



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 02:03 AM UTC

PDB ID : 2P6F / pdb_00002p6f
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

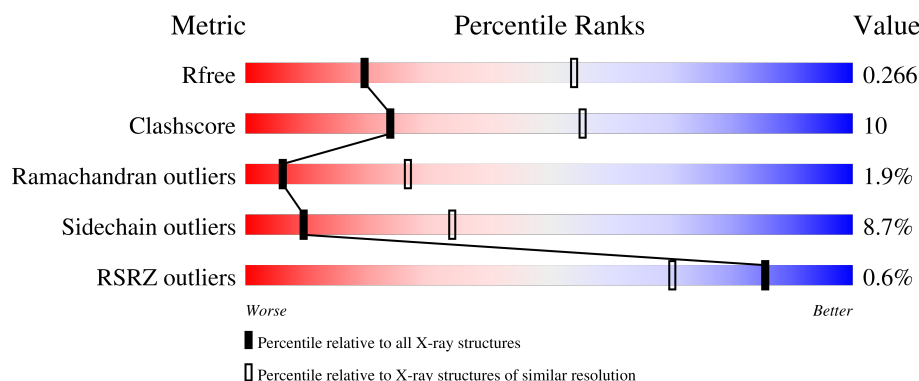
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 ≥ 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	 68% 24% . .
1	B	455	 67% 25% . .
1	C	455	 68% 25% . .
1	D	455	 67% 23% 5% .
1	E	455	 69% 25% . .

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Mol	Chain	Length	Quality of chain
1	F	455	% 70%23% • •

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	-	-	-

2 Entry composition [i](#)

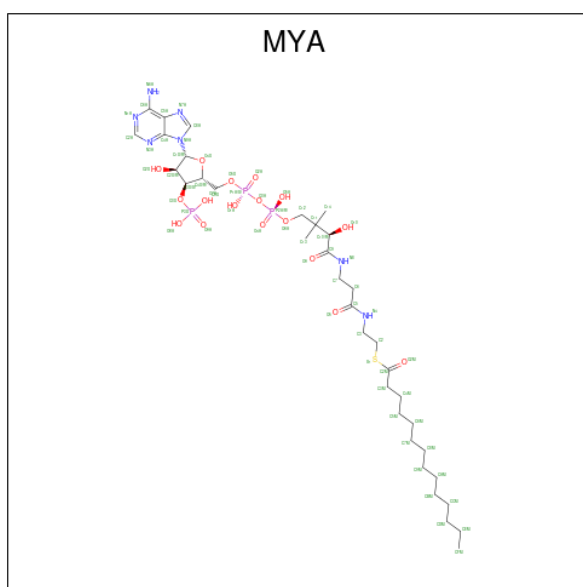
There are 3 unique types of molecules in this entry. The entry contains 21988 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

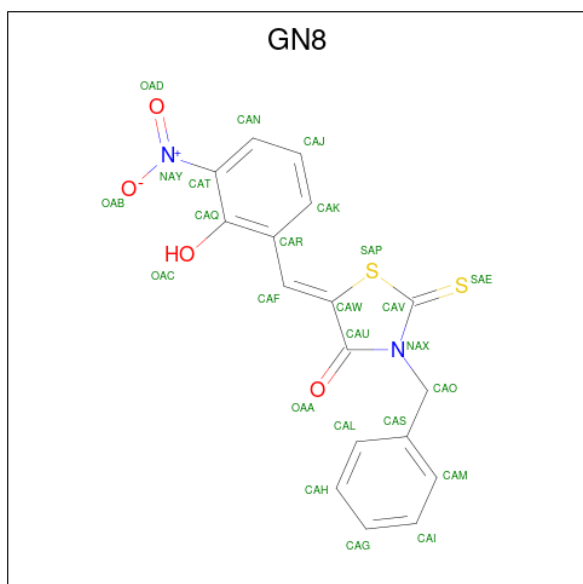
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3578	2318	596	655	9			
1	B	436	Total	C	N	O	S	0	0	0
			3578	2318	596	655	9			
1	C	436	Total	C	N	O	S	0	0	0
			3578	2318	596	655	9			
1	D	436	Total	C	N	O	S	0	0	0
			3578	2318	596	655	9			
1	E	436	Total	C	N	O	S	0	0	0
			3578	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 (CCD ID: MYA) (formula: $C_{35}H_{62}N_7O_{17}P_3S$).



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

- Molecule 3 is (Z)-3-BENZYL-5-(2-HYDROXY-3-NITROBENZYLIDENE)-2-THIOXOTHIAZOLIDIN-4-ONE (CCD ID: GN8) (formula: C₁₇H₁₂N₂O₄S₂).



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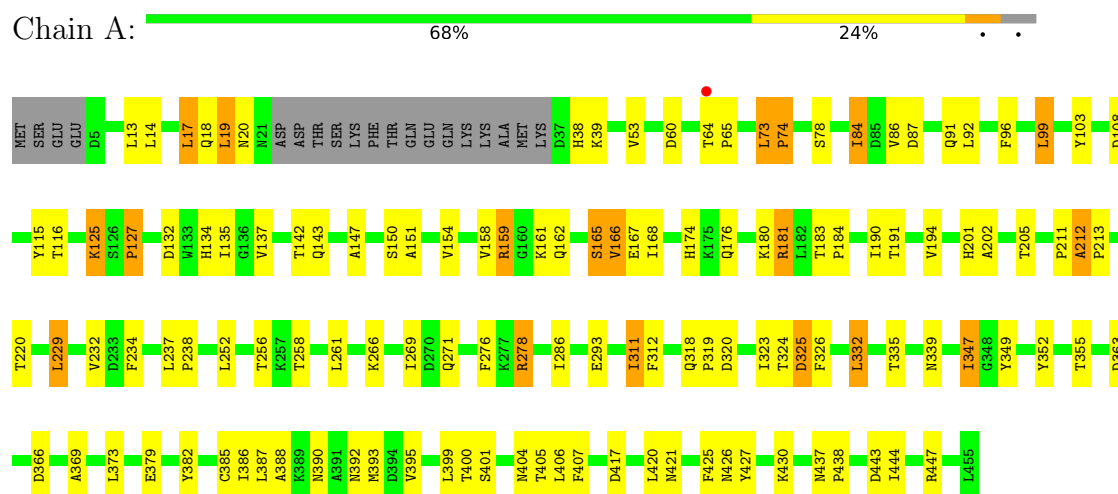
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	S	0	0
			25	17	2	4	2		

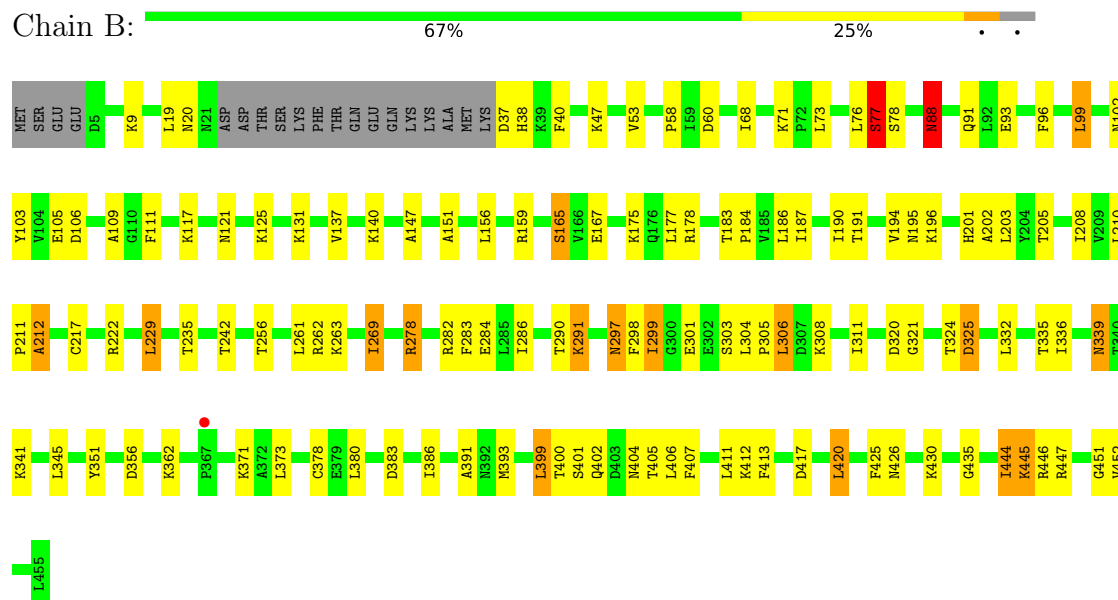
3 Residue-property plots

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.

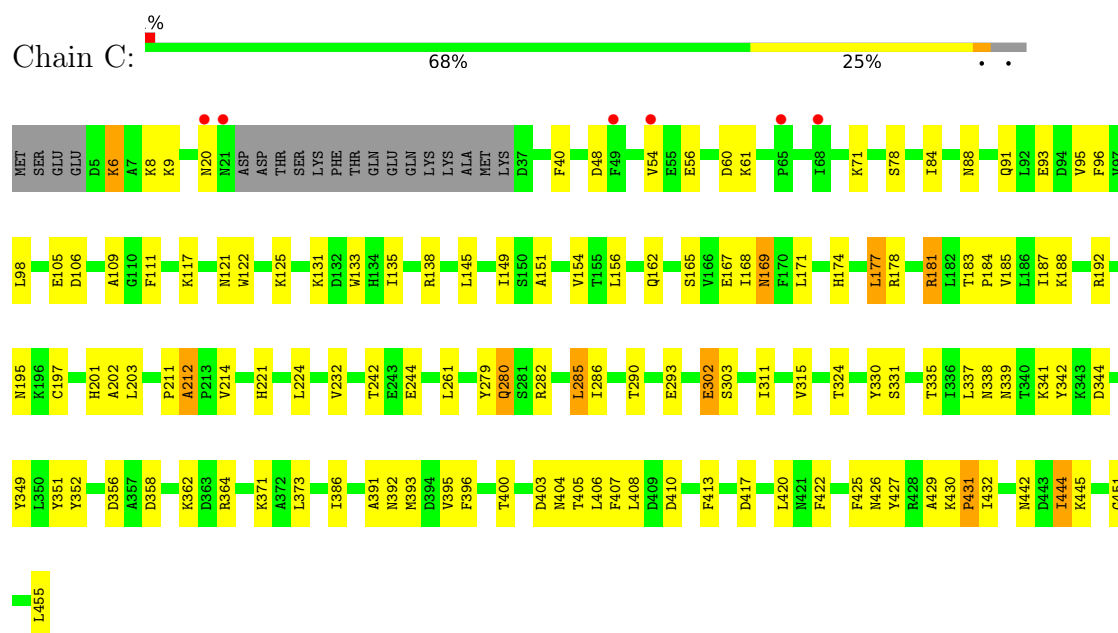
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase



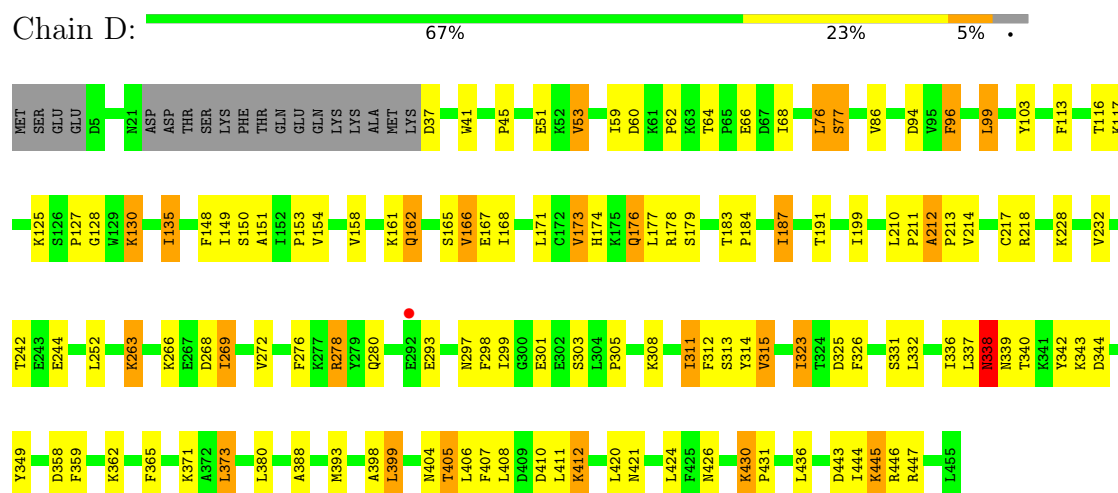
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase



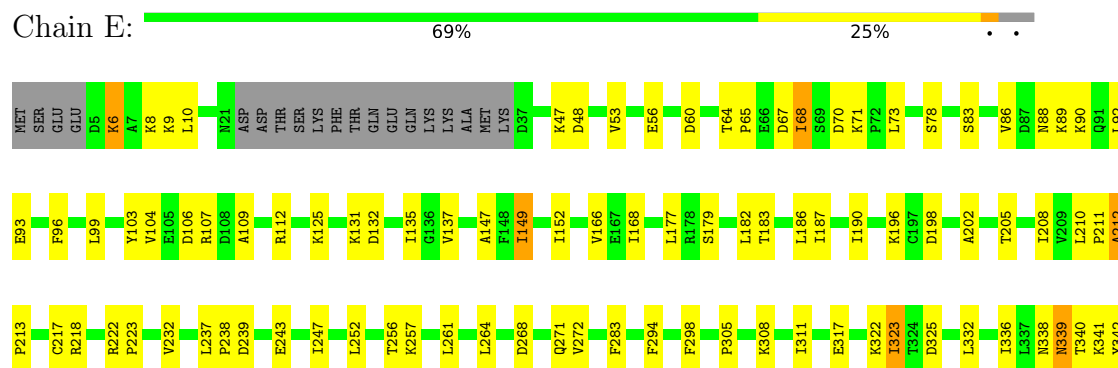
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase

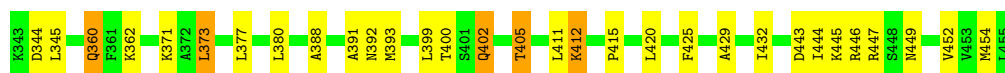


• Molecule 1: Glycylpeptide N-tetradecanoyltransferase

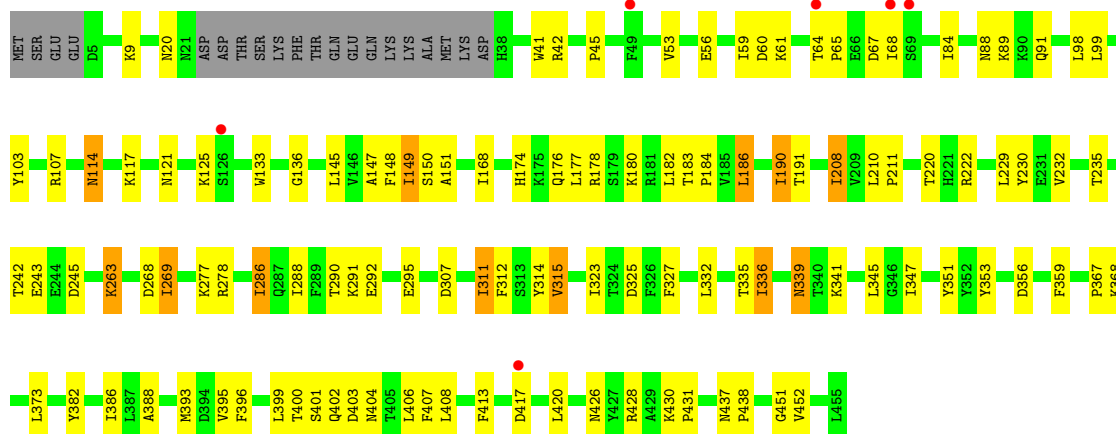


• Molecule 1: Glycylpeptide N-tetradecanoyltransferase





• 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, α , β , γ	188.76Å 151.49Å 133.94Å 90.00° 107.46° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 20.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.00-3.10) 96.8 (20.00-3.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.91Å)	Xtrriage
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 (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtrriage
Anisotropy	0.435	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 13.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	21988	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.46	1/3666 (0.0%)	0.78	1/4957 (0.0%)
1	B	0.45	0/3666	0.77	0/4957
1	C	0.48	0/3666	0.79	0/4957
1	D	0.46	0/3666	0.80	0/4957
1	E	0.45	0/3666	0.78	1/4957 (0.0%)
1	F	0.46	0/3658	0.79	2/4946 (0.0%)
All	All	0.46	1/21988 (0.0%)	0.79	4/29731 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	HIS	CE1-NE2	5.63	1.38	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	399	LEU	N-CA-C	5.34	119.95	113.38
1	A	165	SER	N-CA-C	5.19	115.23	108.07
1	F	61	LYS	CA-C-N	5.05	125.33	119.93
1	F	61	LYS	C-N-CA	5.05	125.33	119.93

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3578	0	3573	75	0
1	B	3578	0	3573	70	0
1	C	3578	0	3573	81	0
1	D	3578	0	3573	77	0
1	E	3578	0	3573	65	0
1	F	3570	0	3569	63	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	441	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 (441) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:331:SER:HB2	1:C:393:MET:HE1	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:88:ASN:C	1:E:88:ASN:HD22	2.06	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:CYS:HB3	1:B:399:LEU:O	2.04	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
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: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:A:161:LYS:HG3	1:A:162:GLN:N	2.19	0.56
1:B:411:LEU:O	1:B:412:LYS:HB2	2.05	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:F:290:THR:C	1:F:292:GLU:H	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:114:ASN:C	1:F:114:ASN:HD22	2.14	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
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:A:405:THR:HG21	1:A:443:ASP:C	2.33	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:A:399:LEU:C	1:A:401:SER:H	2.17	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:D:96:PHE:CD1	1:D:96:PHE:C	2.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:282:ARG:HH22	1:C:358:ASP:CG	2.19	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: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
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: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:D:338:ASN:C	1:D:338:ASN:HD22	2.21	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:F:178:ARG:C	1:F:180:LYS:H	2.21	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:D:331:SER:HB2	1:D:393:MET:HE1	1.93	0.49
1:A:84:ILE:HG23	1:A:91:GLN:HB3	1.94	0.49
1:B:229:LEU:HB3	1:B:235:THR:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:D:96:PHE:C	1:D:96:PHE:HD1	2.21	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:D:64:THR:C	1:D:66:GLU:H	2.21	0.47
1:B:165:SER:HB3	1:B:201:HIS:HB2	1.95	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:C:195:ASN:C	1:C:197:CYS:H	2.22	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:F:88:ASN:HD22	1:F:88:ASN:C	2.23	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:96:PHE:CD1	1:A:96:PHE:C	2.94	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:F:404:ASN:C	1:F:406:LEU:H	2.24	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:C:356:ASP:C	1:C:356:ASP:OD1	2.58	0.46
1:E:237:LEU:HA	1:E:238:PRO:HD3	1.84	0.46
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:E:88:ASN:C	1:E:88:ASN:ND2	2.75	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:A:390:ASN:C	1:A:392:ASN:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:290:THR:O	1:B:291:LYS:C	2.60	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
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:C:324:THR:HG23	1:C:356:ASP:CG	2.43	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ASN:ND2	1:B:417:ASP:HB2	2.34	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: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:HZ2	1:F:288:ILE:HA	1.84	0.42
1:B:40:PHE:CD1	1:B:184:PRO:HB3	2.54	0.42
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:F:184:PRO:C	1:F:186:LEU:H	2.27	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:B:76:LEU:O	1:B:77:SER:C	2.62	0.42
1:C:352:TYR:CE1	1:C:451:GLY:O	2.73	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:A:318:GLN:O	1:A:319:PRO:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:C:131:LYS:C	1:C:133:TRP:H	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:339:ASN:C	1:B:341:LYS:H	2.30	0.40
1:C:181:ARG:CG	1:C:181:ARG:NH1	2.78	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:D:405:THR:HG21	1:D:443:ASP:C	2.47	0.40
1:F:290:THR:C	1:F:292:GLU:N	2.79	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
1:D:76:LEU:HB3	1:D:77:SER:H	1.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	6	27
1	B	432/455 (95%)	382 (88%)	38 (9%)	12 (3%)	4	20
1	C	432/455 (95%)	376 (87%)	50 (12%)	6 (1%)	9	34
1	D	432/455 (95%)	376 (87%)	44 (10%)	12 (3%)	4	20
1	E	432/455 (95%)	391 (90%)	35 (8%)	6 (1%)	9	34
1	F	431/455 (95%)	373 (86%)	52 (12%)	6 (1%)	9	34
All	All	2591/2730 (95%)	2289 (88%)	252 (10%)	50 (2%)	6	27

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
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

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Mol	Chain	Res	Type
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 [i](#)

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%)	363 (92%)	31 (8%)	11	37
1	B	394/413 (95%)	358 (91%)	36 (9%)	9	32
1	C	394/413 (95%)	364 (92%)	30 (8%)	12	39
1	D	394/413 (95%)	352 (89%)	42 (11%)	6	25
1	E	394/413 (95%)	361 (92%)	33 (8%)	10	35
1	F	393/413 (95%)	359 (91%)	34 (9%)	9	34
All	All	2363/2478 (95%)	2157 (91%)	206 (9%)	9	34

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	17	LEU
1	A	19	LEU
1	A	53	VAL
1	A	64	THR
1	A	73	LEU
1	A	84	ILE
1	A	99	LEU
1	A	108	ASP
1	A	116	THR

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Mol	Chain	Res	Type
1	A	125	LYS
1	A	132	ASP
1	A	135	ILE
1	A	166	VAL
1	A	168	ILE
1	A	181	ARG
1	A	190	ILE
1	A	220	THR
1	A	229	LEU
1	A	261	LEU
1	A	278	ARG
1	A	286	ILE
1	A	311	ILE
1	A	320	ASP
1	A	325	ASP
1	A	326	PHE
1	A	332	LEU
1	A	335	THR
1	A	339	ASN
1	A	347	ILE
1	A	373	LEU
1	B	9	LYS
1	B	19	LEU
1	B	37	ASP
1	B	53	VAL
1	B	71	LYS
1	B	73	LEU
1	B	77	SER
1	B	88	ASN
1	B	99	LEU
1	B	105	GLU
1	B	125	LYS
1	B	131	LYS
1	B	165	SER
1	B	196	LYS
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	278	ARG

