E	1	Total	C	N	O	0
			28	16	2	10	
6	E	1	Total	C	N	O	0
			28	16	2	10	
6	G	1	Total	C	N	O	0
			14	8	1	5	
6	H	1	Total	C	N	O	0
			28	16	2	10	
6	H	1	Total	C	N	O	0
			28	16	2	10	
6	J	1	Total	C	N	O	0
			14	8	1	5	
6	K	1	Total	C	N	O	0
			28	16	2	10	
6	K	1	Total	C	N	O	0
			28	16	2	10	

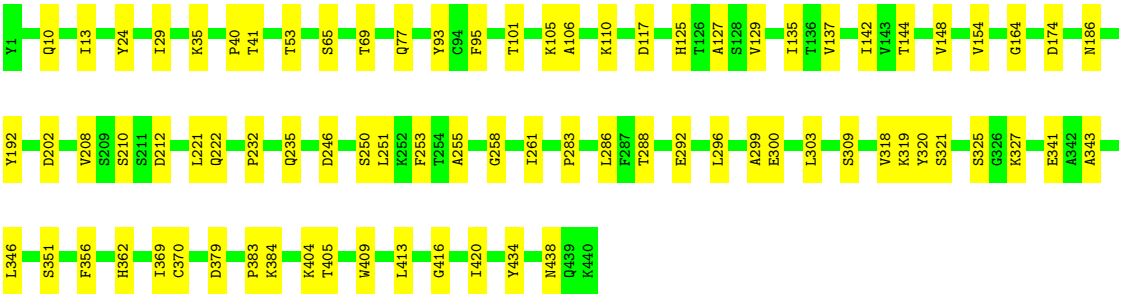
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Spike glycoprotein E1

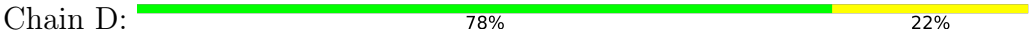
Chain A:

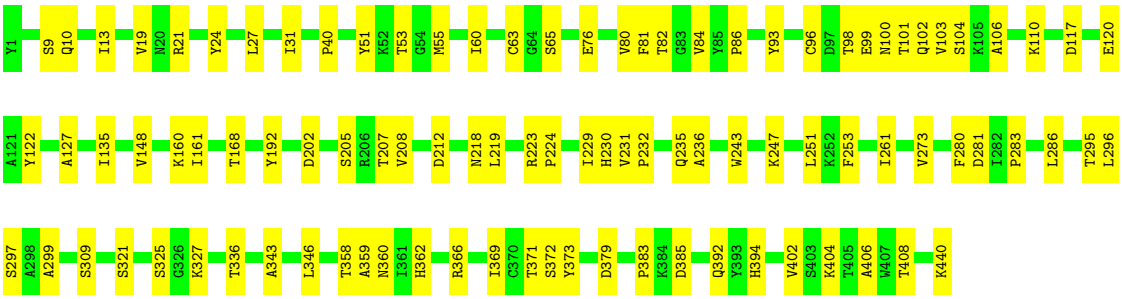




• Molecule 1: Spike glycoprotein E1

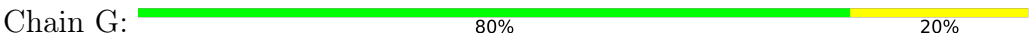
Chain D:





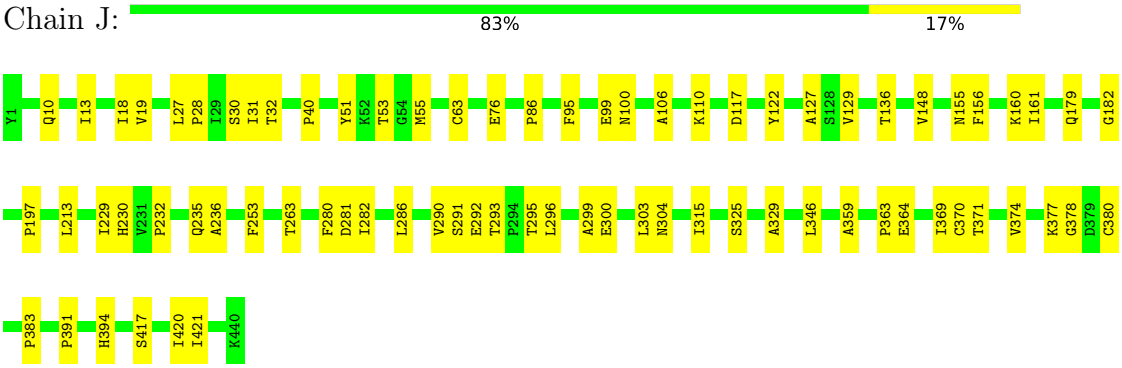
• Molecule 1: Spike glycoprotein E1

Chain G:



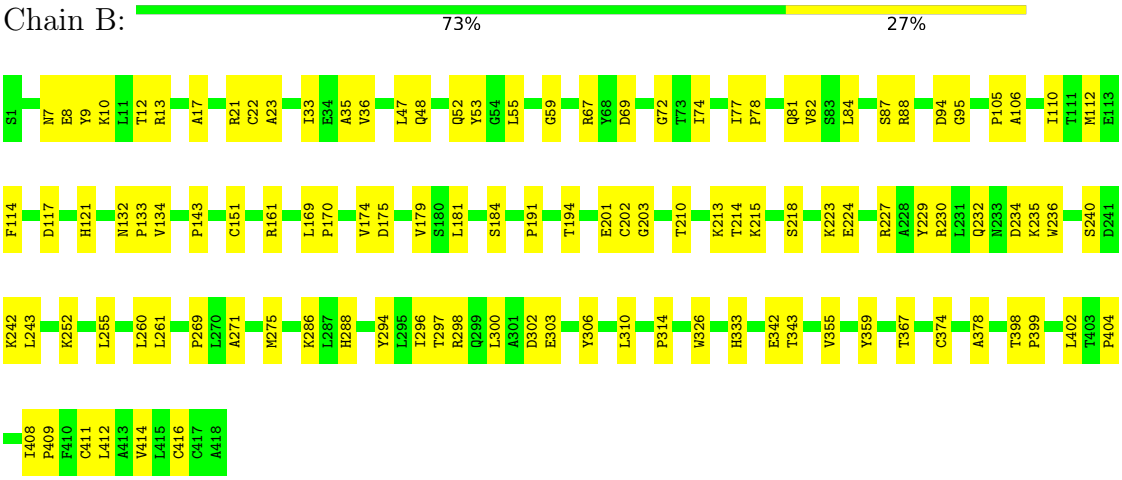
• Molecule 1: Spike glycoprotein E1

Chain J:



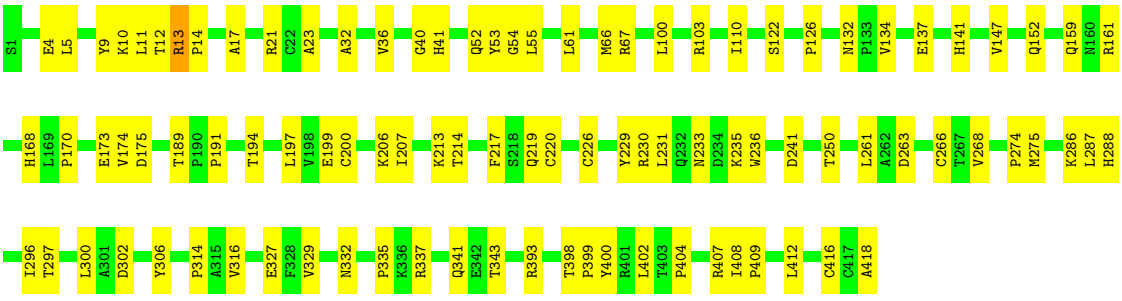
• Molecule 2: Spike glycoprotein E2

Chain B:



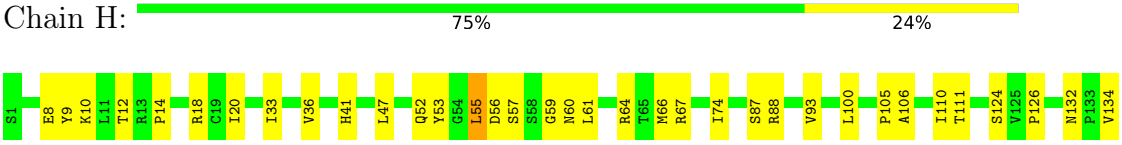
• Molecule 2: Spike glycoprotein E2

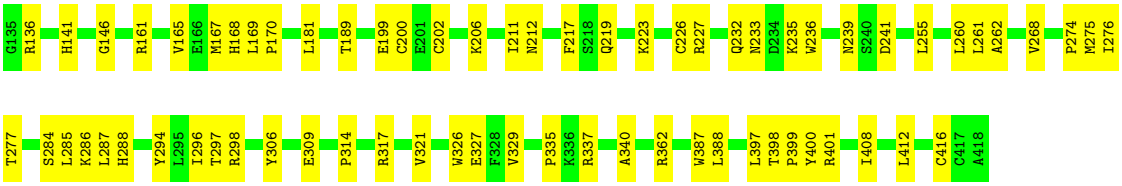
Chain E:



• Molecule 2: Spike glycoprotein E2

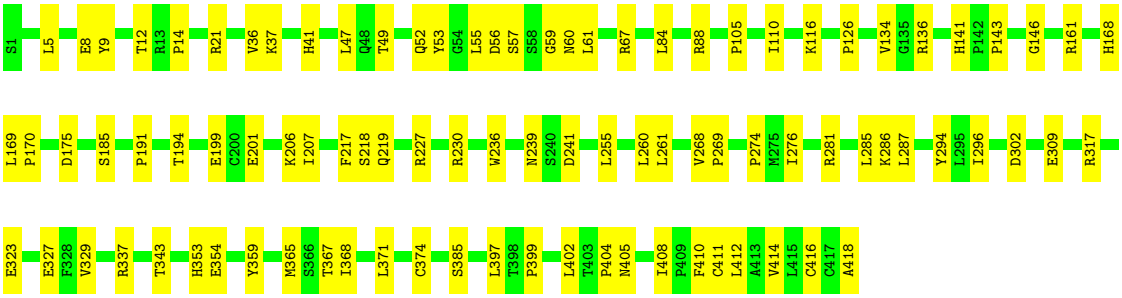
Chain H:





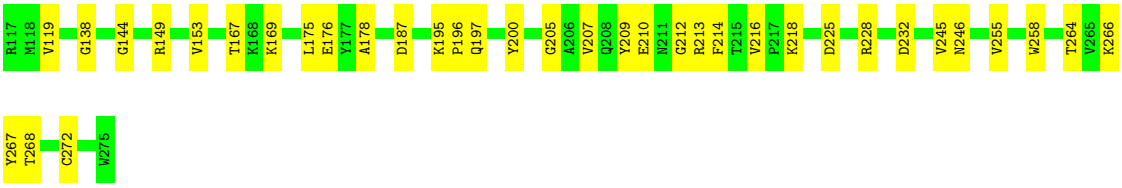
• Molecule 2: Spike glycoprotein E2

Chain K:



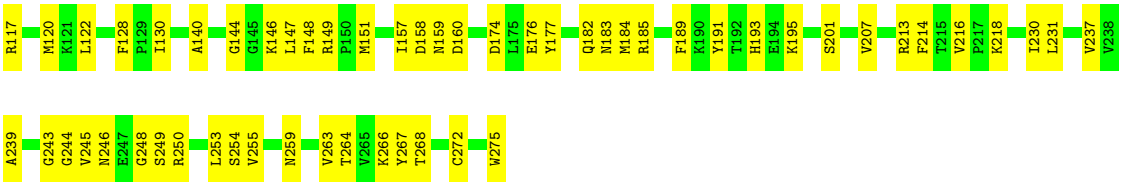
• Molecule 3: Capsid protein

Chain C:



• Molecule 3: Capsid protein

Chain F:

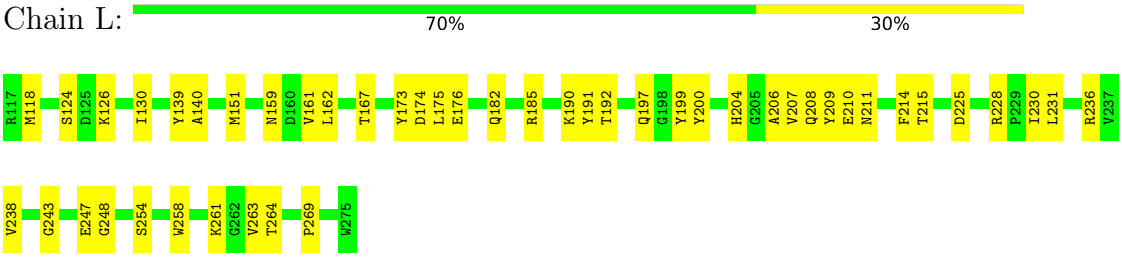


• Molecule 3: Capsid protein

Chain I:

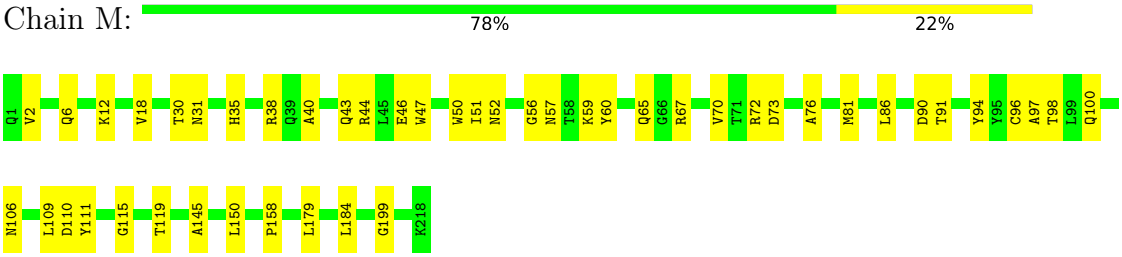
• Molecule 3: Capsid protein

Chain L:



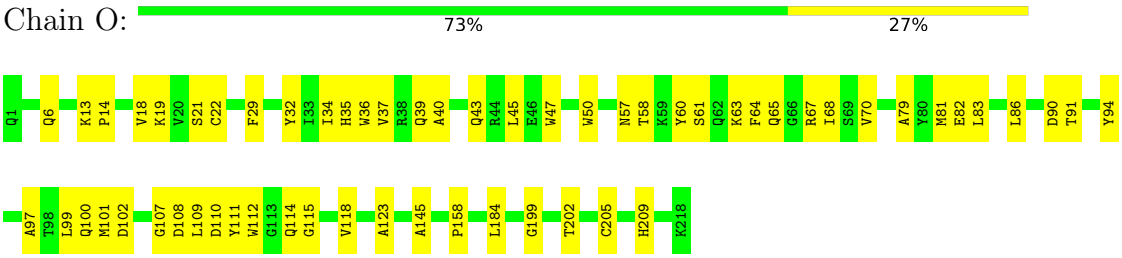
• Molecule 4: hVEEV-63 Fab heavy chain

Chain M:



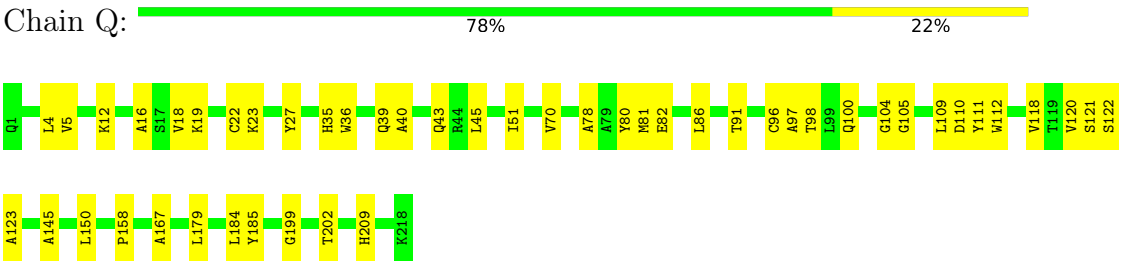
• Molecule 4: hVEEV-63 Fab heavy chain

Chain O:



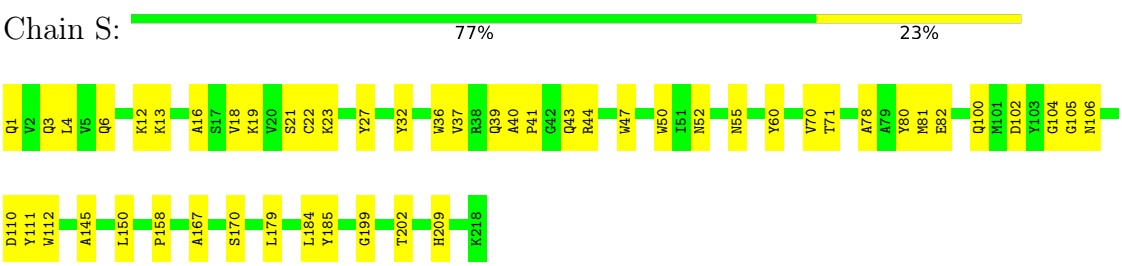
• Molecule 4: hVEEV-63 Fab heavy chain

Chain Q:



