



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:45 PM UTC

PDB ID : 2P6E / pdb_00002p6e
Title : Crystal structures of *Saccharomyces cerevisiae* N-myristoyltransferase with bound myristoyl-CoA
Authors : Wu, J.; Ding, J.
Deposited on : 2007-03-18
Resolution : 2.90 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

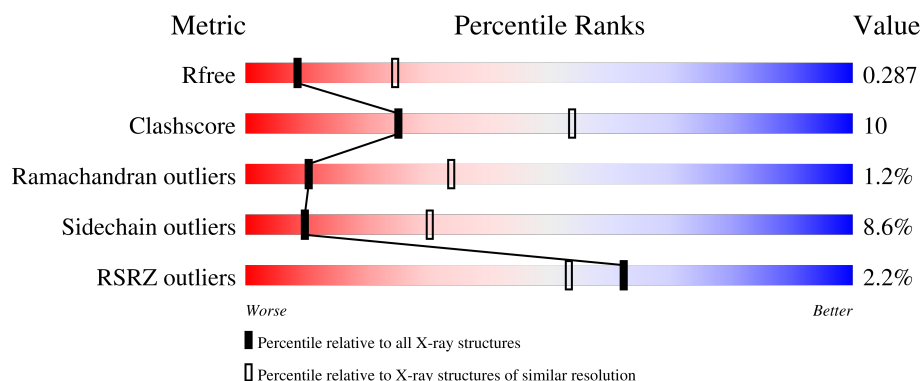
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	2% 73% 21% • •
1	B	455	2% 70% 23% • •
1	C	455	4% 73% 22% • •
1	D	455	2% 74% 20% • •
1	E	455	0% 67% 27% • •

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Mol	Chain	Length	Quality of chain
1	F	455	 2% 71% 22% . .

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](#)

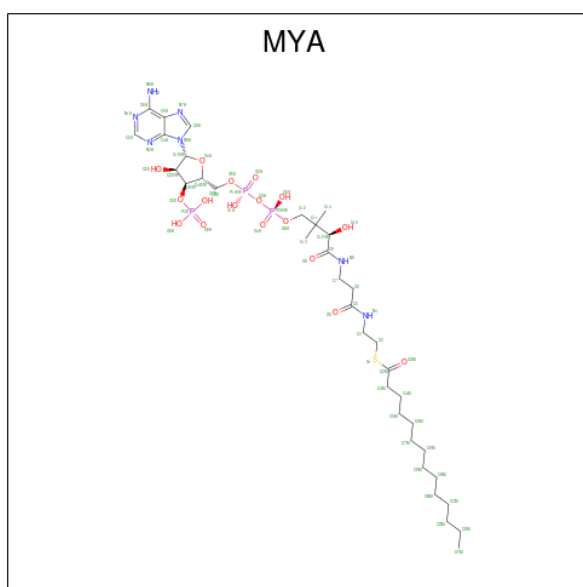
There are 2 unique types of molecules in this entry. The entry contains 22163 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	442	Total	C	N	O	S	0	0	0
			3627	2348	603	667	9			
1	B	443	Total	C	N	O	S	0	0	0
			3634	2352	604	669	9			
1	C	446	Total	C	N	O	S	0	0	0
			3661	2367	608	677	9			
1	D	443	Total	C	N	O	S	0	0	0
			3636	2354	605	668	9			
1	E	443	Total	C	N	O	S	0	0	0
			3634	2352	604	669	9			
1	F	438	Total	C	N	O	S	0	0	0
			3593	2326	598	660	9			

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

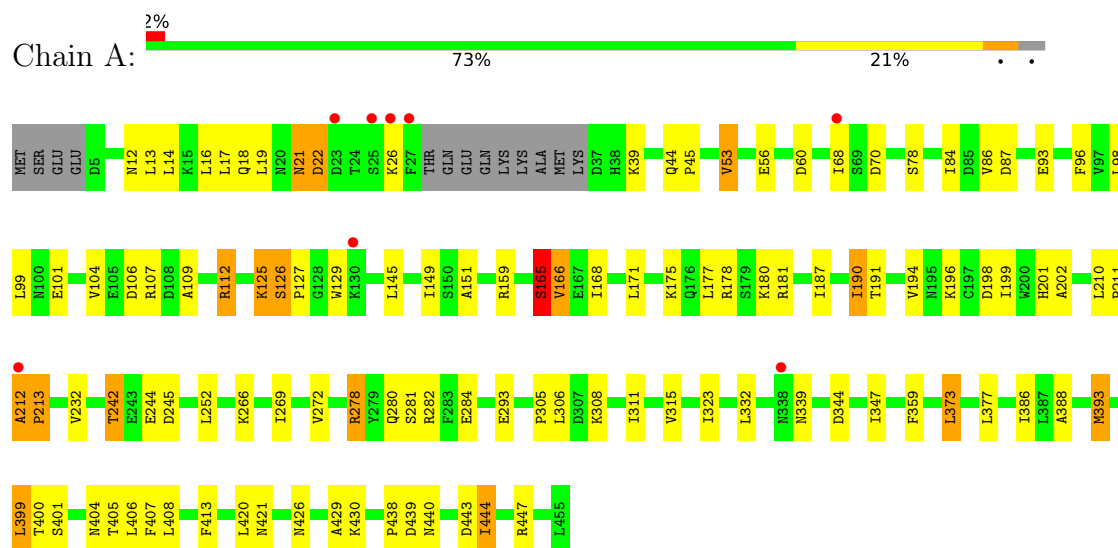


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 63	C 35	N 7	O 17	P 3	S 1	0	0
2	B	1	Total 63	C 35	N 7	O 17	P 3	S 1	0	0
2	C	1	Total 63	C 35	N 7	O 17	P 3	S 1	0	0
2	D	1	Total 63	C 35	N 7	O 17	P 3	S 1	0	0
2	E	1	Total 63	C 35	N 7	O 17	P 3	S 1	0	0
2	F	1	Total 63	C 35	N 7	O 17	P 3	S 1	0	0

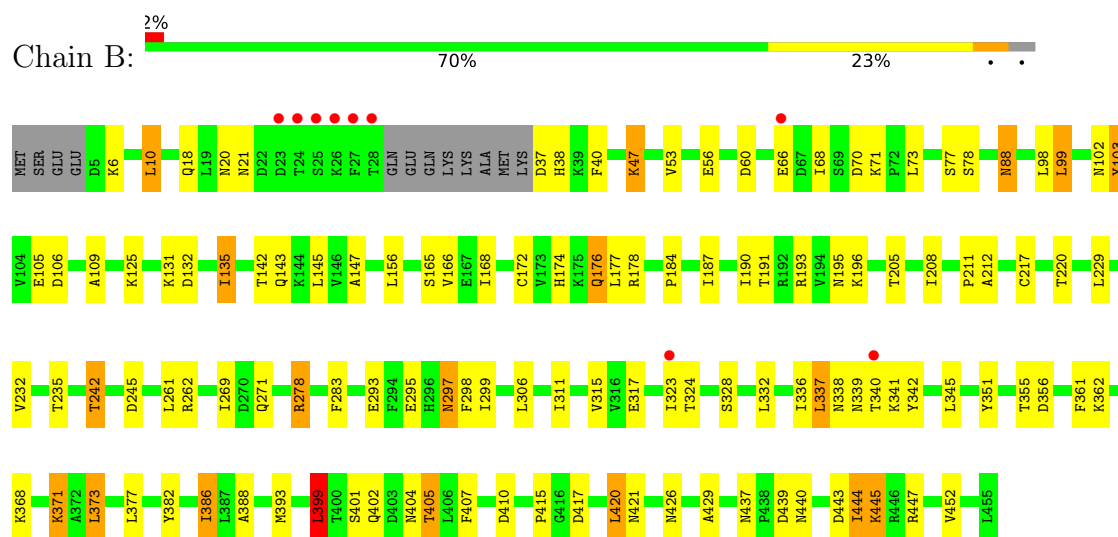
3 Residue-property plots

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.

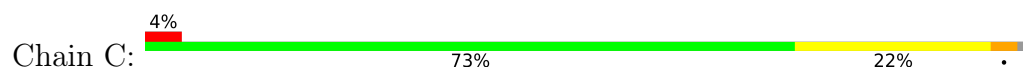
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase

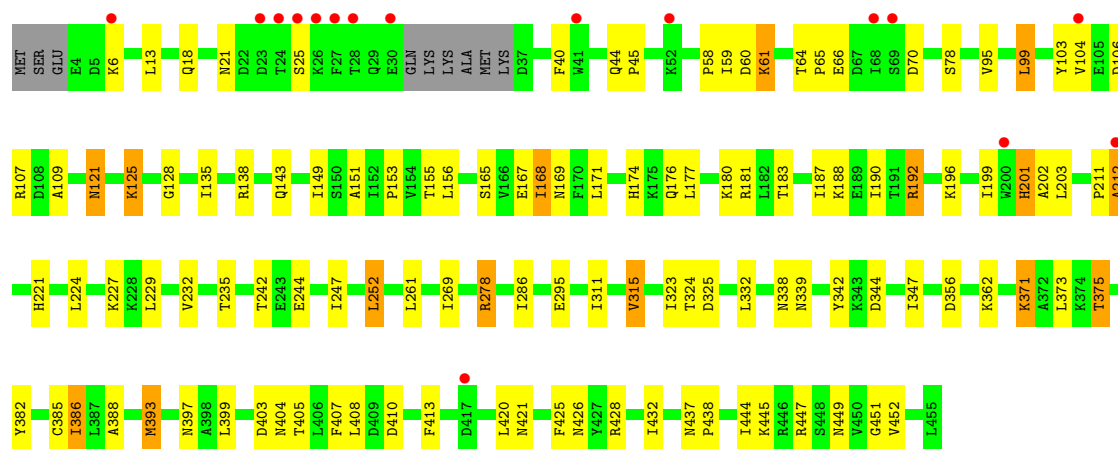


• Molecule 1: Glycylpeptide N-tetradecanoyltransferase

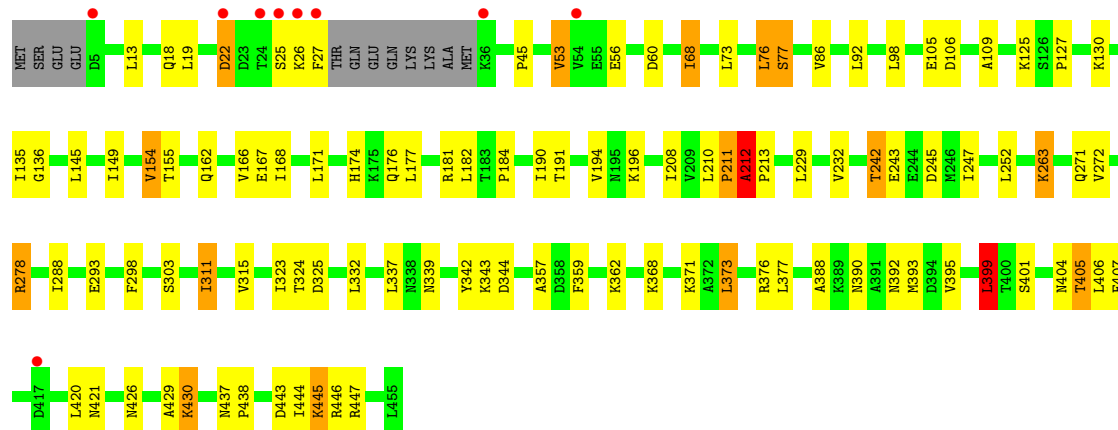
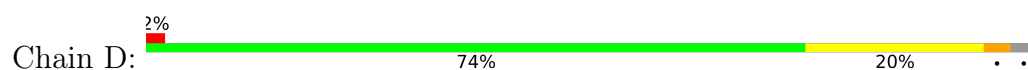


