



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 07:50 PM UTC

PDB ID : 7SFW / pdb_00007sfw
EMDB ID : EMD-25104
Title : CryoEM structure of Venezuelan Equine Encephalitis virus (VEEV) TC-83 strain VLP in complex with Fab hVEEV-63 (focus refine of the asymmetric unit)
Authors : Binshtein, E.; Crowe, J.E.
Deposited on : 2021-10-04
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

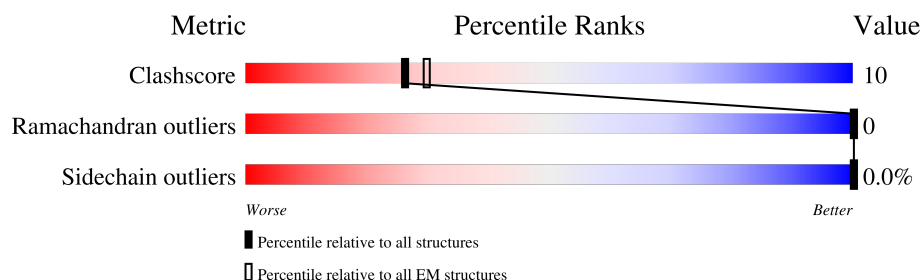
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.



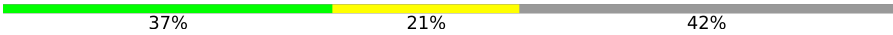
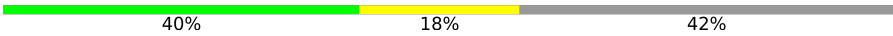
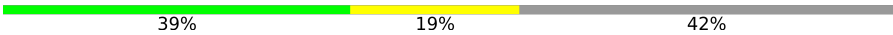
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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

Mol	Chain	Length	Quality of chain
1	A	442	82% 18%
1	D	442	79% 20%
1	G	442	79% 20%
1	J	442	83% 16%
2	B	423	74% 25% .
2	E	423	76% 22% .
2	H	423	77% 22% .
2	K	423	80% 19% .
3	C	275	40% 18% 42%

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Mol	Chain	Length	Quality of chain
3	F	275	
3	I	275	
3	L	275	
4	M	122	
4	O	122	
4	Q	122	
4	S	122	
5	N	107	
5	P	107	
5	R	107	
5	T	107	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 38620 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		

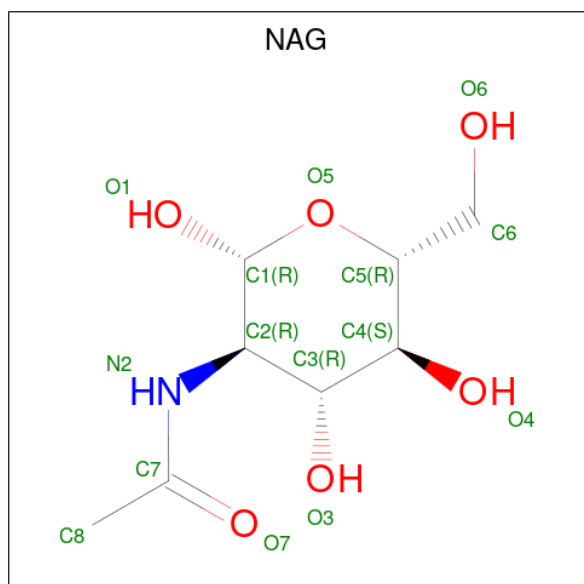
- Molecule 4 is a protein called hVEEV-63 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	122	Total	C	N	O	S	0	0
			941	590	161	185	5		
4	O	122	Total	C	N	O	S	0	0
			941	590	161	185	5		
4	Q	122	Total	C	N	O	S	0	0
			941	590	161	185	5		
4	S	122	Total	C	N	O	S	0	0
			941	590	161	185	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	107	Total	C	N	O	S	0	0
			809	507	130	170	2		
5	P	107	Total	C	N	O	S	0	0
			809	507	130	170	2		
5	R	107	Total	C	N	O	S	0	0
			809	507	130	170	2		
5	T	107	Total	C	N	O	S	0	0
			809	507	130	170	2		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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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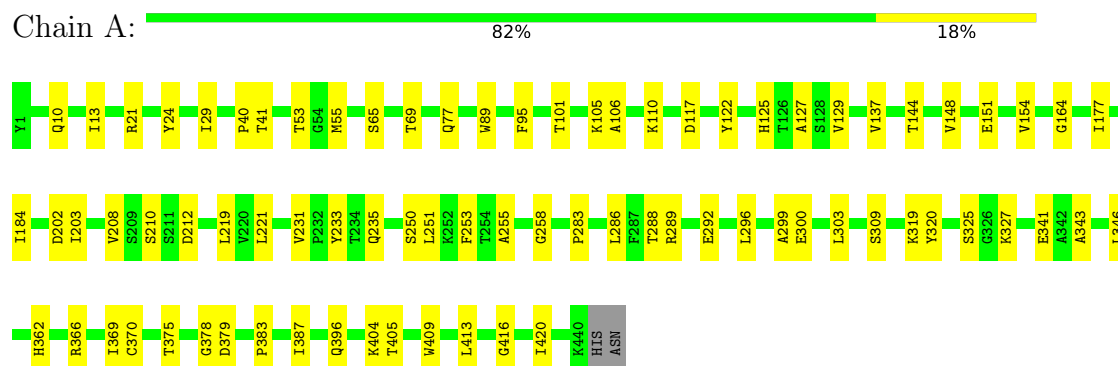
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Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total 14	C 8	N 1	O 5	0
6	B	1	Total 14	C 8	N 1	O 5	0
6	D	1	Total 14	C 8	N 1	O 5	0
6	E	1	Total 14	C 8	N 1	O 5	0
6	E	1	Total 14	C 8	N 1	O 5	0
6	G	1	Total 14	C 8	N 1	O 5	0
6	H	1	Total 14	C 8	N 1	O 5	0
6	H	1	Total 14	C 8	N 1	O 5	0
6	J	1	Total 14	C 8	N 1	O 5	0
6	K	1	Total 14	C 8	N 1	O 5	0
6	K	1	Total 14	C 8	N 1	O 5	0

3 Residue-property plots

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



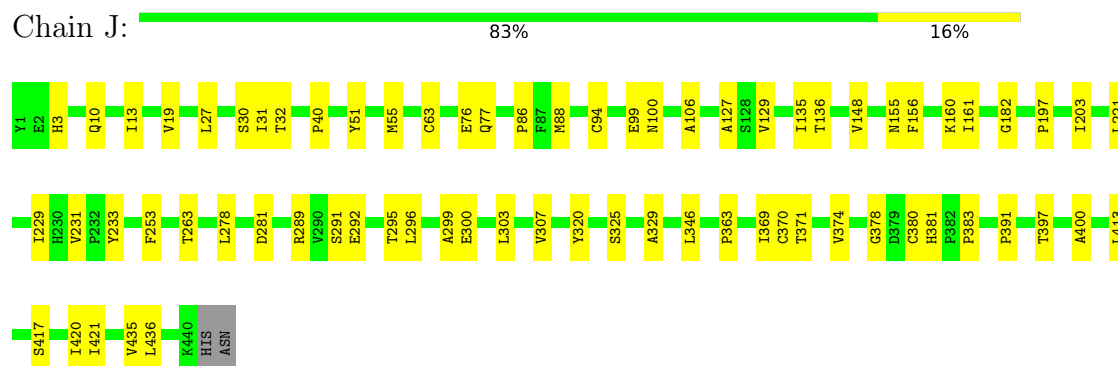
• Molecule 1: Spike glycoprotein E1



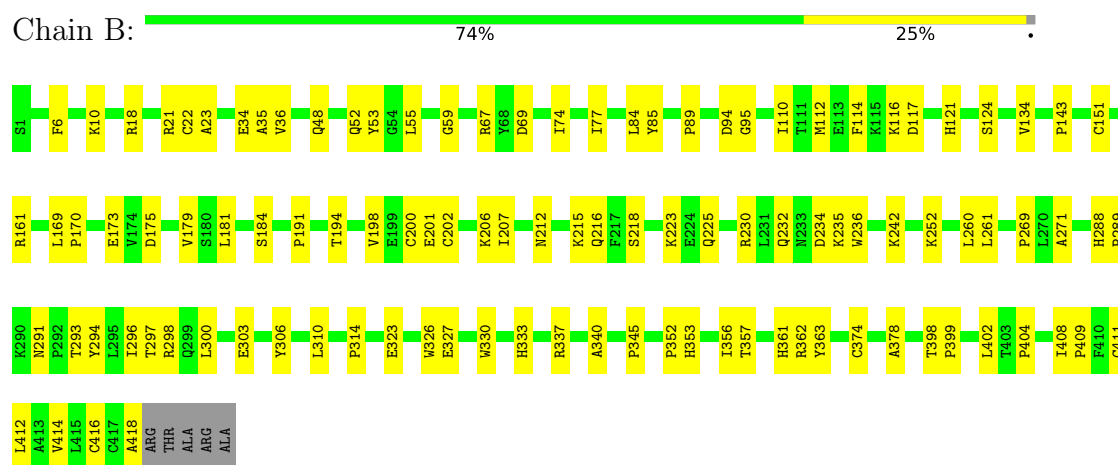
• Molecule 1: Spike glycoprotein E1



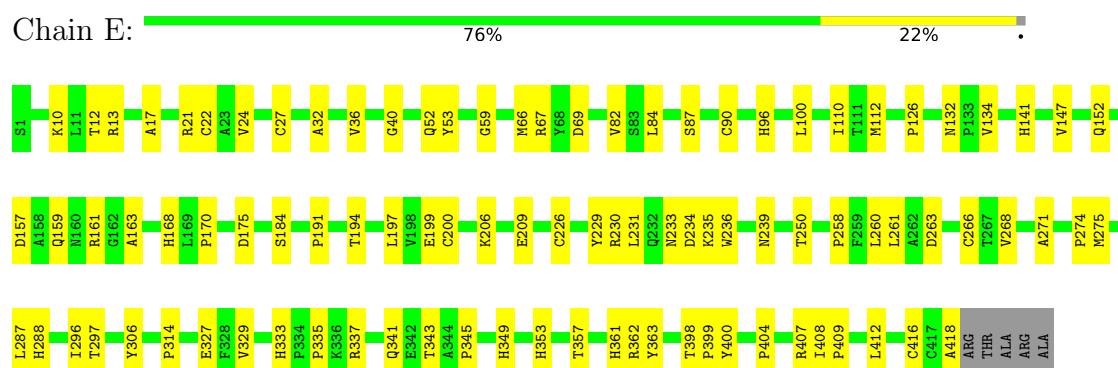
- Molecule 1: Spike glycoprotein E1



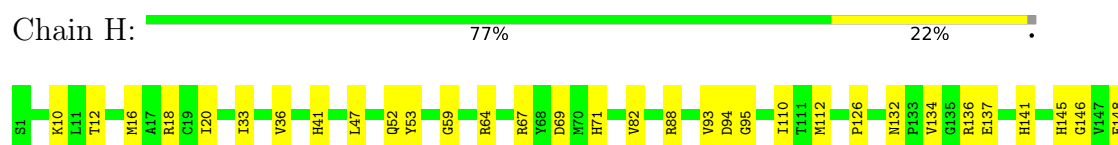
- Molecule 2: Spike glycoprotein E2



- Molecule 2: Spike glycoprotein E2



- Molecule 2: Spike glycoprotein E2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	405000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	0.15	0/3441	0.32	0/4705
1	D	0.16	0/3441	0.33	0/4705
1	G	0.14	0/3441	0.32	0/4705
1	J	0.16	0/3441	0.35	0/4705
2	B	0.16	0/3355	0.38	0/4564
2	E	0.17	0/3355	0.36	0/4564
2	H	0.17	0/3355	0.36	0/4564
2	K	0.17	0/3355	0.35	0/4564
3	C	0.13	0/1276	0.37	0/1720
3	F	0.13	0/1276	0.37	0/1720
3	I	0.13	0/1276	0.34	0/1720
3	L	0.12	0/1276	0.35	0/1720
4	M	0.12	0/961	0.35	0/1301
4	O	0.11	0/961	0.31	0/1301
4	Q	0.11	0/961	0.29	0/1301
4	S	0.11	0/961	0.33	0/1301
5	N	0.11	0/828	0.30	0/1132
5	P	0.11	0/828	0.32	0/1132
5	R	0.13	0/828	0.31	0/1132
5	T	0.11	0/828	0.30	0/1132
All	All	0.15	0/39444	0.34	0/53688