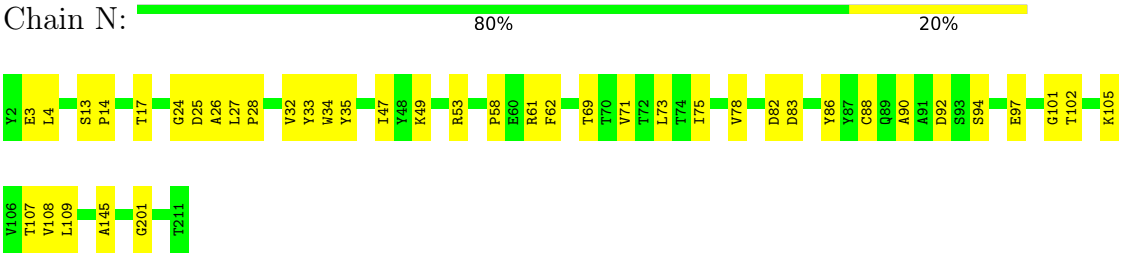
• Molecule 4: hVEEV-63 Fab heavy chain

Chain S:



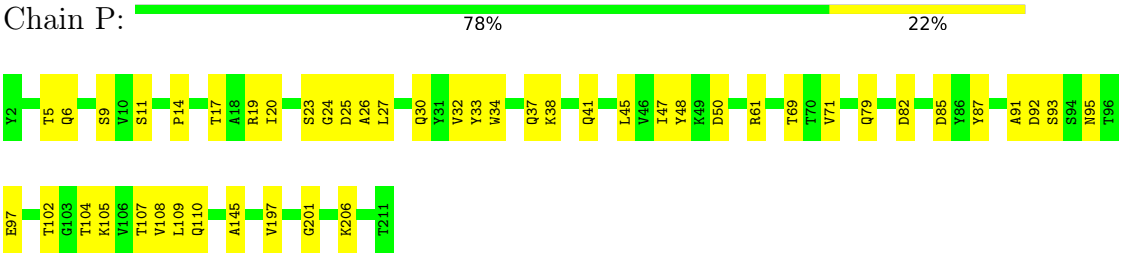
• Molecule 5: hVEEV-63 Fab light chain

Chain N:



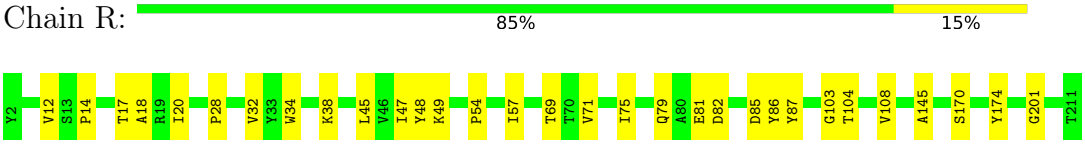
• Molecule 5: hVEEV-63 Fab light chain

Chain P:



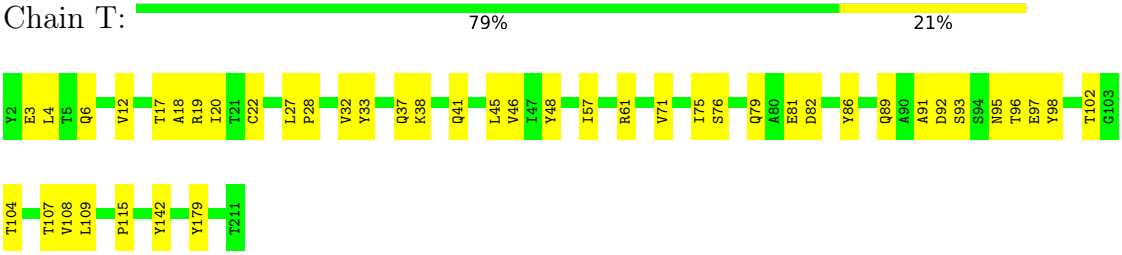
• Molecule 5: hVEEV-63 Fab light chain

Chain R:



• Molecule 5: hVEEV-63 Fab light chain

Chain T:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	17500	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 ($e^-/Å^2$)	40.05	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor

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	0.27	0/3441	0.48	0/4705
1	D	0.28	0/3441	0.51	0/4705
1	G	0.27	0/3441	0.48	0/4705
1	J	0.27	0/3441	0.51	0/4705
2	B	0.27	0/3355	0.51	0/4564
2	E	0.28	0/3355	0.53	0/4564
2	H	0.29	0/3355	0.54	1/4564 (0.0%)
2	K	0.29	0/3355	0.55	0/4564
3	C	0.26	0/1276	0.53	0/1720
3	F	0.26	0/1276	0.54	0/1720
3	I	0.26	0/1276	0.52	0/1720
3	L	0.27	0/1276	0.53	0/1720
4	M	0.24	0/1436	0.48	0/1962
4	O	0.25	0/1433	0.49	0/1957
4	Q	0.29	0/1436	0.51	0/1962
4	S	0.31	0/1433	0.51	0/1957
5	N	0.25	0/1333	0.47	0/1835
5	P	0.26	0/1333	0.48	0/1835
5	R	0.26	0/1333	0.49	0/1835
5	T	0.40	0/1337	0.54	0/1843
All	All	0.28	0/43362	0.51	1/59142 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	55	LEU	CA-CB-CG	6.03	129.17	115.30

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	3351	0	3258	56	0
1	D	3351	0	3258	64	0
1	G	3351	0	3258	58	0
1	J	3351	0	3258	50	0
2	B	3264	0	3198	83	0
2	E	3264	0	3199	83	0
2	H	3264	0	3198	79	0
2	K	3264	0	3198	76	0
3	C	1248	0	1238	23	0
3	F	1248	0	1238	38	0
3	I	1248	0	1238	32	0
3	L	1248	0	1238	30	0
4	M	1415	0	1123	36	0
4	O	1413	0	1117	40	0
4	Q	1415	0	1123	32	0
4	S	1413	0	1117	43	0
5	N	1315	0	995	28	0
5	P	1315	0	995	30	0
5	R	1315	0	995	17	0
5	T	1317	0	1002	28	0
6	A	14	0	13	0	0
6	B	28	0	26	0	0
6	D	14	0	13	0	0
6	E	28	0	26	1	0
6	G	14	0	13	1	0
6	H	28	0	26	1	0
6	J	14	0	13	1	0
6	K	28	0	26	0	0
All	All	42538	0	39400	849	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 10.

