



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 11:28 AM EDT

PDB ID : 2P6F  
Title : Crystal structures of *Saccharomyces cerevisiae* N-myristoyltransferase with bound myristoyl-CoA and inhibitors  
Authors : Wu, J.; Ding, J.  
Deposited on : 2007-03-18  
Resolution : 3.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

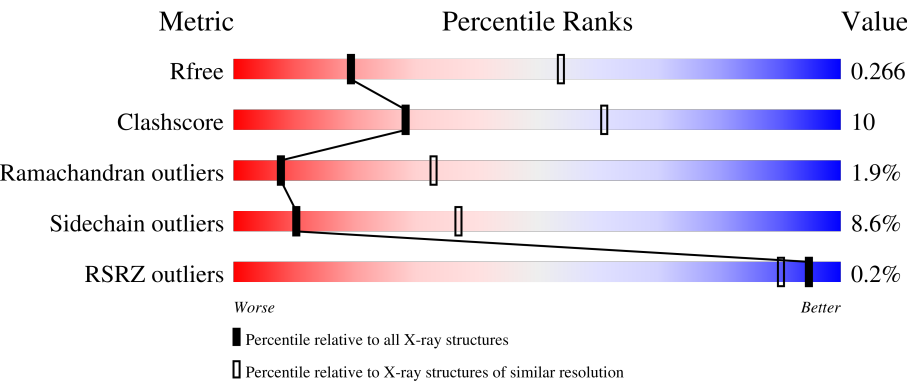
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	455	<div><div>68%</div><div>24%</div><div>.</div><div>.</div></div>
1	B	455	<div><div>69%</div><div>24%</div><div>.</div><div>.</div></div>
1	C	455	<div><div>68%</div><div>25%</div><div>.</div><div>.</div></div>
1	D	455	<div><div>68%</div><div>23%</div><div>5%</div><div>.</div></div>
1	E	455	<div><div>69%</div><div>24%</div><div>.</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
1	F	455	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MYA	A	601	X	-	-	-
2	MYA	B	602	X	-	-	-
2	MYA	C	603	X	-	-	-
2	MYA	D	604	X	-	-	-
2	MYA	E	605	X	-	-	-
2	MYA	F	606	X	-	-	-
3	GN8	D	704	-	-	-	X
3	GN8	E	705	-	-	-	X

## 2 Entry composition [i](#)

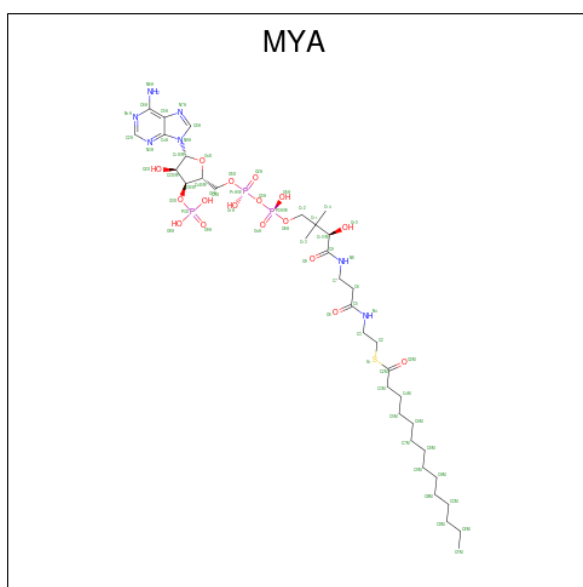
There are 3 unique types of molecules in this entry. The entry contains 21988 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Glycylpeptide N-tetradecanoyltransferase.

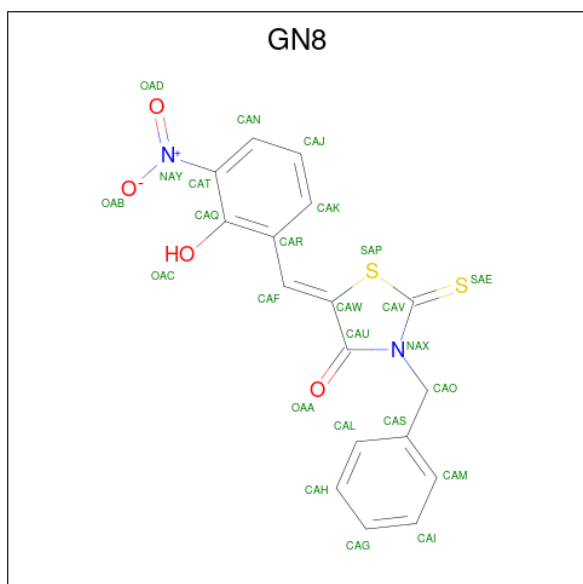
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3578	2318	596	655	9			
1	B	436	Total	C	N	O	S	0	0	0
			3578	2318	596	655	9			
1	C	436	Total	C	N	O	S	0	0	0
			3578	2318	596	655	9			
1	D	436	Total	C	N	O	S	0	0	0
			3578	2318	596	655	9			
1	E	436	Total	C	N	O	S	0	0	0
			3578	2318	596	655	9			
1	F	435	Total	C	N	O	S	0	0	0
			3570	2314	595	652	9			

- Molecule 2 is TETRADECANOYL-COA (three-letter code: MYA) (formula:  $C_{35}H_{62}N_7O_{17}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		

- Molecule 3 is (Z)-3-BENZYL-5-(2-HYDROXY-3-NITROBENZYLIDENE)-2-THIOXOTHIAZOLIDIN-4-ONE (three-letter code: GN8) (formula: C<sub>17</sub>H<sub>12</sub>N<sub>2</sub>O<sub>4</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			25	17	2	4	2		
3	B	1	Total	C	N	O	S	0	0
			25	17	2	4	2		
3	C	1	Total	C	N	O	S	0	0
			25	17	2	4	2		
3	D	1	Total	C	N	O	S	0	0
			25	17	2	4	2		
3	E	1	Total	C	N	O	S	0	0
			25	17	2	4	2		

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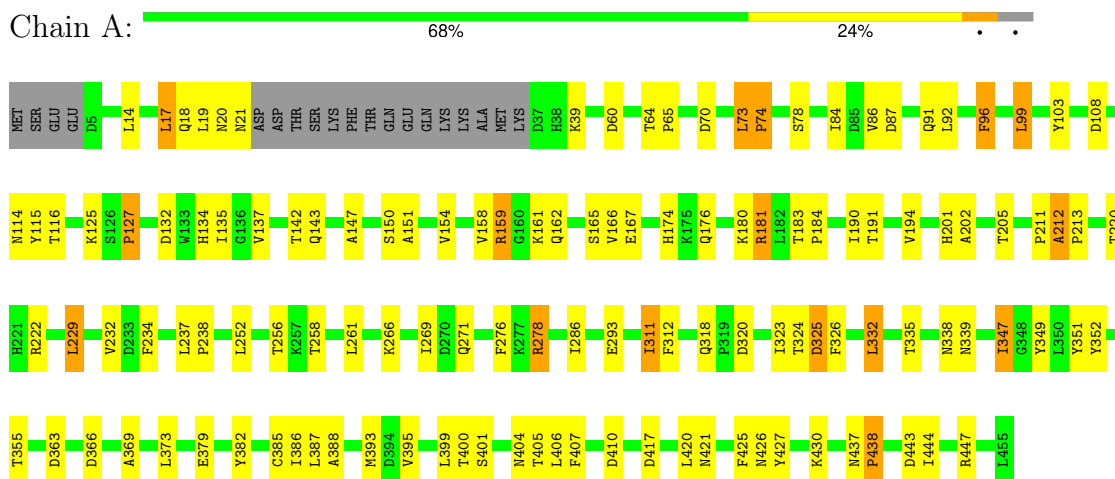
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	S	0	0
			25	17	2	4	2		

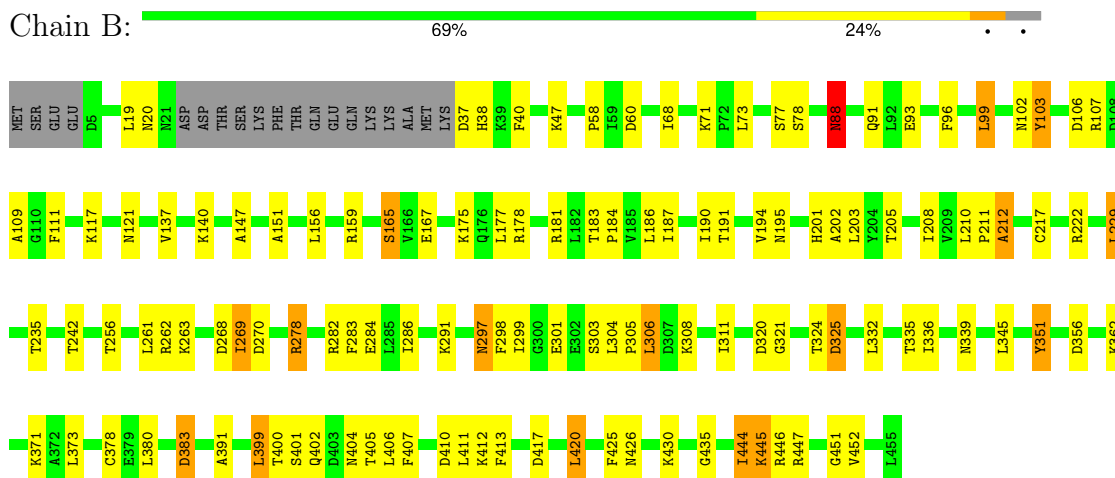
### 3 Residue-property plots

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

- Molecule 1: Glycylpeptide N-tetradecanoyltransferase

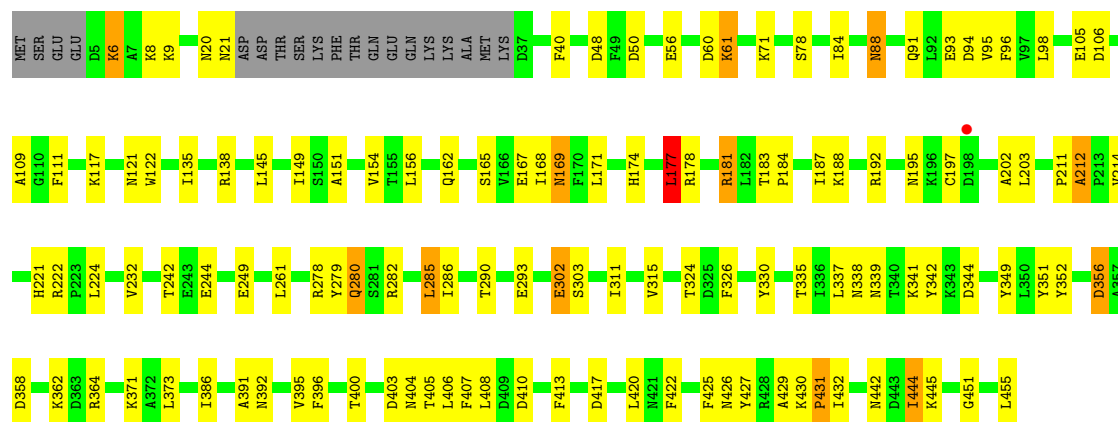


- Molecule 1: Glycylpeptide N-tetradecanoyltransferase

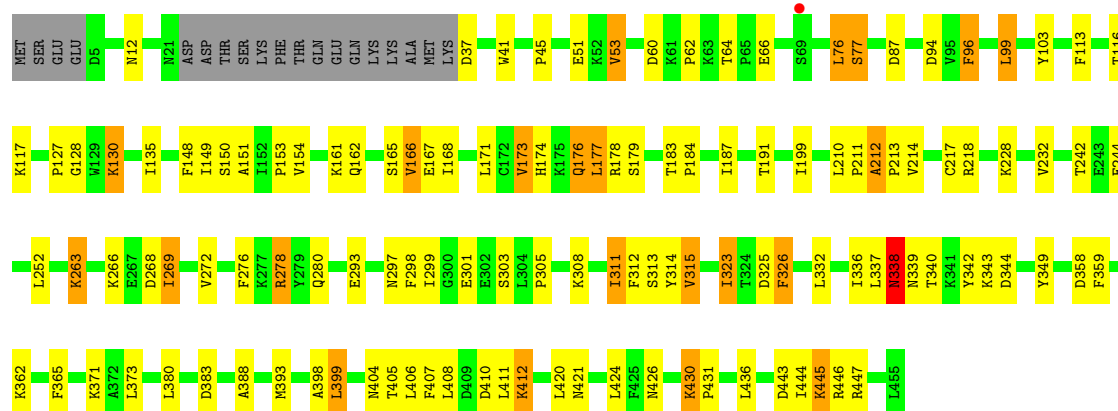


- Molecule 1: Glycylpeptide N-tetradecanoyltransferase

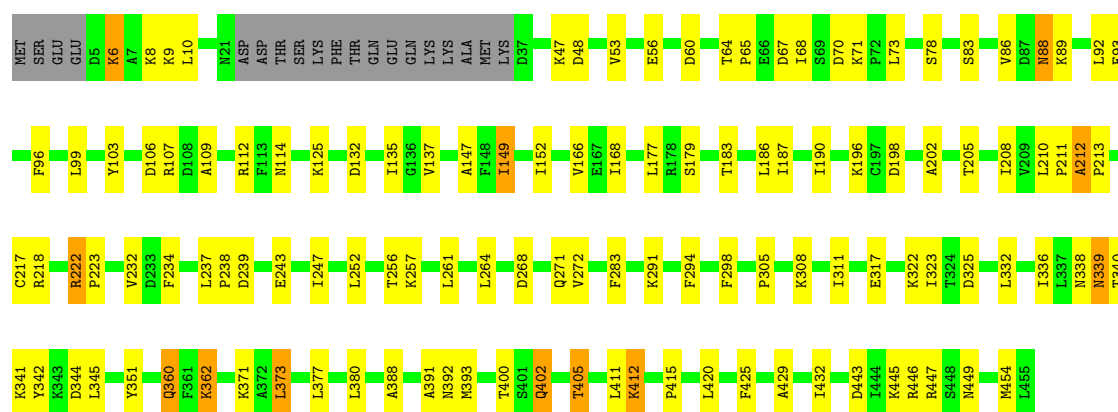




• Molecule 1: Glycylpeptide N-tetradecanoyltransferase



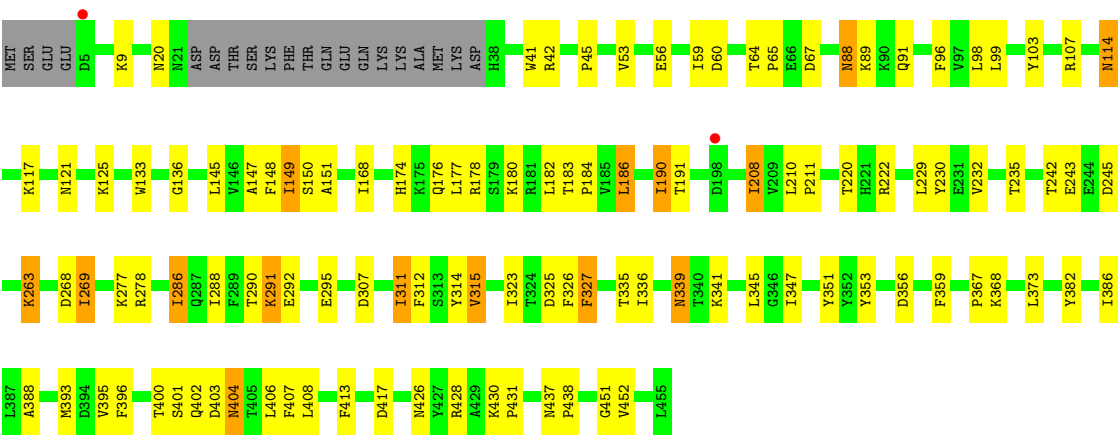
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase



• Molecule 1: Glycylpeptide N-tetradecanoyltransferase







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	188.76Å 151.49Å 133.94Å 90.00° 107.46° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 14.98 – 2.89	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.00-3.10) 97.4 (14.98-2.89)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.270 , 0.332 0.270 , 0.266	Depositor DCC
$R_{free}$ test set	3881 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 12.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	21988	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5840e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GN8, MYA

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	0.38	0/3666	0.51	0/4957
1	B	0.38	0/3666	0.51	0/4957
1	C	0.39	0/3666	0.53	1/4957 (0.0%)
1	D	0.38	0/3666	0.53	1/4957 (0.0%)
1	E	0.38	0/3666	0.52	0/4957
1	F	0.38	0/3658	0.52	0/4946
All	All	0.38	0/21988	0.52	2/29731 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	177	LEU	CA-CB-CG	5.51	127.98	115.30
1	C	177	LEU	CA-CB-CG	5.09	127.00	115.30

