



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:11 PM EDT

PDB ID : 3O9V / pdb_00003o9v
Title : Crystal Structure of Human DPP4 Bound to TAK-986
Authors : Yano, J.K.; Aertgeerts, K.
Deposited on : 2010-08-04
Resolution : 2.75 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

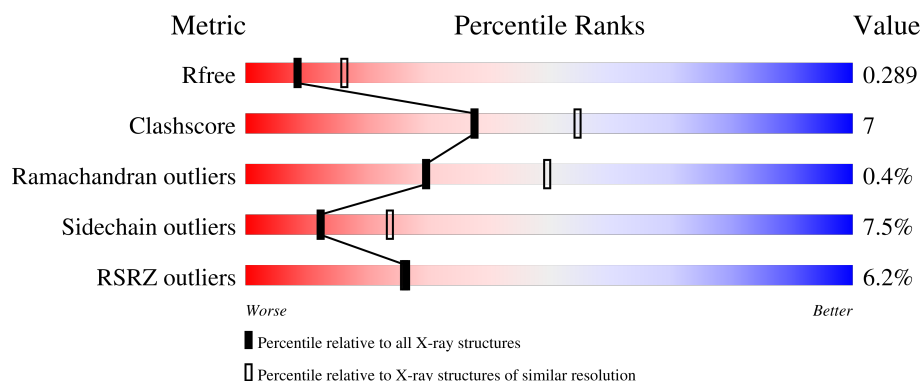
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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.



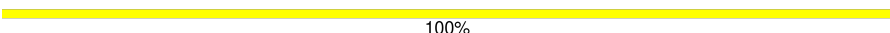
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	6% 75% 21% ..
1	B	740	2% 80% 16% ..
1	C	740	8% 75% 22% ..
1	D	740	8% 81% 15% ..
2	E	2	50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	2	 50%50%
2	G	2	 100%
2	H	2	 100%
2	I	2	 50%50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24702 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	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			
1	D	727	Total	C	N	O	S	0	0	0
			5952	3821	981	1124	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.



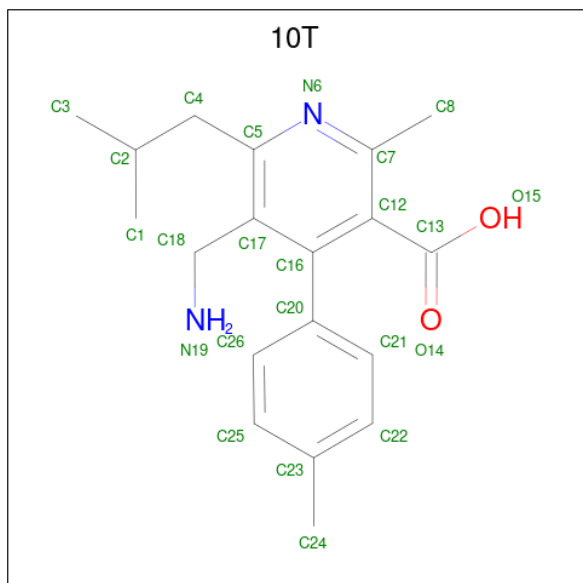
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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			

- Molecule 3 is 5-(aminomethyl)-2-methyl-4-(4-methylphenyl)-6-(2-methylpropyl)pyridine-3-carboxylic acid (CCD ID: 10T) (formula: $C_{19}H_{24}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			23	19	2	2		
3	B	1	Total	C	N	O	0	0
			23	19	2	2		
3	C	1	Total	C	N	O	0	0
			23	19	2	2		
3	D	1	Total	C	N	O	0	0
			23	19	2	2		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	133	Total	O	0	0
			133	133		
5	B	123	Total	O	0	0
			123	123		

Continued on next page...

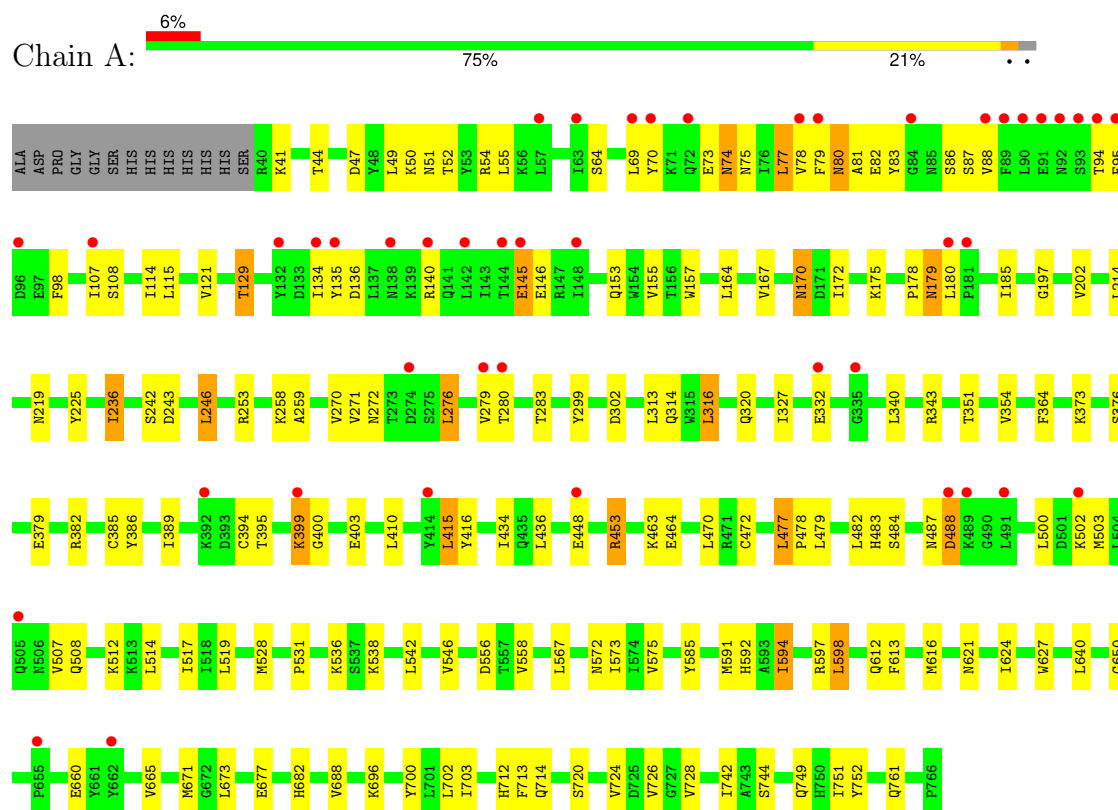
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	83	Total 83	O 83	0	0
5	D	112	Total 112	O 112	0	0

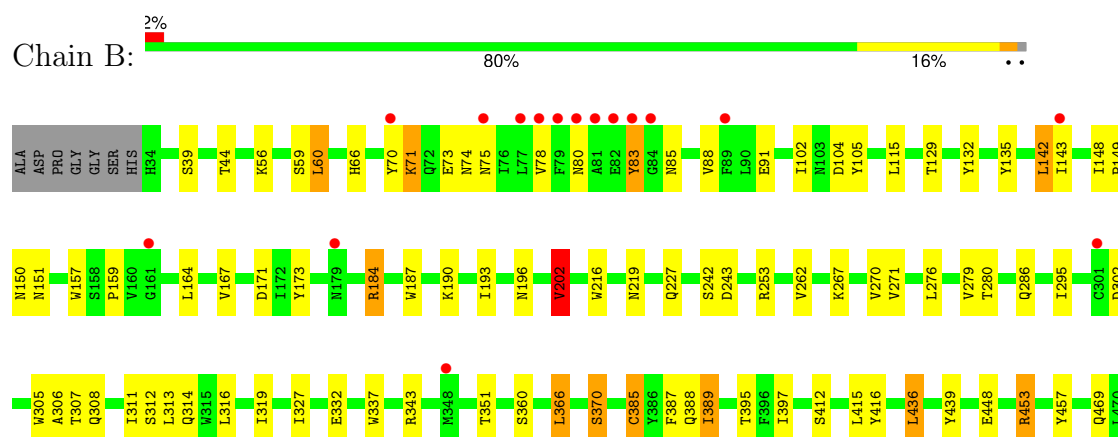
3 Residue-property plots [i](#)

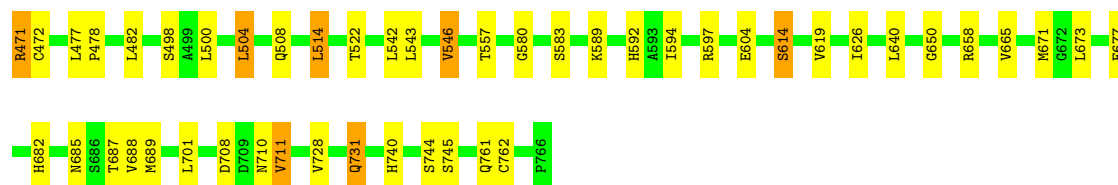
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

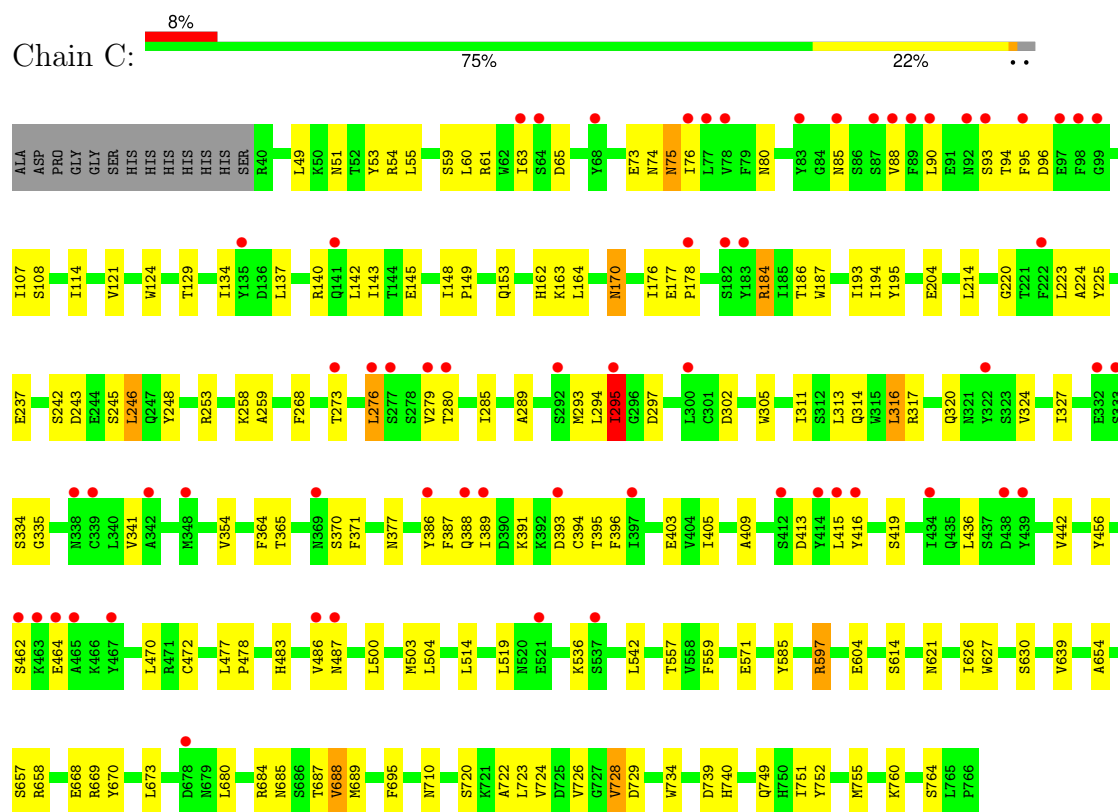


• Molecule 1: Dipeptidyl peptidase 4

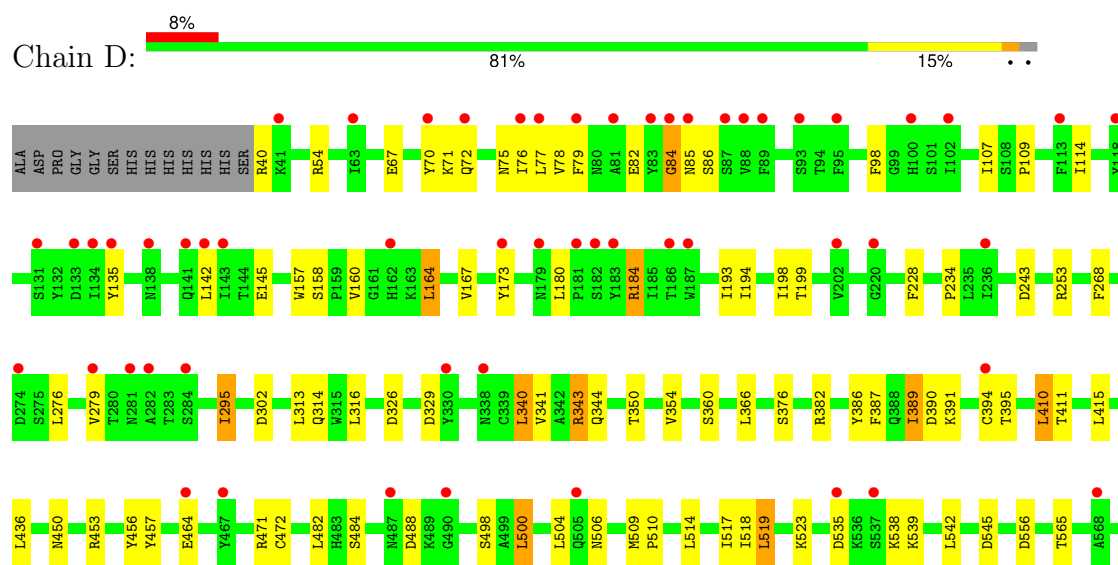


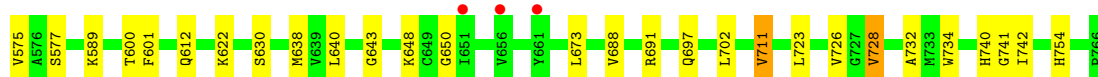


• Molecule 1: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4





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



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



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.17Å 122.89Å 144.91Å 90.00° 114.59° 90.00°	Depositor
Resolution (Å)	35.00 – 2.75 35.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.7 (35.00-2.75) 98.8 (35.00-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.76Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.203 , 0.260 0.248 , 0.289	Depositor DCC
R_{free} test set	5026 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	24702	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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, 10T