• Molecule 1: Glycylpeptide N-tetradecanoyltransferase

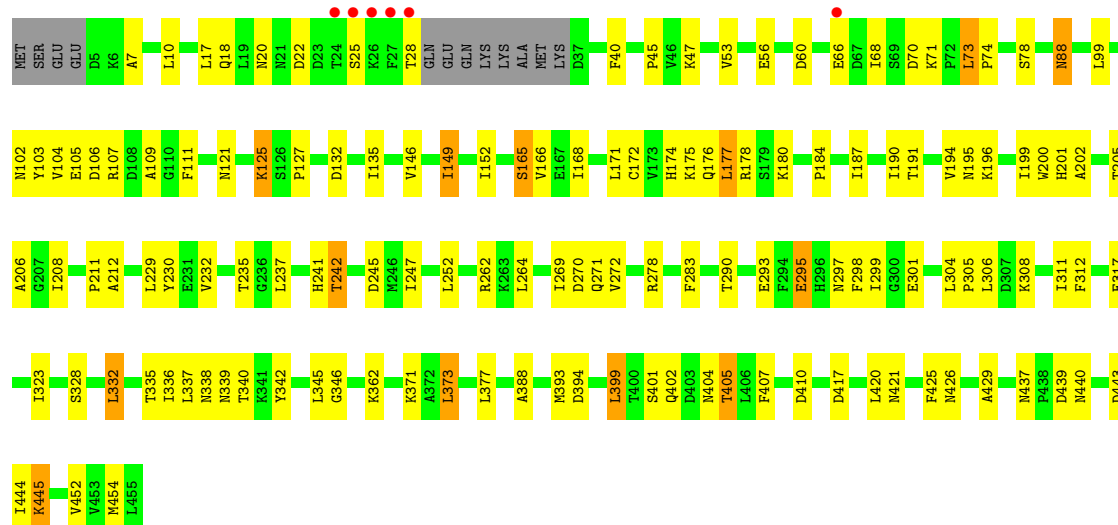




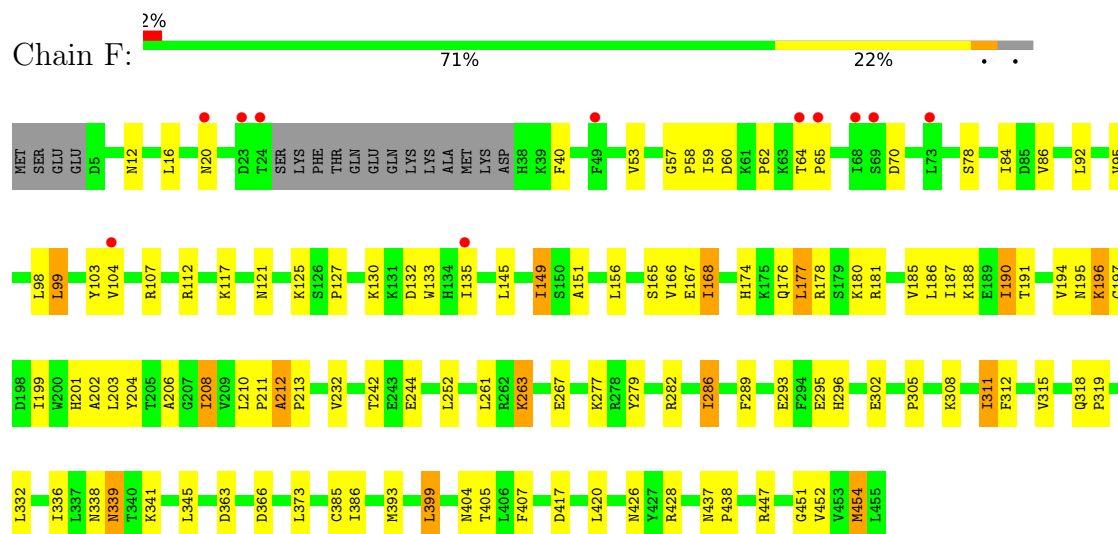
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase



• 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	188.22Å 150.87Å 134.05Å 90.00° 107.65° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-2.90) 98.6 (20.00-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.249 , 0.262 0.245 , 0.287	Depositor DCC
R_{free} test set	5391 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtrriage
Anisotropy	0.494	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.37$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22163	wwPDB-VP
Average B, all atoms (Å ²)	51.0	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 51.56 % 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 5.5100e-05. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.42	0/3716	0.79	2/5024 (0.0%)
1	B	0.44	0/3723	0.80	1/5034 (0.0%)
1	C	0.45	0/3750	0.81	1/5070 (0.0%)
1	D	0.43	0/3725	0.81	2/5035 (0.0%)
1	E	0.43	0/3723	0.81	5/5034 (0.1%)
1	F	0.44	0/3681	0.81	3/4978 (0.1%)
All	All	0.44	0/22318	0.80	14/30175 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	399	LEU	N-CA-C	7.62	121.89	112.59
1	C	399	LEU	N-CA-C	6.72	122.45	113.72
1	A	399	LEU	N-CA-C	6.40	120.73	112.41
1	F	57	GLY	CA-C-N	6.31	127.72	119.84
1	F	57	GLY	C-N-CA	6.31	127.72	119.84
1	E	399	LEU	N-CA-C	5.91	122.47	113.61
1	E	7	ALA	N-CA-C	-5.87	107.93	114.62
1	D	212	ALA	N-CA-C	5.83	122.68	109.81
1	A	165	SER	N-CA-C	5.67	115.77	108.34
1	E	332	LEU	CA-C-N	5.47	125.77	119.92
1	E	332	LEU	C-N-CA	5.47	125.77	119.92
1	F	399	LEU	N-CA-C	5.39	122.21	114.39
1	B	399	LEU	N-CA-C	5.30	121.56	113.61
1	E	165	SER	N-CA-C	5.20	115.01	108.45