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	3578	0	3573	73	0
1	B	3578	0	3573	68	0
1	C	3578	0	3573	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3578	0	3573	75	0
1	E	3578	0	3573	64	0
1	F	3570	0	3569	61	0
2	A	63	0	58	1	0
2	B	63	0	58	6	0
2	C	63	0	58	3	0
2	D	63	0	58	7	0
2	E	63	0	58	3	0
2	F	63	0	58	2	0
3	A	25	0	11	3	0
3	B	25	0	12	1	0
3	C	25	0	12	2	0
3	D	25	0	12	1	0
3	E	25	0	12	1	0
3	F	25	0	12	1	0
All	All	21988	0	21853	429	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 (429) 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)
3:C:703:GN8:SAP	3:C:703:GN8:HAK	1.92	1.09
1:A:278:ARG:HG3	1:A:278:ARG:HH11	1.16	1.05
1:A:212:ALA:H	1:A:213:PRO:HD3	1.18	1.02
3:B:702:GN8:SAP	3:B:702:GN8:HAK	2.09	0.93
3:F:706:GN8:SAP	3:F:706:GN8:HAK	2.10	0.92
3:A:701:GN8:SAP	3:A:701:GN8:HAK	2.13	0.89
1:C:192:ARG:HG2	1:C:192:ARG:HH11	1.37	0.89
1:E:336:ILE:HD11	1:E:345:LEU:HB2	1.57	0.86
3:D:704:GN8:HAK	3:D:704:GN8:SAP	2.15	0.86
1:C:60:ASP:H	1:C:426:ASN:HD21	1.25	0.84
1:C:181:ARG:HH11	1:C:181:ARG:HB3	1.44	0.83
1:D:339:ASN:HD22	1:D:342:TYR:H	1.26	0.82
1:A:278:ARG:HG3	1:A:278:ARG:NH1	1.95	0.80
1:E:149:ILE:HD11	1:E:168:ILE:HG23	1.65	0.79
1:B:60:ASP:H	1:B:426:ASN:HD21	1.32	0.78
1:A:60:ASP:H	1:A:426:ASN:HD21	1.31	0.77
1:E:70:ASP:HB3	1:E:196:LYS:HE3	1.66	0.77
1:B:297:ASN:HD21	1:B:351:TYR:HE2	1.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ALA:O	1:A:393:MET:HG3	1.86	0.75
1:A:18:GLN:HE22	1:A:421:ASN:HD21	1.35	0.75
1:B:137:VAL:HB	1:B:147:ALA:HB3	1.66	0.75
1:D:325:ASP:HB3	1:D:380:LEU:HD11	1.67	0.74
1:B:187:ILE:HG23	2:B:602:MYA:H9MA	1.68	0.74
3:E:705:GN8:HAK	3:E:705:GN8:SAP	2.28	0.74
1:F:60:ASP:N	1:F:426:ASN:HD21	1.88	0.72
1:B:202:ALA:HB2	2:B:602:MYA:HEM	1.71	0.71
1:B:282:ARG:HH12	1:B:373:LEU:HD11	1.55	0.71
1:A:20:ASN:HD21	1:A:417:ASP:HB3	1.55	0.71
1:D:445:LYS:H	1:D:445:LYS:HD2	1.53	0.71
1:A:406:LEU:HG	1:A:447:ARG:HD3	1.73	0.71
1:A:266:LYS:HD2	1:A:269:ILE:HD12	1.73	0.70
1:A:212:ALA:H	1:A:213:PRO:CD	1.99	0.70
1:B:156:LEU:HD11	1:B:203:LEU:HB2	1.74	0.70
1:C:181:ARG:HH11	1:C:181:ARG:CB	2.05	0.69
1:F:41:TRP:HB3	1:F:211:PRO:HG3	1.74	0.69
1:B:278:ARG:HH11	1:B:278:ARG:CG	2.05	0.69
1:F:210:LEU:HB3	1:F:211:PRO:HD2	1.74	0.68
1:B:278:ARG:HH11	1:B:278:ARG:HG3	1.56	0.68
1:B:183:THR:HB	1:B:184:PRO:HD3	1.74	0.68
1:D:443:ASP:OD1	1:D:446:ARG:HG3	1.93	0.68
1:C:339:ASN:HD22	1:C:342:TYR:H	1.40	0.67
1:D:404:ASN:HD22	1:D:407:PHE:HZ	1.42	0.67
1:C:88:ASN:HB3	1:C:91:GLN:HB2	1.77	0.67
1:D:151:ALA:HB1	1:D:166:VAL:HG21	1.77	0.67
1:E:212:ALA:H	1:E:213:PRO:HD2	1.60	0.67
1:F:60:ASP:H	1:F:426:ASN:HD21	1.41	0.67
1:A:212:ALA:N	1:A:213:PRO:HD3	2.02	0.67
1:D:388:ALA:O	1:D:393:MET:HG3	1.93	0.67
1:F:408:LEU:O	1:F:413:PHE:HB2	1.96	0.66
1:C:183:THR:O	1:C:187:ILE:HG12	1.95	0.66
1:A:229:LEU:HD23	1:A:234:PHE:HB3	1.78	0.66
1:B:336:ILE:HD11	1:B:345:LEU:HB2	1.76	0.66
1:D:161:LYS:HG2	1:D:162:GLN:H	1.61	0.65
1:A:39:LYS:HG3	1:A:181:ARG:NH2	2.11	0.65
1:B:404:ASN:HA	1:B:407:PHE:CE2	2.30	0.65
1:E:232:VAL:HG12	1:E:232:VAL:O	1.96	0.65
1:D:405:THR:HG21	1:D:443:ASP:O	1.97	0.64
1:C:181:ARG:HH11	1:C:181:ARG:CG	2.11	0.64
1:E:202:ALA:HB3	1:E:425:PHE:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:ASP:H	1:D:426:ASN:HD21	1.46	0.64
1:E:212:ALA:H	1:E:213:PRO:CD	2.11	0.63
1:B:278:ARG:HG3	1:B:278:ARG:NH1	2.13	0.63
1:C:339:ASN:ND2	1:C:342:TYR:H	1.96	0.63
1:F:437:ASN:HB3	1:F:438:PRO:CD	2.28	0.63
1:D:165:SER:HA	1:D:199:ILE:HG23	1.80	0.63
1:E:205:THR:HG21	1:E:454:MET:HG3	1.81	0.62
1:D:53:VAL:HG13	1:D:430:LYS:HD3	1.81	0.62
1:E:325:ASP:HB3	1:E:380:LEU:HD11	1.81	0.62
1:E:210:LEU:O	1:E:213:PRO:HD3	2.00	0.62
1:E:68:ILE:HG22	1:E:196:LYS:HE2	1.81	0.62
1:D:60:ASP:N	1:D:426:ASN:HD21	1.98	0.62
1:F:263:LYS:HE3	1:F:263:LYS:H	1.65	0.62
1:C:151:ALA:HA	1:C:167:GLU:O	2.00	0.61
1:E:106:ASP:HB3	1:E:109:ALA:HB2	1.83	0.61
1:E:294:PHE:O	1:E:298:PHE:HD1	1.84	0.61
1:F:242:THR:H	1:F:245:ASP:HB2	1.66	0.60
1:D:405:THR:CG2	1:D:444:ILE:HA	2.32	0.60
1:E:211:PRO:O	1:E:212:ALA:HB2	2.01	0.60
1:C:192:ARG:HG2	1:C:192:ARG:NH1	2.13	0.60
1:A:382:TYR:O	1:A:386:ILE:HD12	2.02	0.60
1:B:68:ILE:HG13	1:B:195:ASN:HB3	1.84	0.60
1:D:305:PRO:HG2	1:D:308:LYS:HD3	1.83	0.60
1:E:137:VAL:HB	1:E:147:ALA:HB3	1.84	0.60
1:E:211:PRO:O	1:E:212:ALA:CB	2.50	0.59
1:A:14:LEU:HA	1:A:17:LEU:HD23	1.84	0.59
1:D:263:LYS:H	1:D:263:LYS:HD3	1.66	0.59
1:E:88:ASN:C	1:E:88:ASN:HD22	2.06	0.59
1:A:211:PRO:O	1:A:212:ALA:HB2	2.03	0.59
1:E:6:LYS:H	1:E:6:LYS:HD3	1.68	0.59
1:A:229:LEU:HD11	1:A:395:VAL:HB	1.85	0.59
1:D:96:PHE:HE2	1:D:117:LYS:HB3	1.68	0.59
1:E:388:ALA:O	1:E:393:MET:HG3	2.02	0.58
1:F:147:ALA:HB1	1:F:186:LEU:HD11	1.85	0.58
1:A:405:THR:CG2	1:A:444:ILE:HA	2.33	0.58
1:B:99:LEU:O	1:B:103:TYR:HB2	2.04	0.58
1:B:217:CYS:HB3	1:B:399:LEU:O	2.04	0.58
1:A:161:LYS:HG3	1:A:162:GLN:N	2.19	0.58
1:B:117:LYS:O	1:B:121:ASN:HB2	2.03	0.58
1:D:148:PHE:CZ	1:D:150:SER:HB3	2.37	0.58
1:F:356:ASP:HA	1:F:359:PHE:CD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:404:ASN:HA	1:F:407:PHE:CE2	2.38	0.58
1:B:324:THR:HG23	1:B:356:ASP:OD1	2.04	0.57
1:F:286:ILE:HG22	1:F:451:GLY:HA3	1.85	0.57
1:A:347:ILE:HG23	1:A:395:VAL:HG13	1.87	0.57
1:F:339:ASN:HD22	1:F:341:LYS:H	1.51	0.57
1:C:430:LYS:HG3	1:C:431:PRO:HD2	1.87	0.57
3:C:703:GN8:SAP	3:C:703:GN8:CAK	2.76	0.57
1:F:208:ILE:HD13	1:F:208:ILE:H	1.68	0.57
1:A:166:VAL:HG11	1:A:194:VAL:HG11	1.86	0.57
1:A:137:VAL:HB	1:A:147:ALA:HB3	1.86	0.57
1:A:405:THR:HG21	1:A:443:ASP:O	2.05	0.57
1:D:232:VAL:O	1:D:232:VAL:HG12	2.05	0.57
1:E:56:GLU:HG2	1:E:429:ALA:HA	1.87	0.57
1:B:159:ARG:NH2	1:B:430:LYS:HB2	2.19	0.57
1:D:212:ALA:H	1:D:213:PRO:HD3	1.70	0.57
1:B:444:ILE:HD13	1:B:444:ILE:H	1.69	0.57
1:C:232:VAL:HG12	1:C:232:VAL:O	2.04	0.57
1:E:373:LEU:HD22	1:E:377:LEU:HG	1.86	0.57
1:A:318:GLN:HG2	1:A:324:THR:OG1	2.04	0.56
1:B:229:LEU:HB3	1:B:235:THR:HG22	1.85	0.56
1:B:106:ASP:HB3	1:B:109:ALA:HB2	1.86	0.56
1:B:411:LEU:O	1:B:412:LYS:HB2	2.05	0.56
1:C:224:LEU:HD11	1:C:396:PHE:HB2	1.87	0.56
1:D:278:ARG:HD2	1:D:359:PHE:CE1	2.41	0.56
1:B:58:PRO:HB3	1:B:201:HIS:HE1	1.70	0.56
1:D:218:ARG:HB3	1:D:436:LEU:HD21	1.86	0.56
1:C:286:ILE:HG22	1:C:451:GLY:HA3	1.87	0.56
1:D:211:PRO:O	1:D:212:ALA:CB	2.53	0.56
1:C:202:ALA:HB2	2:C:603:MYA:HDMA	1.87	0.56
1:C:174:HIS:HB3	1:C:177:LEU:HD22	1.88	0.55
1:D:212:ALA:N	1:D:213:PRO:HD3	2.22	0.55
1:C:6:LYS:HE2	1:C:9:LYS:HD3	1.89	0.55
1:B:38:HIS:HA	2:B:602:MYA:P3X	2.47	0.55
1:D:242:THR:HG22	1:D:244:GLU:H	1.70	0.55
1:F:403:ASP:HB3	1:F:406:LEU:HD12	1.87	0.55
1:A:20:ASN:ND2	1:A:417:ASP:HB3	2.20	0.55
1:E:149:ILE:HD11	1:E:168:ILE:CG2	2.36	0.55
1:D:41:TRP:HH2	2:D:604:MYA:H8MA	1.72	0.55
1:D:211:PRO:O	1:D:212:ALA:HB3	2.06	0.55
1:B:102:ASN:HA	1:B:175:LYS:HE3	1.89	0.55
1:B:202:ALA:HB3	1:B:425:PHE:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:PHE:HE2	1:D:446:ARG:HA	1.71	0.55
1:D:406:LEU:HG	1:D:447:ARG:HD3	1.89	0.55
1:D:174:HIS:CD2	1:D:176:GLN:HB2	2.43	0.54
1:E:305:PRO:HG2	1:E:308:LYS:HG3	1.89	0.54
1:C:106:ASP:HB3	1:C:109:ALA:HB2	1.90	0.54
1:A:363:ASP:HB3	1:A:366:ASP:HB2	1.89	0.54
1:A:39:LYS:HG3	1:A:181:ARG:HH21	1.73	0.53
1:C:149:ILE:HD12	1:C:171:LEU:HD13	1.90	0.53
1:F:20:ASN:HB2	1:F:417:ASP:HB2	1.90	0.53
1:A:325:ASP:HB3	1:A:355:THR:HA	1.89	0.53
1:B:47:LYS:HB3	1:B:212:ALA:CB	2.38	0.53
1:D:45:PRO:HB2	1:D:426:ASN:HD22	1.73	0.53
1:C:60:ASP:H	1:C:426:ASN:ND2	2.01	0.53
1:D:127:PRO:HG2	1:D:293:GLU:HA	1.88	0.53
1:F:121:ASN:O	1:F:125:LYS:HB2	2.09	0.53
1:C:98:LEU:HD22	1:C:145:LEU:HG	1.91	0.53
1:D:183:THR:HB	1:D:184:PRO:HD3	1.91	0.53
1:E:205:THR:CG2	1:E:454:MET:HG3	2.39	0.53
1:F:88:ASN:HD22	1:F:89:LYS:N	2.06	0.53
1:B:269:ILE:HD11	1:B:299:ILE:HD13	1.90	0.52
1:B:175:LYS:HA	1:B:178:ARG:HG3	1.91	0.52
1:C:285:LEU:HB2	1:C:432:ILE:HD13	1.90	0.52
1:C:408:LEU:O	1:C:413:PHE:HB2	2.09	0.52
1:F:64:THR:HB	1:F:65:PRO:HD2	1.91	0.52
1:B:111:PHE:HA	1:B:335:THR:O	2.09	0.52
1:E:443:ASP:OD2	1:E:446:ARG:NH2	2.43	0.52
3:A:701:GN8:SAP	3:A:701:GN8:CAK	2.93	0.52
1:C:156:LEU:HD11	1:C:203:LEU:HB2	1.91	0.52
1:C:202:ALA:HB3	1:C:425:PHE:HB3	1.90	0.52
1:E:212:ALA:N	1:E:213:PRO:CD	2.72	0.52
1:C:242:THR:HG22	1:C:244:GLU:H	1.73	0.52
1:C:61:LYS:H	1:C:61:LYS:HD3	1.75	0.52
1:A:151:ALA:HB1	1:A:166:VAL:CG2	2.40	0.52
1:C:20:ASN:HB2	1:C:417:ASP:HB2	1.92	0.51
1:E:243:GLU:O	1:E:247:ILE:HG12	2.10	0.51
1:B:378:CYS:HA	1:B:411:LEU:HD11	1.90	0.51
1:F:315:VAL:HG13	1:F:323:ILE:HG23	1.92	0.51
1:F:336:ILE:HD13	1:F:345:LEU:HB2	1.93	0.51
1:F:290:THR:C	1:F:292:GLU:H	2.13	0.51
1:D:217:CYS:HB3	1:D:399:LEU:O	2.11	0.51
1:E:86:VAL:HG23	1:E:92:LEU:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:LEU:HG	1:C:165:SER:OG	2.10	0.51
1:D:336:ILE:H	1:D:344:ASP:HA	1.76	0.51
1:D:165:SER:HA	1:D:199:ILE:CG2	2.41	0.51
1:D:398:ALA:CB	1:D:408:LEU:HD21	2.41	0.50
1:A:205:THR:HB	1:A:420:LEU:HD22	1.93	0.50
1:C:405:THR:HG23	1:C:442:ASN:HB3	1.92	0.50
1:C:192:ARG:HH11	1:C:192:ARG:CG	2.17	0.50
1:A:405:THR:HG22	1:A:444:ILE:HA	1.94	0.50
1:B:186:LEU:O	1:B:190:ILE:HG22	2.12	0.50
1:C:403:ASP:HB3	1:C:406:LEU:HD12	1.94	0.50
1:F:114:ASN:C	1:F:114:ASN:HD22	2.14	0.50
1:E:360:GLN:HE21	1:E:360:GLN:HA	1.76	0.50
2:F:606:MYA:H2AA	2:F:606:MYA:H6M	1.93	0.50
1:A:134:HIS:ND1	1:A:150:SER:HB2	2.27	0.50
1:C:174:HIS:HB3	1:C:177:LEU:CD2	2.42	0.50
1:D:263:LYS:H	1:D:263:LYS:CD	2.25	0.50
1:C:330:TYR:CE2	1:C:349:TYR:HB2	2.47	0.49
1:E:298:PHE:HA	1:E:311:ILE:HG12	1.94	0.49
1:E:432:ILE:HG23	1:E:449:ASN:HB2	1.94	0.49
1:B:262:ARG:HG2	1:B:263:LYS:N	2.28	0.49
1:A:211:PRO:O	1:A:212:ALA:CB	2.61	0.49
1:E:83:SER:OG	1:E:132:ASP:OD2	2.26	0.49
1:F:59:ILE:HA	1:F:428:ARG:HH12	1.77	0.49
1:C:183:THR:HB	1:C:184:PRO:HD3	1.95	0.49
1:F:278:ARG:HD2	1:F:359:PHE:HE1	1.77	0.49
1:F:437:ASN:HB3	1:F:438:PRO:HD2	1.94	0.49
1:A:202:ALA:HB3	1:A:425:PHE:HB3	1.94	0.49
1:A:84:ILE:HG23	1:A:91:GLN:HB3	1.94	0.49
1:A:405:THR:HG21	1:A:443:ASP:C	2.33	0.49
1:B:229:LEU:HB3	1:B:235:THR:CG2	2.43	0.48
1:E:405:THR:HG21	1:E:443:ASP:O	2.12	0.48
