



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:07 AM UTC

PDB ID : 3G0B / pdb_00003g0b
Title : Crystal structure of dipeptidyl peptidase IV in complex with TAK-322
Authors : Zhang, Z.; Wallace, M.B.; Feng, J.; Stafford, J.A.; Kaldor, S.W.; Shi, L.; Skene, R.J.; Aertgeerts, K.; Lee, B.; Jennings, A.; Xu, R.; Kassel, D.; Webb, D.R.; Gwaltney, S.L.
Deposited on : 2009-01-27
Resolution : 2.25 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

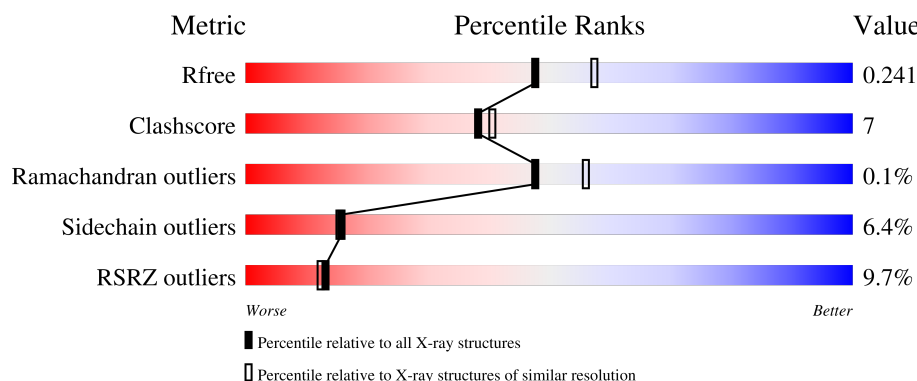
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

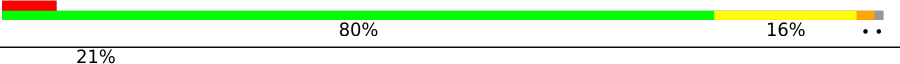
The reported resolution of this entry is 2.25 Å.

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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	740	
1	B	740	
1	C	740	
1	D	740	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	2	 100%
2	F	2	 50% 50%
2	G	2	 50% 50%
2	H	2	 100%
2	I	2	 100%
2	J	2	 50% 50%
2	K	2	 100%
2	L	2	 50% 50%

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
3	NAG	D	804	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24992 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			
1	B	733	Total	C	N	O	S	0	0	0
			6013	3857	997	1133	26			
1	C	726	Total	C	N	O	S	0	0	0
			5946	3818	977	1125	26			
1	D	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	expression tag	UNP P27487
A	28	ASP	-	expression tag	UNP P27487
A	29	PRO	-	expression tag	UNP P27487
A	30	GLY	-	expression tag	UNP P27487
A	31	GLY	-	expression tag	UNP P27487
A	32	SER	-	expression tag	UNP P27487
A	33	HIS	-	expression tag	UNP P27487
A	34	HIS	-	expression tag	UNP P27487
A	35	HIS	-	expression tag	UNP P27487
A	36	HIS	-	expression tag	UNP P27487
A	37	HIS	-	expression tag	UNP P27487
A	38	HIS	-	expression tag	UNP P27487
B	27	ALA	-	expression tag	UNP P27487
B	28	ASP	-	expression tag	UNP P27487
B	29	PRO	-	expression tag	UNP P27487
B	30	GLY	-	expression tag	UNP P27487
B	31	GLY	-	expression tag	UNP P27487
B	32	SER	-	expression tag	UNP P27487
B	33	HIS	-	expression tag	UNP P27487
B	34	HIS	-	expression tag	UNP P27487
B	35	HIS	-	expression tag	UNP P27487

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	36	HIS	-	expression tag	UNP P27487
B	37	HIS	-	expression tag	UNP P27487
B	38	HIS	-	expression tag	UNP P27487
C	27	ALA	-	expression tag	UNP P27487
C	28	ASP	-	expression tag	UNP P27487
C	29	PRO	-	expression tag	UNP P27487
C	30	GLY	-	expression tag	UNP P27487
C	31	GLY	-	expression tag	UNP P27487
C	32	SER	-	expression tag	UNP P27487
C	33	HIS	-	expression tag	UNP P27487
C	34	HIS	-	expression tag	UNP P27487
C	35	HIS	-	expression tag	UNP P27487
C	36	HIS	-	expression tag	UNP P27487
C	37	HIS	-	expression tag	UNP P27487
C	38	HIS	-	expression tag	UNP P27487
D	27	ALA	-	expression tag	UNP P27487
D	28	ASP	-	expression tag	UNP P27487
D	29	PRO	-	expression tag	UNP P27487
D	30	GLY	-	expression tag	UNP P27487
D	31	GLY	-	expression tag	UNP P27487
D	32	SER	-	expression tag	UNP P27487
D	33	HIS	-	expression tag	UNP P27487
D	34	HIS	-	expression tag	UNP P27487
D	35	HIS	-	expression tag	UNP P27487
D	36	HIS	-	expression tag	UNP P27487
D	37	HIS	-	expression tag	UNP P27487
D	38	HIS	-	expression tag	UNP P27487

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



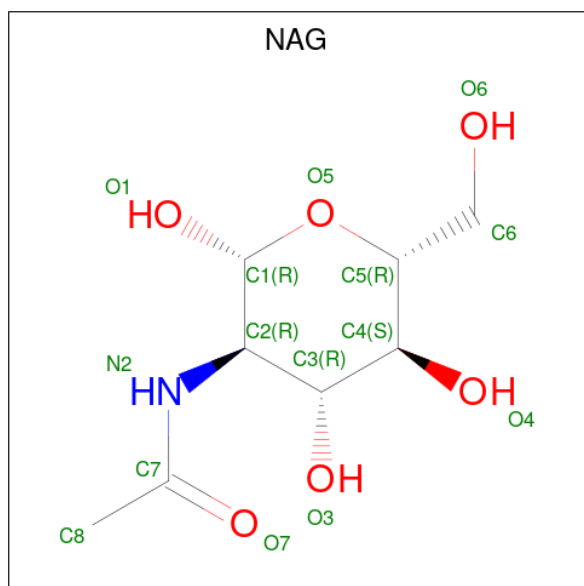
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



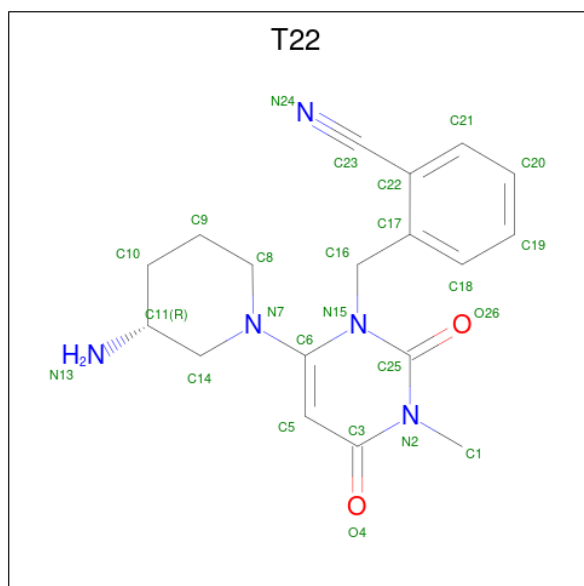
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

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

- Molecule 4 is 2-({6-[(3R)-3-aminopiperidin-1-yl]-3-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl}methyl)benzonitrile (CCD ID: T22) (formula: C₁₈H₂₁N₅O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			25	18	5	2		
4	B	1	Total	C	N	O	0	0
			25	18	5	2		
4	C	1	Total	C	N	O	0	0
			25	18	5	2		
4	D	1	Total	C	N	O	0	0
			25	18	5	2		

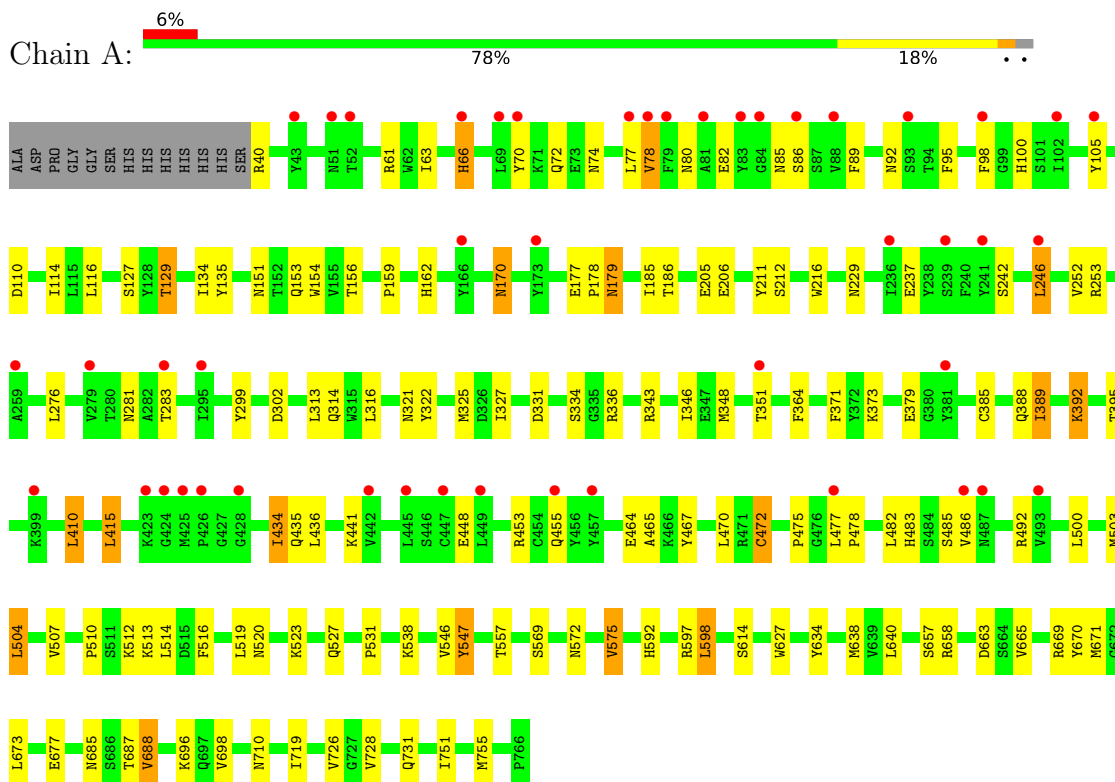
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	166	Total	O	0	0
			166	166		
5	B	166	Total	O	0	0
			166	166		
5	C	80	Total	O	0	0
			80	80		
5	D	145	Total	O	0	0
			145	145		

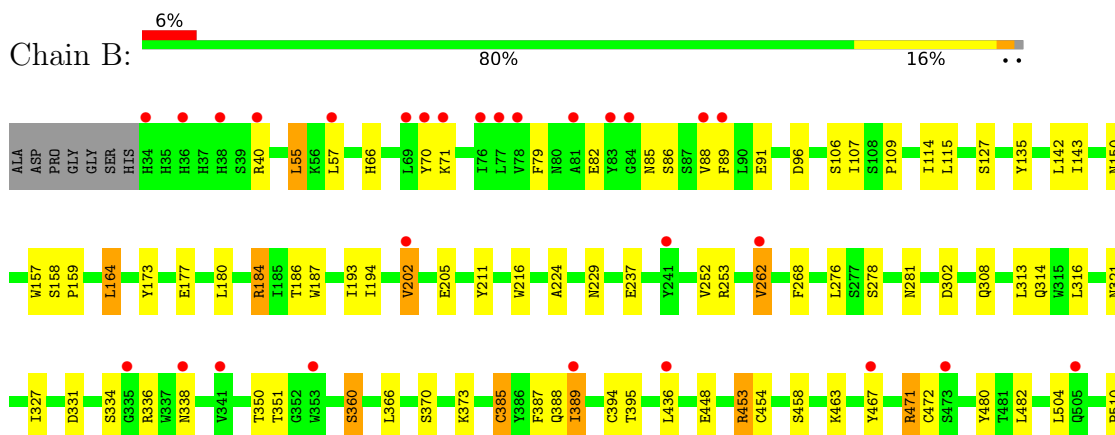
3 Residue-property plots

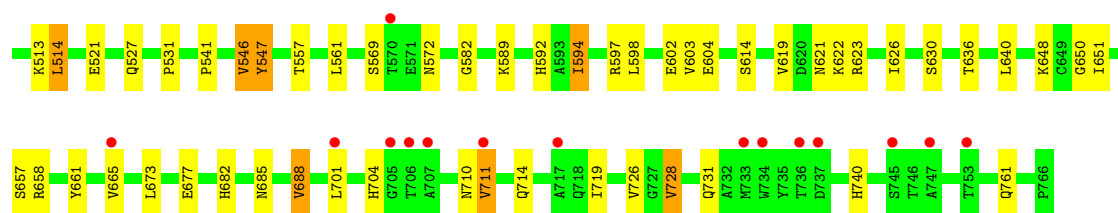
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4

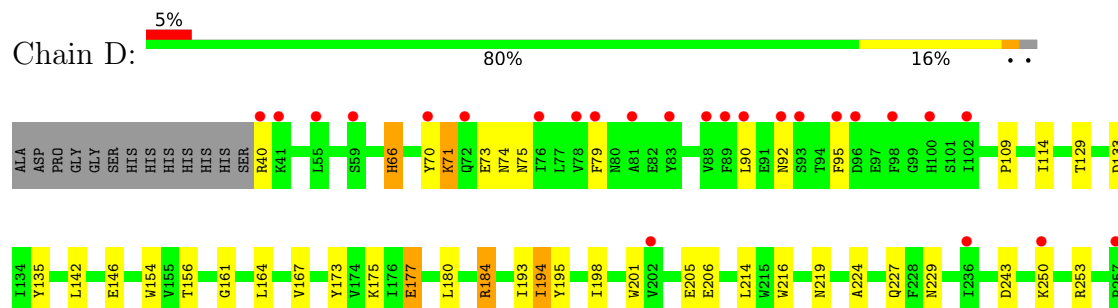


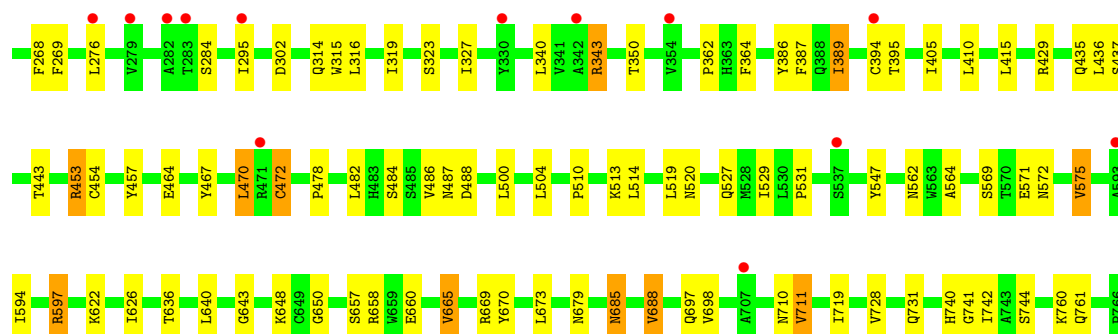


• Molecule 1: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4





- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  50%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

MAG1
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.69Å 122.40Å 144.01Å 90.00° 114.72° 90.00°	Depositor
Resolution (Å)	35.00 – 2.25 35.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	97.0 (35.00-2.25) 97.3 (35.00-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.242 0.204 , 0.241	Depositor DCC
R_{free} test set	8857 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24992	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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: NAG, T22

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	0.58	0/6129	0.81	1/8336 (0.0%)
1	B	0.56	0/6190	0.82	4/8419 (0.0%)
1	C	0.93	28/6118 (0.5%)	0.81	7/8322 (0.1%)
1	D	0.57	0/6129	0.81	0/8336
All	All	0.68	28/24566 (0.1%)	0.81	12/33413 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	338	ASN	CG-ND2	26.56	1.89	1.33
1	C	329	ASP	CG-OD1	21.32	1.65	1.25
1	C	343	ARG	CZ-NH2	16.89	1.55	1.33
1	C	329	ASP	CG-OD2	13.69	1.51	1.25
1	C	343	ARG	CD-NE	13.31	1.64	1.46
1	C	274	ASP	CG-OD1	11.74	1.47	1.25
1	C	274	ASP	CG-OD2	10.75	1.45	1.25
1	C	337	TRP	C-O	10.39	1.36	1.24
1	C	343	ARG	CZ-NH1	9.09	1.45	1.32
1	C	343	ARG	NE-CZ	8.46	1.42	1.33
1	C	331	ASP	CG-OD2	8.22	1.41	1.25
1	C	177	GLU	CD-OE2	7.96	1.40	1.25
1	C	283	THR	C-O	7.95	1.33	1.24
1	C	369	ASN	CG-OD1	7.01	1.36	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	177	GLU	CD-OE1	6.97	1.38	1.25
1	C	390	ASP	CG-OD2	6.85	1.38	1.25
1	C	369	ASN	CG-ND2	6.82	1.47	1.33
1	C	331	ASP	CB-CG	6.48	1.68	1.52
1	C	309	GLU	CG-CD	6.34	1.67	1.52
1	C	338	ASN	C-N	6.20	1.42	1.33
1	C	283	THR	C-N	5.87	1.41	1.33
1	C	338	ASN	CB-CG	5.62	1.66	1.52
1	C	308	GLN	C-O	5.60	1.31	1.24
1	C	331	ASP	CG-OD1	5.49	1.35	1.25
1	C	390	ASP	CG-OD1	5.31	1.35	1.25
1	C	368	GLY	C-O	5.16	1.30	1.24
1	C	338	ASN	C-O	-5.11	1.17	1.24
1	C	336	ARG	C-N	5.10	1.40	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	338	ASN	CB-CG-ND2	-8.90	103.06	116.40
1	C	329	ASP	CB-CG-OD1	-7.71	100.67	118.40
1	B	202	VAL	CB-CA-C	-7.07	100.80	112.26
1	C	338	ASN	OD1-CG-ND2	6.73	129.33	122.60
1	C	343	ARG	NE-CZ-NH1	-6.31	115.19	121.50
1	C	343	ARG	CD-NE-CZ	-6.14	115.80	124.40
1	B	547	TYR	N-CA-C	-5.89	102.56	111.34
1	B	630	SER	CB-CA-C	-5.79	109.36	117.23
1	C	329	ASP	OD1-CG-OD2	5.56	136.24	122.90
1	C	369	ASN	OD1-CG-ND2	5.50	128.10	122.60
1	B	262	VAL	N-CA-CB	5.30	116.83	110.31
1	A	575	VAL	CB-CA-C	5.21	118.43	111.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	338	ASN	Sidechain