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	3627	0	3615	79	0
1	B	3634	0	3622	69	0
1	C	3661	0	3642	70	0
1	D	3636	0	3628	64	0
1	E	3634	0	3622	80	0
1	F	3593	0	3584	64	0
2	A	63	0	58	7	0
2	B	63	0	58	5	0
2	C	63	0	58	6	0
2	D	63	0	58	2	0
2	E	63	0	58	8	0
2	F	63	0	58	5	0
All	All	22163	0	22061	430	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 (430) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:ARG:HG3	1:C:278:ARG:HH11	1.07	1.15
1:B:278:ARG:HH11	1:B:278:ARG:HG3	1.00	1.10
1:A:212:ALA:H	1:A:213:PRO:HD3	1.10	1.07
1:A:151:ALA:HB2	1:A:190:ILE:HD11	1.35	1.05
1:B:47:LYS:HD2	1:B:212:ALA:HB1	1.43	1.01
1:D:76:LEU:HD23	1:D:76:LEU:H	1.36	0.91
1:A:212:ALA:H	1:A:213:PRO:CD	1.83	0.90
1:B:278:ARG:HG3	1:B:278:ARG:NH1	1.80	0.89
1:E:70:ASP:HB3	1:E:196:LYS:HE3	1.54	0.89
1:A:190:ILE:O	1:A:194:VAL:HG23	1.73	0.89
1:A:60:ASP:H	1:A:426:ASN:HD21	1.17	0.87
1:A:112:ARG:CG	1:A:112:ARG:HH11	1.87	0.87
1:C:278:ARG:HG3	1:C:278:ARG:NH1	1.86	0.86
1:E:339:ASN:HD22	1:E:342:TYR:H	1.22	0.85
1:C:437:ASN:HB3	1:C:438:PRO:HD2	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:ASP:H	1:D:426:ASN:HD21	1.25	0.84
1:F:336:ILE:HD11	1:F:345:LEU:HB2	1.59	0.83
1:B:60:ASP:H	1:B:426:ASN:HD21	1.29	0.80
1:C:60:ASP:H	1:C:426:ASN:HD21	1.28	0.80
1:E:339:ASN:ND2	1:E:342:TYR:H	1.81	0.79
1:D:278:ARG:HD2	1:D:359:PHE:CE1	2.18	0.78
1:D:211:PRO:O	1:D:212:ALA:CB	2.31	0.78
1:E:47:LYS:HD2	1:E:212:ALA:HB1	1.66	0.77
1:A:212:ALA:N	1:A:213:PRO:HD3	1.95	0.77
1:D:405:THR:HG21	1:D:443:ASP:O	1.84	0.77
1:A:112:ARG:HH11	1:A:112:ARG:HG2	1.48	0.77
1:B:135:ILE:HD13	1:B:190:ILE:HD13	1.69	0.75
1:A:106:ASP:HB3	1:A:109:ALA:HB2	1.67	0.75
1:E:405:THR:HG21	1:E:443:ASP:O	1.87	0.75
1:F:263:LYS:HE3	1:F:263:LYS:H	1.50	0.74
1:F:339:ASN:HD22	1:F:341:LYS:H	1.33	0.74
1:B:70:ASP:HB3	1:B:196:LYS:HE3	1.69	0.73
1:D:211:PRO:O	1:D:212:ALA:HB2	1.89	0.73
1:E:388:ALA:O	1:E:393:MET:HG3	1.88	0.73
1:A:194:VAL:HG12	1:A:199:ILE:HB	1.70	0.72
1:A:388:ALA:O	1:A:393:MET:HG3	1.89	0.72
1:B:229:LEU:HB3	1:B:235:THR:HG22	1.71	0.72
1:F:212:ALA:H	1:F:213:PRO:HD3	1.55	0.72
1:D:168:ILE:HG13	2:D:604:MYA:HBMA	1.72	0.71
1:F:404:ASN:HA	1:F:407:PHE:CE2	2.25	0.71
1:C:371:LYS:O	1:C:375:THR:HG22	1.91	0.71
1:B:278:ARG:HH11	1:B:278:ARG:CG	1.93	0.70
1:C:339:ASN:HD22	1:C:342:TYR:H	1.36	0.70
1:D:406:LEU:HG	1:D:447:ARG:HD3	1.72	0.70
1:A:405:THR:CG2	1:A:444:ILE:HA	2.22	0.70
1:E:18:GLN:HE22	1:E:421:ASN:HD21	1.39	0.70
1:D:76:LEU:HD23	1:D:76:LEU:N	2.07	0.69
1:A:151:ALA:CB	1:A:190:ILE:HD11	2.16	0.69
1:E:336:ILE:CD1	1:E:345:LEU:HB2	2.22	0.69
1:E:187:ILE:HG12	2:E:605:MYA:H7MA	1.73	0.69
1:A:278:ARG:HD2	1:A:359:PHE:CE1	2.27	0.69
1:D:127:PRO:HG2	1:D:293:GLU:HA	1.75	0.68
1:B:439:ASP:O	1:B:440:ASN:HB2	1.92	0.68
1:A:112:ARG:CG	1:A:112:ARG:NH1	2.55	0.68
1:E:18:GLN:NE2	1:E:421:ASN:HD21	1.91	0.67
1:B:339:ASN:HD22	1:B:341:LYS:H	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:194:VAL:HG12	1:E:199:ILE:HB	1.75	0.67
1:D:212:ALA:O	1:D:213:PRO:C	2.37	0.67
1:A:168:ILE:HG21	2:A:601:MYA:H7M	1.77	0.67
1:B:174:HIS:HD2	1:B:176:GLN:H	1.41	0.66
1:F:202:ALA:HB2	2:F:606:MYA:HDMA	1.77	0.66
1:A:22:ASP:HB3	1:A:26:LYS:HD3	1.78	0.66
1:C:242:THR:HG22	1:C:244:GLU:H	1.60	0.66
1:C:278:ARG:HH11	1:C:278:ARG:CG	1.96	0.66
1:F:20:ASN:HB2	1:F:417:ASP:HB2	1.77	0.66
1:B:174:HIS:CD2	1:B:176:GLN:H	2.14	0.66
1:F:12:ASN:O	1:F:16:LEU:HG	1.95	0.66
1:D:242:THR:HG22	1:D:245:ASP:H	1.60	0.65
1:D:60:ASP:H	1:D:426:ASN:ND2	1.95	0.65
1:E:191:THR:HA	2:E:605:MYA:HDM	1.79	0.65
1:D:53:VAL:HG13	1:D:430:LYS:HD3	1.78	0.65
1:B:388:ALA:O	1:B:393:MET:HG3	1.98	0.64
1:E:68:ILE:HD11	1:E:200:TRP:CH2	2.32	0.64
1:B:339:ASN:ND2	1:B:341:LYS:H	1.96	0.64
1:F:212:ALA:H	1:F:213:PRO:CD	2.10	0.64
1:A:60:ASP:H	1:A:426:ASN:ND2	1.92	0.64
1:D:263:LYS:H	1:D:263:LYS:HD3	1.62	0.64
1:D:388:ALA:O	1:D:393:MET:HG3	1.97	0.64
1:B:336:ILE:HD11	1:B:345:LEU:HB2	1.80	0.63
1:C:18:GLN:HE22	1:C:421:ASN:HD21	1.46	0.63
2:E:605:MYA:H2AA	2:E:605:MYA:H6M	1.79	0.63
1:F:64:THR:HB	1:F:65:PRO:HD2	1.79	0.63
1:C:168:ILE:HD11	2:C:603:MYA:HCM	1.80	0.63
1:E:121:ASN:O	1:E:125:LYS:HB2	1.99	0.63
1:C:59:ILE:HG23	1:C:428:ARG:NH2	2.14	0.63
1:F:405:THR:HG22	1:F:447:ARG:HG2	1.81	0.62
1:C:168:ILE:HG21	2:C:603:MYA:H7M	1.82	0.62
1:A:127:PRO:HG2	1:A:293:GLU:HA	1.81	0.62
1:C:151:ALA:HA	1:C:167:GLU:O	2.00	0.62
1:C:174:HIS:HB3	1:C:177:LEU:HD21	1.80	0.62
1:F:242:THR:HG22	1:F:244:GLU:H	1.65	0.62
1:E:336:ILE:HD11	1:E:345:LEU:HB2	1.81	0.62
1:B:21:ASN:HB3	1:C:107:ARG:HH22	1.65	0.61
1:A:210:LEU:O	1:A:213:PRO:HD3	2.00	0.61
1:C:121:ASN:O	1:C:125:LYS:HB2	2.00	0.61
1:B:20:ASN:HD22	1:B:417:ASP:HB2	1.65	0.61
1:D:404:ASN:HD22	1:D:407:PHE:HZ	1.43	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:LYS:H	1:D:263:LYS:CD	2.13	0.60
1:E:437:ASN:HD21	1:E:445:LYS:HE3	1.65	0.60
1:B:60:ASP:H	1:B:426:ASN:ND2	1.97	0.60
1:D:339:ASN:HD22	1:D:342:TYR:H	1.50	0.60
1:B:242:THR:HB	1:B:245:ASP:H	1.66	0.60
1:C:404:ASN:HA	1:C:407:PHE:CE2	2.37	0.60
1:D:18:GLN:HE22	1:D:421:ASN:HD21	1.48	0.60
1:B:18:GLN:HE22	1:B:421:ASN:HD21	1.49	0.60
1:F:305:PRO:HG2	1:F:308:LYS:HG3	1.82	0.60
1:A:405:THR:HG21	1:A:443:ASP:O	2.03	0.59
1:D:76:LEU:N	1:D:76:LEU:CD2	2.65	0.59
1:C:40:PHE:HE1	1:C:188:LYS:HE3	1.66	0.59
1:C:174:HIS:HB3	1:C:177:LEU:CD2	2.33	0.59
1:B:298:PHE:HA	1:B:311:ILE:HG12	1.85	0.59
1:E:373:LEU:HD22	1:E:377:LEU:HG	1.85	0.59
1:B:405:THR:HG21	1:B:443:ASP:O	2.02	0.59
1:E:405:THR:CG2	1:E:444:ILE:HA	2.33	0.59
1:E:88:ASN:C	1:E:88:ASN:HD22	2.11	0.58
1:F:59:ILE:HG23	1:F:428:ARG:NH2	2.19	0.58
1:F:149:ILE:HD11	1:F:168:ILE:HG23	1.86	0.58
1:F:70:ASP:HB3	1:F:196:LYS:HE3	1.86	0.58
1:A:112:ARG:HH11	1:A:112:ARG:HG3	1.67	0.57
1:E:60:ASP:H	1:E:426:ASN:HD21	1.52	0.57
1:C:347:ILE:C	1:C:393:MET:HE2	2.29	0.57
1:F:437:ASN:HB3	1:F:438:PRO:CD	2.33	0.57
1:A:305:PRO:HG2	1:A:308:LYS:HG3	1.85	0.57
1:D:437:ASN:HD21	1:D:445:LYS:HE3	1.69	0.57
1:B:56:GLU:HG2	1:B:429:ALA:HA	1.86	0.57
1:A:405:THR:HG22	1:A:444:ILE:HA	1.87	0.57
1:E:165:SER:HB3	1:E:201:HIS:HB2	1.87	0.57
1:E:168:ILE:HG13	2:E:605:MYA:HAMA	1.85	0.57
1:F:174:HIS:HB3	1:F:177:LEU:CD2	2.35	0.57
1:A:212:ALA:N	1:A:213:PRO:CD	2.58	0.57
1:E:190:ILE:O	1:E:194:VAL:HG23	2.04	0.57
1:E:232:VAL:HG12	1:E:232:VAL:O	2.05	0.57
1:F:279:TYR:O	1:F:282:ARG:HG2	2.05	0.57
1:E:290:THR:OG1	1:E:293:GLU:HG2	2.05	0.56
1:F:178:ARG:O	1:F:180:LYS:HG3	2.05	0.56
1:F:211:PRO:O	1:F:212:ALA:HB2	2.03	0.56
1:C:61:LYS:H	1:C:61:LYS:HD3	1.70	0.56
1:E:242:THR:HB	1:E:245:ASP:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:THR:HG22	1:A:245:ASP:H	1.70	0.56
1:A:202:ALA:HB2	2:A:601:MYA:HCMA	1.86	0.56
1:C:70:ASP:HB3	1:C:196:LYS:HE3	1.87	0.56
1:D:272:VAL:HG22	1:D:323:ILE:HG21	1.87	0.56
1:F:151:ALA:HA	1:F:167:GLU:O	2.06	0.56
1:A:202:ALA:CB	2:A:601:MYA:HCMA	2.35	0.56
1:F:181:ARG:NH2	2:F:606:MYA:O7A	2.39	0.56
1:B:191:THR:HA	2:B:602:MYA:HDM	1.89	0.55
1:F:211:PRO:O	1:F:212:ALA:CB	2.54	0.55
1:C:437:ASN:HB3	1:C:438:PRO:CD	2.34	0.55
1:C:18:GLN:NE2	1:C:421:ASN:HD21	2.03	0.55
1:A:56:GLU:HG2	1:A:429:ALA:HA	1.89	0.55
1:B:404:ASN:HA	1:B:407:PHE:CE2	2.41	0.55
1:F:204:TYR:HA	1:F:454:MET:HE1	1.88	0.55
1:C:106:ASP:HB3	1:C:109:ALA:HB2	1.89	0.55
1:C:437:ASN:CB	1:C:438:PRO:HD2	2.34	0.55
1:B:18:GLN:NE2	1:B:421:ASN:HD21	2.05	0.55
1:C:40:PHE:CE1	1:C:188:LYS:HE3	2.42	0.54
1:C:99:LEU:O	1:C:103:TYR:HB2	2.07	0.54
1:C:177:LEU:HB2	1:C:180:LYS:HE2	1.89	0.54
1:E:68:ILE:CD1	1:E:195:ASN:HB3	2.37	0.54
1:D:135:ILE:HG22	1:D:136:GLY:H	1.71	0.54
1:C:211:PRO:O	1:C:212:ALA:HB2	2.08	0.54
1:E:298:PHE:HA	1:E:311:ILE:HG12	1.90	0.54
1:A:86:VAL:HG11	1:A:125:LYS:HG3	1.89	0.54
1:B:339:ASN:HD22	1:B:342:TYR:H	1.54	0.54
1:B:444:ILE:HD13	1:B:444:ILE:H	1.73	0.53
1:A:405:THR:HG21	1:A:443:ASP:C	2.34	0.53
1:D:45:PRO:O	1:D:426:ASN:HA	2.08	0.53
1:E:20:ASN:ND2	1:E:22:ASP:HB2	2.23	0.53
2:E:605:MYA:H6M	2:E:605:MYA:C2A	2.38	0.53
1:F:437:ASN:HB3	1:F:438:PRO:HD2	1.90	0.53
1:B:174:HIS:HB3	1:B:177:LEU:HD21	1.91	0.53
1:F:104:VAL:HG21	1:F:112:ARG:HA	1.91	0.53
1:A:439:ASP:O	1:A:440:ASN:HB2	2.09	0.53
1:C:224:LEU:HD12	1:C:393:MET:HB2	1.91	0.53
1:E:68:ILE:HD13	1:E:195:ASN:HB3	1.90	0.53
1:E:301:GLU:HB3	1:E:304:LEU:HG	1.91	0.53
1:B:283:PHE:CE2	1:B:402:GLN:HA	2.44	0.53
1:E:401:SER:O	1:E:404:ASN:HB2	2.08	0.52
1:F:339:ASN:ND2	1:F:341:LYS:H	2.04	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:305:PRO:HG2	1:E:308:LYS:HG3	1.91	0.52
1:E:237:LEU:HD21	1:E:241:HIS:O	2.10	0.52
1:E:102:ASN:O	1:E:178:ARG:NH2	2.42	0.52
1:E:264:LEU:HD11	1:E:272:VAL:HG21	1.92	0.52
1:F:156:LEU:HD11	1:F:203:LEU:HB2	1.91	0.52
1:A:18:GLN:HE22	1:A:421:ASN:HD21	1.57	0.52
1:C:168:ILE:CD1	2:C:603:MYA:HCM	2.40	0.52
1:A:112:ARG:NH1	1:A:112:ARG:HG3	2.24	0.52
1:A:175:LYS:HA	1:A:178:ARG:HG3	1.92	0.52
1:B:371:LYS:HE3	1:B:371:LYS:HA	1.90	0.52
1:E:99:LEU:HD22	1:E:172:CYS:CB	2.40	0.52
1:A:107:ARG:HD3	1:A:175:LYS:HD3	1.91	0.52
1:C:183:THR:O	1:C:187:ILE:HG12	2.10	0.52
1:C:315:VAL:HG22	1:C:323:ILE:CG2	2.40	0.52
1:B:102:ASN:O	1:B:178:ARG:NH2	2.43	0.52
1:B:232:VAL:HG12	1:B:232:VAL:O	2.11	0.52
1:A:211:PRO:O	1:A:212:ALA:HB2	2.09	0.51
1:E:47:LYS:HB3	1:E:212:ALA:CB	2.39	0.51
1:B:156:LEU:HG	1:B:165:SER:OG	2.11	0.51
1:B:205:THR:HB	1:B:420:LEU:HD22	1.93	0.51
1:D:174:HIS:CD2	1:D:176:GLN:H	2.29	0.51
1:E:194:VAL:CG1	1:E:199:ILE:HB	2.40	0.51
1:F:206:ALA:HB1	1:F:208:ILE:HD13	1.93	0.51
1:A:21:ASN:O	1:A:22:ASP:C	2.53	0.51
1:F:99:LEU:O	1:F:103:TYR:HB2	2.11	0.51
1:C:174:HIS:CD2	1:C:176:GLN:H	2.29	0.51
1:A:14:LEU:HD21	1:A:213:PRO:HG2	1.93	0.50
1:D:405:THR:CG2	1:D:444:ILE:HA	2.40	0.50
1:E:404:ASN:HA	1:E:407:PHE:CE2	2.46	0.50
1:F:127:PRO:HG2	1:F:293:GLU:HA	1.92	0.50
1:D:154:VAL:HG21	1:D:167:GLU:HG3	1.92	0.50
1:D:404:ASN:HA	1:D:407:PHE:CE2	2.46	0.50
1:E:132:ASP:O	1:E:135:ILE:HD11	2.10	0.50
1:E:20:ASN:HD22	1:E:417:ASP:HB2	1.77	0.50
1:E:127:PRO:HG2	1:E:293:GLU:HA	1.92	0.50
1:C:339:ASN:ND2	1:C:342:TYR:H	2.06	0.50