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	0.62	0/6129	0.79	2/8336 (0.0%)
1	B	0.62	0/6190	0.79	2/8419 (0.0%)
1	C	0.58	1/6129 (0.0%)	0.78	0/8336
1	D	0.62	0/6124	0.77	2/8329 (0.0%)
All	All	0.61	1/24572 (0.0%)	0.78	6/33420 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	654	ALA	C-O	-5.69	1.21	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	450	ASN	CA-C-N	6.36	125.85	119.24
1	D	450	ASN	C-N-CA	6.36	125.85	119.24
1	A	108	SER	CA-C-N	5.58	125.04	119.24
1	A	108	SER	C-N-CA	5.58	125.04	119.24
1	B	546	VAL	N-CA-C	5.29	116.10	108.48
1	B	202	VAL	CB-CA-C	-5.29	104.93	112.22

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	5957	0	5676	95	0
1	B	6013	0	5715	74	0
1	C	5957	0	5677	96	0
1	D	5952	0	5672	69	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	2	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
3	A	23	0	23	0	0
3	B	23	0	23	0	0
3	C	23	0	23	1	0
3	D	23	0	23	1	0
4	A	28	0	26	0	0
4	B	56	0	52	2	0
4	C	28	0	26	0	0
4	D	28	0	26	0	0
5	A	133	0	0	3	0
5	B	123	0	0	4	0
5	C	83	0	0	2	0
5	D	112	0	0	3	0
All	All	24702	0	23087	331	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 (331) 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:D:518:ILE:O	1:D:519:LEU:HD13	1.66	0.96
1:D:193:ILE:HG22	1:D:194:ILE:HD12	1.53	0.88
1:A:153:GLN:HE22	1:A:170:ASN:H	1.22	0.88
1:A:399:LYS:HD2	1:A:400:GLY:N	1.94	0.83
1:A:500:LEU:HA	1:A:503:MET:HE3	1.60	0.80
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.65	0.78
1:C:193:ILE:HG22	1:C:194:ILE:HD12	1.68	0.76
1:D:193:ILE:HG22	1:D:194:ILE:CD1	2.19	0.73
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.36	0.72
1:C:153:GLN:HE22	1:C:170:ASN:H	1.36	0.71
1:A:77:LEU:HD12	1:A:88:VAL:HA	1.71	0.71