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	5957	0	5679	93	0
1	B	6013	0	5720	73	0
1	C	5946	0	5666	89	0
1	D	5957	0	5676	85	0
2	E	28	0	25	0	0
2	F	28	0	25	2	0
2	G	28	0	25	1	0
2	H	28	0	25	3	0
2	I	28	0	25	0	0
2	J	28	0	25	2	0
2	K	28	0	25	3	0
2	L	28	0	25	5	0
3	A	56	0	52	4	0
3	B	56	0	52	5	0
3	C	56	0	52	3	0
3	D	70	0	65	4	0
4	A	25	0	21	1	0
4	B	25	0	21	1	0
4	C	25	0	21	1	0
4	D	25	0	21	1	0
5	A	166	0	0	0	0
5	B	166	0	0	0	0
5	C	80	0	0	0	0
5	D	145	0	0	1	0
All	All	24992	0	23246	328	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (328) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ASN:HD21	2:F:1:NAG:C1	1.12	1.58
1:C:329:ASP:CG	1:C:329:ASP:OD1	1.65	1.34
1:C:338:ASN:ND2	1:C:338:ASN:CG	1.89	1.31
1:A:229:ASN:ND2	2:F:1:NAG:C1	1.95	1.25
1:D:229:ASN:HD21	2:L:1:NAG:C1	1.69	1.04
1:A:321:ASN:HD21	2:H:1:NAG:C1	1.76	0.99
1:B:229:ASN:HD21	2:J:1:NAG:C1	1.76	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:SER:HB2	1:C:96:ASP:HB3	1.47	0.95
1:C:253:ARG:HH21	1:D:253:ARG:HH21	0.95	0.95
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.07	0.93
1:D:193:ILE:HG22	1:D:194:ILE:HD12	1.49	0.92
1:A:731:GLN:HE22	1:B:731:GLN:HE22	1.12	0.90
1:C:153:GLN:HE22	1:C:170:ASN:H	1.18	0.89
1:A:153:GLN:HE22	1:A:170:ASN:H	1.16	0.89
1:B:150:ASN:HD21	3:B:802:NAG:C1	1.87	0.87
1:A:731:GLN:HE22	1:B:731:GLN:NE2	1.71	0.86
1:A:520:ASN:ND2	3:A:803:NAG:H2	1.92	0.85
1:D:531:PRO:HB3	1:D:572:ASN:HD22	1.42	0.85
1:A:74:ASN:HB3	1:A:92:ASN:HB3	1.59	0.84
1:B:331:ASP:HB2	1:B:338:ASN:HD21	1.40	0.84
1:C:253:ARG:NH2	1:D:253:ARG:HH21	1.76	0.83
1:D:711:VAL:HG13	1:D:740:HIS:CE1	2.13	0.82
1:B:281:ASN:HD21	3:B:803:NAG:C1	1.92	0.81
1:C:253:ARG:HH21	1:D:253:ARG:NH2	1.76	0.80
1:A:731:GLN:NE2	1:B:731:GLN:HE22	1.79	0.79
1:A:325:MET:HE1	1:A:371:PHE:CZ	2.18	0.78
1:B:471:ARG:HG3	1:B:480:TYR:CE1	2.19	0.78
1:A:281:ASN:HD21	2:G:1:NAG:C1	2.00	0.75
1:B:711:VAL:HG13	1:B:740:HIS:CE1	2.23	0.74
1:D:173:TYR:CE1	1:D:184:ARG:HG2	2.23	0.74
1:A:346:ILE:H	1:A:392:LYS:NZ	1.86	0.73
1:A:520:ASN:HD21	3:A:803:NAG:H2	1.52	0.73
1:A:364:PHE:HE2	1:A:389:ILE:HD11	1.54	0.73
1:B:351:THR:OG1	1:B:592:HIS:HD2	1.72	0.72
1:B:321:ASN:HD21	3:B:804:NAG:C1	2.03	0.72
1:B:334:SER:HB3	1:B:336:ARG:HG3	1.72	0.72
1:A:598:LEU:HD22	1:A:671:MET:HG2	1.70	0.71
1:D:219:ASN:HD21	3:D:802:NAG:C1	2.04	0.71
1:A:253:ARG:HH21	1:B:253:ARG:NH2	1.88	0.69
1:A:516:PHE:CD1	1:A:523:LYS:HG2	2.26	0.69
1:B:331:ASP:HB2	1:B:338:ASN:ND2	2.07	0.69
1:A:40:ARG:HH11	1:A:40:ARG:HB3	1.56	0.69
1:A:78:VAL:HG22	1:A:89:PHE:HB2	1.73	0.68
1:B:726:VAL:HG23	1:B:728:VAL:HG12	1.75	0.68
1:D:205:GLU:OE2	4:D:806:T22:N13	2.26	0.68
1:D:229:ASN:ND2	2:L:1:NAG:C1	2.50	0.68
1:B:184:ARG:HD3	1:B:186:THR:O	1.94	0.67
1:C:388:GLN:HB2	1:C:391:LYS:HG2	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:711:VAL:CG1	1:D:740:HIS:CE1	2.78	0.67
1:A:40:ARG:HB3	1:A:40:ARG:NH1	2.10	0.66
1:D:206:GLU:HB3	1:D:665:VAL:HG22	1.77	0.65
1:D:529:ILE:HB	1:D:575:VAL:HG13	1.78	0.65
1:A:415:LEU:HB3	1:A:434:ILE:HG23	1.77	0.65
1:B:205:GLU:OE2	4:B:805:T22:N13	2.30	0.65
1:A:658:ARG:HB2	1:A:687:THR:HG22	1.77	0.65
1:D:643:GLY:HA2	1:D:697:GLN:HE22	1.61	0.65
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.79	0.64
1:B:88:VAL:HG11	1:B:91:GLU:HG3	1.79	0.64
1:B:82:GLU:HG2	1:B:467:TYR:OH	1.97	0.64
1:A:253:ARG:NH2	1:B:253:ARG:HH21	1.88	0.64
1:B:688:VAL:HG22	1:B:719:ILE:HG12	1.80	0.63
1:A:77:LEU:HD12	1:A:86:SER:HB2	1.81	0.63
1:C:710:ASN:C	1:C:710:ASN:HD22	2.06	0.63
1:A:156:THR:HG23	1:A:216:TRP:HE1	1.63	0.63
1:B:602:GLU:HG3	1:B:603:VAL:H	1.64	0.63
1:C:311:ILE:HG22	1:C:337:TRP:CZ3	2.34	0.62
1:D:453:ARG:HG3	1:D:454:CYS:SG	2.39	0.62
1:D:206:GLU:CB	1:D:665:VAL:HG22	2.31	0.61
1:C:731:GLN:HE22	1:D:731:GLN:NE2	1.97	0.61
1:D:340:LEU:HB2	1:D:343:ARG:HG3	1.82	0.61
1:B:173:TYR:CE1	1:B:184:ARG:HG3	2.36	0.60
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.84	0.60
1:C:726:VAL:HG23	1:C:728:VAL:HG12	1.83	0.60
1:C:726:VAL:HG23	1:C:728:VAL:CG1	2.31	0.60
1:C:415:LEU:HB3	1:C:434:ILE:HG23	1.84	0.60
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.83	0.59
1:A:435:GLN:OE1	1:A:441:LYS:HD3	2.02	0.59
1:C:154:TRP:CE2	1:C:212:SER:HB3	2.37	0.59
1:B:327:ILE:HD13	1:B:389:ILE:HG13	1.83	0.59
1:C:90:LEU:HD12	1:C:94:THR:HB	1.84	0.59
1:B:229:ASN:ND2	2:J:1:NAG:C1	2.57	0.59
1:B:385:CYS:HB3	1:B:387:PHE:CE2	2.37	0.59
1:D:133:ASP:HB3	1:D:142:LEU:HD11	1.83	0.59
1:C:205:GLU:OE1	4:C:805:T22:N13	2.36	0.58
1:B:710:ASN:C	1:B:710:ASN:HD22	2.10	0.58
1:C:329:ASP:OD1	1:C:329:ASP:CB	2.47	0.58
1:D:520:ASN:HB2	3:D:804:NAG:H62	1.86	0.58
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.84	0.58
1:C:75:ASN:HB3	1:C:91:GLU:HA	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:ASN:ND2	2:K:1:NAG:O5	2.36	0.58
1:D:74:ASN:HB3	1:D:92:ASN:HD22	1.69	0.57
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.84	0.57
1:D:146:GLU:O	1:D:175:LYS:HE2	2.04	0.57
1:A:327:ILE:HD12	1:A:343:ARG:O	2.04	0.57
1:A:40:ARG:HH11	1:A:40:ARG:CB	2.17	0.57
1:C:343:ARG:HD2	1:C:389:ILE:HG23	1.87	0.57
2:H:1:NAG:H4	2:H:2:NAG:N2	2.20	0.57
1:C:657:SER:HA	1:C:688:VAL:HG13	1.86	0.57
1:C:731:GLN:NE2	1:D:731:GLN:NE2	2.52	0.57
1:A:325:MET:HE3	1:A:327:ILE:HD11	1.87	0.56
1:B:177:GLU:HB2	1:B:180:LEU:HD22	1.86	0.56
1:B:85:ASN:HD21	3:B:801:NAG:C1	2.18	0.56
1:C:598:LEU:HD22	1:C:671:MET:HG2	1.88	0.56
1:C:74:ASN:HD22	1:C:75:ASN:N	2.04	0.56
1:C:731:GLN:HE22	1:D:731:GLN:HE21	1.52	0.56
1:A:346:ILE:H	1:A:392:LYS:HZ1	1.54	0.56
1:D:114:ILE:HG23	1:D:135:TYR:HB3	1.88	0.56
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.89	0.55
1:B:351:THR:OG1	1:B:592:HIS:CD2	2.58	0.55
1:A:321:ASN:HD21	2:H:1:NAG:C2	2.20	0.55
1:D:510:PRO:HD3	1:D:569:SER:HB2	1.88	0.55
1:A:504:LEU:HA	1:A:507:VAL:HG12	1.89	0.55
1:B:614:SER:HA	1:B:619:VAL:HB	1.89	0.54
1:D:685:ASN:ND2	3:D:805:NAG:C1	2.70	0.54
1:D:685:ASN:HD21	3:D:805:NAG:C1	2.21	0.54
1:C:281:ASN:HD21	3:C:802:NAG:C1	2.20	0.54
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.71	0.54
1:D:90:LEU:HD21	1:D:95:PHE:HE2	1.72	0.54
1:A:500:LEU:HA	1:A:503:MET:HE3	1.89	0.54
1:B:360:SER:O	1:B:373:LYS:HE3	2.08	0.54
1:C:115:LEU:HD21	1:C:155:VAL:CG1	2.37	0.54
1:A:343:ARG:HD2	1:A:389:ILE:HG23	1.90	0.54
1:D:194:ILE:HG12	2:L:1:NAG:H82	1.90	0.54
1:C:571:GLU:CD	1:C:760:LYS:HD3	2.34	0.53
1:C:159:PRO:HD3	1:C:216:TRP:HB3	1.89	0.53
1:A:85:ASN:HD21	3:A:801:NAG:C1	2.21	0.53
1:A:546:VAL:HG12	1:A:627:TRP:O	2.08	0.53
1:A:325:MET:HE1	1:A:371:PHE:CE2	2.43	0.53
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.91	0.53
1:C:150:ASN:HD21	3:C:801:NAG:C1	2.22	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:ARG:HD2	1:D:389:ILE:HG23	1.89	0.52
1:A:334:SER:HB3	1:A:336:ARG:HB2	1.90	0.52
1:B:688:VAL:CG2	1:B:719:ILE:HG12	2.38	0.52
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.93	0.51
1:B:626:ILE:HG23	1:B:636:THR:HG23	1.91	0.51
1:C:193:ILE:HG22	1:C:194:ILE:HD12	1.93	0.51
1:C:410:LEU:HD13	1:C:415:LEU:HD23	1.92	0.51
1:D:435:GLN:HE21	1:D:437:SER:HG	1.58	0.51
1:D:229:ASN:ND2	2:L:1:NAG:O5	2.38	0.51
1:D:657:SER:HA	1:D:688:VAL:HG13	1.92	0.51
1:B:546:VAL:HG11	1:B:626:ILE:HD11	1.93	0.51
1:C:184:ARG:HD2	1:C:187:TRP:CE2	2.45	0.51
1:C:351:THR:OG1	1:C:592:HIS:HD2	1.94	0.51
1:C:285:ILE:HG13	1:C:335:GLY:O	2.10	0.51
1:D:710:ASN:C	1:D:710:ASN:HD22	2.20	0.50
1:B:55:LEU:HD13	1:B:561:LEU:HD12	1.91	0.50
1:A:66:HIS:HB3	1:A:467:TYR:HE1	1.76	0.50
1:C:329:ASP:OD1	1:C:329:ASP:N	2.44	0.50
1:B:453:ARG:HG3	1:B:454:CYS:SG	2.51	0.50
1:D:711:VAL:HG13	1:D:740:HIS:ND1	2.26	0.50
1:A:472:CYS:O	1:A:478:PRO:HA	2.12	0.50
1:A:688:VAL:HG22	1:A:719:ILE:HG12	1.94	0.50
1:D:319:ILE:H	1:D:319:ILE:HD12	1.76	0.50
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.94	0.50
1:B:657:SER:HA	1:B:688:VAL:HG13	1.94	0.50
1:C:517:ILE:HD12	1:C:612:GLN:HG3	1.94	0.49
1:B:70:TYR:HB3	1:B:79:PHE:CE1	2.47	0.49
1:A:179:ASN:HD22	1:A:179:ASN:H	1.60	0.49
1:C:184:ARG:HD3	1:C:186:THR:O	2.12	0.49
1:A:129:THR:HG23	1:A:151:ASN:HA	1.94	0.49
1:C:307:THR:OG1	1:C:310:ARG:HB3	2.12	0.49
1:D:364:PHE:HE2	1:D:389:ILE:HD11	1.77	0.49
1:A:74:ASN:HB3	1:A:92:ASN:CB	2.37	0.49
1:B:458:SER:OG	1:B:471:ARG:HD2	2.13	0.49
1:B:711:VAL:CG1	1:B:740:HIS:CE1	2.95	0.49
1:D:486:VAL:C	1:D:487:ASN:HD22	2.21	0.49
1:A:331:ASP:HB3	1:A:334:SER:HB2	1.95	0.49
1:A:513:LYS:O	1:A:527:GLN:HA	2.12	0.48
1:B:531:PRO:HB3	1:B:572:ASN:HD22	1.78	0.48
1:C:598:LEU:HG	1:C:631:TYR:OH	2.12	0.48
1:A:154:TRP:CE2	1:A:212:SER:HB3	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:PHE:CD1	1:A:100:HIS:HB2	2.49	0.48
1:C:115:LEU:HD21	1:C:155:VAL:HG13	1.95	0.48
1:C:310:ARG:NH1	1:C:368:GLY:O	2.41	0.48
1:B:658:ARG:HG2	1:B:661:TYR:CE2	2.49	0.48
1:A:170:ASN:N	1:A:170:ASN:HD22	2.12	0.48
1:B:79:PHE:CD2	1:B:86:SER:HB3	2.49	0.48
1:B:193:ILE:HG22	1:B:194:ILE:HG12	1.96	0.48
1:C:531:PRO:HB3	1:C:572:ASN:HD22	1.79	0.47
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.49	0.47
1:B:321:ASN:HD21	3:B:804:NAG:C2	2.26	0.47
1:A:327:ILE:HD13	1:A:389:ILE:HD12	1.95	0.47
1:C:173:TYR:CE1	1:C:184:ARG:HG3	2.49	0.47
1:D:643:GLY:HA2	1:D:697:GLN:NE2	2.30	0.47
1:D:626:ILE:HG23	1:D:636:THR:HG23	1.97	0.47
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.45	0.46
1:D:75:ASN:N	1:D:75:ASN:HD22	2.13	0.46
1:B:541:PRO:HG3	1:B:623:ARG:CZ	2.44	0.46
1:A:598:LEU:HB2	1:A:671:MET:SD	2.55	0.46
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.96	0.46
1:C:411:THR:C	1:C:413:ASP:H	2.23	0.46
1:D:167:VAL:HG11	1:D:198:ILE:HG12	1.97	0.46
1:D:688:VAL:HG22	1:D:719:ILE:HG12	1.97	0.46
1:A:205:GLU:OE1	4:A:805:T22:N13	2.48	0.46
1:A:206:GLU:OE2	1:A:663:ASP:OD2	2.34	0.46
1:A:657:SER:HA	1:A:688:VAL:HG13	1.97	0.46
1:A:500:LEU:HG	1:A:504:LEU:HD22	1.97	0.46
1:B:109:PRO:HG2	1:B:158:SER:O	2.15	0.46
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.51	0.46
1:D:500:LEU:O	1:D:504:LEU:HB2	2.16	0.45
1:D:472:CYS:O	1:D:478:PRO:HA	2.17	0.45
1:C:159:PRO:HD3	1:C:216:TRP:CB	2.46	0.45
1:A:520:ASN:ND2	3:A:803:NAG:C2	2.73	0.45
1:A:640:LEU:HB3	1:A:698:VAL:HG21	1.99	0.45
1:B:157:TRP:CE3	1:B:164:LEU:HD13	2.51	0.45
1:C:229:ASN:ND2	2:K:1:NAG:C1	2.79	0.45
1:C:306:ALA:HB3	1:C:310:ARG:HG2	1.98	0.45
1:B:387:PHE:CD1	1:B:394:CYS:HB3	2.52	0.45
1:C:510:PRO:HD3	1:C:569:SER:HB2	1.97	0.45
1:C:414:TYR:CE2	1:C:433:LYS:HE3	2.52	0.45
1:C:461:PHE:CD2	1:C:468:TYR:HB3	2.51	0.45
1:D:571:GLU:CD	1:D:760:LYS:HD3	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:512:LYS:HE3	1:C:527:GLN:CD	2.42	0.45
1:D:109:PRO:HD2	1:D:161:GLY:O	2.16	0.45
1:D:640:LEU:HB3	1:D:698:VAL:HG21	1.99	0.45
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.98	0.45
1:D:386:TYR:O	1:D:394:CYS:HB2	2.16	0.45
1:C:472:CYS:O	1:C:478:PRO:HA	2.18	0.44
1:C:259:ALA:HB3	1:C:660:GLU:HA	1.99	0.44
1:C:519:LEU:HB3	3:C:804:NAG:H61	1.99	0.44
1:D:597:ARG:NH2	1:D:679:ASN:OD1	2.50	0.44
1:B:614:SER:HB2	1:B:621:ASN:OD1	2.18	0.44
1:A:322:TYR:CE1	1:A:348:MET:HE2	2.52	0.44
1:C:456:TYR:HB2	1:C:557:THR:OG1	2.17	0.44
1:C:640:LEU:HB3	1:C:698:VAL:HG21	1.99	0.44
1:D:206:GLU:HB3	1:D:665:VAL:CG2	2.46	0.44
1:D:562:ASN:HB2	5:D:980:HOH:O	2.18	0.44
1:A:634:TYR:O	1:A:638:MET:HG2	2.18	0.44
1:D:70:TYR:HB3	1:D:79:PHE:CE1	2.53	0.44
1:A:110:ASP:OD1	1:A:162:HIS:ND1	2.44	0.44
1:D:314:GLN:NE2	1:D:362:PRO:HD3	2.31	0.44
1:D:531:PRO:HB3	1:D:572:ASN:ND2	2.21	0.44
1:A:302:ASP:HB3	1:A:314:GLN:HB2	2.00	0.44
1:A:751:ILE:O	1:A:755:MET:HG3	2.18	0.44
1:D:71:LYS:H	1:D:71:LYS:HD2	1.83	0.44
1:A:82:GLU:HG2	1:A:467:TYR:OH	2.17	0.43
1:B:513:LYS:O	1:B:527:GLN:HA	2.17	0.43
1:C:362:PRO:HA	1:C:373:LYS:HB3	2.00	0.43
1:D:156:THR:HG23	1:D:216:TRP:HE1	1.83	0.43
1:D:405:ILE:HG13	1:D:429:ARG:CD	2.48	0.43
1:A:669:ARG:HD2	1:A:670:TYR:CZ	2.53	0.43
1:C:116:LEU:O	1:C:132:TYR:HA	2.17	0.43
1:A:364:PHE:O	1:A:410:LEU:HD21	2.18	0.43
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.49	0.43
1:B:127:SER:HB3	1:B:211:TYR:CG	2.54	0.43
1:A:185:ILE:HG22	1:A:186:THR:HG23	2.01	0.43
1:A:299:TYR:CE1	1:A:665:VAL:HG22	2.52	0.43
1:A:465:ALA:O	1:A:485:SER:OG	2.26	0.43
1:C:184:ARG:HD2	1:C:187:TRP:CZ2	2.52	0.43
1:C:310:ARG:NH2	1:C:329:ASP:OD2	2.52	0.43
1:D:741:GLY:O	1:D:742:ILE:C	2.62	0.43
1:A:159:PRO:HD3	1:A:216:TRP:HB3	2.00	0.43
1:A:710:ASN:HD22	1:A:710:ASN:C	2.25	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:598:LEU:O	1:B:682:HIS:NE2	2.48	0.43
1:C:471:ARG:HG3	1:C:480:TYR:CE1	2.54	0.43
1:D:114:ILE:CG2	1:D:135:TYR:HB3	2.48	0.43
1:A:80:ASN:ND2	1:A:82:GLU:HB2	2.33	0.43
1:A:237:GLU:HA	1:A:252:VAL:O	2.19	0.43
1:A:455:GLN:HE21	1:A:557:THR:HG21	1.84	0.43
1:D:269:PHE:HB3	1:D:284:SER:HB3	1.99	0.43
1:C:596:ARG:N	1:C:670:TYR:O	2.50	0.42
1:D:315:TRP:O	1:D:323:SER:HB2	2.19	0.42
1:D:484:SER:O	1:D:488:ASP:HA	2.19	0.42
1:B:89:PHE:CE1	1:B:107:ILE:HD13	2.54	0.42
1:D:229:ASN:HD21	2:L:1:NAG:C2	2.27	0.42
1:C:164:LEU:HB2	1:C:175:LYS:HB2	2.00	0.42
1:C:330:TYR:HB2	1:C:337:TRP:CZ2	2.54	0.42
1:D:73:GLU:C	1:D:75:ASN:H	2.27	0.42
1:D:66:HIS:HB3	1:D:467:TYR:HE1	1.85	0.42
1:D:201:TRP:CZ2	1:D:710:ASN:HA	2.55	0.42
1:C:80:ASN:HD22	1:C:80:ASN:C	2.28	0.42
1:C:153:GLN:NE2	1:C:167:VAL:HG12	2.34	0.42
1:D:457:TYR:CD1	1:D:470:LEU:HG	2.54	0.42
1:A:455:GLN:HB2	1:A:475:PRO:HD3	2.02	0.42
1:D:564:ALA:HB1	1:D:575:VAL:HG11	2.02	0.42
1:B:106:SER:HB3	1:B:115:LEU:HB3	2.02	0.42
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.55	0.42
1:C:184:ARG:HH11	1:C:187:TRP:HA	1.85	0.41
1:C:327:ILE:HD13	1:C:389:ILE:HD13	2.02	0.41
1:C:546:VAL:HG12	1:C:627:TRP:O	2.20	0.41
1:A:70:TYR:HD2	1:A:72:GLN:HG2	1.84	0.41
1:A:547:TYR:C	1:A:547:TYR:CD2	2.98	0.41
1:C:325:MET:HE2	1:C:327:ILE:HD11	2.01	0.41
1:B:237:GLU:HG2	1:B:253:ARG:HG2	2.01	0.41
1:B:370:SER:HB2	1:B:387:PHE:O	2.20	0.41
1:C:312:SER:HB2	1:C:325:MET:HE3	2.02	0.41
1:D:658:ARG:HD3	1:D:660:GLU:OE2	2.20	0.41
1:B:237:GLU:HA	1:B:252:VAL:O	2.21	0.41
1:C:115:LEU:HD21	1:C:155:VAL:HG11	2.01	0.41
1:C:63:ILE:HG13	1:C:64:SER:N	2.36	0.41
1:C:640:LEU:HD11	1:C:650:GLY:HA3	2.03	0.41
1:D:513:LYS:O	1:D:527:GLN:HA	2.21	0.41
1:C:320:GLN:O	1:C:354:VAL:HG12	2.20	0.41
1:B:651:ILE:HA	1:B:701:LEU:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:GLU:HB2	1:D:180:LEU:HD22	2.03	0.41
1:D:195:TYR:O	1:D:227:GLN:HA	2.20	0.41
1:D:302:ASP:HB3	1:D:314:GLN:HB2	2.03	0.41
1:A:127:SER:HB3	1:A:211:TYR:CD2	2.56	0.41
1:A:179:ASN:HD22	1:A:179:ASN:N	2.17	0.41
1:A:512:LYS:HE2	1:A:527:GLN:OE1	2.20	0.41
1:B:622:LYS:O	1:B:648:LYS:HD2	2.20	0.41
1:D:154:TRP:HD1	1:D:214:LEU:HD12	1.85	0.41
1:D:405:ILE:HG13	1:D:429:ARG:HD2	2.02	0.41
1:D:622:LYS:O	1:D:648:LYS:HD2	2.20	0.41
1:B:582:GLY:HA2	1:B:594:ILE:HD12	2.01	0.41
1:C:477:LEU:HD23	1:C:497:ASN:HB3	2.02	0.41
1:D:40:ARG:HD2	1:D:40:ARG:HA	1.94	0.41
1:B:602:GLU:HG3	1:B:603:VAL:N	2.32	0.40
1:C:658:ARG:HG2	1:C:661:TYR:CE2	2.56	0.40
1:D:387:PHE:CD1	1:D:394:CYS:HB3	2.56	0.40
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.56	0.40
1:B:308:GLN:OE1	1:B:308:GLN:HA	2.21	0.40
1:B:514:LEU:HD12	1:B:557:THR:HG22	2.03	0.40
1:C:134:ILE:HD13	1:C:178:PRO:HB3	2.03	0.40
1:C:305:TRP:CE2	1:C:311:ILE:HD12	2.56	0.40
1:C:720:SER:O	1:C:724:VAL:HG23	2.21	0.40
1:A:177:GLU:HA	1:A:178:PRO:HD3	1.92	0.40
1:C:338:ASN:ND2	1:C:338:ASN:CB	2.78	0.40
1:C:512:LYS:HE3	1:C:527:GLN:OE1	2.22	0.40
1:D:669:ARG:HD2	1:D:670:TYR:CZ	2.56	0.40
1:A:95:PHE:CE1	1:A:116:LEU:HD11	2.56	0.40
1:C:657:SER:HA	1:C:688:VAL:CG1	2.50	0.40
1:A:134:ILE:HD13	1:A:178:PRO:HB3	2.03	0.40
1:A:322:TYR:HE1	1:A:348:MET:HE2	1.86	0.40
1:A:470:LEU:HD12	1:A:483:HIS:NE2	2.37	0.40
1:C:105:TYR:HB2	1:C:114:ILE:HD11	2.04	0.40
1:C:229:ASN:CG	2:K:1:NAG:C1	2.94	0.40
1:C:731:GLN:NE2	1:D:731:GLN:HE22	2.18	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	725/740 (98%)	697 (96%)	28 (4%)	0	100	100
1	B	731/740 (99%)	704 (96%)	26 (4%)	1 (0%)	48	56
1	C	724/740 (98%)	690 (95%)	32 (4%)	2 (0%)	36	40
1	D	725/740 (98%)	692 (95%)	33 (5%)	0	100	100
All	All	2905/2960 (98%)	2783 (96%)	119 (4%)	3 (0%)	48	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	714	GLN
1	C	73	GLU
1	C	463	LYS

