



Full wwPDB EM Validation Report ⓘ

Jun 2, 2026 – 04:19 PM JST

PDB ID : 9VFR / pdb_00009vfr
EMDB ID : EMD-65032
Title : Structure of mature Cocksackievirus A6 virion complexed with its receptor KREMEN1
Authors : Ke, X.; Li, X.; Liu, Z.; Liu, K.; Yan, X.; Shu, B.; Zhang, C.
Deposited on : 2025-06-11
Resolution : 2.55 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

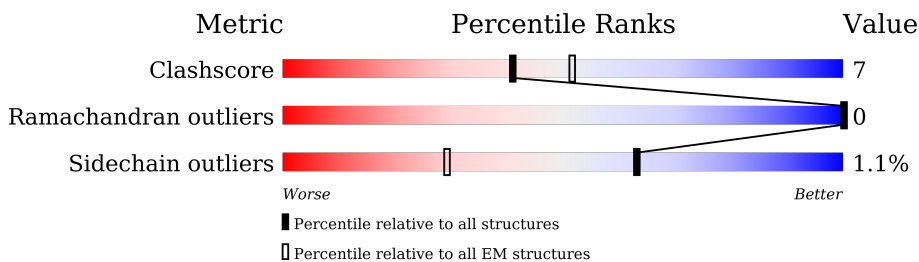
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.55 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	305	
2	B	256	
3	C	240	
4	D	69	
5	G	293	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8479 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 Genome polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	292	Total	C	N	O	S	0	0
			2224	1396	391	426	11		

- Molecule 2 is a protein called Genome polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	249	Total	C	N	O	S	0	0
			1890	1218	318	347	7		

- Molecule 3 is a protein called Genome polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	240	Total	C	N	O	S	0	0
			1823	1174	300	340	9		

- Molecule 4 is a protein called Genome polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	45	Total	C	N	O	0	0
			337	215	59	63		

There is a discrepancy between the modelled and reference sequences:

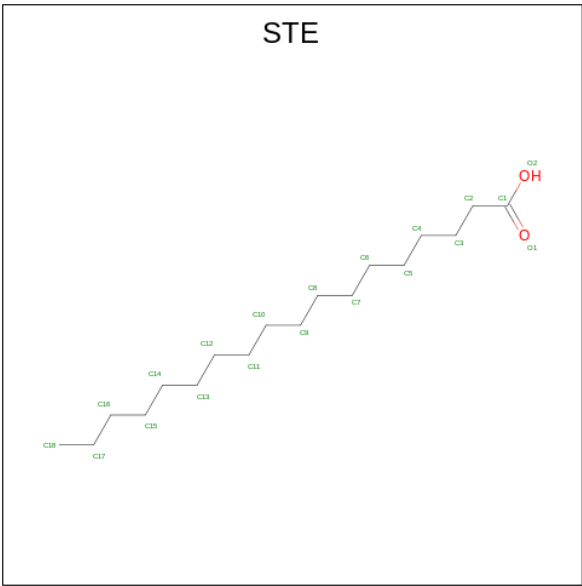
Chain	Residue	Modelled	Actual	Comment	Reference
D	39	ALA	VAL	conflict	UNP E3VJS6

- Molecule 5 is a protein called Kremen protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	293	Total	C	N	O	S	0	0
			2141	1368	374	381	18		

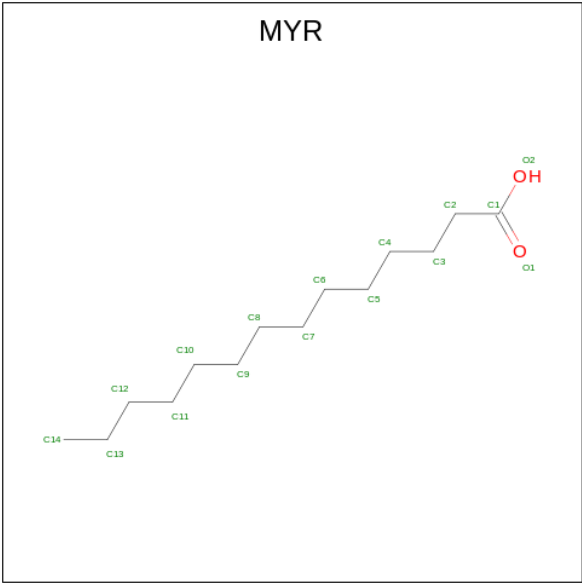
- Molecule 6 is STEARIC ACID (CCD ID: STE) (formula: C₁₈H₃₆O₂) (labeled as "Ligand of

Interest" by depositor).