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	59	0
1	D	3351	0	3258	59	0
1	G	3351	0	3258	59	0
1	J	3351	0	3258	48	0
2	B	3264	0	3198	74	0
2	E	3264	0	3199	68	0
2	H	3264	0	3198	65	0
2	K	3264	0	3198	56	0
3	C	1248	0	1238	31	0
3	F	1248	0	1238	40	0
3	I	1248	0	1238	32	0
3	L	1248	0	1238	31	0
4	M	941	0	907	37	0
4	O	941	0	907	44	0
4	Q	941	0	907	29	0
4	S	941	0	907	28	0
5	N	809	0	767	27	0
5	P	809	0	767	27	0
5	R	809	0	767	11	0
5	T	809	0	767	18	0
6	A	14	0	13	0	0
6	B	28	0	26	1	0
6	D	14	0	13	0	0
6	E	28	0	26	0	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	38620	0	37629	771	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 (771) 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:G:299:ALA:HA	1:G:319:LYS:O	1.65	0.97
5:T:17:THR:HA	5:T:75:ILE:O	1.65	0.96
2:E:200:CYS:HA	2:E:226:CYS:HB2	1.52	0.92
1:J:325:SER:HA	1:J:346:LEU:O	1.69	0.92
2:H:16:MET:HE1	2:H:71:HIS:H	1.36	0.87
1:A:299:ALA:HA	1:A:319:LYS:O	1.76	0.83
4:S:100:GLN:HB2	4:S:111:TYR:HB2	1.60	0.83
2:E:53:TYR:HE1	2:E:66:MET:HG3	1.44	0.83
2:H:200:CYS:HA	2:H:226:CYS:HB2	1.62	0.81
5:T:34:TRP:HB2	5:T:47:ILE:HB	1.63	0.81
2:E:184:SER:O	4:O:31:ASN:ND2	2.13	0.81
5:P:34:TRP:HB2	5:P:47:ILE:HB	1.62	0.80
5:R:34:TRP:HB2	5:R:47:ILE:HB	1.64	0.79
5:N:34:TRP:HB2	5:N:47:ILE:HB	1.65	0.78
4:M:94:TYR:O	4:M:115:GLY:HA2	1.83	0.78
2:H:167:MET:HE2	2:H:236:TRP:HE3	1.49	0.77
4:Q:106:ASN:OD1	4:Q:107:GLY:N	2.18	0.76
4:S:44:ARG:NH2	5:T:3:GLU:OE2	2.18	0.76
3:L:207:VAL:HG21	3:L:230:ILE:HD11	1.67	0.75
2:E:400:TYR:HB3	2:E:408:ILE:HG22	1.68	0.74
2:E:327:GLU:HG3	2:E:337:ARG:HG2	1.68	0.74
1:A:296:LEU:HD11	1:A:320:TYR:HB2	1.70	0.73
5:T:32:VAL:HG21	5:T:71:VAL:HG21	1.70	0.73
2:E:152:GLN:NE2	2:E:263:ASP:OD1	2.22	0.71
3:I:151:MET:HE1	3:I:171:SER:HA	1.72	0.71
3:F:151:MET:HG2	3:F:174:ASP:HA	1.73	0.71
1:D:295:THR:HA	1:D:371:THR:HG21	1.71	0.71
2:H:276:ILE:HG12	2:H:285:LEU:HD23	1.73	0.71
4:O:70:VAL:HG12	4:O:81:MET:HG2	1.73	0.71
4:M:91:THR:HG23	4:M:119:THR:HA	1.72	0.70
1:J:160:LYS:HB2	1:J:281:ASP:HB3	1.73	0.70
3:I:145:GLY:H	3:I:188:THR:HG21	1.57	0.70
3:L:192:THR:HB	3:L:238:VAL:HG12	1.74	0.70
2:B:52:GLN:OE1	2:B:67:ARG:NH2	2.25	0.69
4:O:94:TYR:O	4:O:115:GLY:HA2	1.92	0.69
4:M:44:ARG:NH2	5:N:100:PHE:O	2.25	0.69
1:G:80:VAL:HG22	1:G:103:VAL:HG22	1.73	0.69
5:R:45:LEU:HD21	5:R:48:TYR:HB3	1.75	0.69
4:S:6:GLN:HG2	4:S:22:CYS:HB3	1.75	0.69
1:D:80:VAL:HG22	1:D:103:VAL:HG22	1.75	0.68
2:K:115:LYS:HE3	2:K:120:ARG:HB2	1.75	0.68
4:O:6:GLN:NE2	4:O:96:CYS:SG	2.65	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:400:TYR:HB3	2:H:408:ILE:HG22	1.76	0.68
2:H:161:ARG:HH22	2:H:262:ALA:HB2	1.58	0.68
5:P:85:ASP:OD1	5:P:105:LYS:NZ	2.25	0.68
4:O:99:LEU:HA	4:O:110:ASP:H	1.59	0.67
2:H:202:CYS:SG	2:H:206:LYS:NZ	2.65	0.67
2:B:35:ALA:HB3	2:B:48:GLN:HB3	1.75	0.67
3:C:190:LYS:HE3	3:C:190:LYS:HA	1.77	0.67
3:C:138:GLY:HA3	3:C:153:VAL:HG11	1.77	0.66
5:P:17:THR:HA	5:P:75:ILE:O	1.94	0.66
1:A:53:THR:OG1	1:A:235:GLN:NE2	2.28	0.66
5:P:45:LEU:HD21	5:P:48:TYR:HB3	1.78	0.66
5:N:58:PRO:HG2	5:N:62:PHE:HE2	1.60	0.66
4:O:35:HIS:HB2	4:O:97:ALA:HB3	1.78	0.66
2:E:175:ASP:OD2	2:E:230:ARG:NH2	2.26	0.66
4:M:33:ILE:HG22	4:M:52:ASN:HA	1.78	0.66
4:M:52:ASN:HB3	4:M:56:GLY:H	1.61	0.66
5:N:32:VAL:HG21	5:N:71:VAL:HG21	1.78	0.65
1:J:296:LEU:HD13	1:J:369:ILE:HG21	1.79	0.65
1:G:218:ASN:ND2	2:K:275:MET:SD	2.69	0.65
2:K:184:SER:O	4:S:31:ASN:ND2	2.29	0.65
5:N:18:ALA:HB3	5:N:75:ILE:HB	1.78	0.65
2:B:21:ARG:NH1	2:B:22:CYS:O	2.30	0.65
1:D:96:CYS:O	1:D:100:ASN:ND2	2.30	0.65
1:J:32:THR:HG21	6:J:501:NAG:H82	1.77	0.65
4:M:67:ARG:HE	4:M:83:LEU:HD11	1.61	0.65
5:P:30:GLN:NE2	5:P:95:ASN:OD1	2.30	0.65
3:F:117:ARG:HB3	3:F:120:MET:HE1	1.79	0.64
3:F:193:HIS:O	3:F:195:LYS:NZ	2.27	0.64
1:A:110:LYS:NZ	1:A:208:VAL:O	2.31	0.64
5:N:80:ALA:HA	5:N:108:VAL:HG11	1.79	0.64
2:B:179:VAL:O	2:B:223:LYS:NZ	2.27	0.64
3:I:149:ARG:NH1	3:I:176:GLU:OE2	2.30	0.64
5:R:17:THR:HA	5:R:75:ILE:O	1.98	0.64
1:J:296:LEU:HD21	1:J:299:ALA:HB2	1.80	0.64
4:Q:91:THR:HG23	4:Q:118:VAL:HB	1.78	0.64
2:B:218:SER:H	4:M:105:GLY:HA2	1.62	0.63
4:M:40:ALA:HB3	4:M:43:GLN:HE22	1.61	0.63
4:M:22:CYS:HB2	4:M:79:ALA:HB3	1.79	0.63
2:B:36:VAL:HG21	2:B:110:ILE:HG21	1.80	0.63
4:M:51:ILE:HD13	4:M:70:VAL:HG11	1.80	0.63
1:D:160:LYS:HB2	1:D:281:ASP:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:288:HIS:HD2	2:K:314:PRO:HB3	1.63	0.63
3:C:266:LYS:NZ	3:C:268:THR:OG1	2.32	0.62
4:M:100:GLN:H	4:M:110:ASP:HB2	1.64	0.62
1:A:253:PHE:HB3	2:B:296:ILE:HG21	1.82	0.62
3:L:244:GLY:HA2	3:L:253:LEU:HA	1.81	0.62
2:H:212:ASN:ND2	6:H:501:NAG:O4	2.32	0.62
1:J:155:ASN:HB2	1:J:160:LYS:HZ3	1.64	0.62
4:Q:40:ALA:HB3	4:Q:43:GLN:HB2	1.82	0.62
2:K:84:LEU:HD12	2:K:110:ILE:HD11	1.81	0.62
1:A:69:THR:O	1:A:105:LYS:NZ	2.33	0.62
1:D:358:THR:OG1	1:D:360:ASN:OD1	2.17	0.62
1:G:129:VAL:HG21	1:G:166:LEU:HD22	1.82	0.62
1:G:369:ILE:HG22	1:G:370:CYS:H	1.63	0.62
3:F:244:GLY:HA2	3:F:253:LEU:HA	1.80	0.62
2:E:53:TYR:HE2	2:E:100:LEU:HB2	1.65	0.61
3:C:131:MET:HE1	3:C:136:ILE:HD13	1.83	0.61
1:A:144:THR:HG21	1:A:154:VAL:HG21	1.83	0.61
4:Q:48:MET:HE2	4:Q:68:ILE:HD13	1.82	0.61
3:C:167:THR:HG22	3:C:178:ALA:HB2	1.83	0.61
2:K:402:LEU:HD23	3:L:264:THR:HG21	1.83	0.61
2:B:297:THR:O	2:B:306:TYR:HA	2.00	0.61
1:D:296:LEU:HD21	1:D:299:ALA:HB2	1.83	0.61
4:O:61:SER:O	4:O:65:GLN:NE2	2.34	0.61
3:L:190:LYS:HE2	3:L:236:ARG:HB3	1.82	0.60
2:E:287:LEU:O	2:E:314:PRO:HA	2.01	0.60
3:F:243:GLY:O	3:F:254:SER:N	2.35	0.60
1:G:251:LEU:HB3	1:G:261:ILE:HG13	1.81	0.60
2:K:161:ARG:HB2	2:K:260:LEU:HD12	1.83	0.60
5:T:30:GLN:NE2	5:T:92:ASP:O	2.34	0.60
1:A:24:TYR:CZ	1:G:384:LYS:HG3	2.37	0.60
1:D:325:SER:HA	1:D:346:LEU:O	2.00	0.60
2:H:36:VAL:HG21	2:H:110:ILE:HG21	1.83	0.60
3:C:241:VAL:HG11	3:C:253:LEU:HD23	1.84	0.60
4:S:40:ALA:HB3	4:S:43:GLN:HB2	1.83	0.60
5:T:75:ILE:HD11	5:T:86:TYR:HE1	1.67	0.60
3:F:232:ASP:OD2	3:F:236:ARG:NH1	2.35	0.60
5:R:32:VAL:HG11	5:R:71:VAL:HG21	1.84	0.60
2:K:185:SER:OG	2:K:216:GLN:NE2	2.30	0.60
3:C:157:ILE:HD12	3:C:157:ILE:H	1.66	0.60
3:I:152:HIS:CD2	3:I:275:TRP:HE1	2.20	0.59
2:K:185:SER:HB2	2:K:218:SER:HA	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:69:SER:OG	4:Q:82:GLU:OE1	2.20	0.59
1:G:32:THR:HG21	6:G:501:NAG:H82	1.84	0.59
1:G:59:ALA:O	1:G:66:GLN:NE2	2.35	0.59
3:I:197:GLN:HE22	3:I:210:GLU:HG3	1.68	0.59
4:Q:18:VAL:HG12	4:Q:86:LEU:HD11	1.83	0.59
1:D:283:PRO:HG2	1:D:286:LEU:HD13	1.82	0.59
3:F:266:LYS:NZ	3:F:268:THR:OG1	2.35	0.59
4:S:12:LYS:NZ	4:S:13:LYS:O	2.35	0.59
2:K:186:VAL:HG23	2:K:217:PHE:HB2	1.85	0.59
4:O:44:ARG:HE	5:P:102:THR:HA	1.68	0.59
3:L:257:MET:HG3	3:L:265:VAL:HG13	1.84	0.59
2:H:94:ASP:OD1	2:H:95:GLY:N	2.35	0.59
1:J:291:SER:OG	1:J:292:GLU:OE1	2.19	0.59
1:J:295:THR:HA	1:J:371:THR:HG21	1.85	0.59
1:G:29:ILE:HG12	1:G:137:VAL:HG23	1.84	0.59
1:D:336:THR:OG1	1:D:360:ASN:ND2	2.35	0.58
5:P:92:ASP:OD1	5:P:93:SER:N	2.35	0.58
4:S:37:VAL:HG23	4:S:47:TRP:HA	1.85	0.58
5:T:45:LEU:HD21	5:T:48:TYR:HB3	1.84	0.58
5:N:24:GLY:O	5:N:69:THR:OG1	2.20	0.58
4:Q:37:VAL:HG23	4:Q:47:TRP:HA	1.86	0.58
4:O:40:ALA:HB3	4:O:43:GLN:HB2	1.85	0.58
2:B:116:LYS:HG3	2:B:117:ASP:H	1.67	0.58
3:C:149:ARG:NH2	3:C:153:VAL:O	2.37	0.58
3:I:200:TYR:HD1	3:I:232:ASP:HA	1.69	0.58
4:O:19:LYS:HE3	4:O:80:TYR:HB3	1.85	0.58
1:A:288:THR:OG1	1:A:292:GLU:OE1	2.21	0.58
1:A:405:THR:HG23	1:A:409:TRP:CZ3	2.38	0.58
3:L:241:VAL:HG12	3:L:255:VAL:HG12	1.85	0.58
1:A:325:SER:HA	1:A:346:LEU:O	2.04	0.58
4:O:51:ILE:HG13	4:O:58:THR:HG22	1.85	0.58
2:E:297:THR:O	2:E:306:TYR:HA	2.04	0.58
1:J:77:GLN:HB2	1:J:221:LEU:HD13	1.86	0.57
5:P:17:THR:HG22	5:P:76:SER:HA	1.86	0.57
1:J:30:SER:HB3	1:J:136:THR:HB	1.87	0.57
5:N:14:PRO:HD3	5:N:109:LEU:HB2	1.85	0.57
4:Q:35:HIS:HB2	4:Q:97:ALA:HB3	1.86	0.57
4:O:20:VAL:HG23	4:O:81:MET:HB3	1.85	0.57
4:Q:97:ALA:HB1	4:Q:109:LEU:HB3	1.85	0.57
2:H:232:GLN:HG2	2:H:233:ASN:H	1.68	0.57
2:H:64:ARG:NH2	2:H:93:VAL:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:275:MET:HE1	2:E:288:HIS:CD2	2.40	0.57
3:L:261:LYS:HG3	3:L:263:VAL:HG13	1.87	0.57
4:O:13:LYS:HD2	4:O:14:PRO:HD2	1.87	0.57
3:F:214:PHE:HE2	3:F:230:ILE:HG21	1.69	0.57
1:G:312:PHE:HA	1:G:357:SER:HB2	1.87	0.57
2:B:161:ARG:HB2	2:B:260:LEU:HD12	1.86	0.56
4:O:39:GLN:HB2	4:O:45:LEU:HD23	1.88	0.56
2:B:191:PRO:HG2	2:B:194:THR:HB	1.87	0.56
1:G:59:ALA:HB3	1:G:103:VAL:HB	1.88	0.56
4:M:33:ILE:HD11	4:M:106:ASN:HD22	1.70	0.56
3:F:122:LEU:HD11	3:F:201:SER:HB3	1.86	0.56
1:G:104:SER:HB3	1:G:231:VAL:HG13	1.87	0.56
1:G:21:ARG:NH2	1:G:25:ALA:O	2.38	0.56
1:J:296:LEU:HD12	1:J:346:LEU:HD21	1.88	0.56
4:O:64:PHE:HD2	4:O:68:ILE:HB	1.70	0.56
1:G:53:THR:OG1	1:G:235:GLN:OE1	2.24	0.56
3:C:161:VAL:HG11	3:C:184:MET:HE1	1.88	0.55
1:J:417:SER:O	1:J:421:ILE:HD12	2.06	0.55
1:G:94:CYS:O	2:H:227:ARG:NH1	2.39	0.55
2:K:22:CYS:SG	2:K:29:SER:OG	2.64	0.55
2:K:411:CYS:HA	2:K:414:VAL:HG22	1.88	0.55
4:M:40:ALA:HB3	4:M:43:GLN:NE2	2.20	0.55
4:O:91:THR:HA	4:O:118:VAL:O	2.06	0.55
1:A:95:PHE:HD2	2:B:201:GLU:HG2	1.71	0.55
1:J:182:GLY:HA2	1:J:263:THR:HG21	1.88	0.55
3:L:119:VAL:O	3:L:122:LEU:HD13	2.07	0.55
1:A:210:SER:OG	1:A:212:ASP:OD1	2.20	0.55
1:D:10:GLN:HG2	1:D:13:ILE:HD12	1.87	0.55
3:F:167:THR:HG22	3:F:178:ALA:HB2	1.89	0.55
3:C:214:PHE:HD2	3:C:255:VAL:HG11	1.72	0.55
2:B:18:ARG:H	2:B:242:LYS:HG2	1.71	0.55
2:B:327:GLU:HG3	2:B:337:ARG:HG2	1.89	0.55
2:H:232:GLN:HG2	2:H:233:ASN:N	2.22	0.55
4:M:37:VAL:HG21	4:M:45:LEU:HD23	1.89	0.55
2:K:41:HIS:CD2	2:K:134:VAL:HG22	2.42	0.55
3:I:139:TYR:HD2	3:I:228:ARG:HG2	1.71	0.54
3:L:117:ARG:HB3	3:L:120:MET:HB2	1.89	0.54
1:A:327:LYS:HD2	1:A:343:ALA:HB1	1.89	0.54
1:G:222:GLN:HB2	1:G:232:PRO:HB2	1.87	0.54
4:O:99:LEU:HD11	4:O:101:MET:HB2	1.88	0.54
1:D:364:GLU:HG2	1:D:377:LYS:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:41:HIS:CD2	2:H:134:VAL:HG22	2.43	0.54
4:M:47:TRP:HZ2	4:M:50:TRP:HD1	1.54	0.54
1:D:359:ALA:HB2	1:D:394:HIS:CD2	2.43	0.54
2:E:141:HIS:HD1	2:K:126:PRO:HG3	1.73	0.54
2:B:215:LYS:HE3	5:N:49:LYS:HZ2	1.73	0.54
2:B:291:ASN:O	2:B:293:THR:OG1	2.26	0.54
1:G:21:ARG:HB2	1:G:24:TYR:HB2	1.90	0.54
2:H:329:VAL:HG22	2:H:335:PRO:HB3	1.90	0.54
3:C:195:LYS:NZ	3:C:258:TRP:O	2.40	0.54
1:D:40:PRO:HA	1:D:127:ALA:HA	1.89	0.54
2:B:404:PRO:HB3	3:C:144:GLY:HA3	1.89	0.54
3:I:193:HIS:HB2	3:I:260:GLU:HA	1.90	0.54
4:O:97:ALA:HB1	4:O:109:LEU:HD13	1.90	0.54
1:A:413:LEU:HD21	2:B:378:ALA:HB2	1.90	0.54
1:G:253:PHE:HB3	2:H:296:ILE:HG21	1.89	0.54
1:A:369:ILE:HG22	1:A:370:CYS:H	1.71	0.54
2:B:114:PHE:HD2	2:B:121:HIS:HB2	1.73	0.54
1:D:77:GLN:NE2	1:D:219:LEU:O	2.41	0.54
3:I:185:ARG:HB2	3:I:185:ARG:NH1	2.23	0.54
3:I:241:VAL:HG21	3:I:253:LEU:HD22	1.89	0.54
2:K:309:GLU:OE2	2:K:317:ARG:NH2	2.35	0.54
5:R:92:ASP:OD2	5:R:95:ASN:N	2.41	0.54
1:D:253:PHE:HB3	2:E:296:ILE:HG21	1.90	0.53
2:H:344:ALA:HB2	2:H:362:ARG:HG3	1.89	0.53
3:I:142:VAL:HG22	3:I:188:THR:HG23	1.90	0.53
4:M:36:TRP:CZ3	4:M:70:VAL:HG22	2.43	0.53
5:T:24:GLY:O	5:T:69:THR:OG1	2.24	0.53
2:B:94:ASP:OD2	2:B:95:GLY:N	2.40	0.53
3:F:259:ASN:OD1	3:F:260:GLU:N	2.40	0.53
2:H:212:ASN:N	5:R:31:TYR:OH	2.35	0.53
4:O:44:ARG:NH2	5:P:3:GLU:OE2	2.41	0.53
1:J:156:PHE:HE1	1:J:161:ILE:HD11	1.73	0.53
3:L:195:LYS:NZ	3:L:258:TRP:O	2.29	0.53
3:L:243:GLY:O	3:L:254:SER:N	2.41	0.53
1:D:385:ASP:OD2	2:E:341:GLN:NE2	2.42	0.53
3:F:118:MET:SD	3:F:201:SER:OG	2.58	0.53
2:K:327:GLU:HG3	2:K:337:ARG:HG2	1.91	0.53
5:N:34:TRP:CG	5:N:73:LEU:HD12	2.43	0.53
2:B:412:LEU:HD12	2:B:416:CYS:HA	1.91	0.53
5:R:20:ILE:HG23	5:R:104:THR:HG21	1.90	0.53
4:S:47:TRP:HZ2	4:S:50:TRP:HD1	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:53:TYR:CE1	2:E:66:MET:HG3	2.34	0.53
1:D:362:HIS:CD2	1:D:404:LYS:HG3	2.43	0.53
2:E:345:PRO:HG2	2:E:361:HIS:ND1	2.24	0.53
1:J:135:ILE:HD13	1:J:161:ILE:HD13	1.91	0.53
2:K:136:ARG:HB3	2:K:294:TYR:HB2	1.90	0.53
5:T:96:THR:OG1	5:T:97:GLU:OE1	2.27	0.52
2:H:309:GLU:OE2	2:H:317:ARG:NH2	2.37	0.52
2:H:41:HIS:HA	2:H:132:ASN:HB2	1.91	0.52
4:S:35:HIS:HD2	4:S:47:TRP:HE1	1.55	0.52
5:P:36:GLN:HE21	5:P:44:VAL:HB	1.74	0.52
1:A:55:MET:HE1	1:A:233:TYR:CE1	2.45	0.52
1:A:117:ASP:HB2	2:B:261:LEU:HD23	1.92	0.52
2:E:170:PRO:O	2:E:233:ASN:ND2	2.43	0.52
3:I:202:TRP:CD1	3:I:203:HIS:H	2.28	0.52
2:K:232:GLN:HG2	2:K:233:ASN:H	1.74	0.52
3:I:192:THR:HG22	3:I:194:GLU:H	1.74	0.52
2:K:365:MET:HA	2:K:368:ILE:HG22	1.91	0.52
1:A:250:SER:OG	1:A:251:LEU:N	2.40	0.52
2:H:136:ARG:HB3	2:H:294:TYR:HB2	1.92	0.52
2:K:199:GLU:HA	2:K:206:LYS:O	2.09	0.52
4:Q:23:LYS:HG3	4:Q:78:ALA:HB2	1.91	0.52
1:A:283:PRO:HG2	1:A:286:LEU:HD13	1.92	0.52
1:D:53:THR:OG1	1:D:235:GLN:OE1	2.26	0.52
2:H:408:ILE:N	2:H:409:PRO:HD3	2.25	0.52
1:D:110:LYS:NZ	1:D:208:VAL:O	2.43	0.52
3:I:129:PRO:HA	3:I:139:TYR:HD1	1.74	0.52
1:A:296:LEU:HD13	1:A:346:LEU:HD21	1.92	0.52
2:B:69:ASP:HB3	2:B:74:ILE:HD13	1.91	0.52
3:C:245:VAL:HB	3:C:272:CYS:HA	1.92	0.52
3:I:258:TRP:CD1	3:I:264:THR:HG22	2.45	0.52
1:J:55:MET:HE1	1:J:233:TYR:CE1	2.44	0.52
2:H:52:GLN:OE1	2:H:67:ARG:NH2	2.43	0.51
1:A:40:PRO:HA	1:A:127:ALA:HA	1.92	0.51
2:B:6:PHE:O	2:B:10:LYS:HG3	2.10	0.51
2:H:170:PRO:HD3	2:H:236:TRP:HA	1.91	0.51
1:A:258:GLY:HA3	2:B:300:LEU:HD13	1.92	0.51
2:B:181:LEU:HD13	2:B:223:LYS:HG3	1.92	0.51
1:A:95:PHE:CD2	2:B:201:GLU:HG2	2.46	0.51
2:B:22:CYS:SG	2:B:23:ALA:N	2.83	0.51
2:E:329:VAL:HG22	2:E:335:PRO:HB3	1.91	0.51
2:K:287:LEU:HD23	2:K:330:TRP:CZ3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:41:PRO:O	4:O:43:GLN:NE2	2.43	0.51
5:P:24:GLY:O	5:P:69:THR:OG1	2.28	0.51
4:S:17:SER:HA	4:S:83:LEU:O	2.10	0.51
2:E:200:CYS:HB3	2:E:206:LYS:HB2	1.91	0.51
2:H:397:LEU:O	2:H:401:ARG:N	2.44	0.51
1:J:397:THR:HB	1:J:400:ALA:HB2	1.92	0.51
4:O:37:VAL:HG11	4:O:112:TRP:HZ3	1.74	0.51
2:B:55:LEU:HD12	2:B:59:GLY:HA2	1.92	0.51
2:E:157:ASP:OD1	2:E:161:ARG:NH1	2.43	0.51
1:G:327:LYS:HD2	1:G:343:ALA:HB1	1.93	0.51
3:I:222:ALA:H	3:I:225:ASP:HB2	1.76	0.51
3:F:149:ARG:HG3	3:F:176:GLU:HB2	1.92	0.51
2:H:137:GLU:HG2	2:H:293:THR:HG23	1.92	0.51
4:O:67:ARG:HE	4:O:83:LEU:HD11	1.76	0.51
3:F:207:VAL:HG12	3:F:216:VAL:HG12	1.92	0.51
1:J:303:LEU:HD12	1:J:378:GLY:HA3	1.92	0.51
3:L:202:TRP:CD1	3:L:203:HIS:H	2.29	0.51
5:P:37:GLN:HB3	5:P:85:ASP:HB2	1.93	0.51
2:E:191:PRO:HG2	2:E:194:THR:HB	1.92	0.50
4:M:38:ARG:HD3	4:M:94:TYR:CZ	2.46	0.50
4:S:71:THR:HB	4:S:80:TYR:HB2	1.94	0.50
1:G:168:THR:HG22	1:G:170:TRP:H	1.76	0.50
2:H:146:GLY:HA3	2:H:268:VAL:O	2.11	0.50
3:I:149:ARG:HD2	3:I:157:ILE:HD11	1.92	0.50
1:J:51:TYR:HB3	1:J:203:ILE:HD13	1.94	0.50
1:J:63:CYS:H	1:J:100:ASN:HA	1.74	0.50
5:P:77:GLY:O	5:P:79:GLN:NE2	2.43	0.50
3:I:214:PHE:HE2	3:I:230:ILE:HG12	1.77	0.50
1:J:13:ILE:HD11	1:J:391:PRO:HG2	1.92	0.50
2:B:212:ASN:ND2	6:B:501:NAG:O4	2.39	0.50
1:G:244:LYS:HA	1:G:247:LYS:HG3	1.93	0.50
1:G:362:HIS:ND1	1:G:379:ASP:OD1	2.43	0.50
2:K:412:LEU:HD13	2:K:418:ALA:HB3	1.94	0.50
4:Q:12:LYS:NZ	4:Q:13:LYS:O	2.37	0.50
4:Q:32:TYR:OH	4:Q:105:GLY:O	2.21	0.50
1:G:37:LYS:HE3	1:G:267:ARG:HD2	1.94	0.50
1:A:255:ALA:O	2:B:298:ARG:NH1	2.45	0.50
1:A:300:GLU:HG3	1:A:319:LYS:HB3	1.94	0.50
1:G:435:VAL:O	1:G:439:GLN:HG2	2.12	0.50
4:M:36:TRP:HZ2	4:M:79:ALA:HB1	1.76	0.50
2:B:300:LEU:HD23	2:B:326:TRP:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:197:GLN:NE2	3:C:210:GLU:HA	2.27	0.49
4:S:36:TRP:CZ3	4:S:70:VAL:HG22	2.47	0.49
1:D:361:ILE:HG21	2:E:349:HIS:HE1	1.77	0.49
1:G:142:ILE:HD13	1:G:156:PHE:CG	2.46	0.49
4:Q:100:GLN:H	4:Q:110:ASP:HB2	1.77	0.49
2:B:84:LEU:HD23	2:B:84:LEU:H	1.77	0.49
2:B:411:CYS:HA	2:B:414:VAL:HG22	1.94	0.49
4:Q:2:VAL:HG21	4:Q:100:GLN:HA	1.94	0.49
4:O:101:MET:HE2	4:O:103:TYR:HE2	1.77	0.49
1:A:405:THR:O	1:A:409:TRP:HE3	1.96	0.49
2:B:77:ILE:HD13	2:B:114:PHE:HE1	1.76	0.49
1:D:84:VAL:HG21	1:D:102:GLN:HB2	1.94	0.49
1:D:392:GLN:NE2	1:D:396:GLN:OE1	2.38	0.49
2:E:407:ARG:HG2	2:E:409:PRO:HD3	1.94	0.49
1:D:224:PRO:HA	1:D:232:PRO:HG2	1.95	0.49
2:E:141:HIS:ND1	2:K:126:PRO:HG3	2.28	0.49
2:H:297:THR:O	2:H:306:TYR:HA	2.13	0.49
1:J:40:PRO:HA	1:J:127:ALA:HA	1.94	0.49
2:H:53:TYR:OH	2:H:112:MET:HE1	2.13	0.49
4:O:67:ARG:NH2	4:O:90:ASP:OD1	2.45	0.49
5:P:37:GLN:NE2	5:P:85:ASP:OD2	2.44	0.49
5:T:75:ILE:HD11	5:T:86:TYR:CE1	2.48	0.49
2:B:288:HIS:ND1	2:B:314:PRO:HB3	2.27	0.49
3:F:258:TRP:CD1	3:F:264:THR:HG22	2.47	0.49
3:I:207:VAL:HG22	3:I:216:VAL:HG12	1.95	0.49
4:O:19:LYS:HD3	4:O:82:GLU:HG2	1.94	0.49
2:E:234:ASP:OD1	2:E:235:LYS:N	2.45	0.49
3:L:204:HIS:NE2	3:L:225:ASP:OD1	2.46	0.49
4:M:101:MET:HE1	4:M:103:TYR:CE2	2.48	0.49
2:E:36:VAL:HG21	2:E:110:ILE:HG21	1.95	0.49
2:E:53:TYR:OH	2:E:112:MET:HE1	2.13	0.49
1:J:289:ARG:HG3	1:J:291:SER:H	1.78	0.49
4:S:36:TRP:HZ2	4:S:79:ALA:HB1	1.78	0.49
2:B:169:LEU:HD12	2:B:252:LYS:HE2	1.95	0.48
1:D:404:LYS:O	1:D:408:THR:HG23	2.13	0.48
1:J:10:GLN:HG2	1:J:13:ILE:HD12	1.96	0.48
3:L:247:GLU:HB3	3:L:250:ARG:O	2.13	0.48
4:Q:47:TRP:HZ2	4:Q:50:TRP:HD1	1.61	0.48
1:A:202:ASP:OD1	1:A:202:ASP:N	2.46	0.48
4:O:100:GLN:H	4:O:110:ASP:HB3	1.78	0.48
1:A:413:LEU:HD22	2:B:374:CYS:SG	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:18:VAL:HG22	4:M:86:LEU:HD11	1.95	0.48
5:N:20:ILE:HB	5:N:73:LEU:HB3	1.95	0.48
2:E:362:ARG:HG2	2:E:363:TYR:CD1	2.49	0.48
1:A:303:LEU:HD23	1:A:378:GLY:HA3	1.95	0.48
1:D:31:ILE:HD11	1:D:280:PHE:HZ	1.79	0.48
1:D:360:ASN:HB3	1:D:400:ALA:HB1	1.96	0.48
2:E:22:CYS:O	2:E:24:VAL:N	2.46	0.48
2:E:275:MET:SD	1:J:197:PRO:HG2	2.54	0.48
2:K:206:LYS:HZ1	4:S:103:TYR:HA	1.79	0.48
4:O:94:TYR:O	4:O:115:GLY:CA	2.62	0.48
2:B:10:LYS:NZ	2:B:59:GLY:O	2.41	0.48
1:J:413:LEU:HD23	2:K:374:CYS:SG	2.54	0.48
1:A:77:GLN:HB2	1:A:221:LEU:HD13	1.95	0.47
3:C:213:ARG:NH1	3:C:267:TYR:HB3	2.28	0.47
1:G:51:TYR:HB3	1:G:203:ILE:HD13	1.96	0.47
1:G:265:PRO:HD2	1:G:267:ARG:HH11	1.79	0.47
2:H:82:VAL:HG11	2:H:112:MET:HE3	1.96	0.47
2:H:148:GLU:OE2	2:H:267:THR:OG1	2.29	0.47
1:A:41:THR:OG1	1:A:125:HIS:O	2.26	0.47
2:E:82:VAL:HG11	2:E:112:MET:HE2	1.96	0.47
3:I:208:GLN:HG3	3:I:210:GLU:OE1	2.13	0.47
1:J:300:GLU:HA	1:J:374:VAL:HG21	1.96	0.47
1:G:117:ASP:HB2	2:H:261:LEU:HD23	1.97	0.47
1:J:363:PRO:HD3	1:J:380:CYS:SG	2.54	0.47
3:L:165:LEU:HD11	3:L:181:PRO:HD3	1.97	0.47
1:G:328:CYS:SG	1:G:346:LEU:HD22	2.53	0.47
3:I:270:GLU:OE1	3:I:271:ASN:ND2	2.34	0.47
3:L:167:THR:HB	3:L:176:GLU:HB3	1.96	0.47
4:M:35:HIS:HB2	4:M:97:ALA:HB3	1.95	0.47
4:S:51:ILE:HD13	4:S:70:VAL:HG11	1.96	0.47
1:J:148:VAL:HG12	1:J:148:VAL:O	2.13	0.47
4:M:106:ASN:ND2	5:N:98:TYR:OH	2.48	0.47