1:A:99:LEU:HB3	1:A:115:TYR:HD1	1.77	0.48
1:D:171:LEU:HD22	2:D:604:MYA:H5MA	1.94	0.48
1:D:411:LEU:O	1:D:412:LYS:HB2	2.13	0.48
1:A:399:LEU:C	1:A:401:SER:H	2.17	0.48
1:B:305:PRO:HG2	1:B:308:LYS:HD2	1.96	0.48
1:F:382:TYR:O	1:F:386:ILE:HD12	2.13	0.48
1:D:149:ILE:HD12	1:D:171:LEU:HD13	1.96	0.48
1:A:154:VAL:HG21	1:A:167:GLU:HG3	1.96	0.48
1:B:205:THR:HB	1:B:420:LEU:HD22	1.96	0.48
1:C:187:ILE:HD12	2:C:603:MYA:H6MA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ARG:HD3	1:C:364:ARG:HD2	1.95	0.48
1:D:405:THR:HG21	1:D:444:ILE:HA	1.94	0.48
2:E:605:MYA:H2AA	2:E:605:MYA:H6M	1.95	0.48
1:B:93:GLU:HA	1:B:96:PHE:CZ	2.49	0.48
1:B:286:ILE:HG22	1:B:451:GLY:HA3	1.96	0.48
1:E:99:LEU:O	1:E:103:TYR:HB2	2.13	0.48
1:D:168:ILE:HG21	2:D:604:MYA:H7MA	1.95	0.48
1:A:115:TYR:CE2	1:A:332:LEU:HD21	2.49	0.47
1:A:271:GLN:HB3	1:A:323:ILE:HD12	1.96	0.47
1:F:149:ILE:HB	1:F:186:LEU:HD22	1.95	0.47
1:E:8:LYS:O	1:E:10:LEU:N	2.47	0.47
1:C:404:ASN:HA	1:C:407:PHE:CE2	2.49	0.47
1:F:353:TYR:HE2	1:F:404:ASN:HD21	1.62	0.47
1:B:165:SER:HB3	1:B:201:HIS:HB2	1.95	0.47
1:D:96:PHE:CD1	1:D:96:PHE:C	2.88	0.47
1:A:127:PRO:HG2	1:A:293:GLU:HA	1.96	0.47
1:C:40:PHE:HE1	1:C:188:LYS:HE3	1.79	0.47
1:D:99:LEU:HD13	1:D:103:TYR:CD1	2.49	0.47
1:C:232:VAL:O	1:C:232:VAL:CG1	2.63	0.47
1:E:187:ILE:HG23	2:E:605:MYA:H9M	1.97	0.47
1:E:65:PRO:HD3	1:E:198:ASP:OD2	2.15	0.47
1:A:142:THR:O	1:A:143:GLN:HB2	2.14	0.47
1:D:191:THR:HA	2:D:604:MYA:HDMA	1.97	0.47
1:A:258:THR:HG21	1:A:379:GLU:HB3	1.95	0.46
1:C:290:THR:H	1:C:293:GLU:HG2	1.79	0.46
1:E:222:ARG:NH1	1:E:223:PRO:O	2.47	0.46
1:C:282:ARG:HH22	1:C:358:ASP:CG	2.19	0.46
1:D:312:PHE:HB3	1:D:314:TYR:CE1	2.50	0.46
1:F:174:HIS:HD2	1:F:176:GLN:H	1.63	0.46
1:E:232:VAL:O	1:E:232:VAL:CG1	2.63	0.46
1:E:135:ILE:HG12	1:E:190:ILE:HD13	1.97	0.46
1:A:332:LEU:HB3	1:A:349:TYR:CE1	2.51	0.46
1:E:47:LYS:HG2	1:E:48:ASP:N	2.30	0.46
1:A:276:PHE:CE1	1:A:352:TYR:HB3	2.50	0.46
1:B:47:LYS:HB3	1:B:212:ALA:HB1	1.96	0.46
1:A:87:ASP:OD2	1:A:125:LYS:HE2	2.16	0.46
1:C:84:ILE:HG21	1:C:95:VAL:HG21	1.98	0.46
1:F:339:ASN:ND2	1:F:341:LYS:H	2.14	0.46
1:B:60:ASP:H	1:B:426:ASN:ND2	2.08	0.46
1:B:297:ASN:ND2	1:B:351:TYR:HE2	2.07	0.46
1:E:237:LEU:HA	1:E:238:PRO:HD3	1.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:ASN:ND2	1:E:342:TYR:H	2.13	0.46
1:B:151:ALA:HA	1:B:167:GLU:O	2.16	0.46
1:C:40:PHE:CE1	1:C:188:LYS:HE3	2.51	0.45
1:E:411:LEU:O	1:E:412:LYS:HB2	2.14	0.45
1:F:99:LEU:O	1:F:103:TYR:HB2	2.16	0.45
1:F:191:THR:HA	2:F:606:MYA:HDM	1.97	0.45
1:A:366:ASP:HB3	1:A:369:ALA:HB3	1.98	0.45
1:C:122:TRP:CZ3	1:C:455:LEU:HD21	2.51	0.45
1:F:229:LEU:HB3	1:F:235:THR:HG22	1.98	0.45
1:A:159:ARG:NH2	1:A:430:LYS:O	2.49	0.45
1:A:191:THR:HA	2:A:601:MYA:HDMA	1.97	0.45
1:C:337:LEU:O	1:C:339:ASN:N	2.41	0.45
1:B:435:GLY:HA2	1:B:447:ARG:O	2.17	0.45
1:C:117:LYS:O	1:C:121:ASN:HB2	2.16	0.45
1:D:212:ALA:H	1:D:213:PRO:CD	2.29	0.45
1:B:191:THR:HA	2:B:602:MYA:HDM	1.97	0.45
1:E:93:GLU:HA	1:E:96:PHE:CE2	2.52	0.45
1:F:232:VAL:HG12	1:F:232:VAL:O	2.16	0.45
1:D:154:VAL:HG21	1:D:167:GLU:HG3	1.99	0.45
1:D:315:VAL:HG23	1:D:326:PHE:HB2	1.99	0.45
1:B:88:ASN:HB3	1:B:91:GLN:HB2	1.99	0.45
1:B:325:ASP:HB3	1:B:380:LEU:HD11	1.98	0.45
1:E:218:ARG:HH21	1:E:415:PRO:HB2	1.82	0.45
1:A:19:LEU:HD11	1:B:177:LEU:HD22	1.98	0.45
1:B:298:PHE:HA	1:B:311:ILE:HG12	1.97	0.45
1:D:113:PHE:HD2	1:D:332:LEU:HD21	1.81	0.45
1:E:183:THR:HA	1:E:186:LEU:HD12	1.99	0.45
1:F:53:VAL:HG11	1:F:428:ARG:HD3	1.99	0.45
1:F:88:ASN:HB3	1:F:91:GLN:HB2	1.98	0.45
1:D:338:ASN:C	1:D:338:ASN:HD22	2.21	0.45
1:D:398:ALA:HB3	1:D:408:LEU:HD21	1.98	0.45
1:A:258:THR:CG2	1:A:379:GLU:HB3	2.47	0.44
1:F:178:ARG:C	1:F:180:LYS:H	2.21	0.44
1:C:122:TRP:HZ3	1:C:455:LEU:HD21	1.82	0.44
1:E:71:LYS:O	1:E:71:LYS:HG2	2.17	0.44
1:C:40:PHE:CD1	1:C:184:PRO:HB3	2.52	0.44
1:E:283:PHE:CE2	1:E:402:GLN:HA	2.52	0.44
1:A:183:THR:HB	1:A:184:PRO:HD3	1.99	0.44
1:C:105:GLU:HG3	1:C:178:ARG:HH12	1.82	0.44
1:F:388:ALA:O	1:F:393:MET:HG3	2.17	0.44
1:B:405:THR:HG21	1:B:447:ARG:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:VAL:HB	2:D:604:MYA:H14B	2.00	0.44
1:E:264:LEU:HD12	1:E:268:ASP:HB2	2.00	0.44
1:E:272:VAL:HG22	1:E:323:ILE:HG21	1.99	0.44
1:E:362:LYS:H	1:E:362:LYS:HD2	1.81	0.44
1:F:430:LYS:HB3	1:F:431:PRO:HD2	1.99	0.44
1:B:399:LEU:O	1:B:400:THR:OG1	2.34	0.44
1:E:107:ARG:O	1:E:112:ARG:NH2	2.47	0.44
1:F:174:HIS:CD2	1:F:176:GLN:H	2.35	0.44
1:F:174:HIS:HB3	1:F:177:LEU:HD23	1.99	0.44
1:C:181:ARG:HH11	1:C:181:ARG:HG3	1.81	0.44
1:D:187:ILE:HG23	2:D:604:MYA:HAMA	1.98	0.44
1:E:88:ASN:HD22	1:E:89:LYS:N	2.14	0.44
1:A:232:VAL:O	1:A:232:VAL:CG1	2.65	0.43
1:C:154:VAL:HG21	1:C:167:GLU:HG3	1.99	0.43
1:D:228:LYS:O	1:D:232:VAL:HG23	2.18	0.43
1:D:339:ASN:ND2	1:D:342:TYR:H	2.05	0.43
1:B:159:ARG:HG3	1:B:284:GLU:HB3	1.99	0.43
1:D:191:THR:HA	2:D:604:MYA:CDM	2.48	0.43
1:D:272:VAL:HG22	1:D:323:ILE:HG21	1.99	0.43
1:C:93:GLU:HA	1:C:96:PHE:CZ	2.54	0.43
1:C:195:ASN:C	1:C:197:CYS:H	2.22	0.43
1:C:211:PRO:O	1:C:212:ALA:HB3	2.18	0.43
1:E:179:SER:HA	2:E:605:MYA:O2A	2.18	0.43
1:E:405:THR:HG21	1:E:447:ARG:HA	1.99	0.43
1:F:60:ASP:HB2	1:F:426:ASN:ND2	2.34	0.43
1:B:20:ASN:ND2	1:B:417:ASP:HB2	2.34	0.43
1:B:107:ARG:HD2	1:B:175:LYS:HZ3	1.84	0.43
1:C:138:ARG:HG2	1:C:145:LEU:HA	2.00	0.43
1:D:358:ASP:HB3	1:D:373:LEU:HB2	2.00	0.43
1:F:133:TRP:HB3	1:F:151:ALA:HB3	2.01	0.43
1:F:314:TYR:HB2	1:F:327:PHE:CE2	2.53	0.43
1:B:401:SER:O	1:B:404:ASN:HB2	2.19	0.43
1:C:169:ASN:HD22	1:C:169:ASN:HA	1.56	0.43
1:D:64:THR:C	1:D:66:GLU:H	2.21	0.43
1:D:128:GLY:O	1:D:153:PRO:HG3	2.19	0.43
1:D:212:ALA:N	1:D:213:PRO:CD	2.81	0.43
1:A:99:LEU:O	1:A:103:TYR:HB2	2.19	0.42
1:D:266:LYS:HA	1:D:269:ILE:HD12	2.00	0.42
1:E:391:ALA:O	1:E:392:ASN:HB2	2.19	0.42
1:F:277:LYS:HZ1	1:F:288:ILE:HA	1.84	0.42
1:B:40:PHE:CD1	1:B:184:PRO:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:ILE:HD13	1:C:444:ILE:H	1.83	0.42
1:E:64:THR:O	1:E:67:ASP:HB2	2.19	0.42
1:A:165:SER:HB3	1:A:201:HIS:HB2	2.01	0.42
3:A:701:GN8:CAS	3:A:701:GN8:SAE	3.07	0.42
1:C:324:THR:HG23	1:C:356:ASP:OD1	2.20	0.42
1:C:391:ALA:O	1:C:392:ASN:HB2	2.19	0.42
1:D:332:LEU:HB3	1:D:349:TYR:CE1	2.54	0.42
1:D:404:ASN:HA	1:D:407:PHE:CE2	2.54	0.42
1:A:252:LEU:HD21	1:A:385:CYS:HB3	2.00	0.42
1:B:99:LEU:HD13	1:B:103:TYR:CE1	2.54	0.42
1:B:201:HIS:ND1	1:B:426:ASN:O	2.50	0.42
1:D:214:VAL:HG21	1:D:424:LEU:HD12	2.02	0.42
1:A:99:LEU:HD12	1:A:103:TYR:CD1	2.53	0.42
1:A:232:VAL:O	1:A:232:VAL:HG12	2.18	0.42
1:A:278:ARG:NH1	1:A:278:ARG:CG	2.72	0.42
1:B:425:PHE:CG	2:B:602:MYA:HBMA	2.54	0.42
1:F:88:ASN:HD22	1:F:88:ASN:C	2.23	0.42
1:C:352:TYR:CE1	1:C:451:GLY:O	2.73	0.42
1:D:96:PHE:C	1:D:96:PHE:HD1	2.21	0.42
1:E:10:LEU:H	1:E:10:LEU:HD12	1.83	0.42
1:F:148:PHE:CE2	1:F:150:SER:HB2	2.55	0.42
1:A:311:ILE:HD13	1:A:312:PHE:N	2.35	0.42
1:B:301:GLU:HB3	1:B:304:LEU:HD11	2.01	0.42
1:B:445:LYS:HD2	1:B:446:ARG:H	1.85	0.42
1:D:130:LYS:HE2	1:D:130:LYS:HA	2.02	0.42
1:D:178:ARG:O	1:D:179:SER:HB2	2.20	0.42
1:D:311:ILE:HD13	1:D:312:PHE:N	2.34	0.42
1:F:190:ILE:HD13	1:F:190:ILE:HA	1.92	0.42
1:C:352:TYR:HE1	1:C:451:GLY:O	2.03	0.41
1:D:298:PHE:O	1:D:313:SER:HB2	2.18	0.41
1:C:93:GLU:HA	1:C:96:PHE:CE2	2.55	0.41
1:F:59:ILE:HG23	1:F:428:ARG:NH2	2.35	0.41
1:B:194:VAL:HG11	2:B:602:MYA:HEMA	2.02	0.41
1:B:256:THR:HB	1:B:383:ASP:OD1	2.20	0.41
1:F:136:GLY:HA3	1:F:145:LEU:HD11	2.00	0.41
1:C:111:PHE:HA	1:C:335:THR:O	2.19	0.41
1:C:280:GLN:HG3	1:C:286:ILE:HG21	2.00	0.41
1:A:96:PHE:CD1	1:A:96:PHE:C	2.94	0.41
1:A:437:ASN:HB3	1:A:438:PRO:HD2	2.02	0.41
1:B:406:LEU:HD11	1:B:447:ARG:NH1	2.35	0.41
1:C:214:VAL:HG12	1:C:422:PHE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:TYR:O	1:C:282:ARG:HG2	2.20	0.41
1:E:86:VAL:HG11	1:E:125:LYS:HG2	2.00	0.41
1:E:271:GLN:OE1	1:E:322:LYS:HG2	2.21	0.41
1:F:311:ILE:HD13	1:F:312:PHE:N	2.36	0.41
1:B:406:LEU:HG	1:B:447:ARG:HD3	2.03	0.41
1:C:302:GLU:HG3	1:C:303:SER:N	2.36	0.41
1:F:230:TYR:HD2	1:F:235:THR:O	2.04	0.41
1:A:86:VAL:HG13	1:A:92:LEU:HD13	2.03	0.41
1:C:56:GLU:HG2	1:C:429:ALA:HA	2.01	0.41
1:C:192:ARG:NH1	1:C:192:ARG:CG	2.79	0.41
1:C:356:ASP:OD1	1:C:356:ASP:C	2.58	0.41
1:C:400:THR:HA	1:C:408:LEU:HD11	2.02	0.41
1:F:396:PHE:HD2	1:F:413:PHE:HZ	1.66	0.41
1:C:181:ARG:HB3	1:C:181:ARG:NH1	2.23	0.41
1:E:149:ILE:HD12	1:E:190:ILE:HG21	2.03	0.41
1:E:217:CYS:HB3	1:E:400:THR:OG1	2.21	0.41
1:F:98:LEU:HD22	1:F:145:LEU:HD23	2.03	0.41
1:F:222:ARG:HB2	1:F:413:PHE:CE2	2.55	0.41
1:A:60:ASP:H	1:A:426:ASN:ND2	2.09	0.41
1:A:174:HIS:HD2	1:A:176:GLN:HB2	1.86	0.41
1:A:237:LEU:HA	1:A:238:PRO:HD3	1.95	0.41
1:A:256:THR:HG21	1:A:387:LEU:HG	2.02	0.41
1:F:183:THR:HB	1:F:184:PRO:HD3	2.03	0.41
1:F:347:ILE:HG23	1:F:395:VAL:HG13	2.03	0.41
1:A:73:LEU:HD23	1:A:74:PRO:HD2	2.03	0.41
1:C:168:ILE:HG21	2:C:603:MYA:H7M	2.02	0.41
1:D:276:PHE:O	1:D:280:GLN:HB2	2.21	0.41
1:E:339:ASN:ND2	1:E:341:LYS:H	2.19	0.41
1:A:426:ASN:O	1:A:427:TYR:HB2	2.21	0.40
1:C:339:ASN:ND2	1:C:341:LYS:H	2.19	0.40
1:F:45:PRO:HB2	1:F:426:ASN:HD22	1.86	0.40
1:A:73:LEU:HA	1:A:74:PRO:HD3	1.90	0.40
1:A:180:LYS:HD3	1:A:180:LYS:HA	1.86	0.40
1:A:404:ASN:HA	1:A:407:PHE:CE2	2.56	0.40
1:B:283:PHE:CE2	1:B:402:GLN:HA	2.57	0.40
1:C:181:ARG:CG	1:C:181:ARG:NH1	2.78	0.40
1:F:404:ASN:C	1:F:406:LEU:H	2.24	0.40
1:C:91:GLN:O	1:C:95:VAL:HG23	2.20	0.40
1:D:210:LEU:HB3	1:D:211:PRO:HD2	2.04	0.40
1:F:401:SER:O	1:F:402:GLN:HB2	2.22	0.40
1:B:306:LEU:HD21	1:B:391:ALA:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:LEU:HB3	1:D:77:SER:H	1.61	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	432/455 (95%)	391 (90%)	33 (8%)	8 (2%)	8	33
1	B	432/455 (95%)	382 (88%)	38 (9%)	12 (3%)	5	25
1	C	432/455 (95%)	376 (87%)	50 (12%)	6 (1%)	11	40
1	D	432/455 (95%)	376 (87%)	44 (10%)	12 (3%)	5	25
1	E	432/455 (95%)	391 (90%)	35 (8%)	6 (1%)	11	40
1	F	431/455 (95%)	373 (86%)	52 (12%)	6 (1%)	11	40
All	All	2591/2730 (95%)	2289 (88%)	252 (10%)	50 (2%)	8	33