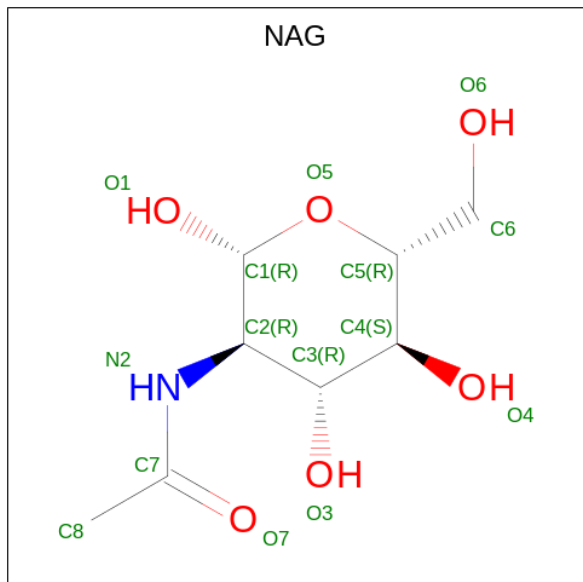
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			20	18	2	

- Molecule 7 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
7	D	1	Total	C	O	0
			16	14	2	

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

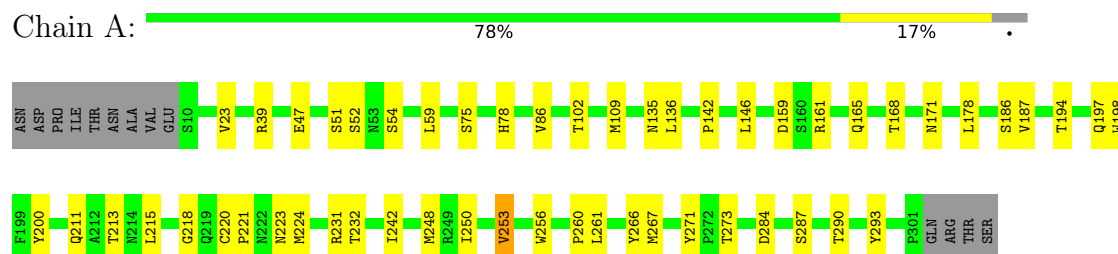


Mol	Chain	Residues	Atoms				AltConf
8	G	1	Total	C	N	O	0
			14	8	1	5	
8	G	1	Total	C	N	O	0
			14	8	1	5	

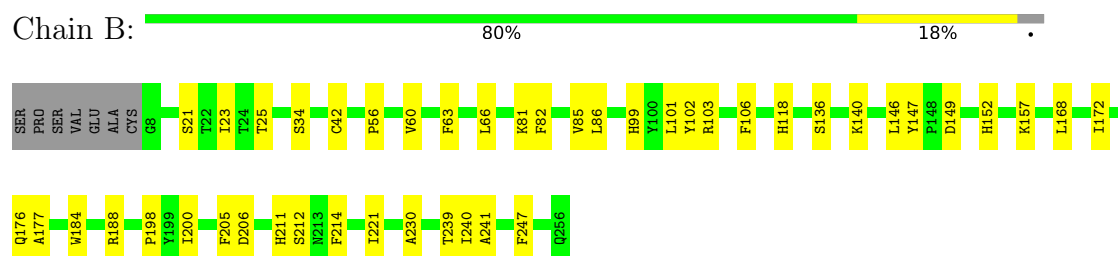
3 Residue-property plots [i](#)

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.