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	2.73	0.71
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.73	0.71
1:C:415:LEU:HB2	1:C:436:LEU:HD11	1.74	0.70
1:D:726:VAL:HG23	1:D:728:VAL:HG12	1.73	0.70
1:D:157:TRP:CZ3	1:D:164:LEU:HD21	2.26	0.69
1:D:391:LYS:HG2	5:D:839:HOH:O	1.92	0.69
1:D:517:ILE:HD13	1:D:612:GLN:HG3	1.74	0.69
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.74	0.68
1:A:80:ASN:HD22	1:A:81:ALA:H	1.42	0.67
1:C:726:VAL:HG23	1:C:728:VAL:HG12	1.76	0.67
1:C:542:LEU:C	1:C:542:LEU:HD23	2.20	0.67
1:D:643:GLY:HA2	1:D:697:GLN:HE22	1.59	0.66
1:A:121:VAL:HB	1:A:129:THR:HG23	1.77	0.66
1:A:327:ILE:HD13	1:A:389:ILE:HD12	1.77	0.66
1:A:598:LEU:HD22	1:A:671:MET:HG2	1.77	0.66
1:A:80:ASN:ND2	5:A:851:HOH:O	2.25	0.66
1:C:597:ARG:HD3	5:C:820:HOH:O	1.94	0.66
1:A:172:ILE:HG22	1:A:185:ILE:HD13	1.79	0.65
1:A:179:ASN:C	1:A:179:ASN:HD22	2.04	0.65
1:A:80:ASN:HD22	1:A:81:ALA:N	1.95	0.65
1:C:295:ILE:HD11	1:C:317:ARG:HE	1.62	0.64
1:A:594:ILE:HD12	1:A:594:ILE:C	2.23	0.64
1:B:59:SER:O	1:B:70:TYR:CD1	2.50	0.64
1:A:157:TRP:CE3	1:A:164:LEU:HD13	2.34	0.63
1:C:90:LEU:HD12	1:C:140:ARG:HH21	1.63	0.63
1:D:386:TYR:O	1:D:394:CYS:HB2	1.99	0.62
1:A:477:LEU:HD12	1:A:477:LEU:H	1.64	0.62
1:A:49:LEU:HD22	1:A:749:GLN:HA	1.80	0.62
1:C:726:VAL:HG23	1:C:728:VAL:CG1	2.29	0.62
1:C:289:ALA:HB3	1:C:294:LEU:HD21	1.81	0.62
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.65	0.61
1:B:542:LEU:C	1:B:542:LEU:HD23	2.24	0.61
1:A:54:ARG:HD3	1:D:40:ARG:HH22	1.64	0.61
1:A:598:LEU:HB2	1:A:671:MET:SD	2.40	0.61
1:D:114:ILE:HG23	1:D:135:TYR:HB3	1.82	0.61
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.82	0.61
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.83	0.61
1:B:267:LYS:HG2	1:B:286:GLN:HE22	1.67	0.60
1:A:487:ASN:O	1:A:488:ASP:HB2	2.01	0.60
1:C:184:ARG:HD3	1:C:186:THR:O	2.01	0.60
1:D:157:TRP:CZ3	1:D:164:LEU:CD2	2.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:ARG:HD3	1:B:389:ILE:HG23	1.84	0.60
1:D:366:LEU:HD23	1:D:366:LEU:C	2.27	0.60
1:D:484:SER:O	1:D:488:ASP:HA	2.02	0.60
2:G:1:NAG:H62	2:G:2:NAG:HN2	1.67	0.60
2:G:1:NAG:H62	2:G:2:NAG:N2	2.16	0.59
1:D:295:ILE:HD13	1:D:295:ILE:O	2.02	0.59
1:A:170:ASN:N	1:A:170:ASN:HD22	2.01	0.59
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.83	0.59
1:A:399:LYS:HD2	1:A:400:GLY:H	1.65	0.59
1:A:453:ARG:NH2	1:A:477:LEU:O	2.36	0.59
1:B:711:VAL:HG13	1:B:740:HIS:CE1	2.38	0.58
1:C:170:ASN:N	1:C:170:ASN:HD22	2.01	0.58
1:D:509:MET:HE3	1:D:510:PRO:HD2	1.85	0.58
1:C:121:VAL:HB	1:C:129:THR:HG22	1.85	0.58
1:D:366:LEU:HD23	1:D:366:LEU:O	2.04	0.58
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.39	0.57
1:C:114:ILE:HB	1:C:137:LEU:HD12	1.85	0.57
1:B:614:SER:HA	1:B:619:VAL:HB	1.87	0.57
1:D:723:LEU:HD22	1:D:728:VAL:HG11	1.86	0.57
1:C:237:GLU:HG2	1:C:253:ARG:HG2	1.87	0.57
1:C:327:ILE:HD13	1:C:389:ILE:HD12	1.87	0.56
1:A:484:SER:O	1:A:488:ASP:HA	2.05	0.56
1:A:134:ILE:HD13	1:A:178:PRO:HB3	1.86	0.56
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.88	0.56
1:C:60:LEU:C	1:C:60:LEU:HD12	2.30	0.56
1:A:95:PHE:HB3	1:A:98:PHE:HB2	1.88	0.56
1:B:327:ILE:HD13	1:B:389:ILE:HG13	1.87	0.55
1:D:389:ILE:HG22	1:D:390:ASP:OD1	2.06	0.55
1:A:594:ILE:C	1:A:594:ILE:CD1	2.79	0.55
1:A:153:GLN:NE2	1:A:170:ASN:H	1.99	0.55
1:B:415:LEU:C	1:B:415:LEU:HD23	2.31	0.55
1:D:542:LEU:HD23	1:D:542:LEU:C	2.32	0.54
1:B:397:ILE:HG22	1:B:439:TYR:CZ	2.41	0.54
1:C:415:LEU:CB	1:C:436:LEU:HD11	2.38	0.54
1:C:80:ASN:HB3	1:C:85:ASN:O	2.07	0.54
1:C:76:ILE:HD12	1:C:90:LEU:HD23	1.90	0.54
1:C:658:ARG:HG2	1:C:689:MET:CE	2.38	0.54
1:C:751:ILE:HG12	1:C:755:MET:HE2	1.90	0.54
1:B:397:ILE:HG22	1:B:439:TYR:CE2	2.43	0.54
1:D:638:MET:HE3	1:D:691:ARG:CZ	2.37	0.54
1:B:196:ASN:ND2	1:B:227:GLN:HG3	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:ARG:NH2	1:B:477:LEU:O	2.41	0.54
1:A:567:LEU:HD22	1:A:573:ILE:HD12	1.90	0.53
1:A:44:THR:HB	5:A:774:HOH:O	2.08	0.53
1:B:761:GLN:HG2	5:B:834:HOH:O	2.07	0.53
1:D:343:ARG:HD2	1:D:389:ILE:HG23	1.90	0.53
1:C:184:ARG:HD2	1:C:187:TRP:CE2	2.44	0.53
1:C:370:SER:HG	1:C:386:TYR:HE2	1.57	0.53
1:A:236:ILE:HD13	1:A:712:HIS:ND1	2.24	0.53
1:A:279:VAL:HG12	1:A:280:THR:HG23	1.91	0.52
1:C:242:SER:HB3	1:C:246:LEU:HD12	1.91	0.52
1:B:242:SER:OG	1:B:243:ASP:N	2.43	0.52
1:C:739:ASP:HB2	5:C:805:HOH:O	2.09	0.52
1:C:657:SER:HA	1:C:688:VAL:CG1	2.40	0.52
1:B:202:VAL:HG22	5:B:814:HOH:O	2.10	0.52
1:B:701:LEU:HD13	1:B:731:GLN:HB3	1.91	0.52
1:D:173:TYR:CE1	1:D:184:ARG:HG2	2.45	0.52
1:C:242:SER:OG	1:C:243:ASP:N	2.43	0.51
1:A:115:LEU:HD21	1:A:155:VAL:HG21	1.90	0.51
1:C:729:ASP:OD1	1:D:754:HIS:ND1	2.35	0.51
1:C:658:ARG:HG2	1:C:689:MET:HE1	1.91	0.51
1:B:313:LEU:N	1:B:313:LEU:HD22	2.25	0.51
1:B:102:ILE:HD12	1:B:102:ILE:H	1.76	0.51
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.37	0.51
1:C:289:ALA:HB3	1:C:294:LEU:CD2	2.41	0.50
1:B:135:TYR:HD1	1:B:142:LEU:HD22	1.76	0.50
1:C:669:ARG:HD2	1:C:670:TYR:CZ	2.46	0.50
1:A:259:ALA:HB3	1:A:660:GLU:HA	1.93	0.50
1:B:415:LEU:HB2	1:B:436:LEU:HD11	1.92	0.50
1:C:214:LEU:HD22	1:C:223:LEU:HD11	1.93	0.50
1:C:316:LEU:HD13	1:C:320:GLN:HG2	1.92	0.50
1:B:83:TYR:CD2	1:B:83:TYR:N	2.79	0.50
1:A:47:ASP:HA	1:A:52:THR:OG1	2.11	0.50
1:D:741:GLY:O	1:D:742:ILE:C	2.54	0.50
1:A:64:SER:HA	1:A:463:LYS:HE2	1.92	0.50
1:C:55:LEU:HD23	1:C:500:LEU:CD2	2.42	0.50
1:C:327:ILE:HD13	1:C:389:ILE:CD1	2.41	0.50
1:C:734:TRP:CZ3	1:D:732:ALA:HB1	2.47	0.50
1:D:142:LEU:HD23	1:D:142:LEU:H	1.77	0.50
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.95	0.50
1:A:700:TYR:OH	1:A:702:LEU:HD13	2.12	0.50
1:D:75:ASN:O	1:D:77:LEU:HD12	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:THR:HG22	1:C:95:PHE:CE1	2.48	0.49
1:D:643:GLY:HA2	1:D:697:GLN:NE2	2.26	0.49
1:A:720:SER:O	1:A:724:VAL:HG23	2.12	0.49
1:C:409:ALA:HB3	1:C:416:TYR:HB2	1.94	0.49
1:D:114:ILE:CG2	1:D:135:TYR:HB3	2.42	0.49
1:C:726:VAL:CG2	1:C:728:VAL:CG1	2.90	0.49
1:D:71:LYS:H	1:D:71:LYS:HD3	1.78	0.49
1:C:253:ARG:HH21	1:D:253:ARG:HH21	1.59	0.49
1:C:630:SER:HB2	1:C:740:HIS:NE2	2.28	0.49
1:C:142:LEU:HD12	1:C:143:ILE:N	2.28	0.49
1:C:273:THR:HA	1:C:276:LEU:HD22	1.93	0.49
1:C:305:TRP:CE2	1:C:311:ILE:HD12	2.48	0.49
1:A:386:TYR:O	1:A:394:CYS:HB2	2.13	0.48
1:A:517:ILE:HD12	1:A:612:GLN:HG3	1.95	0.48
1:B:279:VAL:HG23	1:B:280:THR:HG23	1.95	0.48
1:C:143:ILE:HG22	1:C:143:ILE:O	2.12	0.48
1:B:150:ASN:O	1:B:151:ASN:HB2	2.13	0.48
1:A:546:VAL:HG12	1:A:627:TRP:O	2.14	0.48
1:A:751:ILE:HG23	1:A:752:TYR:N	2.29	0.48
1:C:53:TYR:CD1	1:C:503:MET:HE2	2.48	0.48
1:C:391:LYS:HE3	1:C:393:ASP:HB2	1.94	0.48
1:D:600:THR:OG1	1:D:601:PHE:N	2.46	0.48
1:A:153:GLN:NE2	1:A:167:VAL:HG12	2.29	0.48
1:A:713:PHE:O	1:A:714:GLN:C	2.57	0.48
1:B:514:LEU:HD12	1:B:557:THR:HG22	1.95	0.48
1:D:366:LEU:C	1:D:366:LEU:CD2	2.87	0.48
1:A:55:LEU:HD23	1:A:500:LEU:CD2	2.43	0.47
1:C:626:ILE:HD13	1:C:639:VAL:HG11	1.96	0.47
1:B:305:TRP:CE2	1:B:311:ILE:HD12	2.48	0.47
1:C:657:SER:HA	1:C:688:VAL:HG13	1.96	0.47
1:A:272:ASN:O	1:A:276:LEU:HD13	2.13	0.47
1:D:199:THR:HA	1:D:228:PHE:CE2	2.50	0.47
1:D:410:LEU:HD22	1:D:411:THR:O	2.14	0.47
1:D:500:LEU:HD11	1:D:504:LEU:HD22	1.97	0.47
1:A:80:ASN:ND2	1:A:81:ALA:H	2.08	0.47
1:A:415:LEU:HD13	1:A:416:TYR:N	2.29	0.47
1:B:184:ARG:HD2	1:B:187:TRP:CZ2	2.48	0.47
1:C:658:ARG:HB3	1:C:687:THR:HG22	1.96	0.47
1:B:306:ALA:O	1:B:307:THR:HG23	2.14	0.47
1:B:542:LEU:HD23	1:B:543:LEU:C	2.40	0.47
1:C:93:SER:HA	1:C:96:ASP:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:LYS:NZ	1:C:220:GLY:O	2.45	0.47
1:A:512:LYS:NZ	1:A:558:VAL:O	2.48	0.47
3:C:1:10T:C21	3:C:1:10T:H18	2.44	0.47
1:C:54:ARG:O	1:C:500:LEU:HD22	2.15	0.46
1:D:302:ASP:HB3	1:D:314:GLN:HB2	1.97	0.46
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.96	0.46
1:C:124:TRP:HB2	1:C:204:GLU:OE1	2.15	0.46
1:A:175:LYS:NZ	1:A:180:LEU:O	2.47	0.46
1:A:613:PHE:O	1:A:616:MET:HB2	2.14	0.46
1:B:190:LYS:HG2	1:B:193:ILE:HD12	1.97	0.46
1:D:711:VAL:HG11	1:D:740:HIS:CE1	2.50	0.46
1:A:500:LEU:CA	1:A:503:MET:HE3	2.40	0.46
1:B:167:VAL:HA	1:B:171:ASP:O	2.15	0.46
1:B:415:LEU:HD23	1:B:416:TYR:N	2.30	0.46
1:C:377:ASN:HA	1:C:396:PHE:CZ	2.51	0.46
1:A:597:ARG:HH11	1:A:682:HIS:HB2	1.80	0.46
1:B:658:ARG:HG2	1:B:689:MET:CE	2.46	0.46
1:C:472:CYS:O	1:C:478:PRO:HA	2.16	0.46
1:D:109:PRO:HG2	1:D:158:SER:O	2.14	0.46
1:A:107:ILE:HD11	1:A:114:ILE:HD12	1.98	0.46
1:A:343:ARG:HD2	1:A:389:ILE:CG2	2.45	0.46
1:A:472:CYS:O	1:A:478:PRO:HA	2.16	0.46
1:B:157:TRP:CE3	1:B:164:LEU:HD13	2.51	0.45
1:C:214:LEU:HD23	1:C:225:TYR:HB3	1.97	0.45
1:D:341:VAL:HG12	5:D:836:HOH:O	2.16	0.45
1:A:185:ILE:N	1:A:185:ILE:HD12	2.32	0.45
1:B:302:ASP:HB3	1:B:314:GLN:HE21	1.80	0.45
1:C:415:LEU:C	1:C:415:LEU:HD13	2.42	0.45
1:C:689:MET:HG3	1:C:722:ALA:HB2	1.99	0.45
1:B:44:THR:HB	5:B:819:HOH:O	2.16	0.45
1:B:542:LEU:HD23	1:B:543:LEU:N	2.31	0.45
1:D:340:LEU:HB2	1:D:343:ARG:HG3	1.99	0.45
1:D:376:SER:HA	1:D:382:ARG:HA	1.98	0.45
1:A:415:LEU:HB3	1:A:434:ILE:HG23	1.98	0.45
1:A:453:ARG:NH2	1:A:479:LEU:HB2	2.31	0.45
1:A:470:LEU:HD12	1:A:483:HIS:NE2	2.31	0.45
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.51	0.45
1:C:456:TYR:HB2	1:C:557:THR:OG1	2.17	0.45
1:D:387:PHE:CD1	1:D:394:CYS:HB3	2.52	0.45
1:C:148:ILE:HG23	1:C:149:PRO:HD2	1.98	0.45
1:D:279:VAL:HG12	1:D:279:VAL:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:ILE:HG21	1:A:751:ILE:CD1	2.47	0.45
1:C:405:ILE:HD12	1:C:585:TYR:CD2	2.52	0.45
1:B:306:ALA:O	1:B:307:THR:CG2	2.64	0.45
1:D:360:SER:HA	5:D:840:HOH:O	2.15	0.45
1:C:409:ALA:O	1:C:415:LEU:HD22	2.16	0.44
1:A:382:ARG:HH21	1:A:591:MET:HE1	1.81	0.44
1:C:571:GLU:CD	1:C:760:LYS:HD3	2.42	0.44
1:D:456:TYR:O	1:D:472:CYS:HA	2.16	0.44
1:D:457:TYR:HA	1:D:471:ARG:O	2.18	0.44
1:D:545:ASP:HB3	1:D:577:SER:OG	2.18	0.44
1:A:403:GLU:OE2	1:A:585:TYR:HA	2.17	0.44
1:C:614:SER:HB2	1:C:621:ASN:OD1	2.17	0.44
3:D:1:10T:H18	3:D:1:10T:C21	2.47	0.44
1:C:65:ASP:HA	1:C:462:SER:HB2	1.99	0.44
1:D:734:TRP:CD1	1:D:734:TRP:C	2.96	0.44
1:A:512:LYS:HA	1:A:528:MET:O	2.18	0.44
1:B:71:LYS:HA	1:B:75:ASN:O	2.18	0.44
1:B:351:THR:OG1	1:B:592:HIS:CD2	2.71	0.44
1:A:179:ASN:C	1:A:179:ASN:ND2	2.75	0.44
1:B:219:ASN:HB3	1:B:308:GLN:HE22	1.83	0.44
1:C:302:ASP:HB3	1:C:314:GLN:HB2	1.99	0.44
1:D:84:GLY:O	1:D:86:SER:N	2.46	0.44
1:B:85:ASN:OD1	4:B:851:NAG:H82	2.18	0.43
1:A:172:ILE:HD11	1:A:197:GLY:HA3	1.99	0.43
1:A:316:LEU:HD13	1:A:320:GLN:HG2	1.99	0.43
1:B:385:CYS:HB3	1:B:387:PHE:CE2	2.53	0.43
1:D:556:ASP:C	1:D:556:ASP:OD1	2.61	0.43
1:A:316:LEU:HD21	1:A:354:VAL:CG1	2.48	0.43
1:B:88:VAL:HG11	1:B:91:GLU:HG3	1.99	0.43
1:A:79:PHE:HA	1:A:86:SER:HB3	1.99	0.43
1:B:671:MET:HE1	1:B:682:HIS:HD2	1.83	0.43
1:B:744:SER:O	1:B:745:SER:C	2.60	0.43
1:C:364:PHE:CD2	1:C:371:PHE:HB3	2.53	0.43
1:C:720:SER:O	1:C:724:VAL:HG23	2.19	0.43
1:B:580:GLY:O	1:B:583:SER:OG	2.31	0.43
1:C:470:LEU:HD12	1:C:483:HIS:NE2	2.34	0.43
1:A:316:LEU:HD21	1:A:354:VAL:HG12	2.00	0.43
1:B:85:ASN:CG	4:B:851:NAG:H82	2.44	0.43
1:D:711:VAL:CG1	1:D:740:HIS:ND1	2.81	0.43
1:B:104:ASP:OD1	1:B:105:TYR:N	2.52	0.42
1:C:75:ASN:OD1	1:C:75:ASN:N	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:ILE:HG22	1:C:177:GLU:HG2	2.01	0.42
1:C:370:SER:OG	1:C:386:TYR:HE2	2.02	0.42
1:D:268:PHE:CZ	1:D:313:LEU:HD21	2.54	0.42
1:A:512:LYS:HE2	1:A:556:ASP:O	2.18	0.42
1:B:39:SER:HB3	1:B:508:GLN:HG3	2.01	0.42
1:B:60:LEU:HD21	1:B:469:GLN:CD	2.44	0.42
1:A:145:GLU:O	1:A:146:GLU:HB2	2.18	0.42
1:B:173:TYR:CE1	1:B:184:ARG:HG3	2.54	0.42
1:D:711:VAL:HG12	1:D:740:HIS:CE1	2.53	0.42
1:D:702:LEU:O	1:D:732:ALA:HA	2.20	0.42
1:A:107:ILE:CD1	1:A:114:ILE:HD12	2.49	0.42
1:A:136:ASP:O	1:A:140:ARG:N	2.53	0.42
1:A:70:TYR:HB3	1:A:79:PHE:HE1	1.82	0.42
1:A:219:ASN:ND2	5:A:767:HOH:O	2.51	0.42
1:B:78:VAL:HG13	1:B:78:VAL:O	2.20	0.42
1:B:157:TRP:CZ3	1:B:164:LEU:HD13	2.54	0.42
1:B:500:LEU:O	1:B:504:LEU:HD22	2.20	0.42
1:C:403:GLU:OE2	1:C:585:TYR:HA	2.20	0.42
1:A:415:LEU:C	1:A:415:LEU:CD1	2.93	0.42
1:A:597:ARG:NH1	1:A:682:HIS:HB2	2.34	0.42
1:B:135:TYR:CD1	1:B:142:LEU:HD22	2.54	0.42
1:D:518:ILE:HG22	1:D:519:LEU:N	2.33	0.42
1:A:69:LEU:HD23	1:A:77:LEU:O	2.18	0.42
1:B:302:ASP:HB3	1:B:314:GLN:HB2	2.02	0.42
1:B:312:SER:C	1:B:313:LEU:HD22	2.45	0.42
1:C:751:ILE:HG23	1:C:752:TYR:N	2.35	0.42
1:D:70:TYR:CE2	1:D:79:PHE:HB2	2.55	0.42
1:B:270:VAL:HG11	1:B:337:TRP:CZ2	2.55	0.42
1:B:708:ASP:OD1	1:B:740:HIS:HA	2.20	0.42
1:C:76:ILE:HB	1:C:90:LEU:HB3	2.00	0.41
1:C:134:ILE:HD13	1:C:178:PRO:HB3	2.02	0.41
1:A:299:TYR:CZ	1:A:665:VAL:HG22	2.55	0.41
1:A:364:PHE:HE2	1:A:389:ILE:HD11	1.85	0.41
1:B:626:ILE:O	1:B:650:GLY:HA2	2.21	0.41
1:C:680:LEU:O	1:C:684:ARG:HG3	2.20	0.41
1:B:542:LEU:C	1:B:542:LEU:CD2	2.93	0.41
1:D:622:LYS:O	1:D:648:LYS:HD2	2.21	0.41
1:B:115:LEU:HD11	1:B:132:TYR:HB3	2.01	0.41
1:A:487:ASN:O	1:A:488:ASP:CB	2.68	0.41
1:B:83:TYR:H	1:B:83:TYR:HD2	1.62	0.41
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ASN:HD22	1:A:180:LEU:N	2.19	0.41
1:B:73:GLU:C	1:B:75:ASN:H	2.28	0.41
1:B:457:TYR:HA	1:B:471:ARG:O	2.21	0.41
1:C:53:TYR:HB3	1:C:500:LEU:HD11	2.02	0.41
1:D:54:ARG:O	1:D:500:LEU:HD22	2.20	0.41
1:D:167:VAL:HG11	1:D:198:ILE:HG12	2.03	0.41
1:B:148:ILE:HG23	1:B:149:PRO:HD2	2.02	0.41
1:B:319:ILE:H	1:B:319:ILE:HD12	1.86	0.41
1:C:195:TYR:CD1	1:C:195:TYR:N	2.89	0.41
1:C:248:TYR:OH	1:D:234:PRO:HG2	2.21	0.41
1:C:285:ILE:HG13	1:C:335:GLY:O	2.21	0.41
1:C:387:PHE:CE1	1:C:394:CYS:HB3	2.56	0.41
1:C:486:VAL:HG13	1:C:487:ASN:OD1	2.20	0.41
1:C:695:PHE:CD1	1:C:723:LEU:HD21	2.55	0.41
1:C:293:MET:HE2	1:C:324:VAL:HG23	2.02	0.41
1:A:258:LYS:O	1:A:259:ALA:C	2.63	0.40
1:C:248:TYR:CZ	1:D:234:PRO:HG2	2.55	0.40
1:C:377:ASN:OD1	1:C:377:ASN:C	2.63	0.40
1:D:535:ASP:HB3	1:D:538:LYS:HD2	2.03	0.40
1:B:366:LEU:HD22	1:B:366:LEU:O	2.20	0.40
1:C:55:LEU:HD21	1:C:559:PHE:HE2	1.85	0.40
1:C:162:HIS:NE2	1:C:177:GLU:OE1	2.52	0.40
1:C:542:LEU:HD23	1:C:542:LEU:O	2.22	0.40
1:D:193:ILE:C	1:D:194:ILE:HD12	2.46	0.40
1:D:326:ASP:OD2	1:D:344:GLN:HG2	2.21	0.40
1:A:214:LEU:HD23	1:A:225:TYR:HB3	2.02	0.40
1:A:621:ASN:HA	1:A:624:ILE:HD11	2.04	0.40
1:B:370:SER:HB3	5:B:856:HOH:O	2.20	0.40
1:B:658:ARG:HB3	1:B:687:THR:HG22	2.03	0.40
1:C:49:LEU:HD22	1:C:749:GLN:HA	2.04	0.40
1:C:107:ILE:HG22	1:C:108:SER:O	2.21	0.40
1:D:500:LEU:CD1	1:D:504:LEU:HD22	2.52	0.40
1:C:258:LYS:O	1:C:259:ALA:C	2.63	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%)	679 (94%)	42 (6%)	4 (1%)	21	38
1	B	731/740 (99%)	692 (95%)	37 (5%)	2 (0%)	36	56
1	C	725/740 (98%)	679 (94%)	42 (6%)	4 (1%)	21	38
1	D	725/740 (98%)	675 (93%)	47 (6%)	3 (0%)	30	50
All	All	2906/2960 (98%)	2725 (94%)	168 (6%)	13 (0%)	30	50

