Full wwPDB EM Validation Report ⓘ

Jun 3, 2025 – 06:25 PM JST

PDB ID	:	8ZKT / pdb_00008zkt
EMDB ID	:	EMD-60208
Title	:	Structure of Polycystin-1/Polycystin-2 complex with GOF mutations
Authors	:	Chen, M.Y.; Su, Q.; Shi, Y.G.
Deposited on	:	2024-05-17
Resolution	:	3.34 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:

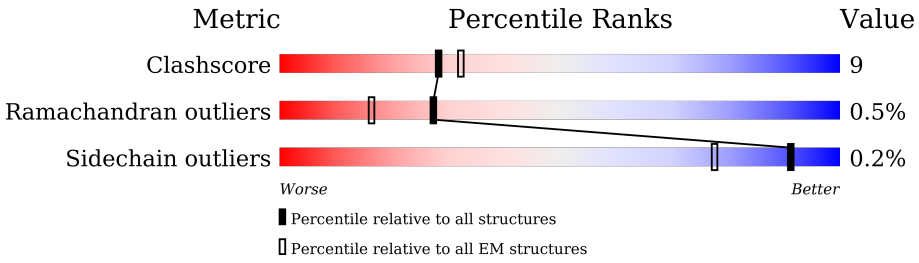
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.34 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1261	49% 10% • 40%
2	B	1007	41% 7% 53%
2	C	1007	40% 7% 53%
2	D	1007	35% 10% 54%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17369 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 Polycystin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	753	Total	C	N	O	S	0	0
			5586	3602	1020	947	17		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3043	MET	-	initiating methionine	UNP P98161
A	3044	ASP	-	expression tag	UNP P98161
A	3045	TYR	-	expression tag	UNP P98161
A	3046	LYS	-	expression tag	UNP P98161
A	3047	ASP	-	expression tag	UNP P98161
A	3048	ASP	-	expression tag	UNP P98161
A	3049	ASP	-	expression tag	UNP P98161
A	3050	ASP	-	expression tag	UNP P98161
A	3051	LYS	-	expression tag	UNP P98161

- Molecule 2 is a protein called Polycystin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	475	Total	C	N	O	S	0	0
			3924	2592	619	693	20		
2	C	475	Total	C	N	O	S	0	0
			3923	2591	619	693	20		
2	D	463	Total	C	N	O	S	0	0
			3810	2517	601	672	20		

There are 117 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-38	MET	-	initiating methionine	UNP Q13563
B	-37	GLY	-	expression tag	UNP Q13563
B	-36	ALA	-	expression tag	UNP Q13563
B	-35	SER	-	expression tag	UNP Q13563

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-34	SER	-	expression tag	UNP Q13563
B	-33	ALA	-	expression tag	UNP Q13563
B	-32	TRP	-	expression tag	UNP Q13563
B	-31	SER	-	expression tag	UNP Q13563
B	-30	HIS	-	expression tag	UNP Q13563
B	-29	PRO	-	expression tag	UNP Q13563
B	-28	GLN	-	expression tag	UNP Q13563
B	-27	PHE	-	expression tag	UNP Q13563
B	-26	GLU	-	expression tag	UNP Q13563
B	-25	LYS	-	expression tag	UNP Q13563
B	-24	GLY	-	expression tag	UNP Q13563
B	-23	GLY	-	expression tag	UNP Q13563
B	-22	GLY	-	expression tag	UNP Q13563
B	-21	SER	-	expression tag	UNP Q13563
B	-20	GLY	-	expression tag	UNP Q13563
B	-19	GLY	-	expression tag	UNP Q13563
B	-18	GLY	-	expression tag	UNP Q13563
B	-17	SER	-	expression tag	UNP Q13563
B	-16	GLY	-	expression tag	UNP Q13563
B	-15	GLY	-	expression tag	UNP Q13563
B	-14	SER	-	expression tag	UNP Q13563
B	-13	ALA	-	expression tag	UNP Q13563
B	-12	TRP	-	expression tag	UNP Q13563
B	-11	SER	-	expression tag	UNP Q13563
B	-10	HIS	-	expression tag	UNP Q13563
B	-9	PRO	-	expression tag	UNP Q13563
B	-8	GLN	-	expression tag	UNP Q13563
B	-7	PHE	-	expression tag	UNP Q13563
B	-6	GLU	-	expression tag	UNP Q13563
B	-5	LYS	-	expression tag	UNP Q13563
B	-4	GLY	-	expression tag	UNP Q13563
B	-3	SER	-	linker	UNP Q13563
B	-2	ALA	-	linker	UNP Q13563
B	-1	ALA	-	linker	UNP Q13563
B	0	ALA	-	linker	UNP Q13563
C	-38	MET	-	initiating methionine	UNP Q13563
C	-37	GLY	-	expression tag	UNP Q13563
C	-36	ALA	-	expression tag	UNP Q13563
C	-35	SER	-	expression tag	UNP Q13563
C	-34	SER	-	expression tag	UNP Q13563
C	-33	ALA	-	expression tag	UNP Q13563
C	-32	TRP	-	expression tag	UNP Q13563

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-31	SER	-	expression tag	UNP Q13563
C	-30	HIS	-	expression tag	UNP Q13563
C	-29	PRO	-	expression tag	UNP Q13563
C	-28	GLN	-	expression tag	UNP Q13563
C	-27	PHE	-	expression tag	UNP Q13563
C	-26	GLU	-	expression tag	UNP Q13563
C	-25	LYS	-	expression tag	UNP Q13563
C	-24	GLY	-	expression tag	UNP Q13563
C	-23	GLY	-	expression tag	UNP Q13563
C	-22	GLY	-	expression tag	UNP Q13563
C	-21	SER	-	expression tag	UNP Q13563
C	-20	GLY	-	expression tag	UNP Q13563
C	-19	GLY	-	expression tag	UNP Q13563
C	-18	GLY	-	expression tag	UNP Q13563
C	-17	SER	-	expression tag	UNP Q13563
C	-16	GLY	-	expression tag	UNP Q13563
C	-15	GLY	-	expression tag	UNP Q13563
C	-14	SER	-	expression tag	UNP Q13563
C	-13	ALA	-	expression tag	UNP Q13563
C	-12	TRP	-	expression tag	UNP Q13563
C	-11	SER	-	expression tag	UNP Q13563
C	-10	HIS	-	expression tag	UNP Q13563
C	-9	PRO	-	expression tag	UNP Q13563
C	-8	GLN	-	expression tag	UNP Q13563
C	-7	PHE	-	expression tag	UNP Q13563
C	-6	GLU	-	expression tag	UNP Q13563
C	-5	LYS	-	expression tag	UNP Q13563
C	-4	GLY	-	expression tag	UNP Q13563
C	-3	SER	-	linker	UNP Q13563
C	-2	ALA	-	linker	UNP Q13563
C	-1	ALA	-	linker	UNP Q13563
C	0	ALA	-	linker	UNP Q13563
D	-38	MET	-	initiating methionine	UNP Q13563
D	-37	GLY	-	expression tag	UNP Q13563
D	-36	ALA	-	expression tag	UNP Q13563
D	-35	SER	-	expression tag	UNP Q13563
D	-34	SER	-	expression tag	UNP Q13563
D	-33	ALA	-	expression tag	UNP Q13563
D	-32	TRP	-	expression tag	UNP Q13563
D	-31	SER	-	expression tag	UNP Q13563
D	-30	HIS	-	expression tag	UNP Q13563
D	-29	PRO	-	expression tag	UNP Q13563

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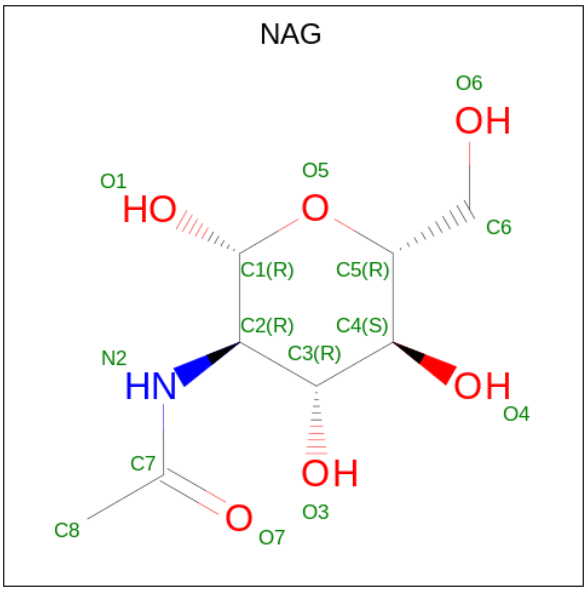
Chain	Residue	Modelled	Actual	Comment	Reference
D	-28	GLN	-	expression tag	UNP Q13563
D	-27	PHE	-	expression tag	UNP Q13563
D	-26	GLU	-	expression tag	UNP Q13563
D	-25	LYS	-	expression tag	UNP Q13563
D	-24	GLY	-	expression tag	UNP Q13563
D	-23	GLY	-	expression tag	UNP Q13563
D	-22	GLY	-	expression tag	UNP Q13563
D	-21	SER	-	expression tag	UNP Q13563
D	-20	GLY	-	expression tag	UNP Q13563
D	-19	GLY	-	expression tag	UNP Q13563
D	-18	GLY	-	expression tag	UNP Q13563
D	-17	SER	-	expression tag	UNP Q13563
D	-16	GLY	-	expression tag	UNP Q13563
D	-15	GLY	-	expression tag	UNP Q13563
D	-14	SER	-	expression tag	UNP Q13563
D	-13	ALA	-	expression tag	UNP Q13563
D	-12	TRP	-	expression tag	UNP Q13563
D	-11	SER	-	expression tag	UNP Q13563
D	-10	HIS	-	expression tag	UNP Q13563
D	-9	PRO	-	expression tag	UNP Q13563
D	-8	GLN	-	expression tag	UNP Q13563
D	-7	PHE	-	expression tag	UNP Q13563
D	-6	GLU	-	expression tag	UNP Q13563
D	-5	LYS	-	expression tag	UNP Q13563
D	-4	GLY	-	expression tag	UNP Q13563
D	-3	SER	-	linker	UNP Q13563
D	-2	ALA	-	linker	UNP Q13563
D	-1	ALA	-	linker	UNP Q13563
D	0	ALA	-	linker	UNP Q13563