4:M:2:VAL:HG13	4:M:27:TYR:CE1	2.49	0.47
5:R:24:GLY:HA3	5:R:27:LEU:HD23	1.96	0.47
1:A:362:HIS:CD2	1:A:404:LYS:HG2	2.50	0.47
3:C:207:VAL:HG22	3:C:216:VAL:HG12	1.95	0.47
1:D:9:SER:OG	1:D:273:VAL:O	2.32	0.47
1:D:51:TYR:OH	1:D:236:ALA:O	2.33	0.47
1:D:205:SER:OG	1:D:207:THR:O	2.31	0.47
3:F:117:ARG:HH21	3:F:120:MET:HE3	1.80	0.47
3:F:243:GLY:HA2	3:F:275:TRP:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:33:ILE:HG12	2:H:47:LEU:HD21	1.96	0.47
2:H:218:SER:O	4:Q:31:ASN:ND2	2.44	0.47
3:F:195:LYS:HE2	3:F:257:MET:HB2	1.97	0.47
4:M:60:TYR:HE1	4:M:70:VAL:HG23	1.78	0.47
5:N:86:TYR:O	5:N:103:GLY:HA2	2.14	0.47
4:O:99:LEU:HB2	4:O:108:ASP:O	2.15	0.47
4:S:4:LEU:HB2	4:S:23:LYS:O	2.15	0.47
5:T:46:VAL:HG23	5:T:57:ILE:HD12	1.96	0.47
1:A:21:ARG:HB2	1:A:24:TYR:HB2	1.97	0.47
2:B:353:HIS:O	2:B:357:THR:HG23	2.14	0.47
2:B:408:ILE:N	2:B:409:PRO:HD2	2.30	0.47
3:F:189:PHE:HE1	3:F:231:LEU:HD11	1.79	0.47
1:G:217:THR:OG1	1:G:235:GLN:NE2	2.44	0.47
1:G:294:PRO:HG3	1:G:326:GLY:HA3	1.95	0.47
5:N:25:ASP:OD1	5:N:26:ALA:N	2.47	0.47
3:C:147:LEU:O	3:C:177:TYR:HA	2.15	0.47
3:C:197:GLN:HE21	3:C:210:GLU:HA	1.79	0.47
1:D:60:ILE:HG21	1:D:86:PRO:HG2	1.96	0.47
2:E:126:PRO:HB3	2:H:141:HIS:HB3	1.98	0.46
1:G:176:LYS:HB3	1:G:189:PHE:CE2	2.50	0.46
3:I:187:ASP:OD1	3:I:187:ASP:N	2.45	0.46
4:S:6:GLN:HE22	4:S:95:TYR:HA	1.79	0.46
1:A:29:ILE:HG23	1:A:137:VAL:HG22	1.97	0.46
2:E:271:ALA:O	2:E:333:HIS:NE2	2.41	0.46
3:F:147:LEU:O	3:F:177:TYR:HA	2.16	0.46
4:O:3:GLN:NE2	4:O:25:SER:HB2	2.30	0.46
1:A:65:SER:HA	1:A:101:THR:HG21	1.96	0.46
2:K:218:SER:O	4:S:31:ASN:HB3	2.15	0.46
3:L:151:MET:HE3	3:L:169:LYS:HD2	1.98	0.46
4:S:37:VAL:HG11	4:S:112:TRP:HZ3	1.80	0.46
3:F:192:THR:OG1	3:F:236:ARG:NH1	2.49	0.46
5:P:32:VAL:HG21	5:P:71:VAL:HG11	1.96	0.46
2:K:288:HIS:CD2	2:K:314:PRO:HB3	2.46	0.46
4:O:47:TRP:HZ2	4:O:50:TRP:HD1	1.64	0.46
4:Q:19:LYS:HE2	4:Q:80:TYR:HB3	1.96	0.46
1:A:366:ARG:NH1	1:A:375:THR:OG1	2.44	0.46
2:H:387:TRP:HE3	2:H:388:LEU:HD12	1.81	0.46
2:K:169:LEU:HD12	2:K:170:PRO:HD2	1.98	0.46
5:R:12:VAL:HG11	5:R:18:ALA:HB2	1.97	0.46
1:A:106:ALA:HB3	1:A:221:LEU:HD11	1.97	0.46
1:A:309:SER:HB3	1:A:383:PRO:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:100:GLN:HB2	4:O:111:TYR:HD2	1.80	0.46
4:S:33:ILE:CG2	4:S:50:TRP:HB2	2.46	0.46
2:E:53:TYR:CE2	2:E:100:LEU:HB2	2.48	0.46
2:E:168:HIS:CD2	2:E:239:ASN:HB2	2.51	0.46
2:H:327:GLU:HB3	2:H:337:ARG:HG2	1.98	0.46
2:K:36:VAL:HG21	2:K:110:ILE:HG21	1.98	0.46
3:L:259:ASN:HD21	3:L:263:VAL:HG22	1.80	0.46
1:D:148:VAL:HG12	1:D:148:VAL:O	2.16	0.45
1:D:218:ASN:ND2	2:H:275:MET:SD	2.89	0.45
3:F:259:ASN:HB2	3:F:265:VAL:HG23	1.99	0.45
2:H:169:LEU:HD12	2:H:170:PRO:HD2	1.97	0.45
5:N:63:SER:HB2	5:N:74:THR:HB	1.98	0.45
5:R:65:SER:OG	5:R:72:THR:OG1	2.33	0.45
2:B:289:PRO:HG3	2:B:330:TRP:HH2	1.81	0.45
2:H:348:PRO:HG3	2:H:358:HIS:CD2	2.51	0.45
3:I:258:TRP:HD1	3:I:264:THR:HG22	1.80	0.45
2:K:137:GLU:HG2	2:K:293:THR:HG23	1.98	0.45
5:R:5:THR:OG1	5:R:23:SER:OG	2.34	0.45
3:F:130:ILE:HD11	3:F:140:ALA:HB2	1.99	0.45
1:G:86:PRO:HB3	1:G:229:ILE:HG12	1.99	0.45
1:D:21:ARG:HB3	1:D:24:TYR:HD2	1.82	0.45
2:H:216:GLN:O	4:Q:106:ASN:N	2.33	0.45
2:E:17:ALA:HB3	2:E:32:ALA:HB3	1.98	0.45
2:E:197:LEU:HA	2:E:209:GLU:HA	1.98	0.45
2:B:198:VAL:O	2:B:207:ILE:HA	2.17	0.45
2:B:200:CYS:SG	2:B:206:LYS:NZ	2.86	0.45
1:D:241:GLU:HG3	1:D:245:LYS:HE3	1.99	0.45
2:E:84:LEU:HD13	2:E:112:MET:HG3	1.98	0.45
1:J:86:PRO:HB3	1:J:229:ILE:HG12	1.98	0.45
2:K:84:LEU:HG	2:K:90:CYS:HB2	1.99	0.45
2:K:359:TYR:HB3	2:K:367:THR:HG21	1.97	0.45
4:O:27:TYR:OH	4:O:98:THR:HG21	2.15	0.45
4:O:107:GLY:HA3	5:P:33:TYR:CD1	2.52	0.45
2:B:175:ASP:OD2	2:B:230:ARG:NH2	2.39	0.45
3:C:143:VAL:HG22	3:C:189:PHE:HB2	1.99	0.45
3:F:202:TRP:CD1	3:F:203:HIS:H	2.35	0.45
2:K:146:GLY:HA3	2:K:268:VAL:O	2.16	0.45
4:M:58:THR:HG21	4:M:70:VAL:HG21	1.99	0.45
2:B:303:GLU:O	2:B:303:GLU:HG2	2.16	0.45
2:B:352:PRO:O	2:B:356:ILE:HG12	2.17	0.45
1:D:362:HIS:NE2	1:D:404:LYS:HG3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:199:GLU:HB2	2:E:229:TYR:HE1	1.80	0.45
2:K:216:GLN:NE2	2:K:218:SER:OG	2.34	0.45
4:O:27:TYR:CE1	4:O:29:PHE:HD1	2.34	0.45
5:P:20:ILE:HG23	5:P:104:THR:HG21	1.98	0.45
4:S:101:MET:HE1	4:S:103:TYR:CE2	2.51	0.45
1:A:122:TYR:HB2	1:A:177:ILE:HG13	1.98	0.45
1:A:148:VAL:O	1:A:164:GLY:HA3	2.17	0.45
3:C:196:PRO:O	3:C:200:TYR:OH	2.32	0.45
2:E:274:PRO:HB3	2:E:287:LEU:HD23	1.98	0.45
1:G:160:LYS:HB3	1:G:281:ASP:HB3	1.99	0.45
3:I:117:ARG:NH1	3:I:199:TYR:OH	2.50	0.45
5:T:36:GLN:OE1	5:T:86:TYR:HE2	1.99	0.45
1:A:89:TRP:NE1	2:B:173:GLU:OE2	2.43	0.45
1:D:86:PRO:HB3	1:D:229:ILE:HG12	1.99	0.45
2:E:134:VAL:HG21	2:E:266:CYS:SG	2.57	0.45
2:E:412:LEU:HD12	2:E:416:CYS:HA	1.99	0.45
1:G:10:GLN:HG2	1:G:13:ILE:HD12	1.99	0.45
1:J:94:CYS:O	2:K:227:ARG:NH1	2.50	0.45
4:Q:36:TRP:CE2	4:Q:81:MET:HB2	2.52	0.45
2:H:275:MET:HE1	2:H:288:HIS:CD2	2.52	0.44
2:B:85:TYR:HB2	2:B:89:PRO:HA	1.99	0.44
2:B:271:ALA:O	2:B:333:HIS:NE2	2.45	0.44
2:K:200:CYS:HB3	2:K:220:CYS:SG	2.57	0.44
3:L:130:ILE:HD11	3:L:140:ALA:HB2	1.99	0.44
3:F:182:GLN:OE1	3:F:185:ARG:NH1	2.51	0.44
4:M:67:ARG:NH2	4:M:90:ASP:OD1	2.50	0.44
5:P:80:ALA:HA	5:P:108:VAL:HG11	1.99	0.44
4:Q:101:MET:HG3	4:Q:110:ASP:OD2	2.17	0.44
4:S:6:GLN:HA	4:S:22:CYS:HA	1.99	0.44
2:B:234:ASP:OD1	2:B:235:LYS:N	2.50	0.44
2:E:84:LEU:HB3	2:E:90:CYS:HB2	1.98	0.44
2:E:159:GLN:HB2	2:E:161:ARG:HH11	1.82	0.44
1:G:105:LYS:HB2	1:G:105:LYS:HE2	1.82	0.44
1:J:63:CYS:HA	1:J:99:GLU:O	2.18	0.44
2:K:302:ASP:OD1	2:K:302:ASP:N	2.50	0.44
2:E:52:GLN:OE1	2:E:67:ARG:NH2	2.38	0.44
1:G:265:PRO:O	1:G:267:ARG:HG3	2.18	0.44
1:D:368:GLN:HG2	1:D:373:TYR:CD1	2.52	0.44
2:E:168:HIS:HB3	2:E:250:THR:HG22	2.00	0.44
1:G:88:MET:HE1	2:H:173:GLU:HG2	1.99	0.44
1:G:162:THR:HB	1:G:279:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:250:ARG:HD2	3:I:250:ARG:HA	1.76	0.44
1:J:76:GLU:HA	1:J:106:ALA:O	2.17	0.44
1:A:55:MET:SD	1:A:231:VAL:HB	2.57	0.44
1:D:81:PHE:HB3	1:D:223:ARG:NH1	2.32	0.44
2:B:134:VAL:HG11	2:B:151:CYS:SG	2.58	0.44
3:C:195:LYS:HB3	3:C:209:TYR:CE2	2.53	0.44
2:E:96:HIS:HB3	2:E:258:PRO:HG3	1.99	0.44
2:E:163:ALA:HB3	2:E:260:LEU:HD11	2.00	0.44
3:I:184:MET:HE2	3:I:184:MET:HB2	1.85	0.44
3:L:121:LYS:HA	3:L:121:LYS:HD3	1.76	0.44
3:L:209:TYR:HB2	3:L:214:PHE:CE1	2.53	0.44
5:P:63:SER:O	5:P:73:LEU:HD12	2.18	0.44
1:A:369:ILE:O	1:A:370:CYS:C	2.61	0.44
1:D:202:ASP:N	1:D:202:ASP:OD1	2.51	0.44
3:F:143:VAL:HG12	3:F:189:PHE:HB2	1.99	0.44
1:G:142:ILE:HD13	1:G:156:PHE:CD2	2.53	0.44
2:H:364:PRO:C	2:H:366:SER:H	2.26	0.44
3:I:131:MET:HA	3:I:131:MET:HE2	1.99	0.44
3:L:161:VAL:HG13	3:L:162:LEU:HD12	1.99	0.44
3:L:200:TYR:HB3	3:L:231:LEU:O	2.17	0.44
5:N:28:PRO:HG3	5:N:69:THR:HA	1.99	0.44
5:P:30:GLN:NE2	5:P:91:ALA:HB3	2.33	0.44
2:E:159:GLN:HB2	2:E:161:ARG:NH1	2.32	0.43
2:E:197:LEU:HB2	2:E:231:LEU:HD11	2.00	0.43
1:G:296:LEU:HD11	1:G:320:TYR:HB2	2.00	0.43
1:G:416:GLY:O	1:G:420:ILE:HG12	2.18	0.43
5:N:34:TRP:CZ3	5:N:88:CYS:HB3	2.53	0.43
5:P:27:LEU:HD11	5:P:32:VAL:CG2	2.48	0.43
1:A:219:LEU:HA	1:A:235:GLN:HB3	2.00	0.43
3:C:169:LYS:HE2	3:C:169:LYS:HB2	1.89	0.43
1:D:76:GLU:HA	1:D:106:ALA:O	2.19	0.43
1:J:19:VAL:CG2	1:J:27:LEU:HB3	2.48	0.43
2:K:191:PRO:HG2	2:K:194:THR:HB	2.00	0.43
4:O:48:MET:HE1	4:O:81:MET:HE2	2.00	0.43
5:P:6:GLN:HB3	5:P:102:THR:OG1	2.17	0.43
4:Q:96:CYS:O	4:Q:112:TRP:HA	2.17	0.43
4:S:20:VAL:HG23	4:S:81:MET:HB3	2.00	0.43
1:A:387:ILE:HD13	2:B:340:ALA:HA	1.99	0.43
3:F:213:ARG:NH1	3:F:267:TYR:HB3	2.33	0.43
2:H:126:PRO:HB3	2:K:141:HIS:HB3	1.99	0.43
4:M:44:ARG:NH1	5:N:3:GLU:OE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:17:THR:HA	5:N:75:ILE:O	2.18	0.43
4:S:36:TRP:CZ2	4:S:79:ALA:HB1	2.52	0.43
5:T:36:GLN:N	5:T:44:VAL:O	2.44	0.43
1:D:77:GLN:HE22	1:D:219:LEU:C	2.27	0.43
2:E:398:THR:OG1	2:E:399:PRO:HD3	2.18	0.43
3:F:187:ASP:OD1	3:F:187:ASP:N	2.51	0.43
3:I:218:LYS:HE2	3:I:218:LYS:HB3	1.77	0.43
4:O:30:THR:O	4:O:54:GLY:HA3	2.18	0.43
5:P:60:GLU:OE1	5:P:60:GLU:N	2.51	0.43
2:B:402:LEU:HA	3:C:146:LYS:HE2	1.99	0.43
2:E:13:ARG:NH2	2:E:69:ASP:OD2	2.52	0.43
1:G:76:GLU:OE2	1:G:105:LYS:HG3	2.18	0.43
1:G:361:ILE:HD13	1:G:403:SER:HB3	2.00	0.43
1:J:417:SER:HA	1:J:420:ILE:HD13	2.00	0.43
3:C:225:ASP:OD1	3:C:228:ARG:HD2	2.18	0.43
2:E:404:PRO:HD3	3:F:258:TRP:NE1	2.34	0.43
2:H:200:CYS:HA	2:H:226:CYS:CB	2.42	0.43
1:J:88:MET:HE2	1:J:88:MET:HB3	1.90	0.43
2:K:211:ILE:HG22	5:T:49:LYS:HE3	2.01	0.43
3:L:194:GLU:OE2	3:L:236:ARG:NH2	2.52	0.43
3:L:207:VAL:CG1	3:L:216:VAL:HG12	2.48	0.43
1:G:130:GLN:HG2	1:G:147:TYR:CD1	2.53	0.43
2:K:206:LYS:NZ	2:K:219:GLN:OE1	2.42	0.43
3:L:254:SER:OG	3:L:269:PRO:HD2	2.18	0.43
4:O:47:TRP:CD2	5:P:98:TYR:HB2	2.54	0.43
5:P:92:ASP:HB2	5:P:97:GLU:HB3	2.00	0.43
1:A:416:GLY:O	1:A:420:ILE:HG12	2.19	0.43
2:E:21:ARG:HD2	2:H:141:HIS:CE1	2.53	0.43
1:G:387:ILE:HD13	2:H:340:ALA:HA	2.01	0.43
4:Q:94:TYR:O	4:Q:115:GLY:HA2	2.19	0.43
1:A:319:LYS:HD2	1:A:319:LYS:HA	1.87	0.43
2:B:143:PRO:HG3	2:B:269:PRO:HD3	2.00	0.43
1:D:117:ASP:HB2	2:E:261:LEU:HD23	2.00	0.43
2:E:22:CYS:SG	2:E:27:CYS:N	2.91	0.43
3:F:148:PHE:CD2	3:F:175:LEU:HD13	2.53	0.43
2:H:134:VAL:HG21	2:H:266:CYS:SG	2.58	0.43
3:F:239:ALA:HB1	3:F:255:VAL:HG22	2.00	0.42
2:K:82:VAL:HG23	2:K:114:PHE:HB3	2.01	0.42
2:K:116:LYS:HA	2:K:116:LYS:HD3	1.76	0.42
4:S:99:LEU:HD12	4:S:100:GLN:H	1.83	0.42
1:D:251:LEU:HD23	1:D:251:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:97:ASP:N	1:G:97:ASP:OD1	2.52	0.42
2:H:168:HIS:CD2	2:H:239:ASN:HB3	2.55	0.42
2:K:88:ARG:HB2	2:K:105:PRO:HG3	2.00	0.42
2:K:371:LEU:HA	2:K:374:CYS:HB3	2.01	0.42
4:M:109:LEU:HB2	5:N:35:TYR:OH	2.18	0.42
5:N:6:GLN:HB3	5:N:102:THR:OG1	2.20	0.42
3:C:146:LYS:HB2	3:C:148:PHE:CE1	2.54	0.42
1:D:232:PRO:HB3	2:H:145:HIS:CG	2.54	0.42
4:O:22:CYS:HB2	4:O:36:TRP:CH2	2.54	0.42
1:A:341:GLU:N	1:A:341:GLU:OE1	2.51	0.42
1:A:362:HIS:ND1	1:A:379:ASP:OD1	2.51	0.42
2:B:345:PRO:HG2	2:B:361:HIS:ND1	2.34	0.42
1:D:168:THR:HG21	1:D:273:VAL:HG22	2.01	0.42
2:E:12:THR:HA	2:E:236:TRP:O	2.19	0.42
2:H:12:THR:HA	2:H:236:TRP:O	2.19	0.42
1:J:296:LEU:HD11	1:J:320:TYR:HB2	2.02	0.42
4:Q:47:TRP:CZ2	4:Q:50:TRP:HD1	2.37	0.42
1:D:63:CYS:HA	1:D:99:GLU:HG2	2.01	0.42
3:F:269:PRO:HG2	3:F:272:CYS:HB2	2.01	0.42
2:H:16:MET:HE2	2:H:69:ASP:O	2.20	0.42
4:O:17:SER:HA	4:O:84:SER:HA	2.02	0.42
4:O:63:LYS:NZ	4:O:64:PHE:HE1	2.17	0.42
4:Q:27:TYR:OH	4:Q:98:THR:HG21	2.18	0.42
1:A:129:VAL:HB	1:A:148:VAL:HB	2.02	0.42
2:B:53:TYR:OH	2:B:112:MET:HE1	2.19	0.42
1:D:19:VAL:CG2	1:D:27:LEU:HB3	2.49	0.42
2:K:14:PRO:HG3	2:K:52:GLN:HG3	2.02	0.42
1:A:151:GLU:HG3	1:D:191:GLU:OE2	2.20	0.42
3:C:151:MET:N	3:C:151:MET:HE2	2.34	0.42
1:G:325:SER:HA	1:G:346:LEU:O	2.18	0.42
5:N:83:ASP:HB2	5:N:108:VAL:HG12	2.02	0.42
4:Q:55:ASN:C	4:Q:55:ASN:HD22	2.28	0.42
1:A:289:ARG:HD2	1:G:305:GLU:OE2	2.20	0.42
3:F:148:PHE:HD2	3:F:175:LEU:HD13	1.84	0.42
1:J:253:PHE:HB3	2:K:296:ILE:HG21	2.02	0.42
4:M:36:TRP:CZ2	4:M:79:ALA:HB1	2.55	0.42
4:Q:73:ASP:OD1	4:Q:73:ASP:N	2.53	0.42
1:A:396:GLN:NE2	2:B:323:GLU:OE1	2.44	0.42
2:B:362:ARG:HG2	2:B:363:TYR:CD2	2.55	0.42
1:D:51:TYR:HB3	1:D:203:ILE:HD13	2.02	0.42
1:D:88:MET:HE2	1:D:88:MET:HB3	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:435:VAL:HG23	1:J:436:LEU:HD22	2.01	0.42
2:K:404:PRO:HD3	3:L:258:TRP:CH2	2.55	0.42
2:B:260:LEU:HD23	2:B:260:LEU:HA	1.87	0.42
3:C:202:TRP:CD1	3:C:203:HIS:H	2.37	0.42
3:F:146:LYS:HB3	3:F:148:PHE:HE1	1.84	0.42
3:F:245:VAL:HB	3:F:272:CYS:HA	2.01	0.42
1:J:55:MET:HG3	2:K:241:ASP:HB3	2.02	0.42
3:L:199:TYR:HA	3:L:208:GLN:HA	2.02	0.42
4:M:4:LEU:HB3	4:M:111:TYR:CE2	2.55	0.42
4:M:15:GLY:N	4:M:86:LEU:O	2.52	0.42
4:O:114:GLN:H	4:O:114:GLN:CD	2.28	0.42
5:T:2:TYR:CE2	5:T:92:ASP:HA	2.54	0.42
2:B:34:GLU:HG2	2:B:48:GLN:OE1	2.20	0.41
3:C:117:ARG:HA	3:C:120:MET:HE2	2.02	0.41
2:E:147:VAL:O	2:E:268:VAL:HG22	2.20	0.41
3:L:157:ILE:H	3:L:157:ILE:HD12	1.84	0.41
1:D:65:SER:HA	1:D:101:THR:HG21	2.02	0.41
2:B:21:ARG:HA	2:B:21:ARG:HD2	1.75	0.41
2:B:398:THR:OG1	2:B:399:PRO:HD3	2.21	0.41
2:E:141:HIS:CE1	2:K:21:ARG:HD3	2.55	0.41
2:E:288:HIS:ND1	2:E:314:PRO:HB3	2.35	0.41
2:E:412:LEU:HD13	2:E:418:ALA:HB3	2.01	0.41
3:F:230:ILE:HG22	3:F:239:ALA:O	2.19	0.41
1:G:134:ASN:OD1	1:G:143:VAL:HG12	2.20	0.41
2:H:10:LYS:HE2	2:H:59:GLY:O	2.21	0.41
2:H:288:HIS:ND1	2:H:314:PRO:HB3	2.35	0.41
1:J:31:ILE:HD13	1:J:278:LEU:HD23	2.02	0.41
4:Q:2:VAL:HB	4:Q:100:GLN:NE2	2.35	0.41
4:Q:22:CYS:HB2	4:Q:36:TRP:CH2	2.55	0.41
1:D:300:GLU:OE1	1:D:300:GLU:N	2.53	0.41
1:G:300:GLU:O	1:G:318:VAL:HA	2.21	0.41
1:J:369:ILE:HG22	1:J:370:CYS:H	1.85	0.41
2:K:207:ILE:HG22	2:K:207:ILE:O	2.20	0.41
5:T:14:PRO:HG3	5:T:108:VAL:HG22	2.02	0.41
2:H:398:THR:OG1	2:H:399:PRO:HD3	2.20	0.41
3:L:126:LYS:HE2	3:L:126:LYS:HB3	1.91	0.41
4:S:33:ILE:HG21	4:S:50:TRP:HB2	2.01	0.41
2:B:114:PHE:CD2	2:B:121:HIS:HB2	2.53	0.41
2:B:170:PRO:HD3	2:B:236:TRP:HA	2.02	0.41
1:D:309:SER:HB3	1:D:383:PRO:HB3	2.02	0.41
2:E:260:LEU:HD23	2:E:260:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:5:THR:HG23	1:G:278:LEU:HB2	2.03	0.41
1:G:202:ASP:OD1	1:G:202:ASP:N	2.54	0.41
2:H:321:VAL:HG13	2:H:326:TRP:HB3	2.03	0.41
1:A:327:LYS:HA	1:A:327:LYS:HD3	1.84	0.41
1:G:310:SER:HB3	1:G:392:GLN:HA	2.03	0.41
2:H:200:CYS:CA	2:H:226:CYS:HB2	2.43	0.41
3:I:209:TYR:OH	3:I:212:GLY:HA2	2.21	0.41
1:J:329:ALA:N	1:J:370:CYS:HB3	2.36	0.41
5:P:85:ASP:HB3	5:P:87:TYR:CE2	2.55	0.41
2:B:21:ARG:HB3	2:B:124:SER:HB3	2.02	0.41
2:B:218:SER:O	4:M:31:ASN:ND2	2.49	0.41
2:E:10:LYS:HE3	2:E:59:GLY:O	2.20	0.41
2:E:40:GLY:O	2:E:132:ASN:ND2	2.39	0.41
3:F:168:LYS:HD2	3:F:177:TYR:CZ	2.55	0.41
3:F:250:ARG:H	3:F:250:ARG:HD3	1.86	0.41
1:G:40:PRO:HA	1:G:127:ALA:HA	2.02	0.41
1:G:231:VAL:HB	2:H:241:ASP:OD1	2.21	0.41
2:H:161:ARG:HB2	2:H:260:LEU:HD12	2.03	0.41
3:I:132:LEU:O	3:I:135:LYS:HG2	2.21	0.41
2:K:37:LYS:HA	2:K:37:LYS:HD3	1.85	0.41
2:K:78:PRO:HG2	2:K:81:GLN:HG3	2.02	0.41
4:M:99:LEU:HD13	4:M:108:ASP:O	2.21	0.41
1:A:184:ILE:O	1:A:250:SER:OG	2.31	0.41
2:B:215:LYS:NZ	4:M:104:GLY:O	2.54	0.41
3:C:130:ILE:O	3:C:131:MET:HE2	2.21	0.41
1:D:321:SER:HB3	1:D:349:GLN:HE22	1.85	0.41
2:E:87:SER:HA	2:H:88:ARG:HD2	2.02	0.41
2:E:353:HIS:O	2:E:357:THR:HG23	2.21	0.41
1:G:129:VAL:HB	1:G:148:VAL:HB	2.02	0.41
1:G:148:VAL:O	1:G:148:VAL:HG12	2.20	0.41
3:I:118:MET:SD	3:I:118:MET:N	2.89	0.41
1:J:307:VAL:HG23	1:J:381:HIS:O	2.21	0.41
5:N:61:ARG:NH2	5:N:82:ASP:OD1	2.45	0.41
4:Q:99:LEU:HD13	4:Q:108:ASP:HB3	2.03	0.41
4:S:40:ALA:HA	4:S:92:ALA:HB1	2.02	0.41
1:A:148:VAL:O	1:A:148:VAL:HG12	2.21	0.41
1:D:296:LEU:HD12	1:D:346:LEU:HD13	2.03	0.41
1:D:383:PRO:HG2	2:E:343:THR:HG22	2.03	0.41
4:S:106:ASN:ND2	5:T:98:TYR:OH	2.50	0.41
2:B:184:SER:OG	4:M:31:ASN:OD1	2.22	0.40
2:B:216:GLN:O	4:M:105:GLY:HA3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:132:LEU:HD13	3:C:154:GLU:HG2	2.02	0.40
3:C:145:GLY:O	3:C:180:VAL:HG22	2.20	0.40
2:H:238:TYR:O	2:H:240:SER:N	2.55	0.40
1:J:55:MET:SD	1:J:231:VAL:HB	2.61	0.40
1:J:383:PRO:HG2	2:K:343:THR:HG22	2.02	0.40
4:M:47:TRP:CD1	5:N:98:TYR:HB2	2.56	0.40
4:O:119:THR:OG1	4:O:120:VAL:N	2.54	0.40
5:T:9:SER:HA	5:T:105:LYS:H	1.86	0.40
2:B:77:ILE:HD13	2:B:114:PHE:CE1	2.56	0.40
1:D:148:VAL:O	1:D:164:GLY:HA3	2.22	0.40
3:F:184:MET:HE3	3:F:184:MET:O	2.22	0.40
1:J:3:HIS:CG	1:J:19:VAL:HG12	2.56	0.40
4:O:44:ARG:NE	5:P:102:THR:HA	2.35	0.40
1:A:203:ILE:O	1:A:203:ILE:HG13	2.21	0.40
2:B:202:CYS:HB3	2:B:225:GLN:NE2	2.36	0.40
2:B:412:LEU:HD13	2:B:418:ALA:HB3	2.03	0.40
1:D:192:TYR:OH	1:D:212:ASP:OD1	2.20	0.40
1:D:329:ALA:H	1:D:370:CYS:HB3	1.86	0.40
3:I:149:ARG:NH2	3:I:153:VAL:O	2.54	0.40
1:J:129:VAL:HB	1:J:148:VAL:HB	2.02	0.40
2:K:168:HIS:CD2	2:K:239:ASN:HB2	2.57	0.40
5:N:58:PRO:HG2	5:N:62:PHE:CE2	2.48	0.40
2:E:408:ILE:N	2:E:409:PRO:HD3	2.36	0.40
2:K:56:ASP:O	2:K:67:ARG:HD3	2.22	0.40
5:N:7:PRO:HA	5:N:8:PRO:HD3	1.97	0.40
5:N:35:TYR:HD1	5:N:45:LEU:HA	1.87	0.40
1:A:10:GLN:HG2	1:A:13:ILE:HD12	2.03	0.40
2:B:294:TYR:CE1	2:B:310:LEU:HB2	2.56	0.40
3:F:151:MET:HE3	3:F:175:LEU:H	1.87	0.40
2:H:18:ARG:HH22	2:H:20:ILE:HD13	1.87	0.40
2:H:297:THR:HB	2:H:307:THR:OG1	2.21	0.40
4:O:50:TRP:HZ3	4:O:52:ASN:HB2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	438/442 (99%)	423 (97%)	15 (3%)	0	100	100
1	D	438/442 (99%)	424 (97%)	14 (3%)	0	100	100
1	G	438/442 (99%)	421 (96%)	17 (4%)	0	100	100
1	J	438/442 (99%)	423 (97%)	15 (3%)	0	100	100
2	B	416/423 (98%)	397 (95%)	19 (5%)	0	100	100
2	E	416/423 (98%)	393 (94%)	23 (6%)	0	100	100
2	H	416/423 (98%)	387 (93%)	29 (7%)	0	100	100
2	K	416/423 (98%)	395 (95%)	21 (5%)	0	100	100
3	C	157/275 (57%)	153 (98%)	4 (2%)	0	100	100
3	F	157/275 (57%)	153 (98%)	4 (2%)	0	100	100
3	I	157/275 (57%)	154 (98%)	3 (2%)	0	100	100
3	L	157/275 (57%)	150 (96%)	7 (4%)	0	100	100
4	M	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
4	O	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
4	Q	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
4	S	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
5	N	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
5	P	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
5	R	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
5	T	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
All	All	4944/5476 (90%)	4729 (96%)	215 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/368 (100%)	366 (100%)	0	100	100
1	D	366/368 (100%)	366 (100%)	0	100	100
1	G	366/368 (100%)	366 (100%)	0	100	100
1	J	366/368 (100%)	366 (100%)	0	100	100
2	B	361/364 (99%)	360 (100%)	1 (0%)	86	88
2	E	361/364 (99%)	361 (100%)	0	100	100
2	H	361/364 (99%)	361 (100%)	0	100	100
2	K	361/364 (99%)	361 (100%)	0	100	100
3	C	132/230 (57%)	132 (100%)	0	100	100
3	F	132/230 (57%)	132 (100%)	0	100	100
3	I	132/230 (57%)	132 (100%)	0	100	100
3	L	132/230 (57%)	132 (100%)	0	100	100
4	M	100/100 (100%)	100 (100%)	0	100	100
4	O	100/100 (100%)	99 (99%)	1 (1%)	68	80
4	Q	100/100 (100%)	100 (100%)	0	100	100
4	S	100/100 (100%)	100 (100%)	0	100	100
5	N	91/91 (100%)	91 (100%)	0	100	100
5	P	91/91 (100%)	91 (100%)	0	100	100
5	R	91/91 (100%)	91 (100%)	0	100	100
5	T	91/91 (100%)	91 (100%)	0	100	100
All	All	4200/4612 (91%)	4198 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	232	GLN
4	O	114	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	16	ASN
1	A	140	HIS
1	A	157	ASN