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	GLU
1	A	488	ASP
1	C	73	GLU
1	D	82	GLU
1	A	74	ASN
1	C	334	SER
1	B	74	ASN
1	A	508	GLN
1	C	297	ASP
1	D	85	ASN
1	B	478	PRO
1	C	295	ILE
1	D	84	GLY

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%)	594 (91%)	58 (9%)	9	17
1	B	658/662 (99%)	607 (92%)	51 (8%)	11	21
1	C	652/662 (98%)	609 (93%)	43 (7%)	15	29
1	D	651/662 (98%)	608 (93%)	43 (7%)	15	29
All	All	2613/2648 (99%)	2418 (92%)	195 (8%)	12	24

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	50	LYS
1	A	51	ASN
1	A	73	GLU
1	A	74	ASN
1	A	75	ASN
1	A	77	LEU
1	A	78	VAL
1	A	80	ASN
1	A	82	GLU
1	A	83	TYR
1	A	87	SER
1	A	94	THR
1	A	129	THR
1	A	145	GLU
1	A	170	ASN
1	A	179	ASN
1	A	202	VAL
1	A	236	ILE
1	A	243	ASP
1	A	246	LEU
1	A	270	VAL
1	A	271	VAL
1	A	276	LEU
1	A	283	THR
1	A	313	LEU
1	A	316	LEU
1	A	340	LEU
1	A	373	LYS
1	A	376	SER
1	A	379	GLU
1	A	385	CYS
1	A	395	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	399	LYS
1	A	410	LEU
1	A	415	LEU
1	A	436	LEU
1	A	448	GLU
1	A	453	ARG
1	A	464	GLU
1	A	477	LEU
1	A	482	LEU
1	A	502	LYS
1	A	507	VAL
1	A	514	LEU
1	A	519	LEU
1	A	536	LYS
1	A	538	LYS
1	A	542	LEU
1	A	575	VAL
1	A	594	ILE
1	A	598	LEU
1	A	673	LEU
1	A	677	GLU
1	A	688	VAL
1	A	742	ILE
1	A	744	SER
1	A	761	GLN
1	B	56	LYS
1	B	60	LEU
1	B	66	HIS
1	B	71	LYS
1	B	80	ASN
1	B	83	TYR
1	B	129	THR
1	B	142	LEU
1	B	143	ILE
1	B	184	ARG
1	B	202	VAL
1	B	262	VAL
1	B	271	VAL
1	B	276	LEU
1	B	295	ILE
1	B	316	LEU
1	B	332	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	360	SER
1	B	366	LEU
1	B	370	SER
1	B	385	CYS
1	B	388	GLN
1	B	389	ILE
1	B	395	THR
1	B	412	SER
1	B	436	LEU
1	B	448	GLU
1	B	453	ARG
1	B	471	ARG
1	B	472	CYS
1	B	482	LEU
1	B	498	SER
1	B	504	LEU
1	B	514	LEU
1	B	522	THR
1	B	546	VAL
1	B	589	LYS
1	B	594	ILE
1	B	597	ARG
1	B	604	GLU
1	B	614	SER
1	B	665	VAL
1	B	673	LEU
1	B	677	GLU
1	B	685	ASN
1	B	688	VAL
1	B	710	ASN
1	B	711	VAL
1	B	728	VAL
1	B	731	GLN
1	B	762	CYS
1	C	51	ASN
1	C	59	SER
1	C	61	ARG
1	C	63	ILE
1	C	74	ASN
1	C	75	ASN
1	C	88	VAL
1	C	145	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	164	LEU
1	C	170	ASN
1	C	184	ARG
1	C	245	SER
1	C	246	LEU
1	C	276	LEU
1	C	279	VAL
1	C	280	THR
1	C	295	ILE
1	C	313	LEU
1	C	316	LEU
1	C	341	VAL
1	C	354	VAL
1	C	365	THR
1	C	388	GLN
1	C	395	THR
1	C	413	ASP
1	C	419	SER
1	C	442	VAL
1	C	464	GLU
1	C	477	LEU
1	C	504	LEU
1	C	514	LEU
1	C	519	LEU
1	C	536	LYS
1	C	597	ARG
1	C	604	GLU
1	C	627	TRP
1	C	668	GLU
1	C	673	LEU
1	C	685	ASN
1	C	688	VAL
1	C	710	ASN
1	C	728	VAL
1	C	764	SER
1	D	67	GLU
1	D	72	GLN
1	D	76	ILE
1	D	78	VAL
1	D	98	PHE
1	D	107	ILE
1	D	145	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	160	VAL
1	D	164	LEU
1	D	180	LEU
1	D	184	ARG
1	D	243	ASP
1	D	276	LEU
1	D	295	ILE
1	D	316	LEU
1	D	329	ASP
1	D	340	LEU
1	D	343	ARG
1	D	350	THR
1	D	354	VAL
1	D	389	ILE
1	D	395	THR
1	D	410	LEU
1	D	415	LEU
1	D	436	LEU
1	D	453	ARG
1	D	464	GLU
1	D	482	LEU
1	D	498	SER
1	D	500	LEU
1	D	506	ASN
1	D	514	LEU
1	D	519	LEU
1	D	523	LYS
1	D	539	LYS
1	D	565	THR
1	D	575	VAL
1	D	589	LYS
1	D	630	SER
1	D	673	LEU
1	D	688	VAL
1	D	711	VAL
1	D	728	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	153	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	169	ASN
1	A	170	ASN
1	A	179	ASN
1	A	344	GLN
1	A	388	GLN
1	A	572	ASN
1	A	592	HIS
1	A	606	GLN
1	A	710	ASN
1	A	748	HIS
1	A	749	GLN
1	A	757	HIS
1	A	761	GLN
1	B	38	HIS
1	B	72	GLN
1	B	80	ASN
1	B	119	ASN
1	B	169	ASN
1	B	196	ASN
1	B	286	GLN
1	B	338	ASN
1	B	344	GLN
1	B	505	GLN
1	B	572	ASN
1	B	592	HIS
1	B	710	ASN
1	C	74	ASN
1	C	138	ASN
1	C	153	GLN
1	C	169	ASN
1	C	170	ASN
1	C	179	ASN
1	C	196	ASN
1	C	344	GLN
1	C	450	ASN
1	C	455	GLN
1	C	572	ASN
1	C	685	ASN
1	C	710	ASN
1	C	731	GLN
1	D	51	ASN
1	D	123	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	169	ASN
1	D	196	ASN
1	D	227	GLN
1	D	344	GLN
1	D	435	GLN
1	D	606	GLN
1	D	685	ASN
1	D	694	ASN
1	D	697	GLN
1	D	710	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

10 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	2,1	14,14,15	0.58	0	17,19,21	0.95	1 (5%)
2	NAG	E	2	2	14,14,15	0.48	0	17,19,21	0.84	0
2	NAG	F	1	2,1	14,14,15	0.63	0	17,19,21	1.23	1 (5%)
2	NAG	F	2	2	14,14,15	0.69	0	17,19,21	1.00	0
2	NAG	G	1	2,1	14,14,15	0.82	0	17,19,21	1.27	3 (17%)
2	NAG	G	2	2	14,14,15	0.50	0	17,19,21	1.67	3 (17%)
2	NAG	H	1	2,1	14,14,15	0.52	0	17,19,21	1.25	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	H	2	2	14,14,15	0.35	0	17,19,21	1.28	2 (11%)
2	NAG	I	1	2,1	14,14,15	0.57	0	17,19,21	1.41	3 (17%)
2	NAG	I	2	2	14,14,15	0.50	0	17,19,21	0.88	0

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	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NAG	O5-C1-C2	-4.15	104.87	111.29
2	G	2	NAG	C1-C2-N2	3.92	116.61	110.43
2	F	1	NAG	C1-O5-C5	3.64	117.06	112.19
2	I	1	NAG	C3-C4-C5	3.18	116.00	110.23
2	H	2	NAG	C1-O5-C5	3.02	116.23	112.19
2	H	1	NAG	O5-C1-C2	-2.76	107.02	111.29
2	G	1	NAG	C1-O5-C5	2.70	115.80	112.19
2	G	1	NAG	O5-C1-C2	-2.61	107.26	111.29
2	H	2	NAG	O4-C4-C5	2.60	115.72	109.32
2	I	1	NAG	C4-C3-C2	2.52	114.71	111.02
2	G	2	NAG	C4-C3-C2	-2.50	107.35	111.02
2	H	1	NAG	O3-C3-C4	-2.40	104.73	110.38
2	G	1	NAG	O5-C5-C6	-2.31	103.17	107.66
2	I	1	NAG	O5-C1-C2	-2.28	107.76	111.29
2	E	1	NAG	O5-C1-C2	-2.05	108.12	111.29

There are no chirality outliers.

All (14) torsion outliers are listed below:

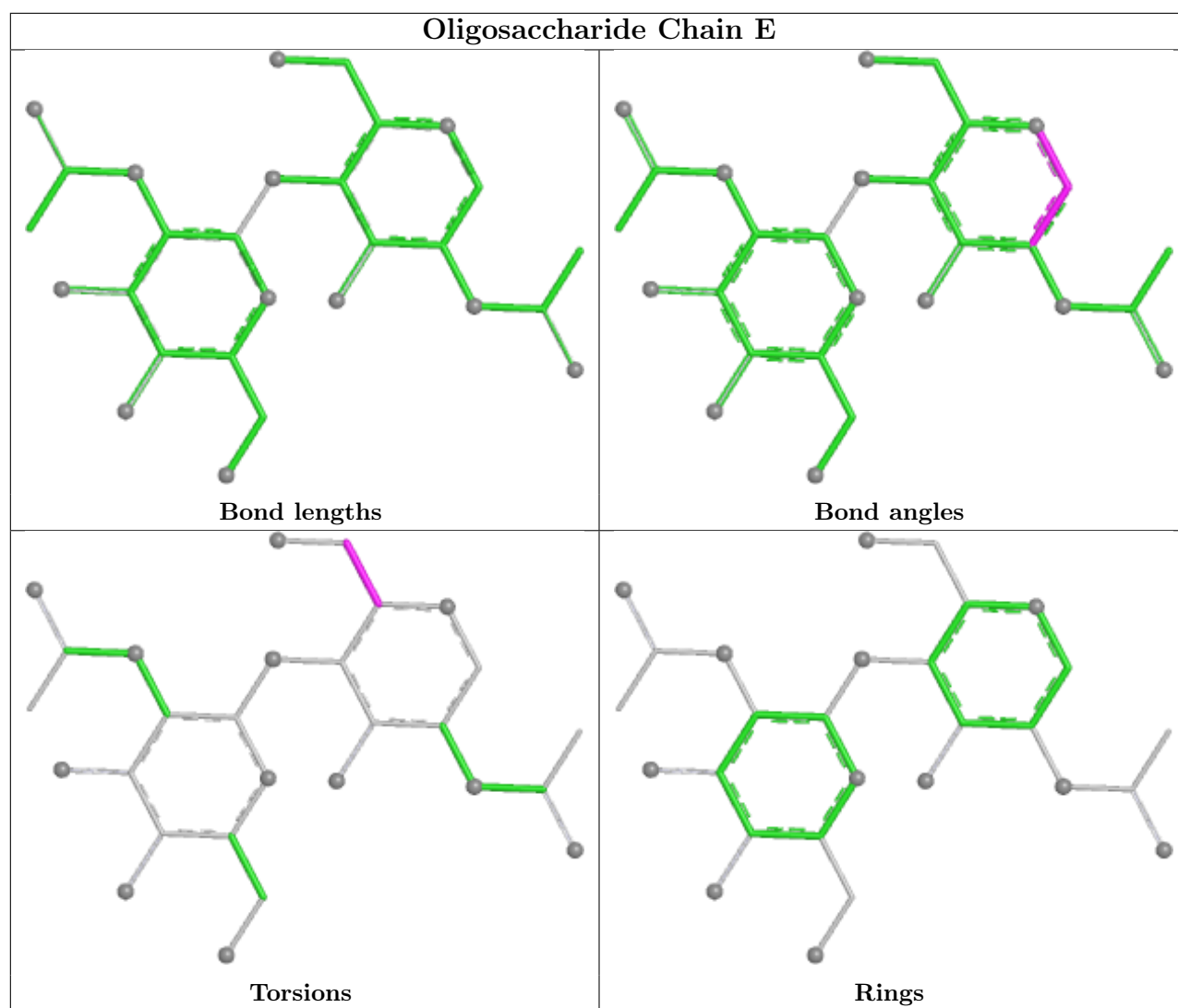
Mol	Chain	Res	Type	Atoms
2	G	1	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	G	2	NAG	C8-C7-N2-C2
2	I	2	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	G	2	NAG	O7-C7-N2-C2
2	I	2	NAG	C4-C5-C6-O6
2	I	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C1-C2-N2-C7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