1:E:312:PHE:O	1:E:328:SER:HA	2.12	0.50
1:A:151:ALA:HB2	1:A:190:ILE:CD1	2.23	0.50
1:F:191:THR:HA	2:F:606:MYA:HEMA	1.93	0.50
1:A:165:SER:HB3	1:A:201:HIS:HB2	1.93	0.50
1:C:382:TYR:O	1:C:386:ILE:HD12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:LEU:HB3	1:E:235:THR:HG22	1.94	0.49
1:C:211:PRO:O	1:C:212:ALA:CB	2.60	0.49
1:D:68:ILE:O	1:D:196:LYS:HE2	2.12	0.49
1:D:155:THR:HG22	1:D:288:ILE:HD12	1.93	0.49
1:E:269:ILE:HD13	1:E:295:GLU:HB2	1.93	0.49
1:D:22:ASP:HB2	1:D:26:LYS:HB2	1.94	0.49
1:D:135:ILE:HG22	1:D:136:GLY:N	2.28	0.49
1:C:95:VAL:O	1:C:99:LEU:HD23	2.12	0.49
1:C:232:VAL:HG12	1:C:232:VAL:O	2.12	0.49
1:C:315:VAL:HG22	1:C:323:ILE:HG23	1.93	0.49
1:E:202:ALA:HB2	2:E:605:MYA:HEM	1.94	0.49
1:D:208:ILE:H	1:D:208:ILE:HD12	1.78	0.49
1:F:336:ILE:CD1	1:F:345:LEU:HB2	2.37	0.49
1:D:181:ARG:HG3	1:D:184:PRO:HG2	1.94	0.49
1:E:439:ASP:O	1:E:440:ASN:HB2	2.12	0.49
1:F:311:ILE:HD13	1:F:312:PHE:H	1.77	0.49
1:B:88:ASN:C	1:B:88:ASN:HD22	2.20	0.48
1:E:99:LEU:HD22	1:E:172:CYS:HB2	1.95	0.48
1:E:339:ASN:ND2	1:E:342:TYR:N	2.58	0.48
1:F:60:ASP:H	1:F:426:ASN:HD21	1.60	0.48
1:A:168:ILE:HG22	2:A:601:MYA:H3MA	1.95	0.48
1:C:227:LYS:HD3	1:C:247:ILE:HD11	1.95	0.48
1:D:68:ILE:HG22	1:D:196:LYS:HG2	1.96	0.48
1:E:107:ARG:HH11	1:E:175:LYS:HZ2	1.59	0.48
1:B:99:LEU:O	1:B:103:TYR:HB2	2.13	0.48
1:B:99:LEU:HD13	1:B:103:TYR:CE1	2.49	0.48
1:B:328:SER:OG	1:B:351:TYR:HB3	2.13	0.48
1:E:232:VAL:O	1:E:232:VAL:CG1	2.61	0.48
1:F:187:ILE:O	1:F:190:ILE:HG22	2.14	0.48
1:A:399:LEU:C	1:A:401:SER:H	2.22	0.48
1:F:187:ILE:HG12	2:F:606:MYA:H7M	1.95	0.48
1:D:106:ASP:HB3	1:D:109:ALA:HB2	1.96	0.48
1:E:174:HIS:CD2	1:E:176:GLN:H	2.32	0.48
1:A:272:VAL:HG22	1:A:323:ILE:HG21	1.94	0.48
1:B:315:VAL:HG22	1:B:323:ILE:HG23	1.96	0.47
1:C:202:ALA:HB3	1:C:425:PHE:HB3	1.95	0.47
1:F:174:HIS:CD2	1:F:176:GLN:H	2.32	0.47
1:A:39:LYS:HG2	1:A:181:ARG:NH2	2.28	0.47
1:A:191:THR:HA	2:A:601:MYA:HDMA	1.96	0.47
1:C:58:PRO:HG3	1:C:201:HIS:HE1	1.79	0.47
1:B:217:CYS:HB3	1:B:399:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LYS:HD3	1:C:61:LYS:N	2.28	0.47
1:D:127:PRO:HG2	1:D:293:GLU:CA	2.44	0.47
1:F:252:LEU:HD21	1:F:385:CYS:HB3	1.97	0.47
1:A:12:ASN:O	1:A:16:LEU:HG	2.14	0.47
1:A:232:VAL:HG12	1:A:232:VAL:O	2.13	0.47
1:C:432:ILE:CG2	1:C:449:ASN:HB2	2.44	0.47
1:E:45:PRO:HB2	1:E:426:ASN:HD22	1.79	0.47
1:A:191:THR:HG23	2:A:601:MYA:HEM	1.97	0.47
1:B:220:THR:HG22	1:B:415:PRO:HA	1.96	0.47
1:C:149:ILE:HD12	1:C:171:LEU:HD13	1.95	0.47
1:C:269:ILE:HG13	1:C:295:GLU:HG3	1.97	0.47
1:F:194:VAL:O	1:F:197:CYS:N	2.48	0.47
1:F:242:THR:HG22	1:F:244:GLU:N	2.27	0.47
1:A:187:ILE:HG12	2:A:601:MYA:H7MA	1.97	0.47
1:C:408:LEU:O	1:C:413:PHE:HB2	2.15	0.47
1:B:38:HIS:HA	2:B:602:MYA:P3X	2.55	0.47
1:B:373:LEU:HD22	1:B:377:LEU:HG	1.97	0.47
1:E:146:VAL:HB	1:E:177:LEU:HD21	1.96	0.47
1:F:58:PRO:O	1:F:428:ARG:NH1	2.46	0.47
1:E:187:ILE:HG23	2:E:605:MYA:H9M	1.97	0.46
1:C:138:ARG:NH1	1:C:143:GLN:O	2.43	0.46
1:C:187:ILE:O	1:C:190:ILE:HG22	2.15	0.46
1:D:232:VAL:O	1:D:232:VAL:CG1	2.64	0.46
1:E:106:ASP:HB3	1:E:109:ALA:HB2	1.96	0.46
1:A:93:GLU:HA	1:A:96:PHE:CZ	2.50	0.46
1:C:432:ILE:HG23	1:C:449:ASN:HB2	1.96	0.46
1:A:22:ASP:OD1	1:A:22:ASP:N	2.49	0.46
1:D:263:LYS:HD3	1:D:263:LYS:N	2.29	0.46
1:E:337:LEU:O	1:E:339:ASN:N	2.40	0.46
1:E:283:PHE:CE2	1:E:402:GLN:HA	2.50	0.46
1:A:39:LYS:HG2	1:A:181:ARG:HH22	1.79	0.46
1:B:106:ASP:HB3	1:B:109:ALA:HB2	1.97	0.46
1:F:165:SER:HB3	1:F:201:HIS:HB2	1.98	0.46
1:A:406:LEU:HD21	1:A:447:ARG:HH11	1.80	0.46
1:E:40:PHE:CD1	1:E:184:PRO:HB3	2.51	0.46
1:C:252:LEU:HD21	1:C:385:CYS:HB3	1.98	0.46
1:D:271:GLN:HB3	1:D:323:ILE:HD12	1.97	0.46
1:F:86:VAL:HG13	1:F:92:LEU:HD13	1.98	0.46
1:B:401:SER:O	1:B:404:ASN:HB2	2.16	0.45
1:C:388:ALA:O	1:C:393:MET:HG2	2.16	0.45
1:D:149:ILE:HD12	1:D:171:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LEU:HD22	1:A:145:LEU:HG	1.98	0.45
1:D:243:GLU:O	1:D:247:ILE:HG12	2.16	0.45
1:E:205:THR:CG2	1:E:454:MET:HG3	2.46	0.45
1:A:166:VAL:HG13	1:A:168:ILE:HD12	1.98	0.45
1:E:171:LEU:HB3	2:E:605:MYA:H3A	1.99	0.45
1:B:132:ASP:O	1:B:135:ILE:HD11	2.17	0.45
1:E:262:ARG:HH21	1:E:317:GLU:HB2	1.82	0.45
1:F:339:ASN:HD22	1:F:339:ASN:C	2.25	0.45
1:B:324:THR:HG23	1:B:356:ASP:OD1	2.16	0.45
1:E:56:GLU:HG2	1:E:429:ALA:HA	1.99	0.45
1:A:242:THR:HG22	1:A:244:GLU:N	2.31	0.45
1:B:98:LEU:HD22	1:B:145:LEU:HG	1.97	0.45
1:D:25:SER:HA	1:D:105:GLU:HB2	1.98	0.45
1:D:324:THR:HG22	1:D:325:ASP:OD2	2.16	0.45
1:A:280:GLN:C	1:A:282:ARG:H	2.25	0.45
1:C:25:SER:HB2	1:C:104:VAL:HA	1.99	0.45
1:C:165:SER:HB3	1:C:201:HIS:HB2	1.99	0.45
1:A:210:LEU:HB3	1:A:211:PRO:HD2	1.99	0.45
1:B:147:ALA:HA	1:B:172:CYS:O	2.17	0.44
1:C:156:LEU:HD11	1:C:203:LEU:HB2	1.98	0.44
1:D:18:GLN:NE2	1:D:421:ASN:HD21	2.15	0.44
1:C:324:THR:HG23	1:C:356:ASP:OD1	2.17	0.44
1:D:210:LEU:O	1:D:213:PRO:HD3	2.16	0.44
1:E:107:ARG:HD2	1:E:175:LYS:HZ3	1.83	0.44
1:A:278:ARG:HG3	1:A:278:ARG:HH11	1.82	0.44
1:B:437:ASN:HD21	1:B:445:LYS:HE3	1.81	0.44
1:B:339:ASN:ND2	1:B:342:TYR:H	2.13	0.44
1:F:127:PRO:HD3	1:F:296:HIS:CD2	2.53	0.44
1:F:363:ASP:HB2	1:F:366:ASP:HB2	2.00	0.44
1:D:191:THR:HA	2:D:604:MYA:HEMA	2.00	0.44
1:F:130:LYS:HG3	1:F:132:ASP:HB2	2.00	0.44
1:F:195:ASN:C	1:F:197:CYS:H	2.25	0.44
1:A:126:SER:O	1:A:129:TRP:HB3	2.17	0.44
1:B:361:PHE:HE2	1:B:368:LYS:HG3	1.81	0.44
1:B:47:LYS:HD2	1:B:212:ALA:CB	2.31	0.44
1:F:117:LYS:O	1:F:121:ASN:HB2	2.18	0.44
1:D:56:GLU:HG2	1:D:429:ALA:HA	2.00	0.44
1:A:404:ASN:HA	1:A:407:PHE:CE2	2.53	0.43
1:E:269:ILE:HD11	1:E:299:ILE:HD13	1.99	0.43
1:F:166:VAL:O	1:F:202:ALA:HA	2.18	0.43
1:C:59:ILE:H	1:C:426:ASN:ND2	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:PRO:O	1:A:426:ASN:HA	2.18	0.43
1:A:87:ASP:OD2	1:A:125:LYS:HE2	2.19	0.43
1:A:211:PRO:O	1:A:212:ALA:CB	2.67	0.43
1:B:187:ILE:HG23	2:B:602:MYA:H9M	2.01	0.43
1:D:390:ASN:C	1:D:392:ASN:H	2.25	0.43
1:E:346:GLY:HA3	1:E:393:MET:HA	2.01	0.43
1:A:53:VAL:HG13	1:A:430:LYS:HG2	2.00	0.43
1:B:6:LYS:O	1:B:10:LEU:HD12	2.19	0.43
1:D:76:LEU:O	1:D:77:SER:C	2.61	0.43
1:D:405:THR:HG21	1:D:443:ASP:C	2.43	0.43
2:B:602:MYA:H12A	2:B:602:MYA:N7A	2.34	0.43
1:E:202:ALA:HB3	1:E:425:PHE:HB3	2.01	0.43
1:B:135:ILE:HD11	1:B:193:ARG:HD2	2.01	0.43
1:B:382:TYR:O	1:B:386:ILE:HD12	2.18	0.43
1:C:181:ARG:NH2	2:C:603:MYA:O7A	2.52	0.43
1:C:192:ARG:HG2	1:C:192:ARG:HH11	1.84	0.43
1:C:232:VAL:O	1:C:232:VAL:CG1	2.67	0.43
1:D:86:VAL:HG13	1:D:92:LEU:HD13	2.01	0.43
1:A:405:THR:HG21	1:A:444:ILE:HA	1.97	0.43
1:C:128:GLY:O	1:C:153:PRO:HG3	2.19	0.43
1:D:98:LEU:HD22	1:D:145:LEU:HG	2.01	0.43
1:A:166:VAL:O	1:A:202:ALA:HA	2.19	0.43
1:A:408:LEU:O	1:A:413:PHE:HB2	2.18	0.43
1:C:168:ILE:HG22	2:C:603:MYA:H3MA	2.00	0.43
1:D:229:LEU:HD21	1:D:395:VAL:HB	2.01	0.43
1:E:149:ILE:HD11	1:E:168:ILE:CG2	2.48	0.43
1:E:269:ILE:O	1:E:270:ASP:C	2.61	0.43
1:A:127:PRO:HG2	1:A:293:GLU:CA	2.49	0.42
1:E:111:PHE:HA	1:E:335:THR:O	2.19	0.42
1:E:345:LEU:HD12	1:E:394:ASP:OD1	2.19	0.42
1:E:71:LYS:O	1:E:71:LYS:HG2	2.18	0.42
1:F:53:VAL:HG21	1:F:428:ARG:HB3	2.00	0.42
1:F:135:ILE:HD11	1:F:190:ILE:HD13	2.01	0.42
1:F:174:HIS:HB3	1:F:177:LEU:HD21	2.01	0.42
1:E:20:ASN:ND2	1:E:417:ASP:O	2.52	0.42
1:A:373:LEU:HD22	1:A:377:LEU:HG	2.01	0.42
1:A:406:LEU:HG	1:A:447:ARG:HD2	2.00	0.42
1:B:405:THR:HG21	1:B:447:ARG:HA	2.02	0.42
1:D:357:ALA:HB2	1:D:376:ARG:HG2	2.01	0.42
1:D:426:ASN:O	1:D:426:ASN:CG	2.62	0.42
1:A:180:LYS:HA	1:A:180:LYS:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:LEU:HD22	1:D:377:LEU:HG	2.00	0.42
1:F:40:PHE:HE1	1:F:188:LYS:HE3	1.84	0.42
1:F:286:ILE:HG22	1:F:451:GLY:HA3	2.02	0.42
1:A:278:ARG:HD2	1:A:359:PHE:CZ	2.55	0.42
1:E:68:ILE:HD11	1:E:200:TRP:HH2	1.78	0.42
1:E:205:THR:O	1:E:206:ALA:HB2	2.20	0.42
1:A:266:LYS:HD2	1:A:269:ILE:HD12	2.02	0.42
1:F:84:ILE:HG12	1:F:95:VAL:CG2	2.50	0.42
1:F:133:TRP:HH2	1:F:199:ILE:HD12	1.85	0.42
1:B:40:PHE:CD1	1:B:184:PRO:HB3	2.55	0.41
1:A:45:PRO:HB3	1:A:426:ASN:HD22	1.85	0.41
1:A:149:ILE:HD12	1:A:171:LEU:HD13	2.01	0.41
1:E:177:LEU:O	1:E:180:LYS:HG2	2.21	0.41
1:A:44:GLN:HA	1:A:45:PRO:HD3	1.87	0.41
1:C:64:THR:HG23	1:C:66:GLU:HB3	2.01	0.41
2:C:603:MYA:H6MA	2:C:603:MYA:H2AA	2.02	0.41
1:A:159:ARG:HG3	1:A:284:GLU:HB3	2.02	0.41
1:B:71:LYS:O	1:B:71:LYS:HG2	2.20	0.41
1:C:44:GLN:HA	1:C:45:PRO:HD3	1.83	0.41
1:D:298:PHE:HA	1:D:311:ILE:HD12	2.02	0.41
1:F:277:LYS:NZ	1:F:289:PHE:H	2.18	0.41
1:B:142:THR:O	1:B:143:GLN:HB2	2.21	0.41
1:D:190:ILE:O	1:D:194:VAL:HG23	2.20	0.41
1:B:174:HIS:CD2	1:B:176:GLN:HB2	2.55	0.41
1:B:337:LEU:O	1:B:339:ASN:N	2.45	0.41
1:F:98:LEU:HD22	1:F:145:LEU:HG	2.03	0.41
1:B:293:GLU:O	1:B:297:ASN:HB2	2.21	0.41
1:D:212:ALA:H	1:D:213:PRO:HD3	1.85	0.41
1:B:262:ARG:HH21	1:B:317:GLU:HB2	1.85	0.41
1:C:221:HIS:ND1	1:C:397:ASN:ND2	2.68	0.41
1:C:229:LEU:HB3	1:C:235:THR:HG22	2.03	0.41
1:C:286:ILE:HG22	1:C:451:GLY:HA3	2.03	0.41
1:E:230:TYR:C	1:E:232:VAL:H	2.29	0.41
1:F:318:GLN:HB3	1:F:319:PRO:HD2	2.03	0.41
1:E:73:LEU:HA	1:E:74:PRO:HD3	1.89	0.41
1:F:210:LEU:HB3	1:F:211:PRO:HD2	2.03	0.41
1:B:232:VAL:O	1:B:232:VAL:CG1	2.68	0.40
1:B:339:ASN:HD22	1:B:341:LYS:N	2.16	0.40
2:B:602:MYA:O5	2:B:602:MYA:N8	2.53	0.40
1:D:232:VAL:O	1:D:232:VAL:HG12	2.20	0.40
1:D:399:LEU:C	1:D:401:SER:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:ALA:CB	2:F:606:MYA:HDMA	2.45	0.40
1:B:68:ILE:HG13	1:B:195:ASN:HB3	2.03	0.40
1:C:403:ASP:OD2	1:C:447:ARG:HD2	2.20	0.40
1:D:278:ARG:HD2	1:D:359:PHE:CZ	2.55	0.40
1:E:149:ILE:HD12	1:E:190:ILE:HG21	2.04	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	438/455 (96%)	400 (91%)	31 (7%)	7 (2%)	7	27
1	B	439/455 (96%)	410 (93%)	24 (6%)	5 (1%)	11	36
1	C	442/455 (97%)	390 (88%)	47 (11%)	5 (1%)	11	36
1	D	439/455 (96%)	399 (91%)	33 (8%)	7 (2%)	7	27
1	E	439/455 (96%)	407 (93%)	29 (7%)	3 (1%)	18	48
1	F	434/455 (95%)	387 (89%)	42 (10%)	5 (1%)	10	34
All	All	2631/2730 (96%)	2393 (91%)	206 (8%)	32 (1%)	10	34