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	652/662 (98%)	608 (93%)	44 (7%)	15	14
1	B	658/662 (99%)	610 (93%)	48 (7%)	13	12
1	C	651/662 (98%)	615 (94%)	36 (6%)	19	20
1	D	652/662 (98%)	612 (94%)	40 (6%)	17	17
All	All	2613/2648 (99%)	2445 (94%)	168 (6%)	16	15

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ARG
1	A	63	ILE
1	A	66	HIS
1	A	78	VAL
1	A	129	THR
1	A	170	ASN
1	A	179	ASN
1	A	246	LEU
1	A	276	LEU
1	A	283	THR
1	A	313	LEU
1	A	316	LEU
1	A	373	LYS
1	A	379	GLU
1	A	385	CYS
1	A	388	GLN
1	A	389	ILE
1	A	392	LYS
1	A	395	THR
1	A	410	LEU
1	A	415	LEU
1	A	434	ILE
1	A	436	LEU
1	A	448	GLU
1	A	453	ARG
1	A	464	GLU
1	A	472	CYS
1	A	477	LEU
1	A	482	LEU
1	A	486	VAL
1	A	492	ARG
1	A	504	LEU
1	A	514	LEU
1	A	519	LEU
1	A	538	LYS
1	A	547	TYR
1	A	575	VAL
1	A	597	ARG
1	A	598	LEU
1	A	614	SER
1	A	673	LEU
1	A	677	GLU
1	A	685	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	688	VAL
1	B	40	ARG
1	B	55	LEU
1	B	57	LEU
1	B	66	HIS
1	B	71	LYS
1	B	96	ASP
1	B	142	LEU
1	B	143	ILE
1	B	164	LEU
1	B	184	ARG
1	B	202	VAL
1	B	262	VAL
1	B	276	LEU
1	B	278	SER
1	B	313	LEU
1	B	316	LEU
1	B	350	THR
1	B	360	SER
1	B	366	LEU
1	B	385	CYS
1	B	388	GLN
1	B	389	ILE
1	B	395	THR
1	B	436	LEU
1	B	448	GLU
1	B	453	ARG
1	B	463	LYS
1	B	471	ARG
1	B	472	CYS
1	B	482	LEU
1	B	504	LEU
1	B	514	LEU
1	B	521	GLU
1	B	546	VAL
1	B	547	TYR
1	B	589	LYS
1	B	594	ILE
1	B	597	ARG
1	B	604	GLU
1	B	665	VAL
1	B	673	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	677	GLU
1	B	685	ASN
1	B	688	VAL
1	B	704	HIS
1	B	711	VAL
1	B	728	VAL
1	B	761	GLN
1	C	59	SER
1	C	74	ASN
1	C	75	ASN
1	C	77	LEU
1	C	80	ASN
1	C	92	ASN
1	C	129	THR
1	C	164	LEU
1	C	246	LEU
1	C	276	LEU
1	C	279	VAL
1	C	280	THR
1	C	283	THR
1	C	313	LEU
1	C	316	LEU
1	C	341	VAL
1	C	360	SER
1	C	365	THR
1	C	370	SER
1	C	385	CYS
1	C	413	ASP
1	C	464	GLU
1	C	482	LEU
1	C	486	VAL
1	C	502	LYS
1	C	504	LEU
1	C	506	ASN
1	C	514	LEU
1	C	519	LEU
1	C	547	TYR
1	C	597	ARG
1	C	598	LEU
1	C	627	TRP
1	C	688	VAL
1	C	710	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	728	VAL
1	D	66	HIS
1	D	71	LYS
1	D	129	THR
1	D	164	LEU
1	D	177	GLU
1	D	184	ARG
1	D	194	ILE
1	D	243	ASP
1	D	250	LYS
1	D	276	LEU
1	D	295	ILE
1	D	316	LEU
1	D	327	ILE
1	D	343	ARG
1	D	350	THR
1	D	389	ILE
1	D	395	THR
1	D	410	LEU
1	D	415	LEU
1	D	436	LEU
1	D	443	THR
1	D	453	ARG
1	D	464	GLU
1	D	470	LEU
1	D	472	CYS
1	D	482	LEU
1	D	514	LEU
1	D	519	LEU
1	D	547	TYR
1	D	575	VAL
1	D	594	ILE
1	D	597	ARG
1	D	665	VAL
1	D	673	LEU
1	D	685	ASN
1	D	688	VAL
1	D	711	VAL
1	D	728	VAL
1	D	744	SER
1	D	761	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	85	ASN
1	A	153	GLN
1	A	169	ASN
1	A	170	ASN
1	A	179	ASN
1	A	227	GLN
1	A	229	ASN
1	A	281	ASN
1	A	321	ASN
1	A	338	ASN
1	A	344	GLN
1	A	455	GLN
1	A	520	ASN
1	A	572	ASN
1	A	586	GLN
1	A	592	HIS
1	A	595	ASN
1	A	606	GLN
1	A	685	ASN
1	A	710	ASN
1	A	748	HIS
1	B	150	ASN
1	B	169	ASN
1	B	196	ASN
1	B	227	GLN
1	B	229	ASN
1	B	281	ASN
1	B	321	ASN
1	B	338	ASN
1	B	344	GLN
1	B	345	HIS
1	B	450	ASN
1	B	505	GLN
1	B	572	ASN
1	B	592	HIS
1	B	606	GLN
1	B	710	ASN
1	B	731	GLN
1	C	74	ASN
1	C	75	ASN
1	C	80	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	119	ASN
1	C	150	ASN
1	C	153	GLN
1	C	169	ASN
1	C	170	ASN
1	C	179	ASN
1	C	281	ASN
1	C	314	GLN
1	C	455	GLN
1	C	520	ASN
1	C	572	ASN
1	C	592	HIS
1	C	606	GLN
1	C	710	ASN
1	C	731	GLN
1	C	748	HIS
1	C	749	GLN
1	D	51	ASN
1	D	66	HIS
1	D	75	ASN
1	D	80	ASN
1	D	92	ASN
1	D	169	ASN
1	D	196	ASN
1	D	219	ASN
1	D	227	GLN
1	D	229	ASN
1	D	344	GLN
1	D	345	HIS
1	D	487	ASN
1	D	572	ASN
1	D	586	GLN
1	D	606	GLN
1	D	685	ASN
1	D	697	GLN
1	D	710	ASN
1	D	731	GLN
1	D	749	GLN
1	D	757	HIS

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 ⓘ

16 monosaccharides 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	NAG	E	1	1,2	14,14,15	0.53	0	17,19,21	1.84	3 (17%)
2	NAG	E	2	2	14,14,15	0.59	0	17,19,21	1.19	1 (5%)
2	NAG	F	1	2	14,14,15	0.70	0	17,19,21	1.34	1 (5%)
2	NAG	F	2	2	14,14,15	0.44	0	17,19,21	1.55	3 (17%)
2	NAG	G	1	2	14,14,15	0.59	0	17,19,21	1.51	3 (17%)
2	NAG	G	2	2	14,14,15	0.55	0	17,19,21	0.65	0
2	NAG	H	1	2	14,14,15	0.54	0	17,19,21	1.66	4 (23%)
2	NAG	H	2	2	14,14,15	0.66	0	17,19,21	1.18	1 (5%)
2	NAG	I	1	2	14,14,15	0.51	0	17,19,21	0.89	0
2	NAG	I	2	2	14,14,15	0.49	0	17,19,21	0.82	0
2	NAG	J	1	2	14,14,15	0.69	0	17,19,21	1.15	2 (11%)
2	NAG	J	2	2	14,14,15	0.52	0	17,19,21	1.18	3 (17%)
2	NAG	K	1	2	14,14,15	0.60	0	17,19,21	0.94	0
2	NAG	K	2	2	14,14,15	0.52	0	17,19,21	1.63	3 (17%)
2	NAG	L	1	2	14,14,15	0.64	0	17,19,21	1.64	2 (11%)
2	NAG	L	2	2	14,14,15	0.54	0	17,19,21	1.41	3 (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	NAG	E	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	NAG	F	1	2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
2	NAG	G	1	2	-	3/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	NAG	H	1	2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	3/6/23/26	0/1/1/1
2	NAG	I	1	2	-	4/6/23/26	0/1/1/1
2	NAG	I	2	2	-	4/6/23/26	0/1/1/1
2	NAG	J	1	2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	4/6/23/26	0/1/1/1
2	NAG	K	1	2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C1-O5-C5	5.72	119.85	112.19
2	K	2	NAG	C1-O5-C5	4.64	118.41	112.19
2	F	2	NAG	C1-O5-C5	4.64	118.40	112.19
2	L	1	NAG	O5-C1-C2	-4.06	105.01	111.29
2	L	1	NAG	C3-C4-C5	4.06	117.59	110.23
2	F	1	NAG	C1-O5-C5	-3.65	107.29	112.19
2	H	1	NAG	C3-C4-C5	3.61	116.77	110.23
2	E	2	NAG	C4-C3-C2	3.58	116.27	111.02
2	G	1	NAG	O5-C1-C2	-3.40	106.04	111.29
2	G	1	NAG	C3-C4-C5	3.25	116.13	110.23
2	H	1	NAG	O5-C1-C2	-3.08	106.52	111.29
2	L	2	NAG	C2-N2-C7	2.97	126.88	122.90
2	H	1	NAG	C1-O5-C5	2.93	116.11	112.19
2	E	1	NAG	C2-N2-C7	2.92	126.82	122.90
2	J	2	NAG	C1-O5-C5	2.92	116.10	112.19
2	H	2	NAG	C4-C3-C2	2.91	115.29	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	NAG	O5-C1-C2	-2.88	106.84	111.29
2	L	2	NAG	C4-C3-C2	2.76	115.06	111.02
2	L	2	NAG	C8-C7-N2	2.69	120.57	116.12
2	K	2	NAG	C8-C7-N2	2.65	120.52	116.12
2	F	2	NAG	C8-C7-N2	2.56	120.37	116.12
2	K	2	NAG	O7-C7-C8	-2.53	117.55	122.05
2	G	1	NAG	C4-C3-C2	2.49	114.67	111.02
2	H	1	NAG	O5-C5-C4	2.41	116.69	110.83
2	J	1	NAG	C3-C4-C5	2.41	114.59	110.23
2	E	1	NAG	C1-C2-N2	2.19	113.88	110.43
2	J	2	NAG	C2-N2-C7	2.18	125.83	122.90
2	J	2	NAG	C8-C7-N2	2.18	119.74	116.12
2	F	2	NAG	O7-C7-C8	-2.10	118.32	122.05

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C3-C2-N2-C7
2	H	2	NAG	O7-C7-N2-C2
2	I	2	NAG	C8-C7-N2-C2
2	I	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	I	2	NAG	O5-C5-C6-O6
2	H	1	NAG	C8-C7-N2-C2
2	E	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	H	1	NAG	O7-C7-N2-C2
2	K	2	NAG	C8-C7-N2-C2
2	K	2	NAG	O7-C7-N2-C2
2	I	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	J	2	NAG	C8-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2
2	L	2	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

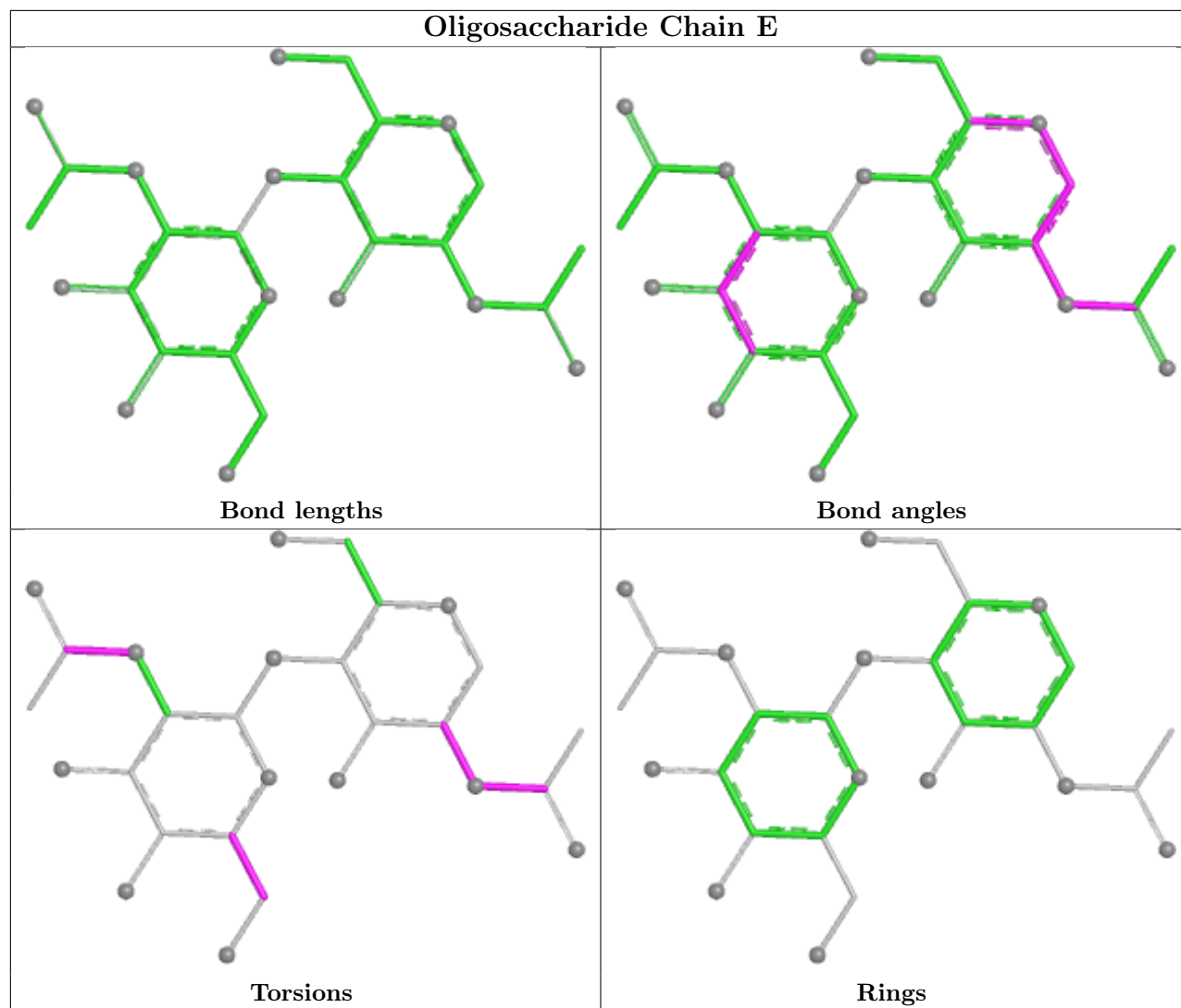
Mol	Chain	Res	Type	Atoms
2	L	2	NAG	O7-C7-N2-C2
2	G	2	NAG	O5-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O5-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O7-C7-N2-C2
2	E	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	L	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C3-C2-N2-C7
2	I	1	NAG	C8-C7-N2-C2
2	E	1	NAG	C1-C2-N2-C7
2	I	1	NAG	O7-C7-N2-C2
2	I	1	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6