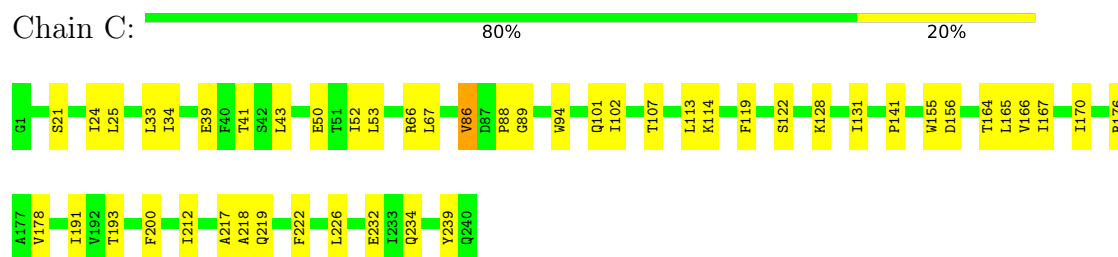
- Molecule 1: Genome polyprotein



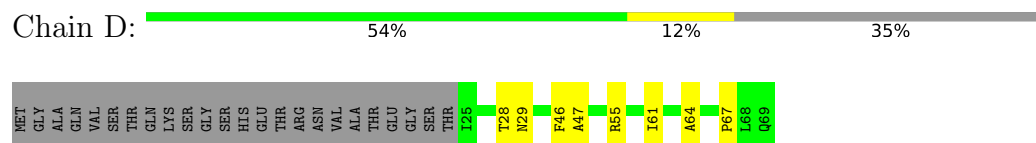
- Molecule 2: Genome polyprotein



- Molecule 3: Genome polyprotein



- Molecule 4: Genome polyprotein

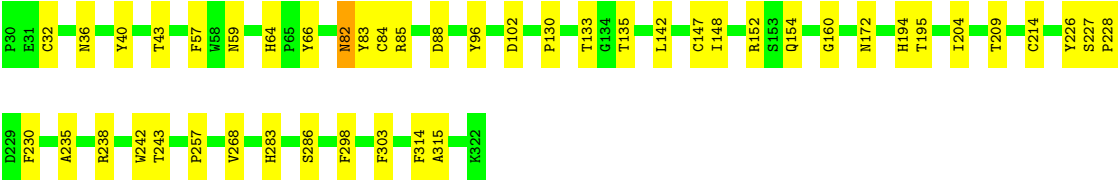


- Molecule 5: Kremen protein 1

Chain G:

84%

15%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	19306	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/2281	0.32	0/3118
2	B	0.32	0/1948	0.31	0/2675
3	C	0.35	0/1873	0.36	0/2569
4	D	0.25	0/345	0.28	0/469
5	G	0.24	0/2214	0.31	0/3026
All	All	0.30	0/8661	0.32	0/11857

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2224	0	2131	42	0
2	B	1890	0	1801	29	0
3	C	1823	0	1786	35	0
4	D	337	0	310	6	0
5	G	2141	0	1839	27	0
6	A	20	0	35	1	0
7	D	16	0	27	0	0
8	G	28	0	26	1	0
All	All	8479	0	7955	114	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 7.