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



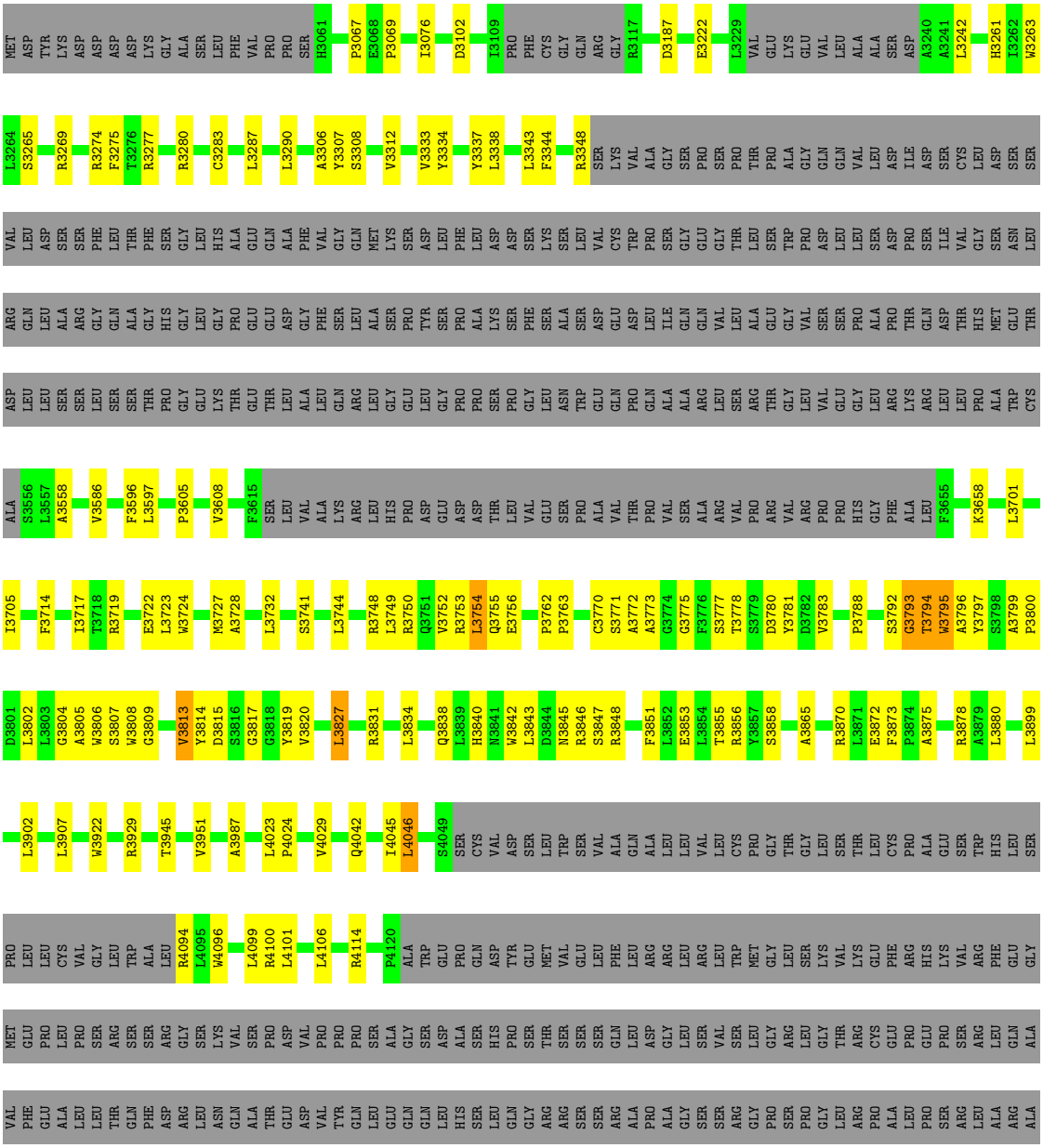
Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3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

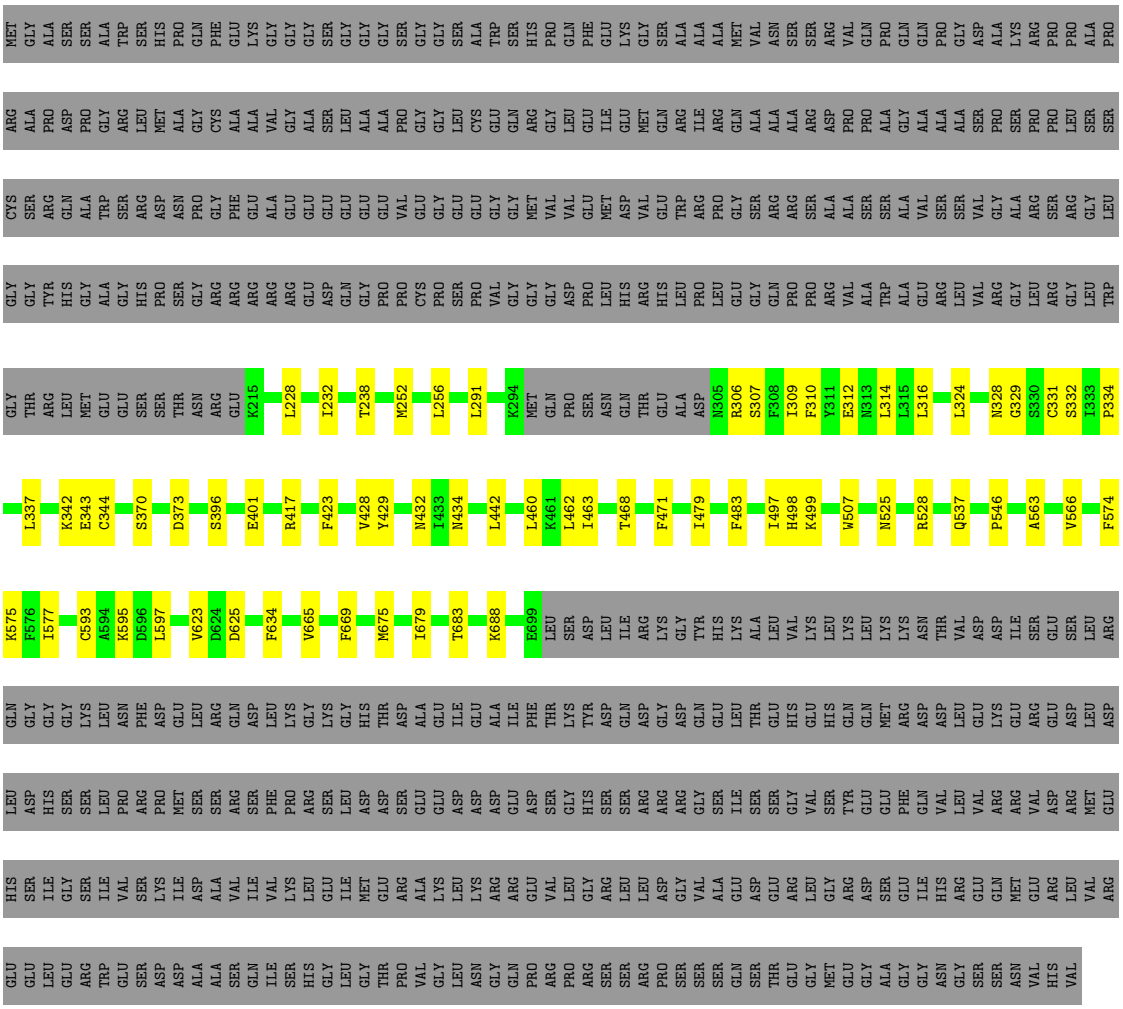
- Molecule 1: Polycystin-1

Chain A:



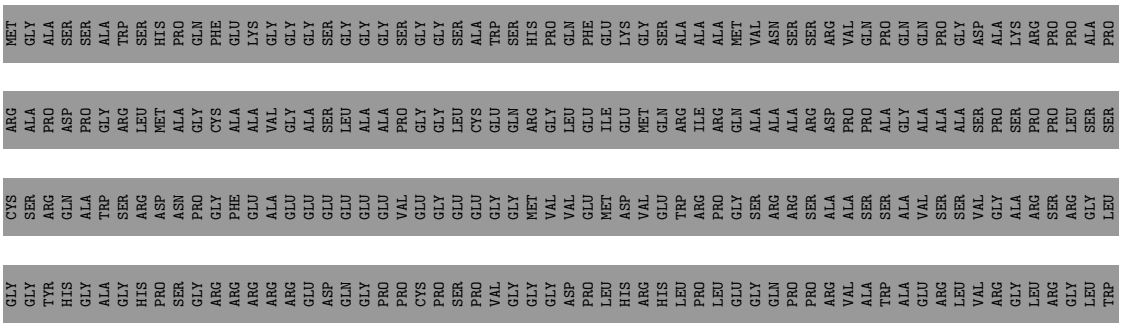
• Molecule 2: Polycystin-2

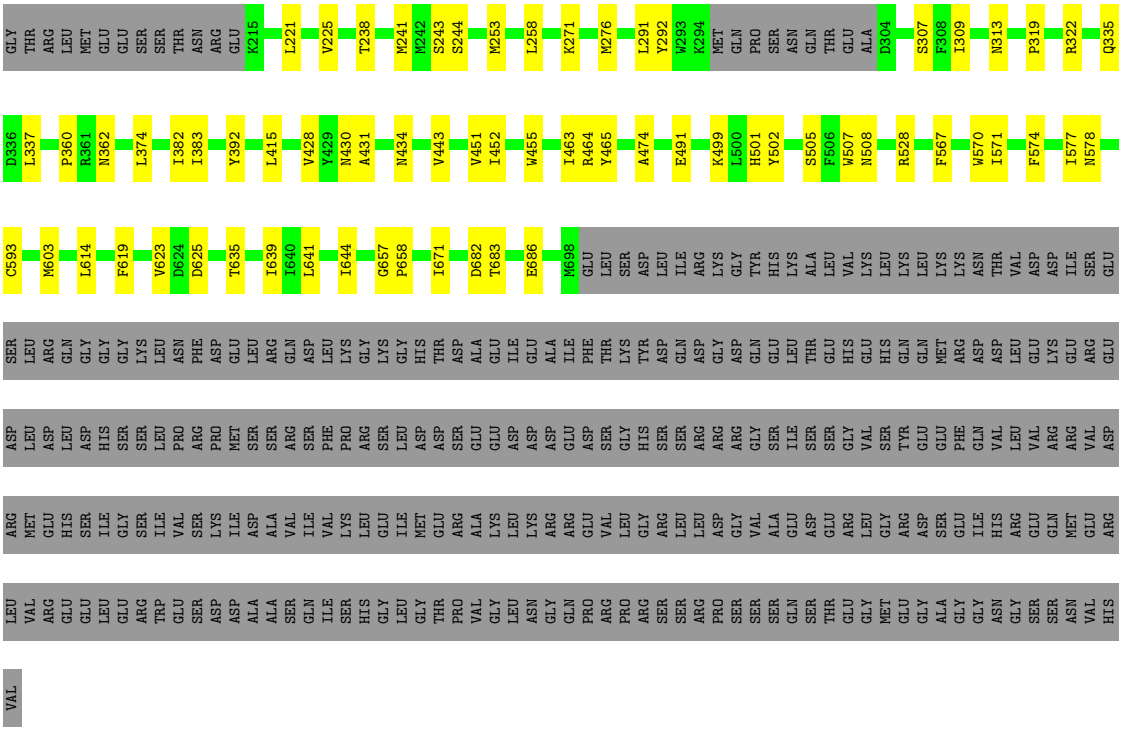
Chain B:



• Molecule 2: Polycystin-2

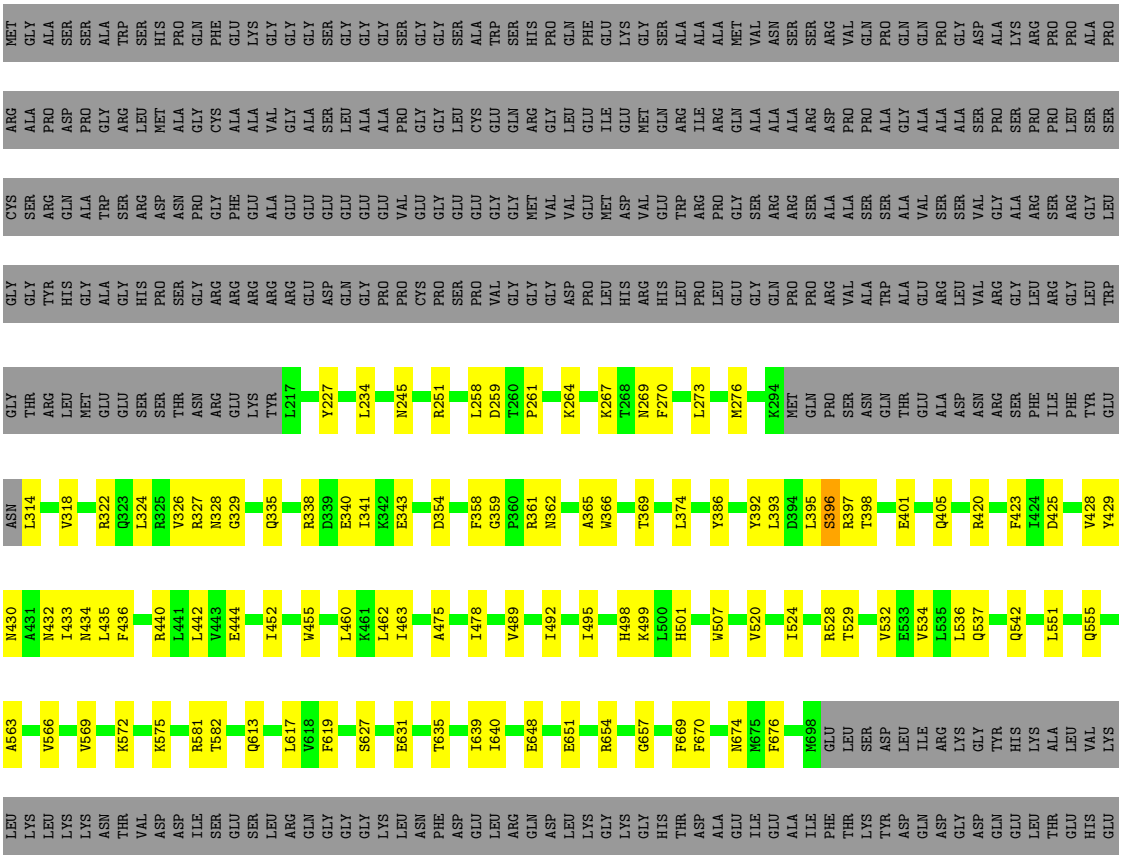
Chain C:





• Molecule 2: Polycystin-2

Chain D:



HIS GLN GLN MET ARG ASP ASP LEU GLU LYS GLU ARG GLU ASP LEU ASP LEU ASP HIS SER SER LEU PRO ARG PRO MET SER SER ARG SER PHE PRO ARG SER LEU ASP ASP SER GLU GLU ASP ASP ASP ASP GLU ASP SER GLY HIS SER SER ARG ARG ARG GLY SER ILE SER SER GLY VAL

SER TYR GLU GLU PHE GLN VAL LEU VAL ARG ARG VAL ASP ARG MET GLU HIS SER ILE GLY SER ILE VAL SER LYS ILE ASP ALA ALA VAL ILE VAL LYS LEU GLU ILE MET GLU ARG ALA LYS LEU LYS ARG ARG GLU VAL LEU GLY ARG LEU LEU ASP GLY VAL ALA GLU ASP GLU ARG LEU

GLY ARG ASP SER GLU ILE HIS ARG GLU GLN MET GLU ARG LEU VAL ARG GLU GLU LEU GLU ARG TRP GLU SER ASP ASP ALA ALA SER GLN ILE SER HIS GLY LEU GLY THR PRO VAL GLY LEU ASN GLY GLN PRO ARG PRO ARG SER SER ARG PRO SER SER SER GLN SER THR GLU GLY

MET GLU GLY ALA GLY GLY ASN GLY SER SER ASN VAL HIS VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	276741	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k 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	0.19	0/5716	0.43	0/7793
2	B	0.21	0/4028	0.39	0/5463
2	C	0.19	0/4027	0.34	0/5462
2	D	0.17	0/3910	0.38	0/5305
All	All	0.19	0/17681	0.39	0/24023

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	5586	0	5410	134	0
2	B	3924	0	3875	49	0
2	C	3923	0	3871	47	0
2	D	3810	0	3771	104	0
3	B	42	0	39	2	0
3	C	42	0	39	0	0
3	D	42	0	39	2	0
All	All	17369	0	17044	319	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 9.