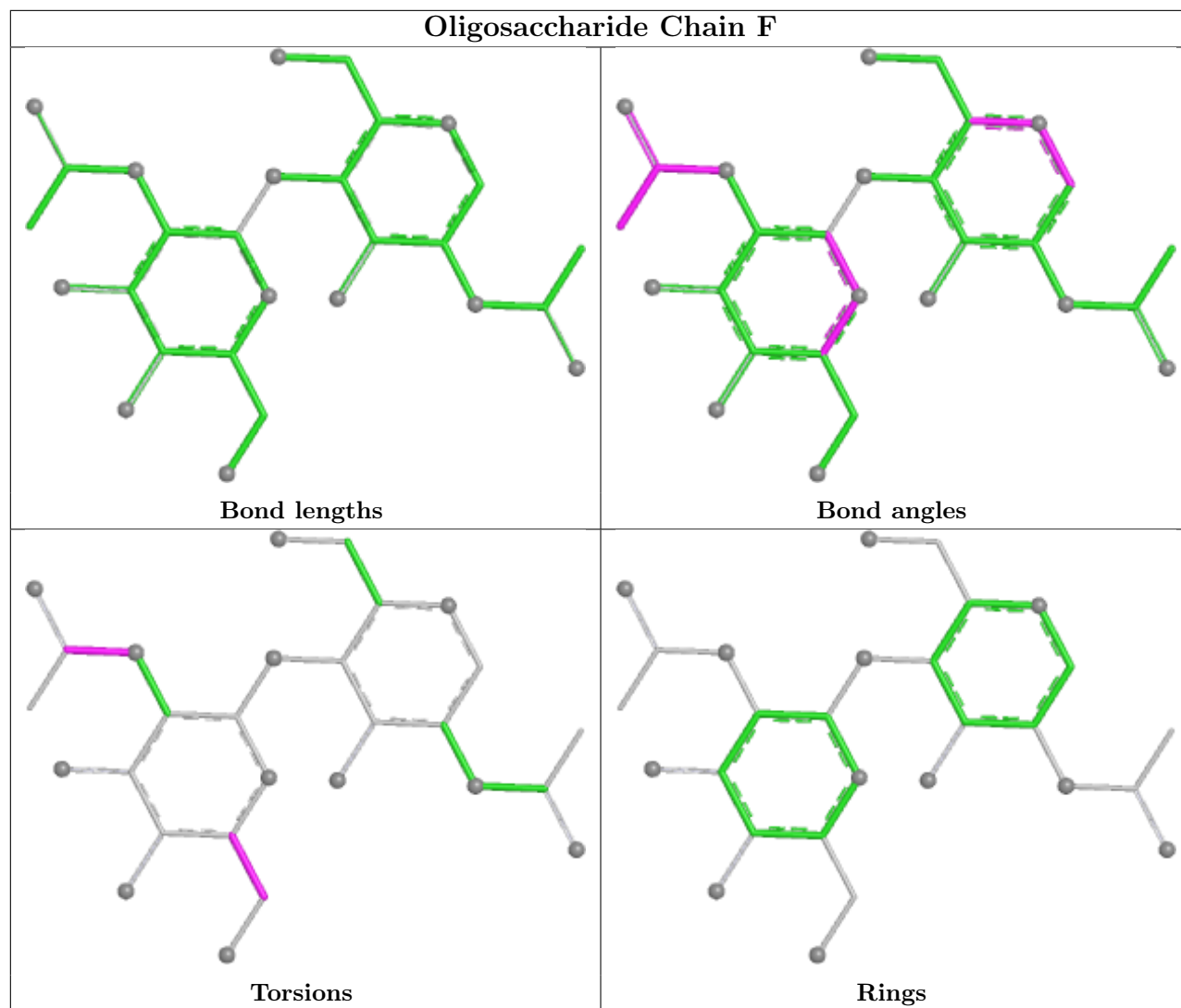
There are no ring outliers.

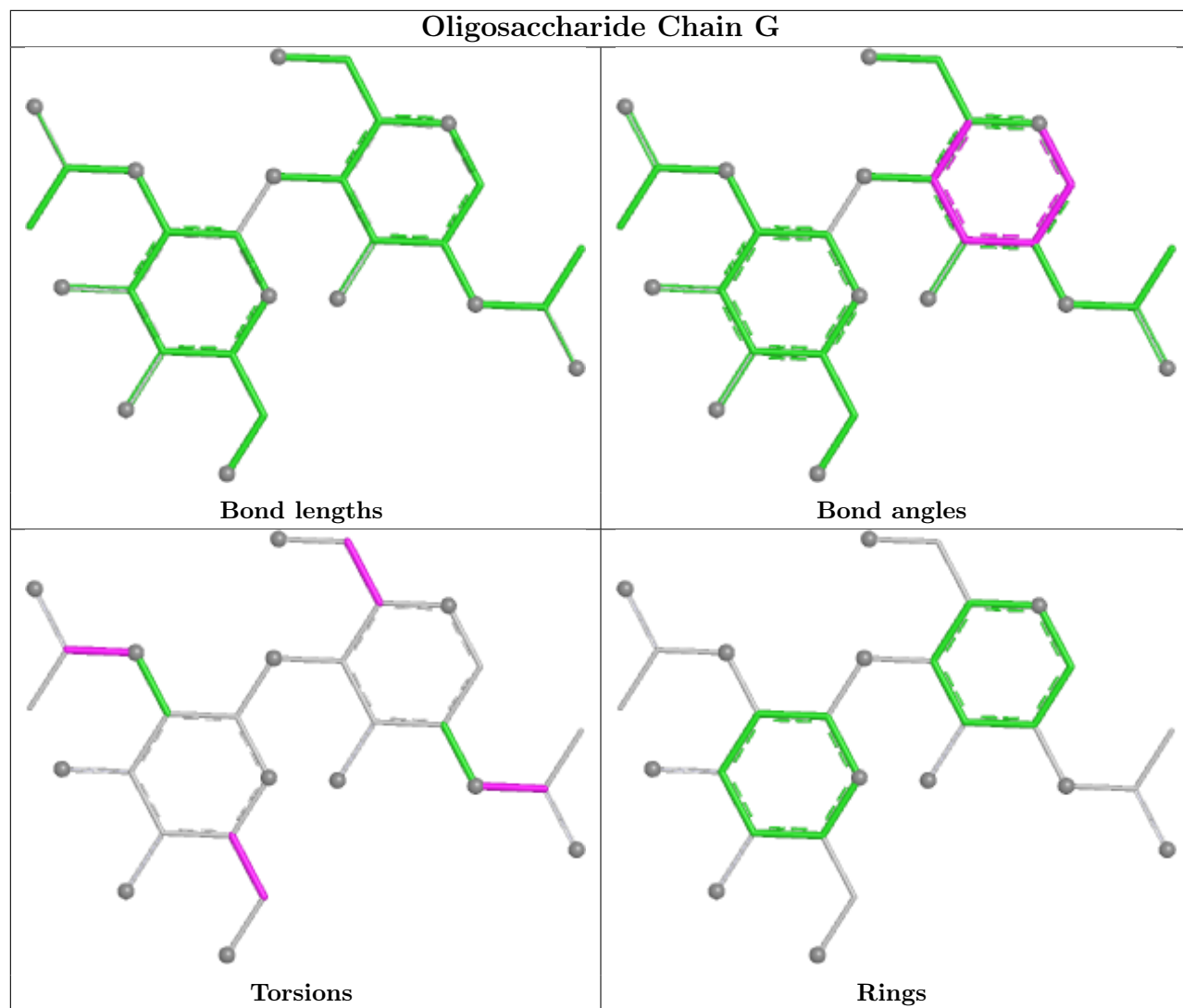
7 monomers are involved in 16 short contacts:

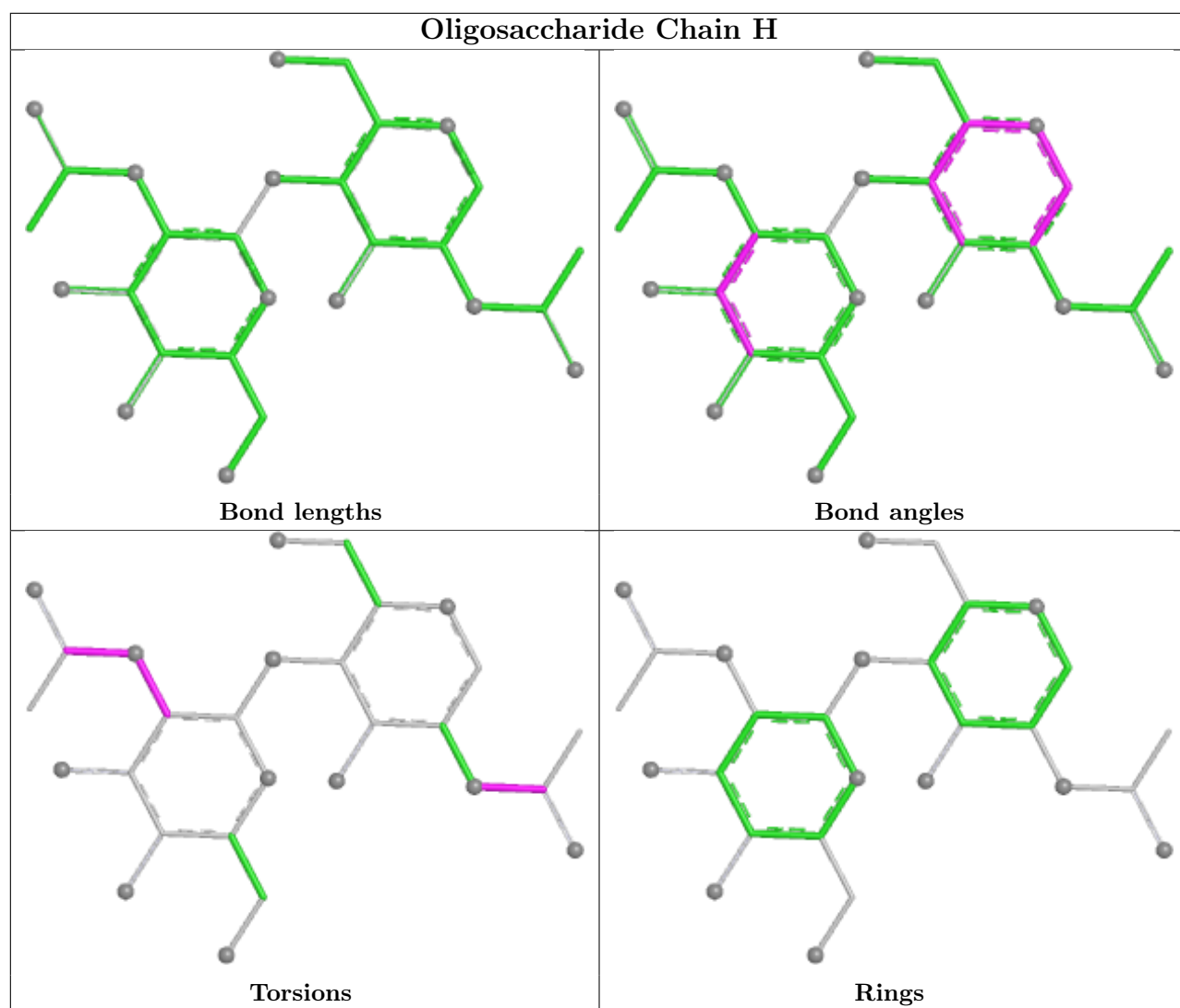
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAG	2	0
2	J	1	NAG	2	0
2	L	1	NAG	5	0
2	K	1	NAG	3	0
2	H	1	NAG	3	0
2	H	2	NAG	1	0
2	G	1	NAG	1	0

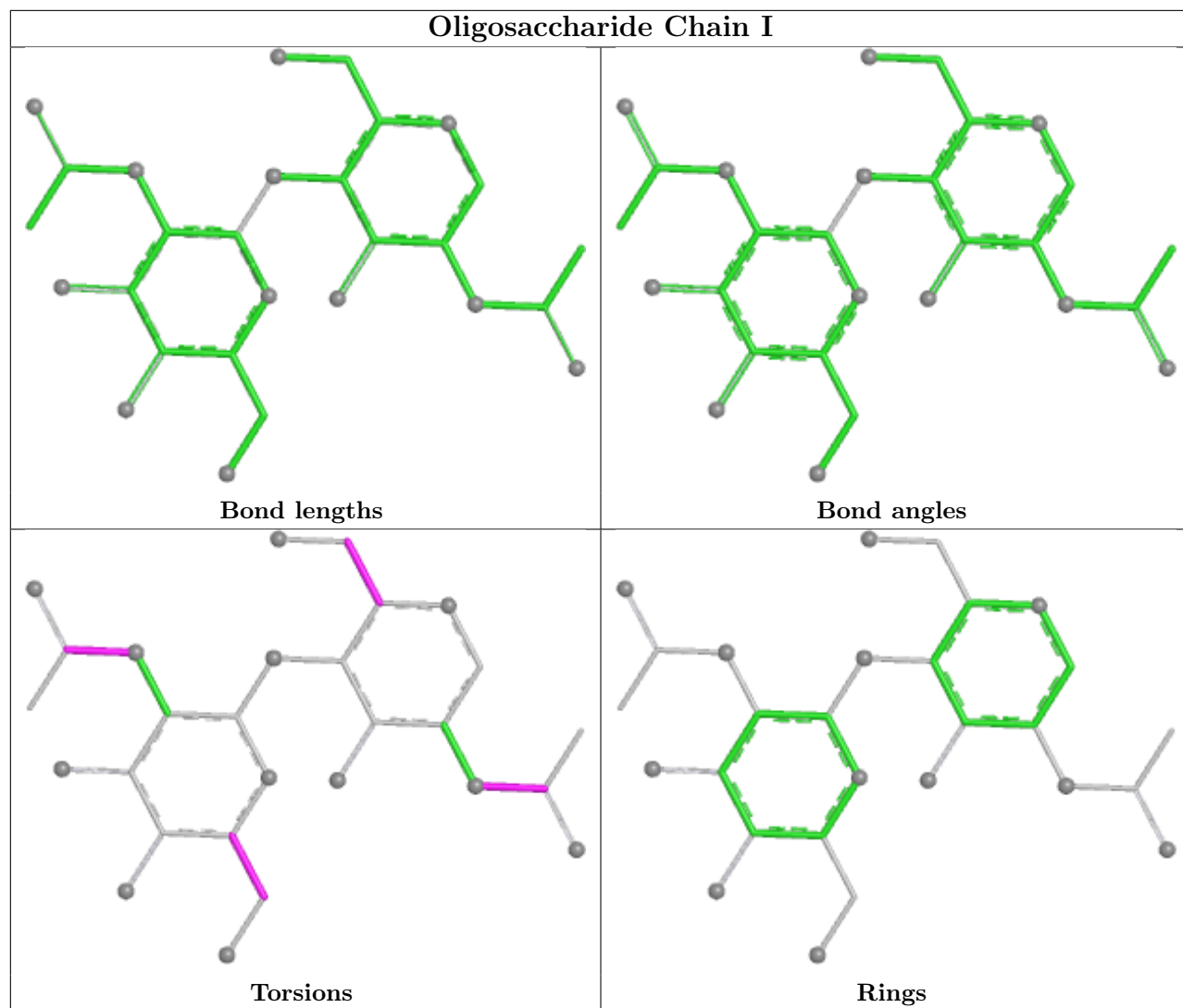
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