All (849) 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)
2:E:200:CYS:HA	2:E:226:CYS:HB2	1.48	0.95
1:G:299:ALA:HA	1:G:319:LYS:O	1.69	0.93
2:H:8:GLU:HA	2:H:255:LEU:HD22	1.55	0.89
1:J:325:SER:HA	1:J:346:LEU:O	1.75	0.86
4:O:94:TYR:O	4:O:115:GLY:HA2	1.75	0.86
4:Q:122:SER:HB3	4:Q:123:ALA:HB2	1.60	0.84
1:A:299:ALA:HA	1:A:319:LYS:O	1.76	0.84
5:N:34:TRP:HB2	5:N:47:ILE:HB	1.60	0.83
2:E:9:TYR:CD2	2:E:55:LEU:HD13	2.13	0.83
3:I:197:GLN:HE22	3:I:210:GLU:HG3	1.44	0.80
5:P:34:TRP:HB2	5:P:47:ILE:HB	1.63	0.80
1:D:218:ASN:ND2	2:H:275:MET:SD	2.55	0.80
5:R:34:TRP:HB2	5:R:47:ILE:HB	1.63	0.79
4:M:97:ALA:HB1	4:M:109:LEU:HB3	1.62	0.79
2:K:9:TYR:OH	2:K:56:ASP:O	2.00	0.79
2:H:9:TYR:OH	2:H:56:ASP:O	2.01	0.78
4:O:35:HIS:HB2	4:O:97:ALA:HB3	1.66	0.78
2:E:55:LEU:HG	2:E:61:LEU:HA	1.66	0.77
5:P:32:VAL:HG21	5:P:71:VAL:HG11	1.65	0.77
1:J:160:LYS:HB2	1:J:281:ASP:HB3	1.67	0.77
2:E:400:TYR:HB3	2:E:408:ILE:HG22	1.67	0.74
1:J:383:PRO:HG2	2:K:343:THR:HG22	1.68	0.74
2:E:327:GLU:HG3	2:E:337:ARG:HG2	1.67	0.73
4:S:100:GLN:HB2	4:S:111:TYR:HB2	1.70	0.73
1:D:53:THR:OG1	1:D:235:GLN:NE2	2.21	0.73
2:H:400:TYR:HB3	2:H:408:ILE:HG22	1.70	0.72
2:B:36:VAL:HG21	2:B:110:ILE:HG21	1.70	0.72
4:S:19:LYS:HD2	4:S:80:TYR:HB3	1.71	0.71
5:T:33:TYR:HB2	5:T:89:GLN:HE21	1.54	0.71
2:B:22:CYS:SG	2:B:23:ALA:N	2.64	0.71
4:O:123:ALA:HB2	4:O:205:CYS:H	1.56	0.71
4:Q:39:GLN:HB3	4:Q:45:LEU:HD13	1.73	0.71
1:D:80:VAL:HG22	1:D:103:VAL:HG22	1.73	0.70
2:E:12:THR:OG1	2:E:52:GLN:OE1	2.08	0.70
5:T:17:THR:HA	5:T:75:ILE:O	1.92	0.70
2:K:219:GLN:NE2	4:S:104:GLY:O	2.25	0.70
2:B:359:TYR:O	2:B:367:THR:OG1	2.07	0.70
4:S:71:THR:HB	4:S:80:TYR:HB2	1.74	0.70
3:I:145:GLY:H	3:I:188:THR:HG21	1.57	0.69
4:M:94:TYR:O	4:M:115:GLY:HA2	1.92	0.69
2:H:200:CYS:HA	2:H:226:CYS:HB2	1.75	0.69
5:N:17:THR:HA	5:N:75:ILE:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:152:GLN:NE2	2:E:263:ASP:OD1	2.26	0.69
4:O:99:LEU:HA	4:O:110:ASP:H	1.57	0.68
1:D:327:LYS:HD2	1:D:343:ALA:HB1	1.74	0.68
1:J:32:THR:HG21	6:J:501:NAG:H82	1.76	0.68
4:S:202:THR:HA	4:S:209:HIS:HA	1.76	0.68
1:A:144:THR:HG21	1:A:154:VAL:HG21	1.74	0.68
1:D:283:PRO:HG2	1:D:286:LEU:HD13	1.76	0.68
2:E:4:GLU:OE2	2:E:159:GLN:NE2	2.27	0.68
5:P:38:LYS:HB2	5:P:41:GLN:HE22	1.57	0.68
2:H:181:LEU:HG	2:H:223:LYS:HG3	1.76	0.68
5:P:30:GLN:NE2	5:P:95:ASN:OD1	2.27	0.68
1:A:53:THR:OG1	1:A:235:GLN:NE2	2.28	0.67
4:Q:91:THR:HG23	4:Q:118:VAL:HB	1.76	0.67
2:E:12:THR:OG1	2:E:67:ARG:NH2	2.26	0.67
2:E:9:TYR:HA	2:E:12:THR:HB	1.76	0.67
3:I:202:TRP:HE1	3:I:228:ARG:HB3	1.60	0.67
2:H:202:CYS:SG	2:H:206:LYS:NZ	2.65	0.67
4:O:19:LYS:HE3	4:O:82:GLU:OE2	1.95	0.67
2:E:141:HIS:CE1	2:K:21:ARG:HD3	2.30	0.66
2:B:402:LEU:HD11	3:C:264:THR:HG21	1.77	0.66
5:N:24:GLY:O	5:N:69:THR:OG1	2.13	0.66
2:B:8:GLU:HA	2:B:255:LEU:HD22	1.76	0.66
1:A:296:LEU:HD11	1:A:320:TYR:HB2	1.76	0.66
2:E:175:ASP:OD2	2:E:230:ARG:NH2	2.29	0.66
1:G:21:ARG:HB2	1:G:24:TYR:HB2	1.78	0.65
2:B:21:ARG:NH1	2:B:22:CYS:O	2.30	0.65
2:E:200:CYS:HA	2:E:226:CYS:CB	2.24	0.65
4:S:1:GLN:HG2	4:S:3:GLN:HE22	1.61	0.65
2:B:69:ASP:HB3	2:B:74:ILE:HD13	1.77	0.65
1:A:253:PHE:HB3	2:B:296:ILE:HG21	1.80	0.64
1:D:336:THR:OG1	1:D:360:ASN:ND2	2.30	0.64
2:H:212:ASN:ND2	6:H:501:NAG:O4	2.30	0.64
4:M:52:ASN:ND2	4:M:57:ASN:OD1	2.29	0.64
1:A:383:PRO:HG2	2:B:343:THR:HG22	1.79	0.64
4:M:35:HIS:HB2	4:M:97:ALA:HB3	1.78	0.64
3:F:122:LEU:HD11	3:F:201:SER:HB3	1.79	0.64
1:J:295:THR:HA	1:J:371:THR:HG21	1.78	0.63
4:M:52:ASN:ND2	4:M:57:ASN:O	2.31	0.63
2:K:88:ARG:HB2	2:K:105:PRO:HG3	1.81	0.63
4:S:40:ALA:HB3	4:S:43:GLN:HB2	1.80	0.63
2:E:9:TYR:HD2	2:E:55:LEU:HD13	1.60	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:61:ARG:HH12	5:P:79:GLN:HB2	1.62	0.63
4:Q:40:ALA:HB3	4:Q:43:GLN:HB2	1.80	0.63
5:R:32:VAL:HG21	5:R:71:VAL:HG21	1.79	0.63
4:S:100:GLN:HB3	4:S:110:ASP:HB2	1.80	0.63
2:B:55:LEU:HD23	2:B:59:GLY:HA2	1.81	0.63
1:G:80:VAL:HG22	1:G:103:VAL:HG22	1.79	0.63
4:Q:202:THR:HA	4:Q:209:HIS:HA	1.81	0.62
1:G:59:ALA:O	1:G:66:GLN:NE2	2.32	0.62
5:P:108:VAL:O	5:P:110:GLN:N	2.32	0.62
5:R:17:THR:HA	5:R:75:ILE:O	1.99	0.62
5:T:32:VAL:HG21	5:T:71:VAL:HG11	1.80	0.62
2:B:52:GLN:OE1	2:B:67:ARG:NH2	2.33	0.62
1:A:325:SER:HA	1:A:346:LEU:O	2.00	0.61
3:C:266:LYS:NZ	3:C:268:THR:OG1	2.33	0.61
4:Q:19:LYS:HE2	4:Q:80:TYR:HB3	1.81	0.61
2:B:114:PHE:HD2	2:B:121:HIS:HB2	1.64	0.61
2:B:77:ILE:HG21	2:B:114:PHE:HE1	1.66	0.61
3:F:266:LYS:NZ	3:F:268:THR:OG1	2.34	0.61
4:M:65:GLN:O	4:M:67:ARG:NH1	2.33	0.61
1:J:291:SER:OG	1:J:292:GLU:OE1	2.19	0.60
1:J:296:LEU:HD21	1:J:299:ALA:HB2	1.82	0.60
4:S:106:ASN:ND2	5:T:98:TYR:OH	2.34	0.60
3:I:241:VAL:HG21	3:I:253:LEU:HD22	1.83	0.60
1:J:155:ASN:HB2	1:J:160:LYS:HZ3	1.67	0.60
4:O:61:SER:O	4:O:65:GLN:NE2	2.34	0.60
1:G:21:ARG:NH2	1:G:25:ALA:O	2.35	0.60
1:A:24:TYR:CZ	1:G:384:LYS:HG3	2.37	0.60
3:L:161:VAL:HG13	3:L:162:LEU:HD12	1.83	0.60
1:D:362:HIS:ND1	1:D:379:ASP:OD1	2.34	0.60
2:H:10:LYS:O	2:H:235:LYS:NZ	2.31	0.59
4:S:170:SER:HA	5:T:179:TYR:HA	1.84	0.59
1:J:31:ILE:HD11	1:J:280:PHE:HZ	1.66	0.59
4:Q:35:HIS:HB2	4:Q:97:ALA:HB3	1.82	0.59
1:G:361:ILE:HG21	1:G:403:SER:H	1.67	0.59
1:A:10:GLN:HG2	1:A:13:ILE:HD12	1.85	0.59
4:O:67:ARG:HE	4:O:83:LEU:HD11	1.67	0.59
2:H:9:TYR:HE1	2:H:59:GLY:HA2	1.67	0.59
3:I:250:ARG:HE	3:I:251:THR:H	1.51	0.59
1:A:362:HIS:ND1	1:A:379:ASP:OD1	2.31	0.59
2:H:167:MET:HE2	2:H:236:TRP:HB2	1.84	0.59
5:N:94:SER:OG	5:N:97:GLU:OE1	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:ARG:HB2	2:B:260:LEU:HD12	1.84	0.59
2:E:12:THR:HG21	2:E:67:ARG:HH12	1.68	0.59
2:B:297:THR:O	2:B:306:TYR:HA	2.02	0.59
5:R:45:LEU:HD21	5:R:48:TYR:HB3	1.83	0.59
3:C:214:PHE:HD2	3:C:255:VAL:HG11	1.66	0.59
1:D:251:LEU:HB3	1:D:261:ILE:HG13	1.85	0.59
2:H:217:PHE:HA	4:Q:105:GLY:HA2	1.83	0.59
2:K:402:LEU:HD23	3:L:264:THR:HG21	1.85	0.59
5:N:61:ARG:NH1	5:N:82:ASP:OD2	2.35	0.59
1:D:96:CYS:O	1:D:100:ASN:ND2	2.35	0.58
3:I:149:ARG:NH1	3:I:176:GLU:OE2	2.32	0.58
5:P:92:ASP:OD1	5:P:93:SER:N	2.36	0.58
2:B:179:VAL:O	2:B:223:LYS:NZ	2.29	0.58
2:H:161:ARG:HH22	2:H:262:ALA:HB2	1.68	0.58
1:G:32:THR:HG21	6:G:501:NAG:H82	1.85	0.58
1:A:210:SER:OG	1:A:212:ASP:OD1	2.20	0.58
3:F:214:PHE:HD2	3:F:255:VAL:HG11	1.67	0.58
2:H:327:GLU:HB3	2:H:337:ARG:HG2	1.86	0.58
4:S:12:LYS:HZ3	4:S:16:ALA:HB3	1.69	0.58
5:T:45:LEU:HD21	5:T:48:TYR:HB3	1.85	0.58
2:B:35:ALA:HB3	2:B:48:GLN:HB3	1.85	0.58
2:E:287:LEU:O	2:E:314:PRO:HA	2.03	0.58
3:F:244:GLY:HA2	3:F:253:LEU:HA	1.83	0.58
5:P:24:GLY:O	5:P:69:THR:OG1	2.22	0.58
3:F:151:MET:HG2	3:F:174:ASP:HA	1.84	0.58
4:S:44:ARG:NH2	5:T:3:GLU:OE2	2.36	0.58
5:N:105:LYS:HE3	5:N:107:THR:HG22	1.86	0.58
5:N:75:ILE:HD11	5:N:86:TYR:HE2	1.68	0.57
2:E:52:GLN:OE1	2:E:67:ARG:NH2	2.37	0.57
1:D:82:THR:HG22	1:D:101:THR:HG22	1.86	0.57
2:E:54:GLY:O	2:E:55:LEU:HD12	2.05	0.57
2:E:297:THR:O	2:E:306:TYR:HA	2.04	0.57
1:G:59:ALA:HB3	1:G:103:VAL:HB	1.87	0.57
1:D:366:ARG:HH12	1:D:373:TYR:HB3	1.69	0.57
2:E:191:PRO:HG2	2:E:194:THR:HB	1.85	0.57
4:S:4:LEU:H	4:S:111:TYR:HE2	1.51	0.57
2:B:84:LEU:HD12	2:B:110:ILE:HD11	1.85	0.57
2:E:53:TYR:CE1	2:E:66:MET:HG3	2.40	0.57
2:K:219:GLN:HA	4:S:32:TYR:HE1	1.68	0.57
4:M:44:ARG:HH12	5:N:102:THR:HG22	1.70	0.57
4:Q:18:VAL:HG12	4:Q:86:LEU:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:PRO:HD3	2:B:236:TRP:HA	1.87	0.57
1:G:312:PHE:HA	1:G:357:SER:HB2	1.87	0.57
5:T:17:THR:HG22	5:T:76:SER:HA	1.86	0.57
1:J:182:GLY:HA2	1:J:263:THR:HG21	1.86	0.57
1:D:358:THR:OG1	1:D:360:ASN:OD1	2.23	0.57
2:E:402:LEU:HD11	3:F:264:THR:HG21	1.85	0.57
3:F:182:GLN:OE1	3:F:185:ARG:NH1	2.38	0.57
2:B:12:THR:OG1	2:B:52:GLN:OE1	2.23	0.57
2:E:11:LEU:HD13	2:E:236:TRP:CZ3	2.40	0.57
4:M:2:VAL:HB	4:M:100:GLN:HE21	1.70	0.57
4:M:47:TRP:HZ2	4:M:50:TRP:HD1	1.52	0.57
3:F:246:ASN:ND2	3:F:248:GLY:O	2.35	0.56
3:C:197:GLN:HE21	3:C:210:GLU:HA	1.70	0.56
2:K:9:TYR:HE1	2:K:59:GLY:HA2	1.70	0.56
5:R:145:ALA:HA	5:R:201:GLY:H	1.71	0.56
2:E:13:ARG:NH2	2:E:173:GLU:OE1	2.38	0.56
2:H:55:LEU:HD13	2:H:61:LEU:HD22	1.87	0.56
3:I:216:VAL:O	3:I:250:ARG:NH2	2.37	0.56
2:K:14:PRO:HG2	2:K:67:ARG:HG2	1.88	0.56
1:A:95:PHE:HD2	2:B:201:GLU:HG2	1.71	0.56
2:B:12:THR:HG21	2:B:67:ARG:HH12	1.70	0.56
4:O:60:TYR:HE1	4:O:70:VAL:HG12	1.69	0.56
3:I:200:TYR:HD1	3:I:232:ASP:HA	1.70	0.56
1:G:251:LEU:HB3	1:G:261:ILE:HG13	1.86	0.56
2:K:199:GLU:HA	2:K:206:LYS:O	2.05	0.56
3:F:193:HIS:O	3:F:195:LYS:NZ	2.27	0.56
3:F:243:GLY:O	3:F:254:SER:N	2.39	0.56
2:H:232:GLN:HG2	2:H:233:ASN:H	1.69	0.56
2:B:175:ASP:OD2	2:B:230:ARG:NH2	2.39	0.56
2:K:411:CYS:HA	2:K:414:VAL:HG22	1.88	0.56
2:B:215:LYS:NZ	5:N:33:TYR:OH	2.38	0.56
1:D:110:LYS:NZ	1:D:208:VAL:O	2.39	0.56
4:M:98:THR:O	4:M:110:ASP:N	2.35	0.56
2:B:412:LEU:HD12	2:B:416:CYS:HA	1.88	0.55
1:G:294:PRO:HG3	1:G:326:GLY:HA3	1.87	0.55
1:J:417:SER:O	1:J:421:ILE:HD12	2.06	0.55
2:H:288:HIS:ND1	2:H:314:PRO:HB3	2.21	0.55
2:H:329:VAL:HG22	2:H:335:PRO:HB3	1.88	0.55
3:L:243:GLY:O	3:L:254:SER:N	2.39	0.55
1:G:362:HIS:ND1	1:G:379:ASP:OD1	2.39	0.55
3:I:245:VAL:HB	3:I:273:GLU:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:61:ARG:NH2	5:P:82:ASP:OD1	2.39	0.55
4:Q:5:VAL:HG23	4:Q:23:LYS:HB2	1.89	0.55
2:E:5:LEU:HD13	2:E:55:LEU:HD11	1.87	0.55
3:I:208:GLN:HG3	3:I:210:GLU:OE1	2.07	0.55
2:E:13:ARG:NH1	2:E:14:PRO:O	2.39	0.55
3:I:258:TRP:CD1	3:I:264:THR:HG22	2.40	0.55
4:O:13:LYS:HD2	4:O:14:PRO:HD2	1.89	0.55
1:J:13:ILE:HD11	1:J:391:PRO:HG2	1.88	0.55
3:L:199:TYR:HA	3:L:208:GLN:HA	1.89	0.55
5:N:145:ALA:HA	5:N:201:GLY:H	1.72	0.55
3:C:218:LYS:NZ	3:C:246:ASN:HD21	2.05	0.55
5:N:25:ASP:OD1	5:N:26:ALA:N	2.40	0.55
2:B:288:HIS:ND1	2:B:314:PRO:HB3	2.22	0.55
2:E:329:VAL:HG22	2:E:335:PRO:HB3	1.88	0.55
3:C:138:GLY:HA3	3:C:153:VAL:HG11	1.89	0.54
1:J:296:LEU:HD13	1:J:369:ILE:HG21	1.88	0.54
1:A:110:LYS:NZ	1:A:208:VAL:O	2.40	0.54
1:D:296:LEU:HD21	1:D:299:ALA:HB2	1.89	0.54
4:S:158:PRO:HA	4:S:199:GLY:HA2	1.89	0.54
3:C:225:ASP:OD1	3:C:228:ARG:NH1	2.37	0.54
1:D:359:ALA:HB2	1:D:394:HIS:CD2	2.43	0.54
4:Q:12:LYS:HD2	4:Q:16:ALA:HB3	1.89	0.54
2:B:275:MET:SD	2:B:286:LYS:NZ	2.80	0.54
1:D:40:PRO:HA	1:D:127:ALA:HA	1.89	0.54
1:G:253:PHE:HB3	2:H:296:ILE:HG21	1.89	0.54
1:A:65:SER:HA	1:A:101:THR:HG21	1.89	0.54
2:K:219:GLN:HE22	4:S:102:ASP:HB2	1.73	0.54
5:P:17:THR:HG22	5:P:19:ARG:NH1	2.22	0.54
2:E:12:THR:HG23	2:E:13:ARG:H	1.72	0.54
2:H:55:LEU:HB2	2:H:60:ASN:O	2.08	0.54
4:S:19:LYS:HE2	4:S:82:GLU:HB3	1.89	0.54
2:E:10:LYS:O	2:E:235:LYS:NZ	2.23	0.54
2:H:232:GLN:HG2	2:H:233:ASN:N	2.23	0.54
2:K:41:HIS:CD2	2:K:134:VAL:HG22	2.43	0.54
4:M:18:VAL:HG22	4:M:86:LEU:HD21	1.90	0.54
2:E:206:LYS:NZ	2:E:220:CYS:SG	2.80	0.54
5:N:32:VAL:HG11	5:N:71:VAL:HG21	1.88	0.54
3:C:197:GLN:NE2	3:C:210:GLU:HA	2.23	0.54
2:K:136:ARG:HB3	2:K:294:TYR:HB2	1.89	0.54
1:A:40:PRO:HA	1:A:127:ALA:HA	1.90	0.53
1:A:117:ASP:HB2	2:B:261:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:97:ALA:HB1	4:O:109:LEU:HD13	1.90	0.53
3:I:217:PRO:HG2	3:I:220:VAL:HG21	1.90	0.53
2:K:309:GLU:OE2	2:K:317:ARG:NH2	2.36	0.53
1:A:77:GLN:HB2	1:A:221:LEU:HD13	1.90	0.53
2:E:286:LYS:HG3	2:E:316:VAL:HG22	1.91	0.53
1:G:255:ALA:O	2:H:298:ARG:NH1	2.41	0.53
2:H:87:SER:HA	2:K:88:ARG:HD3	1.90	0.53
1:J:40:PRO:HA	1:J:127:ALA:HA	1.90	0.53
2:K:84:LEU:HD12	2:K:110:ILE:HD11	1.91	0.53
5:R:14:PRO:HG3	5:R:108:VAL:HB	1.90	0.53
2:B:191:PRO:HG2	2:B:194:THR:HB	1.90	0.53
1:G:53:THR:OG1	1:G:235:GLN:OE1	2.26	0.53
3:I:129:PRO:HA	3:I:139:TYR:HD1	1.71	0.53
4:M:12:LYS:HD3	4:M:18:VAL:HG12	1.89	0.53
4:Q:97:ALA:HB1	4:Q:109:LEU:HB3	1.91	0.53
3:C:195:LYS:NZ	3:C:258:TRP:O	2.41	0.53
1:A:95:PHE:CD2	2:B:201:GLU:HG2	2.44	0.53
1:A:258:GLY:HA3	2:B:300:LEU:HD13	1.91	0.53
2:K:9:TYR:CG	2:K:55:LEU:HD21	2.44	0.53
1:A:369:ILE:HG22	1:A:370:CYS:H	1.72	0.53
3:C:149:ARG:NH2	3:C:153:VAL:O	2.41	0.53
1:D:325:SER:HA	1:D:346:LEU:O	2.08	0.53
2:H:309:GLU:OE2	2:H:317:ARG:NH2	2.38	0.53
4:O:91:THR:HA	4:O:118:VAL:O	2.08	0.53
1:A:29:ILE:HG23	1:A:137:VAL:HG22	1.90	0.53
3:F:151:MET:HE2	3:F:176:GLU:HG3	1.91	0.53
1:G:94:CYS:O	2:H:227:ARG:NH1	2.42	0.53
2:H:277:THR:OG1	2:H:284:SER:HB3	2.08	0.53
3:I:149:ARG:HD2	3:I:157:ILE:HD11	1.91	0.53
3:I:185:ARG:HB2	3:I:185:ARG:NH1	2.24	0.53
1:G:73:ARG:HB2	1:G:76:GLU:HG3	1.91	0.53
4:M:6:GLN:NE2	4:M:96:CYS:SG	2.82	0.53
2:B:9:TYR:HE1	2:B:52:GLN:HB3	1.74	0.52
1:G:231:VAL:N	2:H:241:ASP:OD1	2.42	0.52
2:K:217:PHE:HA	4:S:105:GLY:HA3	1.89	0.52
5:P:5:THR:OG1	5:P:23:SER:OG	2.24	0.52
2:K:412:LEU:HD12	2:K:416:CYS:HA	1.90	0.52
3:L:192:THR:HB	3:L:238:VAL:HG12	1.92	0.52
4:S:18:VAL:O	4:S:82:GLU:HA	2.09	0.52
1:A:69:THR:O	1:A:105:LYS:NZ	2.35	0.52
1:D:385:ASP:OD1	2:E:341:GLN:NE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:VAL:HB	1:G:148:VAL:HB	1.91	0.52
2:H:161:ARG:HD2	2:H:260:LEU:HD12	1.90	0.52
2:H:200:CYS:HA	2:H:226:CYS:CB	2.39	0.52
5:R:28:PRO:HD3	5:R:69:THR:HA	1.91	0.52
1:D:296:LEU:HD13	1:D:369:ILE:HG21	1.90	0.52
2:H:33:ILE:HG12	2:H:47:LEU:HD21	1.92	0.52
2:H:67:ARG:HD2	2:H:74:ILE:HG21	1.92	0.52
3:I:192:THR:HG22	3:I:194:GLU:H	1.74	0.52
1:A:413:LEU:HD21	2:B:378:ALA:HB2	1.91	0.52
1:G:160:LYS:HB3	1:G:281:ASP:HB3	1.92	0.52
3:I:207:VAL:HG22	3:I:216:VAL:HG12	1.90	0.52
2:H:136:ARG:HB3	2:H:294:TYR:HB2	1.92	0.52
2:E:168:HIS:HB3	2:E:250:THR:HG22	1.91	0.52
4:O:67:ARG:NH2	4:O:90:ASP:OD1	2.43	0.52
3:I:193:HIS:HB2	3:I:260:GLU:HA	1.92	0.52
3:L:261:LYS:HG3	3:L:263:VAL:HG13	1.90	0.52
5:P:145:ALA:HA	5:P:201:GLY:H	1.75	0.52
1:A:255:ALA:O	2:B:298:ARG:NH1	2.43	0.52
3:C:167:THR:HG22	3:C:178:ALA:HB2	1.92	0.52
2:E:219:GLN:NE2	4:O:102:ASP:OD1	2.43	0.52
2:H:9:TYR:CG	2:H:55:LEU:HD21	2.45	0.51
2:H:14:PRO:HG3	2:H:52:GLN:HG3	1.93	0.51
2:K:302:ASP:OD1	2:K:302:ASP:N	2.43	0.51
4:O:29:PHE:HE1	4:O:34:ILE:HD11	1.75	0.51
1:A:413:LEU:HD22	2:B:374:CYS:SG	2.50	0.51
2:B:88:ARG:HB2	2:B:105:PRO:HG3	1.91	0.51
1:G:387:ILE:HD13	2:H:340:ALA:HA	1.92	0.51
2:K:185:SER:HB2	2:K:218:SER:HA	1.91	0.51
4:O:70:VAL:HG23	4:O:81:MET:HB3	1.92	0.51
5:T:61:ARG:NH1	5:T:82:ASP:OD2	2.43	0.51
4:O:40:ALA:HB3	4:O:43:GLN:HB2	1.91	0.51
1:A:288:THR:OG1	1:A:292:GLU:OE1	2.28	0.51
2:B:402:LEU:HD22	3:C:175:LEU:HD11	1.92	0.51
1:D:60:ILE:HG21	1:D:86:PRO:HG2	1.92	0.51
4:O:100:GLN:HB2	4:O:111:TYR:HD2	1.76	0.51
2:H:170:PRO:HD3	2:H:236:TRP:HA	1.93	0.51
1:J:117:ASP:HB2	2:K:261:LEU:HD23	1.92	0.51
2:K:8:GLU:HA	2:K:255:LEU:HD22	1.93	0.51
4:Q:158:PRO:HA	4:Q:199:GLY:HA2	1.93	0.51
1:G:217:THR:OG1	1:G:235:GLN:NE2	2.41	0.51
1:A:251:LEU:HB3	1:A:261:ILE:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:ALA:HB1	2:B:242:LYS:HD3	1.92	0.51
2:E:407:ARG:HG2	2:E:409:PRO:HD3	1.92	0.51
2:K:161:ARG:HB2	2:K:260:LEU:HD12	1.93	0.51
3:L:197:GLN:HE22	3:L:210:GLU:HA	1.75	0.51
4:M:100:GLN:N	4:M:110:ASP:OD2	2.43	0.51
5:P:11:SER:HA	5:P:107:THR:HB	1.92	0.51
5:T:92:ASP:OD1	5:T:93:SER:N	2.39	0.51
1:A:106:ALA:HB3	1:A:221:LEU:HD11	1.93	0.51
3:C:245:VAL:HB	3:C:272:CYS:HA	1.92	0.51
1:G:21:ARG:HH21	1:G:24:TYR:HB3	1.76	0.51
4:M:91:THR:HG23	4:M:119:THR:HG22	1.93	0.51
2:B:9:TYR:HA	2:B:12:THR:HB	1.92	0.51
1:D:440:LYS:HA	3:F:259:ASN:HD21	1.75	0.51
2:H:64:ARG:NH2	2:H:93:VAL:O	2.44	0.51
3:F:130:ILE:HD11	3:F:140:ALA:HB2	1.93	0.51
5:N:58:PRO:HG2	5:N:62:PHE:HE1	1.76	0.51
5:P:45:LEU:HD21	5:P:48:TYR:HB3	1.93	0.51
4:M:60:TYR:HE1	4:M:70:VAL:HG12	1.76	0.50
4:O:6:GLN:HE22	4:O:115:GLY:N	2.09	0.50
5:P:92:ASP:HB2	5:P:97:GLU:HB3	1.92	0.50
4:M:100:GLN:OE1	4:M:111:TYR:HB2	2.11	0.50
4:O:202:THR:HA	4:O:209:HIS:HA	1.93	0.50
5:P:25:ASP:OD1	5:P:26:ALA:N	2.45	0.50
3:F:117:ARG:HE	3:F:120:MET:HE3	1.76	0.50
4:S:47:TRP:HZ2	4:S:50:TRP:HD1	1.60	0.50
2:K:274:PRO:HB3	2:K:287:LEU:HD23	1.93	0.50
4:Q:23:LYS:HG3	4:Q:78:ALA:HB2	1.93	0.50
1:G:435:VAL:O	1:G:439:GLN:HG2	2.11	0.50
4:S:41:PRO:O	4:S:43:GLN:NE2	2.44	0.50
1:A:362:HIS:CD2	1:A:404:LYS:HG2	2.47	0.50
2:H:53:TYR:CE2	2:H:66:MET:HG3	2.46	0.50
2:H:397:LEU:O	2:H:401:ARG:N	2.45	0.50
5:N:14:PRO:HD3	5:N:109:LEU:H	1.76	0.50
2:B:342:GLU:O	2:B:342:GLU:HG2	2.12	0.50
2:H:169:LEU:HD12	2:H:170:PRO:HD2	1.93	0.50
3:I:142:VAL:HG22	3:I:188:THR:HG23	1.93	0.50
2:K:365:MET:HA	2:K:368:ILE:HG22	1.93	0.50
3:L:208:GLN:HE21	3:L:215:THR:HG23	1.77	0.50
2:E:412:LEU:HD12	2:E:416:CYS:HA	1.93	0.49
2:H:41:HIS:CD2	2:H:134:VAL:HG22	2.47	0.49
2:K:168:HIS:CD2	2:K:239:ASN:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:158:PRO:HA	4:M:199:GLY:HA2	1.93	0.49
1:D:297:SER:O	1:D:321:SER:OG	2.29	0.49
1:G:142:ILE:HD13	1:G:156:PHE:CG	2.47	0.49
1:G:298:ALA:HB3	1:G:321:SER:HB2	1.94	0.49
5:T:17:THR:OG1	5:T:19:ARG:NH1	2.44	0.49
1:D:31:ILE:HD11	1:D:280:PHE:HZ	1.77	0.49
2:B:300:LEU:HD23	2:B:326:TRP:N	2.26	0.49
1:A:192:TYR:OH	1:A:212:ASP:OD2	2.25	0.49
1:D:117:ASP:HB2	2:E:261:LEU:HD23	1.93	0.49
1:A:41:THR:OG1	1:A:125:HIS:O	2.30	0.49
1:G:29:ILE:HG12	1:G:137:VAL:HG23	1.95	0.49
1:J:296:LEU:HD12	1:J:346:LEU:HD21	1.95	0.49
4:Q:145:ALA:HB2	4:Q:184:LEU:HA	1.94	0.49
2:B:240:SER:HB3	2:B:243:LEU:HD23	1.94	0.49
2:B:294:TYR:CE1	2:B:310:LEU:HB2	2.48	0.49
1:D:76:GLU:HA	1:D:106:ALA:O	2.12	0.49
3:F:160:ASP:OD1	3:F:160:ASP:N	2.46	0.49
1:G:117:ASP:HB2	2:H:261:LEU:HD23	1.93	0.49
1:G:222:GLN:HB2	1:G:232:PRO:HB2	1.95	0.49
3:I:243:GLY:O	3:I:254:SER:N	2.45	0.49
1:D:202:ASP:N	1:D:202:ASP:OD1	2.46	0.49
1:D:253:PHE:HB3	2:E:296:ILE:HG21	1.95	0.49
3:F:149:ARG:HG3	3:F:176:GLU:HB2	1.94	0.49
3:I:118:MET:SD	3:I:118:MET:N	2.84	0.49
3:L:207:VAL:HG21	3:L:230:ILE:HD11	1.95	0.49
5:P:61:ARG:NH1	5:P:79:GLN:OE1	2.45	0.49
2:B:411:CYS:HA	2:B:414:VAL:HG22	1.95	0.49
1:D:205:SER:OG	1:D:207:THR:O	2.28	0.49
2:E:404:PRO:HB3	3:F:144:GLY:HA3	1.94	0.49
1:J:300:GLU:HA	1:J:374:VAL:HG21	1.95	0.49
4:M:52:ASN:HB2	4:M:56:GLY:H	1.78	0.49
1:A:246:ASP:OD1	1:A:246:ASP:N	2.43	0.49
2:H:41:HIS:HA	2:H:132:ASN:HB2	1.94	0.49
1:J:364:GLU:OE1	1:J:377:LYS:NZ	2.39	0.49
4:S:4:LEU:HG	4:S:111:TYR:CE2	2.48	0.49
2:B:302:ASP:OD1	2:B:302:ASP:N	2.46	0.48
2:E:53:TYR:CE1	2:E:100:LEU:HD13	2.48	0.48
2:H:298:ARG:NE	2:H:327:GLU:OE2	2.36	0.48
5:N:83:ASP:OD1	5:N:108:VAL:N	2.45	0.48
2:B:8:GLU:OE1	2:B:255:LEU:HB3	2.13	0.48
4:M:38:ARG:NH1	4:M:90:ASP:OD1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:64:PHE:HB3	4:O:68:ILE:HG21	1.95	0.48
4:O:107:GLY:HA3	5:P:33:TYR:CD1	2.48	0.48
2:E:206:LYS:HE3	2:E:217:PHE:CD2	2.48	0.48
2:H:12:THR:HA	2:H:236:TRP:O	2.14	0.48
1:D:55:MET:HG3	2:E:241:ASP:HB3	1.94	0.48
1:J:303:LEU:HD12	1:J:378:GLY:HA3	1.95	0.48
4:M:59:LYS:NZ	5:N:97:GLU:HG3	2.28	0.48
2:B:181:LEU:HB2	2:B:223:LYS:HD2	1.94	0.48
1:D:21:ARG:HB3	1:D:24:TYR:HD1	1.78	0.48
1:D:230:HIS:CD2	1:D:232:PRO:HG3	2.49	0.48
4:O:39:GLN:HB2	4:O:45:LEU:HD23	1.96	0.48
4:S:52:ASN:HB3	4:S:55:ASN:HB3	1.95	0.48
1:A:300:GLU:HG3	1:A:319:LYS:HB3	1.96	0.48
2:B:87:SER:OG	2:B:106:ALA:O	2.25	0.48
1:D:84:VAL:HG21	1:D:102:GLN:HB2	1.96	0.48
4:M:145:ALA:HB2	4:M:184:LEU:HA	1.95	0.48
5:N:92:ASP:OD1	5:N:92:ASP:N	2.47	0.48
2:B:224:GLU:O	2:B:227:ARG:NH2	2.47	0.48
2:E:274:PRO:HB3	2:E:287:LEU:HD23	1.95	0.48
3:I:138:GLY:HA3	3:I:153:VAL:HG11	1.95	0.48
2:K:296:ILE:HB	2:K:329:VAL:HG22	1.96	0.48
2:E:126:PRO:HB3	2:H:141:HIS:HB3	1.96	0.48
2:E:137:GLU:HG3	2:E:332:ASN:ND2	2.29	0.48
2:H:36:VAL:HG21	2:H:110:ILE:HG21	1.96	0.47
2:H:146:GLY:HA3	2:H:268:VAL:O	2.14	0.47
1:J:51:TYR:OH	1:J:236:ALA:O	2.29	0.47
5:P:105:LYS:HA	5:P:105:LYS:HE2	1.97	0.47
1:A:202:ASP:OD1	1:A:202:ASP:N	2.47	0.47
1:D:98:THR:HG23	1:D:99:GLU:OE1	2.13	0.47
3:F:140:ALA:HB1	3:F:147:LEU:HD11	1.96	0.47
1:G:176:LYS:HB3	1:G:189:PHE:CE2	2.49	0.47
2:H:168:HIS:CD2	2:H:239:ASN:HB3	2.49	0.47
2:K:146:GLY:HA3	2:K:268:VAL:O	2.14	0.47
2:K:201:GLU:HG3	2:K:201:GLU:O	2.14	0.47
4:M:47:TRP:CZ2	4:M:50:TRP:HD1	2.31	0.47
2:H:321:VAL:HG13	2:H:326:TRP:HB3	1.96	0.47
4:M:38:ARG:NE	4:M:46:GLU:OE2	2.42	0.47
1:A:250:SER:OG	1:A:251:LEU:N	2.45	0.47
1:D:192:TYR:OH	1:D:212:ASP:OD2	2.23	0.47