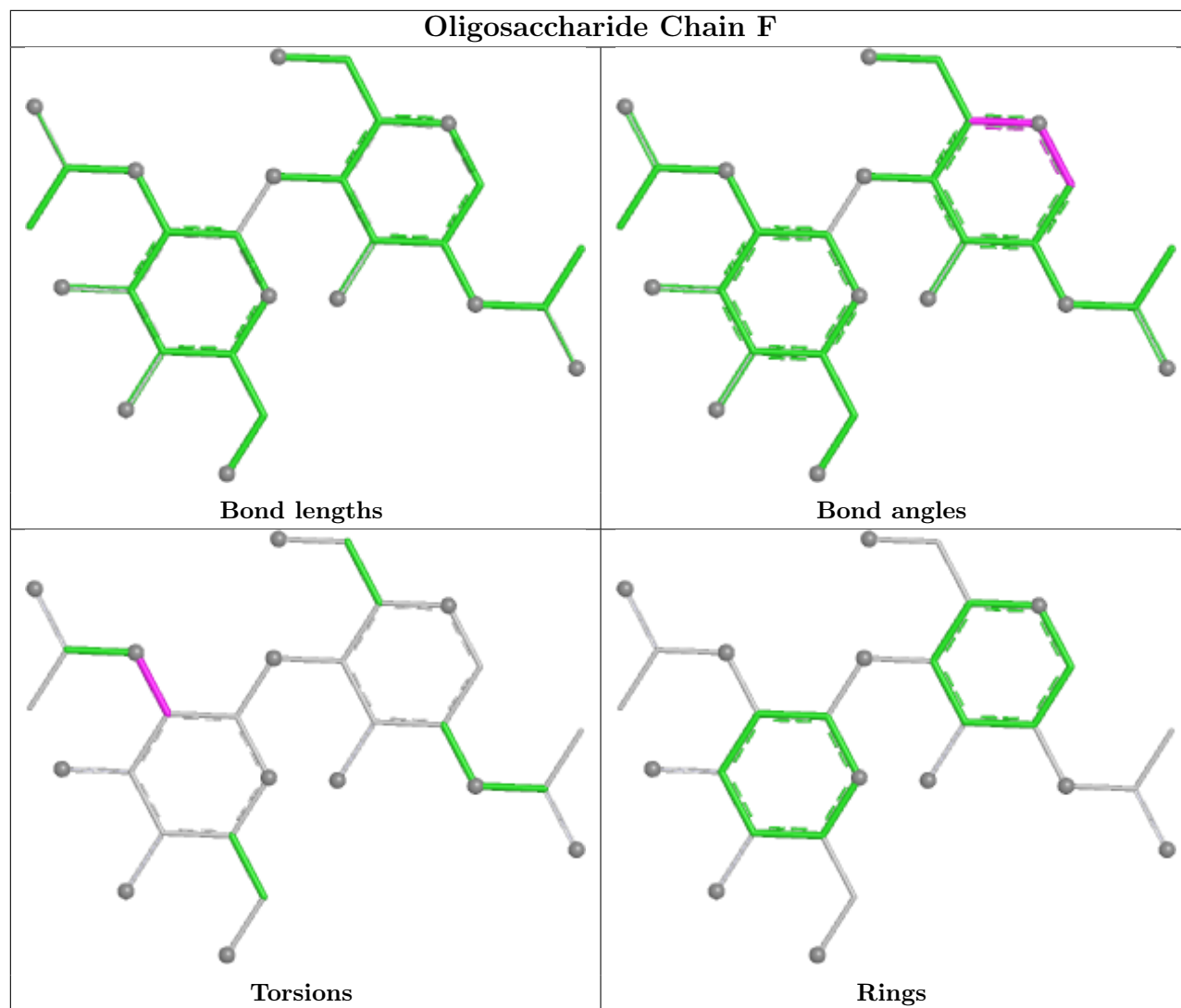
There are no ring outliers.

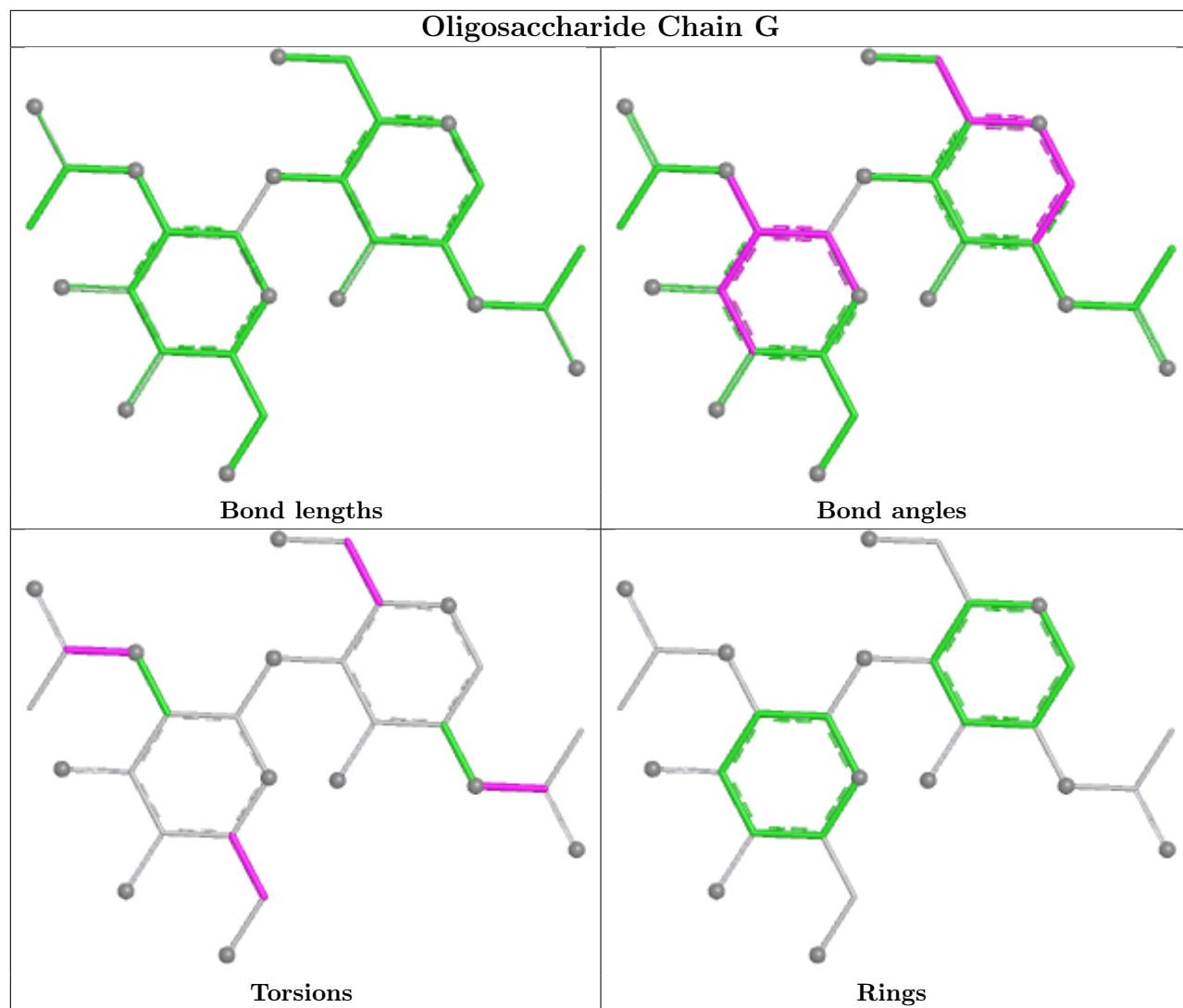
2 monomers are involved in 2 short contacts:

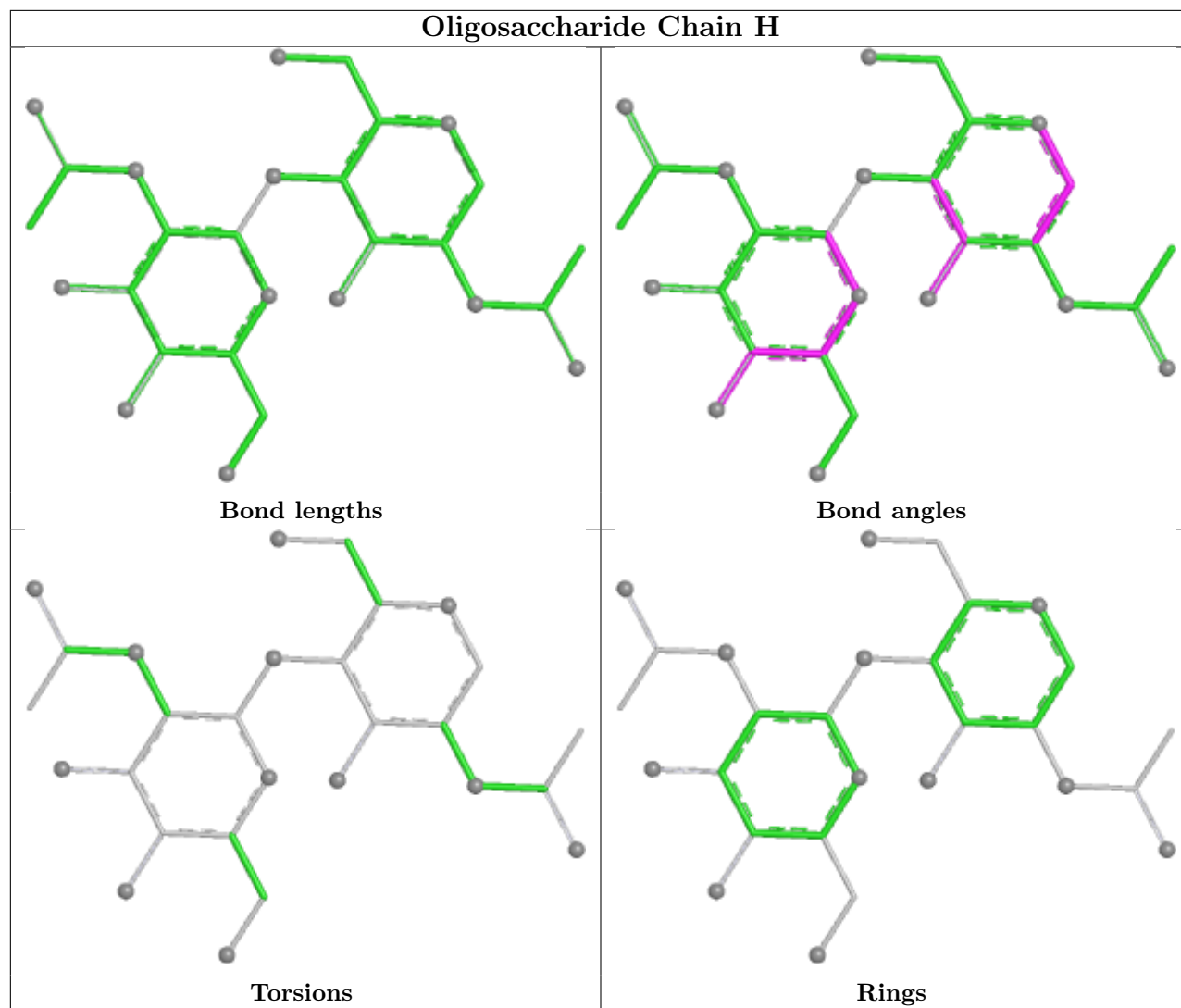
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NAG	2	0
2	G	1	NAG	2	0