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Mol	Chain	Res	Type
1	B	297	ASN
1	B	299	ILE
1	B	320	ASP
1	B	325	ASP
1	B	332	LEU
1	B	339	ASN
1	B	362	LYS
1	B	371	LYS
1	B	386	ILE
1	B	393	MET
1	B	399	LEU
1	B	420	LEU
1	B	444	ILE
1	B	445	LYS
1	B	452	VAL
1	C	6	LYS
1	C	8	LYS
1	C	48	ASP
1	C	54	VAL
1	C	71	LYS
1	C	125	LYS
1	C	135	ILE
1	C	162	GLN
1	C	169	ASN
1	C	177	LEU
1	C	181	ARG
1	C	185	VAL
1	C	201	HIS
1	C	221	HIS
1	C	261	LEU
1	C	280	GLN
1	C	285	LEU
1	C	311	ILE
1	C	315	VAL
1	C	344	ASP
1	C	351	TYR
1	C	362	LYS
1	C	371	LYS
1	C	373	LEU
1	C	386	ILE
1	C	395	VAL
1	C	410	ASP

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Mol	Chain	Res	Type
1	C	420	LEU
1	C	444	ILE
1	C	445	LYS
1	D	37	ASP
1	D	53	VAL
1	D	59	ILE
1	D	68	ILE
1	D	86	VAL
1	D	94	ASP
1	D	96	PHE
1	D	99	LEU
1	D	116	THR
1	D	125	LYS
1	D	130	LYS
1	D	135	ILE
1	D	158	VAL
1	D	162	GLN
1	D	166	VAL
1	D	173	VAL
1	D	176	GLN
1	D	177	LEU
1	D	187	ILE
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	338	ASN
1	D	340	THR
1	D	343	LYS
1	D	362	LYS
1	D	371	LYS
1	D	373	LEU
1	D	399	LEU
1	D	405	THR
1	D	410	ASP
1	D	420	LEU

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Mol	Chain	Res	Type
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	68	ILE
1	E	73	LEU
1	E	90	LYS
1	E	104	VAL
1	E	131	LYS
1	E	149	ILE
1	E	152	ILE
1	E	166	VAL
1	E	177	LEU
1	E	182	LEU
1	E	208	ILE
1	E	239	ASP
1	E	252	LEU
1	E	256	THR
1	E	257	LYS
1	E	261	LEU
1	E	317	GLU
1	E	323	ILE
1	E	332	LEU
1	E	339	ASN
1	E	340	THR
1	E	344	ASP
1	E	360	GLN
1	E	371	LYS
1	E	373	LEU
1	E	405	THR
1	E	420	LEU
1	E	444	ILE
1	E	445	LYS
1	E	452	VAL
1	F	9	LYS
1	F	67	ASP
1	F	68	ILE
1	F	84	ILE
1	F	107	ARG
1	F	114	ASN

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Mol	Chain	Res	Type
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	295	GLU
1	F	307	ASP
1	F	311	ILE
1	F	315	VAL
1	F	325	ASP
1	F	332	LEU
1	F	335	THR
1	F	336	ILE
1	F	339	ASN
1	F	351	TYR
1	F	368	LYS
1	F	373	LEU
1	F	399	LEU
1	F	420	LEU
1	F	452	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	18	GLN
1	A	44	GLN
1	A	174	HIS
1	A	225	ASN
1	A	339	ASN
1	A	397	ASN
1	A	404	ASN
1	A	426	ASN
1	A	437	ASN

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Mol	Chain	Res	Type
1	B	20	ASN
1	B	88	ASN
1	B	114	ASN
1	B	174	HIS
1	B	195	ASN
1	B	297	ASN
1	B	318	GLN
1	B	338	ASN
1	B	339	ASN
1	B	397	ASN
1	B	404	ASN
1	B	421	ASN
1	B	426	ASN
1	C	20	ASN
1	C	44	GLN
1	C	88	ASN
1	C	91	GLN
1	C	114	ASN
1	C	134	HIS
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	C	449	ASN
1	D	18	GLN
1	D	20	ASN
1	D	21	ASN
1	D	44	GLN
1	D	88	ASN
1	D	114	ASN
1	D	162	GLN
1	D	176	GLN
1	D	221	HIS
1	D	338	ASN
1	D	339	ASN
1	D	397	ASN
1	D	402	GLN

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Mol	Chain	Res	Type
1	D	421	ASN
1	D	426	ASN
1	D	437	ASN
1	D	442	ASN
1	E	88	ASN
1	E	114	ASN
1	E	121	ASN
1	E	143	GLN
1	E	174	HIS
1	E	195	ASN
1	E	339	ASN
1	E	360	GLN
1	E	397	ASN
1	E	402	GLN
1	E	404	ASN
1	E	421	ASN
1	E	437	ASN
1	F	88	ASN
1	F	91	GLN
1	F	114	ASN
1	F	121	ASN
1	F	143	GLN
1	F	174	HIS
1	F	176	GLN
1	F	195	ASN
1	F	241	HIS
1	F	296	HIS
1	F	339	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MYA	E	605	-	63,65,65	0.95	5 (7%)	85,91,91	1.61	15 (17%)
2	MYA	D	604	-	63,65,65	0.96	4 (6%)	85,91,91	1.64	15 (17%)
3	GN8	B	702	-	27,27,27	3.80	6 (22%)	34,38,38	3.92	14 (41%)
3	GN8	D	704	-	27,27,27	3.82	6 (22%)	34,38,38	3.98	13 (38%)
2	MYA	B	602	-	63,65,65	0.93	5 (7%)	85,91,91	1.80	16 (18%)
3	GN8	E	705	-	27,27,27	4.03	11 (40%)	34,38,38	4.02	14 (41%)
2	MYA	F	606	-	63,65,65	1.00	6 (9%)	85,91,91	1.66	15 (17%)
2	MYA	C	603	-	63,65,65	0.93	4 (6%)	85,91,91	1.63	14 (16%)
2	MYA	A	601	-	63,65,65	0.93	5 (7%)	85,91,91	1.61	15 (17%)
3	GN8	C	703	-	27,27,27	3.79	6 (22%)	34,38,38	3.83	12 (35%)
3	GN8	A	701	-	27,27,27	3.84	6 (22%)	34,38,38	3.95	14 (41%)
3	GN8	F	706	-	27,27,27	3.83	7 (25%)	34,38,38	3.84	14 (41%)

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
2	MYA	E	605	-	1/1/12/14	17/64/80/80	0/3/3/3
2	MYA	D	604	-	1/1/12/14	14/64/80/80	0/3/3/3
3	GN8	B	702	-	-	2/10/28/28	0/3/3/3
3	GN8	D	704	-	-	2/10/28/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MYA	B	602	-	1/1/12/14	24/64/80/80	0/3/3/3
3	GN8	E	705	-	-	2/10/28/28	0/3/3/3
2	MYA	F	606	-	1/1/12/14	21/64/80/80	0/3/3/3
2	MYA	C	603	-	1/1/12/14	9/64/80/80	0/3/3/3
2	MYA	A	601	-	1/1/12/14	22/64/80/80	0/3/3/3
3	GN8	C	703	-	-	2/10/28/28	0/3/3/3
3	GN8	A	701	-	-	2/10/28/28	0/3/3/3
3	GN8	F	706	-	-	2/10/28/28	0/3/3/3

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	705	GN8	CAF-CAW	14.50	1.50	1.34
3	A	701	GN8	CAF-CAW	14.34	1.49	1.34
3	D	704	GN8	CAF-CAW	14.29	1.49	1.34
3	F	706	GN8	CAF-CAW	14.25	1.49	1.34
3	B	702	GN8	CAF-CAW	14.15	1.49	1.34
3	C	703	GN8	CAF-CAW	14.03	1.49	1.34
3	C	703	GN8	OAD-NAY	10.06	1.40	1.22
3	D	704	GN8	OAD-NAY	9.99	1.40	1.22
3	A	701	GN8	OAD-NAY	9.94	1.39	1.22
3	F	706	GN8	OAD-NAY	9.93	1.39	1.22
3	E	705	GN8	OAD-NAY	9.92	1.39	1.22
3	B	702	GN8	OAD-NAY	9.91	1.39	1.22
3	E	705	GN8	CAU-CAW	-4.95	1.39	1.48
3	A	701	GN8	CAT-NAY	-4.89	1.36	1.45
3	A	701	GN8	CAU-CAW	-4.86	1.39	1.48
3	F	706	GN8	CAT-NAY	-4.86	1.36	1.45
3	F	706	GN8	CAU-CAW	-4.82	1.39	1.48
3	B	702	GN8	CAT-NAY	-4.78	1.37	1.45
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	E	705	GN8	CAT-NAY	-4.66	1.37	1.45
3	D	704	GN8	CAV-SAE	4.66	1.77	1.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	703	GN8	CAT-NAY	-4.65	1.37	1.45
3	D	704	GN8	CAT-NAY	-4.60	1.37	1.45
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
3	E	705	GN8	CAM-CAS	3.68	1.46	1.38
3	E	705	GN8	CAH-CAG	3.55	1.46	1.38
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
3	E	705	GN8	CAG-CAI	2.77	1.44	1.38
3	E	705	GN8	CAL-CAS	2.72	1.44	1.38
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
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	F	606	MYA	C3M-C2M	2.23	1.53	1.50
2	C	603	MYA	P2A-O3A	2.21	1.61	1.59
2	F	606	MYA	P2A-O3A	2.21	1.61	1.59
2	E	605	MYA	C5A-N7A	-2.20	1.35	1.39
2	A	601	MYA	C5A-N7A	-2.18	1.35	1.39
2	D	604	MYA	C5A-N7A	-2.15	1.35	1.39
2	E	605	MYA	C8A-N7A	2.15	1.35	1.31
2	C	603	MYA	C8A-N7A	2.10	1.35	1.31
2	B	602	MYA	C8A-N7A	2.09	1.35	1.31
2	B	602	MYA	C5A-N7A	-2.07	1.35	1.39
2	F	606	MYA	C8A-N7A	2.06	1.35	1.31
2	F	606	MYA	C5A-N7A	-2.06	1.35	1.39
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	MYA	C8A-N7A	2.02	1.35	1.31