2:E:36:VAL:HG21	2:E:110:ILE:HG21	1.96	0.47
1:G:104:SER:HB3	1:G:231:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:168:THR:HG22	1:G:170:TRP:H	1.78	0.47
2:H:88:ARG:HB2	2:H:105:PRO:HG3	1.96	0.47
3:L:139:TYR:CD2	3:L:228:ARG:HD3	2.50	0.47
3:L:247:GLU:HG2	3:L:248:GLY:H	1.80	0.47
5:R:12:VAL:HG11	5:R:18:ALA:HB2	1.95	0.47
4:S:6:GLN:HA	4:S:22:CYS:HA	1.95	0.47
2:B:408:ILE:N	2:B:409:PRO:HD2	2.30	0.47
2:H:275:MET:HB2	2:H:286:LYS:HB3	1.96	0.47
5:N:13:SER:HB3	5:N:109:LEU:HD12	1.95	0.47
5:T:6:GLN:O	5:T:102:THR:OG1	2.30	0.47
2:E:40:GLY:O	2:E:132:ASN:ND2	2.34	0.47
2:E:408:ILE:N	2:E:409:PRO:HD3	2.30	0.47
3:F:147:LEU:O	3:F:177:TYR:HA	2.15	0.47
2:K:9:TYR:CZ	2:K:55:LEU:HG	2.49	0.47
3:L:151:MET:HB3	3:L:174:ASP:OD1	2.15	0.47
1:D:65:SER:HA	1:D:101:THR:HG21	1.96	0.47
2:H:387:TRP:HE3	2:H:388:LEU:HD12	1.79	0.47
2:K:14:PRO:HG3	2:K:52:GLN:HG3	1.96	0.47
2:K:405:ASN:HB2	3:L:191:TYR:OH	2.14	0.47
3:L:204:HIS:NE2	3:L:225:ASP:OD2	2.48	0.47
2:B:7:ASN:OD1	2:B:8:GLU:N	2.47	0.47
2:B:169:LEU:HD12	2:B:252:LYS:HE2	1.96	0.47
2:B:271:ALA:O	2:B:333:HIS:NE2	2.43	0.47
2:E:197:LEU:HB2	2:E:231:LEU:HD11	1.97	0.47
2:E:5:LEU:HD13	2:E:55:LEU:CD1	2.45	0.47
4:O:21:SER:HA	4:O:79:ALA:O	2.14	0.47
4:O:100:GLN:HB2	4:O:111:TYR:CD2	2.50	0.47
4:Q:51:ILE:HG13	4:Q:70:VAL:HG11	1.97	0.47
1:D:148:VAL:HG12	1:D:148:VAL:O	2.15	0.47
2:E:288:HIS:ND1	2:E:314:PRO:HB3	2.30	0.47
1:G:148:VAL:O	1:G:148:VAL:HG12	2.15	0.47
1:G:296:LEU:HD11	1:G:320:TYR:HB2	1.97	0.47
2:K:14:PRO:HD3	2:K:67:ARG:NH2	2.29	0.47
2:K:327:GLU:HG3	2:K:337:ARG:HG2	1.97	0.47
3:L:182:GLN:HA	3:L:185:ARG:NH1	2.29	0.47
5:T:4:LEU:HD23	5:T:22:CYS:SG	2.55	0.47
1:A:321:SER:O	1:A:321:SER:OG	2.34	0.46
5:P:27:LEU:HD21	5:P:71:VAL:HG23	1.97	0.46
1:A:174:ASP:HB2	1:A:186:ASN:OD1	2.15	0.46
1:G:250:SER:OG	1:G:251:LEU:N	2.49	0.46
2:K:169:LEU:HD12	2:K:170:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:64:PHE:HD2	4:O:68:ILE:HB	1.81	0.46
5:T:27:LEU:HD11	5:T:32:VAL:CG1	2.46	0.46
2:E:141:HIS:HD1	2:K:126:PRO:HG3	1.80	0.46
3:F:189:PHE:HE1	3:F:231:LEU:HD11	1.80	0.46
1:D:9:SER:OG	1:D:273:VAL:O	2.30	0.46
1:G:328:CYS:SG	1:G:346:LEU:HD22	2.56	0.46
2:K:55:LEU:HB2	2:K:60:ASN:O	2.15	0.46
2:K:402:LEU:HD21	3:L:175:LEU:HD21	1.98	0.46
5:R:85:ASP:HB3	5:R:87:TYR:CE1	2.50	0.46
3:C:213:ARG:NH1	3:C:267:TYR:HB3	2.31	0.46
2:K:12:THR:HA	2:K:236:TRP:O	2.15	0.46
4:S:12:LYS:HD2	4:S:13:LYS:O	2.16	0.46
2:E:159:GLN:HB2	2:E:161:ARG:HH11	1.79	0.46
1:G:369:ILE:HG22	1:G:370:CYS:H	1.80	0.46
3:I:223:LYS:HA	3:I:275:TRP:HE3	1.81	0.46
1:J:363:PRO:HD3	1:J:380:CYS:SG	2.55	0.46
5:P:20:ILE:HG23	5:P:104:THR:HG21	1.97	0.46
1:G:3:HIS:HD2	1:G:4:ALA:H	1.64	0.46
3:L:209:TYR:HB2	3:L:214:PHE:CE1	2.50	0.46
5:N:3:GLU:OE2	5:N:4:LEU:N	2.49	0.46
5:P:30:GLN:NE2	5:P:91:ALA:HB3	2.31	0.46
5:T:96:THR:OG1	5:T:97:GLU:OE1	2.26	0.46
5:T:115:PRO:HA	5:T:142:TYR:HA	1.98	0.46
1:A:327:LYS:HD2	1:A:343:ALA:HB1	1.98	0.46
2:B:143:PRO:HG3	2:B:269:PRO:HD3	1.97	0.46
2:H:9:TYR:CE1	2:H:59:GLY:HA2	2.49	0.46
2:B:10:LYS:O	2:B:235:LYS:NZ	2.39	0.46
2:B:12:THR:HG23	2:B:13:ARG:H	1.81	0.46
2:E:159:GLN:HB2	2:E:161:ARG:NH1	2.31	0.46
1:G:19:VAL:HG23	1:G:21:ARG:NH1	2.31	0.46
4:Q:100:GLN:HB3	4:Q:110:ASP:HB2	1.97	0.46
5:N:34:TRP:CG	5:N:73:LEU:HD12	2.51	0.46
5:P:92:ASP:N	5:P:97:GLU:O	2.48	0.46
1:D:63:CYS:HA	1:D:99:GLU:HG2	1.98	0.45
2:E:54:GLY:C	2:E:55:LEU:HD12	2.36	0.45
3:F:189:PHE:CE1	3:F:231:LEU:HD11	2.51	0.45
2:H:9:TYR:CZ	2:H:55:LEU:HG	2.50	0.45
4:S:37:VAL:HG11	4:S:112:TRP:HZ3	1.79	0.45
1:A:222:GLN:HB2	1:A:232:PRO:HB2	1.97	0.45
2:K:5:LEU:HD13	2:K:55:LEU:HD22	1.99	0.45
4:Q:100:GLN:H	4:Q:110:ASP:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:21:SER:HB2	4:S:80:TYR:CD1	2.51	0.45
5:T:91:ALA:HB1	5:T:95:ASN:HA	1.99	0.45
3:L:159:ASN:HD21	3:L:162:LEU:HD13	1.80	0.45
5:T:46:VAL:HG23	5:T:57:ILE:HD12	1.99	0.45
1:A:409:TRP:HZ3	2:B:355:VAL:HG21	1.81	0.45
2:H:14:PRO:HG3	2:H:52:GLN:HB2	1.98	0.45
5:P:37:GLN:HB3	5:P:85:ASP:HB2	1.99	0.45
1:D:160:LYS:HB2	1:D:281:ASP:HB2	1.99	0.45
1:G:156:PHE:HE1	1:G:161:ILE:HD11	1.82	0.45
2:H:412:LEU:HD12	2:H:416:CYS:HA	1.98	0.45
3:L:192:THR:OG1	3:L:236:ARG:HD2	2.16	0.45
4:M:94:TYR:O	4:M:115:GLY:CA	2.64	0.45
1:G:86:PRO:HB3	1:G:229:ILE:HG12	1.98	0.45
2:K:37:LYS:HA	2:K:37:LYS:HD3	1.76	0.45
2:K:371:LEU:HA	2:K:374:CYS:HB3	1.98	0.45
5:P:6:GLN:HB3	5:P:102:THR:OG1	2.17	0.45
4:Q:70:VAL:HG22	4:Q:81:MET:HG2	1.98	0.45
4:Q:100:GLN:HB2	4:Q:111:TYR:HB2	1.97	0.45
4:S:13:LYS:HA	4:S:13:LYS:HD3	1.75	0.45
2:B:303:GLU:O	2:B:303:GLU:HG2	2.15	0.45
3:C:207:VAL:HG22	3:C:216:VAL:HG12	1.99	0.45
1:D:51:TYR:OH	1:D:236:ALA:O	2.32	0.45
1:D:404:LYS:O	1:D:408:THR:HG23	2.17	0.45
1:J:359:ALA:HB2	1:J:394:HIS:CD2	2.52	0.45
4:O:145:ALA:HB2	4:O:184:LEU:HA	1.98	0.45
4:Q:27:TYR:OH	4:Q:98:THR:HG21	2.17	0.45
4:S:36:TRP:CZ3	4:S:70:VAL:HG22	2.51	0.45
2:H:14:PRO:HD3	2:H:67:ARG:NH2	2.32	0.45
1:J:76:GLU:HA	1:J:106:ALA:O	2.17	0.45
5:N:4:LEU:HD11	5:N:90:ALA:HB3	1.96	0.45
4:O:57:ASN:OD1	4:O:58:THR:N	2.49	0.45
3:F:213:ARG:NH1	3:F:267:TYR:HB3	2.32	0.45
1:G:300:GLU:O	1:G:318:VAL:HA	2.17	0.45
2:H:199:GLU:O	2:H:226:CYS:HB2	2.17	0.45
4:M:40:ALA:HB3	4:M:43:GLN:HB2	1.98	0.45
5:T:6:GLN:NE2	5:T:86:TYR:O	2.44	0.45
2:B:9:TYR:HB3	2:B:55:LEU:HD22	1.99	0.44
3:C:119:VAL:HG11	3:C:205:GLY:HA2	1.99	0.44
2:K:219:GLN:HG2	4:S:32:TYR:CE1	2.51	0.44
2:K:353:HIS:CE1	2:K:354:GLU:HG2	2.52	0.44
3:L:167:THR:HB	3:L:176:GLU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:27:LEU:N	5:N:28:PRO:HD2	2.32	0.44
4:Q:120:VAL:HG22	4:Q:121:SER:H	1.82	0.44
1:A:93:TYR:HA	2:B:174:VAL:HG11	1.99	0.44
1:D:10:GLN:HG2	1:D:13:ILE:HD12	1.99	0.44
1:D:392:GLN:NE2	1:D:394:HIS:O	2.44	0.44
4:M:73:ASP:HB3	4:M:76:ALA:HB3	1.98	0.44
1:A:283:PRO:HG2	1:A:286:LEU:HD13	1.97	0.44
1:A:341:GLU:OE1	1:A:341:GLU:N	2.46	0.44
2:B:82:VAL:HG21	2:B:112:MET:HE2	1.99	0.44
1:D:243:TRP:O	1:D:247:LYS:HB3	2.17	0.44
2:E:17:ALA:HB3	2:E:32:ALA:HB3	2.00	0.44
2:E:219:GLN:HG2	4:O:32:TYR:OH	2.17	0.44
3:F:146:LYS:HB3	3:F:148:PHE:HE1	1.81	0.44
3:I:214:PHE:CD1	3:I:255:VAL:HG11	2.52	0.44
2:K:276:ILE:HG12	2:K:285:LEU:HD23	1.98	0.44
4:M:59:LYS:HZ2	5:N:97:GLU:HG3	1.82	0.44
5:R:20:ILE:HG23	5:R:104:THR:HG21	1.99	0.44
4:S:36:TRP:HZ3	4:S:70:VAL:HG22	1.82	0.44
2:E:170:PRO:O	2:E:233:ASN:ND2	2.51	0.44
1:J:19:VAL:CG2	1:J:27:LEU:HB3	2.48	0.44
5:T:6:GLN:HG2	5:T:104:THR:HG23	1.99	0.44
1:A:148:VAL:O	1:A:164:GLY:HA3	2.18	0.44
3:F:216:VAL:HG13	3:F:253:LEU:HD22	1.99	0.44
2:B:12:THR:HG23	2:B:13:ARG:N	2.33	0.44
1:G:13:ILE:HD11	1:G:391:PRO:HG2	2.00	0.44
4:M:70:VAL:HA	4:M:81:MET:HA	1.99	0.44
1:D:86:PRO:HB3	1:D:229:ILE:HG12	1.99	0.44
4:Q:100:GLN:N	4:Q:110:ASP:HB2	2.33	0.44
3:C:218:LYS:HZ2	3:C:246:ASN:HD21	1.64	0.44
2:E:199:GLU:HB2	2:E:229:TYR:HE1	1.83	0.44
3:F:259:ASN:HB2	3:F:263:VAL:HG22	2.00	0.44
1:J:53:THR:OG1	1:J:235:GLN:OE1	2.36	0.44
1:G:96:CYS:O	1:G:100:ASN:ND2	2.44	0.44
2:H:165:VAL:HG23	2:H:255:LEU:HB2	2.00	0.44
3:L:182:GLN:HA	3:L:185:ARG:HH12	1.83	0.44
3:F:207:VAL:HG12	3:F:216:VAL:HG12	1.99	0.43
1:J:18:ILE:HG22	1:J:28:PRO:HA	2.00	0.43
1:J:369:ILE:HG22	1:J:370:CYS:H	1.82	0.43
4:M:30:THR:O	4:M:31:ASN:ND2	2.51	0.43
2:E:147:VAL:O	2:E:268:VAL:HG22	2.18	0.43
3:F:245:VAL:HB	3:F:272:CYS:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:200:CYS:HB2	2:H:206:LYS:HE2	1.99	0.43
3:I:274:GLN:HG3	3:I:275:TRP:CD1	2.53	0.43
2:K:55:LEU:HB3	2:K:61:LEU:HA	2.00	0.43
1:D:219:LEU:HA	1:D:235:GLN:HB3	1.99	0.43
2:H:52:GLN:OE1	2:H:67:ARG:NH2	2.42	0.43
3:I:129:PRO:HA	3:I:139:TYR:CD1	2.51	0.43
1:J:304:ASN:HB2	1:J:315:ILE:HG23	1.99	0.43
5:R:38:LYS:NZ	5:R:81:GLU:O	2.51	0.43
2:B:184:SER:OG	4:M:31:ASN:OD1	2.35	0.43
3:I:203:HIS:HB3	3:I:228:ARG:NH1	2.33	0.43
3:L:124:SER:O	3:L:126:LYS:NZ	2.34	0.43
4:O:158:PRO:HA	4:O:199:GLY:HA2	2.00	0.43
4:S:167:ALA:HB1	4:S:185:TYR:HA	1.99	0.43
1:A:327:LYS:HA	1:A:327:LYS:HD3	1.85	0.43
1:J:63:CYS:H	1:J:100:ASN:HA	1.82	0.43
1:J:95:PHE:CE1	2:K:201:GLU:HB2	2.52	0.43
2:K:359:TYR:HB3	2:K:367:THR:HG21	2.00	0.43
3:C:169:LYS:HD3	3:C:176:GLU:HG3	2.00	0.43
2:E:41:HIS:ND1	2:E:134:VAL:HG22	2.33	0.43
2:E:275:MET:SD	1:J:197:PRO:HG2	2.59	0.43
3:I:187:ASP:OD1	3:I:187:ASP:N	2.48	0.43
1:J:19:VAL:HG23	1:J:27:LEU:HB3	2.00	0.43
1:J:63:CYS:HA	1:J:100:ASN:HA	2.00	0.43
4:S:36:TRP:CE3	4:S:81:MET:HG3	2.53	0.43
2:E:134:VAL:HG21	2:E:266:CYS:SG	2.59	0.43
2:E:207:ILE:HG22	2:E:207:ILE:O	2.19	0.43
2:H:18:ARG:HH22	2:H:20:ILE:HD13	1.84	0.43
2:H:57:SER:HA	2:H:67:ARG:HD3	2.01	0.43
2:H:87:SER:OG	2:H:106:ALA:O	2.31	0.43
1:J:253:PHE:HB3	2:K:296:ILE:HG21	2.01	0.43
1:J:290:VAL:HA	1:J:293:THR:HG22	2.01	0.43
2:K:57:SER:HA	2:K:67:ARG:HD2	2.00	0.43
4:S:4:LEU:HA	4:S:23:LYS:O	2.19	0.43
3:F:151:MET:CE	3:F:176:GLU:HG3	2.48	0.43
1:G:192:TYR:OH	1:G:212:ASP:OD2	2.19	0.43
2:H:297:THR:O	2:H:306:TYR:HA	2.19	0.43
1:J:329:ALA:N	1:J:370:CYS:HB3	2.33	0.43
5:N:14:PRO:HA	5:N:78:VAL:HG13	2.01	0.43
4:Q:81:MET:SD	4:Q:82:GLU:N	2.91	0.43
1:A:35:LYS:HB2	1:A:35:LYS:HE2	1.76	0.43
1:A:135:ILE:HB	1:A:142:ILE:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:TYR:HB3	2:B:55:LEU:CD2	2.49	0.43
2:E:21:ARG:HD2	2:H:141:HIS:CE1	2.54	0.43
2:E:170:PRO:HD3	2:E:236:TRP:HA	2.01	0.43
3:F:264:THR:O	3:F:264:THR:HG22	2.19	0.43
1:G:416:GLY:O	1:G:420:ILE:HG12	2.19	0.43
1:J:10:GLN:HG2	1:J:13:ILE:HD12	2.01	0.43
4:O:18:VAL:HG12	4:O:86:LEU:HD11	2.01	0.43
4:Q:150:LEU:HA	4:Q:179:LEU:H	1.83	0.43
5:R:54:PRO:HD2	5:R:57:ILE:HG13	2.00	0.43
4:S:4:LEU:HG	4:S:111:TYR:HE2	1.84	0.43
4:S:60:TYR:HE1	4:S:70:VAL:HG23	1.84	0.43
1:D:120:GLU:HG3	1:D:122:TYR:CE2	2.54	0.43
3:F:128:PHE:HB2	3:F:157:ILE:HD11	1.99	0.43
3:F:158:ASP:OD1	3:F:159:ASN:N	2.52	0.43
1:G:402:VAL:O	1:G:406:ALA:HB3	2.18	0.43
2:K:175:ASP:OD2	2:K:230:ARG:NH1	2.51	0.43
2:K:281:ARG:NH2	2:K:323:GLU:OE1	2.42	0.43
4:O:22:CYS:HB2	4:O:36:TRP:CH2	2.54	0.43
4:Q:167:ALA:HB1	4:Q:185:TYR:HA	2.01	0.43
5:T:38:LYS:HB2	5:T:41:GLN:HB2	2.01	0.43
2:B:9:TYR:CG	2:B:55:LEU:HD13	2.53	0.42
3:C:196:PRO:O	3:C:200:TYR:OH	2.24	0.42
1:D:104:SER:HB2	1:D:231:VAL:HG22	1.99	0.42
1:G:328:CYS:SG	1:G:369:ILE:HG22	2.59	0.42
1:J:31:ILE:HD11	1:J:280:PHE:CZ	2.50	0.42
2:K:143:PRO:HG3	2:K:269:PRO:HD3	2.01	0.42
2:K:399:PRO:HG3	3:L:173:TYR:OH	2.18	0.42
5:N:88:CYS:O	5:N:101:GLY:N	2.51	0.42
5:P:197:VAL:HA	5:P:206:LYS:HA	2.00	0.42
1:G:10:GLN:HG2	1:G:13:ILE:HD12	2.01	0.42
1:G:148:VAL:O	1:G:164:GLY:HA3	2.19	0.42
2:H:398:THR:OG1	2:H:399:PRO:HD3	2.20	0.42
2:K:191:PRO:HG2	2:K:194:THR:HB	2.00	0.42
1:A:303:LEU:HD11	1:A:356:PHE:CZ	2.55	0.42
1:A:318:VAL:O	1:A:351:SER:HA	2.19	0.42
2:E:302:ASP:N	2:E:302:ASP:OD1	2.51	0.42
2:E:404:PRO:HG2	3:F:191:TYR:CG	2.54	0.42
2:K:55:LEU:HD13	2:K:61:LEU:HD12	2.02	0.42
2:K:404:PRO:HD3	3:L:258:TRP:CH2	2.54	0.42
3:L:197:GLN:HE22	3:L:211:ASN:H	1.65	0.42
5:R:170:SER:N	5:R:174:TYR:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:GLY:O	1:A:420:ILE:HG12	2.19	0.42
2:B:232:GLN:HG2	2:B:234:ASP:OD1	2.20	0.42
2:E:393:ARG:HH21	2:E:418:ALA:HA	1.85	0.42
3:I:169:LYS:HD3	3:I:169:LYS:N	2.35	0.42
2:K:408:ILE:O	2:K:410:PHE:N	2.53	0.42
3:L:130:ILE:HD11	3:L:140:ALA:HB2	2.00	0.42
4:O:47:TRP:HZ2	4:O:50:TRP:HD1	1.67	0.42
4:S:39:GLN:HE22	5:T:37:GLN:HE22	1.66	0.42
4:S:145:ALA:HB2	4:S:184:LEU:HA	2.01	0.42
5:T:12:VAL:HG21	5:T:18:ALA:HB2	2.00	0.42
5:T:27:LEU:N	5:T:28:PRO:HD2	2.35	0.42
2:E:11:LEU:HA	2:E:235:LYS:HD2	2.02	0.42
2:E:141:HIS:ND1	2:K:126:PRO:HG3	2.34	0.42
1:G:97:ASP:OD1	1:G:97:ASP:N	2.53	0.42
1:J:282:ILE:HG23	1:J:286:LEU:HD12	2.01	0.42
1:D:362:HIS:NE2	1:D:404:LYS:HG2	2.34	0.42
2:K:397:LEU:HD23	2:K:397:LEU:HA	1.90	0.42
4:O:99:LEU:HD12	4:O:110:ASP:HB2	2.02	0.42
5:P:14:PRO:HD3	5:P:109:LEU:H	1.84	0.42
1:D:295:THR:HA	1:D:371:THR:HG21	2.00	0.42
1:D:296:LEU:HD22	1:D:372:SER:HB2	2.01	0.42
2:K:55:LEU:CB	2:K:61:LEU:HA	2.50	0.42
5:T:79:GLN:NE2	5:T:81:GLU:OE2	2.53	0.42
2:B:134:VAL:HG11	2:B:151:CYS:SG	2.60	0.42
1:D:135:ILE:HG21	1:D:161:ILE:CD1	2.49	0.42
2:E:213:LYS:HE3	6:E:501:NAG:H83	2.02	0.42
3:F:191:TYR:HA	3:F:237:VAL:O	2.19	0.42
1:G:325:SER:HA	1:G:346:LEU:O	2.19	0.42
2:H:9:TYR:CZ	2:H:67:ARG:CZ	3.03	0.42
5:N:53:ARG:NH2	5:N:62:PHE:O	2.52	0.42
4:S:27:TYR:CE2	4:S:32:TYR:HD2	2.38	0.42
1:A:309:SER:HB3	1:A:383:PRO:HB3	2.02	0.42
2:B:94:ASP:OD1	2:B:95:GLY:N	2.51	0.42
2:B:132:ASN:HA	2:B:133:PRO:HD3	1.83	0.42
1:D:366:ARG:NH1	1:D:373:TYR:HB3	2.33	0.42
2:E:398:THR:OG1	2:E:399:PRO:HD3	2.20	0.42
2:H:53:TYR:CE2	2:H:100:LEU:HD13	2.55	0.42
3:L:200:TYR:HB3	3:L:231:LEU:O	2.20	0.42
1:D:230:HIS:NE2	1:D:232:PRO:HG3	2.34	0.42
1:G:244:LYS:HA	1:G:247:LYS:HG3	2.02	0.42
3:I:152:HIS:CE1	3:I:275:TRP:HE1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:86:PRO:HB3	1:J:229:ILE:HG12	2.02	0.42
1:A:148:VAL:O	1:A:148:VAL:HG12	2.19	0.41
1:A:300:GLU:O	1:A:318:VAL:HA	2.20	0.41
2:B:210:THR:HG23	5:N:49:LYS:HD3	2.02	0.41
2:B:218:SER:H	4:M:106:ASN:HB2	1.85	0.41
2:E:12:THR:HG23	2:E:13:ARG:N	2.35	0.41
2:H:397:LEU:HD23	2:H:397:LEU:HA	1.87	0.41
4:O:37:VAL:HG21	4:O:112:TRP:HZ3	1.84	0.41
5:T:20:ILE:HG23	5:T:104:THR:HG21	2.01	0.41
5:T:86:TYR:HB2	5:T:104:THR:OG1	2.20	0.41
1:A:405:THR:HG22	1:A:409:TRP:CZ3	2.55	0.41
1:A:434:TYR:HE1	1:A:438:ASN:HD21	1.68	0.41
2:E:174:VAL:HA	2:E:229:TYR:HA	2.01	0.41
1:G:77:GLN:NE2	1:G:219:LEU:O	2.53	0.41
1:J:110:LYS:HG3	1:J:213:LEU:HD13	2.03	0.41
2:B:404:PRO:HB3	3:C:144:GLY:HA3	2.02	0.41
1:D:402:VAL:O	1:D:406:ALA:HB3	2.20	0.41
3:F:183:ASN:OD1	3:F:184:MET:N	2.53	0.41
2:H:126:PRO:HB3	2:K:141:HIS:HB3	2.00	0.41
3:L:247:GLU:HG2	3:L:248:GLY:N	2.35	0.41
1:D:168:THR:HG21	1:D:273:VAL:HG22	2.02	0.41
1:D:383:PRO:HG2	2:E:343:THR:HG22	2.01	0.41
3:F:218:LYS:HE3	3:F:249:SER:HA	2.02	0.41
3:F:230:ILE:HG22	3:F:239:ALA:O	2.20	0.41
3:F:239:ALA:HB1	3:F:255:VAL:HG22	2.01	0.41
2:H:362:ARG:HD2	2:H:362:ARG:HA	1.77	0.41
2:K:397:LEU:HD11	2:K:418:ALA:HB2	2.01	0.41
4:O:6:GLN:HE22	4:O:115:GLY:C	2.23	0.41
2:B:78:PRO:HG2	2:B:81:GLN:HG3	2.01	0.41
3:C:187:ASP:OD1	3:C:187:ASP:N	2.44	0.41
1:D:224:PRO:HA	1:D:232:PRO:HG2	2.01	0.41
2:E:9:TYR:CE2	2:E:55:LEU:HD13	2.53	0.41
2:E:23:ALA:HB2	2:E:122:SER:HB3	2.02	0.41
1:J:55:MET:HG3	2:K:241:ASP:HB3	2.03	0.41
2:K:116:LYS:HD3	2:K:116:LYS:HA	1.89	0.41
4:O:99:LEU:HD11	4:O:101:MET:HB2	2.02	0.41
4:Q:36:TRP:CE2	4:Q:81:MET:HB2	2.55	0.41
1:D:161:ILE:HG12	1:D:280:PHE:HD2	1.86	0.41
1:D:309:SER:HB3	1:D:383:PRO:HB3	2.02	0.41
1:J:30:SER:HB3	1:J:136:THR:OG1	2.20	0.41
1:J:63:CYS:HB2	1:J:99:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:150:LEU:HA	4:M:179:LEU:H	1.86	0.41
4:O:6:GLN:NE2	4:O:114:GLN:HG2	2.36	0.41
4:Q:96:CYS:O	4:Q:112:TRP:HA	2.20	0.41
2:B:117:ASP:OD1	2:B:117:ASP:N	2.53	0.41
2:B:398:THR:OG1	2:B:399:PRO:HD3	2.21	0.41
3:C:200:TYR:HD2	3:C:232:ASP:HA	1.85	0.41
2:E:103:ARG:HD2	2:K:21:ARG:CZ	2.51	0.41
2:K:36:VAL:HG22	2:K:47:LEU:HD12	2.03	0.41
2:E:275:MET:HB2	2:E:286:LYS:HB3	2.03	0.41
2:H:189:THR:O	2:H:189:THR:OG1	2.33	0.41
2:H:274:PRO:HB3	2:H:287:LEU:HD23	2.03	0.41
3:I:196:PRO:HD2	3:I:200:TYR:OH	2.20	0.41
4:O:18:VAL:O	4:O:82:GLU:HA	2.21	0.41
4:Q:4:LEU:H	4:Q:111:TYR:HE2	1.68	0.41
1:A:129:VAL:HB	1:A:148:VAL:HB	2.03	0.41
2:B:9:TYR:OH	2:B:53:TYR:O	2.33	0.41
2:B:202:CYS:SG	2:B:203:GLY:N	2.88	0.41
2:B:236:TRP:CZ2	2:B:252:LYS:HD2	2.56	0.41
1:D:19:VAL:CG1	1:D:27:LEU:HB3	2.51	0.41
1:D:93:TYR:HA	2:E:174:VAL:HG11	2.03	0.41
1:D:161:ILE:HG12	1:D:280:PHE:CD2	2.55	0.41
1:G:362:HIS:CD2	1:G:404:LYS:HG3	2.56	0.41
2:H:111:THR:HG23	2:H:124:SER:HB2	2.03	0.41
3:I:258:TRP:HD1	3:I:264:THR:HG22	1.83	0.41
2:K:36:VAL:HG22	2:K:47:LEU:CD1	2.51	0.41
2:K:49:THR:HG21	2:K:53:TYR:OH	2.21	0.41
2:K:207:ILE:HG22	2:K:207:ILE:O	2.21	0.41
2:K:219:GLN:NE2	4:S:102:ASP:HB2	2.36	0.41
4:Q:45:LEU:HD23	5:R:87:TYR:CZ	2.56	0.41
4:S:150:LEU:HA	4:S:179:LEU:CB	2.50	0.41
2:B:174:VAL:HA	2:B:229:TYR:HA	2.03	0.41
2:E:189:THR:HG22	2:E:214:THR:HG23	2.02	0.41
1:J:230:HIS:NE2	1:J:232:PRO:HG3	2.36	0.41
1:J:417:SER:HA	1:J:420:ILE:HD13	2.03	0.41
3:L:118:MET:SD	3:L:206:ALA:HB2	2.61	0.41
4:O:99:LEU:HB2	4:O:108:ASP:O	2.20	0.41
4:Q:22:CYS:HB2	4:Q:36:TRP:CH2	2.56	0.41
4:S:23:LYS:HA	4:S:78:ALA:HA	2.03	0.41
5:T:79:GLN:OE1	5:T:81:GLU:HG3	2.21	0.41
1:G:360:ASN:ND2	1:G:400:ALA:HA	2.36	0.40
4:O:99:LEU:HB2	4:O:109:LEU:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:9:SER:HB2	5:P:105:LYS:HB2	2.02	0.40
4:S:6:GLN:HB3	4:S:22:CYS:HB3	2.04	0.40
2:B:12:THR:HG21	2:B:67:ARG:HH22	1.87	0.40
2:H:276:ILE:HG12	2:H:285:LEU:HD23	2.02	0.40
1:J:129:VAL:HB	1:J:148:VAL:HB	2.02	0.40
1:J:420:ILE:HG22	2:K:385:SER:OG	2.21	0.40
4:M:109:LEU:O	5:N:35:TYR:OH	2.27	0.40
5:P:85:ASP:HB3	5:P:87:TYR:CE2	2.57	0.40
5:R:79:GLN:N	5:R:82:ASP:OD2	2.43	0.40
2:B:33:ILE:HG12	2:B:47:LEU:HD21	2.02	0.40
1:D:81:PHE:HB3	1:D:223:ARG:NH1	2.36	0.40
1:J:156:PHE:HE1	1:J:161:ILE:HD11	1.86	0.40
2:K:14:PRO:HD3	2:K:67:ARG:CZ	2.51	0.40
4:M:30:THR:OG1	4:M:31:ASN:N	2.54	0.40
5:P:32:VAL:HG22	5:P:50:ASP:OD1	2.22	0.40
2:B:72:GLY:HA3	2:B:230:ARG:NH1	2.37	0.40
2:B:213:LYS:O	2:B:214:THR:OG1	2.32	0.40
3:C:209:TYR:CZ	3:C:212:GLY:HA2	2.56	0.40
2:E:300:LEU:HD21	2:E:327:GLU:HB2	2.04	0.40
1:G:402:VAL:HG13	1:G:407:TRP:HE1	1.86	0.40
2:H:211:ILE:HG22	5:R:49:LYS:HE3	2.04	0.40
2:K:227:ARG:HA	2:K:227:ARG:HD3	1.91	0.40
5:R:86:TYR:O	5:R:103:GLY:HA2	2.22	0.40
3:F:243:GLY:HA2	3:F:275:TRP:HB2	2.02	0.40
2:H:219:GLN:NE2	4:Q:104:GLY:HA2	2.37	0.40
1:J:122:TYR:HE2	1:J:179:GLN:HE21	1.69	0.40
3:L:254:SER:OG	3:L:269:PRO:HD2	2.21	0.40
4:M:51:ILE:HG13	4:M:52:ASN:N	2.35	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	438/440 (100%)	419 (96%)	19 (4%)	0	100	100
1	D	438/440 (100%)	414 (94%)	24 (6%)	0	100	100
1	G	438/440 (100%)	423 (97%)	15 (3%)	0	100	100
1	J	438/440 (100%)	416 (95%)	22 (5%)	0	100	100
2	B	416/418 (100%)	384 (92%)	32 (8%)	0	100	100
2	E	416/418 (100%)	388 (93%)	28 (7%)	0	100	100
2	H	416/418 (100%)	385 (92%)	31 (8%)	0	100	100
2	K	416/418 (100%)	383 (92%)	33 (8%)	0	100	100
3	C	157/159 (99%)	149 (95%)	8 (5%)	0	100	100
3	F	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
3	I	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
3	L	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
4	M	216/218 (99%)	200 (93%)	16 (7%)	0	100	100
4	O	216/218 (99%)	199 (92%)	17 (8%)	0	100	100
4	Q	216/218 (99%)	201 (93%)	15 (7%)	0	100	100
4	S	216/218 (99%)	197 (91%)	19 (9%)	0	100	100
5	N	205/209 (98%)	197 (96%)	8 (4%)	0	100	100
5	P	205/209 (98%)	200 (98%)	5 (2%)	0	100	100
5	R	205/209 (98%)	201 (98%)	4 (2%)	0	100	100
5	T	207/209 (99%)	190 (92%)	17 (8%)	0	100	100
All	All	5730/5776 (99%)	5406 (94%)	324 (6%)	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	366/366 (100%)	365 (100%)	1 (0%)	92	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	366/366 (100%)	366 (100%)	0	100 100
1	G	366/366 (100%)	364 (100%)	2 (0%)	88 93
1	J	366/366 (100%)	366 (100%)	0	100 100
2	B	361/361 (100%)	361 (100%)	0	100 100
2	E	361/361 (100%)	360 (100%)	1 (0%)	92 95
2	H	361/361 (100%)	361 (100%)	0	100 100
2	K	361/361 (100%)	360 (100%)	1 (0%)	92 95
3	C	132/132 (100%)	132 (100%)	0	100 100
3	F	132/132 (100%)	131 (99%)	1 (1%)	81 89
3	I	132/132 (100%)	132 (100%)	0	100 100
3	L	132/132 (100%)	131 (99%)	1 (1%)	81 89
4	M	101/182 (56%)	100 (99%)	1 (1%)	76 86
4	O	100/182 (55%)	99 (99%)	1 (1%)	76 86
4	Q	101/182 (56%)	101 (100%)	0	100 100
4	S	100/182 (55%)	100 (100%)	0	100 100
5	N	91/179 (51%)	91 (100%)	0	100 100
5	P	91/179 (51%)	91 (100%)	0	100 100
5	R	91/179 (51%)	91 (100%)	0	100 100
5	T	92/179 (51%)	89 (97%)	3 (3%)	38 62
All	All	4203/4880 (86%)	4191 (100%)	12 (0%)	92 95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	384	LYS
2	E	13	ARG
3	F	250	ARG
1	G	21	ARG
1	G	289	ARG
2	K	286	LYS
3	L	190	LYS
4	M	72	ARG
4	O	63	LYS
5	T	107	THR
5	T	108	VAL