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Mol	Chain	Res	Type
1	A	179	GLN
1	A	270	ASN
1	A	381	HIS
2	B	28	HIS
2	B	232	GLN
3	C	197	GLN
1	D	16	ASN
1	D	77	GLN
1	D	179	GLN
2	E	81	GLN
2	E	149	GLN
2	E	159	GLN
2	E	358	HIS
3	F	137	ASN
1	G	140	HIS
1	G	157	ASN
1	G	392	GLN
1	G	396	GLN
2	H	121	HIS
2	H	358	HIS
2	H	361	HIS
3	I	152	HIS
3	I	182	GLN
3	I	274	GLN
1	J	16	ASN
1	J	179	GLN
1	J	218	ASN
1	J	331	HIS
1	J	386	HIS
1	J	438	ASN
2	K	80	HIS
2	K	121	HIS
2	K	145	HIS
2	K	239	ASN
2	K	288	HIS
2	K	361	HIS
4	M	55	ASN
4	M	106	ASN
5	N	41	GLN
5	N	89	GLN
4	O	52	ASN
5	P	30	GLN

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Mol	Chain	Res	Type
4	Q	55	ASN
5	R	16	GLN
4	S	3	GLN
4	S	55	ASN
4	S	65	GLN
4	S	106	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	E	502	-	14,14,15	0.26	0	17,19,21	0.43	0
6	NAG	D	501	1	14,14,15	0.25	0	17,19,21	0.57	0
6	NAG	B	502	2	14,14,15	0.23	0	17,19,21	0.57	0
6	NAG	A	501	1	14,14,15	0.19	0	17,19,21	0.51	0
6	NAG	G	501	1	14,14,15	0.21	0	17,19,21	0.47	0
6	NAG	H	502	2	14,14,15	0.39	0	17,19,21	0.38	0
6	NAG	J	501	1	14,14,15	0.19	0	17,19,21	0.45	0
6	NAG	K	501	-	14,14,15	0.45	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	E	501	-	14,14,15	0.47	0	17,19,21	0.39	0
6	NAG	B	501	-	14,14,15	0.47	0	17,19,21	0.38	0
6	NAG	H	501	-	14,14,15	0.48	0	17,19,21	0.38	0
6	NAG	K	502	2	14,14,15	0.28	0	17,19,21	0.40	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	E	502	-	-	2/6/23/26	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	A	501	1	-	1/6/23/26	0/1/1/1
6	NAG	G	501	1	-	0/6/23/26	0/1/1/1
6	NAG	H	502	2	-	3/6/23/26	0/1/1/1
6	NAG	J	501	1	-	2/6/23/26	0/1/1/1
6	NAG	K	501	-	-	2/6/23/26	0/1/1/1
6	NAG	E	501	-	-	2/6/23/26	0/1/1/1
6	NAG	B	501	-	-	2/6/23/26	0/1/1/1
6	NAG	H	501	-	-	2/6/23/26	0/1/1/1
6	NAG	K	502	2	-	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 (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	502	NAG	O5-C5-C6-O6
6	E	502	NAG	O5-C5-C6-O6
6	H	501	NAG	O5-C5-C6-O6
6	B	502	NAG	C4-C5-C6-O6
6	J	501	NAG	C4-C5-C6-O6
6	B	501	NAG	O5-C5-C6-O6
6	B	501	NAG	C4-C5-C6-O6
6	J	501	NAG	O5-C5-C6-O6
6	H	501	NAG	C4-C5-C6-O6