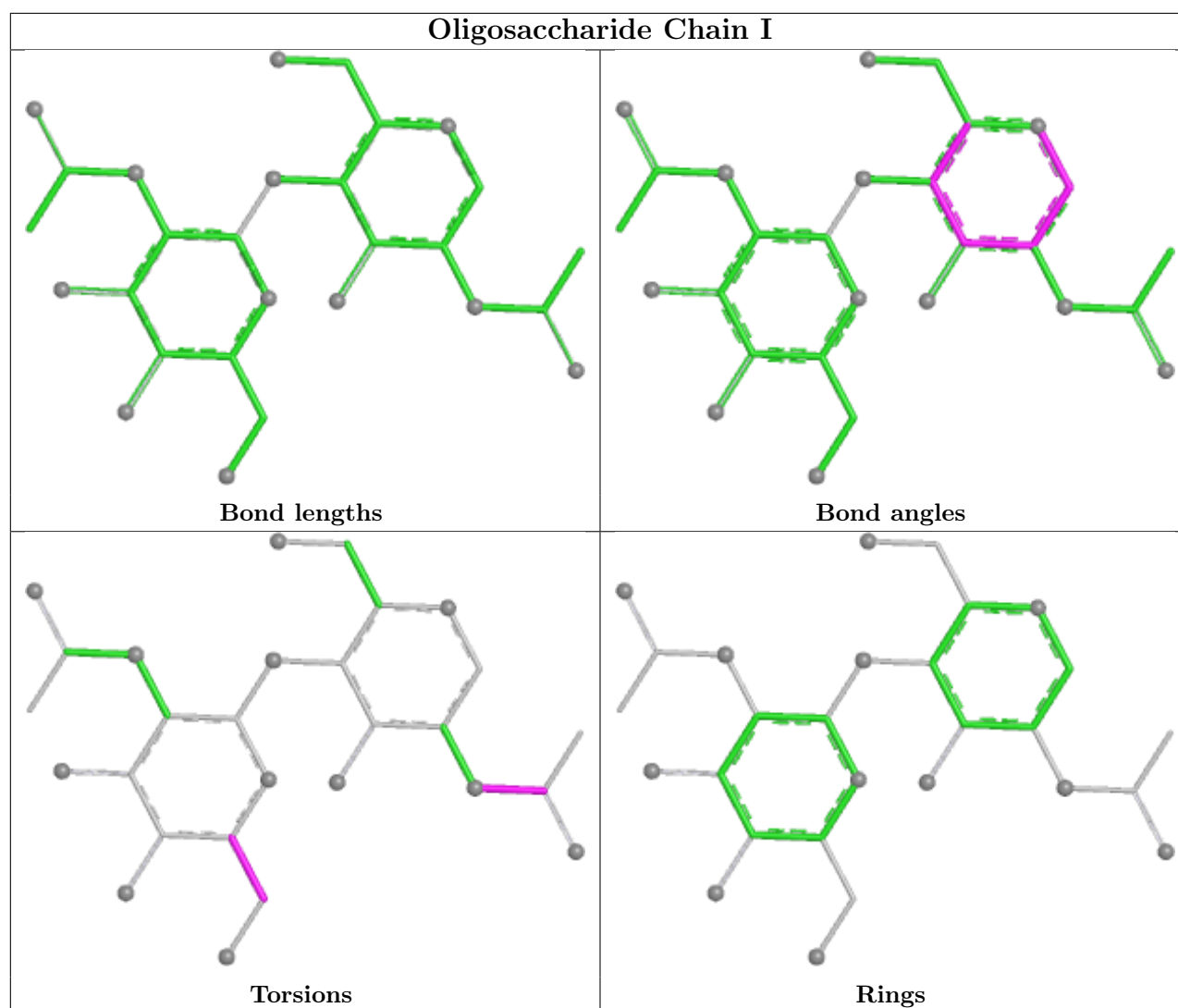
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	10T	D	1	-	24,24,24	0.71	0	31,34,34	1.57	4 (12%)
4	NAG	C	1501	1	14,14,15	0.58	0	17,19,21	1.68	2 (11%)
4	NAG	B	2811	1	14,14,15	0.61	0	17,19,21	1.16	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	2811	1	14,14,15	0.78	1 (7%)	17,19,21	1.53	3 (17%)
3	10T	C	1	-	24,24,24	0.78	0	31,34,34	1.40	4 (12%)
4	NAG	D	2811	1	14,14,15	0.73	0	17,19,21	1.21	2 (11%)
4	NAG	A	1501	1	14,14,15	0.58	0	17,19,21	1.84	2 (11%)
4	NAG	B	851	1	14,14,15	0.59	0	17,19,21	1.63	4 (23%)
4	NAG	D	1501	1	14,14,15	0.56	0	17,19,21	1.44	1 (5%)
4	NAG	A	3211	1	14,14,15	0.62	0	17,19,21	0.99	1 (5%)
4	NAG	B	2191	1	14,14,15	0.75	1 (7%)	17,19,21	1.20	1 (5%)
3	10T	A	1	-	24,24,24	0.71	0	31,34,34	1.26	3 (9%)
3	10T	B	1	-	24,24,24	0.73	0	31,34,34	1.46	5 (16%)
4	NAG	B	1501	1	14,14,15	0.49	0	17,19,21	1.46	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	10T	D	1	-	-	0/13/14/14	0/2/2/2
4	NAG	C	1501	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2811	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2811	1	-	2/6/23/26	0/1/1/1
3	10T	C	1	-	-	1/13/14/14	0/2/2/2
4	NAG	D	2811	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1501	1	-	4/6/23/26	0/1/1/1
4	NAG	B	851	1	-	4/6/23/26	0/1/1/1
4	NAG	D	1501	1	-	4/6/23/26	0/1/1/1
4	NAG	A	3211	1	-	4/6/23/26	0/1/1/1
4	NAG	B	2191	1	-	2/6/23/26	0/1/1/1
3	10T	A	1	-	-	1/13/14/14	0/2/2/2
3	10T	B	1	-	-	0/13/14/14	0/2/2/2
4	NAG	B	1501	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2191	NAG	C1-C2	2.17	1.55	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2811	NAG	C1-C2	2.13	1.55	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1501	NAG	C1-O5-C5	5.25	119.22	112.19
4	D	1501	NAG	C1-O5-C5	5.19	119.14	112.19
4	A	1501	NAG	C1-O5-C5	5.01	118.90	112.19
4	B	1501	NAG	C1-O5-C5	4.97	118.85	112.19
3	D	1	10T	C17-C5-N6	-4.62	119.92	123.48
3	C	1	10T	C17-C5-N6	-4.61	119.93	123.48
3	A	1	10T	C17-C5-N6	-4.13	120.30	123.48
3	B	1	10T	C17-C5-N6	-3.87	120.50	123.48
4	B	851	NAG	C4-C3-C2	3.70	116.45	111.02
4	D	2811	NAG	C1-O5-C5	3.65	117.08	112.19
4	B	2811	NAG	C1-O5-C5	3.64	117.07	112.19
4	C	2811	NAG	C4-C3-C2	3.47	116.10	111.02
4	A	1501	NAG	C4-C3-C2	-3.34	106.12	111.02
4	B	2191	NAG	C1-O5-C5	3.34	116.66	112.19
3	D	1	10T	C7-N6-C5	3.27	122.83	118.66
3	D	1	10T	C12-C7-N6	-3.18	118.70	121.87
4	B	851	NAG	O5-C5-C6	3.07	113.64	107.66
3	C	1	10T	C7-N6-C5	2.99	122.47	118.66
4	C	2811	NAG	O5-C5-C6	2.97	113.44	107.66
4	C	2811	NAG	C2-N2-C7	2.86	126.73	122.90
3	A	1	10T	C7-N6-C5	2.86	122.30	118.66
3	D	1	10T	C8-C7-N6	2.82	120.90	116.53
3	C	1	10T	C12-C7-N6	-2.73	119.15	121.87
3	B	1	10T	C8-C7-N6	2.61	120.59	116.53
4	B	851	NAG	C1-C2-N2	-2.55	106.41	110.43
3	A	1	10T	C12-C7-N6	-2.55	119.33	121.87
3	B	1	10T	C12-C7-N6	-2.51	119.37	121.87
4	B	851	NAG	C1-O5-C5	2.39	115.38	112.19
4	A	3211	NAG	C1-O5-C5	2.27	115.23	112.19
3	B	1	10T	C7-N6-C5	2.13	121.37	118.66
3	C	1	10T	C8-C7-N6	2.10	119.80	116.53
4	C	1501	NAG	O7-C7-N2	2.10	125.69	121.98
3	B	1	10T	O14-C13-C12	-2.07	116.24	121.18
4	D	2811	NAG	C4-C3-C2	2.02	113.98	111.02

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1501	NAG	O7-C7-N2-C2
4	B	851	NAG	C8-C7-N2-C2
4	B	851	NAG	O7-C7-N2-C2
4	A	1501	NAG	C8-C7-N2-C2
4	B	851	NAG	O5-C5-C6-O6
4	B	2191	NAG	C8-C7-N2-C2
4	B	2191	NAG	O7-C7-N2-C2
4	B	851	NAG	C4-C5-C6-O6
4	B	2811	NAG	C8-C7-N2-C2
4	D	2811	NAG	C8-C7-N2-C2
4	D	2811	NAG	O7-C7-N2-C2
4	A	1501	NAG	C4-C5-C6-O6
4	C	2811	NAG	C4-C5-C6-O6
4	B	2811	NAG	O7-C7-N2-C2
4	A	3211	NAG	O5-C5-C6-O6
4	A	1501	NAG	O5-C5-C6-O6
4	C	2811	NAG	O5-C5-C6-O6
4	A	3211	NAG	C4-C5-C6-O6
4	D	1501	NAG	C4-C5-C6-O6
4	D	1501	NAG	O5-C5-C6-O6
4	B	1501	NAG	C4-C5-C6-O6
4	D	2811	NAG	C4-C5-C6-O6
4	D	1501	NAG	C8-C7-N2-C2
3	A	1	10T	C16-C17-C18-N19
4	D	1501	NAG	O7-C7-N2-C2
4	D	2811	NAG	O5-C5-C6-O6
4	C	1501	NAG	C8-C7-N2-C2
4	C	1501	NAG	O7-C7-N2-C2
4	B	1501	NAG	O5-C5-C6-O6
3	C	1	10T	C3-C2-C4-C5
4	A	3211	NAG	C8-C7-N2-C2
4	A	3211	NAG	O7-C7-N2-C2

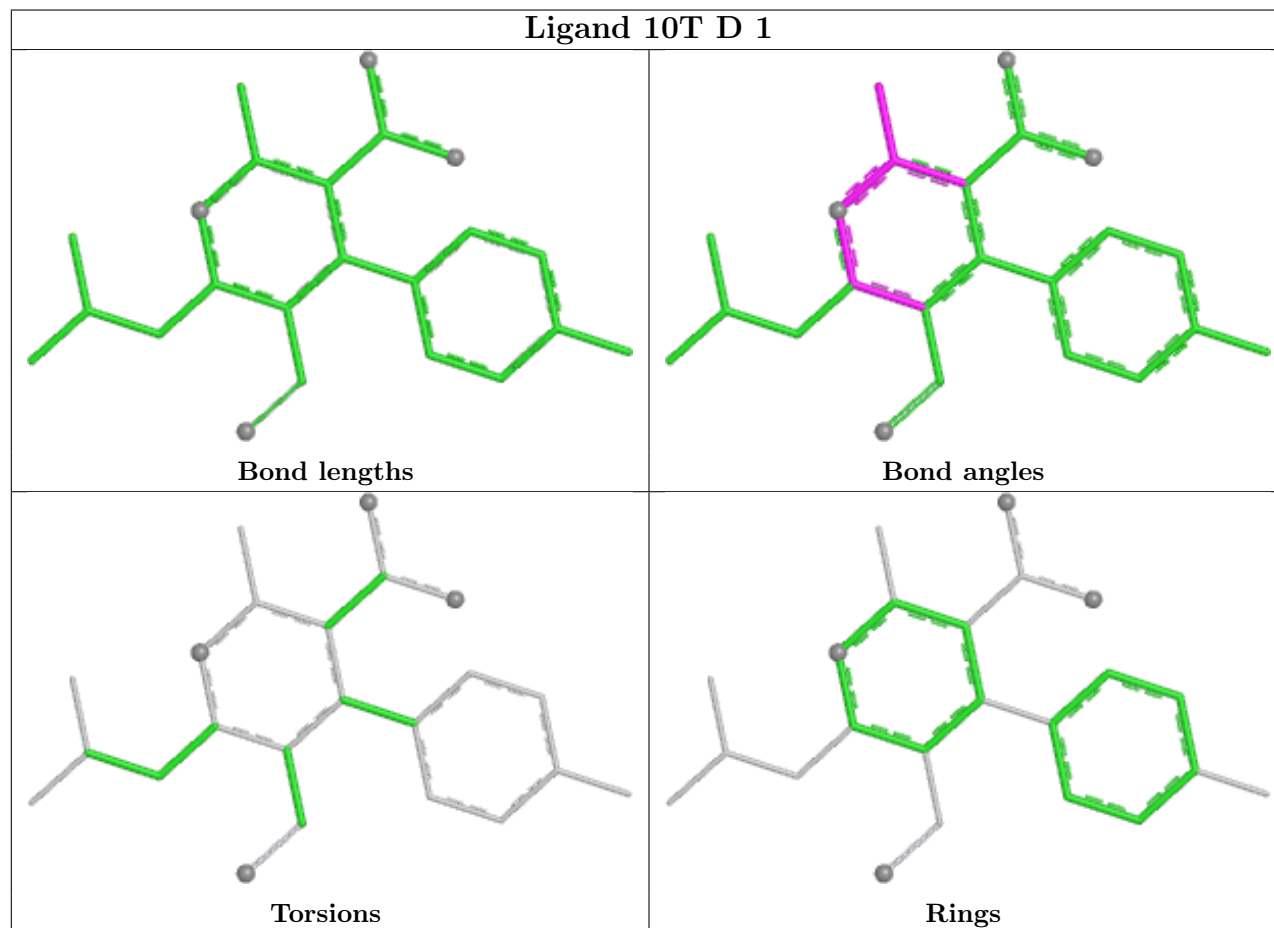
There are no ring outliers.