All (319) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4045:ILE:O	1:A:4046:LEU:HG	1.15	1.32
1:A:3756:GLU:HB2	1:A:3845:ASN:O	1.36	1.25
1:A:4099:LEU:HD12	1:A:4099:LEU:O	1.28	1.24
2:D:397:ARG:HH21	2:D:542:GLN:CA	1.63	1.12
2:B:331:CYS:SG	2:B:344:CYS:CB	2.38	1.10
2:D:397:ARG:HH21	2:D:542:GLN:N	1.52	1.08
1:A:3797:TYR:HB2	1:A:3819:TYR:HE2	1.20	1.07
2:D:397:ARG:NE	2:D:542:GLN:HB3	1.70	1.07
2:B:331:CYS:SG	2:B:344:CYS:SG	1.06	1.04
1:A:4045:ILE:O	1:A:4046:LEU:CG	2.10	1.00
2:D:397:ARG:CZ	2:D:542:GLN:HB3	1.92	0.99
2:D:397:ARG:HE	2:D:542:GLN:HB3	1.26	0.99
2:D:397:ARG:HB2	2:D:542:GLN:OE1	1.62	0.98
1:A:3781:TYR:O	1:A:3793:GLY:O	1.82	0.98
1:A:3753:ARG:HD2	1:A:3846:ARG:CB	1.94	0.97
1:A:3754:LEU:HB3	1:A:3775:GLY:O	1.65	0.97
2:D:397:ARG:CB	2:D:542:GLN:OE1	2.13	0.97
1:A:4099:LEU:HD12	1:A:4101:LEU:HG	1.46	0.96
2:D:397:ARG:NH2	2:D:542:GLN:HB3	1.81	0.94
1:A:4099:LEU:O	1:A:4099:LEU:CD1	2.16	0.93
1:A:3750:ARG:NH2	1:A:3815:ASP:O	2.02	0.93
1:A:4042:GLN:O	1:A:4046:LEU:HD21	1.69	0.93
2:D:397:ARG:HH21	2:D:542:GLN:CB	1.82	0.92
1:A:3797:TYR:HB2	1:A:3819:TYR:CE2	2.05	0.91
2:D:397:ARG:NH2	2:D:542:GLN:N	2.19	0.89
1:A:3756:GLU:OE1	1:A:3845:ASN:HA	1.72	0.89
1:A:3806:TRP:CZ3	1:A:3815:ASP:OD1	2.25	0.89
1:A:3753:ARG:HD2	1:A:3846:ARG:HB2	1.53	0.88
1:A:4099:LEU:CD1	1:A:4101:LEU:HG	2.03	0.88
2:B:331:CYS:CB	2:B:344:CYS:HG	1.87	0.87
1:A:3806:TRP:CE3	1:A:3815:ASP:OD1	2.29	0.86
1:A:3753:ARG:HH11	1:A:3847:SER:H	1.23	0.83
1:A:3756:GLU:CB	1:A:3845:ASN:O	2.23	0.83
1:A:3797:TYR:CB	1:A:3819:TYR:HE2	1.92	0.82
1:A:4045:ILE:C	1:A:4046:LEU:HG	2.05	0.82
2:D:397:ARG:NH2	2:D:542:GLN:CA	2.42	0.81
2:D:397:ARG:HE	2:D:542:GLN:CB	1.95	0.78
1:A:4099:LEU:CD1	1:A:4101:LEU:CG	2.62	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3753:ARG:HD2	1:A:3846:ARG:HB3	1.67	0.76
2:D:318:VAL:HG21	2:D:395:LEU:O	1.87	0.75
1:A:3756:GLU:CD	1:A:3845:ASN:HA	2.12	0.75
2:D:397:ARG:NH2	2:D:542:GLN:H	1.82	0.75
1:A:3756:GLU:OE1	1:A:3845:ASN:CA	2.34	0.75
2:D:397:ARG:HH21	2:D:542:GLN:HB3	1.43	0.75
2:D:640:ILE:HA	2:D:669:PHE:HZ	1.51	0.74
2:C:574:PHE:HA	2:C:577:ILE:HG22	1.70	0.74
2:D:397:ARG:NH2	2:D:542:GLN:CB	2.47	0.74
1:A:3856:ARG:HB3	1:A:3865:ALA:HB3	1.70	0.74
1:A:3705:ILE:HD11	1:A:3856:ARG:HH11	1.52	0.73
2:B:331:CYS:CB	2:B:344:CYS:SG	2.71	0.73
1:A:4099:LEU:HD13	1:A:4101:LEU:HD21	1.70	0.73
2:D:358:PHE:HB2	2:D:366:TRP:HB3	1.72	0.72
2:D:397:ARG:HB3	2:D:542:GLN:OE1	1.86	0.72
1:A:3724:TRP:CD1	1:A:3838:GLN:HE22	2.09	0.71
1:A:3265:SER:OG	1:A:3280:ARG:NH1	2.24	0.70
2:D:401:GLU:O	2:D:405:GLN:NE2	2.24	0.70
1:A:3770:CYS:SG	1:A:3878:ARG:NH2	2.65	0.69
2:B:252:MET:HB3	2:B:310:PHE:HE2	1.56	0.69
2:D:314:LEU:N	2:D:430:ASN:OD1	2.27	0.68
2:D:318:VAL:HG23	2:D:396:SER:O	1.93	0.68
2:B:312:GLU:OE1	2:B:432:ASN:ND2	2.27	0.67
2:C:309:ILE:HB	2:C:313:ASN:HB2	1.76	0.67
2:D:234:LEU:HD21	2:D:566:VAL:HG22	1.77	0.66
1:A:3807:SER:O	1:A:3809:GLY:N	2.29	0.66
2:D:432:ASN:OD1	2:D:433:ILE:N	2.29	0.65
1:A:3794:THR:O	1:A:3796:ALA:N	2.27	0.65
2:B:434:ASN:HD21	2:B:463:ILE:HB	1.61	0.65
2:B:498:HIS:CE1	2:B:499:LYS:HE3	2.32	0.64
1:A:4099:LEU:HD11	1:A:4101:LEU:HD11	1.79	0.64
1:A:3755:GLN:O	1:A:3755:GLN:HG2	1.95	0.64
2:B:593:CYS:HB3	2:B:683:THR:HG21	1.80	0.63
1:A:4046:LEU:HD12	2:D:563:ALA:HB2	1.80	0.62
2:C:292:TYR:O	2:C:307:SER:OG	2.18	0.62
1:A:3290:LEU:HB3	1:A:3333:VAL:HG21	1.80	0.62
1:A:4099:LEU:HD22	2:D:676:PHE:CD2	2.34	0.62
2:D:358:PHE:O	2:D:361:ARG:NH2	2.32	0.62
1:A:3343:LEU:HD22	1:A:3558:ALA:HB2	1.82	0.61
2:B:228:LEU:O	2:B:232:ILE:HD12	2.00	0.61
2:D:397:ARG:HE	2:D:542:GLN:CG	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:429:TYR:HD1	2:D:436:PHE:HB3	1.64	0.60
2:B:343:GLU:OE2	2:B:417:ARG:NH2	2.35	0.60
2:D:318:VAL:CG2	2:D:395:LEU:O	2.49	0.60
1:A:4042:GLN:O	1:A:4046:LEU:CD2	2.46	0.59
1:A:3872:GLU:HB2	1:A:3880:LEU:HB3	1.84	0.59
1:A:3813:VAL:HG12	1:A:3813:VAL:O	2.02	0.59
1:A:3102:ASP:OD2	1:A:3269:ARG:NH2	2.36	0.59
2:B:460:LEU:HD23	2:B:462:LEU:HD21	1.84	0.59
2:D:327:ARG:HB2	2:D:354:ASP:HB3	1.84	0.58
2:D:259:ASP:HA	2:D:269:ASN:HD22	1.68	0.58
3:D:1003:NAG:H83	3:D:1003:NAG:H3	1.85	0.58
1:A:3752:VAL:O	1:A:3753:ARG:HB3	2.04	0.58
1:A:3756:GLU:OE1	1:A:3845:ASN:O	2.21	0.58
1:A:4099:LEU:CD1	1:A:4101:LEU:HD11	2.34	0.58
1:A:4099:LEU:HD11	1:A:4101:LEU:CD1	2.33	0.58
2:D:581:ARG:HG3	2:D:582:THR:HG23	1.86	0.58
1:A:3802:LEU:N	1:A:3802:LEU:HD12	2.19	0.57
1:A:4099:LEU:O	1:A:4101:LEU:HG	2.04	0.57
2:D:397:ARG:O	2:D:397:ARG:HG2	2.03	0.57
1:A:3275:PHE:HE1	1:A:3344:PHE:HB3	1.69	0.57
2:D:434:ASN:ND2	2:D:462:LEU:HB3	2.20	0.57
2:C:505:SER:OG	2:C:508:ASN:N	2.37	0.57
1:A:4029:VAL:HG11	1:A:4096:TRP:CZ3	2.39	0.56
2:D:245:ASN:HD21	2:D:433:ILE:HD13	1.70	0.56
2:D:396:SER:CB	2:D:401:GLU:HG3	2.35	0.56
3:B:1002:NAG:H3	3:B:1002:NAG:H83	1.88	0.56
2:D:528:ARG:NH1	2:D:555:GLN:OE1	2.39	0.56
1:A:3067:PRO:HB2	1:A:3069:PRO:HD3	1.88	0.56
1:A:3807:SER:OG	1:A:3814:TYR:HB2	2.04	0.56
1:A:3274:ARG:HD2	1:A:3348:ARG:HG3	1.88	0.56
1:A:3306:ALA:O	1:A:3307:TYR:HB2	2.07	0.55
2:C:313:ASN:HD22	2:C:430:ASN:HB2	1.71	0.55
1:A:3795:TRP:CZ3	1:A:3842:TRP:HD1	2.24	0.55
1:A:4099:LEU:CD1	1:A:4101:LEU:CD1	2.84	0.55
1:A:3269:ARG:HE	1:A:3277:ARG:HB2	1.71	0.55
2:D:227:TYR:OH	2:D:569:VAL:O	2.25	0.55
2:B:396:SER:OG	2:B:401:GLU:OE1	2.24	0.55
2:D:396:SER:HB3	2:D:401:GLU:HG3	1.87	0.55
1:A:3750:ARG:CZ	1:A:3815:ASP:O	2.55	0.55
2:D:670:PHE:O	2:D:674:ASN:ND2	2.40	0.55
2:B:370:SER:OG	2:B:373:ASP:OD1	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3799:ALA:O	1:A:3800:PRO:C	2.48	0.54
2:B:507:TRP:HB3	2:B:575:LYS:HD2	1.90	0.54
2:D:258:LEU:HA	2:D:270:PHE:HB3	1.90	0.54
2:B:574:PHE:HE1	2:C:603:MET:HB3	1.72	0.54
1:A:3724:TRP:CG	1:A:3838:GLN:HE22	2.24	0.54
1:A:3809:GLY:HA2	1:A:3870:ARG:CZ	2.38	0.54
2:B:342:LYS:HB3	2:B:343:GLU:OE1	2.08	0.54
2:C:434:ASN:ND2	2:C:463:ILE:O	2.41	0.54
2:D:534:VAL:O	2:D:537:GLN:NE2	2.37	0.54
2:D:365:ALA:HB2	2:D:393:LEU:HB2	1.90	0.53
2:D:322:ARG:HD2	2:D:374:LEU:HD13	1.91	0.53
1:A:3797:TYR:CB	1:A:3819:TYR:CE2	2.80	0.53
2:D:463:ILE:HD11	2:D:529:THR:HG23	1.91	0.53
2:C:313:ASN:ND2	2:C:430:ASN:HB2	2.24	0.53
1:A:3261:HIS:CE1	1:A:3263:TRP:HB2	2.44	0.53
2:B:423:PHE:CE2	2:B:442:LEU:HD13	2.44	0.53
2:D:227:TYR:CE1	2:D:572:LYS:HD3	2.44	0.53
2:D:492:ILE:HA	2:D:495:ILE:HG22	1.90	0.52
1:A:3605:PRO:HA	1:A:3608:VAL:HG12	1.91	0.52
2:D:386:TYR:OH	2:D:444:GLU:OE1	2.26	0.52
2:C:502:TYR:CZ	2:C:508:ASN:HB3	2.44	0.52
2:B:238:THR:HG21	2:B:566:VAL:HG21	1.92	0.52
2:C:593:CYS:HB3	2:C:683:THR:HG21	1.91	0.52
2:D:397:ARG:O	2:D:398:THR:HG23	2.09	0.52
1:A:3287:LEU:HD21	1:A:3337:TYR:CG	2.45	0.52
1:A:4106:LEU:HD13	2:B:675:MET:HG2	1.92	0.51
1:A:4114:ARG:HG3	1:A:4114:ARG:HH11	1.74	0.51
2:B:623:VAL:HG12	2:B:625:ASP:H	1.75	0.51
2:D:429:TYR:CD1	2:D:436:PHE:HB3	2.45	0.51
1:A:3732:LEU:HD12	1:A:3827:LEU:HD13	1.92	0.51
1:A:3780:ASP:HB3	1:A:3793:GLY:HA3	1.93	0.51
2:D:397:ARG:O	2:D:398:THR:CG2	2.59	0.51
1:A:3797:TYR:HA	1:A:3819:TYR:CD2	2.46	0.51
2:D:397:ARG:C	2:D:398:THR:HG23	2.36	0.51
2:C:570:TRP:NE1	2:D:613:GLN:HE22	2.09	0.50
1:A:4094:ARG:HG3	1:A:4096:TRP:H	1.76	0.50
2:C:443:VAL:HG13	2:C:451:VAL:HG13	1.94	0.50
2:D:436:PHE:HE1	2:D:460:LEU:HD12	1.75	0.50
2:B:468:THR:HA	2:B:471:PHE:HD2	1.77	0.50
2:C:639:ILE:HG12	2:C:644:ILE:HG22	1.94	0.50
2:D:267:LYS:O	2:D:267:LYS:NZ	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:383:ILE:HD11	2:C:452:ILE:HD12	1.94	0.50