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	ALA
1	C	212	ALA
1	D	77	SER
1	D	212	ALA
1	F	212	ALA
1	A	78	SER
1	A	281	SER

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Mol	Chain	Res	Type
1	A	400	THR
1	B	78	SER
1	C	21	ASN
1	C	78	SER
1	E	78	SER
1	E	338	ASN
1	F	196	LYS
1	A	22	ASP
1	C	192	ARG
1	D	303	SER
1	B	337	LEU
1	B	338	ASN
1	D	22	ASP
1	D	337	LEU
1	E	211	PRO
1	B	211	PRO
1	F	78	SER
1	F	338	ASN
1	D	211	PRO
1	C	65	PRO
1	D	438	PRO
1	A	213	PRO
1	A	438	PRO
1	B	269	ILE
1	F	62	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	400/413 (97%)	365 (91%)	35 (9%)	9	29
1	B	401/413 (97%)	361 (90%)	40 (10%)	7	24
1	C	404/413 (98%)	371 (92%)	33 (8%)	10	32
1	D	401/413 (97%)	368 (92%)	33 (8%)	10	32
1	E	401/413 (97%)	364 (91%)	37 (9%)	8	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	396/413 (96%)	368 (93%)	28 (7%)	13	40
All	All	2403/2478 (97%)	2197 (91%)	206 (9%)	10	30

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	21	ASN
1	A	53	VAL
1	A	68	ILE
1	A	70	ASP
1	A	84	ILE
1	A	99	LEU
1	A	101	GLU
1	A	104	VAL
1	A	112	ARG
1	A	125	LYS
1	A	126	SER
1	A	165	SER
1	A	166	VAL
1	A	177	LEU
1	A	190	ILE
1	A	196	LYS
1	A	198	ASP
1	A	242	THR
1	A	252	LEU
1	A	278	ARG
1	A	306	LEU
1	A	311	ILE
1	A	315	VAL
1	A	332	LEU
1	A	339	ASN
1	A	344	ASP
1	A	347	ILE
1	A	373	LEU
1	A	386	ILE
1	A	393	MET
1	A	420	LEU
1	A	444	ILE
1	B	10	LEU

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Mol	Chain	Res	Type
1	B	37	ASP
1	B	47	LYS
1	B	53	VAL
1	B	66	GLU
1	B	73	LEU
1	B	77	SER
1	B	88	ASN
1	B	99	LEU
1	B	103	TYR
1	B	105	GLU
1	B	125	LYS
1	B	131	LYS
1	B	135	ILE
1	B	166	VAL
1	B	168	ILE
1	B	176	GLN
1	B	208	ILE
1	B	242	THR
1	B	261	LEU
1	B	271	GLN
1	B	278	ARG
1	B	295	GLU
1	B	297	ASN
1	B	299	ILE
1	B	306	LEU
1	B	332	LEU
1	B	340	THR
1	B	355	THR
1	B	362	LYS
1	B	371	LYS
1	B	373	LEU
1	B	386	ILE
1	B	399	LEU
1	B	405	THR
1	B	410	ASP
1	B	420	LEU
1	B	444	ILE
1	B	445	LYS
1	B	452	VAL
1	C	6	LYS
1	C	13	LEU
1	C	61	LYS

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Mol	Chain	Res	Type
1	C	99	LEU
1	C	121	ASN
1	C	125	LYS
1	C	135	ILE
1	C	155	THR
1	C	168	ILE
1	C	169	ASN
1	C	199	ILE
1	C	201	HIS
1	C	252	LEU
1	C	261	LEU
1	C	278	ARG
1	C	311	ILE
1	C	315	VAL
1	C	325	ASP
1	C	332	LEU
1	C	338	ASN
1	C	344	ASP
1	C	362	LYS
1	C	371	LYS
1	C	373	LEU
1	C	375	THR
1	C	386	ILE
1	C	393	MET
1	C	405	THR
1	C	410	ASP
1	C	420	LEU
1	C	444	ILE
1	C	445	LYS
1	C	452	VAL
1	D	13	LEU
1	D	19	LEU
1	D	27	PHE
1	D	53	VAL
1	D	68	ILE
1	D	73	LEU
1	D	76	LEU
1	D	125	LYS
1	D	130	LYS
1	D	154	VAL
1	D	162	GLN
1	D	166	VAL

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Mol	Chain	Res	Type
1	D	177	LEU
1	D	182	LEU
1	D	242	THR
1	D	252	LEU
1	D	263	LYS
1	D	278	ARG
1	D	311	ILE
1	D	315	VAL
1	D	332	LEU
1	D	343	LYS
1	D	344	ASP
1	D	362	LYS
1	D	368	LYS
1	D	371	LYS
1	D	373	LEU
1	D	399	LEU
1	D	405	THR
1	D	420	LEU
1	D	430	LYS
1	D	445	LYS
1	D	446	ARG
1	E	10	LEU
1	E	17	LEU
1	E	25	SER
1	E	28	THR
1	E	53	VAL
1	E	66	GLU
1	E	73	LEU
1	E	88	ASN
1	E	103	TYR
1	E	104	VAL
1	E	105	GLU
1	E	125	LYS
1	E	149	ILE
1	E	152	ILE
1	E	166	VAL
1	E	177	LEU
1	E	208	ILE
1	E	242	THR
1	E	247	ILE
1	E	252	LEU
1	E	271	GLN

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Mol	Chain	Res	Type
1	E	278	ARG
1	E	295	GLU
1	E	297	ASN
1	E	306	LEU
1	E	323	ILE
1	E	332	LEU
1	E	340	THR
1	E	362	LYS
1	E	371	LYS
1	E	373	LEU
1	E	399	LEU
1	E	405	THR
1	E	410	ASP
1	E	420	LEU
1	E	445	LYS
1	E	452	VAL
1	F	99	LEU
1	F	107	ARG
1	F	125	LYS
1	F	149	ILE
1	F	168	ILE
1	F	177	LEU
1	F	185	VAL
1	F	186	LEU
1	F	190	ILE
1	F	208	ILE
1	F	232	VAL
1	F	261	LEU
1	F	263	LYS
1	F	267	GLU
1	F	286	ILE
1	F	295	GLU
1	F	302	GLU
1	F	311	ILE
1	F	315	VAL
1	F	332	LEU
1	F	339	ASN
1	F	373	LEU
1	F	386	ILE
1	F	393	MET
1	F	399	LEU
1	F	420	LEU

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Mol	Chain	Res	Type
1	F	452	VAL
1	F	454	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	88	ASN
1	A	174	HIS
1	A	176	GLN
1	A	297	ASN
1	A	339	ASN
1	A	397	ASN
1	A	404	ASN
1	A	421	ASN
1	A	426	ASN
1	A	437	ASN
1	B	20	ASN
1	B	21	ASN
1	B	88	ASN
1	B	114	ASN
1	B	174	HIS
1	B	195	ASN
1	B	339	ASN
1	B	397	ASN
1	B	404	ASN
1	B	421	ASN
1	B	426	ASN
1	B	437	ASN
1	C	29	GLN
1	C	44	GLN
1	C	114	ASN
1	C	174	HIS
1	C	195	ASN
1	C	201	HIS
1	C	339	ASN
1	C	397	ASN
1	C	404	ASN
1	C	421	ASN
1	C	426	ASN
1	D	88	ASN
1	D	114	ASN

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Mol	Chain	Res	Type
1	D	143	GLN
1	D	162	GLN
1	D	174	HIS
1	D	176	GLN
1	D	339	ASN
1	D	397	ASN
1	D	404	ASN
1	D	421	ASN
1	D	426	ASN
1	D	437	ASN
1	E	20	ASN
1	E	88	ASN
1	E	174	HIS
1	E	176	GLN
1	E	195	ASN
1	E	297	ASN
1	E	339	ASN
1	E	397	ASN
1	E	404	ASN
1	E	421	ASN
1	E	426	ASN
1	E	437	ASN
1	F	44	GLN
1	F	88	ASN
1	F	121	ASN
1	F	162	GLN
1	F	174	HIS
1	F	195	ASN
1	F	201	HIS
1	F	241	HIS
1	F	296	HIS
1	F	339	ASN
1	F	390	ASN
1	F	397	ASN
1	F	404	ASN
1	F	421	ASN
1	F	426	ASN
1	F	437	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	1.42	11 (17%)	85,91,91	1.51	15 (17%)
2	MYA	A	601	-	63,65,65	1.41	10 (15%)	85,91,91	1.55	13 (15%)
2	MYA	C	603	-	63,65,65	1.48	8 (12%)	85,91,91	1.53	12 (14%)
2	MYA	D	604	-	63,65,65	1.40	10 (15%)	85,91,91	1.55	12 (14%)
2	MYA	F	606	-	63,65,65	1.36	9 (14%)	85,91,91	1.54	13 (15%)
2	MYA	B	602	-	63,65,65	1.35	10 (15%)	85,91,91	1.64	15 (17%)

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	15/64/80/80	0/3/3/3
2	MYA	A	601	-	1/1/12/14	21/64/80/80	0/3/3/3
2	MYA	C	603	-	1/1/12/14	14/64/80/80	0/3/3/3
2	MYA	D	604	-	1/1/12/14	24/64/80/80	0/3/3/3
2	MYA	F	606	-	1/1/12/14	22/64/80/80	0/3/3/3
2	MYA	B	602	-	1/1/12/14	27/64/80/80	0/3/3/3

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	603	MYA	P1A-O3A	4.84	1.64	1.59
2	E	605	MYA	P1A-O3A	4.16	1.64	1.59
2	A	601	MYA	P1A-O3A	4.15	1.64	1.59
2	F	606	MYA	P2A-O4A	4.05	1.64	1.50
2	D	604	MYA	P1A-O3A	3.92	1.63	1.59
2	C	603	MYA	P2A-O4A	3.91	1.64	1.50
2	B	602	MYA	P3X-O9A	3.80	1.62	1.50
2	C	603	MYA	P3X-O9A	3.77	1.62	1.50
2	B	602	MYA	P2A-O4A	3.77	1.63	1.50
2	D	604	MYA	P3X-O9A	3.75	1.62	1.50
2	D	604	MYA	P2A-O4A	3.75	1.63	1.50
2	E	605	MYA	P3X-O9A	3.74	1.62	1.50
2	F	606	MYA	P3X-O9A	3.72	1.62	1.50
2	E	605	MYA	P2A-O4A	3.70	1.63	1.50
2	A	601	MYA	P3X-O9A	3.69	1.61	1.50
2	A	601	MYA	P2A-O4A	3.63	1.63	1.50
2	B	602	MYA	P1A-O3A	3.47	1.63	1.59
2	C	603	MYA	P1A-O2A	3.46	1.62	1.50
2	E	605	MYA	P1A-O2A	3.39	1.62	1.50
2	C	603	MYA	P2A-O3A	3.37	1.63	1.59
2	E	605	MYA	C5A-N7A	-3.36	1.33	1.39
2	D	604	MYA	C5A-N7A	-3.35	1.33	1.39
2	A	601	MYA	C5A-N7A	-3.27	1.33	1.39
2	D	604	MYA	P1A-O2A	3.23	1.62	1.50
2	C	603	MYA	C5A-N7A	-3.23	1.33	1.39
2	F	606	MYA	C5A-N7A	-3.20	1.33	1.39
2	F	606	MYA	P1A-O3A	3.19	1.62	1.59
2	A	601	MYA	P1A-O2A	3.18	1.61	1.50
2	F	606	MYA	P1A-O2A	3.18	1.61	1.50
2	B	602	MYA	C5A-N7A	-3.15	1.33	1.39
2	A	601	MYA	P2A-O3A	3.14	1.62	1.59
2	B	602	MYA	P1A-O2A	3.10	1.61	1.50
2	C	603	MYA	C3M-C2M	2.93	1.53	1.50
2	E	605	MYA	P2A-O3A	2.78	1.62	1.59
2	E	605	MYA	C3M-C2M	2.77	1.53	1.50
2	E	605	MYA	P3X-O3X	2.71	1.64	1.59
2	B	602	MYA	C3M-C2M	2.68	1.53	1.50
2	F	606	MYA	C3M-C2M	2.58	1.53	1.50
2	A	601	MYA	C3M-C2M	2.47	1.53	1.50
2	D	604	MYA	P2A-O3A	2.41	1.62	1.59
2	D	604	MYA	C3M-C2M	2.35	1.53	1.50
2	E	605	MYA	C4A-N9A	-2.26	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	604	MYA	P3X-O8A	2.24	1.63	1.54
2	D	604	MYA	C8A-N9A	-2.22	1.33	1.37
2	A	601	MYA	P3X-O8A	2.19	1.62	1.54
2	A	601	MYA	C4A-N9A	-2.17	1.33	1.37
2	D	604	MYA	C4A-N9A	-2.17	1.33	1.37
2	B	602	MYA	C4A-N9A	-2.14	1.33	1.37
2	E	605	MYA	P3X-O8A	2.12	1.62	1.54
2	B	602	MYA	P3X-O8A	2.11	1.62	1.54
2	F	606	MYA	P2A-O3A	2.10	1.61	1.59
2	F	606	MYA	P3X-O3X	2.09	1.63	1.59
2	A	601	MYA	C8A-N9A	-2.08	1.34	1.37
2	B	602	MYA	C8A-N9A	-2.06	1.34	1.37
2	E	605	MYA	C8A-N9A	-2.04	1.34	1.37
2	F	606	MYA	P3X-O8A	2.03	1.62	1.54
2	C	603	MYA	C8A-N9A	-2.01	1.34	1.37
2	B	602	MYA	P3X-O3X	2.01	1.63	1.59