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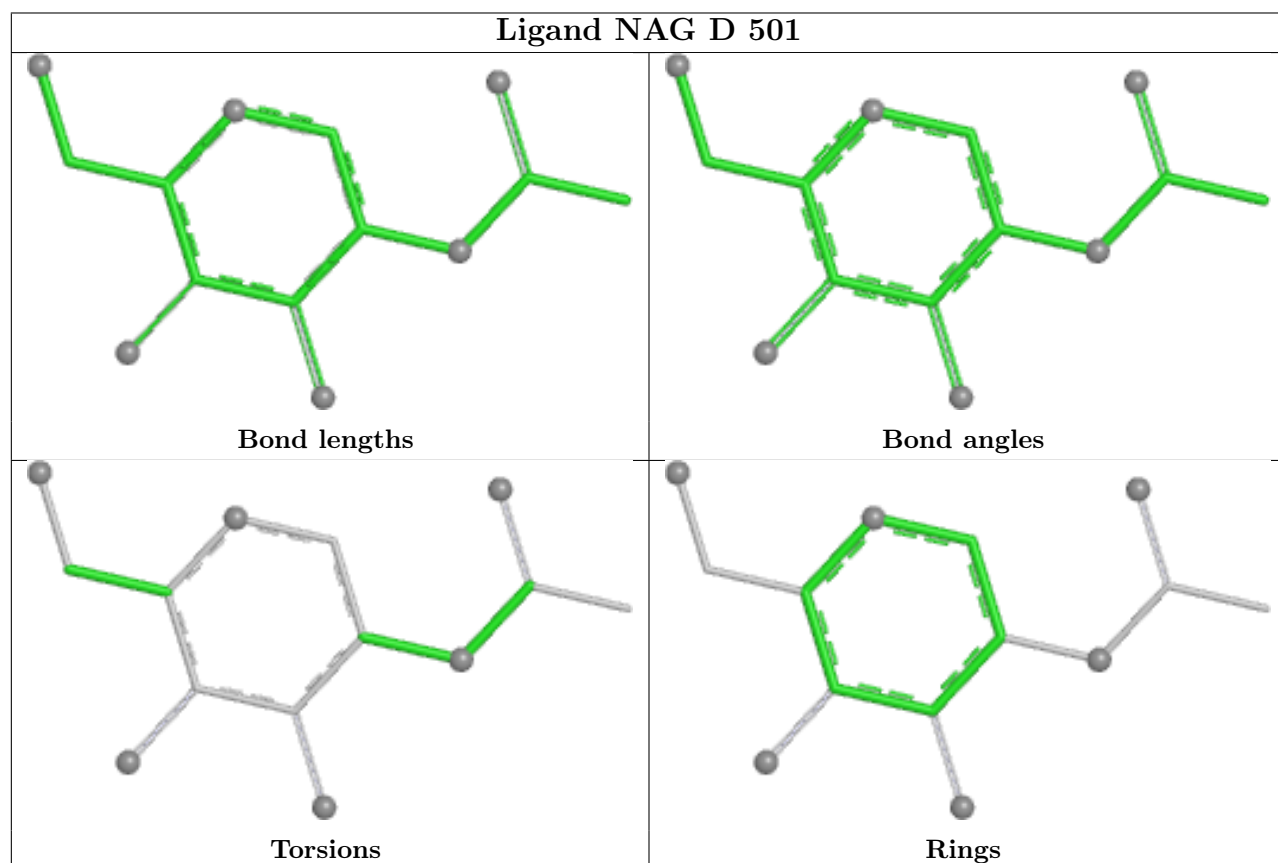
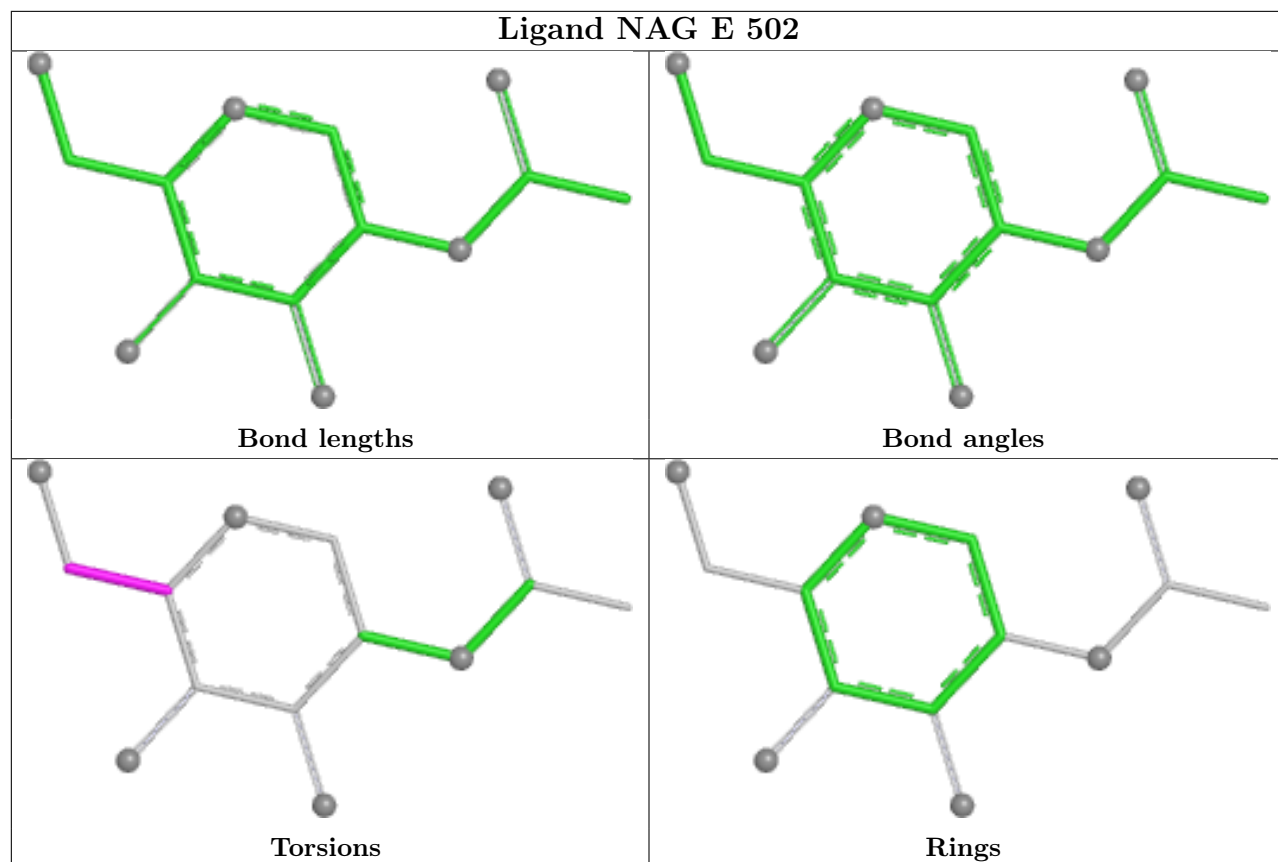
Mol	Chain	Res	Type	Atoms
6	E	501	NAG	O5-C5-C6-O6
6	K	501	NAG	O5-C5-C6-O6
6	E	501	NAG	C4-C5-C6-O6
6	E	502	NAG	C4-C5-C6-O6
6	K	501	NAG	C4-C5-C6-O6
6	K	502	NAG	O5-C5-C6-O6
6	H	502	NAG	O5-C5-C6-O6
6	K	502	NAG	C4-C5-C6-O6
6	H	502	NAG	C4-C5-C6-O6
6	A	501	NAG	C1-C2-N2-C7
6	H	502	NAG	C3-C2-N2-C7