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Mol	Chain	Res	Type
5	T	109	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
3	C	197	GLN
1	D	235	GLN
2	E	159	GLN
1	G	3	HIS
3	I	197	GLN
2	K	219	GLN
3	L	208	GLN
4	O	6	GLN
4	O	65	GLN
5	P	30	GLN
5	P	37	GLN
5	P	41	GLN
4	Q	3	GLN
4	Q	55	ASN
5	T	89	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

12 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	$\#\|Z\| > 2$
6	NAG	A	501	1	14,14,15	0.20	0	17,19,21	0.47	0
6	NAG	E	501	-	14,14,15	0.49	0	17,19,21	0.38	0
6	NAG	B	501	-	14,14,15	0.48	0	17,19,21	0.36	0
6	NAG	E	502	-	14,14,15	0.31	0	17,19,21	0.39	0
6	NAG	H	501	-	14,14,15	0.50	0	17,19,21	0.37	0
6	NAG	H	502	2	14,14,15	0.32	0	17,19,21	0.36	0
6	NAG	J	501	1	14,14,15	0.21	0	17,19,21	0.41	0
6	NAG	D	501	1	14,14,15	0.20	0	17,19,21	0.53	0
6	NAG	B	502	2	14,14,15	0.20	0	17,19,21	0.49	0
6	NAG	K	502	2	14,14,15	0.29	0	17,19,21	0.40	0
6	NAG	G	501	1	14,14,15	0.21	0	17,19,21	0.44	0
6	NAG	K	501	-	14,14,15	0.48	0	17,19,21	0.38	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
6	NAG	A	501	1	-	0/6/23/26	0/1/1/1
6	NAG	E	501	-	-	2/6/23/26	0/1/1/1
6	NAG	B	501	-	-	0/6/23/26	0/1/1/1
6	NAG	E	502	-	-	2/6/23/26	0/1/1/1
6	NAG	H	501	-	-	2/6/23/26	0/1/1/1
6	NAG	H	502	2	-	3/6/23/26	0/1/1/1
6	NAG	J	501	1	-	1/6/23/26	0/1/1/1
6	NAG	D	501	1	-	0/6/23/26	0/1/1/1
6	NAG	B	502	2	-	2/6/23/26	0/1/1/1
6	NAG	K	502	2	-	2/6/23/26	0/1/1/1
6	NAG	G	501	1	-	1/6/23/26	0/1/1/1
6	NAG	K	501	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	501	NAG	O5-C5-C6-O6
6	B	502	NAG	O5-C5-C6-O6
6	K	502	NAG	O5-C5-C6-O6
6	K	501	NAG	O5-C5-C6-O6
6	E	501	NAG	O5-C5-C6-O6
6	B	502	NAG	C4-C5-C6-O6
6	H	501	NAG	C4-C5-C6-O6
6	E	501	NAG	C4-C5-C6-O6
6	K	501	NAG	C4-C5-C6-O6
6	E	502	NAG	O5-C5-C6-O6
6	K	502	NAG	C4-C5-C6-O6
6	H	502	NAG	O5-C5-C6-O6
6	E	502	NAG	C4-C5-C6-O6
6	J	501	NAG	O5-C5-C6-O6
6	H	502	NAG	C4-C5-C6-O6
6	H	502	NAG	C1-C2-N2-C7
6	G	501	NAG	C4-C5-C6-O6