All (171) 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	8.66	132.01	122.38
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	8.03	131.30	122.38
3	A	701	GN8	CAO-NAX-CAV	8.02	131.29	122.38
3	C	703	GN8	CAF-CAW-CAU	7.91	129.11	120.37
3	B	702	GN8	CAO-NAX-CAV	7.72	130.95	122.38
3	C	703	GN8	CAW-CAU-NAX	7.56	117.56	110.20
3	C	703	GN8	CAF-CAW-SAP	-7.30	119.87	129.25
3	F	706	GN8	CAO-NAX-CAV	7.27	130.46	122.38
3	B	702	GN8	CAV-SAP-CAW	-6.90	86.33	92.67
3	A	701	GN8	CAF-CAW-CAU	6.87	127.96	120.37
3	F	706	GN8	CAF-CAW-CAU	6.84	127.92	120.37
3	D	704	GN8	CAV-SAP-CAW	-6.83	86.39	92.67
3	B	702	GN8	CAF-CAW-CAU	6.81	127.89	120.37
3	A	701	GN8	CAV-SAP-CAW	-6.81	86.41	92.67
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
3	D	704	GN8	CAF-CAW-CAU	6.62	127.68	120.37
2	B	602	MYA	C3M-C2M-S1	6.47	121.12	113.40
3	B	702	GN8	CAF-CAW-SAP	-6.23	121.25	129.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	706	GN8	CAF-CAW-SAP	-6.19	121.29	129.25
3	A	701	GN8	CAF-CAW-SAP	-6.16	121.33	129.25
3	D	704	GN8	CAF-CAW-SAP	-6.01	121.53	129.25
3	C	703	GN8	CAO-NAX-CAV	5.73	128.75	122.38
3	E	705	GN8	CAF-CAW-CAU	5.48	126.42	120.37
2	D	604	MYA	C3M-C2M-S1	5.43	119.87	113.40
2	F	606	MYA	C3M-C2M-S1	5.38	119.81	113.40
2	C	603	MYA	C5A-C4A-N3A	-5.35	119.35	126.72
2	F	606	MYA	C5A-C4A-N3A	-5.33	119.38	126.72
3	D	704	GN8	CAN-CAT-CAQ	-5.27	119.11	121.86
2	B	602	MYA	C5A-C4A-N3A	-5.25	119.49	126.72
2	E	605	MYA	C5A-C4A-N3A	-5.23	119.51	126.72
2	B	602	MYA	N3A-C2A-N1A	-5.17	120.75	128.58
2	D	604	MYA	C5A-C4A-N3A	-5.13	119.66	126.72
2	A	601	MYA	C5A-C4A-N3A	-5.11	119.68	126.72
3	E	705	GN8	CAN-CAT-CAQ	-5.04	119.23	121.86
2	C	603	MYA	N3A-C2A-N1A	-4.97	121.05	128.58
2	D	604	MYA	N3A-C2A-N1A	-4.93	121.11	128.58
2	F	606	MYA	N3A-C2A-N1A	-4.88	121.20	128.58
2	A	601	MYA	N3A-C2A-N1A	-4.83	121.26	128.58
2	E	605	MYA	N3A-C2A-N1A	-4.83	121.27	128.58
2	A	601	MYA	C3M-C2M-S1	4.81	119.13	113.40
3	E	705	GN8	CAF-CAW-SAP	-4.72	123.18	129.25
2	C	603	MYA	C3M-C2M-S1	4.64	118.93	113.40
3	E	705	GN8	OAA-CAU-CAW	-4.58	119.73	126.45
3	F	706	GN8	CAN-CAT-CAQ	-4.50	119.52	121.86
2	B	602	MYA	O2M-C2M-C3M	-4.47	118.83	123.98
3	E	705	GN8	CAR-CAQ-CAT	4.38	120.79	117.20
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	B	702	GN8	CAN-CAT-CAQ	-4.29	119.62	121.86
3	A	701	GN8	OAA-CAU-CAW	-4.24	120.22	126.45
3	C	703	GN8	CAN-CAT-CAQ	-4.23	119.66	121.86
3	D	704	GN8	CAR-CAQ-CAT	4.22	120.66	117.20
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	A	701	GN8	CAR-CAQ-CAT	4.07	120.54	117.20
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	F	706	GN8	CAR-CAQ-CAT	4.03	120.50	117.20
3	A	701	GN8	CAN-CAT-CAQ	-3.95	119.80	121.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	703	GN8	CAR-CAQ-CAT	3.90	120.40	117.20
3	B	702	GN8	CAR-CAQ-CAT	3.88	120.38	117.20
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
3	E	705	GN8	CAS-CAO-NAX	3.74	119.35	113.09
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	SAP-CAV-SAE	-3.59	116.73	122.98
2	C	603	MYA	O2M-C2M-C3M	-3.59	119.83	123.98
3	D	704	GN8	CAS-CAO-NAX	3.59	119.11	113.09
2	B	602	MYA	C2A-N3A-C4A	3.56	120.53	111.83
2	C	603	MYA	C2A-N3A-C4A	3.56	120.52	111.83
2	F	606	MYA	C2A-N3A-C4A	3.54	120.47	111.83
2	F	606	MYA	N3A-C4A-N9A	3.53	133.18	127.17
2	B	602	MYA	N9A-C8A-N7A	-3.50	108.97	113.94
2	C	603	MYA	N3A-C4A-N9A	3.47	133.07	127.17
2	B	602	MYA	N3A-C4A-N9A	3.47	133.06	127.17
2	E	605	MYA	C2A-N3A-C4A	3.47	120.30	111.83
2	D	604	MYA	C2A-N3A-C4A	3.45	120.25	111.83
3	C	703	GN8	CAR-CAF-CAW	-3.44	123.46	130.13
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	F	606	MYA	N9A-C8A-N7A	-3.41	109.10	113.94
2	A	601	MYA	C2A-N3A-C4A	3.41	120.15	111.83
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
2	A	601	MYA	N9A-C8A-N7A	-3.40	109.12	113.94
2	A	601	MYA	N3A-C4A-N9A	3.39	132.94	127.17
2	D	604	MYA	N3A-C4A-N9A	3.37	132.90	127.17
2	D	604	MYA	N9A-C8A-N7A	-3.36	109.16	113.94
2	C	603	MYA	N9A-C8A-N7A	-3.33	109.21	113.94
2	F	606	MYA	C2-C3-N4	-3.22	105.70	112.41
2	E	605	MYA	N3A-C4A-N9A	3.19	132.59	127.17
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
2	E	605	MYA	N9A-C8A-N7A	-3.13	109.49	113.94
3	B	702	GN8	CAS-CAO-NAX	3.10	118.29	113.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
3	A	701	GN8	CAS-CAO-NAX	2.81	117.79	113.09
2	C	603	MYA	C7-N8-C9	2.79	127.56	122.55
3	D	704	GN8	CAN-CAT-NAY	2.79	119.45	116.47
2	A	601	MYA	C14-C11-C10	2.78	113.51	108.77
2	C	603	MYA	C4A-C5A-N7A	-2.76	107.43	110.58
2	A	601	MYA	C7-N8-C9	2.75	127.48	122.55
2	B	602	MYA	C4A-C5A-N7A	-2.74	107.45	110.58
2	D	604	MYA	C14-C11-C10	2.70	113.37	108.77
2	B	602	MYA	C5A-N7A-C8A	2.69	107.67	103.45
2	E	605	MYA	C4A-C5A-N7A	-2.67	107.53	110.58
2	C	603	MYA	C5A-N7A-C8A	2.63	107.59	103.45
2	F	606	MYA	C4A-C5A-N7A	-2.61	107.59	110.58
2	B	602	MYA	C4A-N9A-C8A	2.59	108.46	105.74
3	E	705	GN8	CAN-CAT-NAY	2.59	119.24	116.47
2	F	606	MYA	C5A-N7A-C8A	2.59	107.52	103.45
2	A	601	MYA	C4A-C5A-N7A	-2.59	107.62	110.58
3	E	705	GN8	CAM-CAS-CAL	2.58	122.07	118.23
2	D	604	MYA	C4A-C5A-N7A	-2.58	107.64	110.58
2	A	601	MYA	C4A-N9A-C8A	2.57	108.44	105.74
2	E	605	MYA	C3-N4-C5	2.55	127.57	122.82
2	A	601	MYA	C5A-N7A-C8A	2.54	107.44	103.45
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	C5A-N7A-C8A	2.51	107.39	103.45
2	D	604	MYA	C4A-N9A-C8A	2.51	108.37	105.74
2	D	604	MYA	C6-C7-N8	-2.50	106.69	112.00
2	F	606	MYA	C4A-N9A-C8A	2.48	108.35	105.74
2	C	603	MYA	C3-N4-C5	2.48	127.44	122.82
2	E	605	MYA	C5A-N7A-C8A	2.45	107.30	103.45
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
2	C	603	MYA	C4A-N9A-C8A	2.33	108.19	105.74
3	B	702	GN8	CAR-CAF-CAW	-2.29	125.70	130.13
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	CAR-CAF-CAW	-2.22	125.83	130.13
2	F	606	MYA	C14-C11-C10	2.20	112.51	108.77
3	F	706	GN8	CAS-CAO-NAX	2.19	116.75	113.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	GN8	CAN-CAT-NAY	2.12	118.74	116.47
2	E	605	MYA	C3X-C2X-C1X	2.11	104.52	99.89
2	B	602	MYA	O2M-C2M-S1	-2.06	120.06	122.68
3	A	701	GN8	CAR-CAF-CAW	-2.06	126.14	130.13
3	F	706	GN8	CAN-CAT-NAY	2.03	118.64	116.47
3	B	702	GN8	CAN-CAT-NAY	2.03	118.64	116.47
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 (119) 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

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Mol	Chain	Res	Type	Atoms
3	F	706	GN8	CAS-CAO-NAX-CAU
3	F	706	GN8	CAS-CAO-NAX-CAV
3	E	705	GN8	CAS-CAO-NAX-CAU
2	B	602	MYA	C3M-C4M-C5M-C6M
2	D	604	MYA	C4M-C5M-C6M-C7M
2	D	604	MYA	C7M-C8M-C9M-CAM
3	C	703	GN8	CAS-CAO-NAX-CAU
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
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
3	E	705	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

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Mol	Chain	Res	Type	Atoms
2	D	604	MYA	S1-C2M-C3M-C4M
2	D	604	MYA	O2M-C2M-C3M-C4M
2	F	606	MYA	CCM-CDM-CEM-CFM
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
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
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
2	F	606	MYA	C9-C10-C11-C14
2	A	601	MYA	C6M-C7M-C8M-C9M

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Mol	Chain	Res	Type	Atoms
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