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	606	MYA	C5A-C4A-N3A	-5.61	118.99	126.72
2	C	603	MYA	C5A-C4A-N3A	-5.56	119.06	126.72
2	D	604	MYA	C5A-C4A-N3A	-5.27	119.46	126.72
2	A	601	MYA	C3M-C2M-S1	5.23	119.64	113.40
2	B	602	MYA	C5A-C4A-N3A	-5.23	119.52	126.72
2	A	601	MYA	C5A-C4A-N3A	-5.22	119.52	126.72
2	E	605	MYA	C5A-C4A-N3A	-5.21	119.54	126.72
2	B	602	MYA	C3M-C2M-S1	5.18	119.58	113.40
2	D	604	MYA	C3M-C2M-S1	4.98	119.34	113.40
2	F	606	MYA	C3M-C2M-S1	4.90	119.24	113.40
2	F	606	MYA	N3A-C2A-N1A	-4.63	121.57	128.58
2	B	602	MYA	N3A-C2A-N1A	-4.61	121.60	128.58
2	A	601	MYA	N3A-C2A-N1A	-4.61	121.60	128.58
2	D	604	MYA	N3A-C2A-N1A	-4.60	121.61	128.58
2	C	603	MYA	C3M-C2M-S1	4.53	118.80	113.40
2	C	603	MYA	N3A-C2A-N1A	-4.51	121.75	128.58
2	E	605	MYA	N3A-C2A-N1A	-4.51	121.76	128.58
2	F	606	MYA	N3A-C4A-N9A	3.89	133.79	127.17
2	C	603	MYA	N3A-C4A-N9A	3.84	133.69	127.17
2	F	606	MYA	C2A-N3A-C4A	3.69	120.84	111.83
2	A	601	MYA	N3A-C4A-N9A	3.61	133.30	127.17
2	E	605	MYA	C3M-C2M-S1	3.59	117.69	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	603	MYA	C2A-N3A-C4A	3.59	120.60	111.83
2	D	604	MYA	N3A-C4A-N9A	3.53	133.17	127.17
2	A	601	MYA	C2A-N3A-C4A	3.53	120.45	111.83
2	B	602	MYA	C2A-N3A-C4A	3.53	120.45	111.83
2	D	604	MYA	C2A-N3A-C4A	3.51	120.41	111.83
2	B	602	MYA	N3A-C4A-N9A	3.48	133.09	127.17
2	E	605	MYA	C2A-N3A-C4A	3.48	120.33	111.83
2	D	604	MYA	O2M-C2M-C3M	-3.35	120.11	123.98
2	E	605	MYA	N3A-C4A-N9A	3.29	132.76	127.17
2	A	601	MYA	O2M-C2M-C3M	-3.28	120.19	123.98
2	B	602	MYA	O2M-C2M-C3M	-3.27	120.21	123.98
2	B	602	MYA	N9A-C8A-N7A	-3.22	109.37	113.94
2	F	606	MYA	O2M-C2M-C3M	-3.21	120.28	123.98
2	A	601	MYA	N9A-C8A-N7A	-3.21	109.39	113.94
2	B	602	MYA	C10-C9-N8	-3.18	110.45	116.48
2	D	604	MYA	N9A-C8A-N7A	-3.16	109.45	113.94
2	B	602	MYA	C6-C7-N8	-3.10	105.40	112.00
2	C	603	MYA	O2M-C2M-C3M	-3.03	120.49	123.98
2	E	605	MYA	N9A-C8A-N7A	-2.94	109.76	113.94
2	F	606	MYA	N9A-C8A-N7A	-2.93	109.77	113.94
2	D	604	MYA	C5A-N7A-C8A	2.89	107.99	103.45
2	B	602	MYA	C5A-N7A-C8A	2.87	107.96	103.45
2	D	604	MYA	C4A-C5A-N7A	-2.84	107.34	110.58
2	C	603	MYA	N9A-C8A-N7A	-2.84	109.91	113.94
2	E	605	MYA	C4A-C5A-N7A	-2.83	107.34	110.58
2	B	602	MYA	C4A-C5A-N7A	-2.83	107.35	110.58
2	A	601	MYA	C5A-N7A-C8A	2.80	107.85	103.45
2	F	606	MYA	C5A-N7A-C8A	2.76	107.79	103.45
2	C	603	MYA	C5A-N7A-C8A	2.73	107.75	103.45
2	E	605	MYA	C5A-N7A-C8A	2.73	107.75	103.45
2	C	603	MYA	C4A-C5A-N7A	-2.61	107.60	110.58
2	A	601	MYA	C4A-C5A-N7A	-2.61	107.60	110.58
2	F	606	MYA	C4A-C5A-N7A	-2.60	107.61	110.58
2	E	605	MYA	C6-C7-N8	-2.59	106.48	112.00
2	B	602	MYA	C14-C11-C10	2.49	113.02	108.77
2	E	605	MYA	C14-C11-C10	2.42	112.89	108.77
2	C	603	MYA	O1A-P1A-O3A	2.37	113.69	107.27
2	E	605	MYA	C10-C9-N8	-2.34	112.05	116.48
2	A	601	MYA	O1A-P1A-O3A	2.32	113.55	107.27
2	B	602	MYA	O1A-P1A-O3A	2.31	113.51	107.27
2	A	601	MYA	C14-C11-C10	2.29	112.68	108.77
2	E	605	MYA	C2-C3-N4	-2.27	107.68	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	603	MYA	C14-C11-C10	2.26	112.62	108.77
2	F	606	MYA	O7A-P3X-O3X	2.25	114.60	105.85
2	C	603	MYA	O7A-P3X-O3X	2.23	114.56	105.85
2	E	605	MYA	O7A-P3X-O3X	2.23	114.53	105.85
2	B	602	MYA	O7A-P3X-O3X	2.16	114.25	105.85
2	A	601	MYA	C4A-N9A-C8A	2.14	107.99	105.74
2	E	605	MYA	O2M-C2M-C3M	-2.13	121.52	123.98
2	D	604	MYA	O1A-P1A-O3A	2.12	112.99	107.27
2	B	602	MYA	C4A-N9A-C8A	2.08	107.92	105.74
2	F	606	MYA	C14-C11-C10	2.08	112.31	108.77
2	F	606	MYA	O1A-P1A-O3A	2.06	112.85	107.27
2	A	601	MYA	O7A-P3X-O3X	2.04	113.78	105.85
2	F	606	MYA	O3A-P1A-O2A	-2.03	104.59	110.70
2	D	604	MYA	C4A-N9A-C8A	2.02	107.86	105.74
2	D	604	MYA	O7A-P3X-O3X	2.02	113.72	105.85
2	E	605	MYA	O1A-P1A-O3A	2.00	112.69	107.27

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 (123) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	MYA	C5-C6-C7-N8
2	A	601	MYA	C5X-O5X-P1A-O2A
2	A	601	MYA	C12-O6A-P2A-O3A
2	A	601	MYA	C12-O6A-P2A-O4A
2	A	601	MYA	C2M-C3M-C4M-C5M
2	B	602	MYA	C5-C6-C7-N8
2	B	602	MYA	C10-C11-C12-O6A
2	B	602	MYA	C13-C11-C12-O6A
2	B	602	MYA	C14-C11-C12-O6A
2	B	602	MYA	C5X-O5X-P1A-O1A
2	B	602	MYA	C5X-O5X-P1A-O2A
2	B	602	MYA	C12-O6A-P2A-O3A

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Mol	Chain	Res	Type	Atoms
2	B	602	MYA	C12-O6A-P2A-O4A
2	B	602	MYA	C12-O6A-P2A-O5A
2	B	602	MYA	C2M-C3M-C4M-C5M
2	D	604	MYA	C5X-O5X-P1A-O2A
2	D	604	MYA	P1A-O3A-P2A-O6A
2	D	604	MYA	C12-O6A-P2A-O3A
2	D	604	MYA	C12-O6A-P2A-O4A
2	E	605	MYA	C10-C11-C12-O6A
2	E	605	MYA	C13-C11-C12-O6A
2	E	605	MYA	C14-C11-C12-O6A
2	F	606	MYA	C5-C6-C7-N8
2	F	606	MYA	C10-C11-C12-O6A
2	F	606	MYA	C13-C11-C12-O6A
2	F	606	MYA	C14-C11-C12-O6A
2	F	606	MYA	C5X-O5X-P1A-O2A
2	F	606	MYA	C5X-O5X-P1A-O3A
2	F	606	MYA	C12-O6A-P2A-O3A
2	F	606	MYA	C12-O6A-P2A-O4A
2	F	606	MYA	C2M-C3M-C4M-C5M
2	B	602	MYA	C3X-C4X-C5X-O5X
2	F	606	MYA	C6M-C7M-C8M-C9M
2	E	605	MYA	C7M-C8M-C9M-CAM
2	E	605	MYA	CBM-CCM-CDM-CEM
2	E	605	MYA	C9M-CAM-CBM-CCM
2	A	601	MYA	C7M-C8M-C9M-CAM
2	D	604	MYA	C8M-C9M-CAM-CBM
2	B	602	MYA	C5M-C6M-C7M-C8M
2	D	604	MYA	C5M-C6M-C7M-C8M
2	C	603	MYA	C4M-C5M-C6M-C7M
2	F	606	MYA	C5M-C6M-C7M-C8M
2	B	602	MYA	CAM-CBM-CCM-CDM
2	A	601	MYA	C4M-C5M-C6M-C7M
2	B	602	MYA	C3M-C4M-C5M-C6M
2	C	603	MYA	C5-C6-C7-N8
2	E	605	MYA	C5-C6-C7-N8
2	F	606	MYA	C8M-C9M-CAM-CBM
2	B	602	MYA	O4X-C4X-C5X-O5X
2	D	604	MYA	CAM-CBM-CCM-CDM
2	E	605	MYA	C3M-C4M-C5M-C6M
2	F	606	MYA	C3M-C4M-C5M-C6M
2	C	603	MYA	C8M-C9M-CAM-CBM
2	A	601	MYA	O10-C10-C9-O9

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Mol	Chain	Res	Type	Atoms
2	D	604	MYA	O10-C10-C9-O9
2	F	606	MYA	CAM-CBM-CCM-CDM
2	A	601	MYA	C3M-C4M-C5M-C6M
2	E	605	MYA	P1A-O3A-P2A-O4A
2	A	601	MYA	CCM-CDM-CEM-CFM
2	D	604	MYA	C3M-C4M-C5M-C6M
2	D	604	MYA	S1-C2-C3-N4
2	B	602	MYA	C11-C10-C9-N8
2	F	606	MYA	C9M-CAM-CBM-CCM
2	B	602	MYA	C7M-C8M-C9M-CAM
2	E	605	MYA	C4M-C5M-C6M-C7M
2	A	601	MYA	S1-C2M-C3M-C4M
2	A	601	MYA	O2M-C2M-C3M-C4M
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	S1-C2M-C3M-C4M
2	F	606	MYA	O2M-C2M-C3M-C4M
2	C	603	MYA	CAM-CBM-CCM-CDM
2	A	601	MYA	P1A-O3A-P2A-O6A
2	E	605	MYA	C2M-C3M-C4M-C5M
2	D	604	MYA	CBM-CCM-CDM-CEM
2	D	604	MYA	C7M-C8M-C9M-CAM
2	B	602	MYA	C8M-C9M-CAM-CBM
2	C	603	MYA	C6M-C7M-C8M-C9M
2	F	606	MYA	P2A-O3A-P1A-O1A
2	A	601	MYA	CBM-CCM-CDM-CEM
2	B	602	MYA	O10-C10-C9-O9
2	E	605	MYA	O10-C10-C9-O9
2	F	606	MYA	O10-C10-C9-O9
2	A	601	MYA	C14-C11-C12-O6A
2	D	604	MYA	C13-C11-C12-O6A
2	D	604	MYA	C14-C11-C12-O6A
2	E	605	MYA	C8M-C9M-CAM-CBM
2	A	601	MYA	C5X-O5X-P1A-O3A
2	A	601	MYA	C12-O6A-P2A-O5A
2	B	602	MYA	C5X-O5X-P1A-O3A
2	C	603	MYA	C5X-O5X-P1A-O2A
2	D	604	MYA	C12-O6A-P2A-O5A
2	F	606	MYA	C12-O6A-P2A-O5A
2	A	601	MYA	P2A-O3A-P1A-O1A