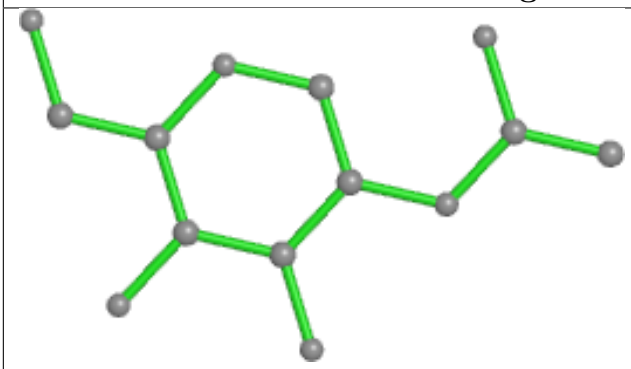
There are no ring outliers.

4 monomers are involved in 4 short contacts:

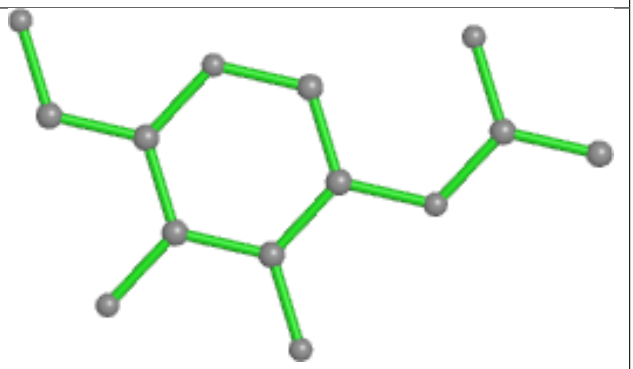
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	501	NAG	1	0
6	H	501	NAG	1	0
6	J	501	NAG	1	0
6	G	501	NAG	1	0

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 then 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.