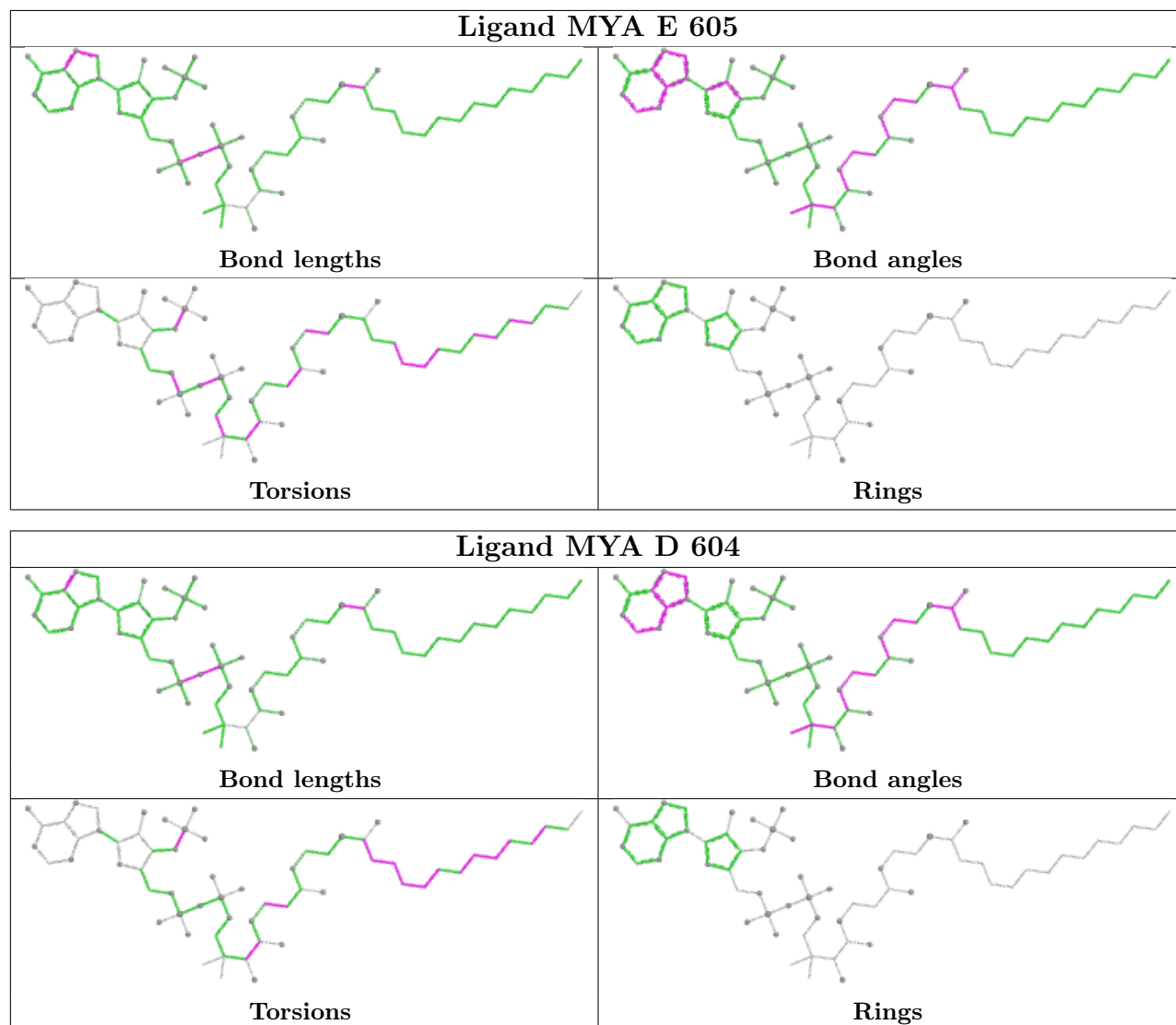
There are no ring outliers.

12 monomers are involved in 31 short contacts:

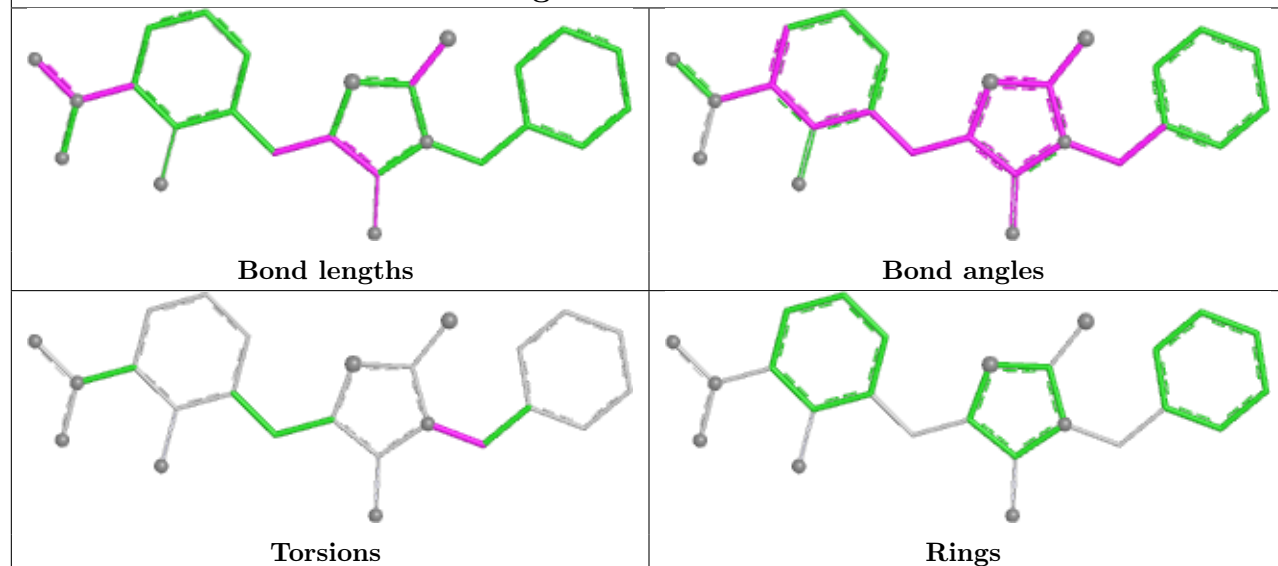
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	605	MYA	3	0
2	D	604	MYA	7	0
3	B	702	GN8	1	0
3	D	704	GN8	1	0
2	B	602	MYA	6	0
3	E	705	GN8	1	0
2	F	606	MYA	2	0
2	C	603	MYA	3	0
2	A	601	MYA	1	0
3	C	703	GN8	2	0
3	A	701	GN8	3	0
3	F	706	GN8	1	0

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

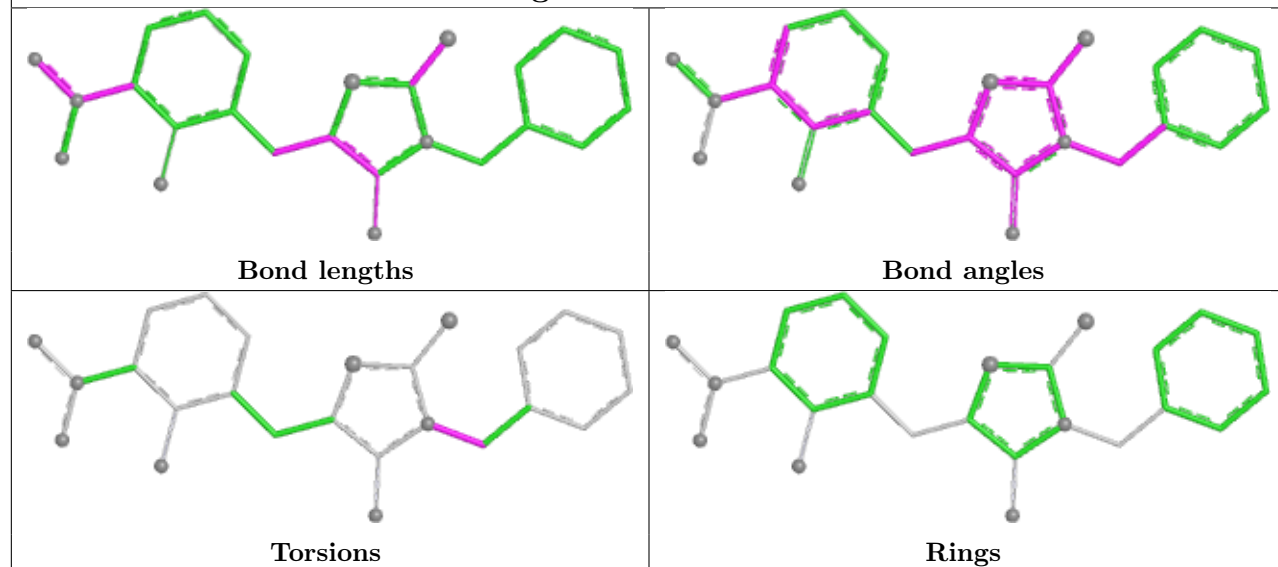
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