2:D:261:PRO:HG3	2:D:267:LYS:HZ3	1.76	0.50
1:A:4099:LEU:HD13	1:A:4101:LEU:CD2	2.40	0.49
2:B:675:MET:O	2:B:679:ILE:HG13	2.12	0.49
1:A:3806:TRP:O	1:A:3814:TYR:O	2.30	0.49
1:A:3334:TYR:CZ	1:A:3338:LEU:HD21	2.47	0.49
2:D:498:HIS:HD2	2:D:499:LYS:HG3	1.77	0.49
2:C:258:LEU:HD23	2:C:271:LYS:HE2	1.93	0.49
1:A:3756:GLU:OE1	1:A:3845:ASN:C	2.55	0.49
2:C:243:SER:OG	2:C:244:SER:N	2.45	0.49
2:C:322:ARG:HD2	2:C:374:LEU:HD21	1.95	0.49
1:A:3875:ALA:HB3	1:A:3878:ARG:HG2	1.95	0.48
2:B:597:LEU:HD13	2:C:671:ILE:HD12	1.95	0.48
2:B:316:LEU:HD23	2:B:429:TYR:HB2	1.95	0.48
1:A:3719:ARG:HH21	1:A:3722:GLU:H	1.61	0.48
1:A:3752:VAL:O	1:A:3848:ARG:HB3	2.13	0.48
1:A:3922:TRP:CZ3	1:A:3929:ARG:HB3	2.48	0.48
2:D:326:VAL:HG13	2:D:420:ARG:HG3	1.94	0.48
2:D:335:GLN:OE1	2:D:338:ARG:NH1	2.46	0.48
2:D:428:VAL:HG23	2:D:429:TYR:N	2.29	0.47
1:A:3802:LEU:N	1:A:3802:LEU:CD1	2.77	0.47
2:C:253:MET:HE2	2:C:428:VAL:HG21	1.95	0.47
2:D:359:GLY:O	2:D:361:ARG:N	2.47	0.47
1:A:3748:ARG:NH2	1:A:3853:GLU:OE2	2.45	0.47
1:A:3804:GLY:O	1:A:3805:ALA:HB3	2.14	0.47
1:A:3805:ALA:O	1:A:3806:TRP:CG	2.68	0.47
2:B:316:LEU:HD12	2:B:546:PRO:HG3	1.96	0.47
2:D:499:LYS:C	2:D:501:HIS:H	2.23	0.47
1:A:3287:LEU:HD21	1:A:3337:TYR:CD1	2.49	0.47
2:B:688:LYS:NZ	2:C:686:GLU:OE1	2.46	0.47
2:C:635:THR:O	2:C:639:ILE:HG13	2.14	0.47
1:A:3308:SER:HA	1:A:3312:VAL:HG12	1.97	0.47
1:A:3762:PRO:HG2	1:A:3763:PRO:HD3	1.97	0.47
2:D:369:THR:HG21	2:D:392:TYR:HE1	1.80	0.47
1:A:3269:ARG:NE	1:A:3277:ARG:HB2	2.29	0.47
1:A:3719:ARG:HH22	1:A:3723:LEU:HD22	1.80	0.46
2:C:335:GLN:OE1	2:C:335:GLN:N	2.48	0.46
1:A:3783:VAL:HG12	1:A:3840:HIS:CE1	2.50	0.46
1:A:3847:SER:O	1:A:3873:PHE:HB2	2.15	0.46
2:B:328:ASN:OD1	2:B:329:GLY:N	2.48	0.46
2:D:264:LYS:HD3	2:D:264:LYS:HA	1.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:498:HIS:HE1	2:B:499:LYS:HE3	1.80	0.46
2:D:619:PHE:HZ	2:D:657:GLY:HA2	1.80	0.46
1:A:3753:ARG:HH11	1:A:3847:SER:N	2.00	0.46
1:A:4099:LEU:HD22	2:D:676:PHE:CE2	2.50	0.46
2:B:334:PRO:HG2	2:B:337:LEU:HD21	1.98	0.46
2:C:360:PRO:O	2:C:362:ASN:N	2.48	0.46
2:D:324:LEU:HD12	2:D:423:PHE:HE2	1.80	0.46
1:A:3752:VAL:HG21	1:A:3814:TYR:HD1	1.81	0.46
1:A:3753:ARG:CD	1:A:3846:ARG:HB2	2.37	0.46
1:A:4045:ILE:C	1:A:4046:LEU:CG	2.79	0.46
1:A:3187:ASP:HA	1:A:3222:GLU:HA	1.97	0.46
2:B:331:CYS:SG	2:B:344:CYS:HB2	2.47	0.46
1:A:3275:PHE:CE2	1:A:3280:ARG:HG2	2.51	0.46
2:C:238:THR:HA	2:C:241:MET:HG2	1.98	0.46
1:A:3724:TRP:CG	1:A:3838:GLN:NE2	2.85	0.45
2:C:464:ARG:HH22	2:C:528:ARG:HH12	1.64	0.45
2:C:491:GLU:OE2	2:C:502:TYR:OH	2.34	0.45
1:A:3596:PHE:HD2	1:A:3597:LEU:HD12	1.82	0.45
2:B:306:ARG:HD2	2:B:314:LEU:HD11	1.98	0.45
2:B:332:SER:O	2:B:332:SER:OG	2.31	0.45
1:A:3242:LEU:HD23	1:A:3242:LEU:H	1.82	0.45
2:B:337:LEU:HD23	2:B:337:LEU:H	1.81	0.45
1:A:3076:ILE:HD11	1:A:3899:LEU:HD22	1.99	0.45
1:A:3752:VAL:HG21	1:A:3814:TYR:CD1	2.52	0.45
2:C:499:LYS:C	2:C:501:HIS:H	2.25	0.45
1:A:3771:SER:O	1:A:3773:ALA:N	2.50	0.44
1:A:3805:ALA:O	1:A:3806:TRP:CD1	2.70	0.44
2:D:627:SER:OG	2:D:631:GLU:OE1	2.33	0.44
2:C:238:THR:HG23	2:D:617:LEU:HD21	1.98	0.44
2:D:258:LEU:HD21	2:D:455:TRP:CG	2.52	0.44
2:D:640:ILE:HA	2:D:669:PHE:CZ	2.40	0.44
1:A:3744:LEU:HB3	1:A:3855:THR:HG23	1.99	0.44
1:A:3814:TYR:CG	1:A:3851:PHE:HZ	2.35	0.44
2:D:425:ASP:OD1	2:D:440:ARG:HG3	2.17	0.44
2:B:634:PHE:CZ	2:C:658:PRO:HB3	2.51	0.44
1:A:3754:LEU:HB2	1:A:3777:SER:N	2.32	0.44
1:A:3797:TYR:CD2	1:A:3797:TYR:O	2.70	0.44
2:B:525:ASN:OD1	2:B:528:ARG:NH2	2.51	0.44
1:A:3741:SER:OG	1:A:3856:ARG:NE	2.48	0.44
1:A:3907:LEU:HD22	1:A:3945:THR:HG23	2.00	0.44
2:B:291:LEU:O	2:B:307:SER:OG	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:563:ALA:HB1	2:C:614:LEU:HD12	1.99	0.44
2:D:507:TRP:CG	2:D:575:LYS:HD3	2.53	0.43
1:A:3658:LYS:HE3	1:A:3658:LYS:HB2	1.88	0.43
2:C:431:ALA:HB2	2:D:341:ILE:HD13	1.99	0.43
2:C:505:SER:C	2:C:507:TRP:H	2.26	0.43
2:D:635:THR:O	2:D:639:ILE:HG13	2.18	0.43
2:D:528:ARG:O	2:D:532:VAL:HG23	2.18	0.43
2:C:221:LEU:O	2:C:225:VAL:HG23	2.18	0.43
1:A:3749:LEU:O	1:A:3820:VAL:HA	2.19	0.43
1:A:4099:LEU:CD1	1:A:4101:LEU:CD2	2.96	0.43
1:A:3275:PHE:HD2	1:A:3280:ARG:CZ	2.32	0.43
1:A:3701:LEU:O	1:A:3705:ILE:HG12	2.19	0.43
2:B:256:LEU:HD22	2:B:310:PHE:CE1	2.54	0.43
2:D:273:LEU:HD23	2:D:273:LEU:HA	1.84	0.43
2:C:567:PHE:O	2:C:571:ILE:HG12	2.19	0.42
1:A:3951:VAL:HG12	1:A:3987:ALA:HB2	2.02	0.42
2:B:665:VAL:O	2:B:669:PHE:HB2	2.20	0.42
2:D:358:PHE:HB3	2:D:359:GLY:H	1.70	0.42
2:D:434:ASN:HD22	2:D:462:LEU:HB3	1.83	0.42
2:D:572:LYS:O	2:D:572:LYS:HG2	2.18	0.42
2:D:640:ILE:HG12	2:D:669:PHE:HE1	1.83	0.42
2:D:475:ALA:HA	2:D:478:ILE:HG12	2.00	0.42
1:A:3754:LEU:H	1:A:3848:ARG:NH2	2.17	0.42
1:A:3800:PRO:HD3	1:A:3817:GLY:HA3	2.02	0.42
2:C:382:ILE:HA	2:D:654:ARG:HH22	1.84	0.42
2:D:245:ASN:ND2	2:D:433:ILE:HG21	2.34	0.42
2:D:328:ASN:OD1	2:D:329:GLY:N	2.53	0.42
1:A:4046:LEU:CD1	2:D:563:ALA:CB	2.97	0.42
2:B:328:ASN:OD1	2:B:343:GLU:HB2	2.20	0.42
2:B:577:ILE:HG13	2:B:577:ILE:O	2.19	0.42
1:A:3714:PHE:HA	1:A:3717:ILE:HG12	2.02	0.42
2:B:688:LYS:HD3	2:C:682:ASP:OD2	2.20	0.42
2:D:276:MET:HE3	2:D:276:MET:HB2	1.97	0.42
2:D:462:LEU:HD21	2:D:536:LEU:HD13	2.02	0.42
1:A:3728:ALA:HB2	1:A:3834:LEU:HD21	2.02	0.41
2:C:337:LEU:H	2:C:337:LEU:HD23	1.85	0.41
2:D:362:ASN:HB2	3:D:1003:NAG:H2	2.02	0.41
2:D:374:LEU:HD21	2:D:392:TYR:CD1	2.54	0.41
2:B:479:ILE:HG22	2:B:483:PHE:CE2	2.55	0.41
2:B:497:ILE:HG22	2:B:498:HIS:CD2	2.55	0.41
2:C:465:TYR:HE1	2:C:474:ALA:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:619:PHE:HB3	2:C:623:VAL:HG21	2.02	0.41
2:D:251:ARG:HG2	2:D:251:ARG:HH11	1.85	0.41
2:C:574:PHE:O	2:C:578:ASN:ND2	2.42	0.41
2:D:405:GLN:H	2:D:405:GLN:HG2	1.76	0.41
2:D:532:VAL:HG22	2:D:551:LEU:HD23	2.03	0.41
1:A:3727:MET:HE1	1:A:3749:LEU:HD21	2.02	0.41
2:C:291:LEU:HD21	2:C:319:PRO:HG3	2.01	0.41
2:D:444:GLU:CG	2:D:452:ILE:HB	2.50	0.41
2:D:489:VAL:O	2:D:492:ILE:HG22	2.21	0.41
1:A:3753:ARG:HB2	1:A:3846:ARG:HB3	2.03	0.41
2:B:309:ILE:HD12	2:B:428:VAL:HG11	2.02	0.41
2:C:322:ARG:HG3	2:C:392:TYR:HB3	2.01	0.41
2:D:648:GLU:HA	2:D:651:GLU:HB3	2.02	0.41
1:A:4023:LEU:HB3	1:A:4024:PRO:HD3	2.02	0.41
2:B:537:GLN:OE1	3:B:1001:NAG:O6	2.30	0.41
1:A:3283:CYS:O	1:A:3287:LEU:HD23	2.21	0.41
1:A:3794:THR:C	1:A:3796:ALA:N	2.77	0.41
1:A:4046:LEU:HD12	2:D:563:ALA:CB	2.48	0.41
2:B:324:LEU:HD12	2:B:423:PHE:HE1	1.86	0.41
2:D:434:ASN:OD1	2:D:435:LEU:N	2.50	0.41
2:D:520:VAL:O	2:D:524:ILE:HG12	2.21	0.41
2:B:595:LYS:H	2:B:595:LYS:HG3	1.69	0.41
2:C:623:VAL:C	2:C:625:ASP:H	2.29	0.41
2:D:328:ASN:OD1	2:D:343:GLU:HB2	2.21	0.41
2:D:423:PHE:CE1	2:D:442:LEU:HD12	2.57	0.41
2:C:619:PHE:HZ	2:C:657:GLY:HA2	1.85	0.40
2:D:338:ARG:C	2:D:340:GLU:H	2.29	0.40
1:A:3827:LEU:HD11	1:A:3831:ARG:HD3	2.04	0.40
1:A:3842:TRP:CE3	1:A:3843:LEU:HB2	2.56	0.40
1:A:4114:ARG:HG3	1:A:4114:ARG:NH1	2.36	0.40
1:A:3858:SER:O	1:A:3858:SER:OG	2.38	0.40
2:C:258:LEU:HD21	2:C:455:TRP:CG	2.56	0.40
1:A:3586:VAL:HG23	1:A:3902:LEU:HD22	2.02	0.40
2:C:276:MET:SD	2:C:415:LEU:HB3	2.62	0.40
2:C:641:LEU:HD22	2:D:669:PHE:HE2	1.87	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	741/1261 (59%)	644 (87%)	87 (12%)	10 (1%)	10 37
2	B	471/1007 (47%)	439 (93%)	32 (7%)	0	100 100
2	C	471/1007 (47%)	436 (93%)	35 (7%)	0	100 100
2	D	459/1007 (46%)	417 (91%)	41 (9%)	1 (0%)	44 72
All	All	2142/4282 (50%)	1936 (90%)	195 (9%)	11 (0%)	27 56