All (114) 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)
5:G:283:HIS:H	5:G:286:SER:HB2	1.53	0.72
3:C:24:ILE:HG13	3:C:25:LEU:HG	1.77	0.65
1:A:260:PRO:HB3	2:B:176:GLN:HB2	1.79	0.64
1:A:52:SER:HB3	3:C:114:LYS:HD2	1.81	0.63
3:C:50:GLU:HA	3:C:217:ALA:HB2	1.81	0.62
2:B:85:VAL:HG23	2:B:157:LYS:HA	1.83	0.61
1:A:54:SER:O	3:C:219:GLN:NE2	2.34	0.61
5:G:130:PRO:HD2	5:G:133:THR:HG22	1.84	0.60
5:G:227:SER:HB3	5:G:314:PHE:H	1.67	0.59
5:G:243:THR:HG23	5:G:298:PHE:HE1	1.67	0.58
5:G:214:CYS:SG	5:G:238:ARG:NH1	2.75	0.58
3:C:88:PRO:HG3	3:C:113:LEU:HD11	1.85	0.57
5:G:226:TYR:HB3	5:G:230:PHE:HB2	1.88	0.56
3:C:41:THR:OG1	4:D:47:ALA:O	2.24	0.56
1:A:168:THR:OG1	1:A:171:ASN:O	2.25	0.55
1:A:47:GLU:HA	2:B:184:TRP:HB2	1.86	0.55
5:G:148:ILE:HG23	5:G:209:THR:HA	1.89	0.55
2:B:66:LEU:HD13	2:B:85:VAL:HG22	1.88	0.55
2:B:82:PHE:O	2:B:85:VAL:HG12	2.07	0.55
2:B:188:ARG:NH1	3:C:122:SER:O	2.40	0.55
2:B:149:ASP:OD1	2:B:152:HIS:ND1	2.40	0.54
5:G:84:CYS:O	5:G:85:ARG:NH1	2.34	0.54
2:B:168:LEU:HD11	2:B:177:ALA:HB2	1.88	0.54
1:A:250:ILE:HG22	1:A:253:VAL:HG22	1.89	0.54
1:A:215:LEU:O	1:A:271:TYR:OH	2.20	0.54
5:G:133:THR:N	5:G:172:ASN:OD1	2.40	0.53
1:A:198:TRP:HZ3	6:A:401:STE:H41	1.74	0.53
2:B:176:GLN:HE22	3:C:101:GLN:HG3	1.73	0.52
2:B:86:LEU:HG	2:B:240:ILE:HD11	1.92	0.52
5:G:32:CYS:SG	5:G:40:TYR:HB2	2.50	0.51
1:A:221:PRO:HB3	1:A:224:MET:HE2	1.92	0.51
1:A:260:PRO:HB2	2:B:172:ILE:HB	1.91	0.51
3:C:89:GLY:HA3	3:C:178:VAL:HG13	1.93	0.50
3:C:128:LYS:NZ	3:C:156:ASP:OD2	2.38	0.50
1:A:200:TYR:O	1:A:218:GLY:HA2	2.12	0.50
1:A:213:THR:O	2:B:147:TYR:HB2	2.11	0.50
2:B:56:PRO:O	2:B:60:VAL:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ASP:OD1	3:C:66:ARG:NH2	2.46	0.49
2:B:42:CYS:HB2	2:B:103:ARG:HD3	1.93	0.49
3:C:86:VAL:HG11	3:C:167:ILE:HG12	1.95	0.49
5:G:268:VAL:HG22	5:G:303:PHE:HD1	1.78	0.49
1:A:51:SER:O	4:D:55:ARG:NH1	2.38	0.49
1:A:293:TYR:HB3	3:C:191:ILE:HD11	1.95	0.48
3:C:52:ILE:HG21	3:C:67:LEU:HB3	1.95	0.48
1:A:186:SER:OG	3:C:21:SER:OG	2.24	0.48
5:G:235:ALA:HB3	5:G:238:ARG:HE	1.78	0.48
1:A:221:PRO:HA	1:A:224:MET:HG3	1.96	0.48
2:B:118:HIS:CE1	2:B:230:ALA:HB1	2.49	0.48
1:A:266:TYR:HB2	3:C:239:TYR:CZ	2.49	0.48
3:C:131:ILE:HG22	3:C:165:LEU:HD22	1.94	0.47
4:D:28:THR:OG1	4:D:29:ASN:N	2.47	0.47
1:A:267:MET:HE2	1:A:273:THR:HG22	1.96	0.47
5:G:43:THR:HG23	5:G:83:TYR:CZ	2.49	0.47
1:A:59:LEU:HD12	3:C:166:VAL:HG13	1.97	0.47
2:B:200:ILE:H	2:B:214:PHE:HZ	1.61	0.47
1:A:142:PRO:O	1:A:178:LEU:HB2	2.15	0.47
5:G:82:ASN:ND2	8:G:401:NAG:O7	2.48	0.46
5:G:257:PRO:HD2	5:G:315:ALA:O	2.16	0.46
5:G:36:ASN:HB3	5:G:195:THR:O	2.15	0.46
2:B:23:ILE:HD11	2:B:239:THR:HG21	1.97	0.46
1:A:287:SER:HB3	1:A:290:THR:HG23	1.97	0.46
5:G:57:PHE:HB3	5:G:59:ASN:OD1	2.16	0.46
2:B:82:PHE:CZ	2:B:106:PHE:HB3	2.51	0.46
3:C:170:ILE:O	3:C:176:ARG:NH2	2.41	0.46