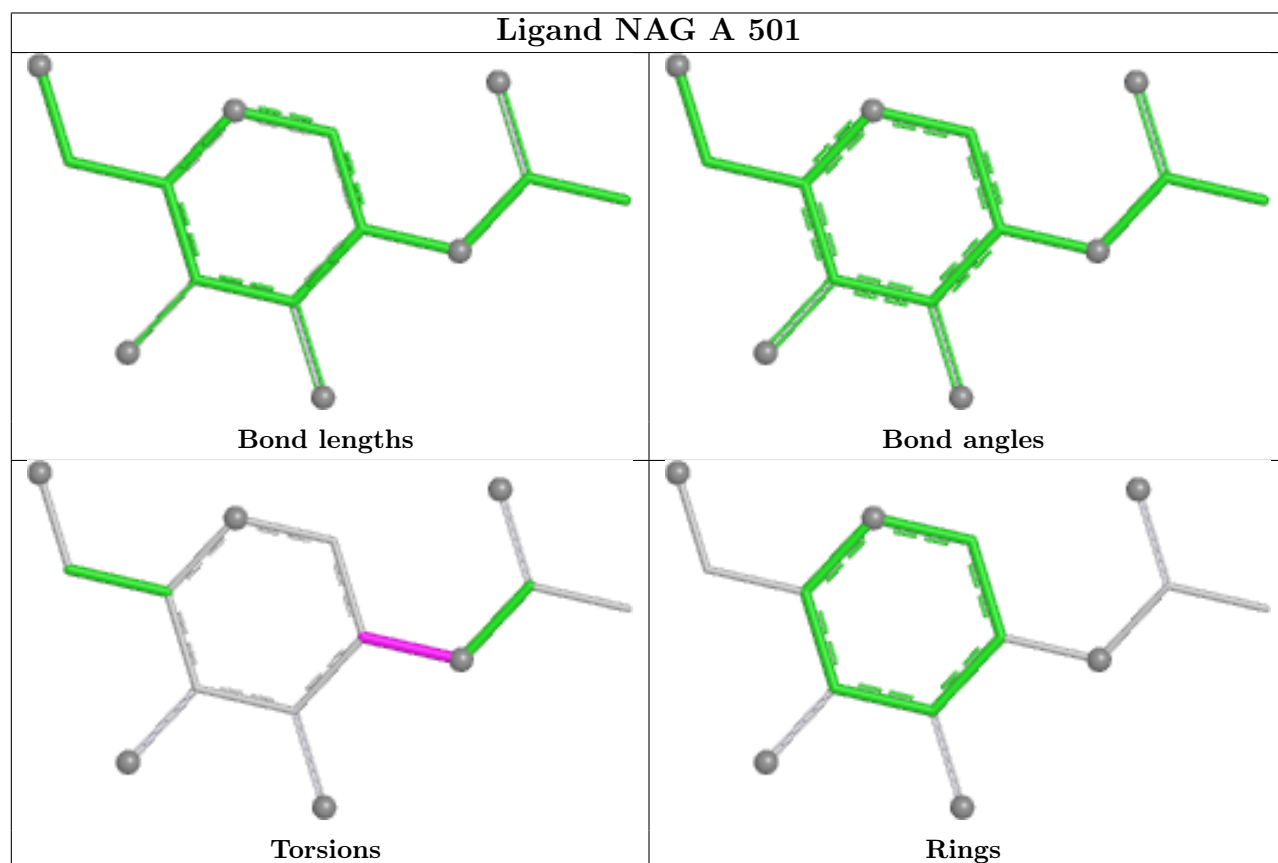
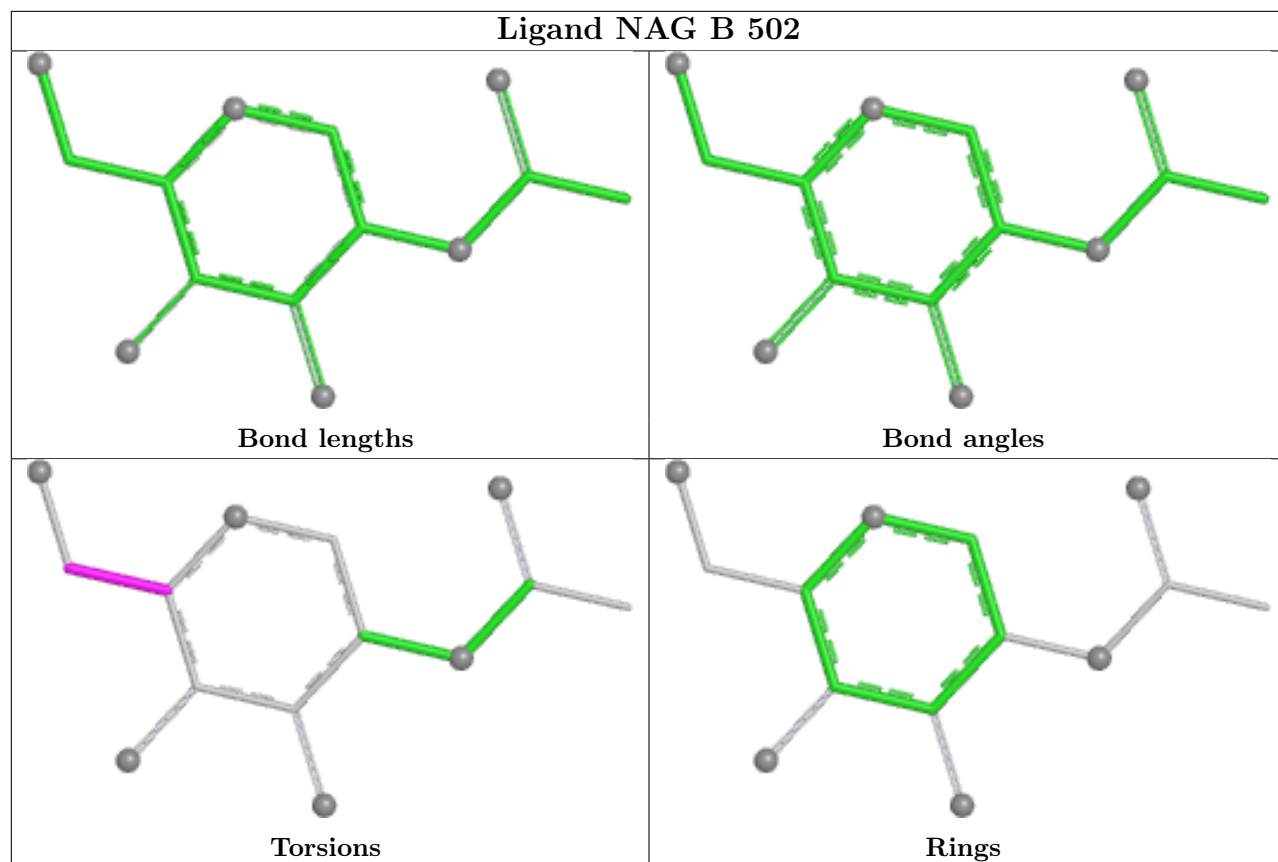
There are no ring outliers.