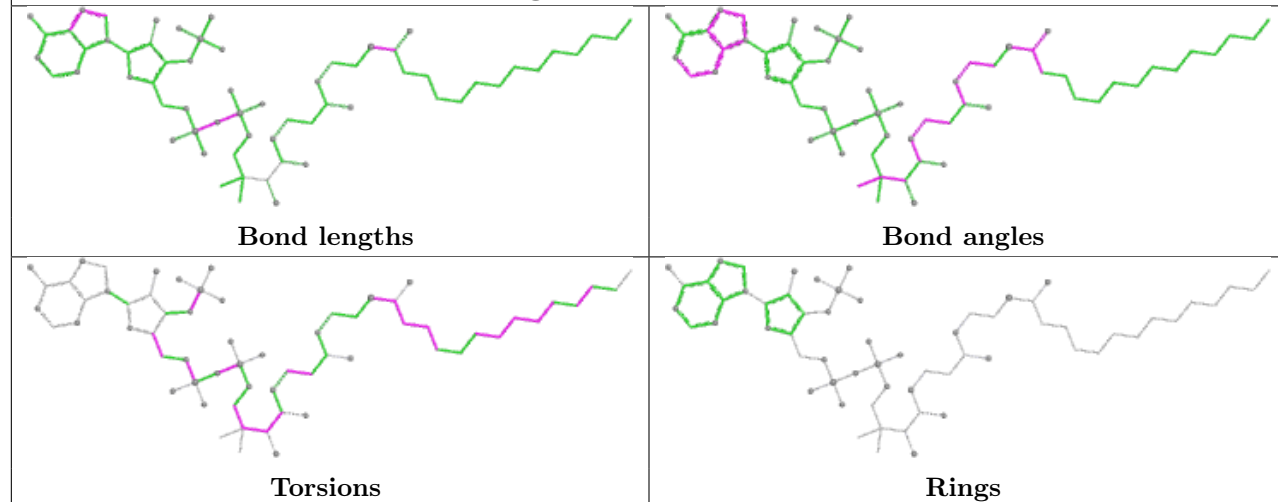
Ligand GN8 B 702



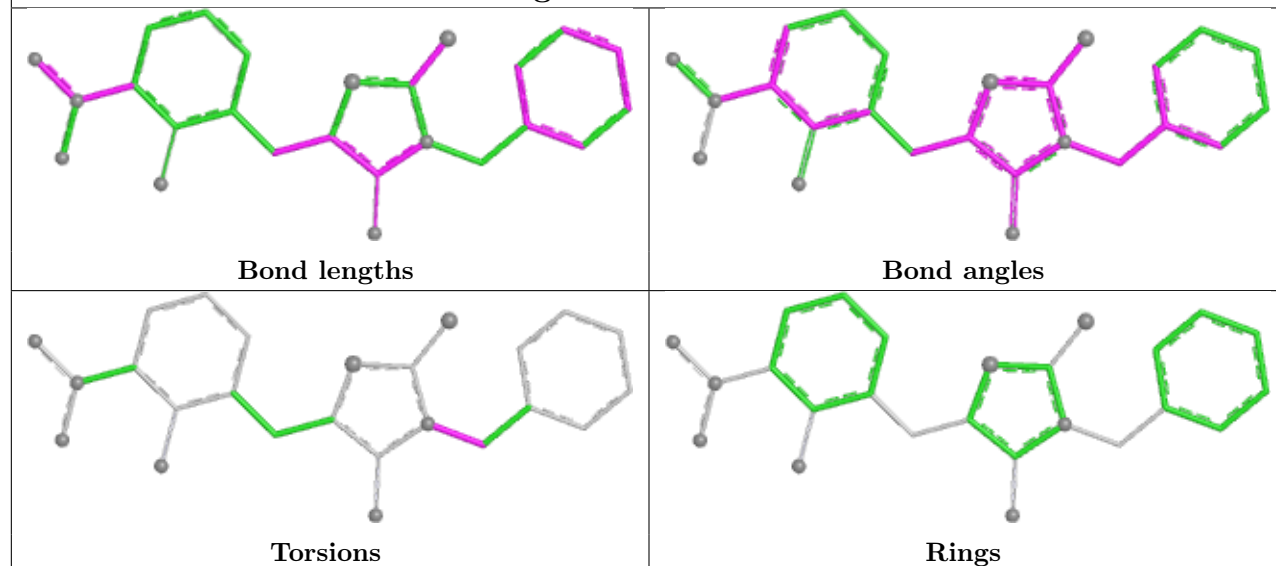
Ligand GN8 D 704



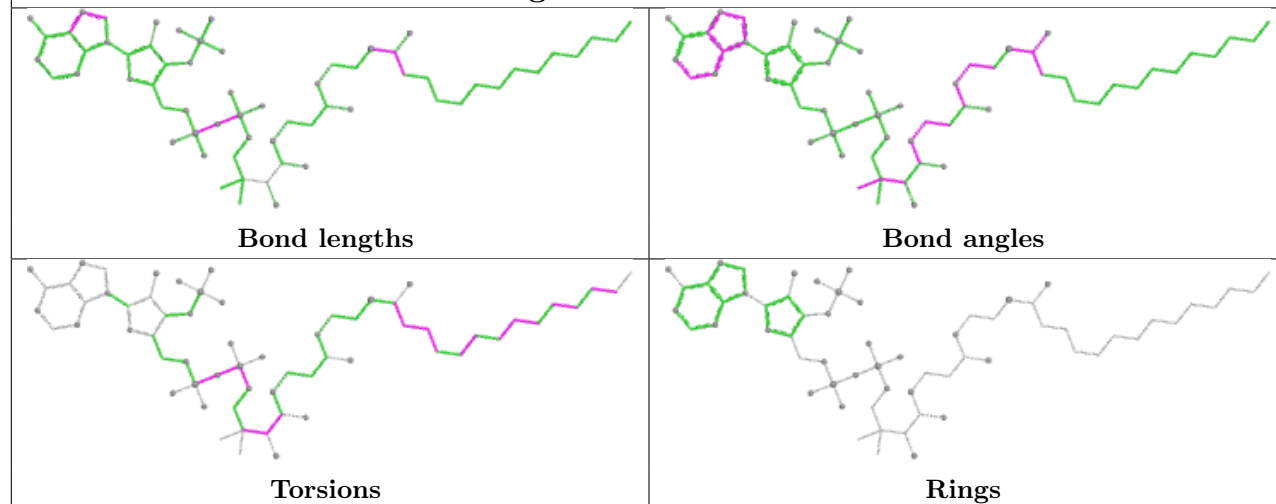
Ligand MYA B 602



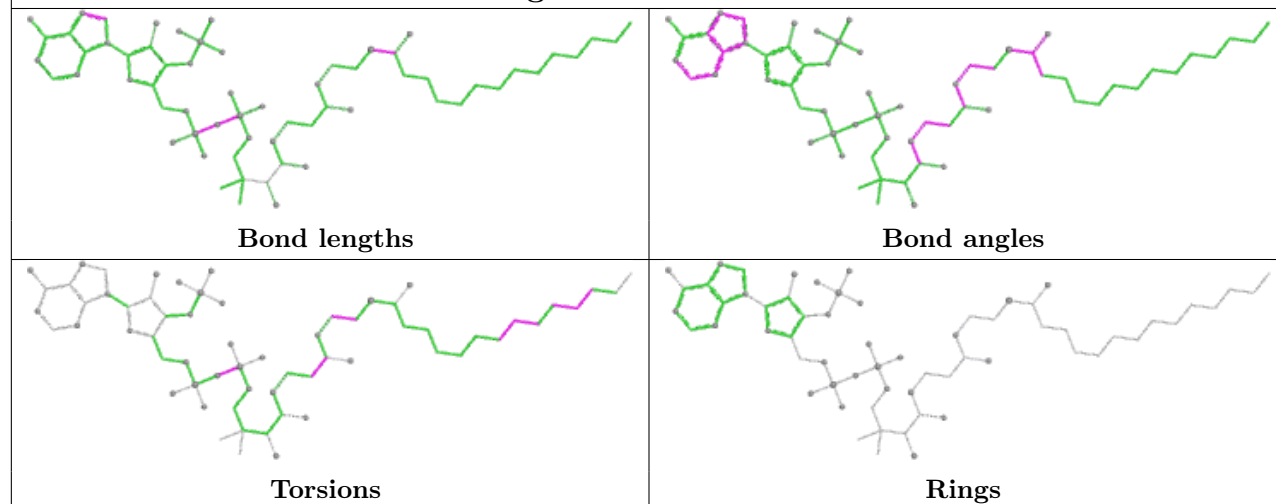
Ligand GN8 E 705

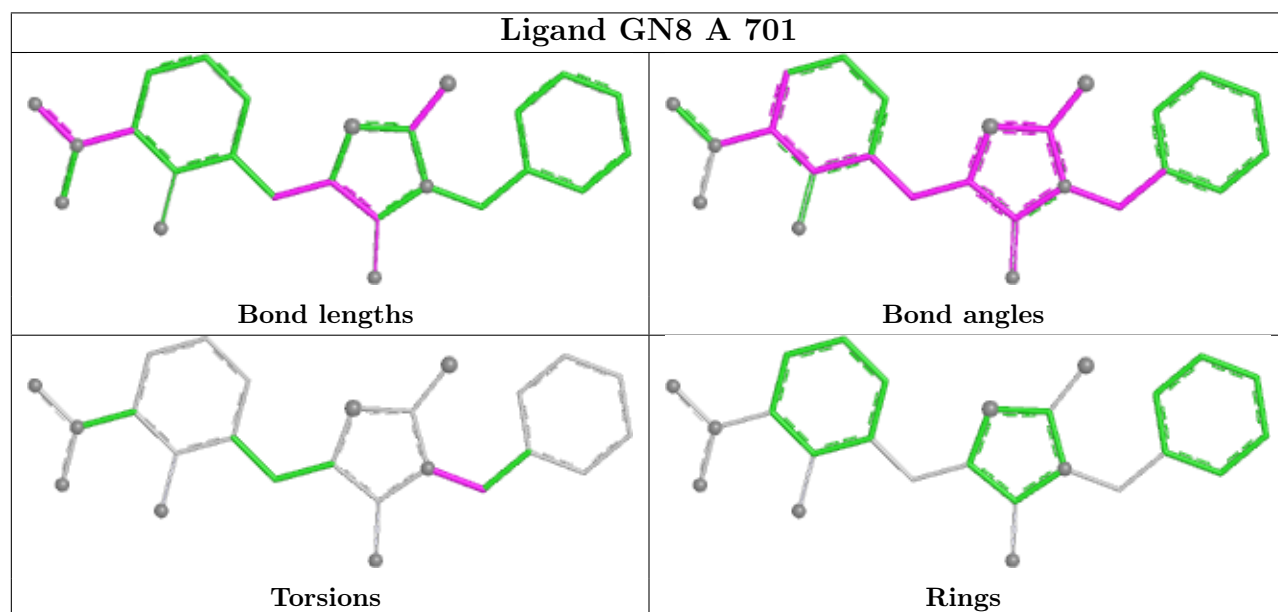
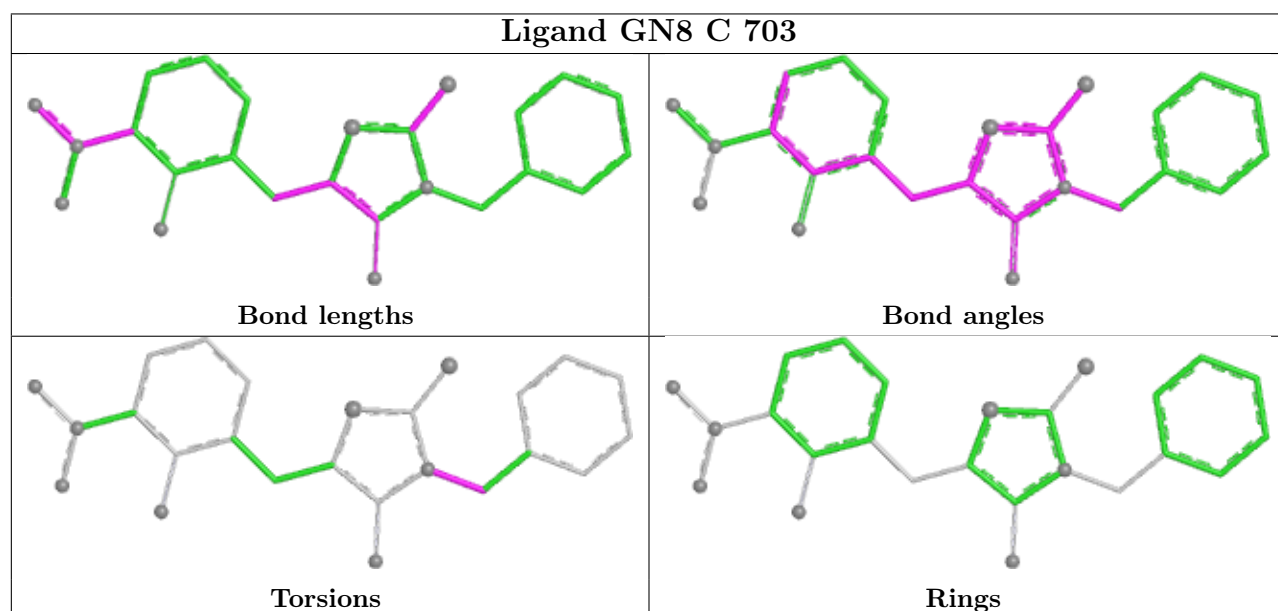
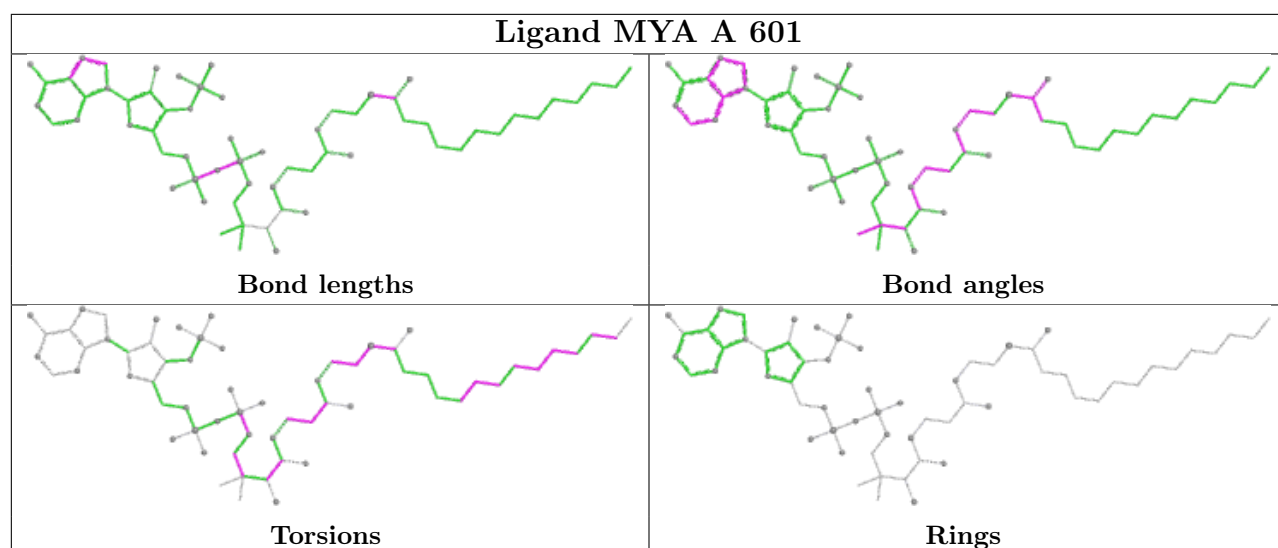