1:A:161:ARG:O	1:A:231:ARG:NH1	2.45	0.46
1:A:256:TRP:CD1	3:C:39:GLU:HB2	2.51	0.46
2:B:184:TRP:CZ3	2:B:221:ILE:HG13	2.51	0.46
3:C:43:LEU:HD23	3:C:102:ILE:HG23	1.97	0.46
1:A:75:SER:OG	1:A:78:HIS:ND1	2.44	0.45
1:A:86:VAL:HG11	1:A:248:MET:HE2	1.98	0.45
1:A:146:LEU:HD11	1:A:242:ILE:HG21	1.97	0.45
5:G:135:THR:HG21	5:G:154:GLN:NE2	2.32	0.45
2:B:101:LEU:HB3	2:B:205:PHE:HB3	1.99	0.45
1:A:75:SER:HB3	4:D:46:PHE:HD1	1.80	0.45
4:D:61:ILE:HD13	4:D:67:PRO:HB3	1.97	0.45
3:C:114:LYS:HG3	3:C:164:THR:HG23	1.97	0.45
1:A:194:THR:HG23	3:C:33:LEU:HA	1.99	0.45
2:B:34:SER:HB2	2:B:198:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:HG3	4:D:64:ALA:HB1	1.98	0.45
1:A:146:LEU:HD23	1:A:232:THR:HA	1.99	0.44
1:A:159:ASP:OD1	1:A:159:ASP:N	2.44	0.44
1:A:197:GLN:O	1:A:223:ASN:ND2	2.50	0.44
3:C:53:LEU:HD21	3:C:94:TRP:CD2	2.53	0.44
2:B:206:ASP:OD2	2:B:211:HIS:ND1	2.46	0.44
5:G:160:GLY:HA3	5:G:204:ILE:HD11	1.99	0.44
2:B:106:PHE:HE2	2:B:214:PHE:CD1	2.35	0.44
2:B:136:SER:HB3	2:B:146:LEU:HD23	2.01	0.43
2:B:21:SER:HB3	2:B:63:PHE:HB2	2.00	0.43
2:B:99:HIS:CG	2:B:247:PHE:HB3	2.54	0.43
2:B:140:LYS:NZ	5:G:88:ASP:OD2	2.49	0.43
5:G:142:LEU:HD11	5:G:147:CYS:HB2	2.00	0.43
3:C:141:PRO:HD2	3:C:193:THR:HG21	2.01	0.43
5:G:152:ARG:NH1	5:G:209:THR:O	2.48	0.43
1:A:194:THR:HG21	3:C:34:ILE:HG12	2.01	0.43
3:C:107:THR:HB	3:C:226:LEU:HB3	2.00	0.43
1:A:261:LEU:HD12	3:C:101:GLN:HB3	2.00	0.42
1:A:109:MET:HE2	1:A:198:TRP:CE3	2.54	0.42
1:A:59:LEU:HD12	3:C:166:VAL:HG22	2.02	0.42
3:C:114:LYS:HE3	3:C:217:ALA:HB3	2.01	0.42
3:C:218:ALA:HB1	3:C:222:PHE:CG	2.55	0.42
1:A:135:ASN:ND2	1:A:136:LEU:O	2.52	0.42
3:C:101:GLN:OE1	3:C:232:GLU:HG3	2.19	0.42
5:G:82:ASN:OD1	5:G:82:ASN:N	2.42	0.41
2:B:63:PHE:CD1	2:B:241:ALA:HB2	2.55	0.41
1:A:187:VAL:HG22	3:C:24:ILE:HD13	2.02	0.41
3:C:155:TRP:HZ3	3:C:212:ILE:HD13	1.85	0.41
1:A:211:GLN:HG3	5:G:194:HIS:HE1	1.85	0.41
5:G:64:HIS:HB3	5:G:96:TYR:CZ	2.55	0.41
1:A:200:TYR:CG	1:A:220:CYS:HB2	2.55	0.40
5:G:66:TYR:CZ	5:G:88:ASP:HB3	2.56	0.40
2:B:81:LYS:HB3	2:B:212:SER:HB3	2.03	0.40
3:C:119:PHE:CZ	3:C:200:PHE:HE1	2.40	0.40
1:A:165:GLN:OE1	1:A:165:GLN:N	2.45	0.40
5:G:228:PRO:HD3	5:G:242:TRP:HH2	1.86	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	290/305 (95%)	278 (96%)	12 (4%)	0	100	100
2	B	247/256 (96%)	241 (98%)	6 (2%)	0	100	100
3	C	238/240 (99%)	231 (97%)	7 (3%)	0	100	100
4	D	43/69 (62%)	42 (98%)	1 (2%)	0	100	100
5	G	291/293 (99%)	262 (90%)	29 (10%)	0	100	100
All	All	1109/1163 (95%)	1054 (95%)	55 (5%)	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	237/260 (91%)	234 (99%)	3 (1%)	61	76
2	B	198/218 (91%)	196 (99%)	2 (1%)	68	80
3	C	197/206 (96%)	195 (99%)	2 (1%)	68	80
4	D	30/55 (54%)	30 (100%)	0	100	100
5	G	194/245 (79%)	192 (99%)	2 (1%)	68	80
All	All	856/984 (87%)	847 (99%)	9 (1%)	63	79