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Mol	Chain	Res	Type	Atoms
2	B	602	MYA	P2A-O3A-P1A-O1A
2	C	603	MYA	P2A-O3A-P1A-O1A
2	D	604	MYA	P2A-O3A-P1A-O1A
2	C	603	MYA	C2X-C1X-N9A-C8A
2	C	603	MYA	C7M-C8M-C9M-CAM
2	D	604	MYA	O2M-C2M-S1-C2
2	D	604	MYA	O5-C5-C6-C7
2	F	606	MYA	CBM-CCM-CDM-CEM
2	E	605	MYA	S1-C2-C3-N4
2	A	601	MYA	P2A-O3A-P1A-O2A
2	B	602	MYA	P2A-O3A-P1A-O2A
2	C	603	MYA	P2A-O3A-P1A-O2A
2	C	603	MYA	C5M-C6M-C7M-C8M
2	B	602	MYA	C11-C10-C9-O9
2	B	602	MYA	C11-C12-O6A-P2A
2	A	601	MYA	C13-C11-C12-O6A
2	C	603	MYA	C13-C11-C12-O6A
2	D	604	MYA	C9-C10-C11-C12
2	A	601	MYA	O10-C10-C9-N8
2	B	602	MYA	O10-C10-C9-N8
2	C	603	MYA	O10-C10-C9-N8
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	C	603	MYA	C3M-C4M-C5M-C6M
2	D	604	MYA	N4-C5-C6-C7
2	D	604	MYA	P2A-O3A-P1A-O2A

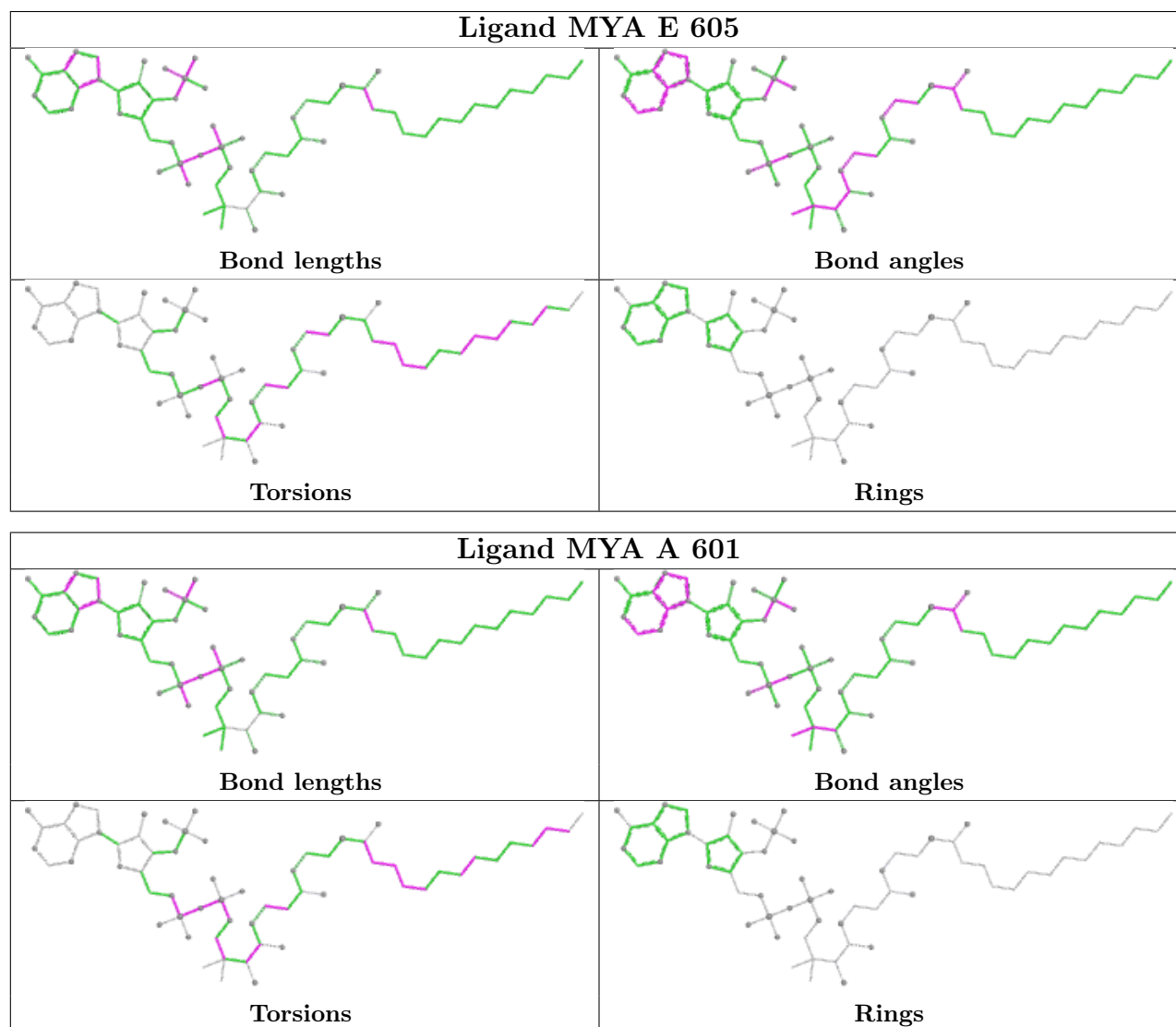
There are no ring outliers.

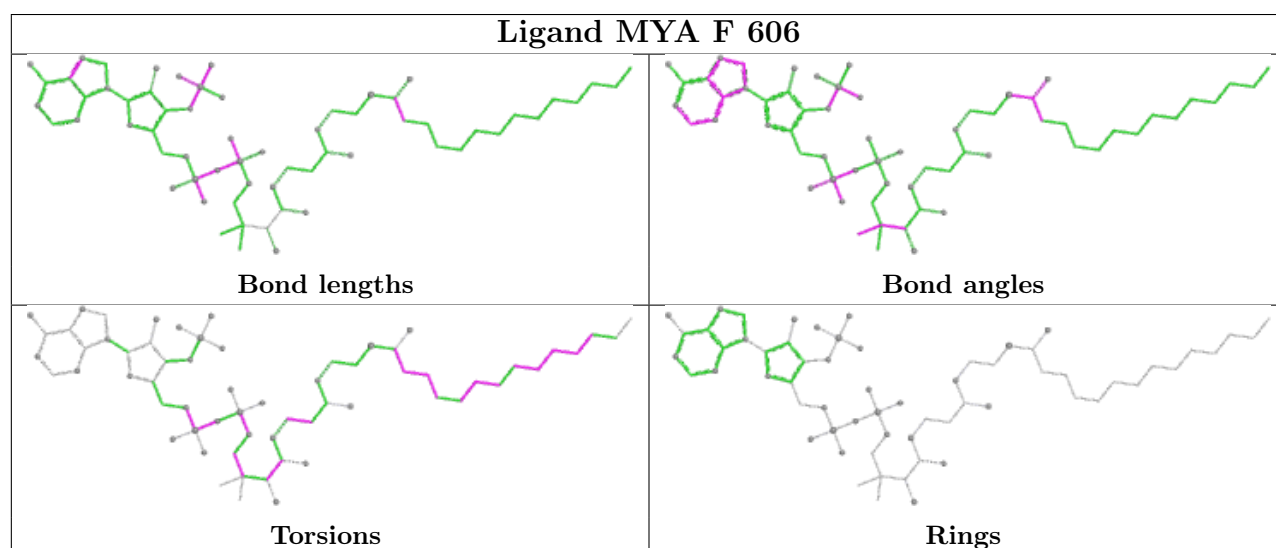
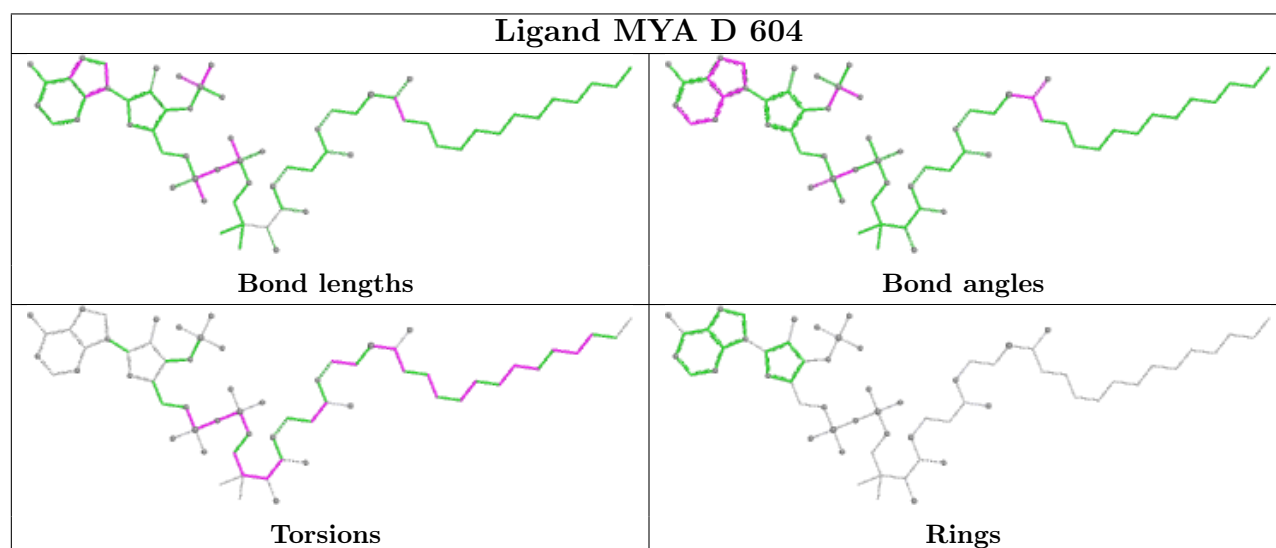
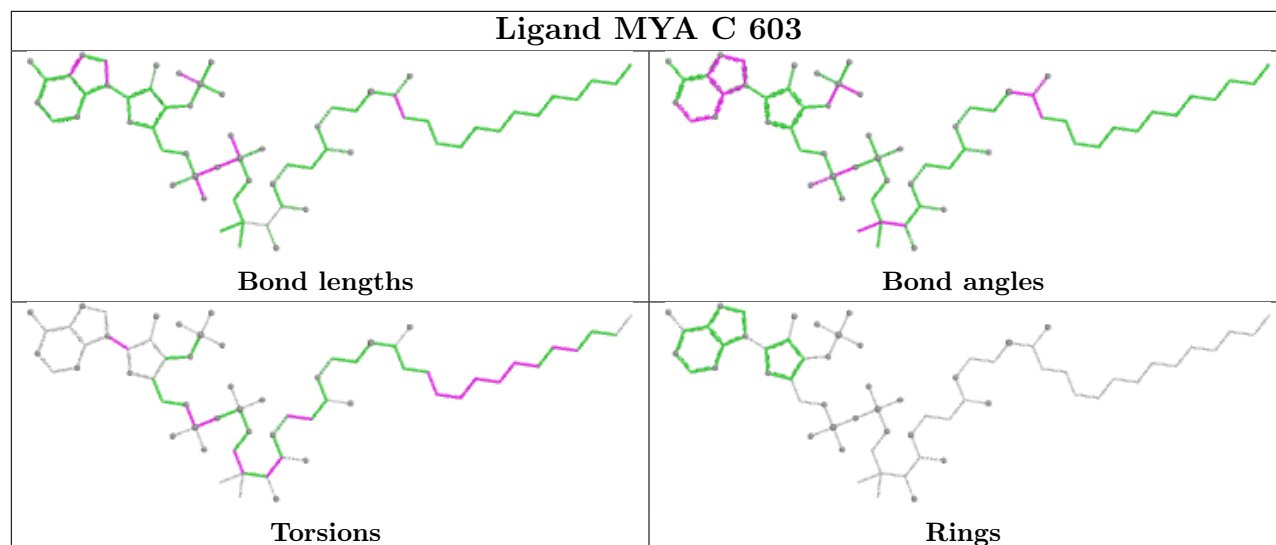
6 monomers are involved in 33 short contacts:

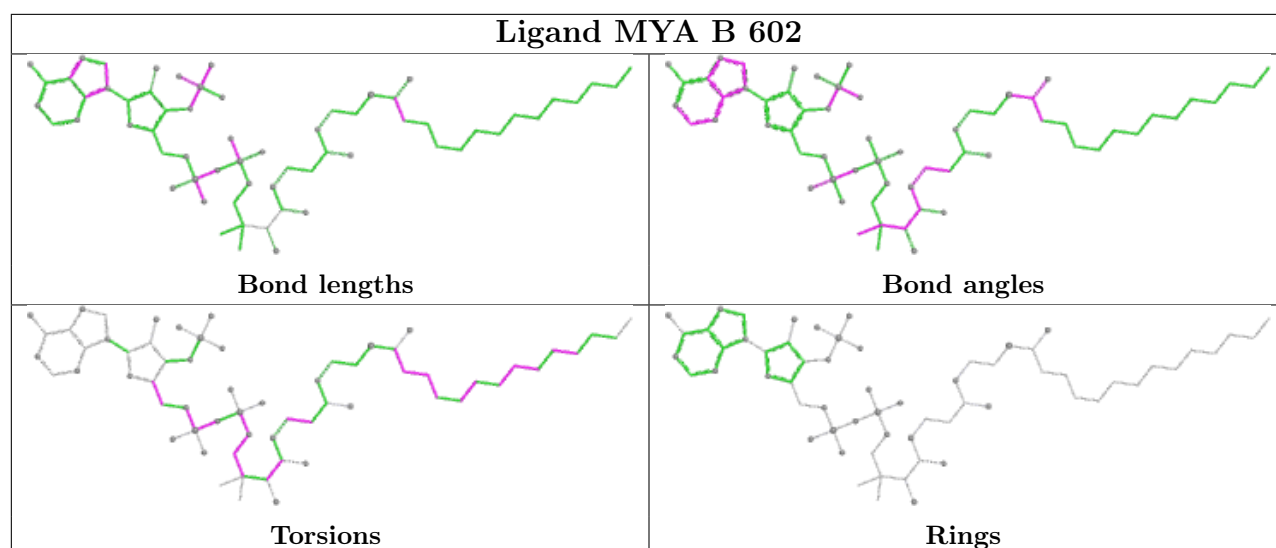
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	605	MYA	8	0
2	A	601	MYA	7	0
2	C	603	MYA	6	0
2	D	604	MYA	2	0
2	F	606	MYA	5	0
2	B	602	MYA	5	0