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	ALA
1	B	78	SER
1	C	302	GLU
1	D	135	ILE
1	D	212	ALA
1	D	301	GLU
1	E	9	LYS
1	E	212	ALA
1	B	77	SER
1	B	413	PHE
1	C	78	SER

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Mol	Chain	Res	Type
1	D	51	GLU
1	D	77	SER
1	B	88	ASN
1	B	140	LYS
1	B	303	SER
1	C	338	ASN
1	C	427	TYR
1	D	76	LEU
1	D	337	LEU
1	E	78	SER
1	E	338	ASN
1	F	56	GLU
1	A	158	VAL
1	B	306	LEU
1	B	321	GLY
1	D	303	SER
1	D	338	ASN
1	D	412	LYS
1	F	42	ARG
1	F	269	ILE
1	F	291	LYS
1	A	65	PRO
1	A	78	SER
1	A	159	ARG
1	B	269	ILE
1	B	291	LYS
1	C	212	ALA
1	C	431	PRO
1	E	402	GLN
1	E	412	LYS
1	F	400	THR
1	A	400	THR
1	D	62	PRO
1	A	74	PRO
1	B	211	PRO
1	D	431	PRO
1	B	212	ALA
1	F	367	PRO
1	A	127	PRO



### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	394/413 (95%)	361 (92%)	33 (8%)	11	38
1	B	394/413 (95%)	361 (92%)	33 (8%)	11	38
1	C	394/413 (95%)	358 (91%)	36 (9%)	9	33
1	D	394/413 (95%)	358 (91%)	36 (9%)	9	33
1	E	394/413 (95%)	362 (92%)	32 (8%)	11	39
1	F	393/413 (95%)	359 (91%)	34 (9%)	10	36
All	All	2363/2478 (95%)	2159 (91%)	204 (9%)	10	37

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	21	ASN
1	A	64	THR
1	A	70	ASP
1	A	73	LEU
1	A	96	PHE
1	A	99	LEU
1	A	108	ASP
1	A	114	ASN
1	A	116	THR
1	A	132	ASP
1	A	135	ILE
1	A	181	ARG
1	A	190	ILE
1	A	220	THR
1	A	222	ARG
1	A	229	LEU
1	A	261	LEU
1	A	278	ARG
1	A	286	ILE
1	A	311	ILE
1	A	320	ASP

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Mol	Chain	Res	Type
1	A	325	ASP
1	A	326	PHE
1	A	332	LEU
1	A	335	THR
1	A	338	ASN
1	A	339	ASN
1	A	347	ILE
1	A	351	TYR
1	A	373	LEU
1	A	410	ASP
1	A	438	PRO
1	B	19	LEU
1	B	37	ASP
1	B	71	LYS
1	B	73	LEU
1	B	88	ASN
1	B	99	LEU
1	B	103	TYR
1	B	165	SER
1	B	181	ARG
1	B	208	ILE
1	B	210	LEU
1	B	222	ARG
1	B	229	LEU
1	B	242	THR
1	B	261	LEU
1	B	268	ASP
1	B	270	ASP
1	B	278	ARG
1	B	297	ASN
1	B	320	ASP
1	B	325	ASP
1	B	332	LEU
1	B	339	ASN
1	B	351	TYR
1	B	362	LYS
1	B	371	LYS
1	B	383	ASP
1	B	399	LEU
1	B	410	ASP
1	B	420	LEU
1	B	444	ILE

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Mol	Chain	Res	Type
1	B	445	LYS
1	B	452	VAL
1	C	6	LYS
1	C	8	LYS
1	C	21	ASN
1	C	48	ASP
1	C	50	ASP
1	C	61	LYS
1	C	71	LYS
1	C	88	ASN
1	C	94	ASP
1	C	135	ILE
1	C	162	GLN
1	C	169	ASN
1	C	177	LEU
1	C	181	ARG
1	C	221	HIS
1	C	222	ARG
1	C	249	GLU
1	C	261	LEU
1	C	278	ARG
1	C	280	GLN
1	C	285	LEU
1	C	311	ILE
1	C	315	VAL
1	C	326	PHE
1	C	344	ASP
1	C	351	TYR
1	C	356	ASP
1	C	362	LYS
1	C	371	LYS
1	C	373	LEU
1	C	386	ILE
1	C	395	VAL
1	C	410	ASP
1	C	420	LEU
1	C	444	ILE
1	C	445	LYS
1	D	12	ASN
1	D	37	ASP
1	D	53	VAL
1	D	87	ASP

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Mol	Chain	Res	Type
1	D	94	ASP
1	D	96	PHE
1	D	99	LEU
1	D	116	THR
1	D	130	LYS
1	D	166	VAL
1	D	173	VAL
1	D	176	GLN
1	D	177	LEU
1	D	252	LEU
1	D	263	LYS
1	D	268	ASP
1	D	269	ILE
1	D	278	ARG
1	D	297	ASN
1	D	299	ILE
1	D	311	ILE
1	D	315	VAL
1	D	323	ILE
1	D	326	PHE
1	D	338	ASN
1	D	340	THR
1	D	343	LYS
1	D	362	LYS
1	D	371	LYS
1	D	383	ASP
1	D	399	LEU
1	D	410	ASP
1	D	420	LEU
1	D	421	ASN
1	D	430	LYS
1	D	445	LYS
1	E	6	LYS
1	E	53	VAL
1	E	60	ASP
1	E	73	LEU
1	E	88	ASN
1	E	114	ASN
1	E	149	ILE
1	E	152	ILE
1	E	166	VAL
1	E	177	LEU

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Mol	Chain	Res	Type
1	E	208	ILE
1	E	222	ARG
1	E	234	PHE
1	E	239	ASP
1	E	252	LEU
1	E	256	THR
1	E	257	LYS
1	E	261	LEU
1	E	291	LYS
1	E	317	GLU
1	E	332	LEU
1	E	339	ASN
1	E	340	THR
1	E	344	ASP
1	E	351	TYR
1	E	360	GLN
1	E	362	LYS
1	E	371	LYS
1	E	373	LEU
1	E	405	THR
1	E	420	LEU
1	E	445	LYS
1	F	9	LYS
1	F	67	ASP
1	F	88	ASN
1	F	96	PHE
1	F	107	ARG
1	F	114	ASN
1	F	117	LYS
1	F	149	ILE
1	F	168	ILE
1	F	182	LEU
1	F	186	LEU
1	F	190	ILE
1	F	208	ILE
1	F	220	THR
1	F	243	GLU
1	F	263	LYS
1	F	268	ASP
1	F	269	ILE
1	F	286	ILE
1	F	291	LYS

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Mol	Chain	Res	Type
1	F	295	GLU
1	F	307	ASP
1	F	311	ILE
1	F	315	VAL
1	F	325	ASP
1	F	326	PHE
1	F	327	PHE
1	F	335	THR
1	F	339	ASN
1	F	351	TYR
1	F	368	LYS
1	F	373	LEU
1	F	404	ASN
1	F	452	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	HIS
1	A	195	ASN
1	A	250	ASN
1	A	338	ASN
1	A	339	ASN
1	A	397	ASN
1	A	404	ASN
1	A	421	ASN
1	A	426	ASN
1	B	20	ASN
1	B	88	ASN
1	B	174	HIS
1	B	176	GLN
1	B	195	ASN
1	B	297	ASN
1	B	318	GLN
1	B	339	ASN
1	B	397	ASN
1	B	404	ASN
1	B	421	ASN
1	B	426	ASN
1	B	442	ASN
1	C	20	ASN
1	C	88	ASN

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Mol	Chain	Res	Type
1	C	91	GLN
1	C	114	ASN
1	C	162	GLN
1	C	169	ASN
1	C	174	HIS
1	C	339	ASN
1	C	397	ASN
1	C	404	ASN
1	C	421	ASN
1	C	426	ASN
1	C	437	ASN
1	D	18	GLN
1	D	20	ASN
1	D	21	ASN
1	D	114	ASN
1	D	176	GLN
1	D	195	ASN
1	D	221	HIS
1	D	241	HIS
1	D	338	ASN
1	D	339	ASN
1	D	397	ASN
1	D	421	ASN
1	D	426	ASN
1	D	442	ASN
1	E	88	ASN
1	E	114	ASN
1	E	121	ASN
1	E	174	HIS
1	E	195	ASN
1	E	339	ASN
1	E	360	GLN
1	E	397	ASN
1	E	404	ASN
1	E	421	ASN
1	E	426	ASN
1	E	437	ASN
1	E	449	ASN
1	F	88	ASN
1	F	91	GLN
1	F	114	ASN
1	F	174	HIS

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Mol	Chain	Res	Type
1	F	176	GLN
1	F	195	ASN
1	F	296	HIS
1	F	338	ASN
1	F	339	ASN
1	F	397	ASN
1	F	404	ASN
1	F	421	ASN
1	F	426	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	GN8	C	703	-	25,27,27	2.96	5 (20%)	28,38,38	3.72	11 (39%)
2	MYA	A	601	-	59,65,65	0.89	4 (6%)	72,91,91	1.40	8 (11%)
3	GN8	B	702	-	25,27,27	2.95	6 (24%)	28,38,38	3.91	12 (42%)
3	GN8	F	706	-	25,27,27	2.97	7 (28%)	28,38,38	3.80	12 (42%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GN8	A	701	-	25,27,27	2.97	6 (24%)	28,38,38	3.96	11 (39%)
2	MYA	F	606	-	59,65,65	0.97	5 (8%)	72,91,91	1.46	8 (11%)
3	GN8	D	704	-	25,27,27	2.98	6 (24%)	28,38,38	3.94	10 (35%)
2	MYA	E	605	-	59,65,65	0.90	3 (5%)	72,91,91	1.42	9 (12%)
2	MYA	B	602	-	59,65,65	0.90	3 (5%)	72,91,91	1.64	9 (12%)
2	MYA	D	604	-	59,65,65	0.93	4 (6%)	72,91,91	1.45	8 (11%)
2	MYA	C	603	-	59,65,65	0.91	4 (6%)	72,91,91	1.41	7 (9%)
3	GN8	E	705	-	25,27,27	3.19	8 (32%)	28,38,38	4.02	9 (32%)

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	GN8	C	703	-	-	3/8/28/28	0/3/3/3
2	MYA	A	601	-	1/1/12/14	22/60/80/80	0/3/3/3
3	GN8	B	702	-	-	3/8/28/28	0/3/3/3
3	GN8	F	706	-	-	3/8/28/28	0/3/3/3
3	GN8	A	701	-	-	3/8/28/28	0/3/3/3
2	MYA	F	606	-	1/1/12/14	21/60/80/80	0/3/3/3
3	GN8	D	704	-	-	2/8/28/28	0/3/3/3
2	MYA	E	605	-	1/1/12/14	17/60/80/80	0/3/3/3
2	MYA	B	602	-	1/1/12/14	24/60/80/80	0/3/3/3
2	MYA	D	604	-	1/1/12/14	14/60/80/80	0/3/3/3
2	MYA	C	603	-	1/1/12/14	9/60/80/80	0/3/3/3
3	GN8	E	705	-	-	3/8/28/28	0/3/3/3

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	703	GN8	OAD-NAY	9.98	1.40	1.22
3	D	704	GN8	OAD-NAY	9.91	1.40	1.22
3	A	701	GN8	OAD-NAY	9.86	1.39	1.22
3	F	706	GN8	OAD-NAY	9.85	1.39	1.22
3	E	705	GN8	OAD-NAY	9.85	1.39	1.22
3	B	702	GN8	OAD-NAY	9.83	1.39	1.22
3	E	705	GN8	CAF-CAW	6.82	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	GN8	CAF-CAW	6.74	1.49	1.35
3	D	704	GN8	CAF-CAW	6.71	1.49	1.35
3	F	706	GN8	CAF-CAW	6.70	1.49	1.35
3	B	702	GN8	CAF-CAW	6.65	1.49	1.35
3	C	703	GN8	CAF-CAW	6.59	1.49	1.35
3	E	705	GN8	CAM-CAS	5.49	1.46	1.36
3	E	705	GN8	CAU-CAW	-4.95	1.39	1.48
3	A	701	GN8	CAU-CAW	-4.86	1.39	1.48
3	F	706	GN8	CAU-CAW	-4.82	1.39	1.48
3	B	702	GN8	CAU-CAW	-4.77	1.39	1.48
3	C	703	GN8	CAU-CAW	-4.75	1.39	1.48
3	D	704	GN8	CAU-CAW	-4.73	1.39	1.48
3	C	703	GN8	CAV-SAE	4.72	1.78	1.66
3	F	706	GN8	CAV-SAE	4.71	1.78	1.66
3	E	705	GN8	CAV-SAE	4.71	1.78	1.66
3	B	702	GN8	CAV-SAE	4.69	1.77	1.66
3	A	701	GN8	CAV-SAE	4.68	1.77	1.66
3	D	704	GN8	CAV-SAE	4.66	1.77	1.66
2	B	602	MYA	C2M-S1	-3.73	1.67	1.76
2	A	601	MYA	C2M-S1	-3.71	1.67	1.76
2	E	605	MYA	C2M-S1	-3.70	1.67	1.76
2	D	604	MYA	C2M-S1	-3.48	1.68	1.76
2	C	603	MYA	C2M-S1	-3.46	1.68	1.76
2	F	606	MYA	C2M-S1	-3.26	1.68	1.76
3	D	704	GN8	OAA-CAU	3.15	1.29	1.23
3	C	703	GN8	OAA-CAU	3.10	1.29	1.23
3	B	702	GN8	OAA-CAU	3.05	1.29	1.23
3	F	706	GN8	OAA-CAU	3.04	1.29	1.23
3	E	705	GN8	OAA-CAU	2.93	1.29	1.23
3	A	701	GN8	OAA-CAU	2.93	1.29	1.23
2	D	604	MYA	P1A-O3A	2.84	1.62	1.59
2	C	603	MYA	P1A-O3A	2.56	1.62	1.59
2	F	606	MYA	P1A-O3A	2.55	1.62	1.59
2	D	604	MYA	P2A-O3A	2.53	1.62	1.59
2	E	605	MYA	P1A-O3A	2.50	1.62	1.59
2	B	602	MYA	P1A-O3A	2.44	1.62	1.59
3	F	706	GN8	CAM-CAS	2.38	1.41	1.36
2	B	602	MYA	P2A-O3A	2.31	1.62	1.59
2	A	601	MYA	P1A-O3A	2.27	1.62	1.59
2	A	601	MYA	P2A-O3A	2.27	1.61	1.59
2	C	603	MYA	O4X-C1X	2.26	1.43	1.40
2	F	606	MYA	C3M-C2M	2.23	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	MYA	O4X-C1X	2.21	1.43	1.40
2	C	603	MYA	P2A-O3A	2.21	1.61	1.59
2	F	606	MYA	P2A-O3A	2.21	1.61	1.59
3	D	704	GN8	CAM-CAS	2.19	1.40	1.36
2	D	604	MYA	O4X-C1X	2.18	1.43	1.40
3	A	701	GN8	CAM-CAS	2.17	1.40	1.36
3	B	702	GN8	CAM-CAS	2.11	1.40	1.36
2	F	606	MYA	O4X-C1X	2.08	1.43	1.40
3	E	705	GN8	CAH-CAG	2.06	1.46	1.40
3	E	705	GN8	CAU-NAX	-2.06	1.35	1.40
2	E	605	MYA	P2A-O3A	2.04	1.61	1.59
3	F	706	GN8	CAU-NAX	-2.03	1.35	1.40