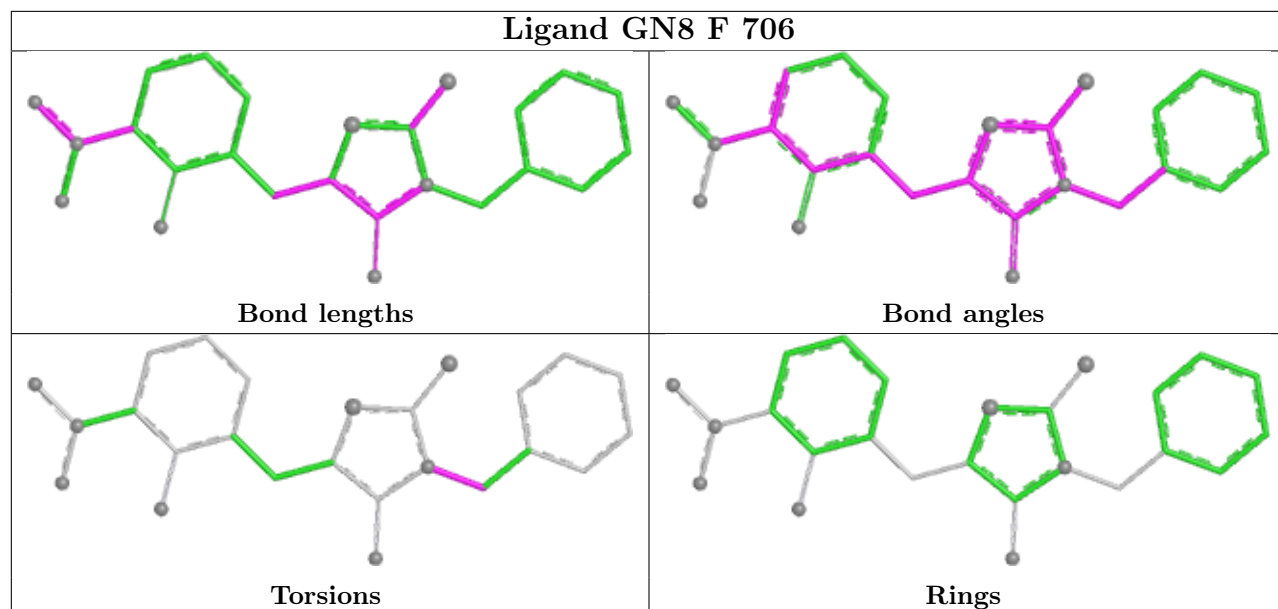
Ligand MYA F 606



Ligand MYA C 603







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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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 ²)	Q<0.9
1	A	436/455 (95%)	-0.18	1 (0%) 91 83	16, 31, 54, 69	0
1	B	436/455 (95%)	-0.25	1 (0%) 91 83	15, 29, 56, 66	0
1	C	436/455 (95%)	0.11	6 (1%) 73 53	15, 42, 65, 104	0
1	D	436/455 (95%)	-0.13	1 (0%) 91 83	17, 34, 54, 69	0
1	E	436/455 (95%)	-0.27	0 100 100	15, 26, 48, 65	0
1	F	435/455 (95%)	0.16	6 (1%) 73 53	17, 47, 66, 106	0
All	All	2615/2730 (95%)	-0.09	15 (0%) 85 70	15, 34, 61, 106	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	69	SER	3.6
1	F	68	ILE	3.6
1	F	49	PHE	2.9
1	C	49	PHE	2.8
1	C	68	ILE	2.5
1	D	292	GLU	2.4
1	A	64	THR	2.2
1	C	20	ASN	2.2
1	C	21	ASN	2.1
1	C	54	VAL	2.1
1	F	126	SER	2.1
1	F	417	ASP	2.1
1	F	64	THR	2.1
1	B	367	PRO	2.1
1	C	65	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

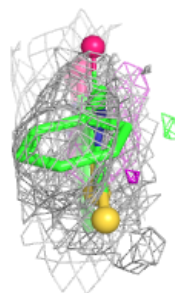
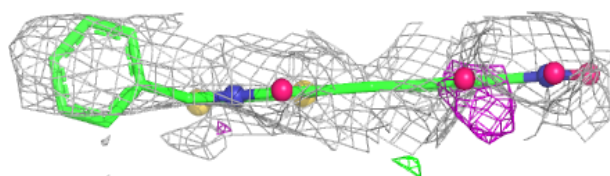
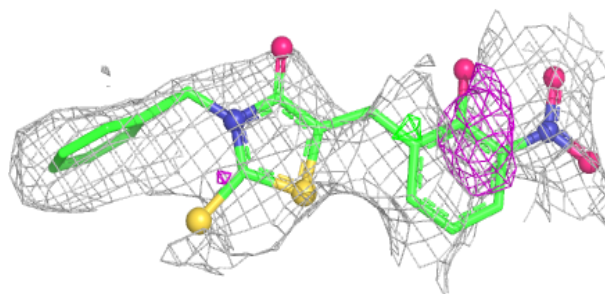
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GN8	D	704	25/25	0.59	0.16	59,68,77,78	0
3	GN8	A	701	25/25	0.65	0.16	50,62,72,73	0
3	GN8	C	703	25/25	0.67	0.15	60,66,73,74	0
3	GN8	E	705	25/25	0.67	0.18	62,67,73,74	0
3	GN8	B	702	25/25	0.68	0.17	67,72,78,78	0
3	GN8	F	706	25/25	0.71	0.16	65,72,76,78	0
2	MYA	C	603	63/63	0.85	0.13	47,50,55,55	0
2	MYA	F	606	63/63	0.87	0.12	53,60,65,66	0
2	MYA	D	604	63/63	0.93	0.10	25,39,43,43	0
2	MYA	E	605	63/63	0.94	0.09	13,25,30,32	0
2	MYA	A	601	63/63	0.95	0.09	21,31,44,46	0
2	MYA	B	602	63/63	0.95	0.08	16,26,29,31	0

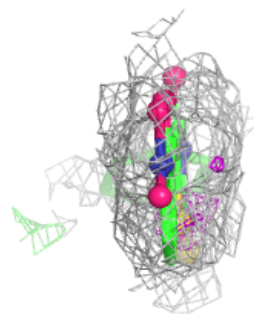
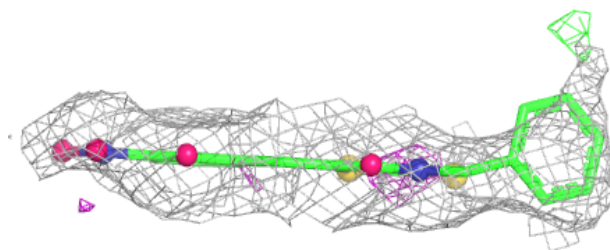
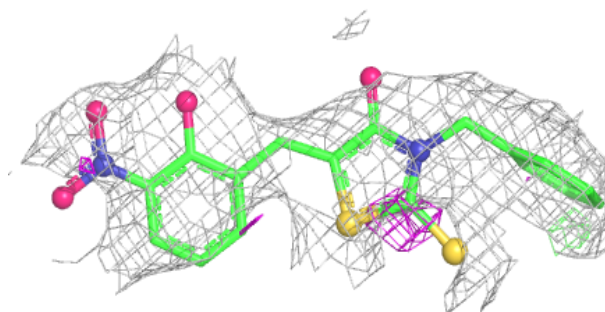
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GN8 D 704:

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

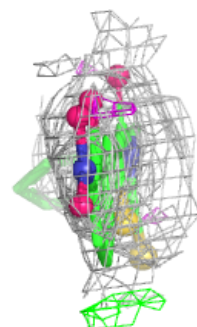
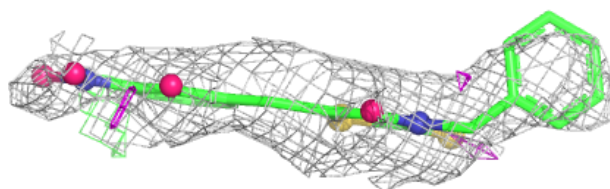
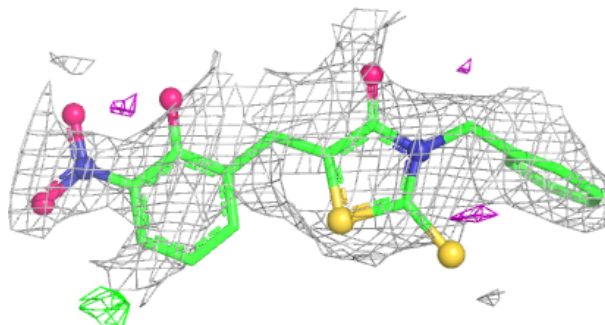
**Electron density around GN8 A 701:**

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

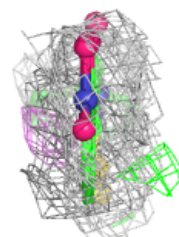
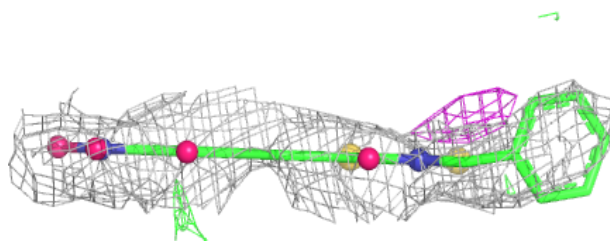
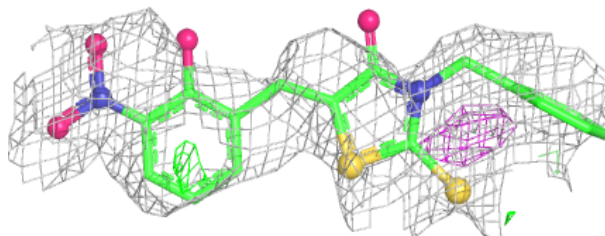


Electron density around GN8 C 703:

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

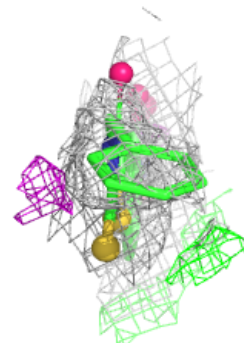
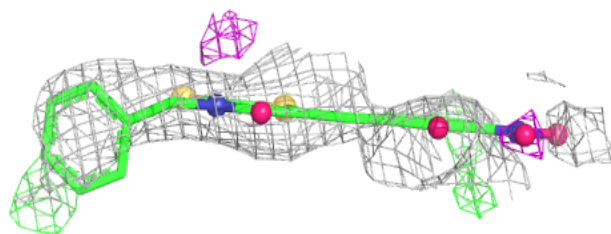
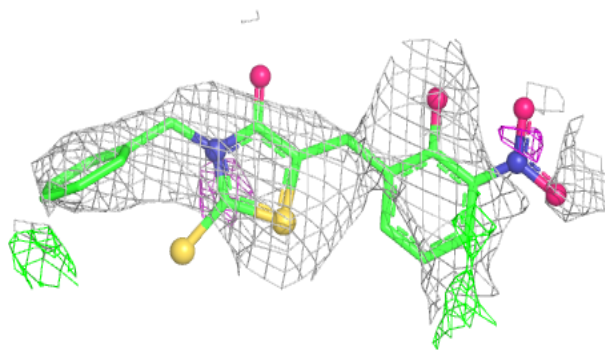
**Electron density around GN8 E 705:**

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

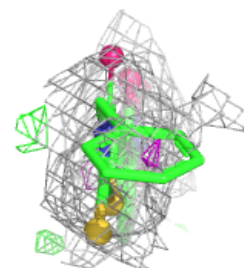
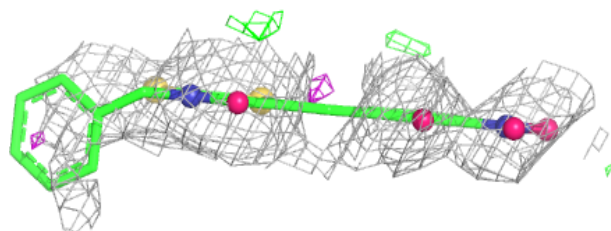
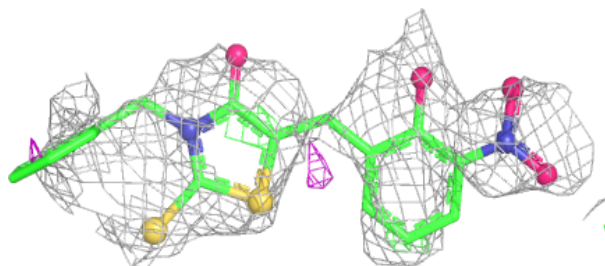


Electron density around GN8 B 702:

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

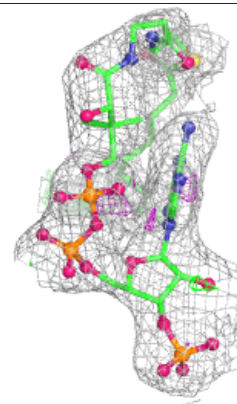
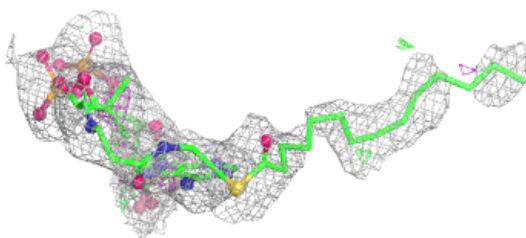
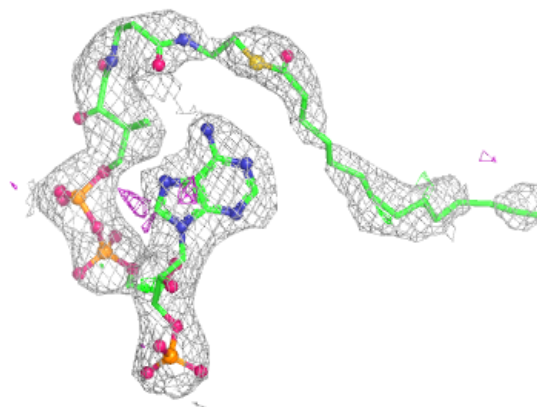
**Electron density around GN8 F 706:**

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

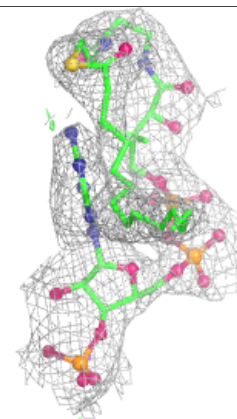
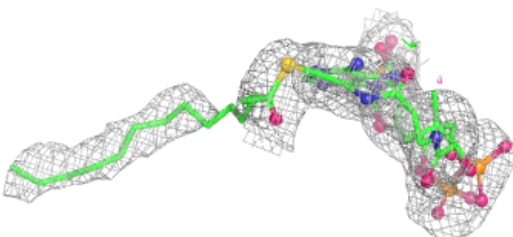
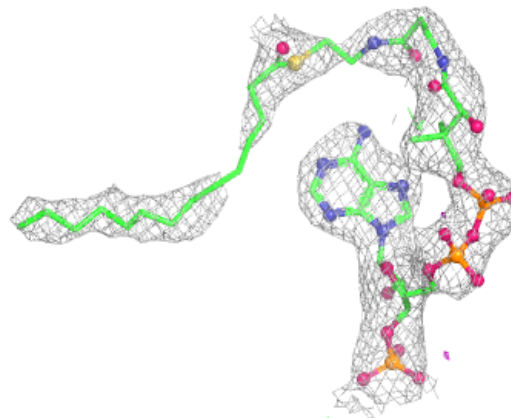


Electron density around MYA C 603:

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

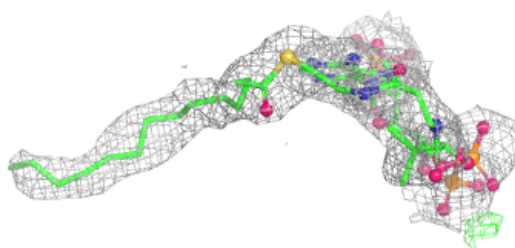
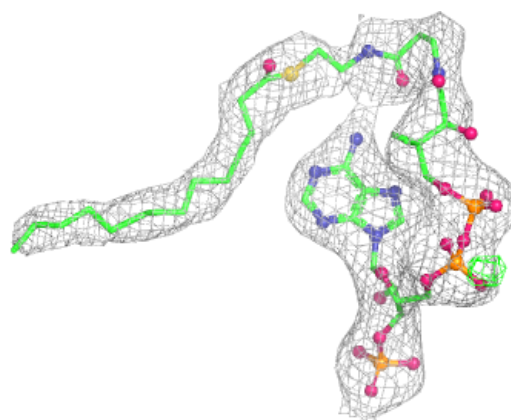
**Electron density around MYA F 606:**

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

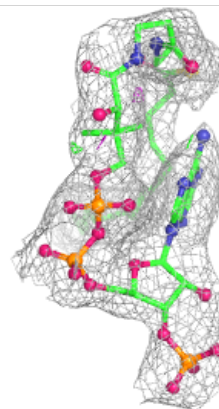
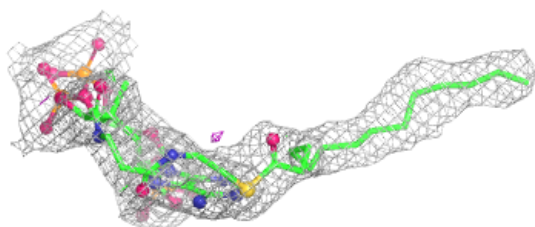
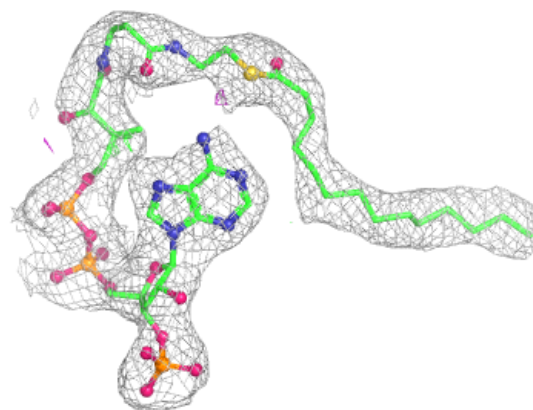


Electron density around MYA D 604:

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

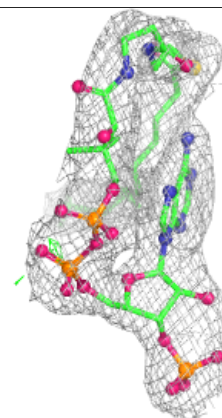
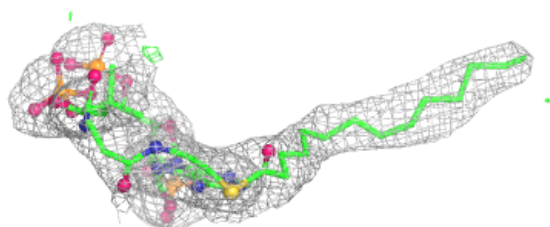
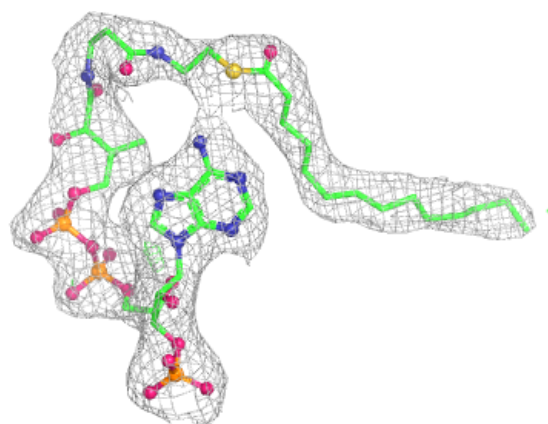
**Electron density around MYA E 605:**

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

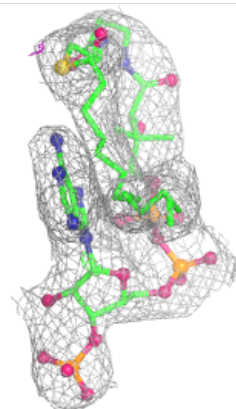
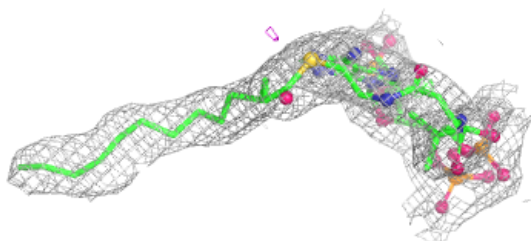
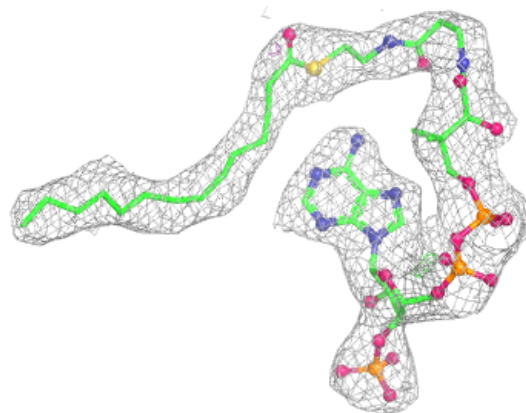


Electron density around MYA A 601:

$2mF_o-DF_c$ (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)



6.5 Other polymers ⓘ

There are no such residues in this entry.