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3808	TRP
1	A	3772	ALA
1	A	3788	PRO
1	A	3794	THR
1	A	3795	TRP
1	A	3792	SER
1	A	4100	ARG
1	A	3754	LEU
2	D	396	SER
1	A	3793	GLY
1	A	3827	LEU

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	518/1041 (50%)	515 (99%)	3 (1%)	84 90
2	B	428/860 (50%)	428 (100%)	0	100 100
2	C	428/860 (50%)	428 (100%)	0	100 100
2	D	416/860 (48%)	416 (100%)	0	100 100
All	All	1790/3621 (49%)	1787 (100%)	3 (0%)	91 95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3778	THR
1	A	3813	VAL
1	A	4046	LEU

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	3751	GLN
1	A	3790	ASN
1	A	3962	GLN
2	B	412	ASN
2	B	434	ASN
2	B	498	HIS
2	B	547	ASN
2	B	653	ASN
2	C	313	ASN
2	C	323	GLN
2	C	379	HIS
2	C	645	ASN
2	D	557	GLN
2	D	559	ASN
2	D	613	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

9 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	$\#\|Z\| > 2$
3	NAG	D	1002	2	14,14,15	0.23	0	17,19,21	0.42	0
3	NAG	C	1001	2	14,14,15	0.32	0	17,19,21	0.53	0
3	NAG	B	1003	2	14,14,15	0.24	0	17,19,21	0.44	0
3	NAG	D	1003	2	14,14,15	0.58	0	17,19,21	1.24	1 (5%)
3	NAG	C	1002	2	14,14,15	0.89	1 (7%)	17,19,21	1.09	1 (5%)
3	NAG	D	1001	2	14,14,15	0.20	0	17,19,21	0.48	0
3	NAG	B	1001	2	14,14,15	0.86	1 (7%)	17,19,21	1.29	1 (5%)
3	NAG	C	1003	2	14,14,15	0.19	0	17,19,21	0.45	0
3	NAG	B	1002	2	14,14,15	0.42	0	17,19,21	1.28	2 (11%)

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
3	NAG	D	1002	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1001	2	-	4/6/23/26	0/1/1/1
3	NAG	B	1003	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1003	2	-	3/6/23/26	0/1/1/1
3	NAG	C	1002	2	-	3/6/23/26	0/1/1/1
3	NAG	D	1001	2	-	3/6/23/26	0/1/1/1
3	NAG	B	1001	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1003	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1002	2	-	5/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	NAG	O5-C1	3.12	1.48	1.43
3	C	1002	NAG	O5-C1	3.05	1.48	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1001	NAG	C1-O5-C5	5.10	119.10	112.19
3	B	1002	NAG	C2-N2-C7	4.31	129.04	122.90
3	D	1003	NAG	C2-N2-C7	4.29	129.01	122.90
3	C	1002	NAG	C1-O5-C5	4.22	117.91	112.19
3	B	1002	NAG	C1-C2-N2	2.06	114.00	110.49

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1002	NAG	O5-C5-C6-O6
3	D	1002	NAG	C4-C5-C6-O6
3	B	1001	NAG	C4-C5-C6-O6
3	B	1002	NAG	C4-C5-C6-O6
3	B	1001	NAG	O5-C5-C6-O6
3	D	1002	NAG	O5-C5-C6-O6
3	B	1002	NAG	C8-C7-N2-C2
3	B	1002	NAG	O7-C7-N2-C2
3	B	1003	NAG	C8-C7-N2-C2
3	B	1003	NAG	O7-C7-N2-C2
3	C	1001	NAG	C8-C7-N2-C2
3	C	1001	NAG	O7-C7-N2-C2
3	C	1002	NAG	C8-C7-N2-C2
3	C	1002	NAG	O7-C7-N2-C2
3	D	1001	NAG	C8-C7-N2-C2
3	D	1001	NAG	O7-C7-N2-C2
3	D	1003	NAG	C8-C7-N2-C2
3	D	1003	NAG	O7-C7-N2-C2
3	C	1001	NAG	C4-C5-C6-O6
3	C	1001	NAG	O5-C5-C6-O6

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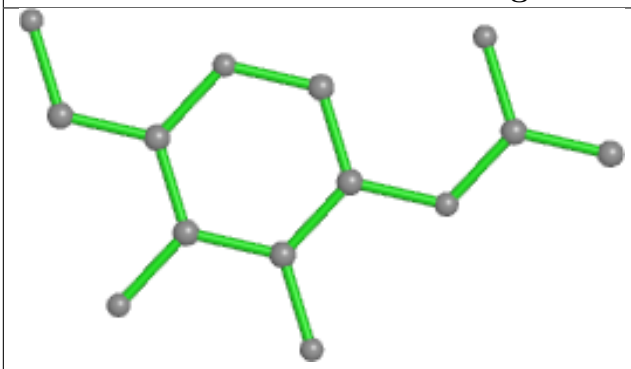
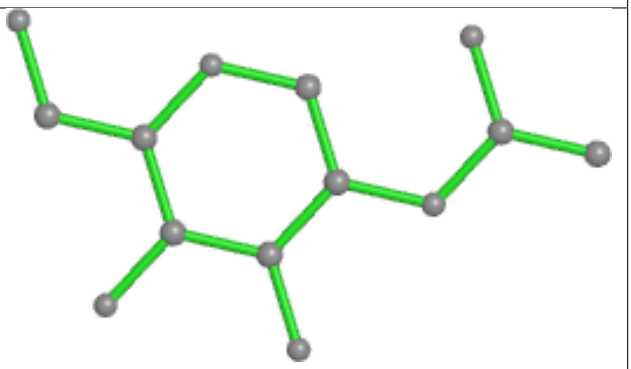
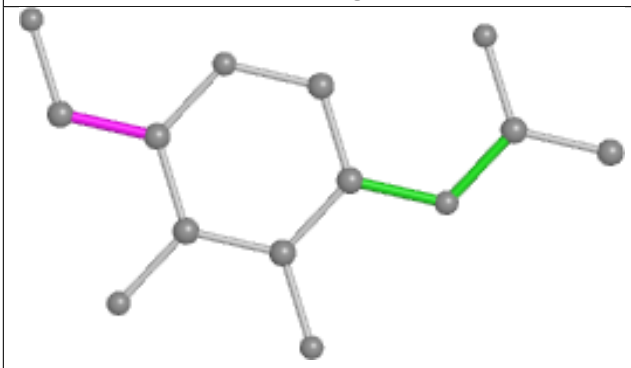
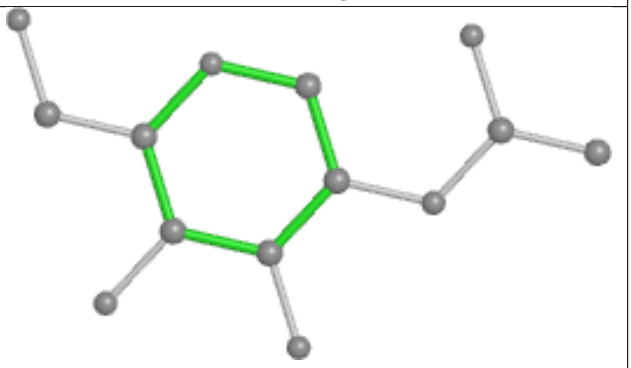
Mol	Chain	Res	Type	Atoms
3	C	1002	NAG	O5-C5-C6-O6
3	D	1001	NAG	O5-C5-C6-O6
3	B	1002	NAG	C3-C2-N2-C7
3	D	1003	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1003	NAG	2	0
3	B	1001	NAG	1	0
3	B	1002	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 D 1002	
 Bond lengths	 Bond angles
 Torsions	 Rings

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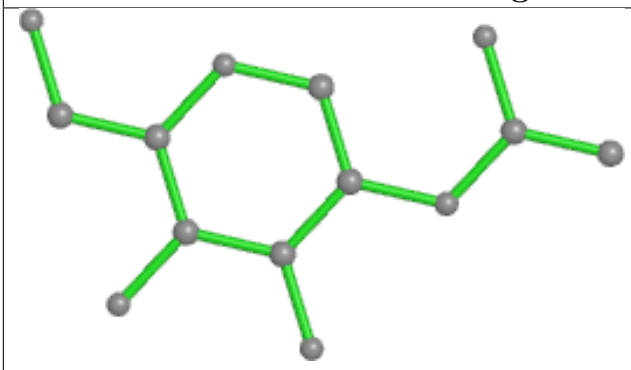
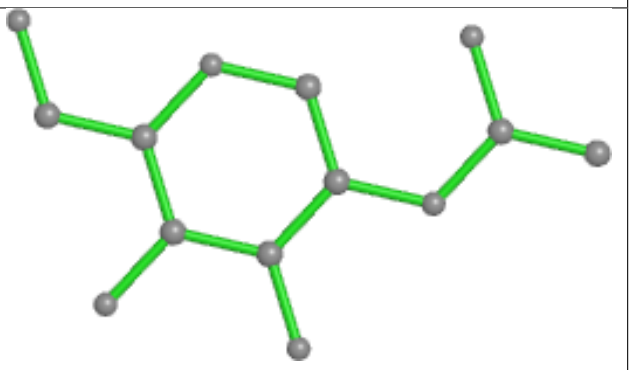
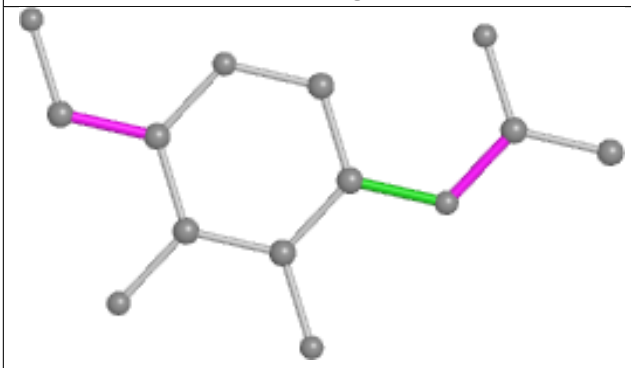
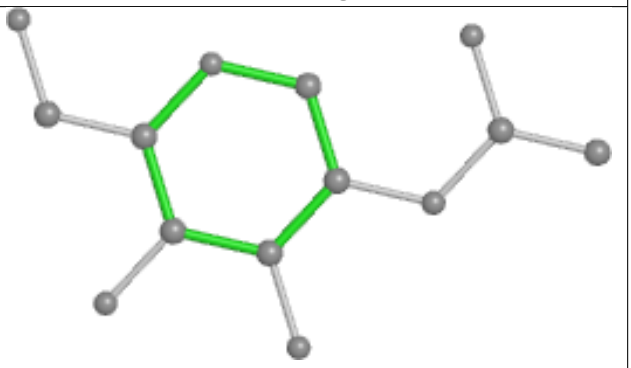
 Bond lengths	 Bond angles
 Torsions	 Rings