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	705	GN8	CAV-NAX-CAU	-10.03	105.77	116.70
3	A	701	GN8	CAV-NAX-CAU	-9.97	105.84	116.70
3	D	704	GN8	CAV-NAX-CAU	-9.81	106.01	116.70
3	B	702	GN8	CAV-NAX-CAU	-9.81	106.01	116.70
3	F	706	GN8	CAV-NAX-CAU	-9.52	106.33	116.70
3	C	703	GN8	CAV-NAX-CAU	-9.38	106.48	116.70
3	E	705	GN8	CAW-CAU-NAX	8.94	118.89	110.20
3	E	705	GN8	CAO-NAX-CAV	8.65	132.01	122.42
3	B	702	GN8	SAP-CAV-NAX	8.52	118.67	110.18
3	A	701	GN8	CAW-CAU-NAX	8.47	118.44	110.20
3	A	701	GN8	SAP-CAV-NAX	8.45	118.60	110.18
3	D	704	GN8	SAP-CAV-NAX	8.45	118.60	110.18
3	C	703	GN8	SAP-CAV-NAX	8.34	118.49	110.18
3	F	706	GN8	SAP-CAV-NAX	8.29	118.44	110.18
3	E	705	GN8	SAP-CAV-NAX	8.27	118.42	110.18
3	D	704	GN8	CAW-CAU-NAX	8.22	118.20	110.20
3	B	702	GN8	CAW-CAU-NAX	8.16	118.13	110.20
3	F	706	GN8	CAW-CAU-NAX	8.03	118.01	110.20
3	D	704	GN8	CAO-NAX-CAV	8.02	131.30	122.42
3	A	701	GN8	CAO-NAX-CAV	8.01	131.29	122.42
3	B	702	GN8	CAO-NAX-CAV	7.70	130.95	122.42
3	C	703	GN8	CAW-CAU-NAX	7.56	117.56	110.20
3	F	706	GN8	CAO-NAX-CAV	7.26	130.46	122.42
3	B	702	GN8	CAV-SAP-CAW	-6.90	86.33	92.67
3	D	704	GN8	CAV-SAP-CAW	-6.83	86.39	92.67
3	A	701	GN8	CAV-SAP-CAW	-6.81	86.41	92.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	706	GN8	CAV-SAP-CAW	-6.79	86.43	92.67
3	C	703	GN8	CAV-SAP-CAW	-6.76	86.45	92.67
3	E	705	GN8	CAV-SAP-CAW	-6.69	86.51	92.67
2	B	602	MYA	C3M-C2M-S1	6.47	121.12	113.40
2	B	602	MYA	N3A-C2A-N1A	-5.83	120.75	128.67
3	C	703	GN8	CAO-NAX-CAV	5.71	128.75	122.42
2	C	603	MYA	N3A-C2A-N1A	-5.61	121.05	128.67
2	D	604	MYA	N3A-C2A-N1A	-5.57	121.11	128.67
2	F	606	MYA	N3A-C2A-N1A	-5.51	121.20	128.67
2	A	601	MYA	N3A-C2A-N1A	-5.46	121.26	128.67
2	E	605	MYA	N3A-C2A-N1A	-5.45	121.27	128.67
2	D	604	MYA	C3M-C2M-S1	5.43	119.87	113.40
3	C	703	GN8	CAF-CAW-CAU	5.41	129.11	120.95
2	F	606	MYA	C3M-C2M-S1	5.38	119.81	113.40
2	A	601	MYA	C3M-C2M-S1	4.81	119.13	113.40
3	A	701	GN8	CAF-CAW-CAU	4.65	127.96	120.95
2	C	603	MYA	C3M-C2M-S1	4.64	118.93	113.40
3	F	706	GN8	CAF-CAW-CAU	4.62	127.92	120.95
3	B	702	GN8	CAF-CAW-CAU	4.61	127.89	120.95
3	E	705	GN8	OAA-CAU-CAW	-4.58	119.73	126.45
2	B	602	MYA	O2M-C2M-C3M	-4.47	118.83	123.98
3	D	704	GN8	CAF-CAW-CAU	4.46	127.68	120.95
2	E	605	MYA	C3M-C2M-S1	4.35	118.59	113.40
2	D	604	MYA	O2M-C2M-C3M	-4.33	118.98	123.98
3	A	701	GN8	OAA-CAU-CAW	-4.24	120.22	126.45
3	D	704	GN8	OAA-CAU-CAW	-4.20	120.28	126.45
2	B	602	MYA	C7-N8-C9	4.12	129.94	122.55
3	E	705	GN8	CAS-CAO-NAX	4.07	119.35	113.32
3	C	703	GN8	OAA-CAU-CAW	-4.06	120.48	126.45
3	F	706	GN8	OAA-CAU-CAW	-4.04	120.51	126.45
3	B	702	GN8	OAA-CAU-CAW	-4.03	120.52	126.45
3	D	704	GN8	CAS-CAO-NAX	3.91	119.11	113.32
2	E	605	MYA	C2-C3-N4	-3.88	104.32	112.41
3	A	701	GN8	SAP-CAV-SAE	-3.87	116.26	122.98
3	D	704	GN8	SAP-CAV-SAE	-3.82	116.34	122.98
3	C	703	GN8	SAP-CAV-SAE	-3.77	116.42	122.98
3	F	706	GN8	SAP-CAV-SAE	-3.76	116.44	122.98
2	A	601	MYA	O2M-C2M-C3M	-3.75	119.65	123.98
2	F	606	MYA	O2M-C2M-C3M	-3.73	119.67	123.98
3	B	702	GN8	SAP-CAV-SAE	-3.65	116.63	122.98
3	E	705	GN8	CAF-CAW-CAU	3.62	126.42	120.95
3	E	705	GN8	SAP-CAV-SAE	-3.59	116.73	122.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	603	MYA	O2M-C2M-C3M	-3.59	119.83	123.98
2	B	602	MYA	C6-C7-N8	-3.43	104.69	112.00
2	C	603	MYA	C2-C3-N4	-3.41	105.28	112.41
2	B	602	MYA	C2-C3-N4	-3.41	105.30	112.41
2	E	605	MYA	O2M-C2M-C3M	-3.40	120.06	123.98
3	B	702	GN8	CAS-CAO-NAX	3.36	118.29	113.32
2	F	606	MYA	C2-C3-N4	-3.22	105.70	112.41
2	D	604	MYA	C7-N8-C9	3.17	128.25	122.55
2	E	605	MYA	C6-C7-N8	-3.17	105.25	112.00
2	A	601	MYA	C2-C3-N4	-3.16	105.81	112.41
3	C	703	GN8	CAR-CAF-CAW	-3.03	123.46	130.90
3	A	701	GN8	CAS-CAO-NAX	3.02	117.79	113.32
2	B	602	MYA	C14-C11-C10	3.00	113.89	108.77
2	F	606	MYA	C7-N8-C9	2.96	127.86	122.55
2	E	605	MYA	C7-N8-C9	2.81	127.59	122.55
2	C	603	MYA	C7-N8-C9	2.79	127.56	122.55
2	A	601	MYA	C14-C11-C10	2.78	113.51	108.77
2	A	601	MYA	C7-N8-C9	2.75	127.48	122.55
2	D	604	MYA	C14-C11-C10	2.70	113.37	108.77
3	C	703	GN8	CAF-CAW-SAP	-2.67	119.87	127.28
2	E	605	MYA	C3-N4-C5	2.55	127.57	122.82
2	F	606	MYA	C6-C7-N8	-2.54	106.60	112.00
2	D	604	MYA	C2-C3-N4	-2.53	107.13	112.41
2	D	604	MYA	C6-C7-N8	-2.50	106.69	112.00
2	C	603	MYA	C3-N4-C5	2.48	127.44	122.82
2	C	603	MYA	C6-C7-N8	-2.44	106.80	112.00
2	A	601	MYA	C3-N4-C5	2.43	127.34	122.82
2	B	602	MYA	C3-N4-C5	2.38	127.25	122.82
3	C	703	GN8	OAC-CAQ-CAR	-2.34	118.86	121.81
3	F	706	GN8	CAS-CAO-NAX	2.32	116.75	113.32
2	E	605	MYA	C14-C11-C10	2.28	112.66	108.77
2	F	606	MYA	C3-N4-C5	2.22	126.96	122.82
3	F	706	GN8	OAC-CAQ-CAR	-2.21	119.03	121.81
2	F	606	MYA	C14-C11-C10	2.20	112.51	108.77
3	B	702	GN8	OAC-CAQ-CAR	-2.19	119.04	121.81
3	B	702	GN8	CAF-CAW-SAP	-2.17	121.25	127.28
3	A	701	GN8	OAC-CAQ-CAR	-2.17	119.07	121.81
3	F	706	GN8	CAF-CAW-SAP	-2.16	121.29	127.28
3	A	701	GN8	CAF-CAW-SAP	-2.14	121.33	127.28
3	B	702	GN8	CAR-CAF-CAW	-2.12	125.70	130.90
2	E	605	MYA	C3X-C2X-C1X	2.11	104.52	99.89
3	D	704	GN8	CAF-CAW-SAP	-2.07	121.53	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	MYA	O2M-C2M-S1	-2.06	120.06	122.68
3	F	706	GN8	CAR-CAF-CAW	-2.06	125.83	130.90
2	D	604	MYA	C3-N4-C5	2.01	126.57	122.82
2	A	601	MYA	C6-C7-N8	-2.01	107.72	112.00

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	MYA	C10
2	B	602	MYA	C10
2	C	603	MYA	C10
2	D	604	MYA	C10
2	E	605	MYA	C10
2	F	606	MYA	C10

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	MYA	C12-O6A-P2A-O5A
2	B	602	MYA	O2M-C2M-S1-C2
2	B	602	MYA	C3M-C2M-S1-C2
2	B	602	MYA	C5-C6-C7-N8
2	B	602	MYA	C5X-O5X-P1A-O2A
2	B	602	MYA	C5X-O5X-P1A-O3A
2	B	602	MYA	C2M-C3M-C4M-C5M
2	C	603	MYA	S1-C2-C3-N4
2	D	604	MYA	C2M-C3M-C4M-C5M
2	F	606	MYA	O10-C10-C11-C12
2	F	606	MYA	O10-C10-C11-C14
2	F	606	MYA	C12-O6A-P2A-O3A
2	F	606	MYA	C12-O6A-P2A-O4A
2	F	606	MYA	C2M-C3M-C4M-C5M
3	A	701	GN8	CAS-CAO-NAX-CAU
3	A	701	GN8	CAS-CAO-NAX-CAV
3	B	702	GN8	CAS-CAO-NAX-CAU
3	B	702	GN8	CAS-CAO-NAX-CAV
3	D	704	GN8	CAS-CAO-NAX-CAU
3	D	704	GN8	CAS-CAO-NAX-CAV
3	E	705	GN8	CAS-CAO-NAX-CAU
3	E	705	GN8	CAS-CAO-NAX-CAV
3	F	706	GN8	CAS-CAO-NAX-CAU
3	F	706	GN8	CAS-CAO-NAX-CAV

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Mol	Chain	Res	Type	Atoms
2	B	602	MYA	C3M-C4M-C5M-C6M
2	D	604	MYA	C4M-C5M-C6M-C7M
2	D	604	MYA	C7M-C8M-C9M-CAM
2	D	604	MYA	C9M-CAM-CBM-CCM
2	E	605	MYA	C5M-C6M-C7M-C8M
2	B	602	MYA	CBM-CCM-CDM-CEM
2	E	605	MYA	CAM-CBM-CCM-CDM
2	F	606	MYA	C7M-C8M-C9M-CAM
2	E	605	MYA	C4M-C5M-C6M-C7M
2	B	602	MYA	C9M-CAM-CBM-CCM
2	B	602	MYA	C7M-C8M-C9M-CAM
2	A	601	MYA	C5-C6-C7-N8
2	A	601	MYA	C8M-C9M-CAM-CBM
3	B	702	GN8	NAX-CAO-CAS-CAM
3	C	703	GN8	NAX-CAO-CAS-CAM
2	A	601	MYA	CAM-CBM-CCM-CDM
2	D	604	MYA	CBM-CCM-CDM-CEM
2	E	605	MYA	C8M-C9M-CAM-CBM
2	D	604	MYA	C3M-C4M-C5M-C6M
2	B	602	MYA	O10-C10-C9-O9
2	E	605	MYA	C3X-O3X-P3X-O9A
2	E	605	MYA	C3M-C4M-C5M-C6M
2	C	603	MYA	CBM-CCM-CDM-CEM
3	C	703	GN8	CAS-CAO-NAX-CAV
2	F	606	MYA	C3M-C4M-C5M-C6M
2	C	603	MYA	C8M-C9M-CAM-CBM
2	F	606	MYA	CAM-CBM-CCM-CDM
2	B	602	MYA	C6M-C7M-C8M-C9M
2	B	602	MYA	O10-C10-C11-C13
2	F	606	MYA	O10-C10-C11-C13
2	A	601	MYA	C5M-C6M-C7M-C8M
2	E	605	MYA	S1-C2-C3-N4
2	D	604	MYA	C5M-C6M-C7M-C8M
2	A	601	MYA	C11-C10-C9-N8
2	A	601	MYA	CCM-CDM-CEM-CFM
2	A	601	MYA	O2M-C2M-S1-C2
2	F	606	MYA	C5M-C6M-C7M-C8M
2	B	602	MYA	S1-C2M-C3M-C4M
2	B	602	MYA	O2M-C2M-C3M-C4M
2	D	604	MYA	S1-C2M-C3M-C4M
2	D	604	MYA	O2M-C2M-C3M-C4M
2	F	606	MYA	CCM-CDM-CEM-CFM

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Mol	Chain	Res	Type	Atoms
2	C	603	MYA	P1A-O3A-P2A-O4A
2	A	601	MYA	O10-C10-C9-O9
2	A	601	MYA	C14-C11-C12-O6A
2	E	605	MYA	C13-C11-C12-O6A
2	E	605	MYA	C14-C11-C12-O6A
2	B	602	MYA	C3X-C4X-C5X-O5X
2	A	601	MYA	C3-C2-S1-C2M
2	B	602	MYA	C3X-O3X-P3X-O9A
2	A	601	MYA	C12-O6A-P2A-O3A
2	A	601	MYA	C12-O6A-P2A-O4A
2	B	602	MYA	O10-C10-C11-C12
2	E	605	MYA	C5X-O5X-P1A-O2A
2	F	606	MYA	C12-O6A-P2A-O5A
2	B	602	MYA	O10-C10-C11-C14
2	C	603	MYA	CAM-CBM-CCM-CDM
2	A	601	MYA	S1-C2-C3-N4
3	A	701	GN8	NAX-CAO-CAS-CAM
3	F	706	GN8	NAX-CAO-CAS-CAM
2	B	602	MYA	C8M-C9M-CAM-CBM
2	C	603	MYA	O5-C5-C6-C7
2	A	601	MYA	O10-C10-C9-N8
2	B	602	MYA	O10-C10-C9-N8
2	D	604	MYA	O10-C10-C9-O9
2	E	605	MYA	O10-C10-C9-O9
3	C	703	GN8	CAS-CAO-NAX-CAU
2	C	603	MYA	C7M-C8M-C9M-CAM
2	D	604	MYA	C3X-O3X-P3X-O9A
2	F	606	MYA	S1-C2M-C3M-C4M
2	F	606	MYA	O2M-C2M-C3M-C4M
2	C	603	MYA	P1A-O3A-P2A-O5A
2	F	606	MYA	P1A-O3A-P2A-O4A
2	E	605	MYA	O5-C5-C6-C7
2	A	601	MYA	C3M-C2M-S1-C2
2	D	604	MYA	C5-C6-C7-N8
2	C	603	MYA	N4-C5-C6-C7
2	E	605	MYA	N4-C5-C6-C7
2	F	606	MYA	C8M-C9M-CAM-CBM
2	D	604	MYA	C8M-C9M-CAM-CBM
2	A	601	MYA	O5-C5-C6-C7
2	A	601	MYA	C9M-CAM-CBM-CCM
3	E	705	GN8	NAX-CAO-CAS-CAM
2	F	606	MYA	C9-C10-C11-C14

*Continued on next page...*



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Mol	Chain	Res	Type	Atoms
2	A	601	MYA	C6M-C7M-C8M-C9M
2	B	602	MYA	P1A-O3A-P2A-O4A
2	E	605	MYA	P1A-O3A-P2A-O5A
2	F	606	MYA	P2A-O3A-P1A-O2A
2	F	606	MYA	P1A-O3A-P2A-O5A
2	A	601	MYA	C11-C10-C9-O9
2	E	605	MYA	C3X-O3X-P3X-O7A
2	A	601	MYA	C13-C11-C12-O6A
2	B	602	MYA	C13-C11-C12-O6A
2	B	602	MYA	C14-C11-C12-O6A
2	D	604	MYA	O10-C10-C9-N8
2	E	605	MYA	O10-C10-C9-N8
2	F	606	MYA	O10-C10-C9-N8
2	E	605	MYA	C10-C11-C12-O6A
2	A	601	MYA	N4-C5-C6-C7
2	F	606	MYA	P2A-O3A-P1A-O1A