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

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	442/455 (97%)	0.07	8 (1%) 67 59	28, 45, 73, 95	0
1	B	443/455 (97%)	0.02	9 (2%) 65 56	29, 44, 71, 92	0
1	C	446/455 (98%)	0.38	16 (3%) 46 38	29, 55, 82, 102	0
1	D	443/455 (97%)	0.09	9 (2%) 65 56	29, 45, 69, 110	0
1	E	443/455 (97%)	-0.04	6 (1%) 73 65	26, 41, 67, 93	0
1	F	438/455 (96%)	0.37	11 (2%) 58 48	35, 60, 92, 119	0
All	All	2655/2730 (97%)	0.15	59 (2%) 62 53	26, 48, 80, 119	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	PHE	7.6
1	C	27	PHE	6.5
1	E	27	PHE	6.0
1	A	27	PHE	5.8
1	D	27	PHE	4.7
1	B	25	SER	4.6
1	E	24	THR	4.0
1	D	26	LYS	3.8
1	E	28	THR	3.7
1	B	24	THR	3.7
1	E	25	SER	3.7
1	F	24	THR	3.5
1	A	26	LYS	3.4
1	A	338	ASN	3.3
1	C	24	THR	3.2
1	C	69	SER	3.2
1	B	28	THR	3.2
1	A	25	SER	3.1
1	A	212	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	41	TRP	3.0
1	C	26	LYS	3.0
1	B	66	GLU	2.9
1	E	26	LYS	2.8
1	D	417	ASP	2.8
1	C	212	ALA	2.8
1	C	68	ILE	2.8
1	F	64	THR	2.7
1	B	26	LYS	2.7
1	F	69	SER	2.7
1	C	25	SER	2.5
1	D	36	LYS	2.5
1	D	24	THR	2.5
1	D	22	ASP	2.4
1	C	52	LYS	2.4
1	B	23	ASP	2.3
1	C	417	ASP	2.3
1	F	68	ILE	2.3
1	E	66	GLU	2.3
1	C	6	LYS	2.3
1	D	25	SER	2.3
1	A	130	LYS	2.3
1	D	5	ASP	2.2
1	F	23	ASP	2.2
1	C	28	THR	2.2
1	F	20	ASN	2.2
1	B	323	ILE	2.2
1	F	104	VAL	2.2
1	F	135	ILE	2.2
1	C	200	TRP	2.2
1	B	340	THR	2.1
1	C	104	VAL	2.1
1	F	49	PHE	2.1
1	C	23	ASP	2.1
1	F	65	PRO	2.0
1	C	30	GLU	2.0
1	F	73	LEU	2.0
1	A	68	ILE	2.0
1	A	23	ASP	2.0
1	D	54	VAL	2.0

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](#)

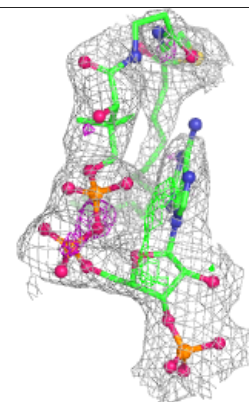
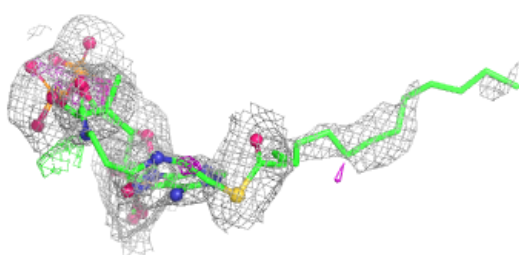
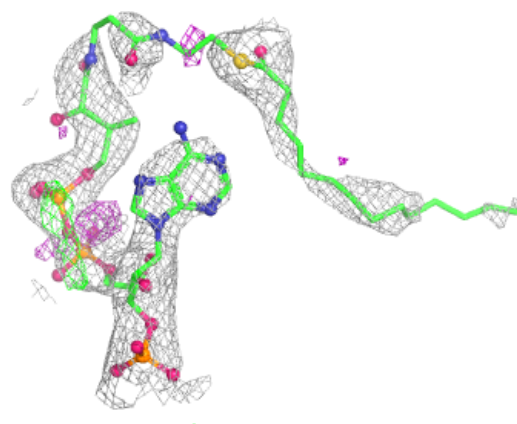
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	MYA	C	603	63/63	0.80	0.16	68,78,82,85	0
2	MYA	D	604	63/63	0.86	0.14	47,62,79,80	0
2	MYA	F	606	63/63	0.86	0.14	74,80,83,83	0
2	MYA	B	602	63/63	0.87	0.14	31,66,72,73	0
2	MYA	A	601	63/63	0.87	0.13	51,65,74,74	0
2	MYA	E	605	63/63	0.88	0.12	32,57,62,62	0

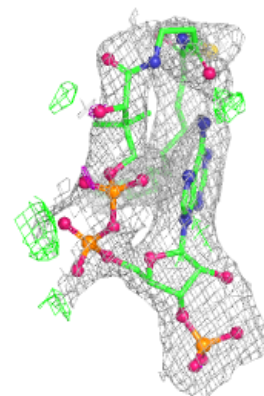
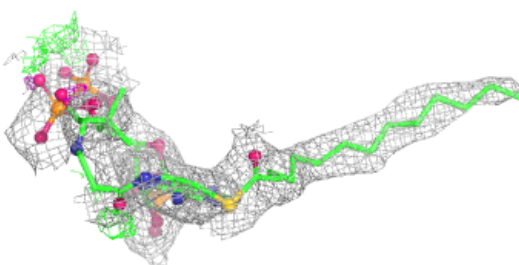
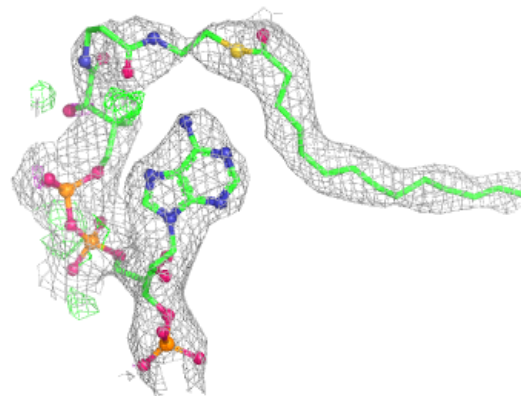
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

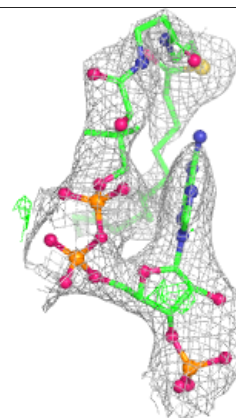
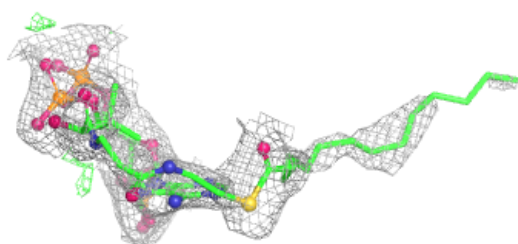
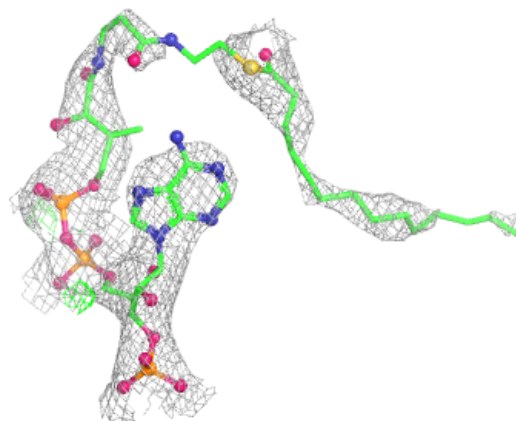
**Electron density around MYA D 604:**

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



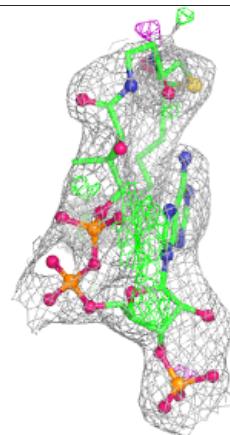
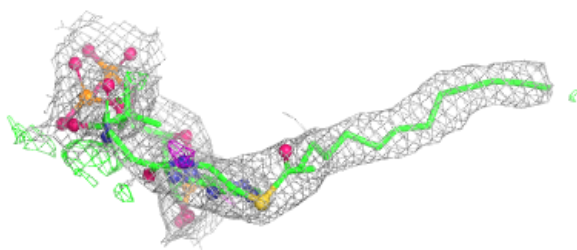
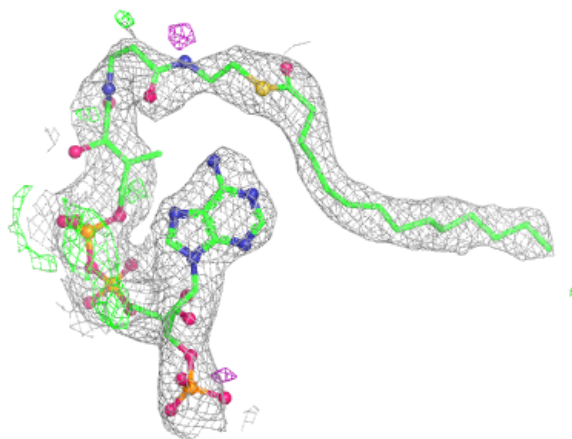
Electron density around MYA F 606:

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



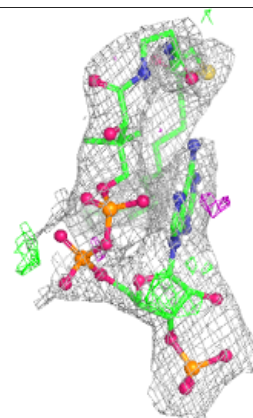
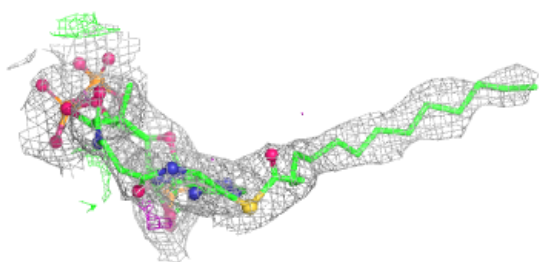
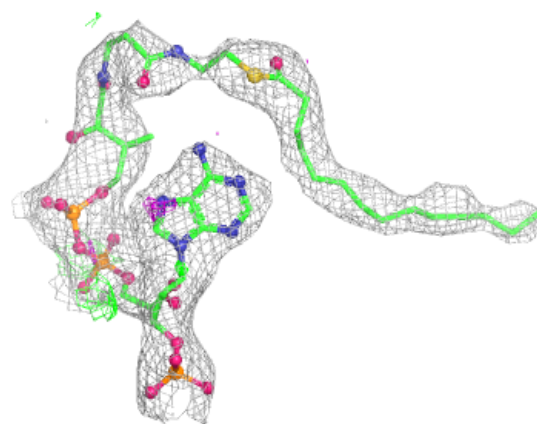
Electron density around MYA B 602:

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



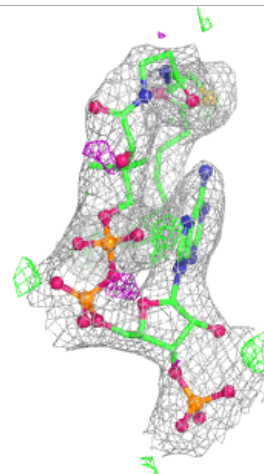
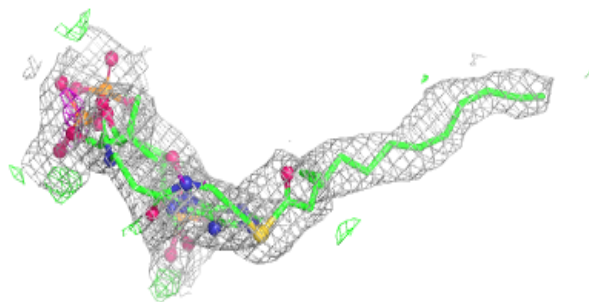
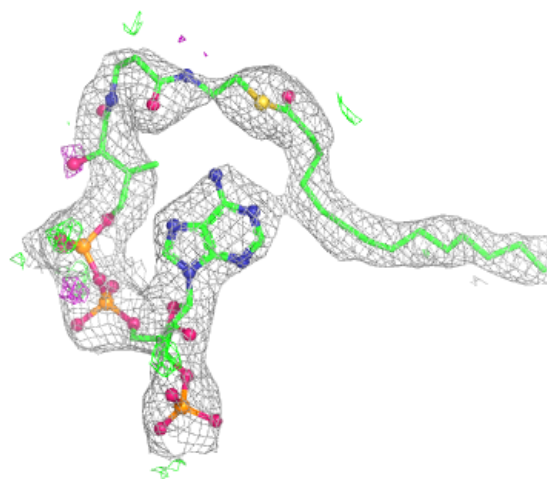
Electron density around MYA A 601:

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



Electron density around MYA 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 ⓘ

There are no such residues in this entry.