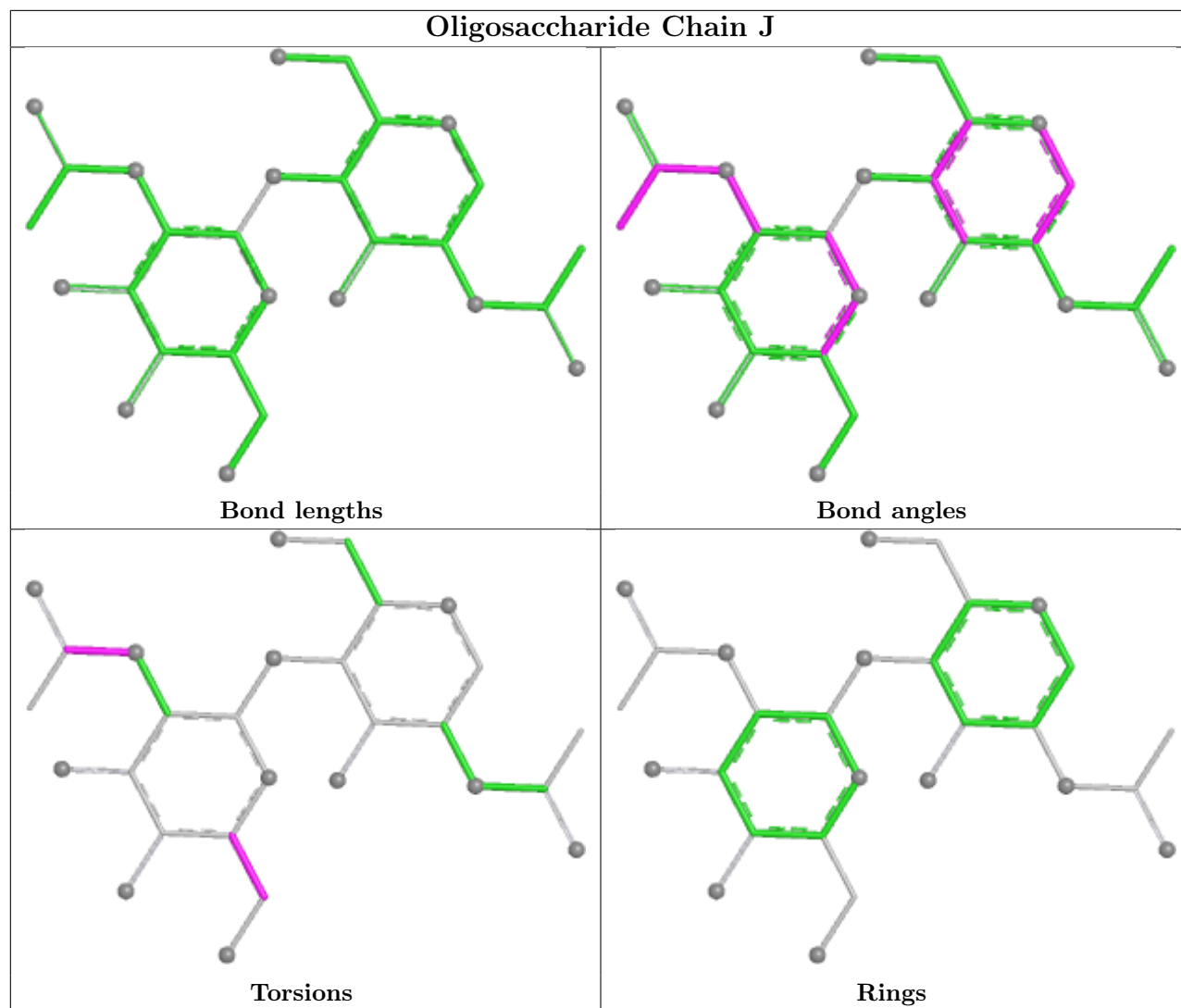


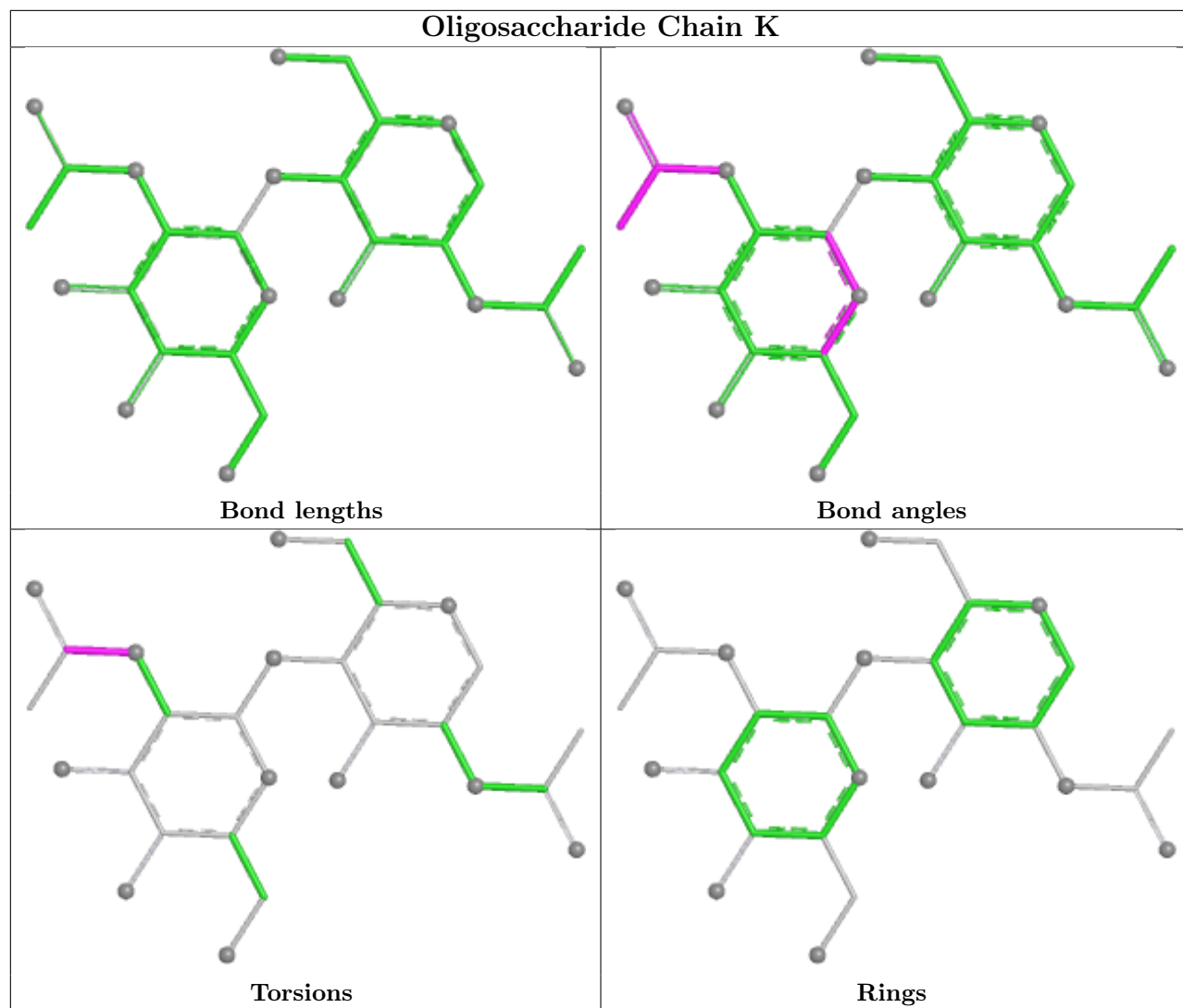


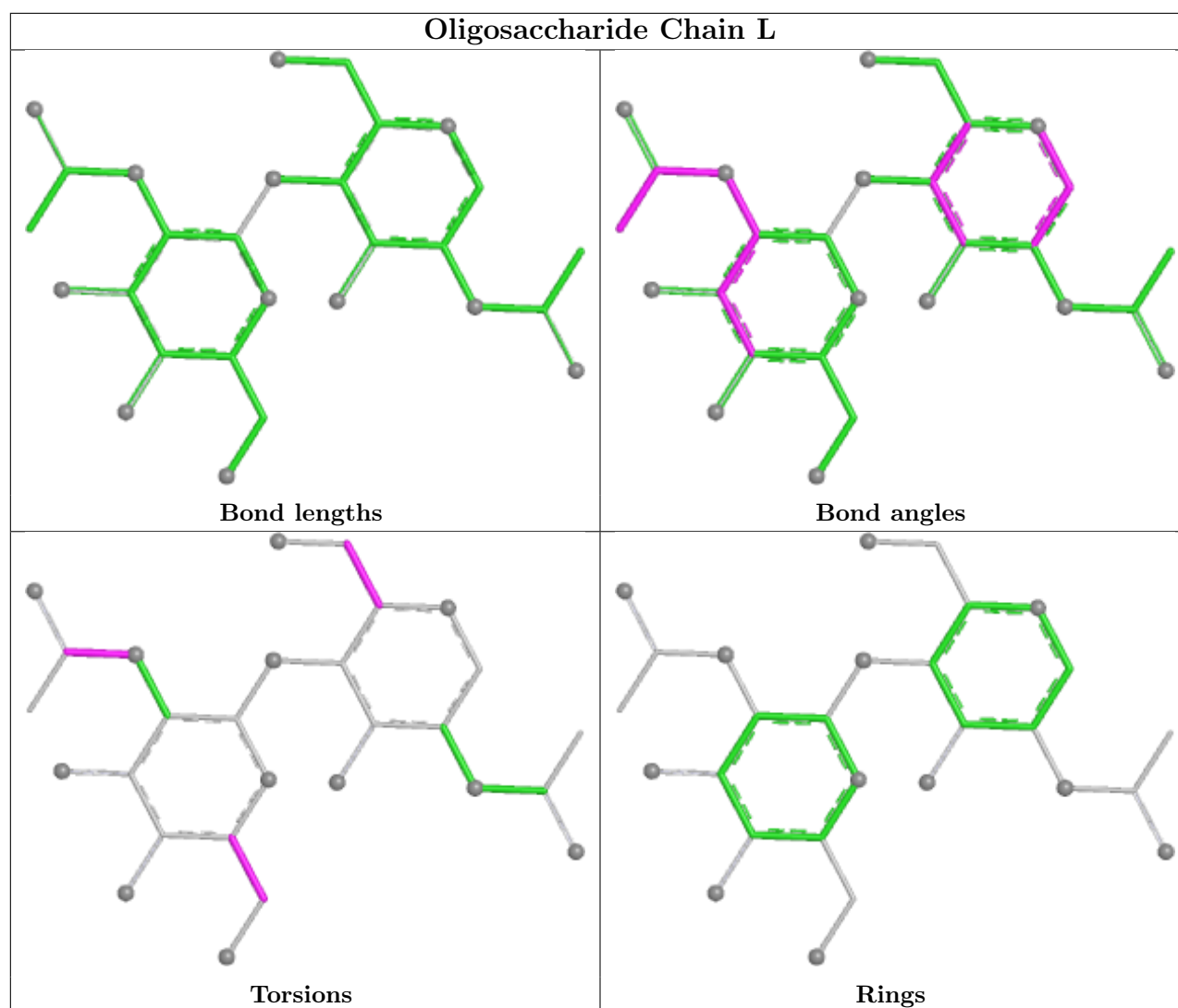












5.6 Ligand geometry [i](#)

21 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	$\# Z > 2$
4	T22	A	805	-	26,27,27	2.15	2 (7%)	31,38,38	2.64	7 (22%)
4	T22	B	805	-	26,27,27	2.15	2 (7%)	31,38,38	2.64	7 (22%)
3	NAG	A	802	-	14,14,15	0.63	0	17,19,21	1.02	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	803	-	14,14,15	0.48	0	17,19,21	0.83	1 (5%)
3	NAG	C	801	-	14,14,15	0.57	0	17,19,21	1.29	2 (11%)
3	NAG	C	804	-	14,14,15	0.64	0	17,19,21	1.42	2 (11%)
3	NAG	B	801	-	14,14,15	0.46	0	17,19,21	0.99	1 (5%)
3	NAG	A	801	-	14,14,15	0.51	0	17,19,21	0.65	0
3	NAG	C	802	-	14,14,15	0.51	0	17,19,21	0.81	0
4	T22	D	806	-	26,27,27	2.15	2 (7%)	31,38,38	2.62	7 (22%)
3	NAG	A	804	-	14,14,15	0.47	0	17,19,21	0.80	0
3	NAG	D	804	1	14,14,15	0.55	0	17,19,21	1.22	2 (11%)
3	NAG	D	802	-	14,14,15	0.60	0	17,19,21	1.28	2 (11%)
3	NAG	D	801	1	14,14,15	1.16	1 (7%)	17,19,21	1.75	5 (29%)
3	NAG	A	803	-	14,14,15	0.54	0	17,19,21	1.43	5 (29%)
3	NAG	D	805	-	14,14,15	0.47	0	17,19,21	1.14	2 (11%)
3	NAG	D	803	1	14,14,15	0.77	0	17,19,21	1.36	2 (11%)
3	NAG	B	804	-	14,14,15	0.54	0	17,19,21	1.19	1 (5%)
3	NAG	C	803	1	14,14,15	0.58	0	17,19,21	1.00	1 (5%)
3	NAG	B	802	-	14,14,15	0.53	0	17,19,21	1.21	1 (5%)
4	T22	C	805	-	26,27,27	2.15	2 (7%)	31,38,38	2.63	7 (22%)

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
4	T22	A	805	-	-	1/10/20/20	0/3/3/3
4	T22	B	805	-	-	1/10/20/20	0/3/3/3
3	NAG	A	802	-	-	3/6/23/26	0/1/1/1
3	NAG	B	803	-	-	4/6/23/26	0/1/1/1
3	NAG	C	801	-	-	3/6/23/26	0/1/1/1
3	NAG	C	804	-	-	2/6/23/26	0/1/1/1
3	NAG	B	801	-	-	4/6/23/26	0/1/1/1
3	NAG	A	801	-	-	2/6/23/26	0/1/1/1
3	NAG	C	802	-	-	4/6/23/26	0/1/1/1
4	T22	D	806	-	-	1/10/20/20	0/3/3/3
3	NAG	A	804	-	-	5/6/23/26	0/1/1/1
3	NAG	D	804	1	1/1/5/7	4/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	802	-	-	3/6/23/26	0/1/1/1
3	NAG	D	801	1	-	3/6/23/26	0/1/1/1
3	NAG	A	803	-	-	4/6/23/26	0/1/1/1
3	NAG	D	805	-	-	2/6/23/26	0/1/1/1
3	NAG	D	803	1	-	2/6/23/26	0/1/1/1
3	NAG	B	804	-	-	0/6/23/26	0/1/1/1
3	NAG	C	803	1	-	2/6/23/26	0/1/1/1
3	NAG	B	802	-	-	4/6/23/26	0/1/1/1
4	T22	C	805	-	-	1/10/20/20	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	805	T22	C22-C23	-9.24	1.31	1.44
4	A	805	T22	C22-C23	-9.24	1.31	1.44
4	D	806	T22	C22-C23	-9.23	1.31	1.44
4	C	805	T22	C22-C23	-9.22	1.31	1.44
3	D	801	NAG	O5-C1	-3.90	1.37	1.43
4	C	805	T22	C3-N2	-2.48	1.35	1.40
4	A	805	T22	C3-N2	-2.46	1.35	1.40
4	B	805	T22	C3-N2	-2.44	1.35	1.40
4	D	806	T22	C3-N2	-2.42	1.35	1.40

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	805	T22	C5-C6-N7	-8.93	114.68	125.28
4	A	805	T22	C5-C6-N7	-8.93	114.69	125.28
4	C	805	T22	C5-C6-N7	-8.91	114.71	125.28
4	D	806	T22	C5-C6-N7	-8.89	114.73	125.28
4	C	805	T22	C5-C3-N2	5.48	120.50	115.36
4	A	805	T22	C5-C3-N2	5.47	120.49	115.36
4	B	805	T22	C5-C3-N2	5.45	120.48	115.36
4	D	806	T22	C5-C3-N2	5.42	120.45	115.36
4	B	805	T22	C3-N2-C25	-5.31	120.31	124.58
4	A	805	T22	C3-N2-C25	-5.26	120.34	124.58
4	C	805	T22	C3-N2-C25	-5.25	120.36	124.58
4	D	806	T22	C3-N2-C25	-5.24	120.36	124.58
3	D	803	NAG	C4-C3-C2	4.39	117.46	111.02
3	C	804	NAG	C4-C3-C2	4.34	117.37	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	805	T22	N15-C25-N2	3.77	121.37	116.72
4	A	805	T22	N15-C25-N2	3.73	121.31	116.72
3	D	801	NAG	C2-N2-C7	3.72	127.88	122.90
4	C	805	T22	N15-C25-N2	3.72	121.30	116.72
4	D	806	T22	N15-C25-N2	3.70	121.28	116.72
4	C	805	T22	O4-C3-C5	-3.32	117.41	125.61
4	A	805	T22	O4-C3-C5	-3.32	117.43	125.61
4	B	805	T22	O4-C3-C5	-3.31	117.44	125.61
4	D	806	T22	O4-C3-C5	-3.29	117.49	125.61
3	D	804	NAG	C1-O5-C5	3.17	116.44	112.19
3	D	801	NAG	C1-O5-C5	3.13	116.38	112.19
4	C	805	T22	C17-C22-C23	3.09	123.04	120.16
4	B	805	T22	C17-C22-C23	3.09	123.04	120.16
3	D	802	NAG	C3-C4-C5	3.07	115.80	110.23
4	A	805	T22	C17-C22-C23	3.07	123.02	120.16
4	D	806	T22	C17-C22-C23	3.03	122.98	120.16
3	C	801	NAG	O5-C1-C2	-2.92	106.77	111.29
3	C	804	NAG	C3-C4-C5	2.86	115.42	110.23
3	B	804	NAG	O5-C1-C2	-2.83	106.92	111.29
3	A	803	NAG	C2-N2-C7	2.81	126.67	122.90
3	D	804	NAG	C2-N2-C7	2.74	126.58	122.90
3	C	801	NAG	C3-C4-C5	2.68	115.10	110.23
3	A	803	NAG	C3-C4-C5	2.64	115.02	110.23
3	A	803	NAG	C1-O5-C5	2.52	115.56	112.19
3	D	801	NAG	C4-C3-C2	-2.46	107.41	111.02
3	C	803	NAG	C1-O5-C5	2.45	115.47	112.19
3	B	802	NAG	O5-C1-C2	-2.42	107.55	111.29
3	A	802	NAG	O5-C5-C6	2.31	112.16	107.66
3	D	805	NAG	C8-C7-N2	2.24	119.84	116.12
3	D	801	NAG	O3-C3-C2	2.21	114.00	109.40
4	B	805	T22	C1-N2-C3	2.20	120.92	117.87
3	D	803	NAG	C3-C4-C5	2.20	114.22	110.23
4	C	805	T22	C1-N2-C3	2.19	120.91	117.87
4	A	805	T22	C1-N2-C3	2.18	120.90	117.87
4	D	806	T22	C1-N2-C3	2.16	120.87	117.87
3	D	805	NAG	O5-C1-C2	-2.12	108.00	111.29
3	A	803	NAG	C4-C3-C2	2.11	114.11	111.02
3	B	803	NAG	C1-O5-C5	2.11	115.01	112.19
3	D	801	NAG	O5-C1-C2	-2.10	108.04	111.29
3	A	803	NAG	C1-C2-N2	2.08	113.71	110.43
3	D	802	NAG	C1-O5-C5	2.05	114.94	112.19
3	B	801	NAG	O5-C1-C2	-2.05	108.12	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	804	NAG	C1

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	NAG	C8-C7-N2-C2
3	A	801	NAG	O7-C7-N2-C2
3	A	802	NAG	C8-C7-N2-C2
3	A	802	NAG	O7-C7-N2-C2
3	A	803	NAG	C1-C2-N2-C7
3	A	803	NAG	C8-C7-N2-C2
3	A	803	NAG	O7-C7-N2-C2
3	A	804	NAG	C8-C7-N2-C2
3	A	804	NAG	O7-C7-N2-C2
3	B	801	NAG	O7-C7-N2-C2
3	B	802	NAG	C8-C7-N2-C2
3	B	802	NAG	O7-C7-N2-C2
3	B	803	NAG	C8-C7-N2-C2
3	B	803	NAG	O7-C7-N2-C2
3	C	801	NAG	C8-C7-N2-C2
3	C	801	NAG	O7-C7-N2-C2
3	D	801	NAG	C1-C2-N2-C7
3	D	802	NAG	O7-C7-N2-C2
3	D	804	NAG	C1-C2-N2-C7
3	D	804	NAG	C8-C7-N2-C2
3	D	804	NAG	O7-C7-N2-C2
3	B	801	NAG	C8-C7-N2-C2
3	D	802	NAG	C8-C7-N2-C2
3	C	802	NAG	C8-C7-N2-C2
3	C	802	NAG	O7-C7-N2-C2
3	D	805	NAG	C8-C7-N2-C2
3	C	804	NAG	O5-C5-C6-O6
3	B	802	NAG	O5-C5-C6-O6
3	C	802	NAG	O5-C5-C6-O6
3	B	803	NAG	O5-C5-C6-O6
3	C	804	NAG	C4-C5-C6-O6
3	B	801	NAG	O5-C5-C6-O6
3	D	805	NAG	O7-C7-N2-C2
3	B	801	NAG	C4-C5-C6-O6
3	B	803	NAG	C4-C5-C6-O6
3	C	802	NAG	C4-C5-C6-O6
3	B	802	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	803	NAG	C4-C5-C6-O6
3	D	803	NAG	O5-C5-C6-O6
3	A	804	NAG	C4-C5-C6-O6
3	A	802	NAG	O5-C5-C6-O6
3	D	804	NAG	O5-C5-C6-O6
3	A	804	NAG	O5-C5-C6-O6
3	A	803	NAG	O5-C5-C6-O6
4	A	805	T22	N15-C16-C17-C22
4	B	805	T22	N15-C16-C17-C22
4	C	805	T22	N15-C16-C17-C22
4	D	806	T22	N15-C16-C17-C22
3	D	802	NAG	C4-C5-C6-O6
3	C	803	NAG	C8-C7-N2-C2
3	C	801	NAG	C1-C2-N2-C7
3	A	804	NAG	C3-C2-N2-C7
3	C	803	NAG	O7-C7-N2-C2
3	D	801	NAG	O7-C7-N2-C2
3	D	801	NAG	C8-C7-N2-C2