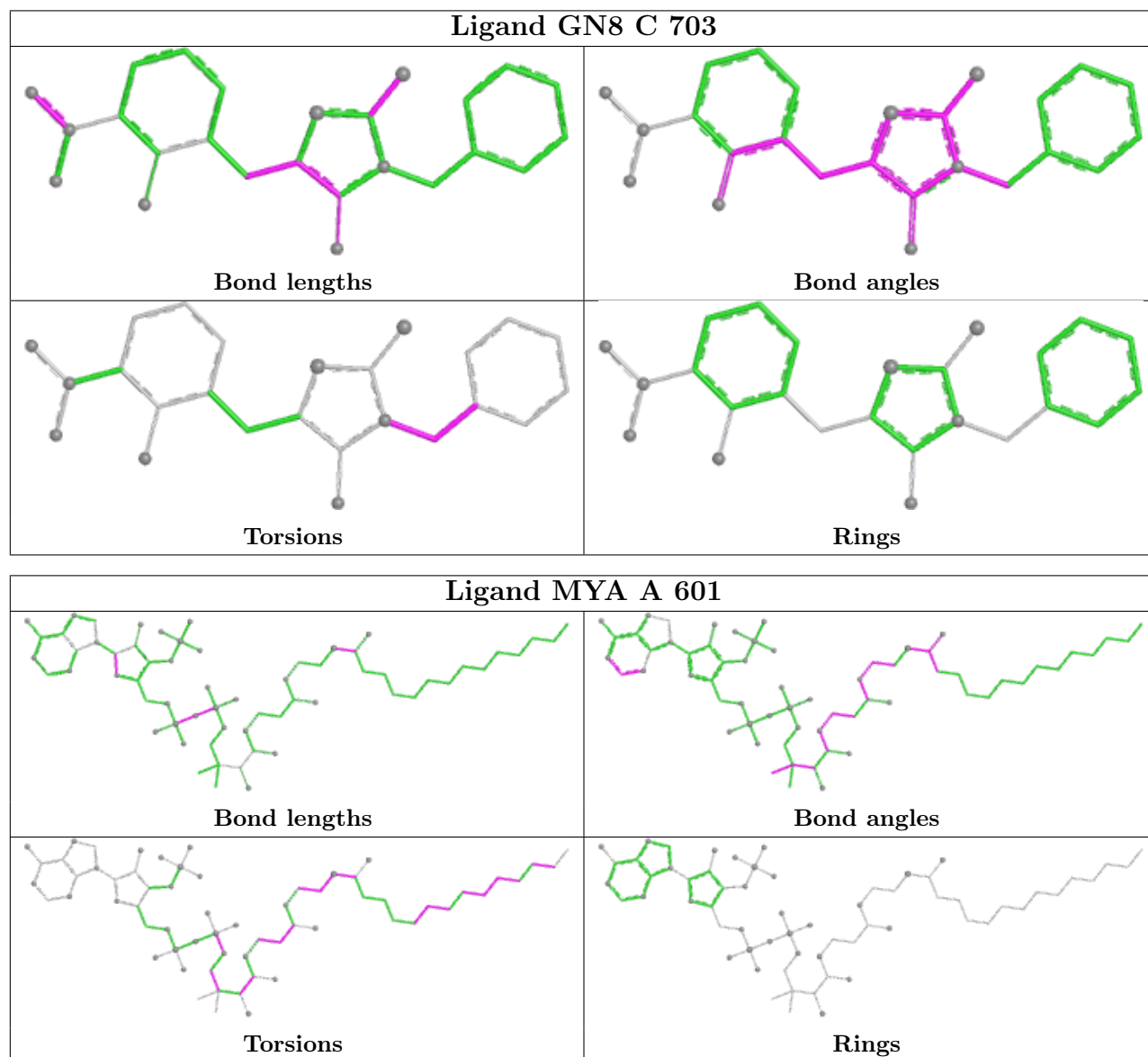
There are no ring outliers.

12 monomers are involved in 31 short contacts:

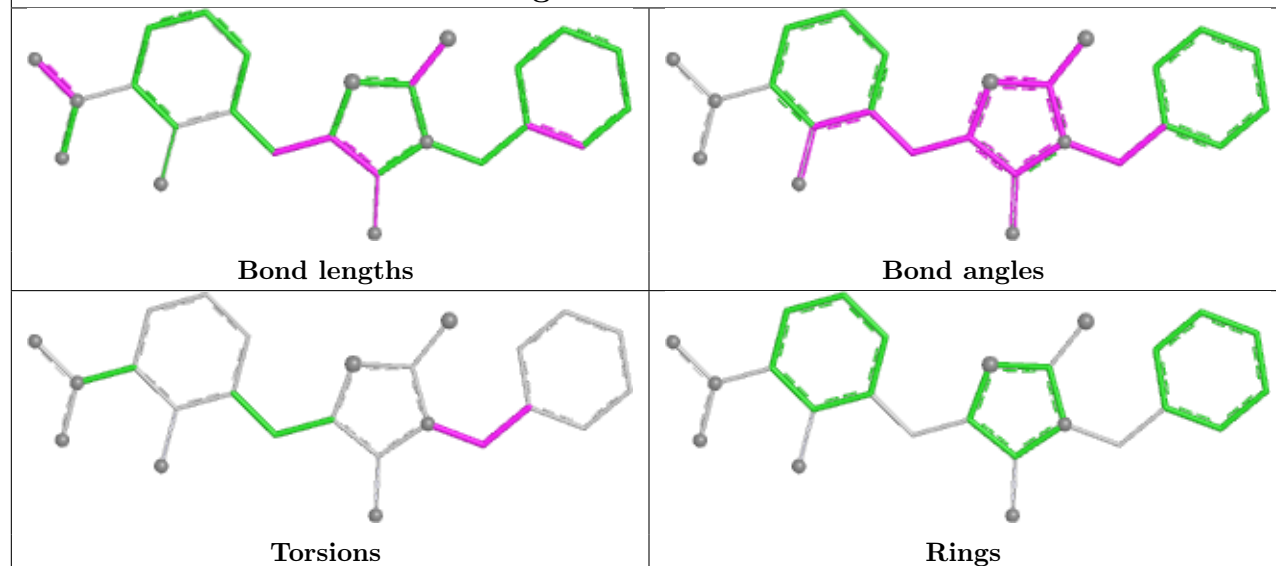
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	703	GN8	2	0
2	A	601	MYA	1	0
3	B	702	GN8	1	0
3	F	706	GN8	1	0
3	A	701	GN8	3	0
2	F	606	MYA	2	0
3	D	704	GN8	1	0
2	E	605	MYA	3	0
2	B	602	MYA	6	0
2	D	604	MYA	7	0
2	C	603	MYA	3	0
3	E	705	GN8	1	0

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

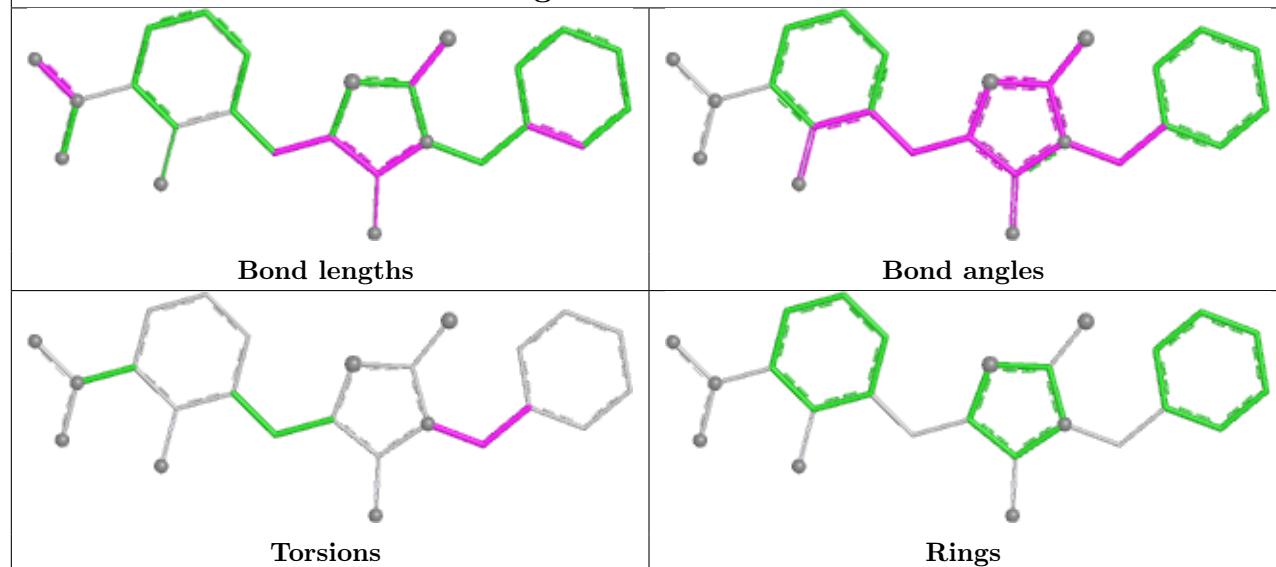
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