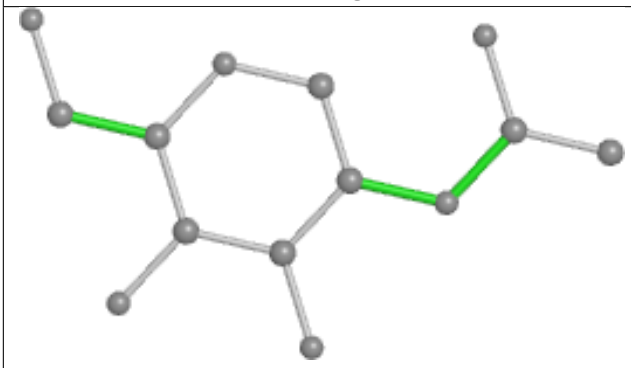
Ligand NAG A 501



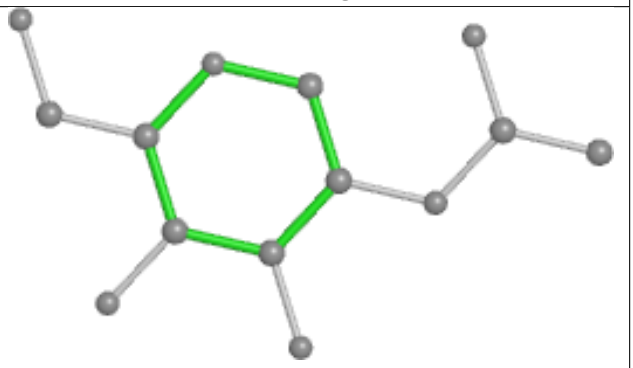
Bond lengths



Bond angles

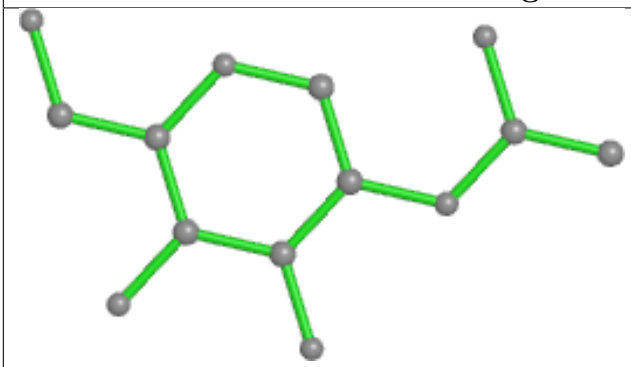


Torsions

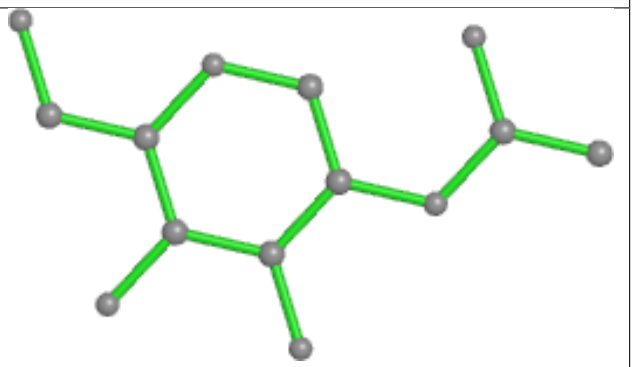


Rings

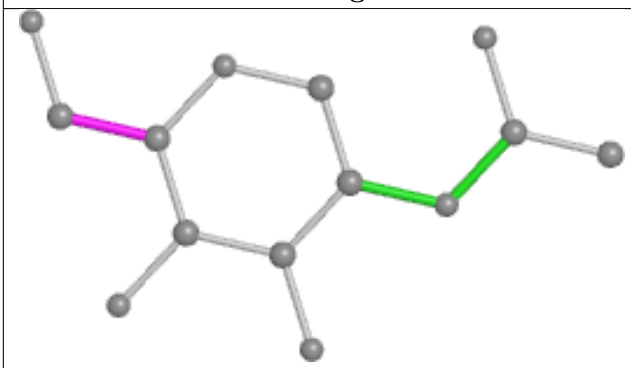
Ligand NAG E 501



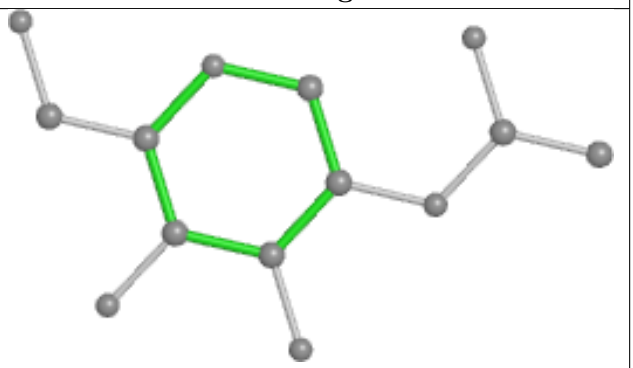
Bond lengths



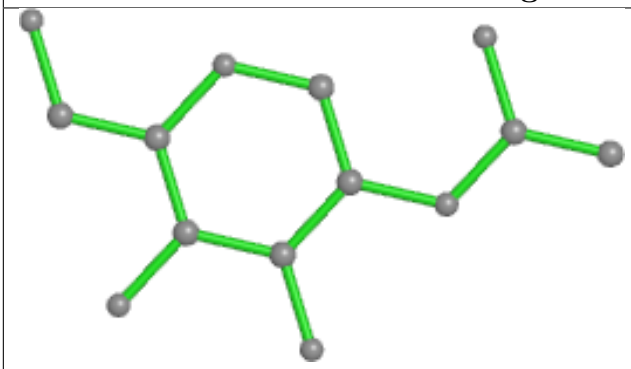
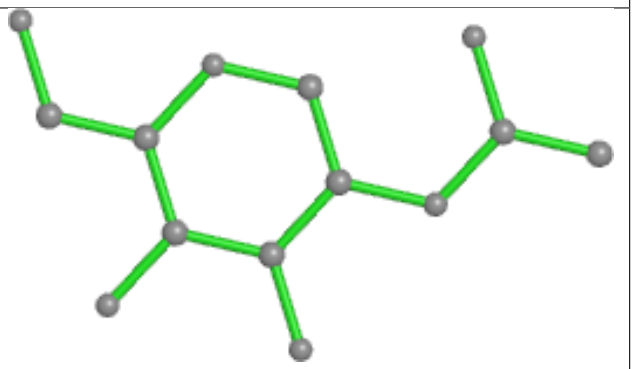
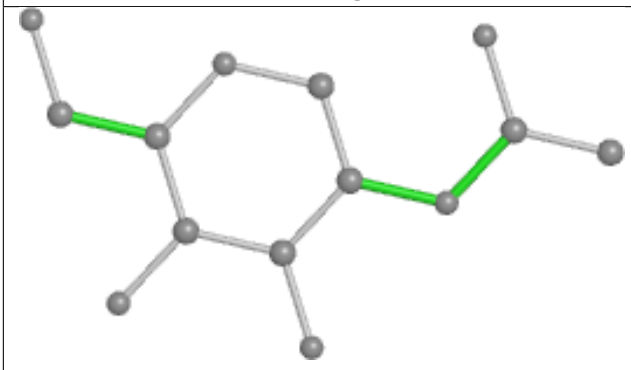
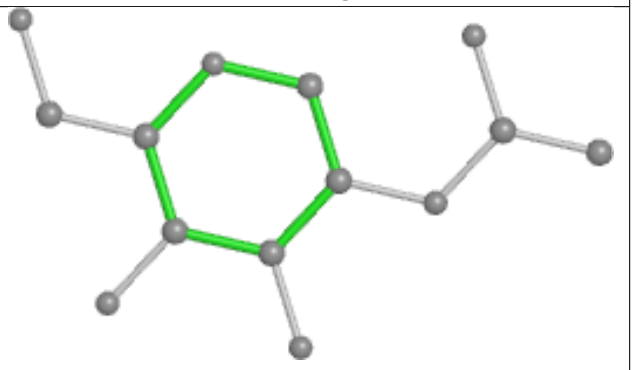
Bond angles

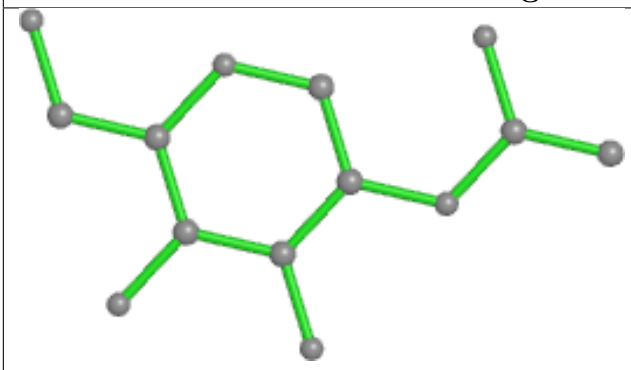
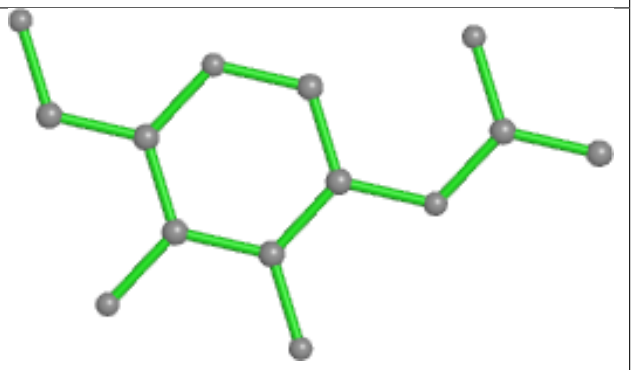
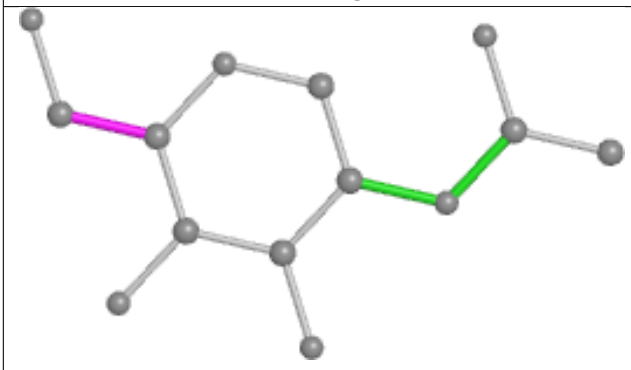
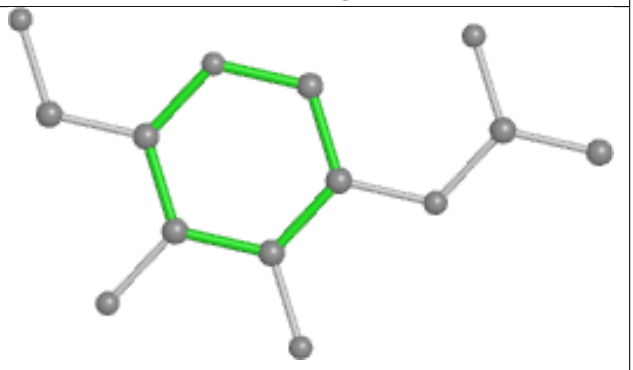


Torsions

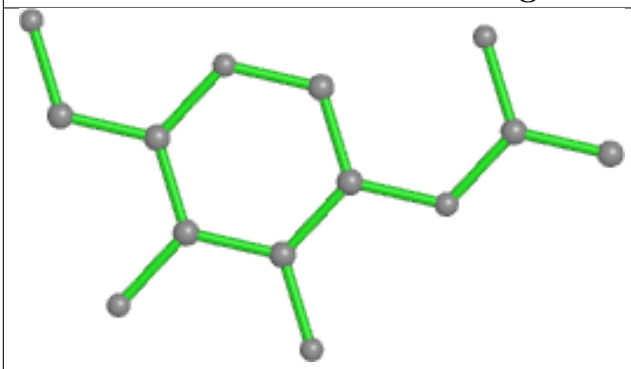


Rings

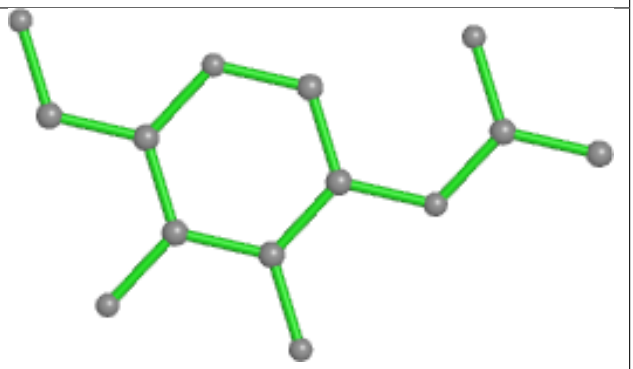
Ligand NAG B 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG E 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

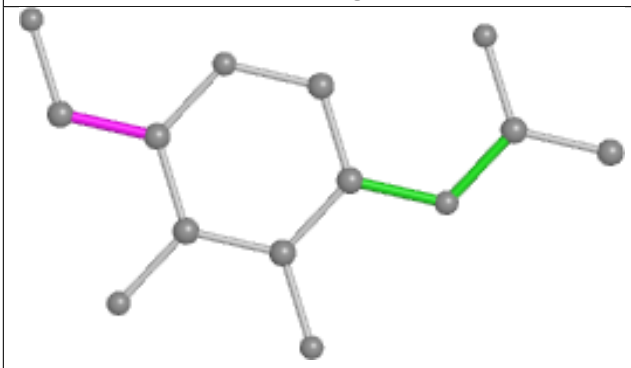
Ligand NAG H 501



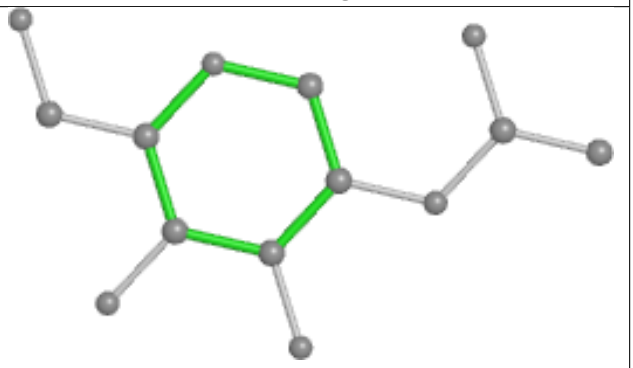
Bond lengths



Bond angles

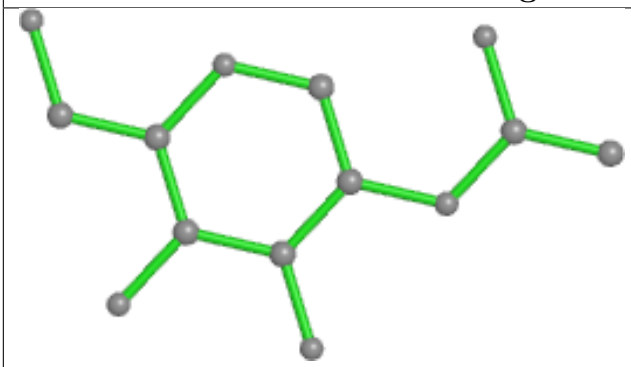


Torsions



Rings

Ligand NAG H 502



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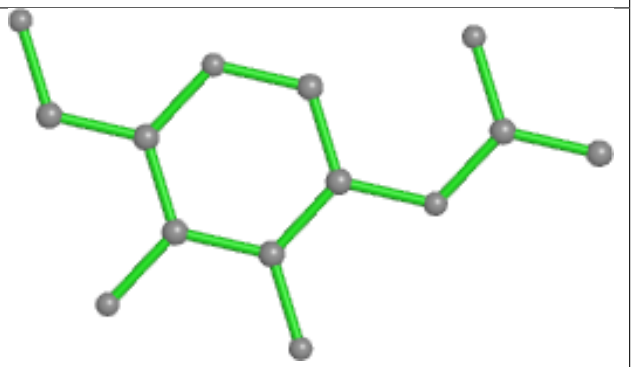

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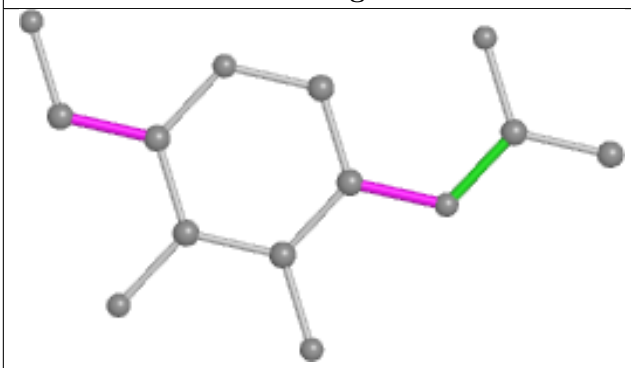

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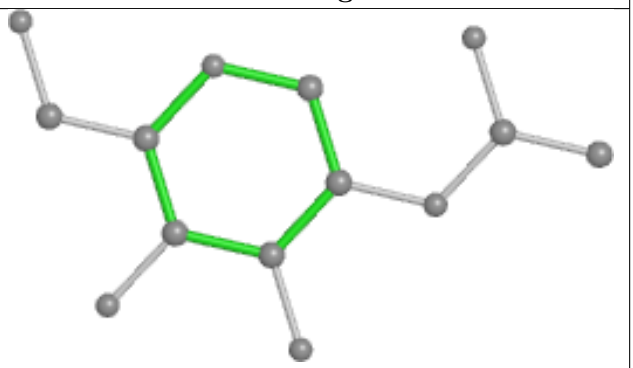
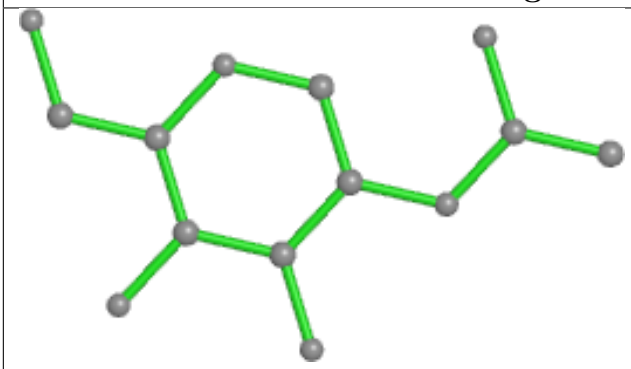