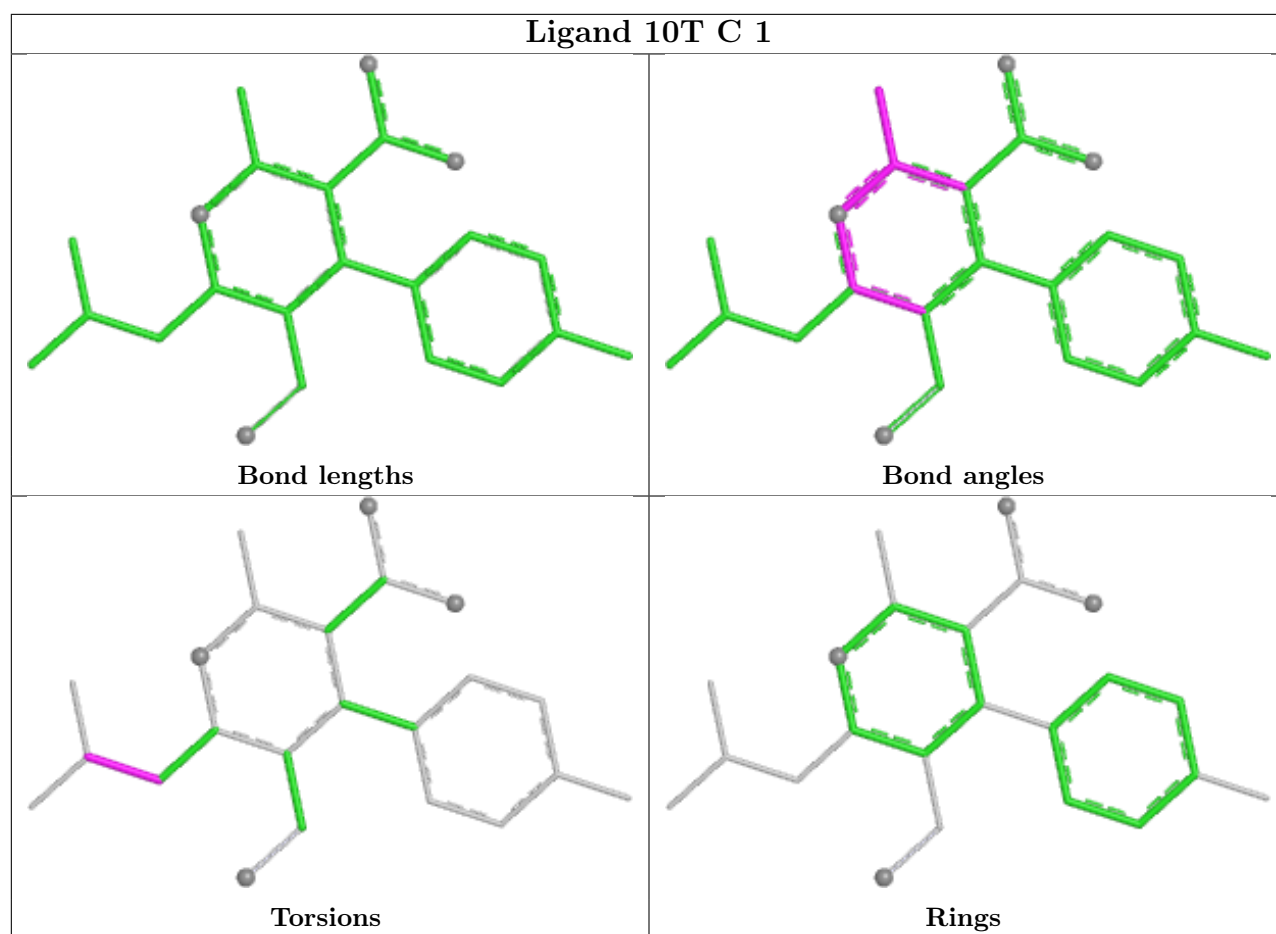
3 monomers are involved in 4 short contacts:

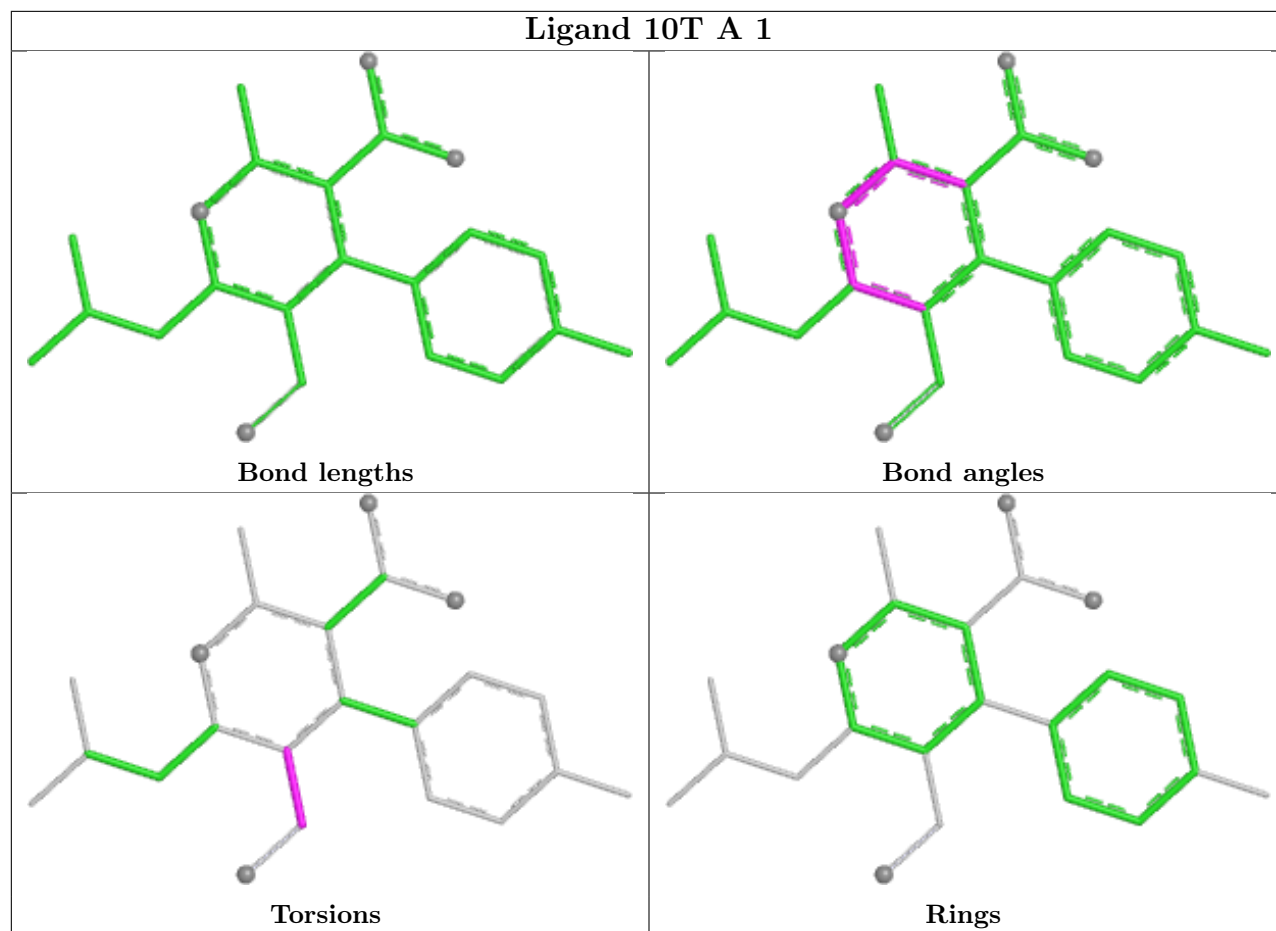
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	10T	1	0
3	C	1	10T	1	0
4	B	851	NAG	2	0

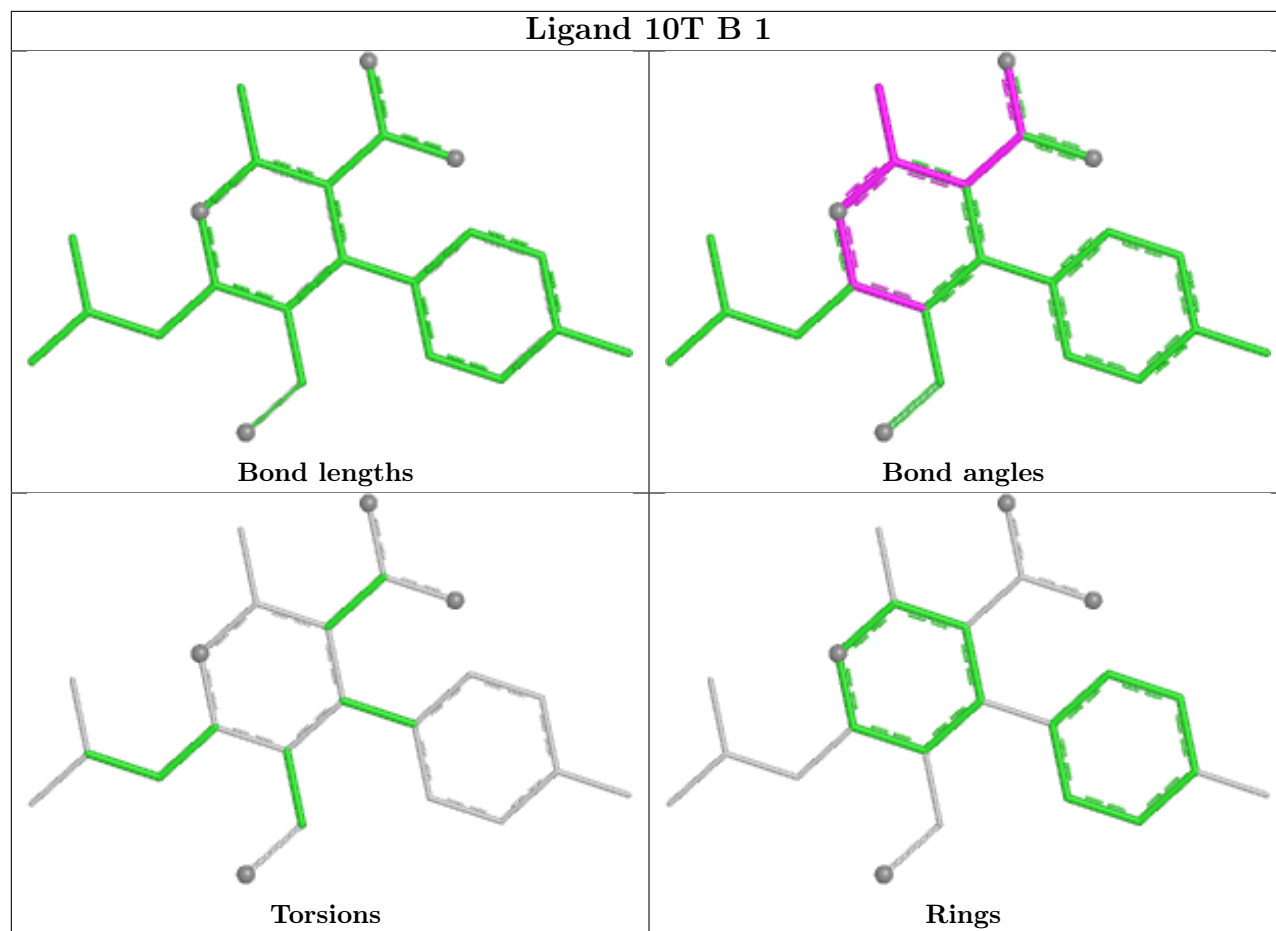
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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	727/740 (98%)	0.76	45 (6%)	26 26	38, 47, 61, 77	0
1	B	733/740 (99%)	0.64	16 (2%)	62 60	36, 46, 60, 83	0
1	C	727/740 (98%)	0.92	62 (8%)	16 17	39, 47, 65, 81	0
1	D	727/740 (98%)	0.89	58 (7%)	18 18	36, 47, 64, 76	0
All	All	2914/2960 (98%)	0.80	181 (6%)	26 26	36, 47, 64, 83	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	88	VAL	5.3
1	A	88	VAL	4.5
1	B	81	ALA	4.3
1	D	79	PHE	4.0
1	A	78	VAL	3.7
1	A	399	LYS	3.6
1	C	438	ASP	3.5
1	B	84	GLY	3.5
1	C	89	PHE	3.4
1	A	489	LYS	3.4
1	B	70	TYR	3.3
1	C	93	SER	3.3
1	A	140	ARG	3.3
1	C	467	TYR	3.3
1	C	83	TYR	3.3
1	D	274	ASP	3.3
1	D	89	PHE	3.2
1	C	87	SER	3.2
1	D	102	ILE	3.2
1	D	394	CYS	3.1
1	D	95	PHE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	462	SER	3.1
1	D	138	ASN	3.1
1	D	84	GLY	3.1
1	C	183	TYR	3.0
1	A	84	GLY	3.0
1	C	77	LEU	3.0
1	A	181	PRO	3.0
1	A	135	TYR	3.0
1	C	439	TYR	3.0
1	D	83	TYR	3.0
1	D	70	TYR	2.9
1	D	186	THR	2.9
1	C	487	ASN	2.9
1	D	179	ASN	2.9
1	B	83	TYR	2.9
1	D	183	TYR	2.9
1	D	141	GLN	2.9
1	C	64	SER	2.9
1	A	92	ASN	2.8
1	A	138	ASN	2.8
1	C	322	TYR	2.8
1	A	90	LEU	2.8
1	D	93	SER	2.8
1	C	90	LEU	2.8
1	C	415	LEU	2.8
1	C	85	ASN	2.8
1	A	142	LEU	2.8
1	A	274	ASP	2.8
1	C	339	CYS	2.7
1	C	412	SER	2.7
1	C	97	GLU	2.7
1	D	41	LYS	2.7
1	C	222	PHE	2.7
1	D	279	VAL	2.7
1	C	78	VAL	2.7
1	C	464	GLU	2.6
1	A	392	LYS	2.6
1	C	98	PHE	2.6
1	A	332	GLU	2.6
1	B	80	ASN	2.6
1	B	89	PHE	2.6
1	C	393	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	678	ASP	2.6
1	D	143	ILE	2.6
1	A	132	TYR	2.6
1	A	279	VAL	2.6
1	C	369	ASN	2.6
1	C	521	GLU	2.6
1	D	162	HIS	2.5
1	A	91	GLU	2.5
1	B	82	GLU	2.5
1	A	655	PRO	2.5
1	B	79	PHE	2.5
1	A	148	ILE	2.5
1	D	142	LEU	2.5
1	B	78	VAL	2.5
1	D	134	ILE	2.5
1	C	279	VAL	2.5
1	C	486	VAL	2.5
1	D	85	ASN	2.5
1	A	93	SER	2.5
1	C	434	ILE	2.5
1	C	537	SER	2.5
1	A	505	GLN	2.5
1	C	388	GLN	2.5
1	C	397	ILE	2.4
1	C	277	SER	2.4
1	D	182	SER	2.4
1	C	135	TYR	2.4
1	D	135	TYR	2.4
1	A	63	ILE	2.4
1	D	76	ILE	2.4
1	D	281	ASN	2.4
1	D	537	SER	2.4
1	A	145	GLU	2.4
1	A	448	GLU	2.4
1	C	292	SER	2.4
1	D	464	GLU	2.4
1	D	505	GLN	2.4
1	C	273	THR	2.4
1	B	161	GLY	2.3
1	D	72	GLN	2.3
1	C	338	ASN	2.3
1	D	133	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	63	ILE	2.3
1	D	118	TYR	2.3
1	D	330	TYR	2.3
1	C	178	PRO	2.3
1	D	88	VAL	2.3
1	C	342	ALA	2.3
1	C	465	ALA	2.3
1	D	284	SER	2.3
1	A	95	PHE	2.3
1	D	100	HIS	2.2
1	A	94	THR	2.2
1	C	141	GLN	2.2
1	C	295	ILE	2.2
1	C	348	MET	2.2
1	D	87	SER	2.2
1	C	95	PHE	2.2
1	B	301	CYS	2.2
1	D	467	TYR	2.2
1	C	300	LEU	2.2
1	D	77	LEU	2.2
1	D	131	SER	2.2
1	C	63	ILE	2.2
1	D	568	ALA	2.2
1	A	72	GLN	2.2
1	B	348	MET	2.2
1	C	333	SER	2.2
1	A	134	ILE	2.2
1	D	651	ILE	2.2
1	D	113	PHE	2.2
1	D	181	PRO	2.1
1	C	92	ASN	2.1
1	D	338	ASN	2.1
1	C	416	TYR	2.1
1	C	463	LYS	2.1
1	B	143	ILE	2.1
1	A	79	PHE	2.1
1	A	57	LEU	2.1
1	A	70	TYR	2.1
1	C	68	TYR	2.1
1	C	276	LEU	2.1
1	C	386	TYR	2.1
1	D	490	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	76	ILE	2.1
1	D	202	VAL	2.1
1	C	182	SER	2.1
1	C	332	GLU	2.1
1	D	187	TRP	2.1
1	A	491	LEU	2.1
1	A	414	TYR	2.1
1	D	220	GLY	2.1
1	A	107	ILE	2.1
1	A	96	ASP	2.1
1	A	488	ASP	2.1
1	A	69	LEU	2.1
1	D	487	ASN	2.1
1	C	99	GLY	2.1
1	D	173	TYR	2.1
1	D	535	ASP	2.0
1	D	282	ALA	2.0
1	A	280	THR	2.0
1	B	77	LEU	2.0
1	B	75	ASN	2.0
1	B	179	ASN	2.0
1	A	335	GLY	2.0
1	C	389	ILE	2.0
1	D	661	TYR	2.0
1	A	89	PHE	2.0
1	A	502	LYS	2.0
1	D	81	ALA	2.0
1	A	144	THR	2.0
1	C	280	THR	2.0
1	A	180	LEU	2.0
1	D	236	ILE	2.0
1	D	656	VAL	2.0
1	A	662	TYR	2.0
1	C	414	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