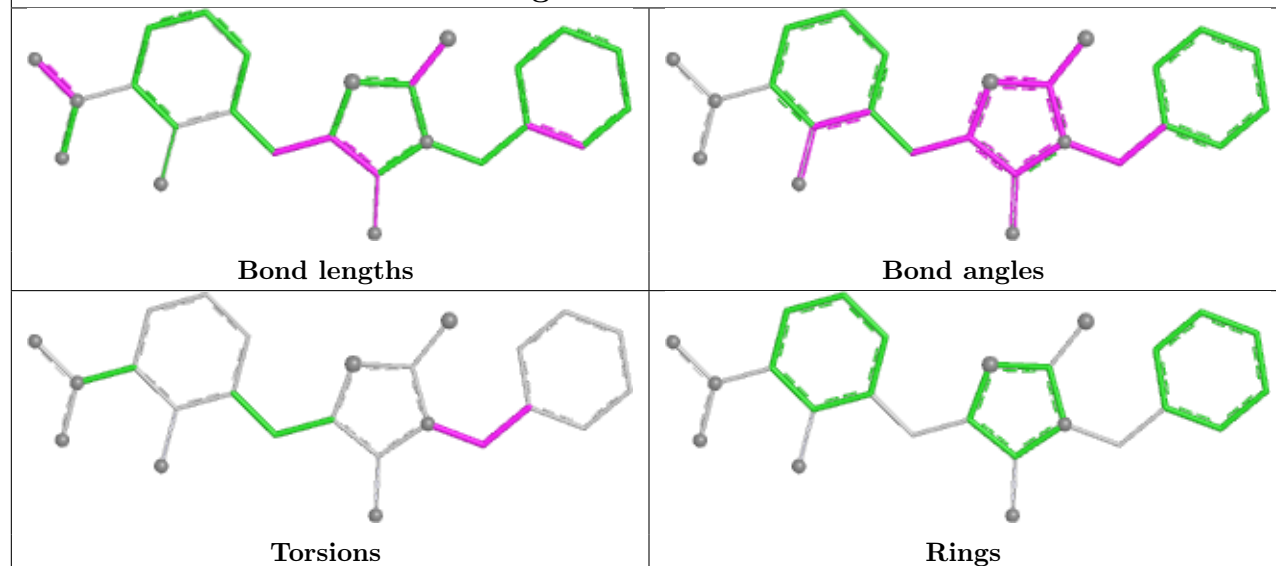
## Ligand GN8 B 702



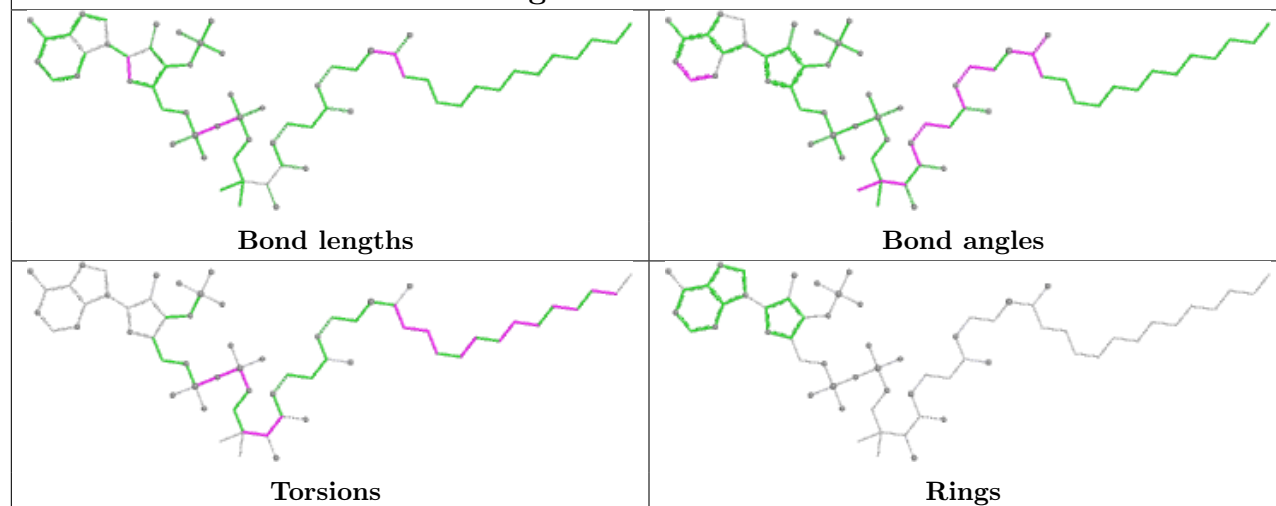
## Ligand GN8 F 706



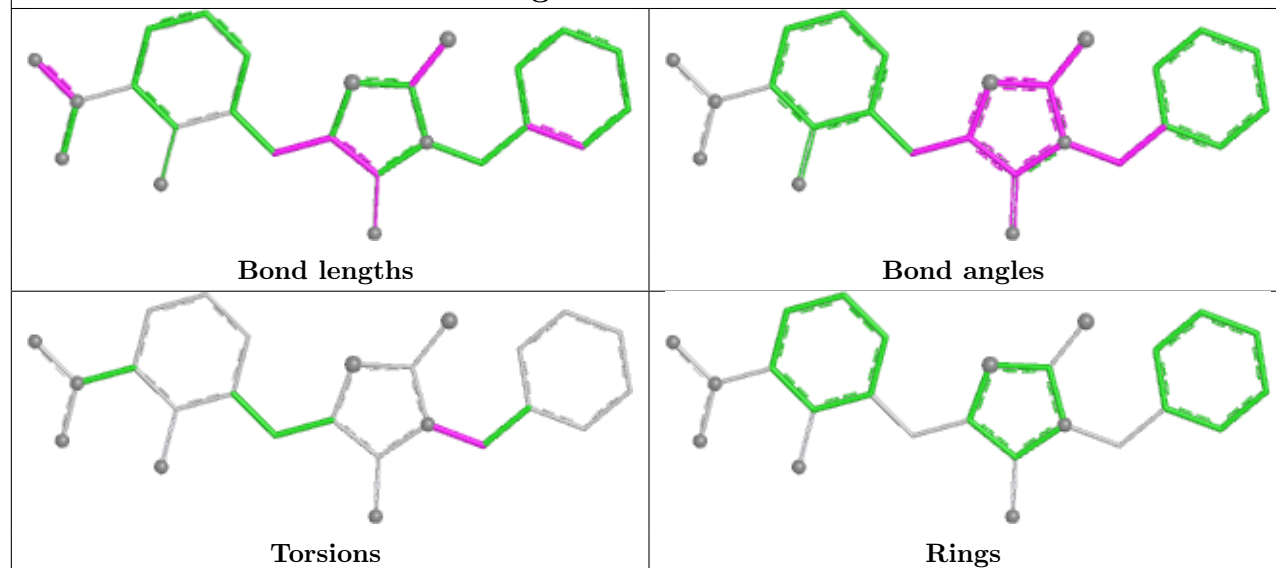
## Ligand GN8 A 701

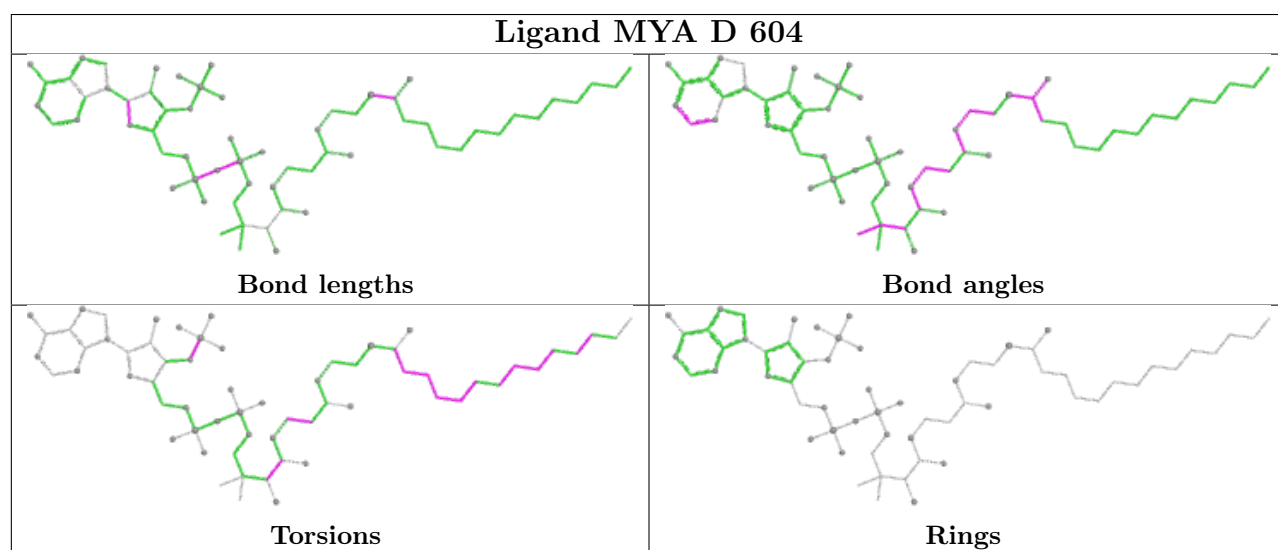
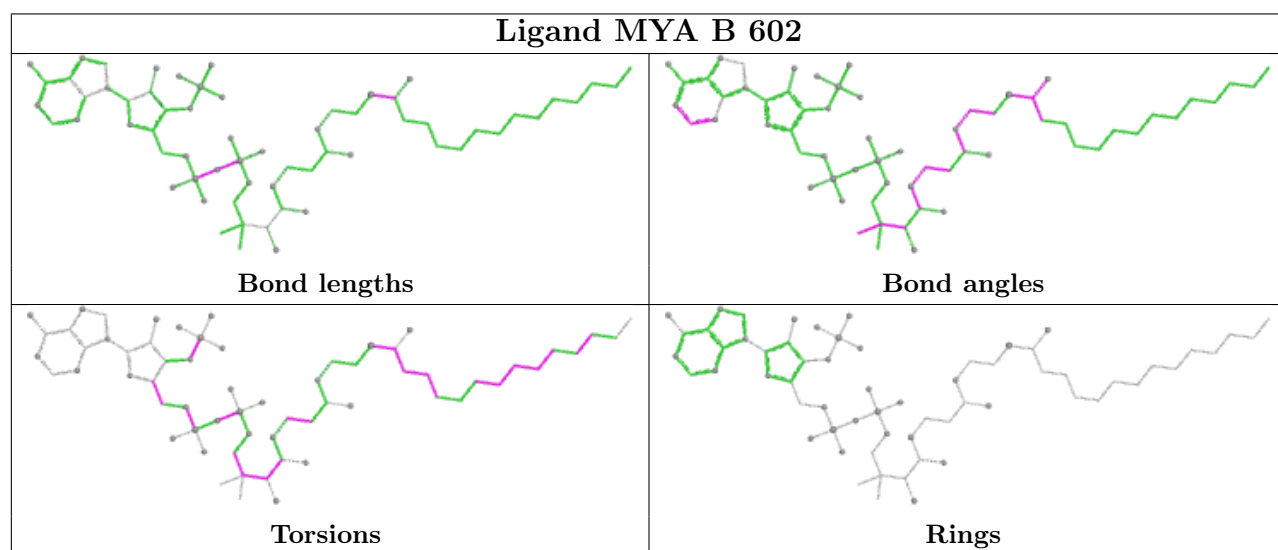
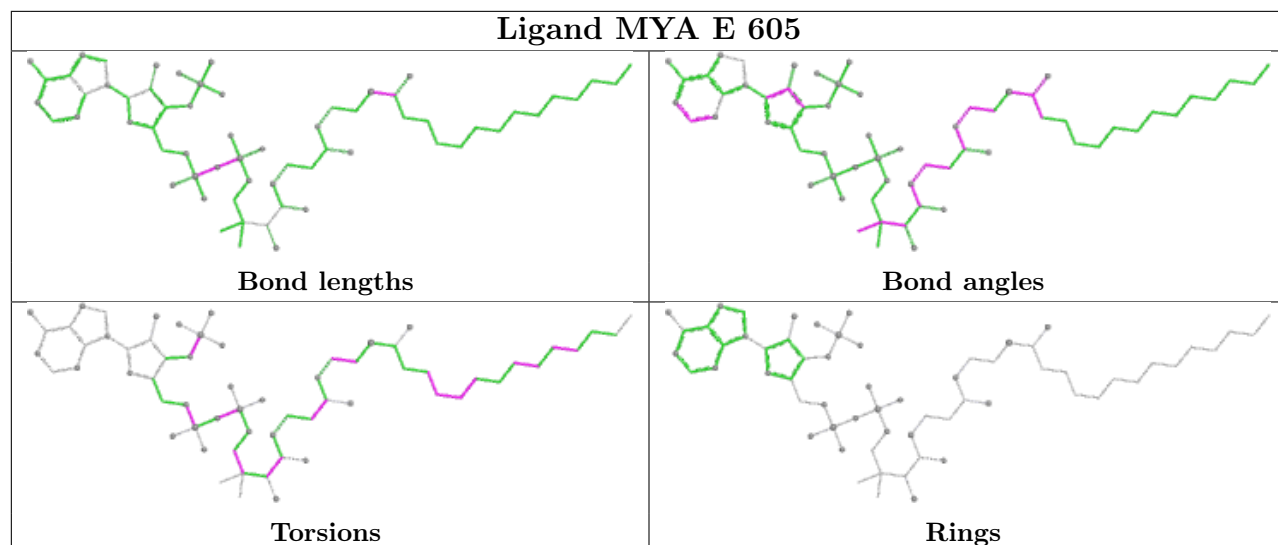


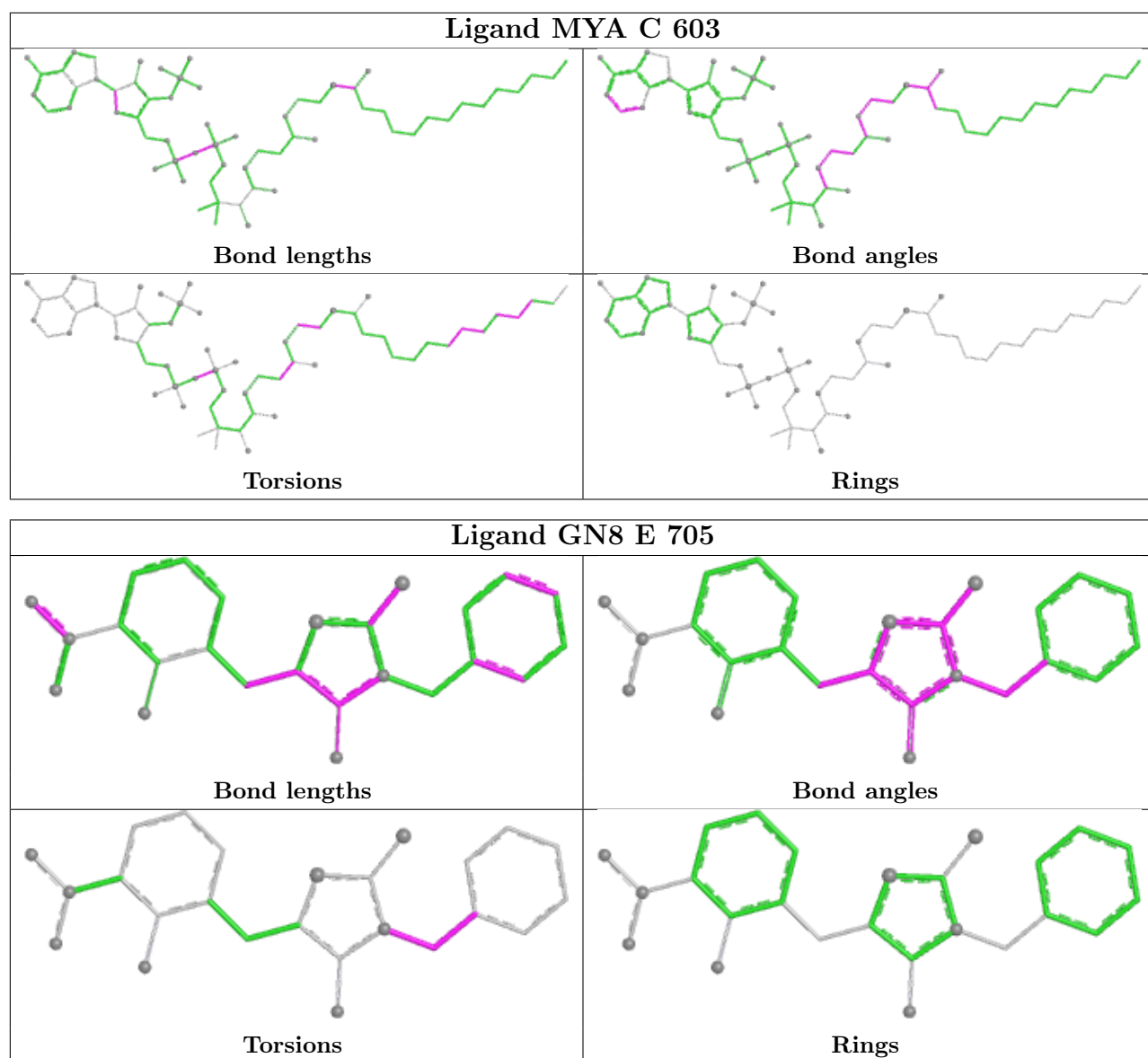
## Ligand MYA F 606



## Ligand GN8 D 704







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	436/455 (95%)	-0.54	0	100	100	16, 31, 54, 69	0
1	B	436/455 (95%)	-0.60	0	100	100	15, 29, 56, 66	0
1	C	436/455 (95%)	-0.38	1 (0%)	95	90	15, 42, 65, 104	0
1	D	436/455 (95%)	-0.51	1 (0%)	95	90	17, 34, 54, 69	0
1	E	436/455 (95%)	-0.62	0	100	100	15, 26, 48, 65	0
1	F	435/455 (95%)	-0.31	2 (0%)	91	81	17, 47, 66, 106	0
All	All	2615/2730 (95%)	-0.49	4 (0%)	95	90	15, 34, 61, 106	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	5	ASP	2.3
1	D	69	SER	2.3
1	F	198	ASP	2.1
1	C	198	ASP	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

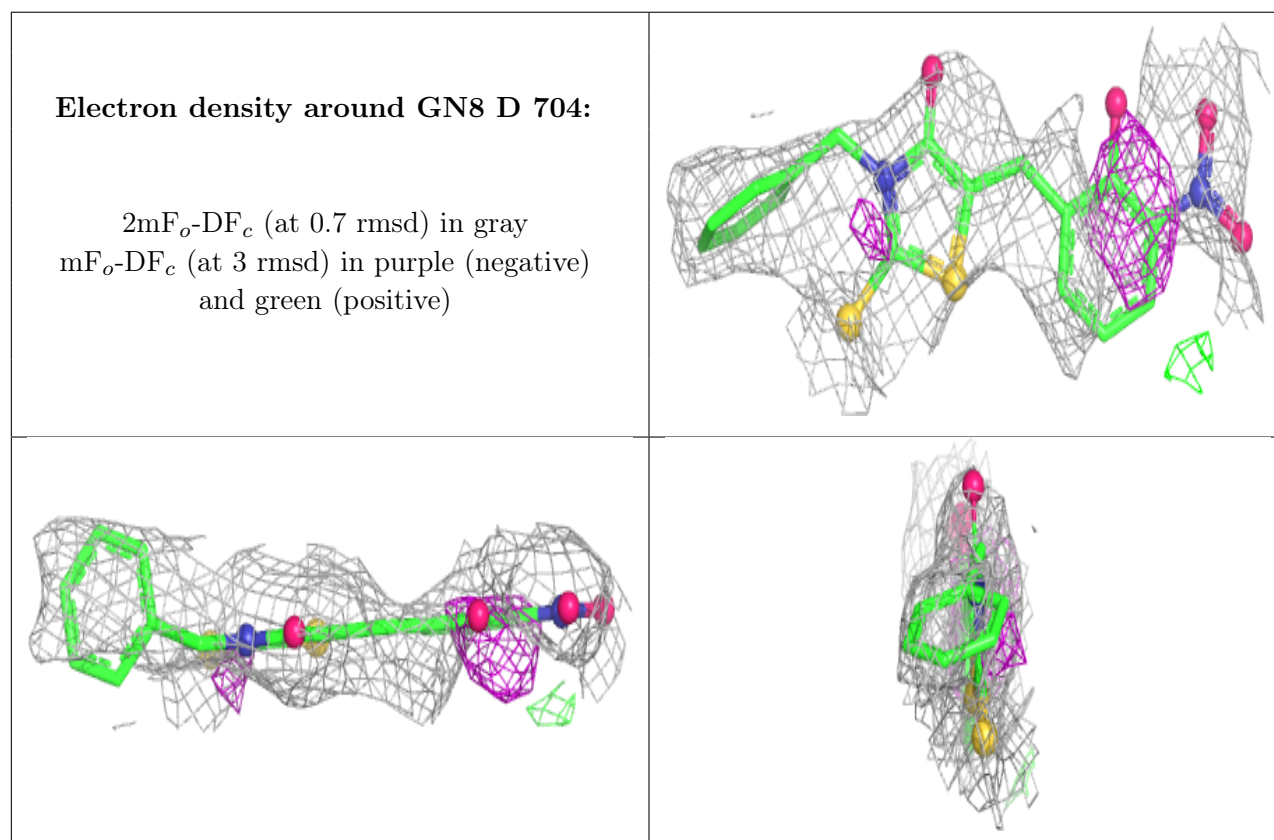
### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GN8	D	704	25/25	0.63	0.42	59,68,77,78	0
3	GN8	B	702	25/25	0.66	0.38	67,72,78,78	0
3	GN8	A	701	25/25	0.67	0.36	50,62,72,73	0
3	GN8	E	705	25/25	0.72	0.42	62,67,73,74	0
3	GN8	F	706	25/25	0.75	0.38	65,72,76,78	0
3	GN8	C	703	25/25	0.76	0.35	60,66,73,74	0
2	MYA	C	603	63/63	0.89	0.21	47,50,55,55	0
2	MYA	F	606	63/63	0.90	0.20	53,60,65,66	0
2	MYA	D	604	63/63	0.94	0.16	25,39,43,43	0
2	MYA	B	602	63/63	0.95	0.13	16,26,29,31	0
2	MYA	E	605	63/63	0.95	0.14	13,25,30,32	0
2	MYA	A	601	63/63	0.95	0.13	21,31,44,46	0

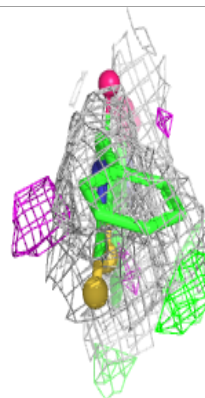
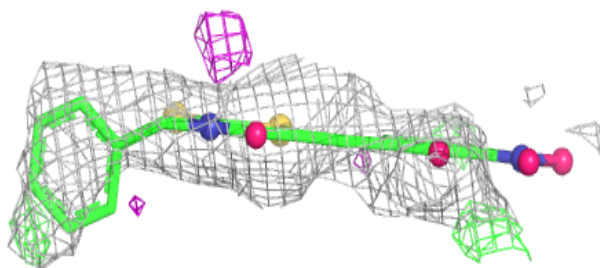
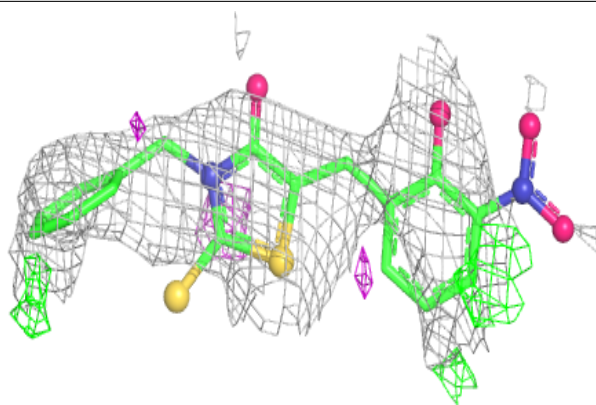
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



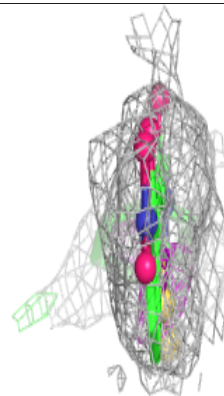
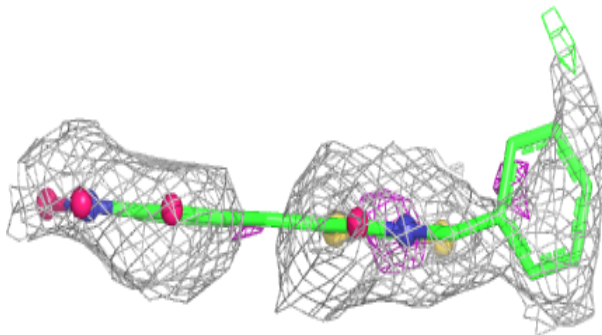
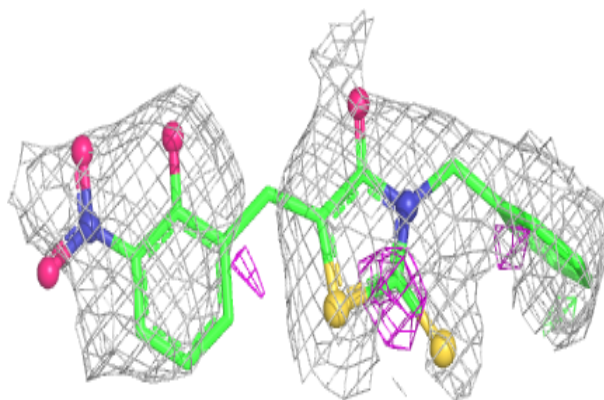