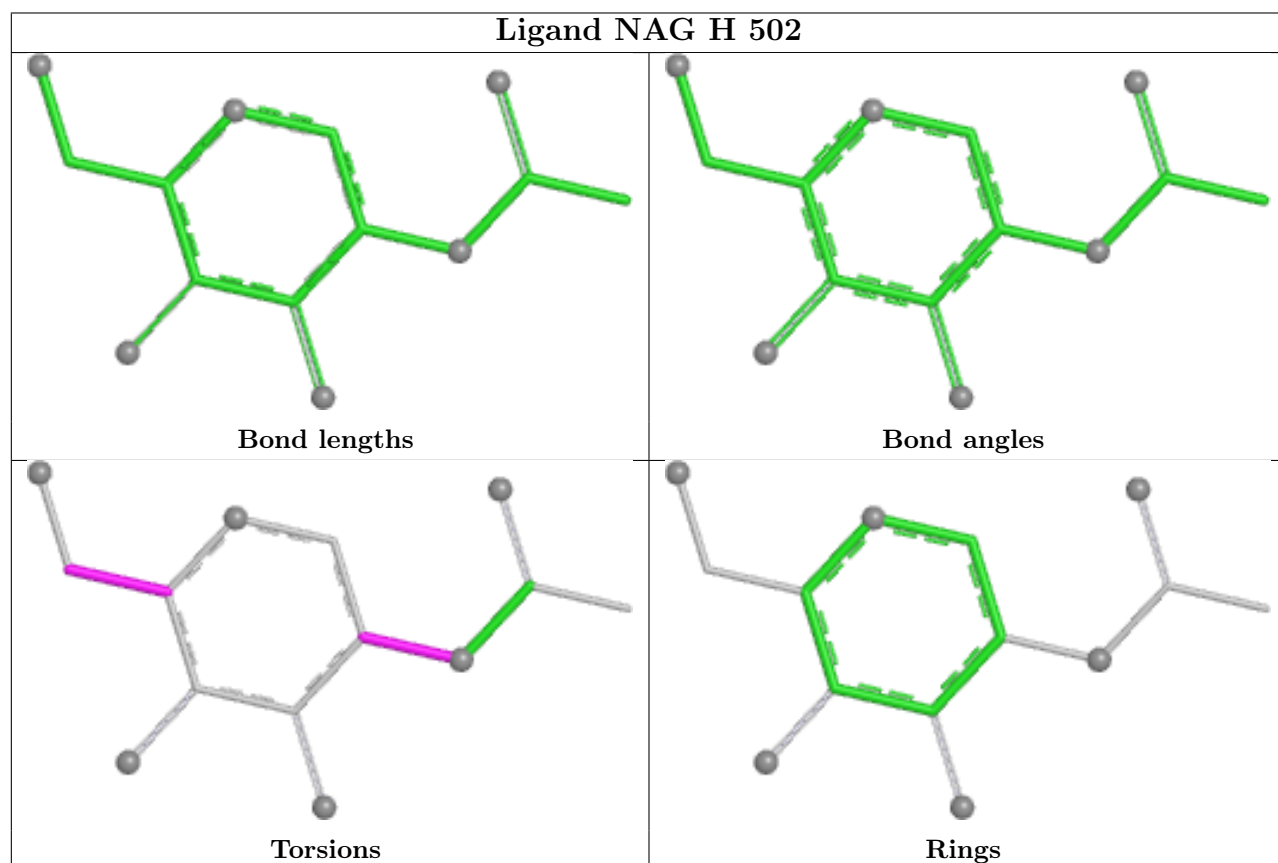
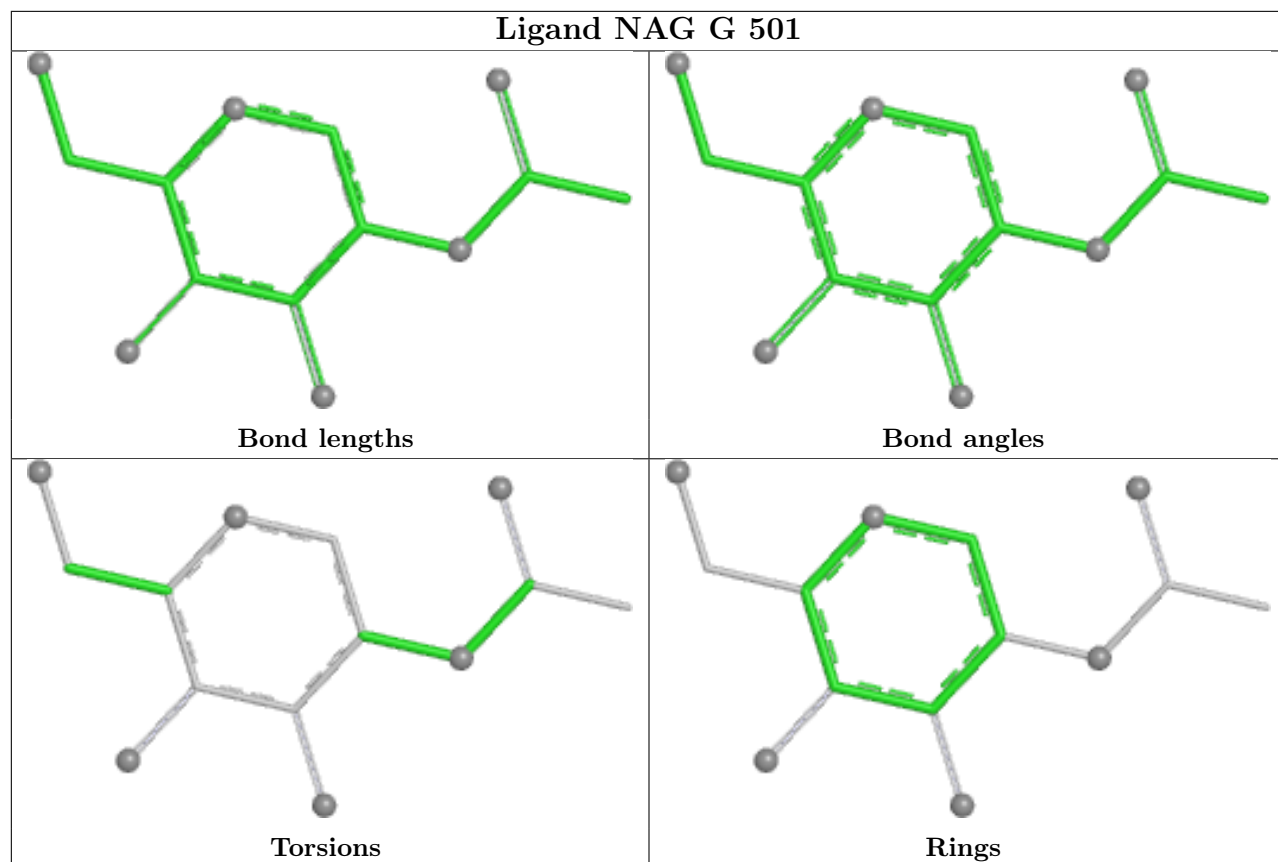
4 monomers are involved in 4 short contacts:

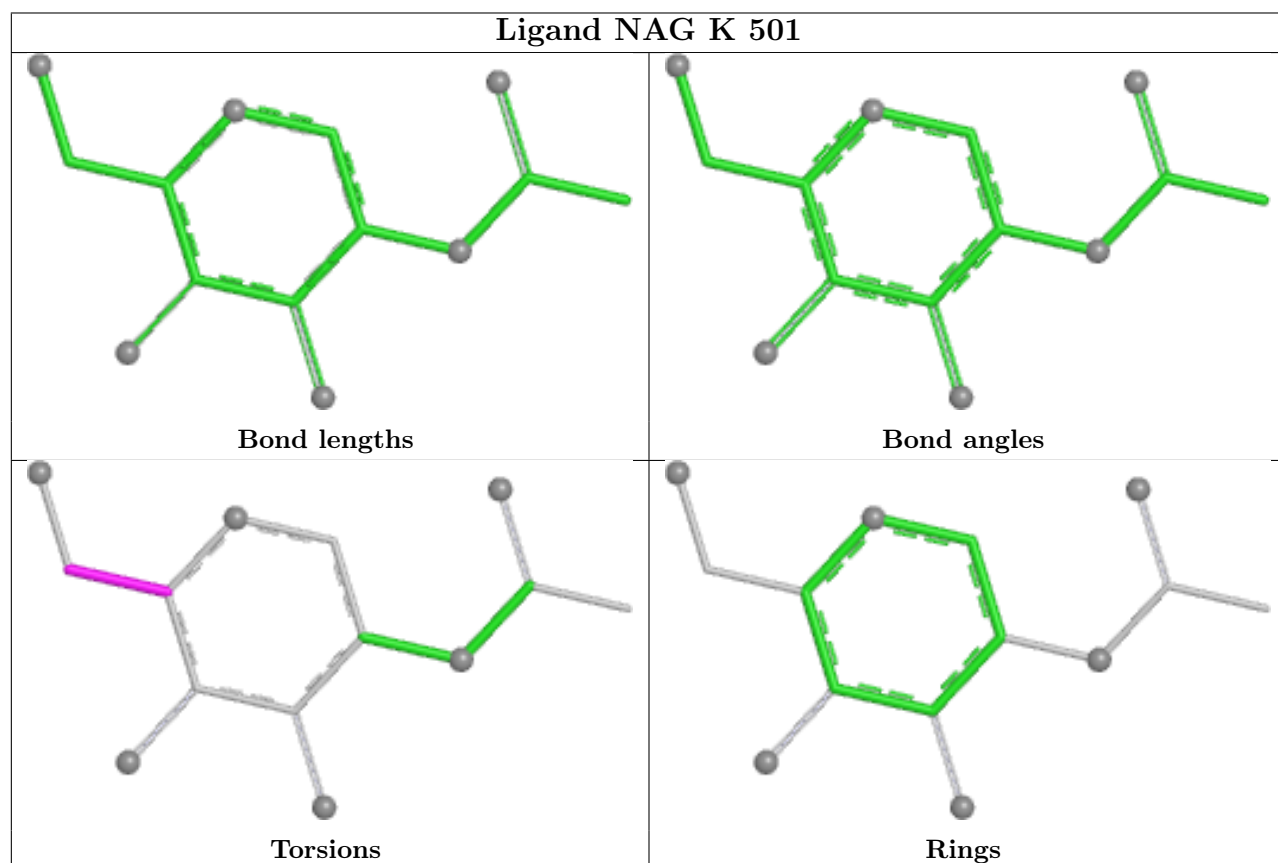
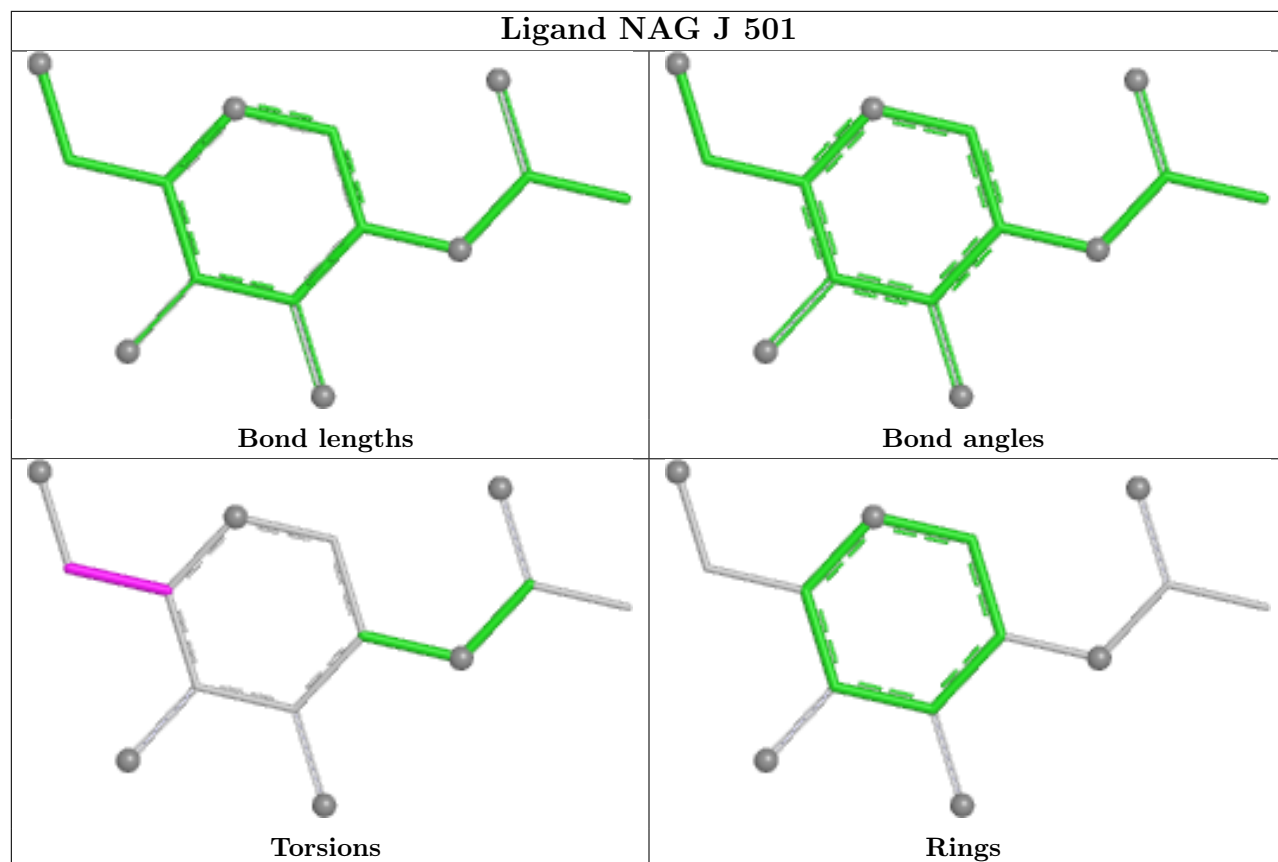
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	501	NAG	1	0
6	J	501	NAG	1	0
6	B	501	NAG	1	0
6	H	501	NAG	1	0