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	102	THR
1	A	253	VAL
2	B	25	THR
2	B	102	TYR
3	C	86	VAL
3	C	234	GLN
5	G	82	ASN
5	G	102	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	135	ASN
1	A	197	GLN
1	A	211	GLN
2	B	142	ASN
2	B	176	GLN
3	C	74	GLN
3	C	85	GLN
3	C	108	GLN
3	C	211	ASN
5	G	64	HIS
5	G	100	HIS
5	G	115	GLN
5	G	140	ASN
5	G	194	HIS

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

4 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	STE	A	401	-	19,19,19	0.53	0	19,19,19	0.52	0
7	MYR	D	101	-	15,15,15	0.61	0	15,15,15	0.74	0
8	NAG	G	402	5	14,14,15	0.19	0	17,19,21	0.45	0
8	NAG	G	401	5	14,14,15	0.20	0	17,19,21	0.42	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	STE	A	401	-	-	11/17/17/17	-
7	MYR	D	101	-	-	6/13/13/13	-
8	NAG	G	402	5	-	0/6/23/26	0/1/1/1
8	NAG	G	401	5	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	401	STE	C1-C2-C3-C4
6	A	401	STE	C2-C3-C4-C5
7	D	101	MYR	C3-C4-C5-C6
7	D	101	MYR	C5-C6-C7-C8
7	D	101	MYR	C2-C3-C4-C5
6	A	401	STE	C9-C10-C11-C12
6	A	401	STE	C7-C8-C9-C10

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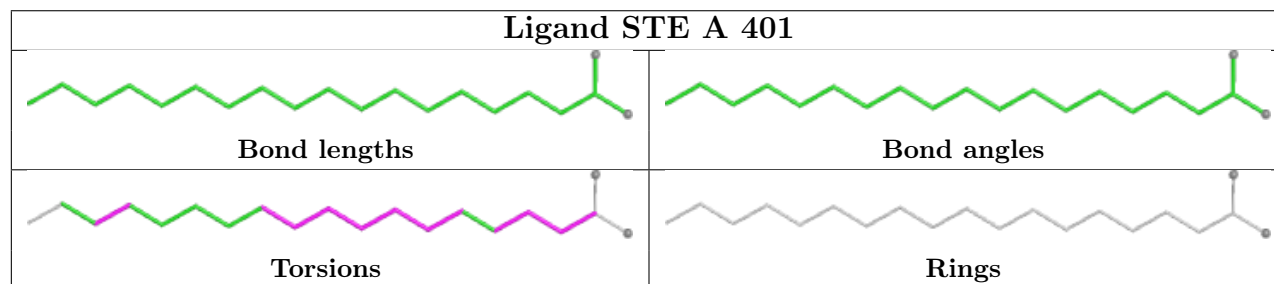
Mol	Chain	Res	Type	Atoms
6	A	401	STE	C14-C15-C16-C17
8	G	401	NAG	O5-C5-C6-O6
7	D	101	MYR	C11-C10-C9-C8
6	A	401	STE	C4-C5-C6-C7
6	A	401	STE	C11-C10-C9-C8
6	A	401	STE	C6-C7-C8-C9
7	D	101	MYR	O1-C1-C2-C3
7	D	101	MYR	O2-C1-C2-C3
6	A	401	STE	O2-C1-C2-C3
6	A	401	STE	O1-C1-C2-C3
6	A	401	STE	C5-C6-C7-C8