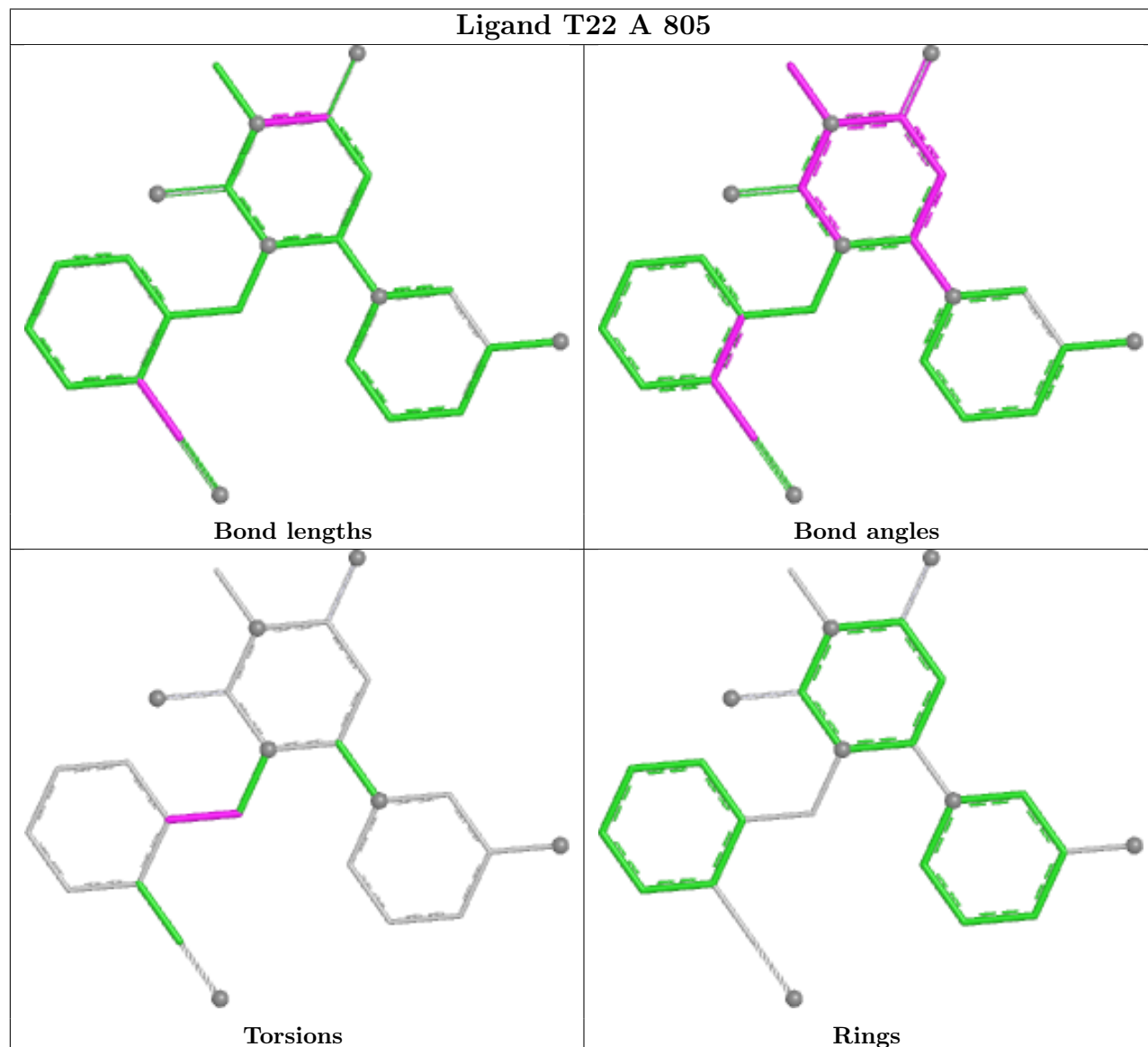
There are no ring outliers.

16 monomers are involved in 20 short contacts:

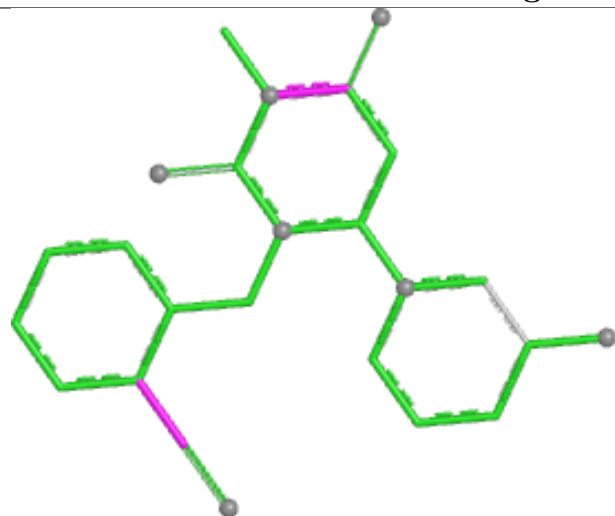
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	805	T22	1	0
4	B	805	T22	1	0
3	B	803	NAG	1	0
3	C	801	NAG	1	0
3	C	804	NAG	1	0
3	B	801	NAG	1	0
3	A	801	NAG	1	0
3	C	802	NAG	1	0
4	D	806	T22	1	0
3	D	804	NAG	1	0
3	D	802	NAG	1	0
3	A	803	NAG	3	0
3	D	805	NAG	2	0
3	B	804	NAG	2	0
3	B	802	NAG	1	0
4	C	805	T22	1	0

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

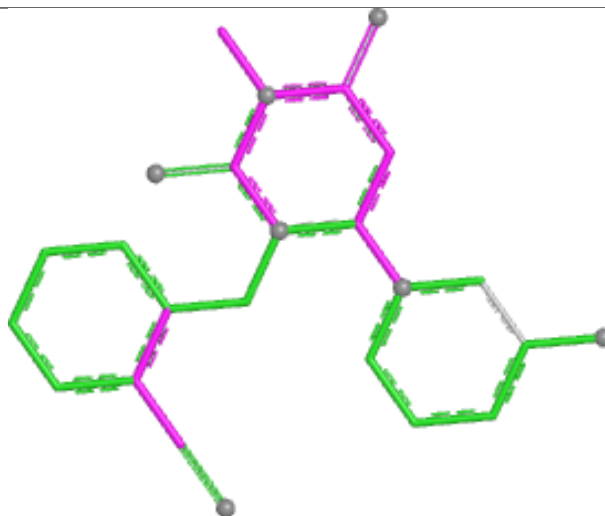
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



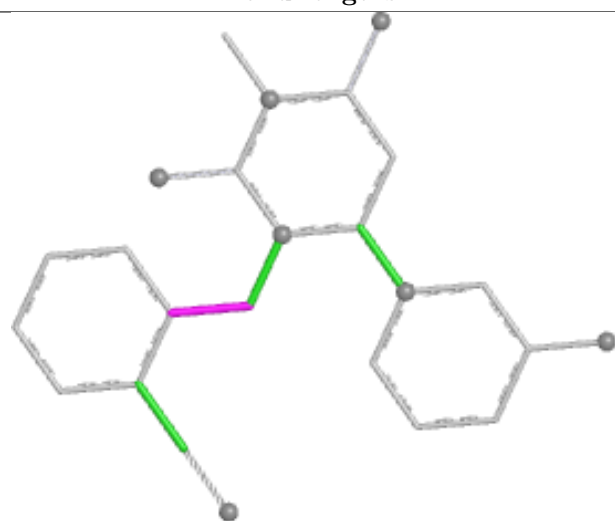
Ligand T22 B 805



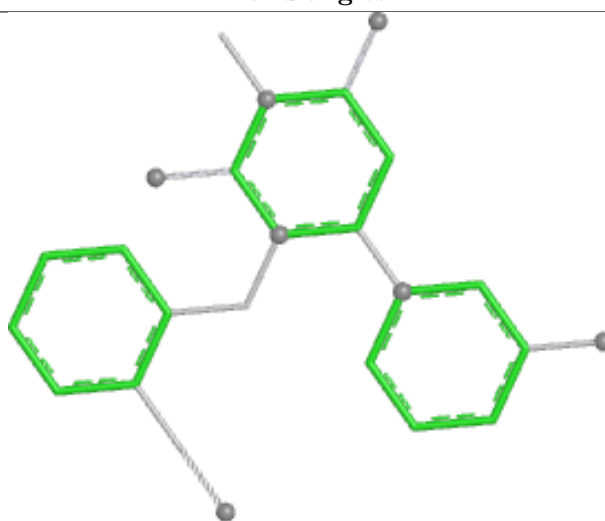
Bond lengths



Bond angles

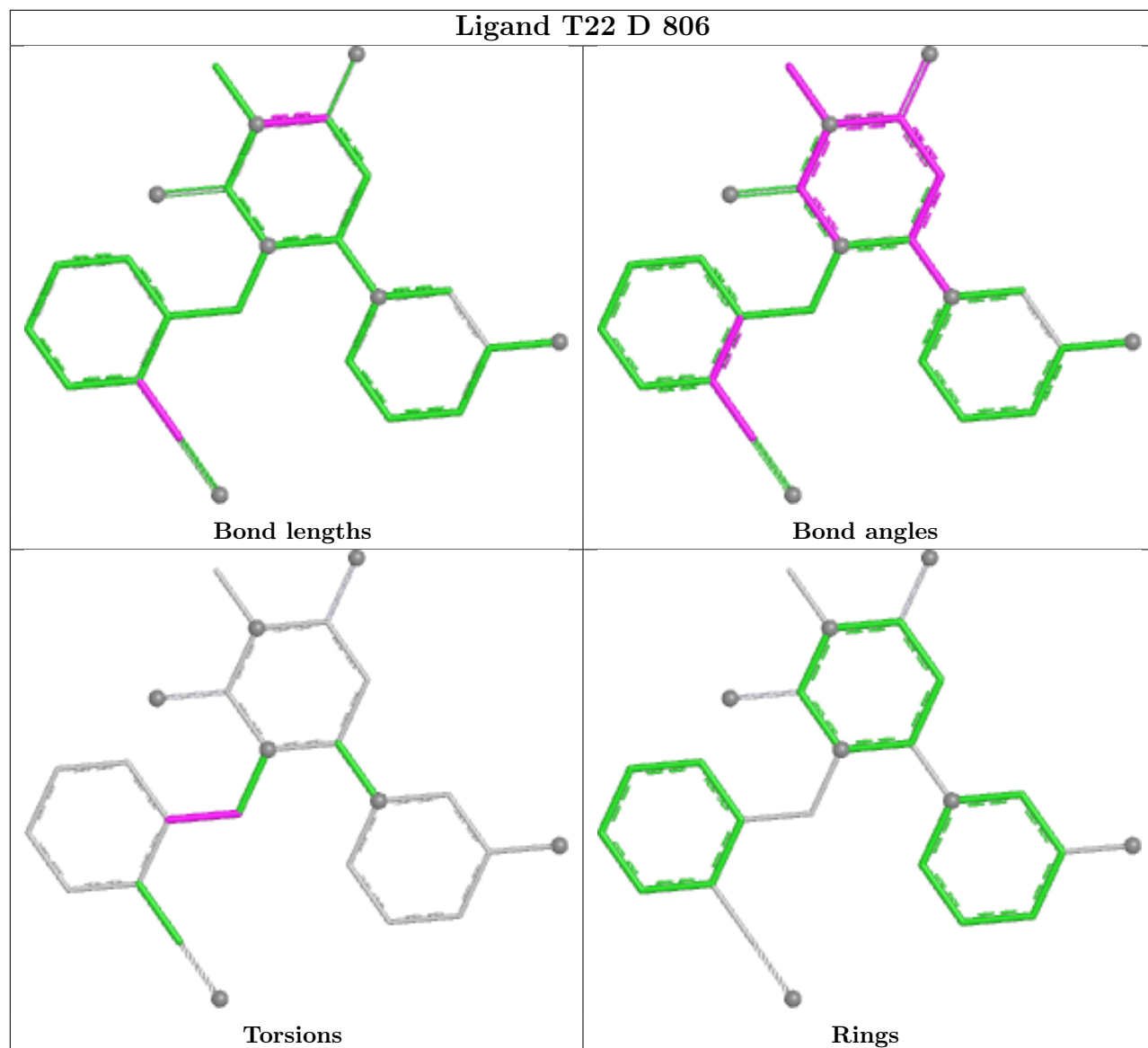


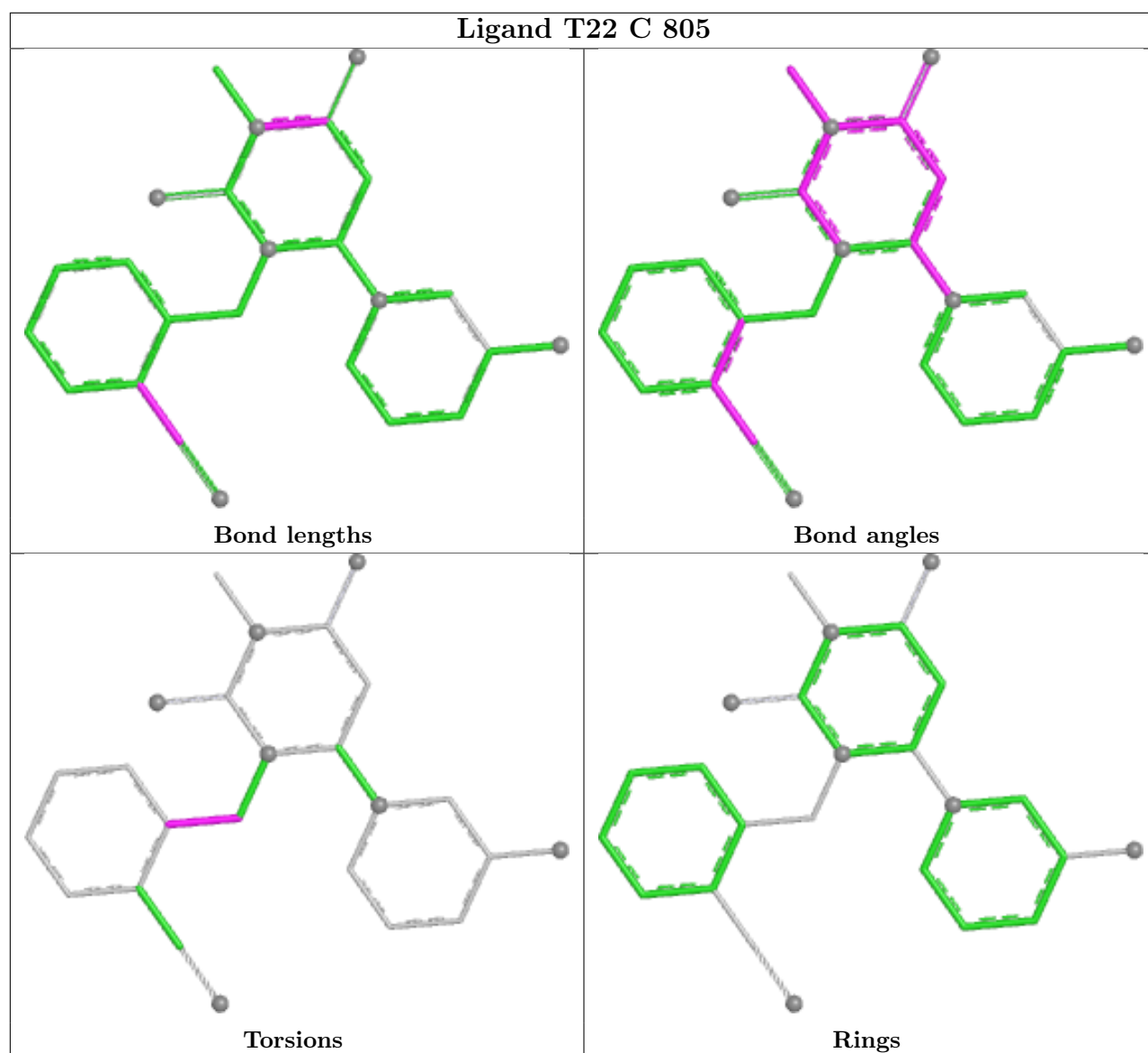
Torsions



Rings

Ligand T22 D 806





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	727/740 (98%)	0.81	46 (6%)	26 24	41, 50, 64, 77	0
1	B	733/740 (99%)	0.83	43 (5%)	28 26	38, 50, 64, 77	0
1	C	726/740 (98%)	1.41	157 (21%)	2 2	44, 51, 73, 88	0
1	D	727/740 (98%)	0.87	38 (5%)	33 31	43, 50, 66, 79	0
All	All	2913/2960 (98%)	0.98	284 (9%)	13 12	38, 50, 67, 88	0