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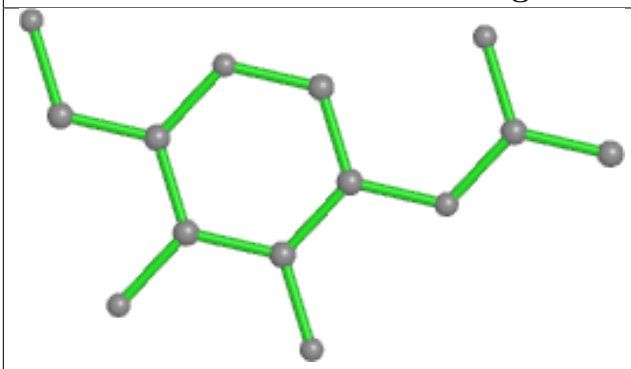

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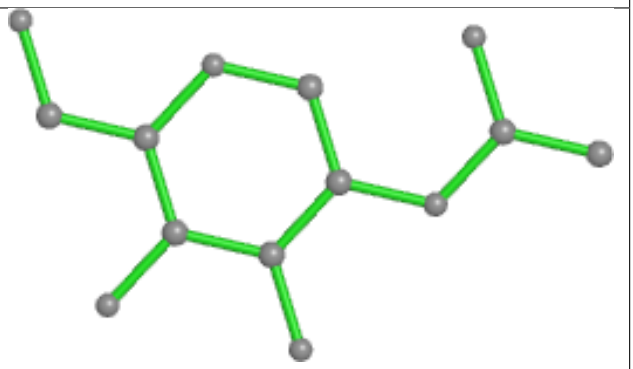

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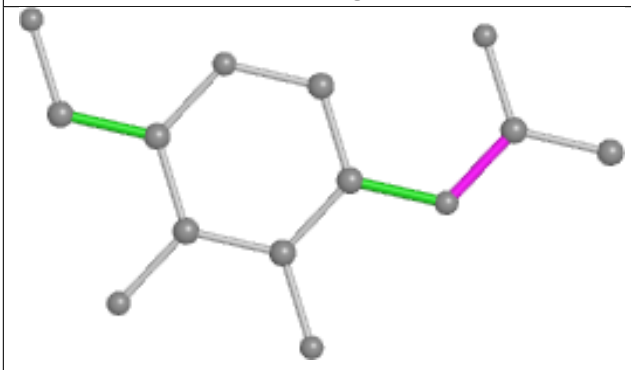

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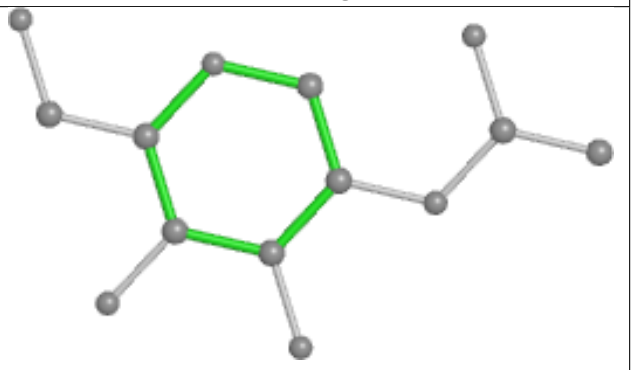

Rings

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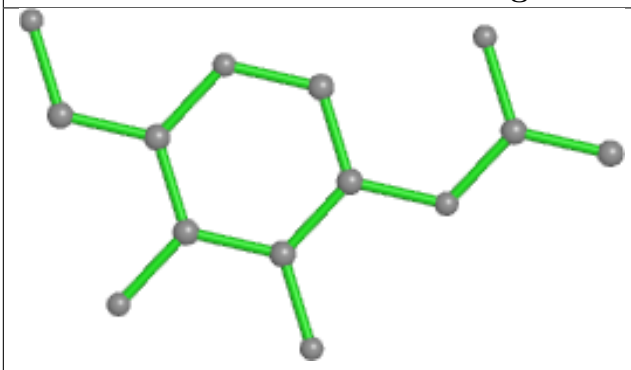

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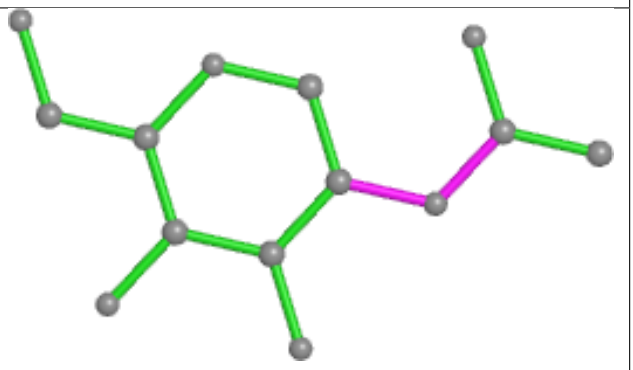

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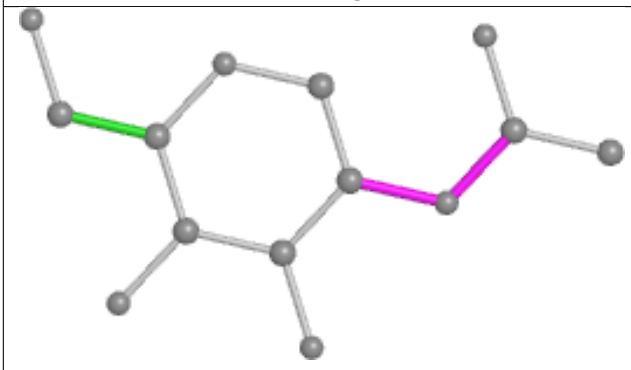

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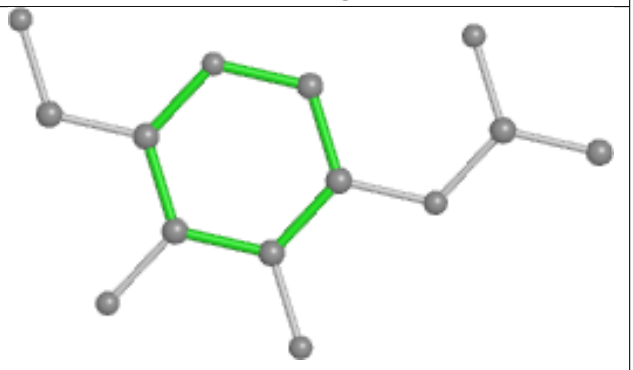

Rings

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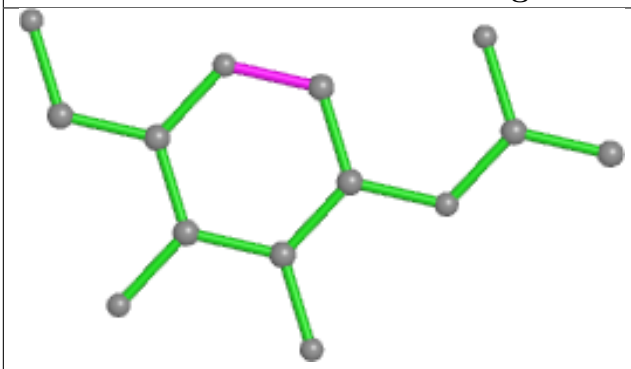

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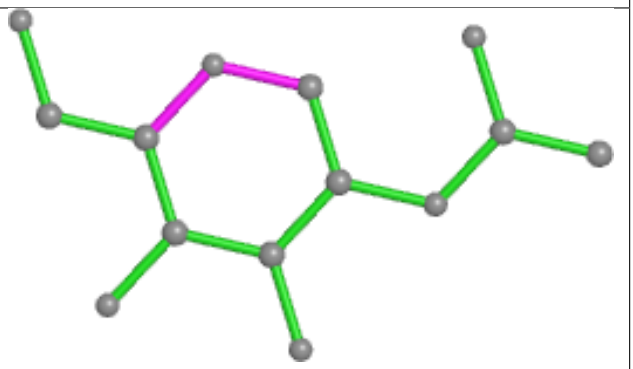

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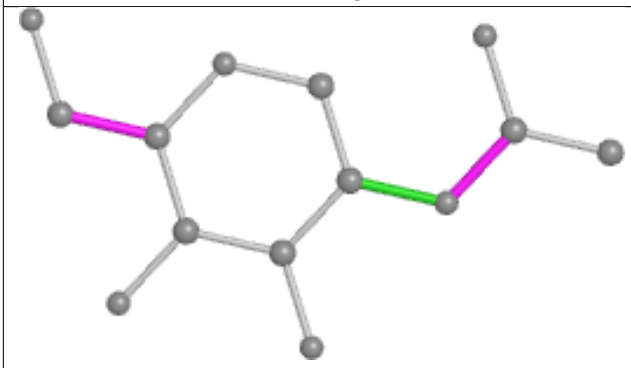

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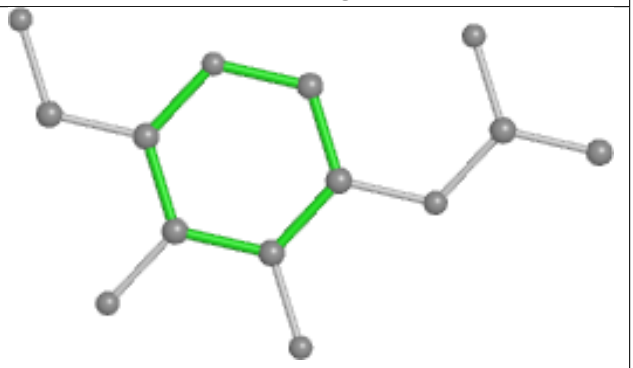

Rings

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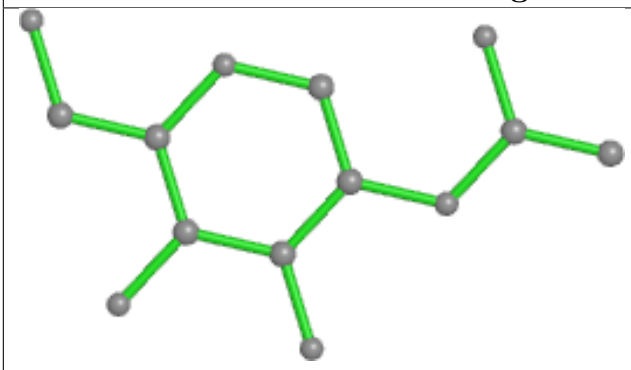

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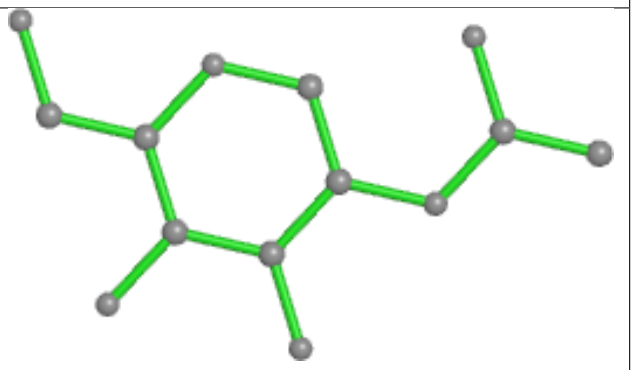