**Electron density around GN8 B 702:**

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

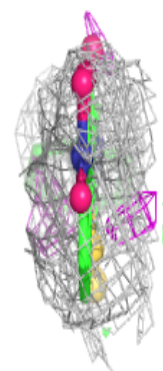
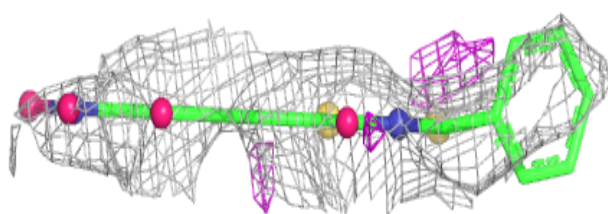
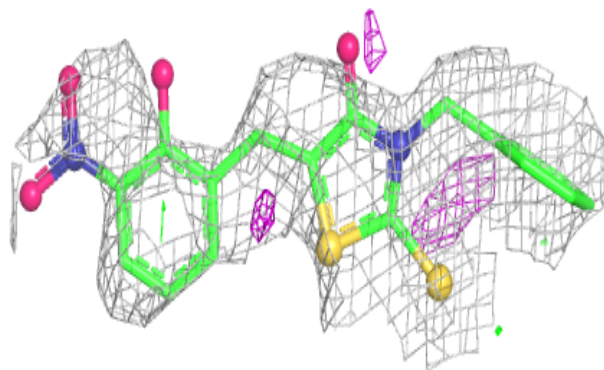
**Electron density around GN8 A 701:**

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

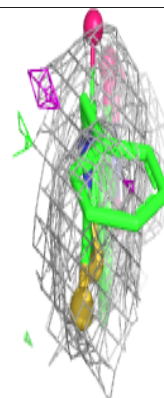
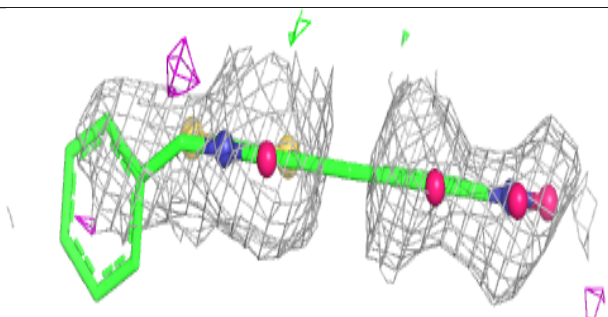
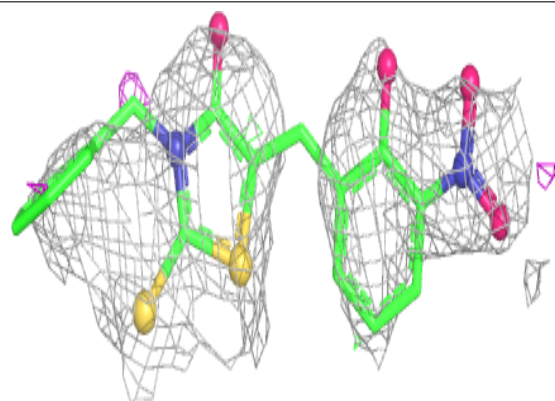


**Electron density around GN8 E 705:**

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

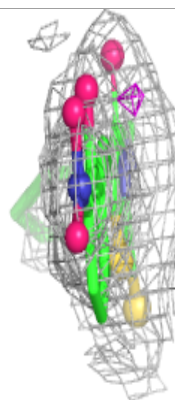
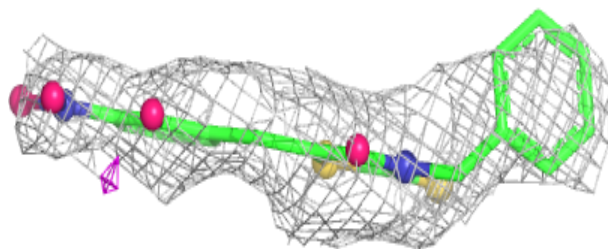
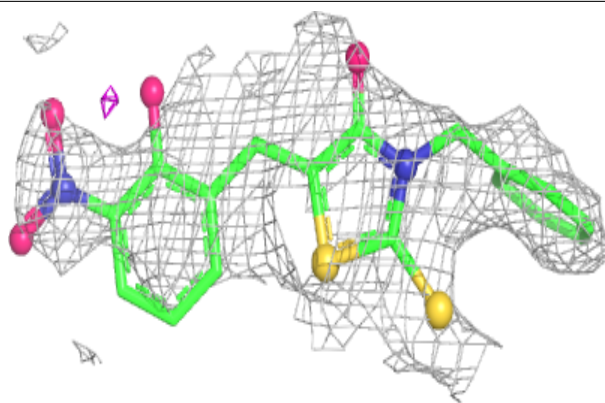
**Electron density around GN8 F 706:**

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

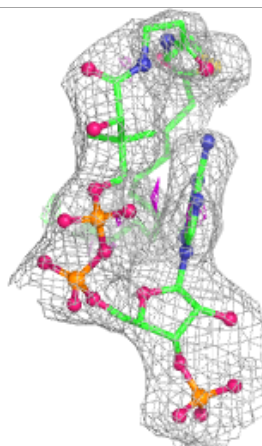
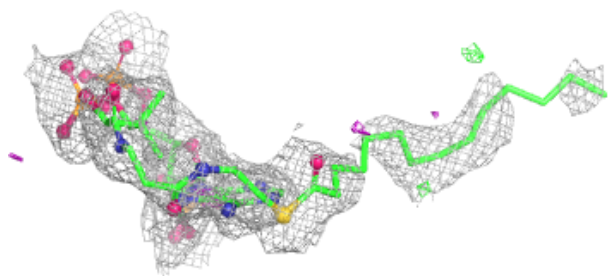
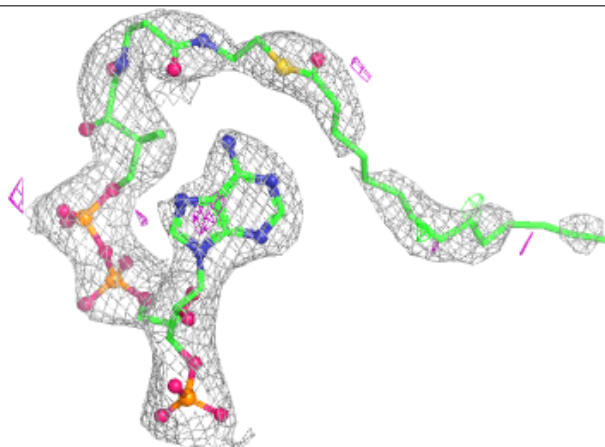


**Electron density around GN8 C 703:**

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

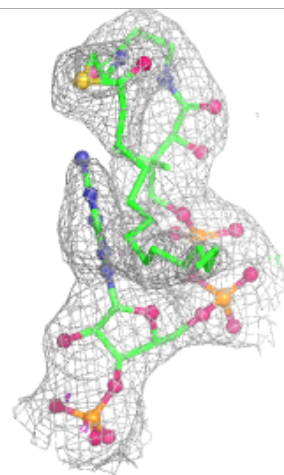
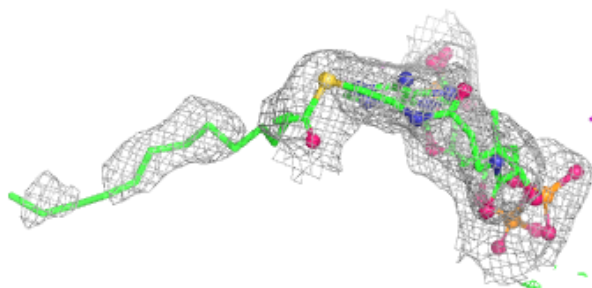
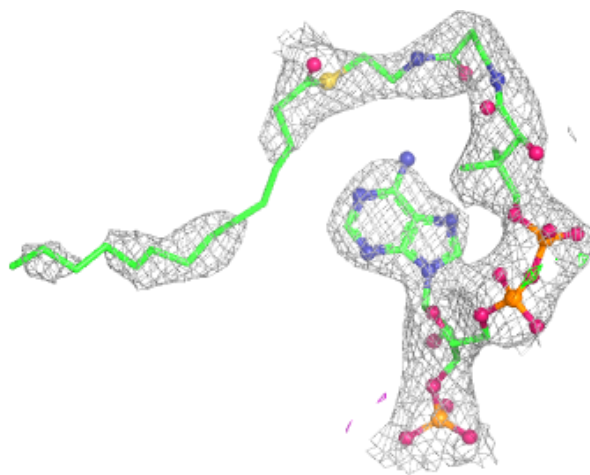
**Electron density around MYA C 603:**

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



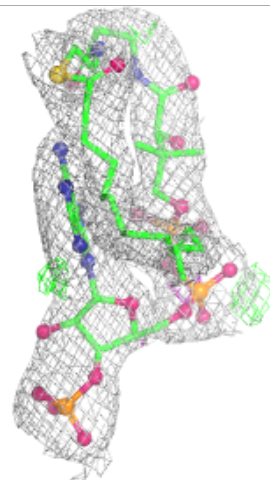
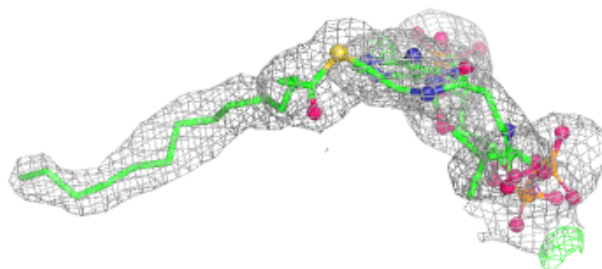
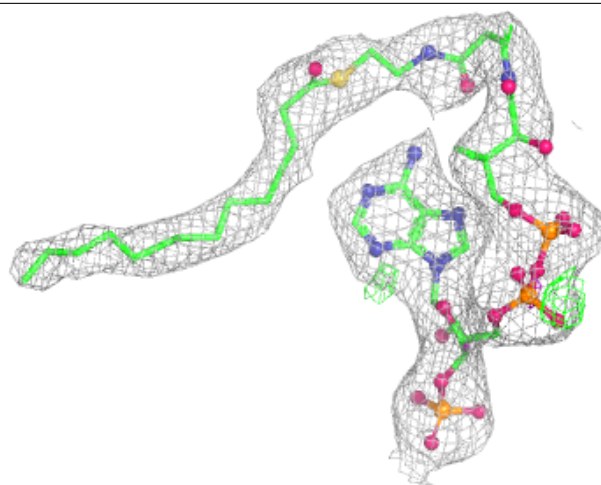
**Electron density around MYA F 606:**

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



**Electron density around MYA D 604:**

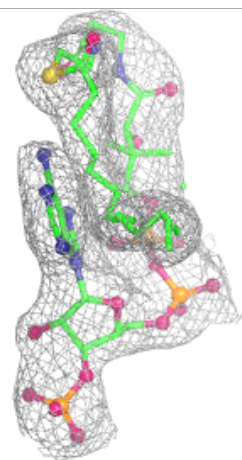
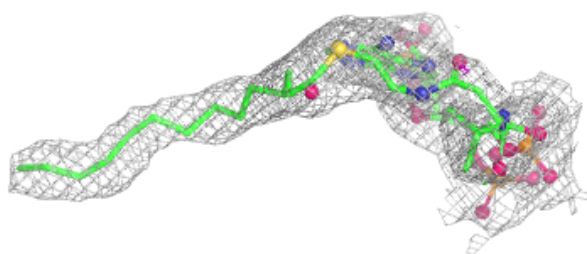
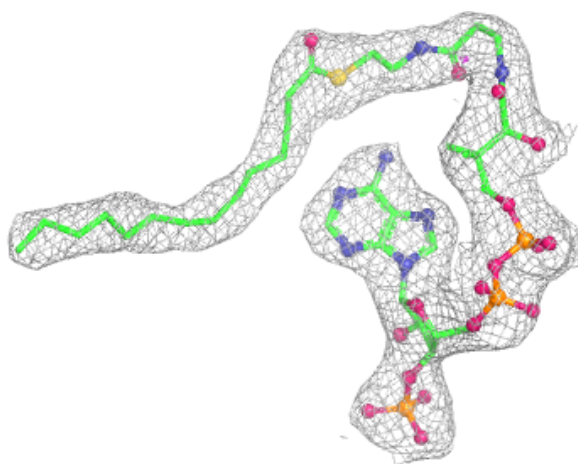
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





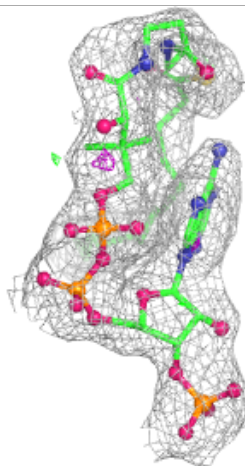
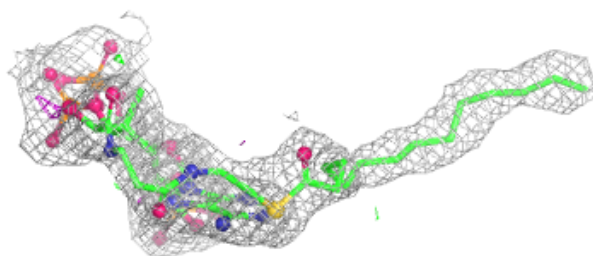
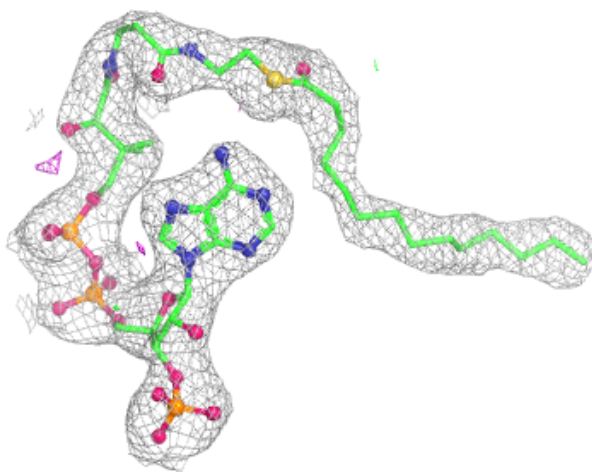
**Electron density around MYA B 602:**

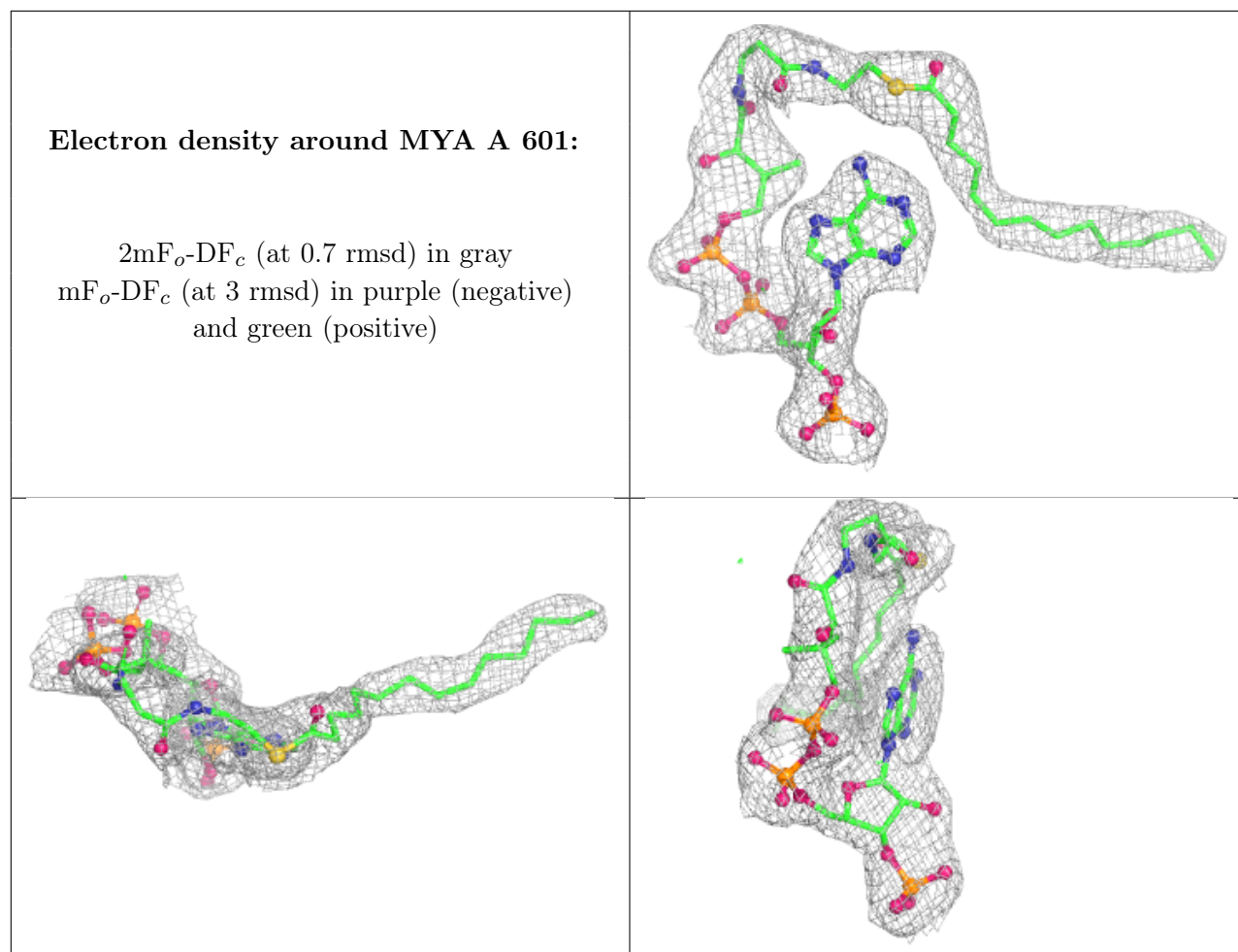
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MYA E 605:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.