All (284) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	90	LEU	5.5
1	C	244	GLU	4.8
1	C	247	GLN	4.5
1	C	241	TYR	4.5
1	C	322	TYR	4.4
1	C	88	VAL	4.4
1	A	69	LEU	4.4
1	C	248	TYR	4.4
1	C	246	LEU	4.4
1	C	148	ILE	4.4
1	C	134	ILE	4.3
1	C	330	TYR	4.3
1	C	89	PHE	4.3
1	C	734	TRP	4.3
1	C	337	TRP	4.2
1	C	95	PHE	4.2
1	C	249	PRO	4.1
1	C	81	ALA	4.0
1	C	69	LEU	4.0
1	B	734	TRP	3.9
1	C	705	GLY	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	79	PHE	3.9
1	C	135	TYR	3.9
1	C	240	PHE	3.9
1	D	81	ALA	3.9
1	C	77	LEU	3.7
1	C	70	TYR	3.6
1	C	242	SER	3.6
1	C	245	SER	3.6
1	C	105	TYR	3.5
1	D	89	PHE	3.5
1	C	385	CYS	3.5
1	B	736	THR	3.4
1	D	40	ARG	3.4
1	C	243	ASP	3.4
1	C	98	PHE	3.3
1	C	736	THR	3.3
1	C	746	THR	3.3
1	A	84	GLY	3.3
1	C	58	TYR	3.3
1	C	59	SER	3.3
1	C	68	TYR	3.3
1	C	250	LYS	3.2
1	C	236	ILE	3.2
1	C	78	VAL	3.2
1	C	99	GLY	3.2
1	C	178	PRO	3.2
1	C	94	THR	3.2
1	B	717	ALA	3.1
1	C	442	VAL	3.1
1	B	83	TYR	3.1
1	B	338	ASN	3.1
1	C	515	ASP	3.1
1	C	335	GLY	3.1
1	A	486	VAL	3.1
1	B	69	LEU	3.1
1	B	70	TYR	3.0
1	C	143	ILE	3.0
1	B	81	ALA	3.0
1	D	282	ALA	3.0
1	C	76	ILE	3.0
1	C	239	SER	3.0
1	D	202	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	142	LEU	2.9
1	C	486	VAL	2.9
1	C	129	THR	2.9
1	B	711	VAL	2.9
1	C	238	TYR	2.9
1	A	449	LEU	2.9
1	D	279	VAL	2.9
1	B	76	ILE	2.9
1	A	51	ASN	2.9
1	C	338	ASN	2.9
1	C	717	ALA	2.9
1	D	79	PHE	2.9
1	A	86	SER	2.8
1	B	34	HIS	2.8
1	C	470	LEU	2.8
1	C	601	PHE	2.8
1	C	397	ILE	2.8
1	A	79	PHE	2.8
1	D	342	ALA	2.8
1	B	707	ALA	2.8
1	D	90	LEU	2.8
1	C	252	VAL	2.8
1	C	346	ILE	2.7
1	C	762	CYS	2.7
1	C	140	ARG	2.7
1	C	735	TYR	2.7
1	C	457	TYR	2.7
1	C	614	SER	2.7
1	C	348	MET	2.7
1	A	399	LYS	2.6
1	A	283	THR	2.6
1	A	455	GLN	2.6
1	C	124	TRP	2.6
1	C	150	ASN	2.6
1	C	174	VAL	2.6
1	C	251	THR	2.6
1	C	57	LEU	2.6
1	C	707	ALA	2.6
1	A	78	VAL	2.6
1	C	706	THR	2.6
1	D	295	ILE	2.6
1	C	339	CYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	425	MET	2.6
1	A	88	VAL	2.6
1	C	324	VAL	2.6
1	D	354	VAL	2.6
1	A	105	TYR	2.6
1	C	83	TYR	2.6
1	D	59	SER	2.6
1	D	70	TYR	2.6
1	D	76	ILE	2.6
1	B	71	LYS	2.6
1	C	494	LEU	2.5
1	C	394	CYS	2.5
1	C	747	ALA	2.5
1	B	737	ASP	2.5
1	C	733	MET	2.5
1	C	737	ASP	2.5
1	C	62	TRP	2.5
1	D	95	PHE	2.5
1	A	83	TYR	2.5
1	B	241	TYR	2.5
1	C	180	LEU	2.5
1	A	424	GLY	2.5
1	B	89	PHE	2.5
1	C	469	GLN	2.5
1	C	665	VAL	2.5
1	C	114	ILE	2.5
1	A	426	PRO	2.5
1	B	705	GLY	2.5
1	C	255	PRO	2.5
1	B	353	TRP	2.5
1	C	477	LEU	2.5
1	C	589	LYS	2.5
1	C	380	GLY	2.5
1	D	72	GLN	2.5
1	D	257	PRO	2.5
1	B	57	LEU	2.4
1	B	77	LEU	2.4
1	C	92	ASN	2.4
1	C	100	HIS	2.4
1	A	81	ALA	2.4
1	C	604	GLU	2.4
1	C	42	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	93	SER	2.4
1	A	236	ILE	2.4
1	D	98	PHE	2.4
1	C	432	TYR	2.4
1	D	330	TYR	2.4
1	C	84	GLY	2.4
1	C	93	SER	2.4
1	A	98	PHE	2.4
1	B	78	VAL	2.4
1	C	375	ILE	2.4
1	C	164	LEU	2.4
1	C	326	ASP	2.4
1	D	41	LYS	2.4
1	C	360	SER	2.4
1	C	485	SER	2.4
1	C	493	VAL	2.4
1	C	711	VAL	2.4
1	D	394	CYS	2.4
1	A	457	TYR	2.3
1	C	132	TYR	2.3
1	C	439	TYR	2.3
1	B	84	GLY	2.3
1	A	52	THR	2.3
1	C	121	VAL	2.3
1	C	198	ILE	2.3
1	C	60	LEU	2.3
1	C	119	ASN	2.3
1	B	467	TYR	2.3
1	B	706	THR	2.3
1	C	63	ILE	2.3
1	C	66	HIS	2.3
1	C	518	ILE	2.3
1	A	246	LEU	2.3
1	D	276	LEU	2.3
1	C	181	PRO	2.3
1	A	428	GLY	2.3
1	D	471	ARG	2.3
1	D	537	SER	2.3
1	A	442	VAL	2.3
1	B	88	VAL	2.3
1	C	516	PHE	2.3
1	C	639	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	88	VAL	2.3
1	C	702	LEU	2.3
1	C	111	GLY	2.3
1	C	468	TYR	2.3
1	D	83	TYR	2.3
1	B	747	ALA	2.3
1	C	443	THR	2.3
1	D	283	THR	2.3
1	A	295	ILE	2.3
1	C	139	LYS	2.3
1	A	445	LEU	2.2
1	C	222	PHE	2.2
1	C	235	LEU	2.2
1	C	396	PHE	2.2
1	C	713	PHE	2.2
1	A	487	ASN	2.2
1	C	51	ASN	2.2
1	C	253	ARG	2.2
1	C	144	THR	2.2
1	C	86	SER	2.2
1	C	41	LYS	2.2
1	D	236	ILE	2.2
1	B	262	VAL	2.2
1	C	279	VAL	2.2
1	B	38	HIS	2.2
1	A	423	LYS	2.2
1	D	707	ALA	2.2
1	A	70	TYR	2.2
1	A	239	SER	2.2
1	A	102	ILE	2.2
1	B	665	VAL	2.2
1	D	96	ASP	2.2
1	B	733	MET	2.2
1	D	593	ALA	2.2
1	A	173	TYR	2.2
1	C	137	LEU	2.2
1	D	102	ILE	2.2
1	C	354	VAL	2.2
1	C	621	ASN	2.2
1	D	92	ASN	2.2
1	C	91	GLU	2.2
1	C	399	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	474	GLY	2.2
1	D	100	HIS	2.2
1	C	210	ALA	2.2
1	A	43	TYR	2.1
1	A	77	LEU	2.1
1	A	477	LEU	2.1
1	C	703	ILE	2.1
1	C	97	GLU	2.1
1	A	66	HIS	2.1
1	B	335	GLY	2.1
1	B	745	SER	2.1
1	C	87	SER	2.1
1	C	283	THR	2.1
1	C	327	ILE	2.1
1	C	496	ASP	2.1
1	D	78	VAL	2.1
1	B	505	GLN	2.1
1	C	364	PHE	2.1
1	A	259	ALA	2.1
1	B	473	SER	2.1
1	C	152	THR	2.1
1	C	481	THR	2.1
1	D	93	SER	2.1
1	C	175	LYS	2.1
1	A	381	TYR	2.1
1	C	107	ILE	2.1
1	C	384	ILE	2.1
1	B	36	HIS	2.1
1	A	279	VAL	2.1
1	B	202	VAL	2.1
1	A	447	CYS	2.1
1	B	701	LEU	2.1
1	C	340	LEU	2.1
1	D	55	LEU	2.1
1	B	389	ILE	2.1
1	C	590	ILE	2.1
1	A	166	TYR	2.1
1	A	241	TYR	2.1
1	B	341	VAL	2.1
1	D	250	LYS	2.0
1	A	351	THR	2.0
1	B	753	THR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	436	LEU	2.0
1	C	96	ASP	2.0
1	C	393	ASP	2.0
1	C	759	ILE	2.0
1	A	493	VAL	2.0
1	B	40	ARG	2.0
1	C	341	VAL	2.0
1	B	570	THR	2.0
1	C	82	GLU	2.0
1	C	504	LEU	2.0
1	C	147	ARG	2.0

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

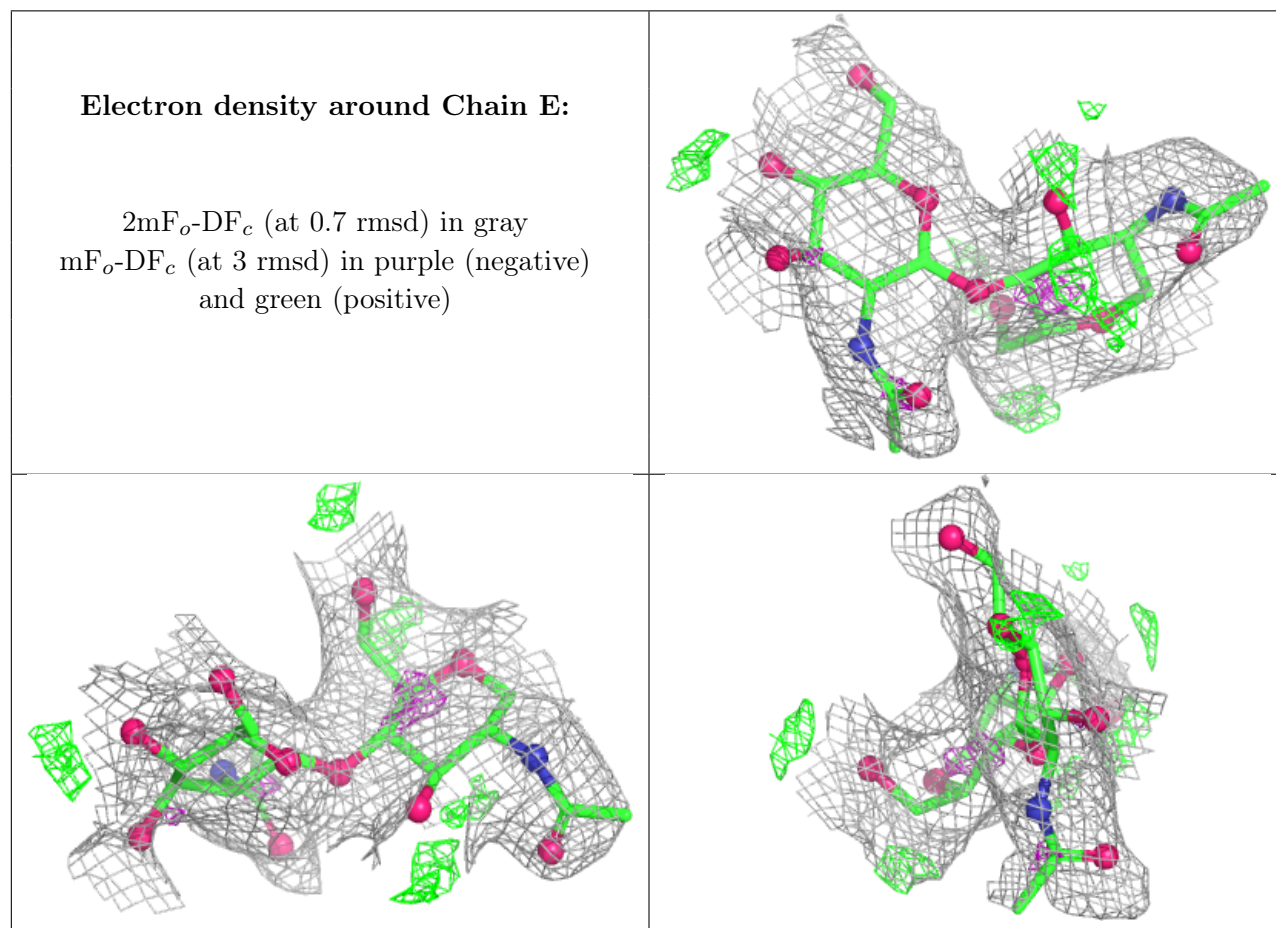
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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.

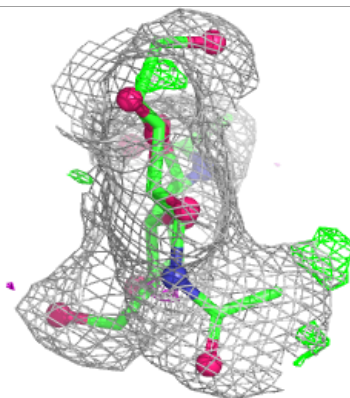
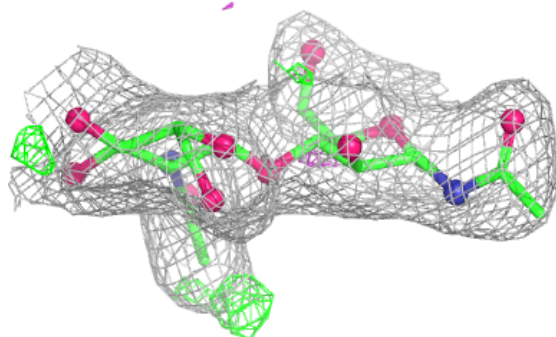
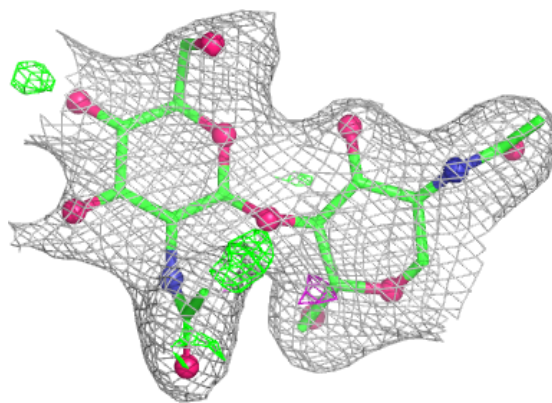
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	G	1	14/15	0.46	0.21	97,101,102,102	0
2	NAG	H	2	14/15	0.48	0.20	106,107,108,108	0
2	NAG	E	2	14/15	0.49	0.17	88,91,91,91	0
2	NAG	J	2	14/15	0.51	0.18	81,85,86,87	0
2	NAG	I	2	14/15	0.59	0.18	117,119,119,119	0
2	NAG	I	1	14/15	0.61	0.18	116,118,119,119	0
2	NAG	E	1	14/15	0.62	0.17	73,78,81,85	0
2	NAG	G	2	14/15	0.62	0.17	102,103,103,103	0
2	NAG	L	2	14/15	0.63	0.17	80,85,87,87	0
2	NAG	K	2	14/15	0.67	0.15	64,65,66,67	0
2	NAG	F	2	14/15	0.69	0.14	71,71,74,74	0
2	NAG	J	1	14/15	0.81	0.14	69,76,79,82	0
2	NAG	H	1	14/15	0.83	0.15	99,102,103,105	0
2	NAG	K	1	14/15	0.84	0.12	54,58,60,62	0
2	NAG	L	1	14/15	0.87	0.12	74,77,79,81	0
2	NAG	F	1	14/15	0.89	0.10	61,66,68,69	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

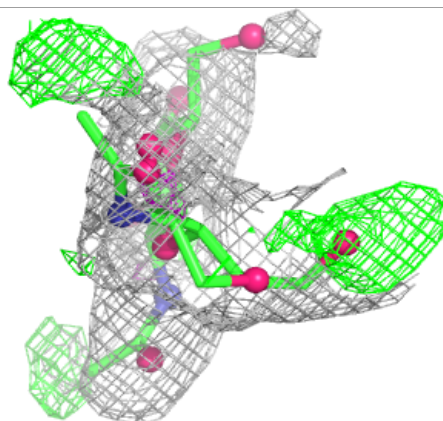
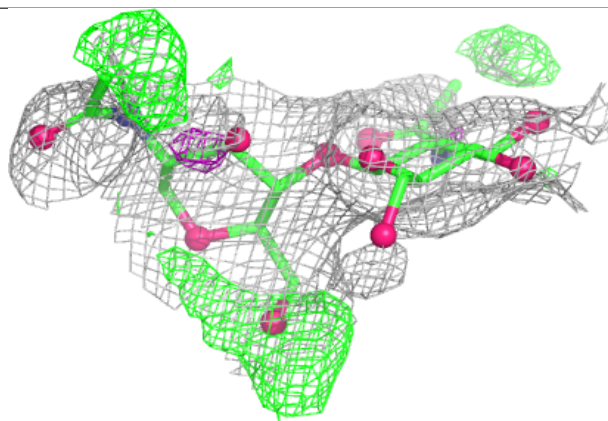
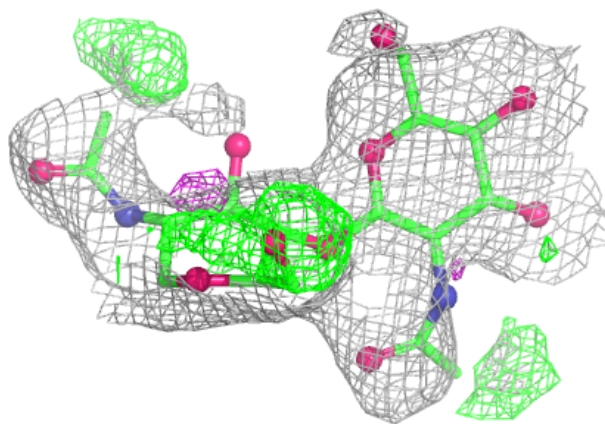


Electron density around Chain F:

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

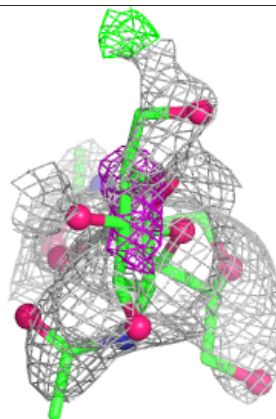
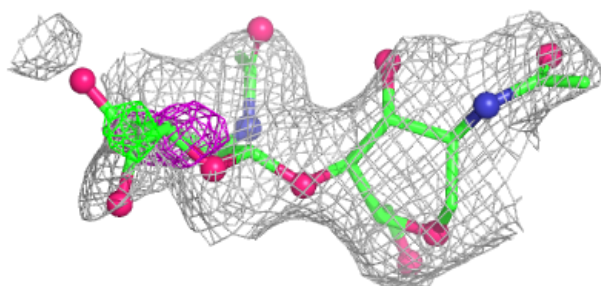
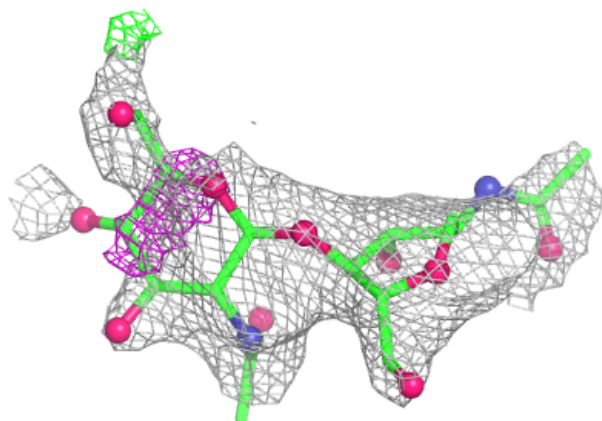
**Electron density around Chain G:**

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



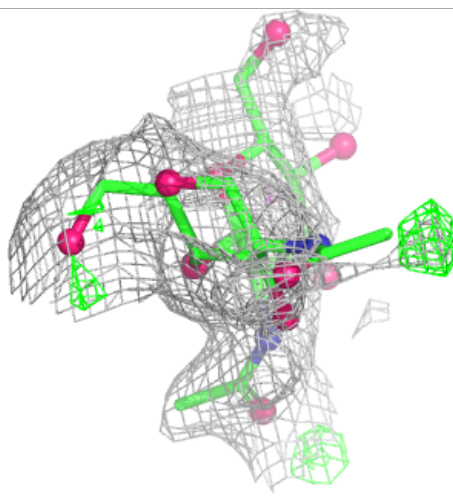
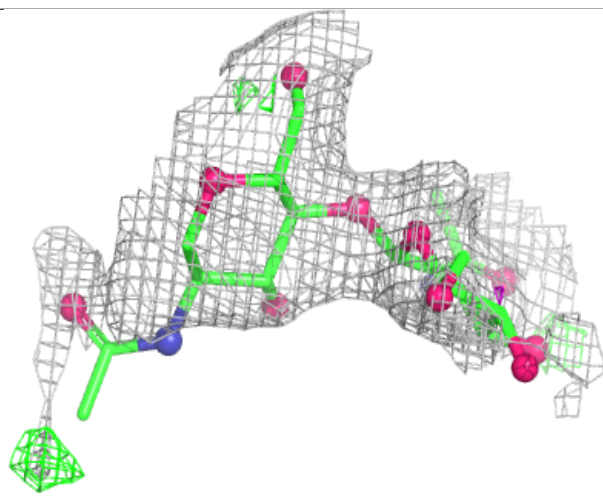
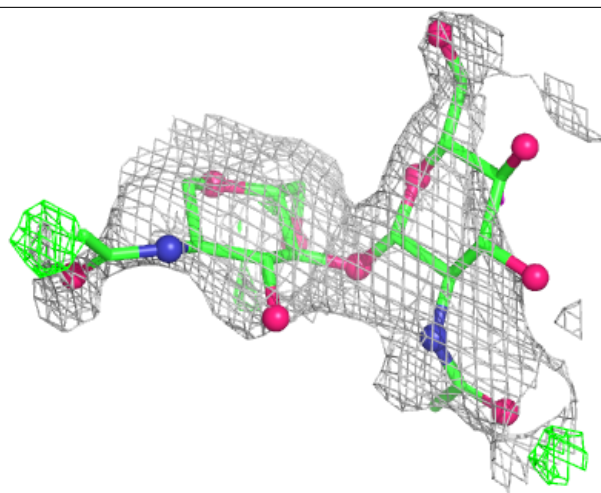
Electron density around Chain H:

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



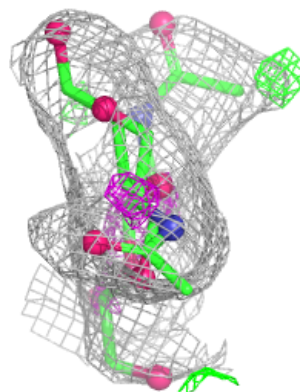
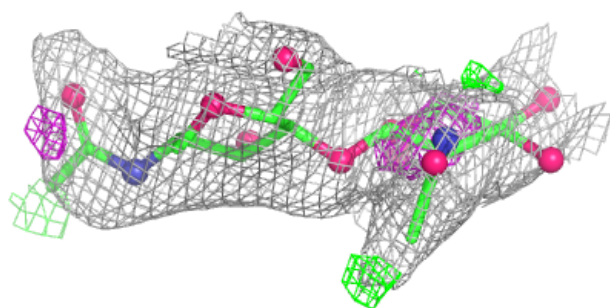
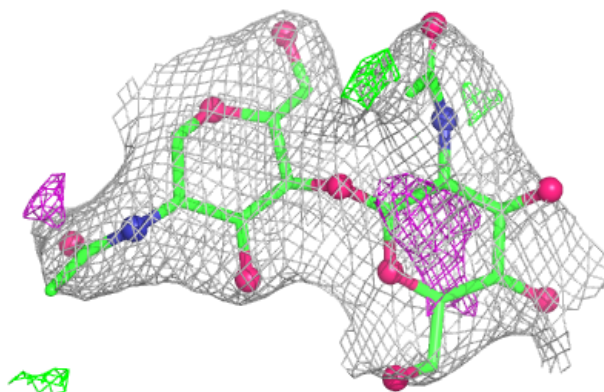
Electron density around Chain I:

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



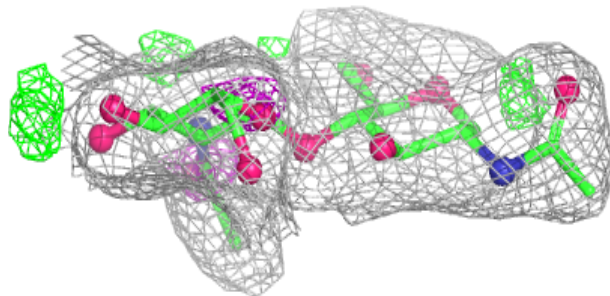
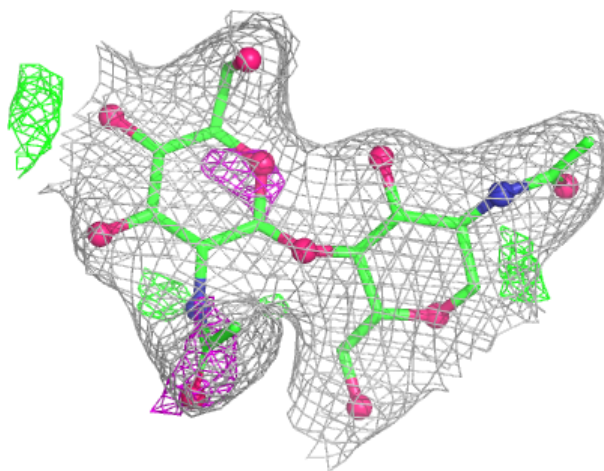
Electron density around Chain J:

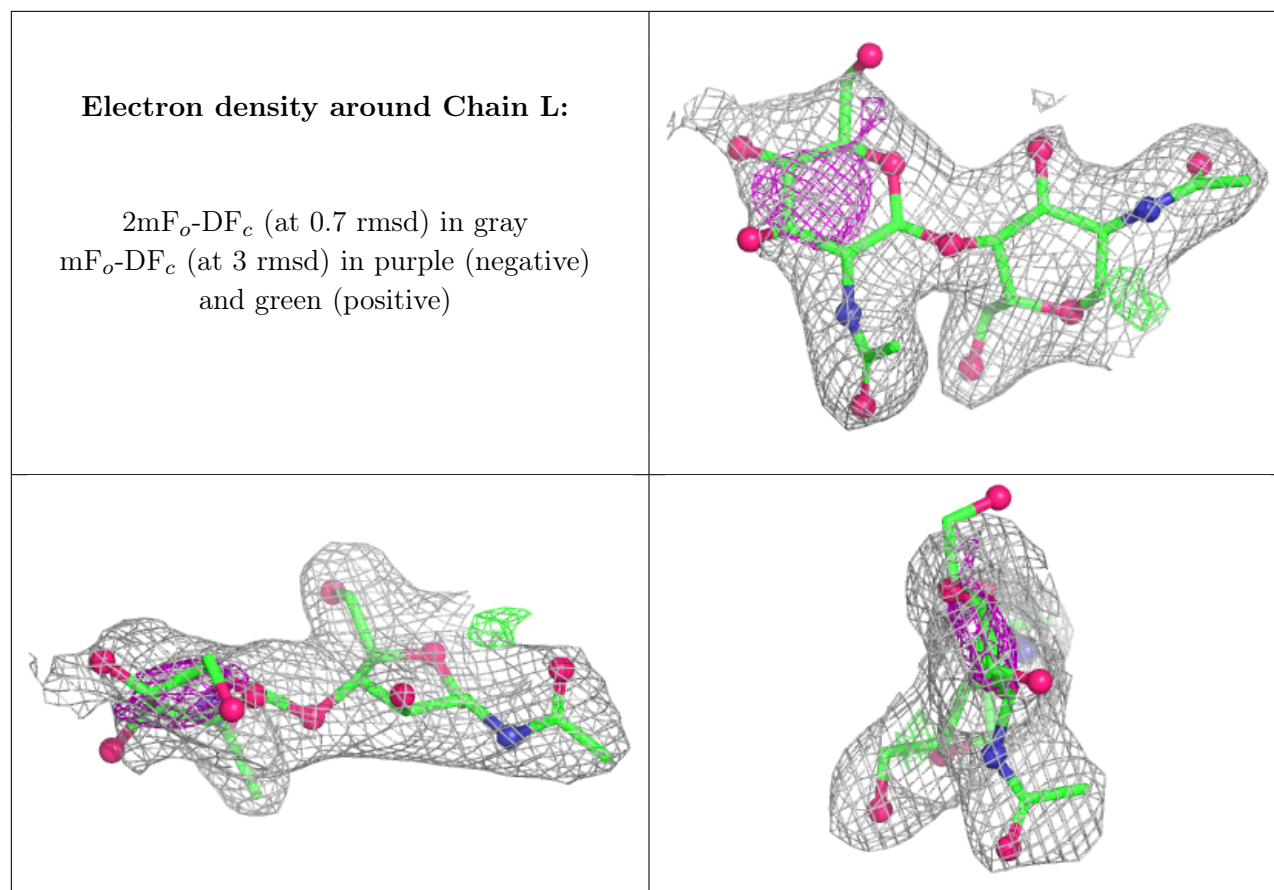
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

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





6.4 Ligands ⓘ

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(Å ²)	Q<0.9
3	NAG	A	804	14/15	0.40	0.19	111,112,114,114	0
3	NAG	A	803	14/15	0.48	0.21	71,75,77,78	0
3	NAG	D	805	14/15	0.51	0.18	91,93,94,94	0
3	NAG	C	804	14/15	0.54	0.21	89,91,92,92	0
3	NAG	A	802	14/15	0.60	0.22	97,98,99,99	0
3	NAG	D	803	14/15	0.62	0.17	70,74,75,76	0
3	NAG	C	801	14/15	0.62	0.19	88,90,90,90	0
3	NAG	D	802	14/15	0.63	0.17	84,85,86,86	0
3	NAG	B	804	14/15	0.64	0.19	90,92,92,92	0
3	NAG	A	801	14/15	0.66	0.17	94,97,97,98	0
3	NAG	D	804	14/15	0.67	0.18	73,75,80,80	0
3	NAG	D	801	14/15	0.67	0.16	66,69,70,71	0
3	NAG	B	801	14/15	0.69	0.16	84,86,86,87	0

Continued on next page...

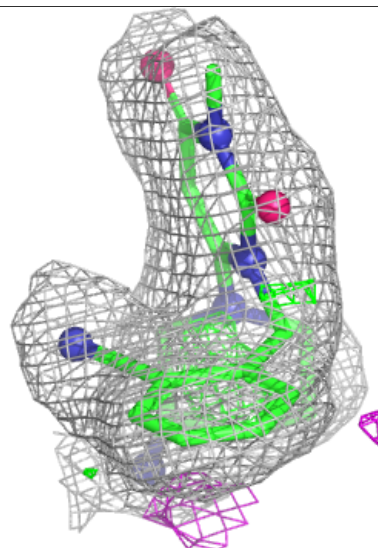
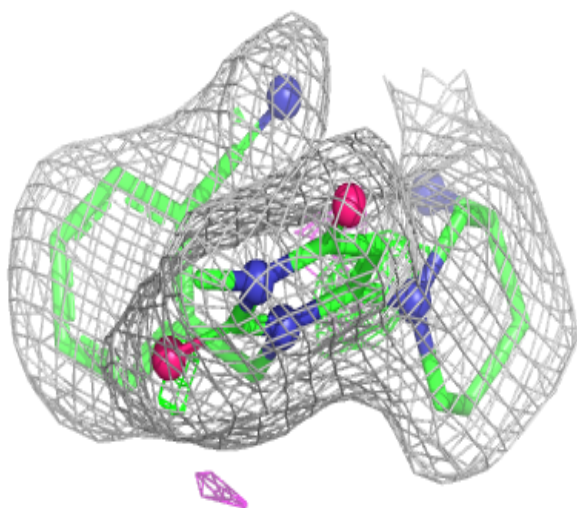
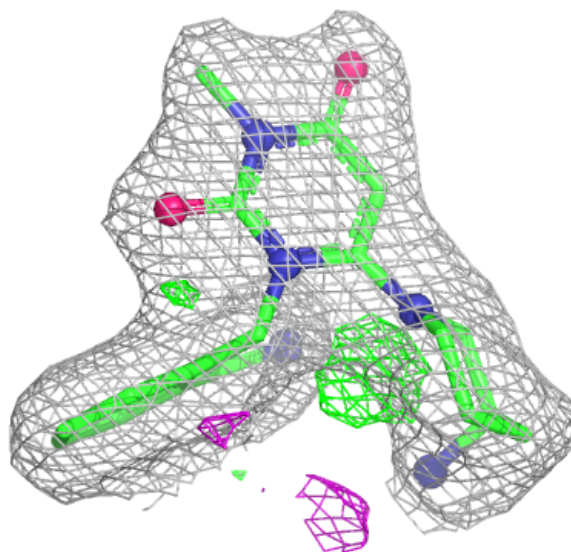
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	C	803	14/15	0.69	0.17	71,75,78,78	0
3	NAG	C	802	14/15	0.71	0.16	92,95,96,96	0
3	NAG	B	802	14/15	0.71	0.17	88,89,90,90	0
3	NAG	B	803	14/15	0.74	0.15	93,94,95,96	0
4	T22	B	805	25/25	0.92	0.11	48,50,51,52	0
4	T22	D	806	25/25	0.93	0.10	48,50,51,52	0
4	T22	C	805	25/25	0.94	0.10	48,50,51,52	0
4	T22	A	805	25/25	0.95	0.09	48,50,51,52	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.

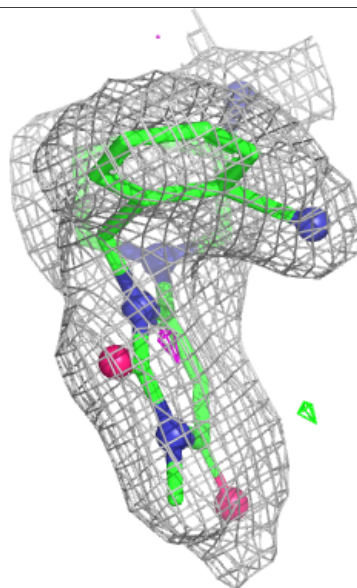
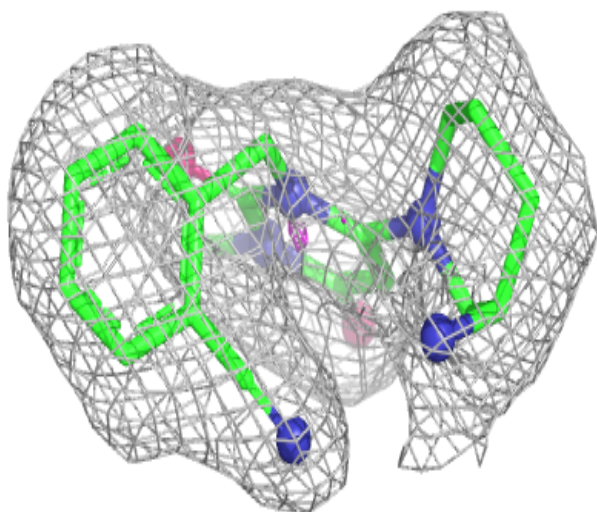
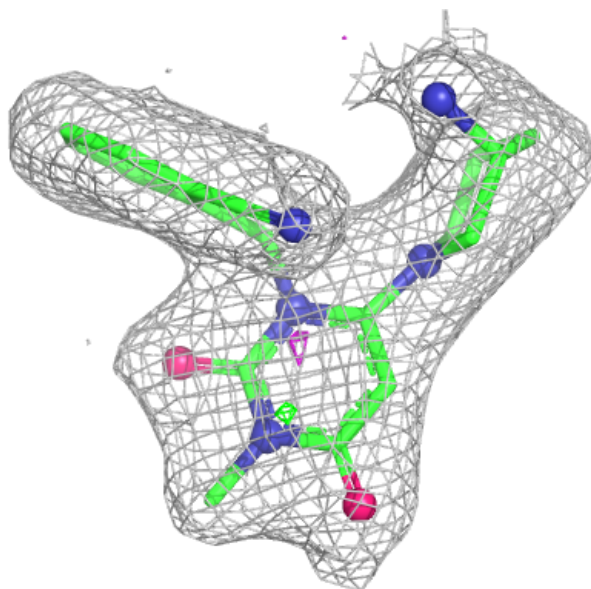
Electron density around T22 B 805:

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



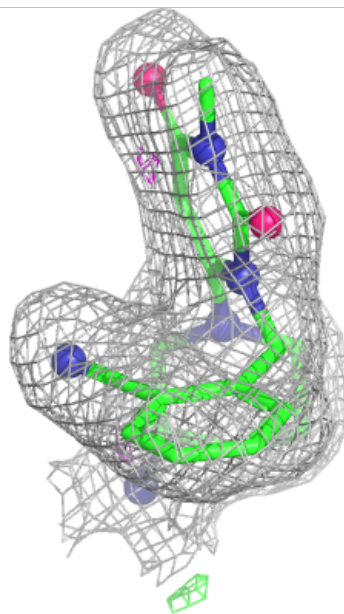
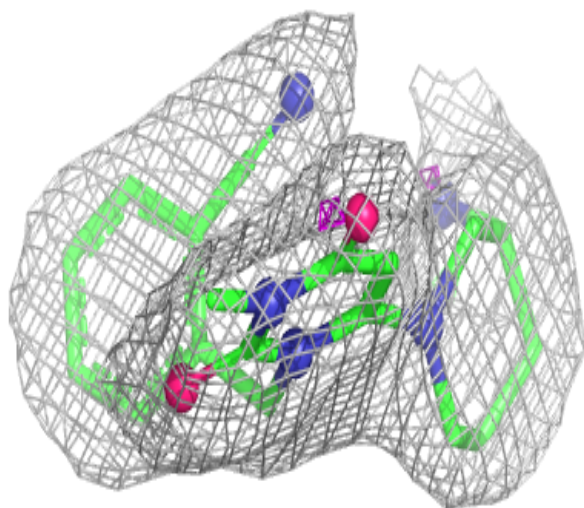
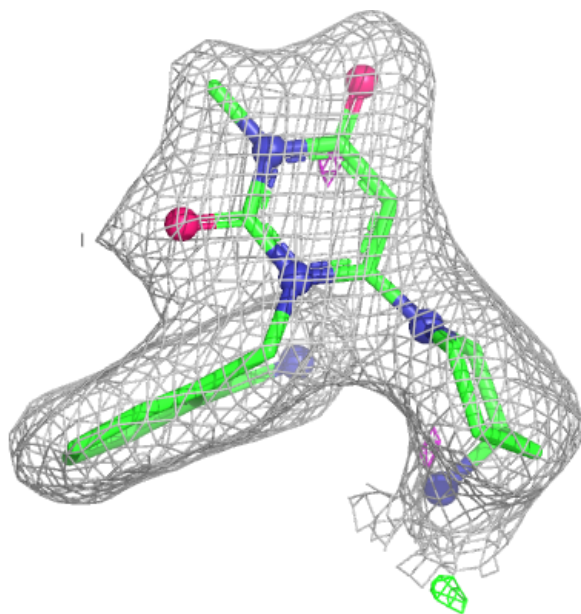
Electron density around T22 D 806:

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



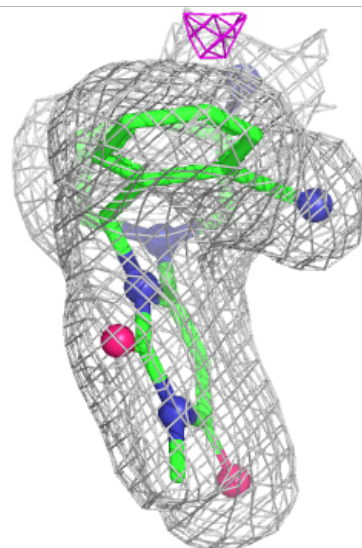
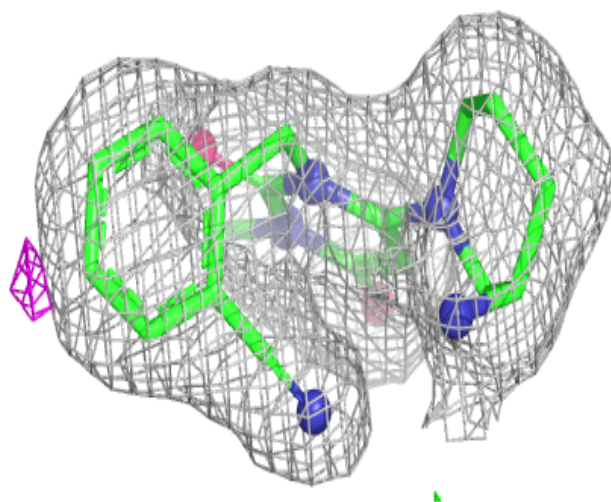
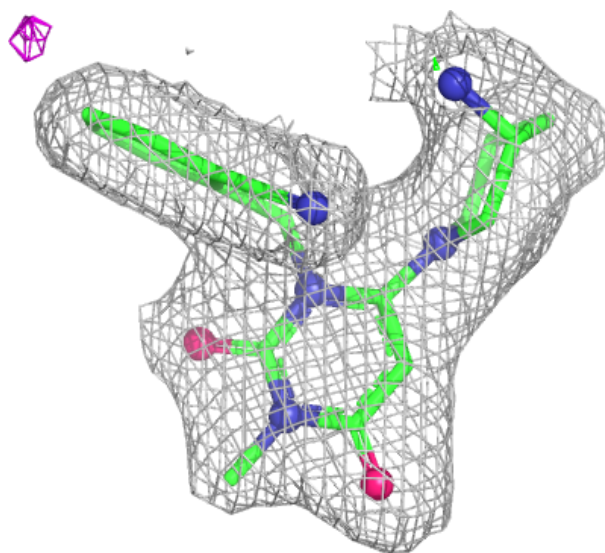
Electron density around T22 C 805:

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



Electron density around T22 A 805:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.