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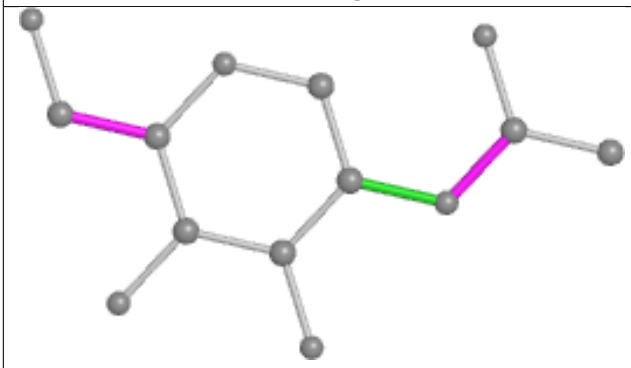

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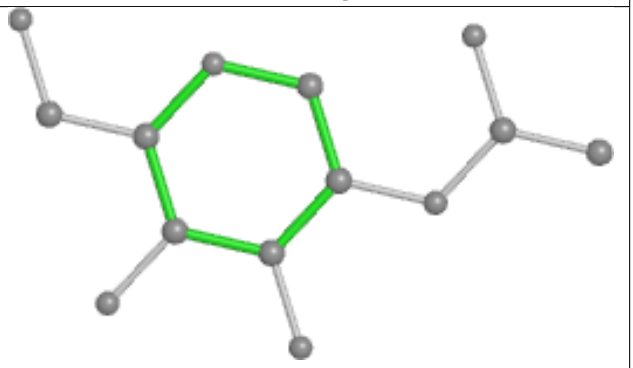

Rings

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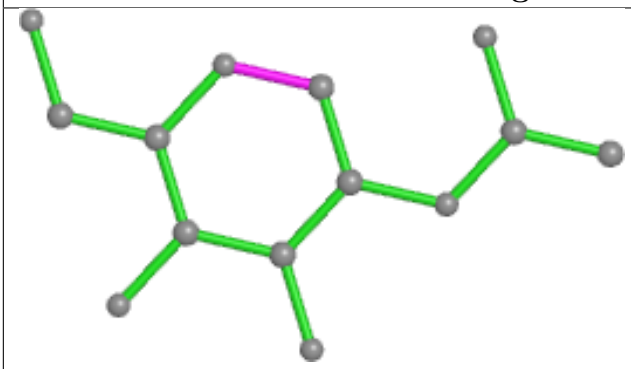
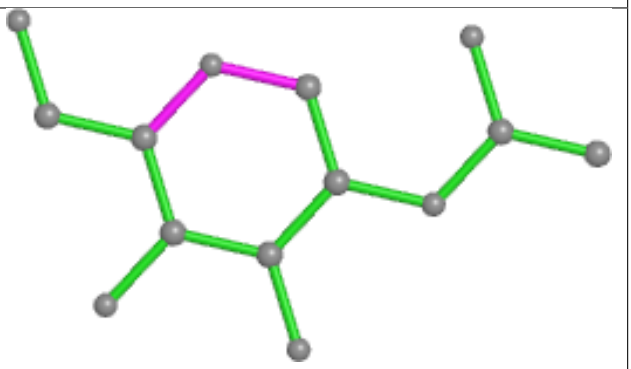
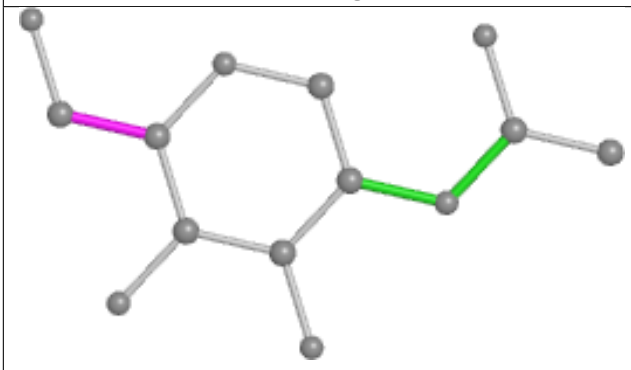
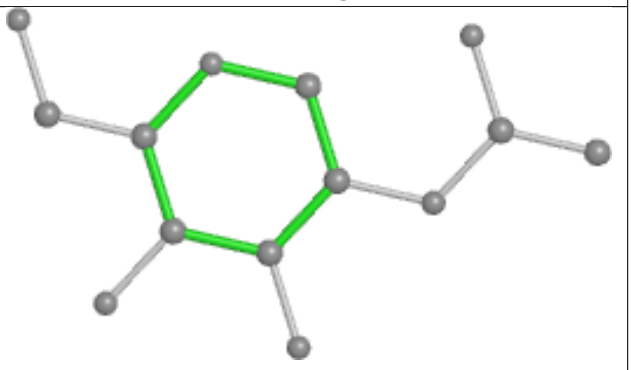
 Bond lengths	 Bond angles
 Torsions	 Rings

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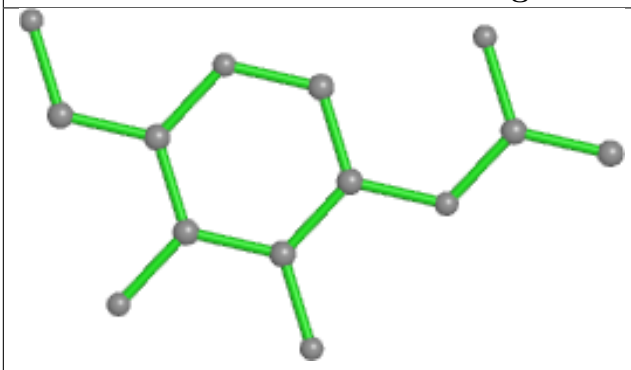
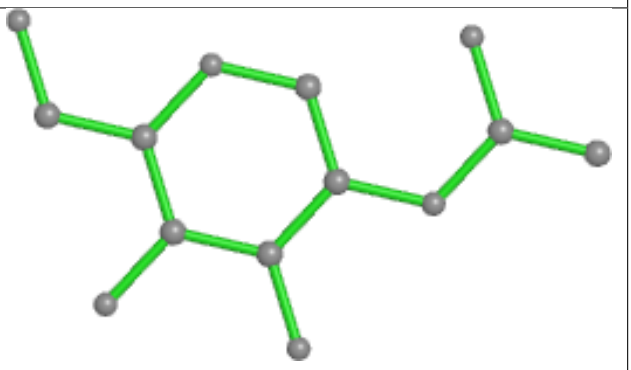
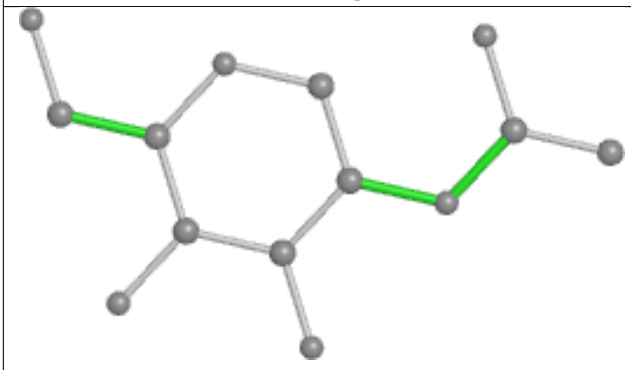
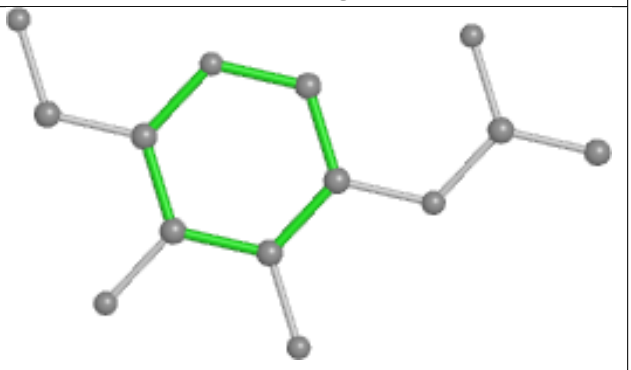
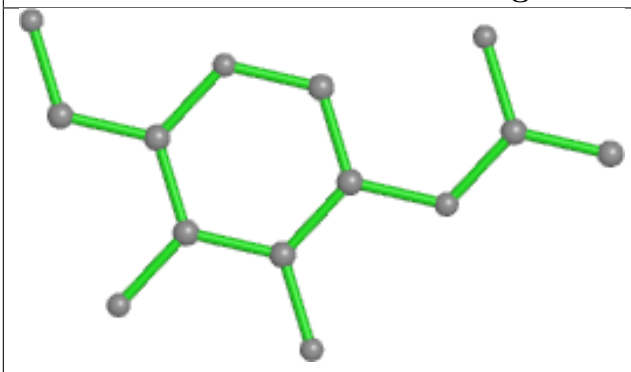
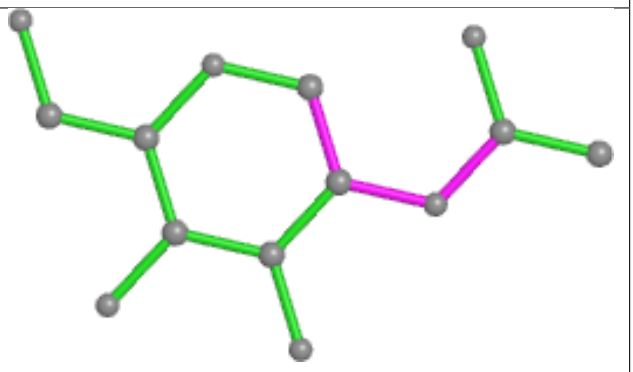
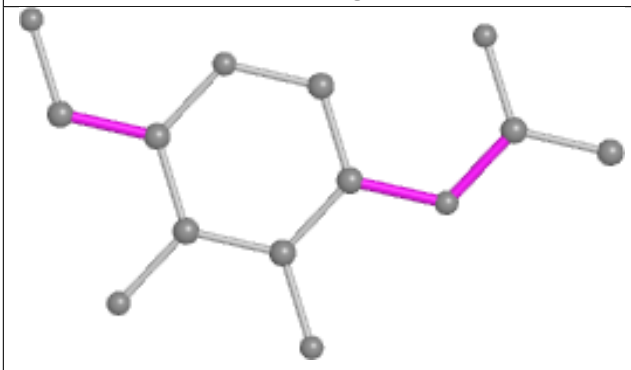
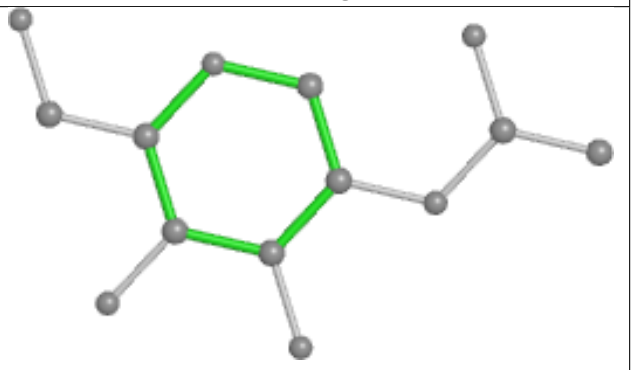
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1002	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.