Rings

Ligand NAG J 501



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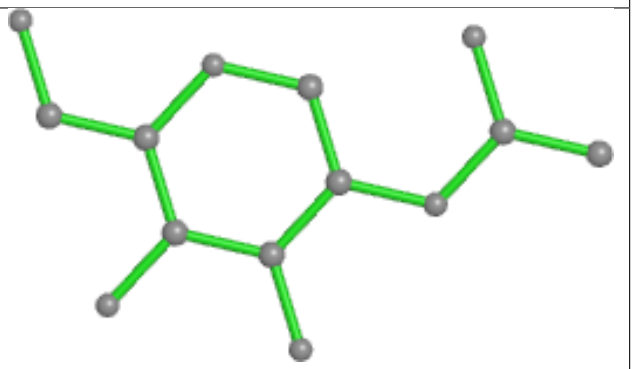
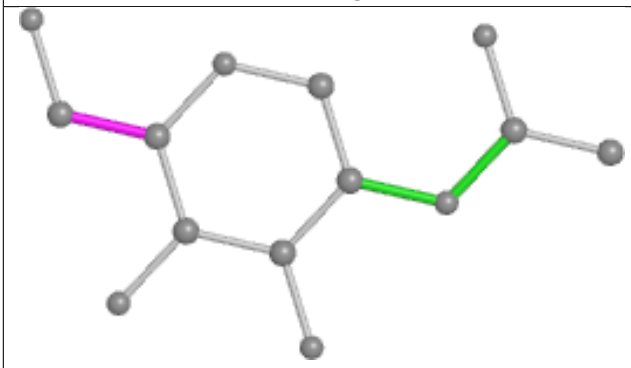
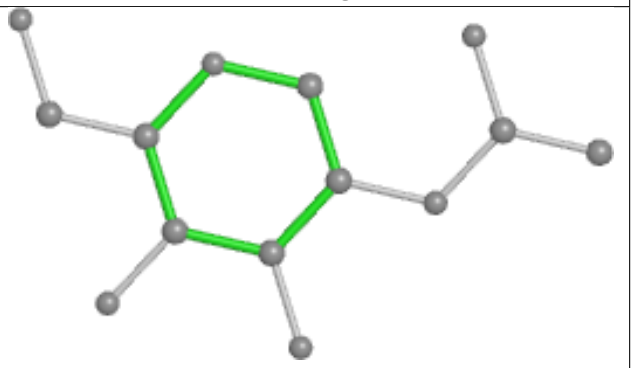


Bond angles

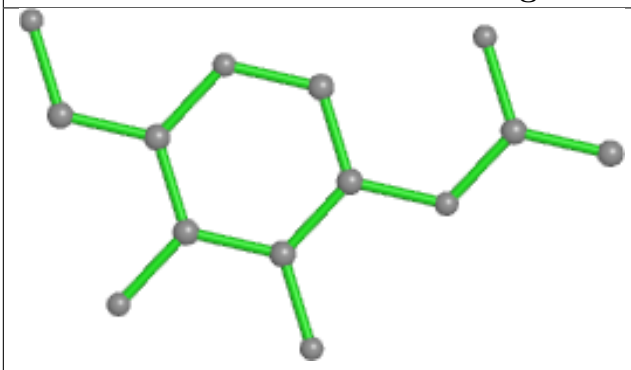


Torsions

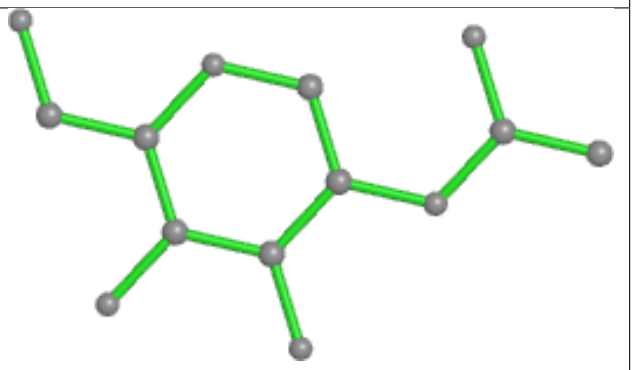


Rings

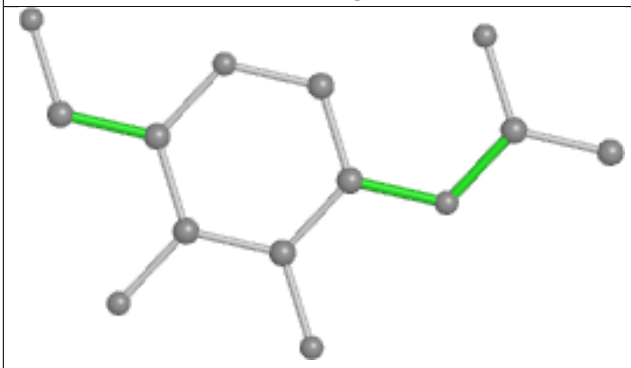
Ligand NAG D 501



Bond lengths



Bond angles



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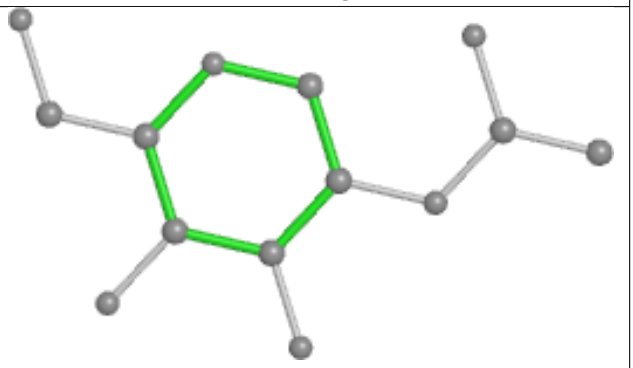
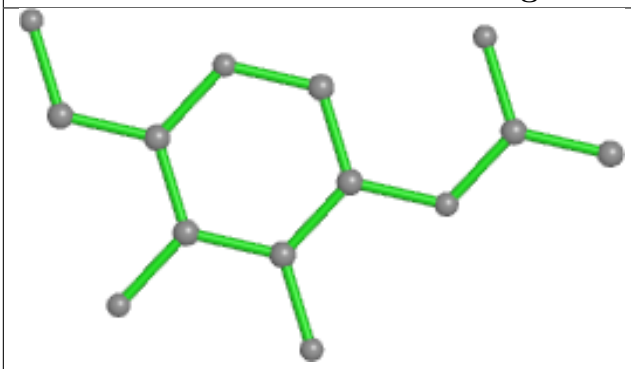
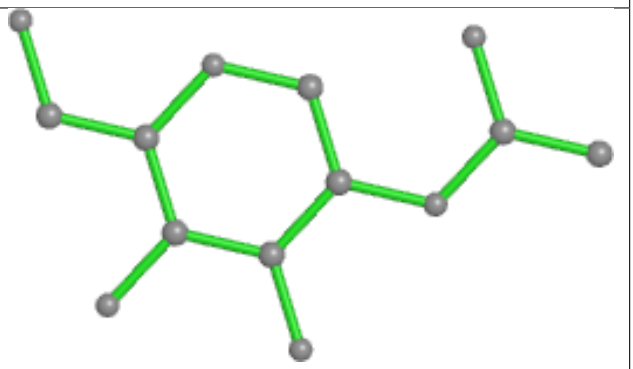


Rings

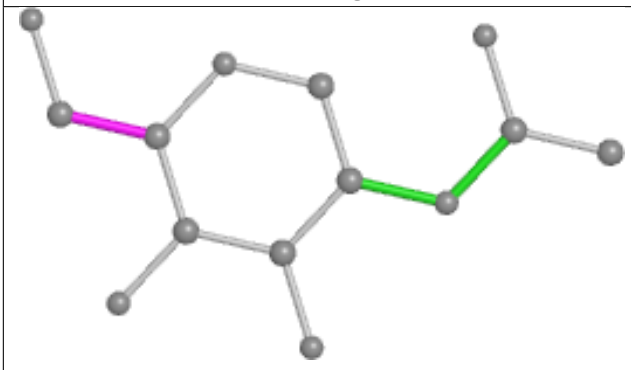
Ligand NAG B 502



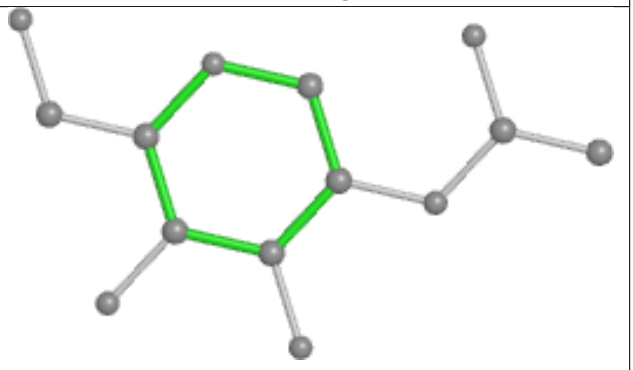
Bond lengths



Bond angles

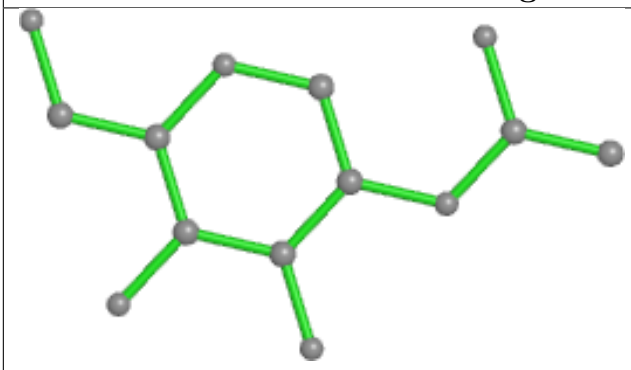


Torsions

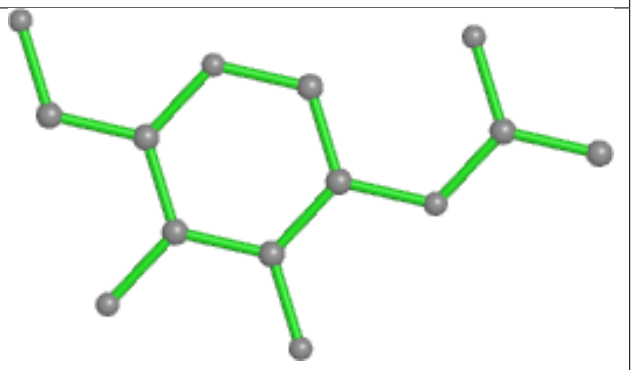


Rings

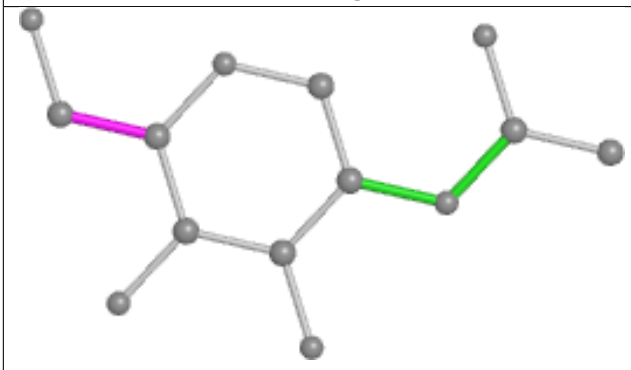
Ligand NAG K 502



Bond lengths



Bond angles



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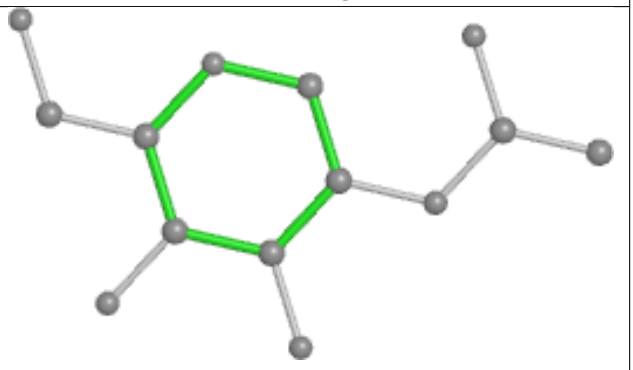
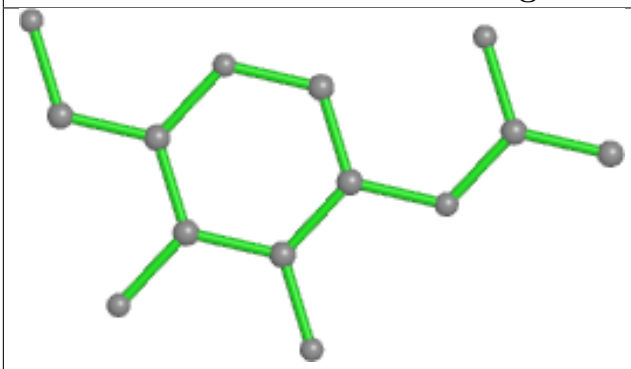
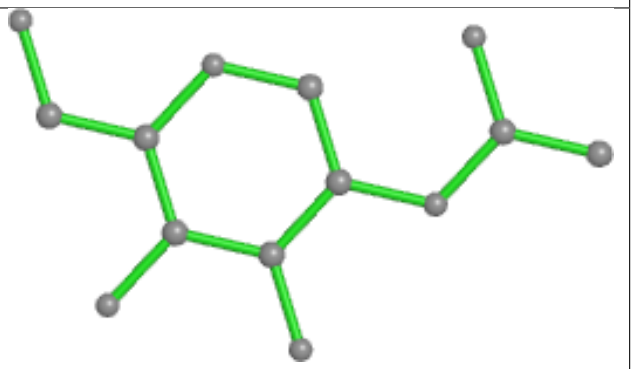
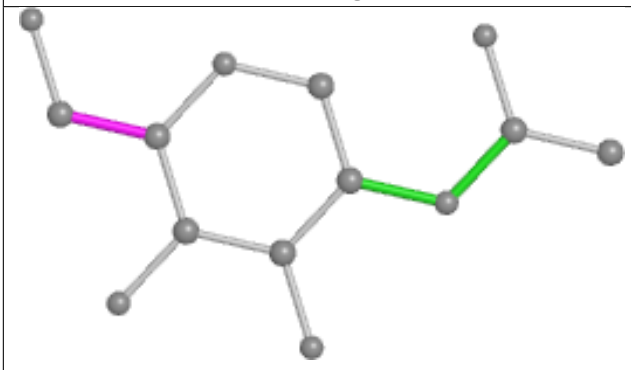
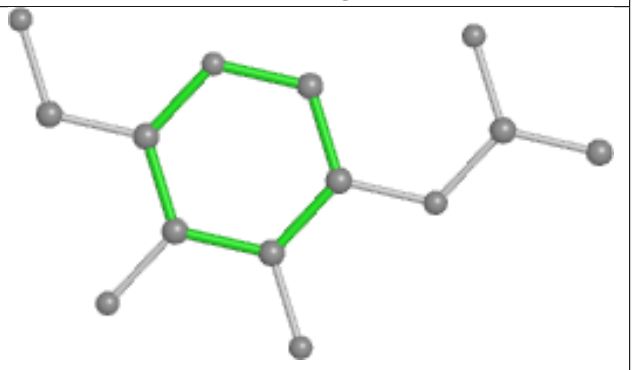
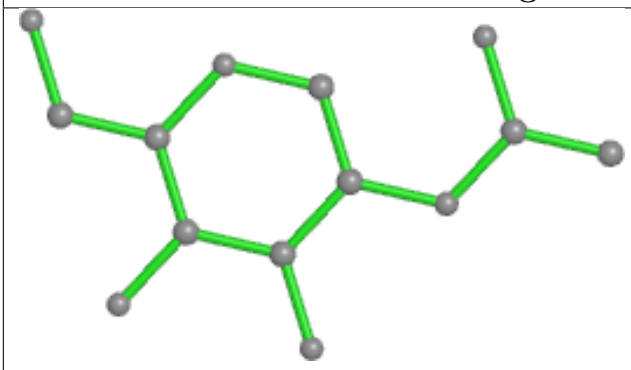
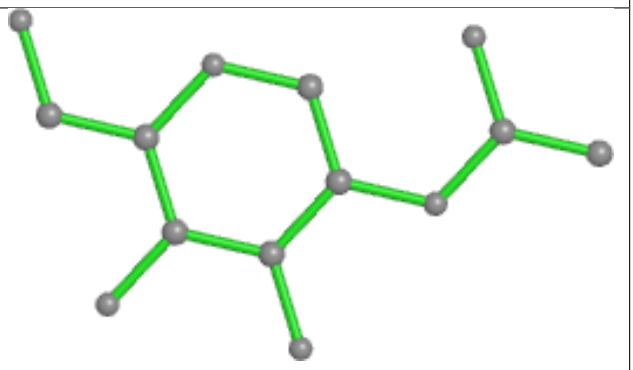
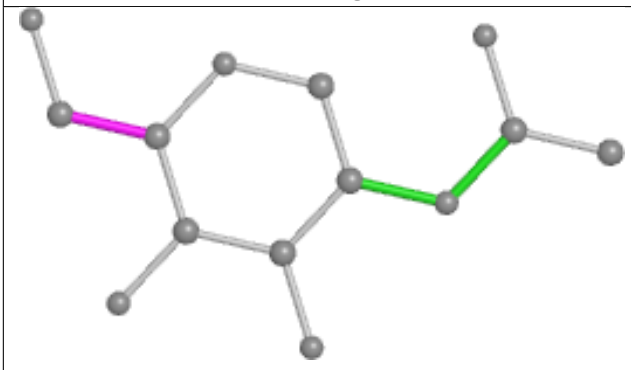
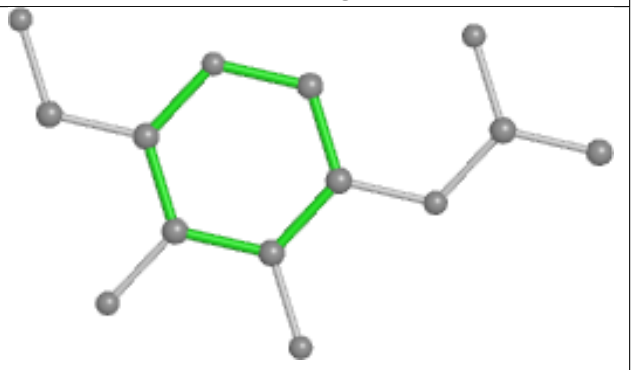


Rings

Ligand NAG G 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NAG K 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	N	1
5	R	1
5	P	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	109:LEU	C	110:GLN	N	3.86
1	R	109:LEU	C	110:GLN	N	3.83
1	P	109:LEU	C	110:GLN	N	3.41

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25103. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

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

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.