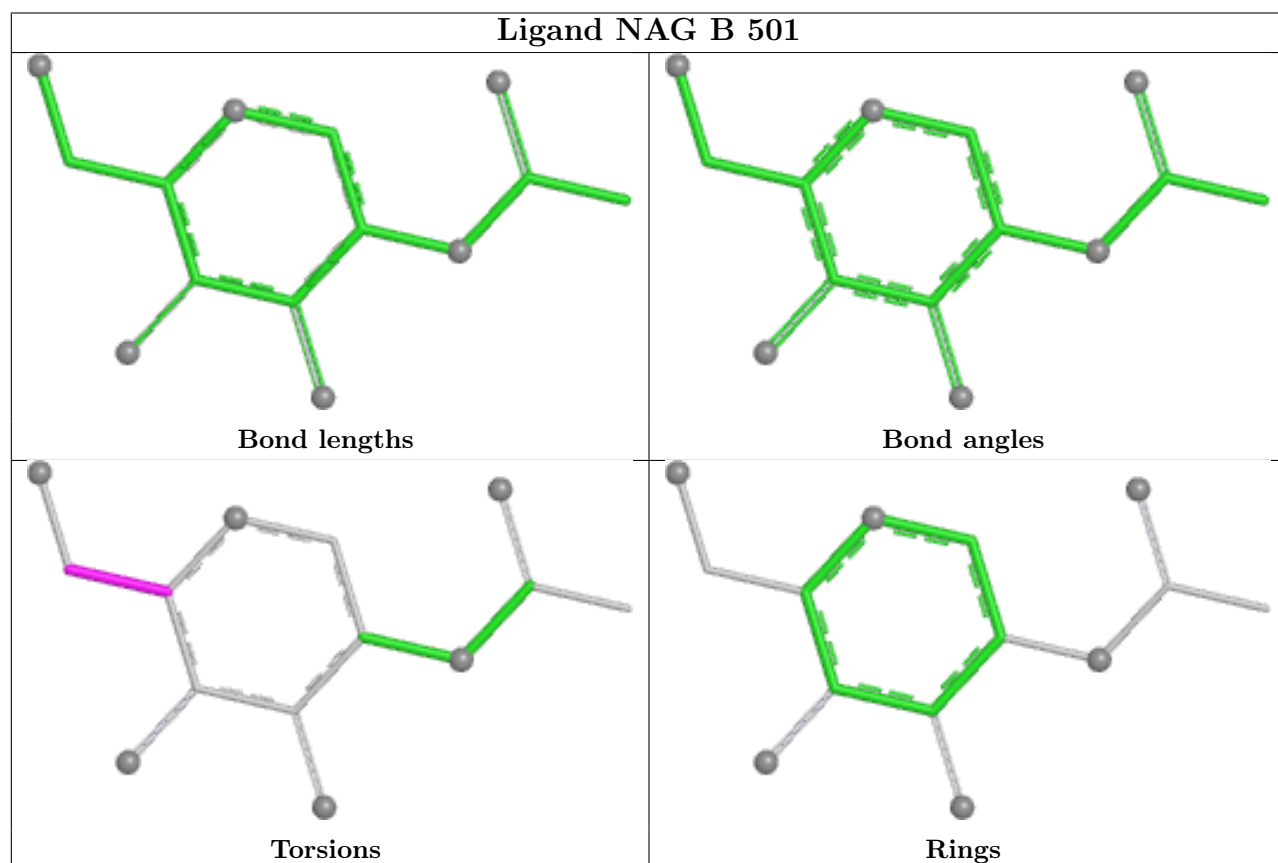
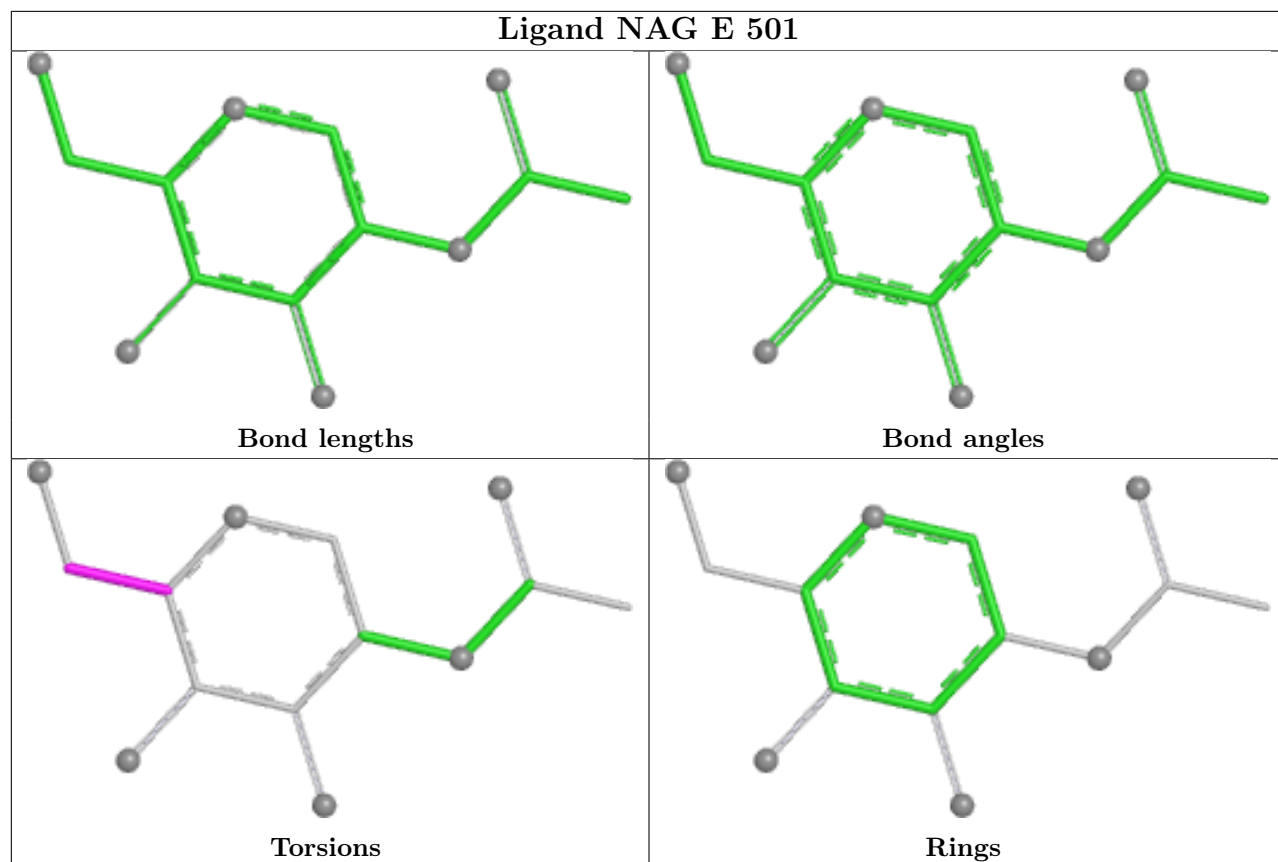
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

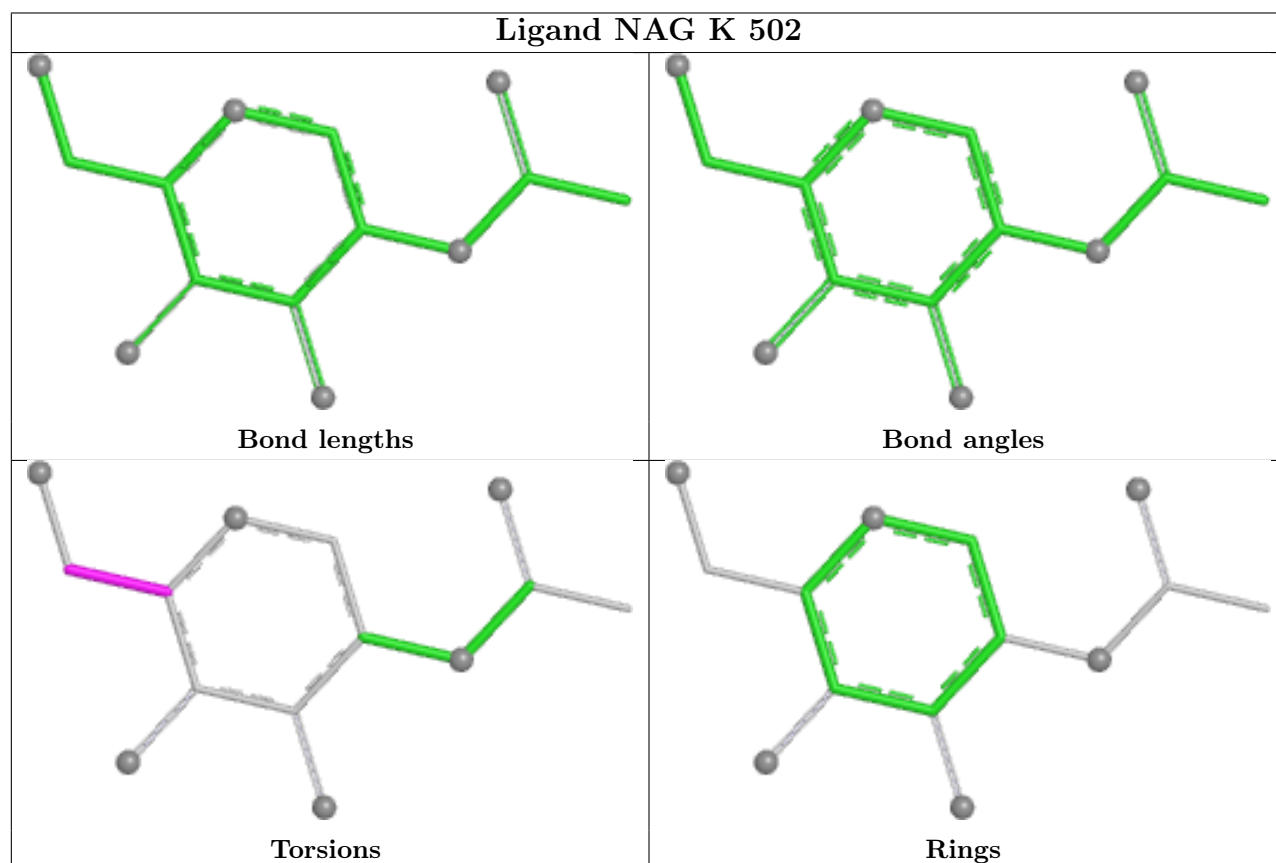
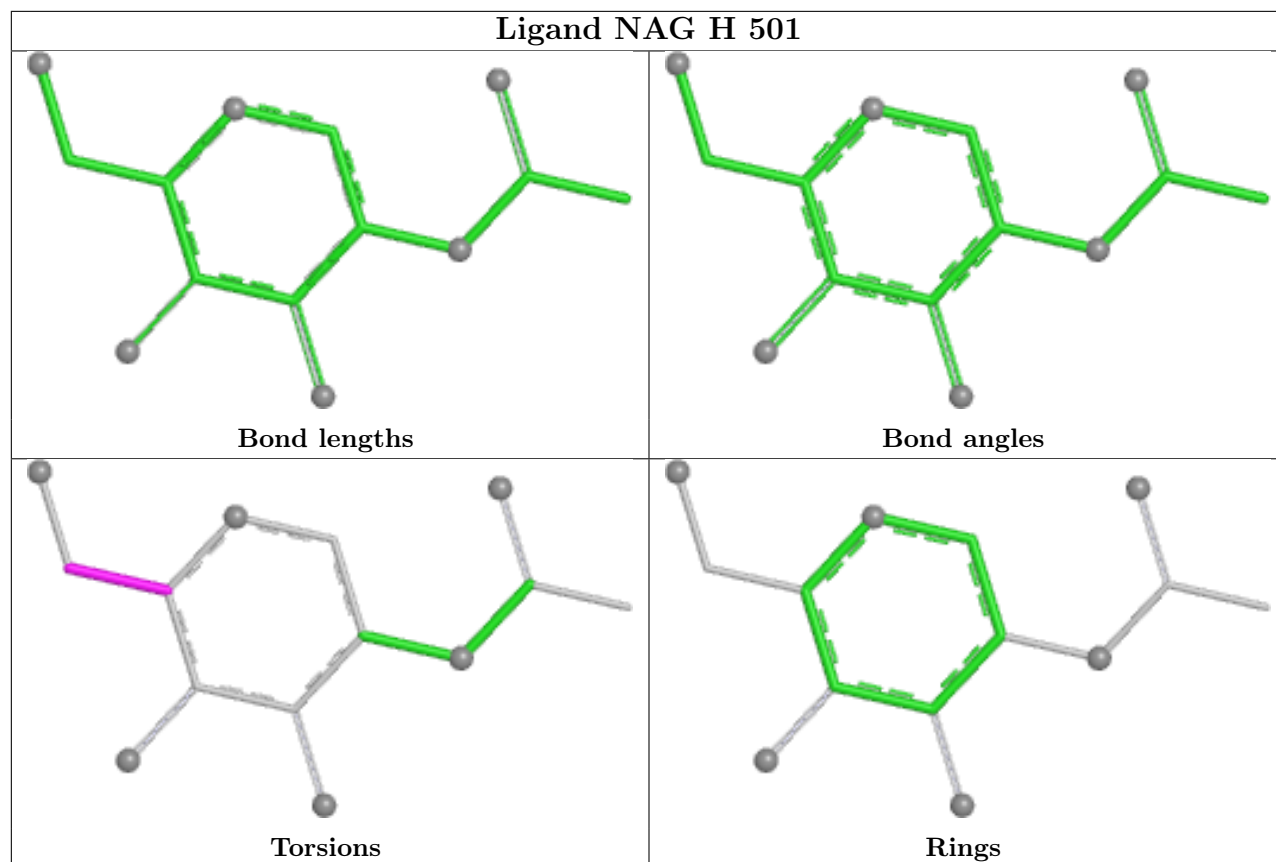












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25104. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

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 standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 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.