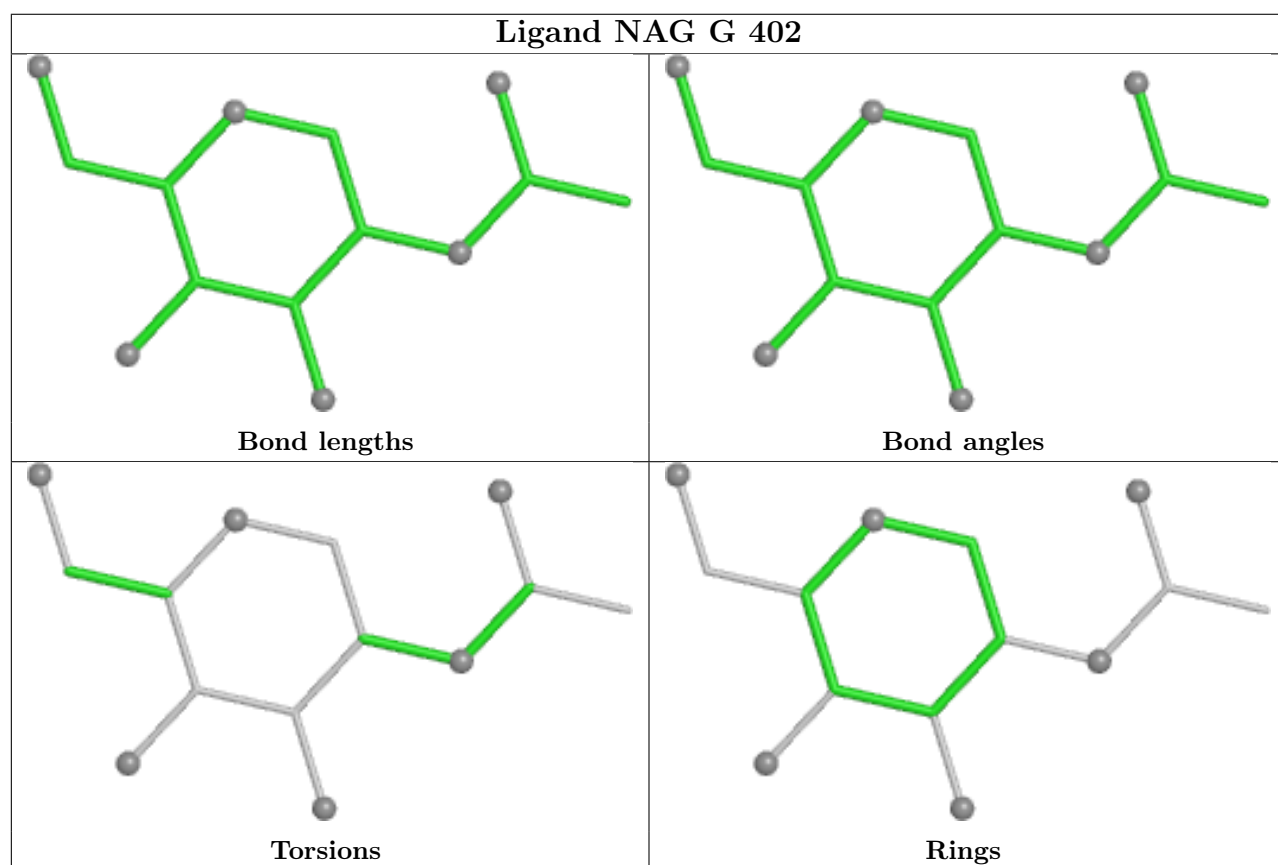
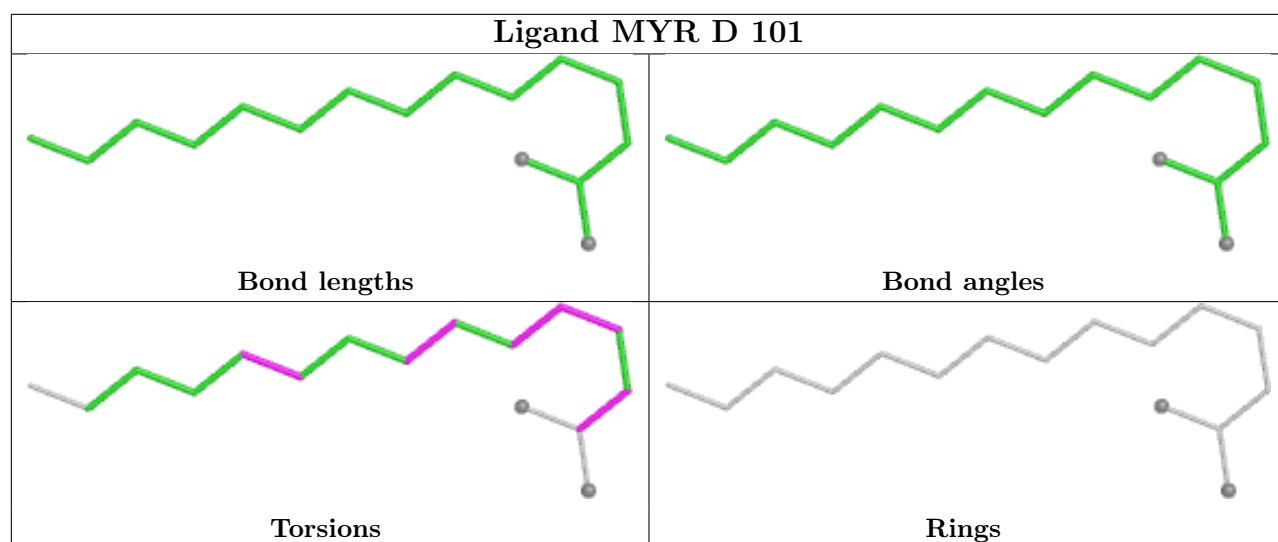
There are no ring outliers.

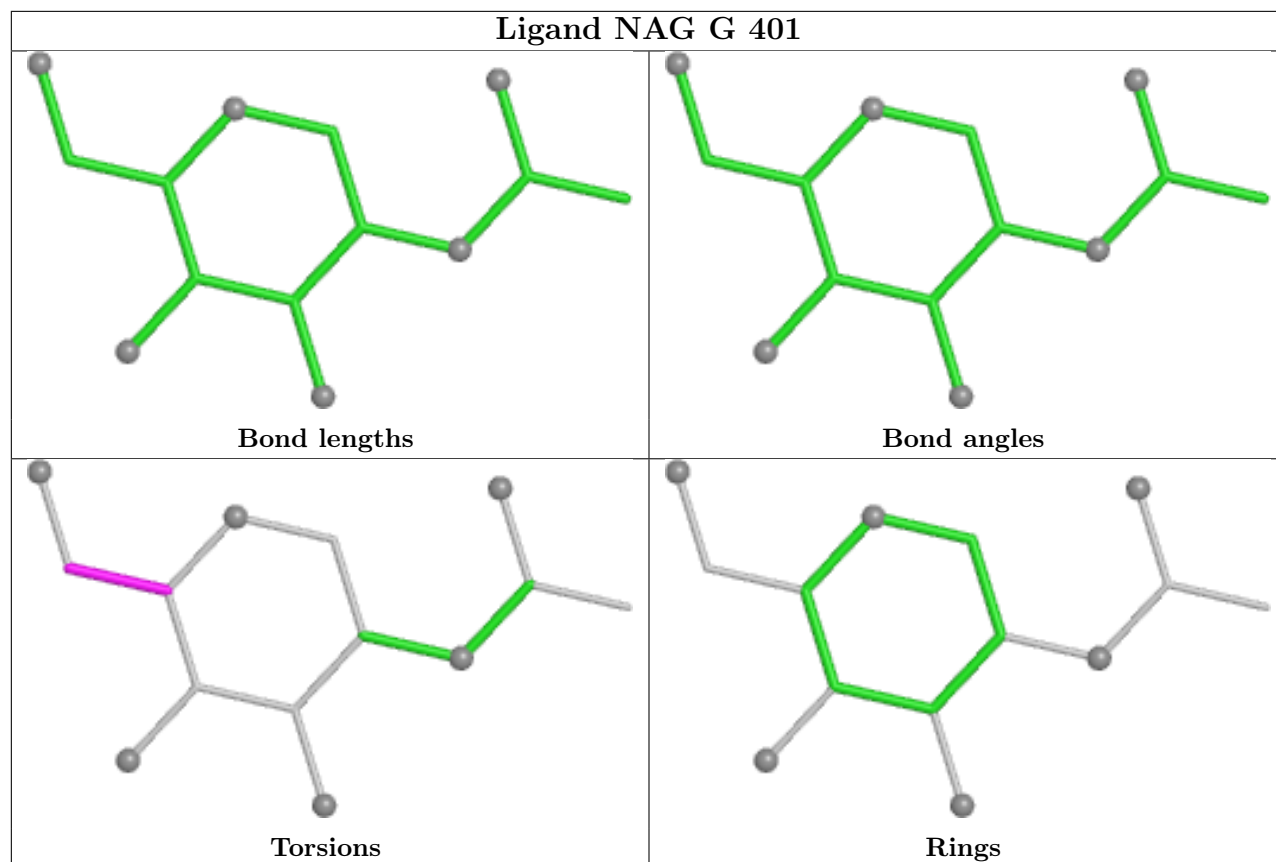
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	401	STE	1	0
8	G	401	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.