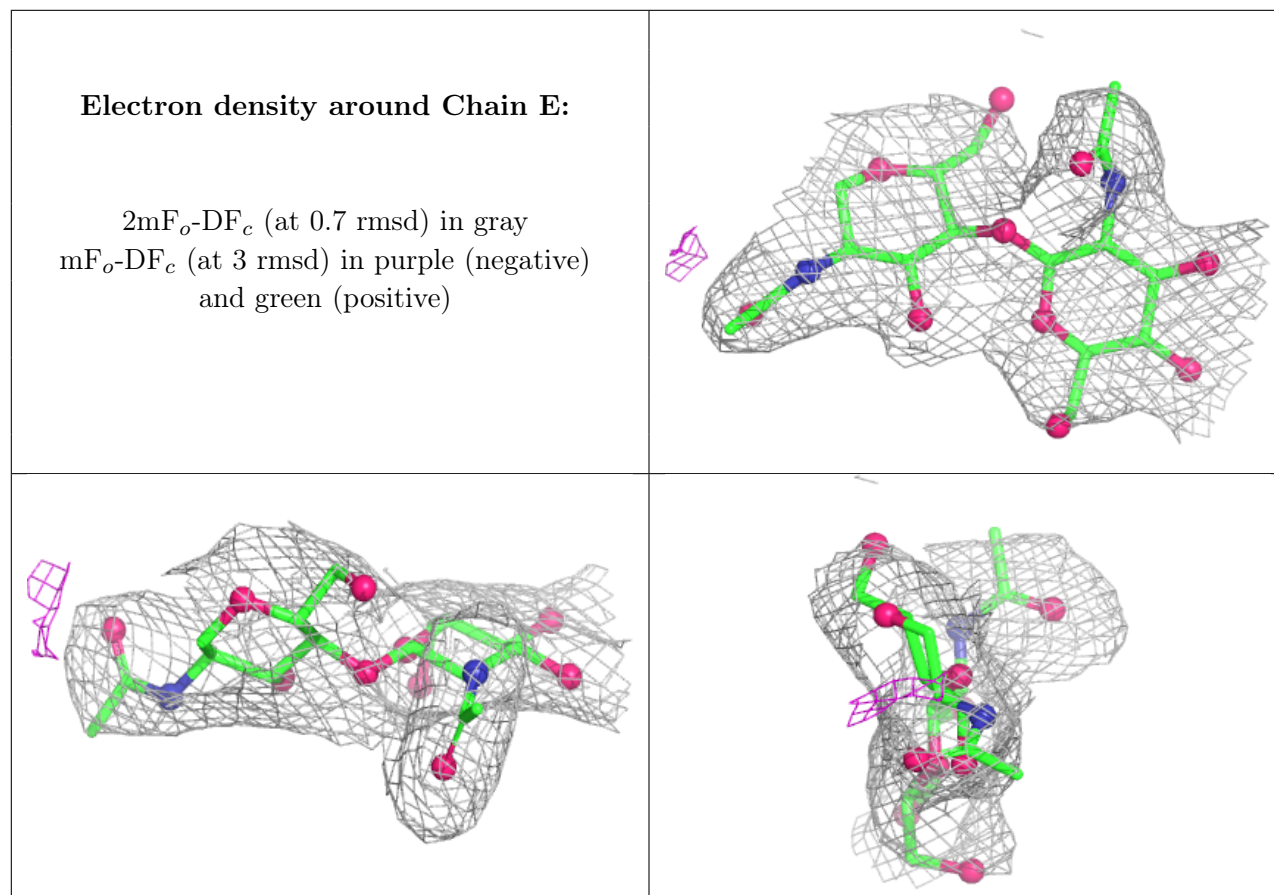
There are no non-standard protein/DNA/RNA residues in this entry.

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.

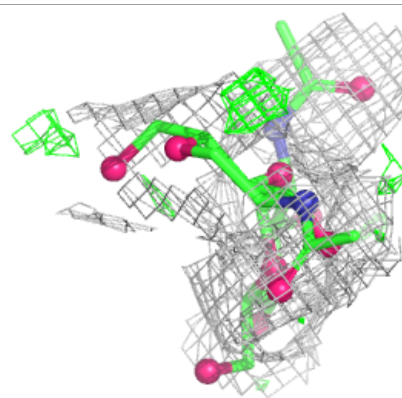
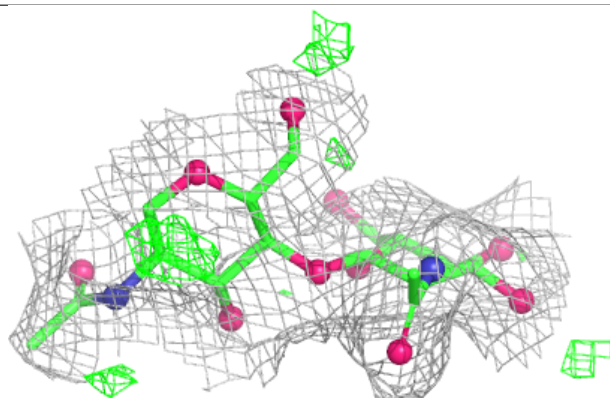
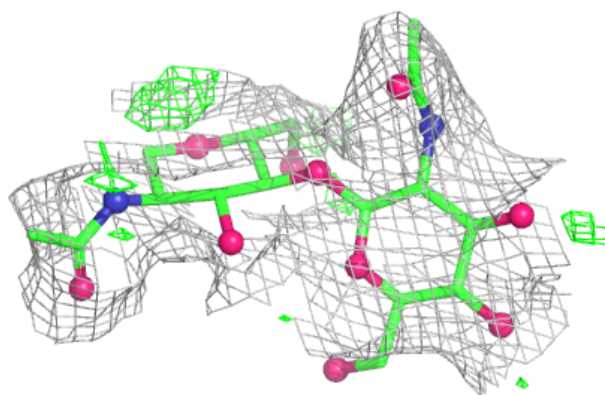
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	G	2	14/15	0.64	0.14	78,79,82,82	0
2	NAG	F	1	14/15	0.72	0.16	67,70,73,74	0
2	NAG	F	2	14/15	0.73	0.15	73,76,78,79	0
2	NAG	I	2	14/15	0.80	0.12	71,73,75,75	0
2	NAG	H	2	14/15	0.82	0.11	55,56,58,58	0
2	NAG	E	2	14/15	0.82	0.12	66,69,70,71	0
2	NAG	G	1	14/15	0.84	0.12	64,66,69,74	0
2	NAG	E	1	14/15	0.89	0.12	59,61,65,66	0
2	NAG	I	1	14/15	0.90	0.09	57,59,63,67	0
2	NAG	H	1	14/15	0.90	0.10	46,50,52,53	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.

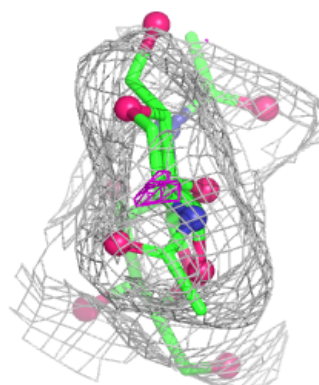
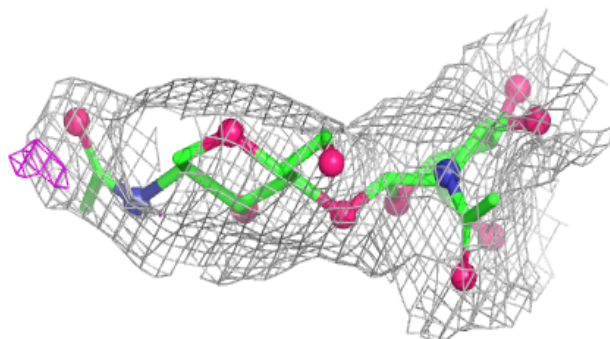
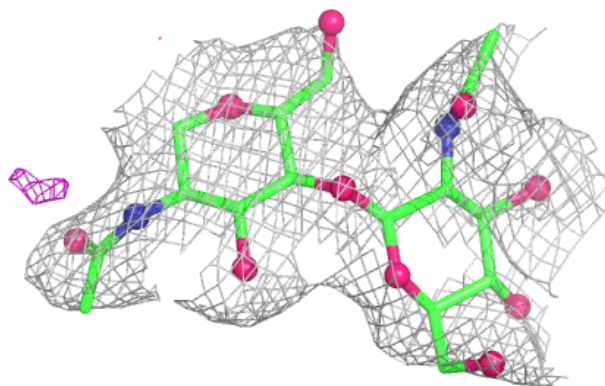


Electron density around Chain F:

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

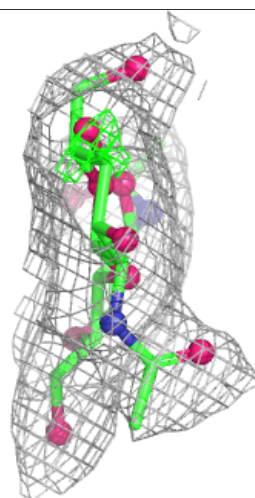
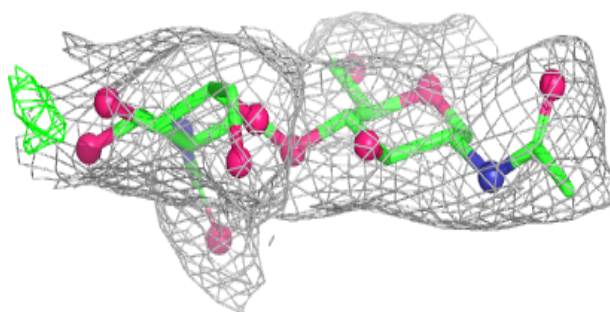
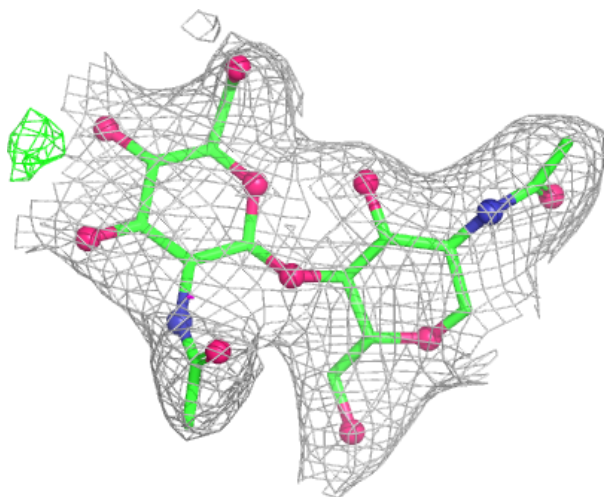
**Electron density around Chain G:**

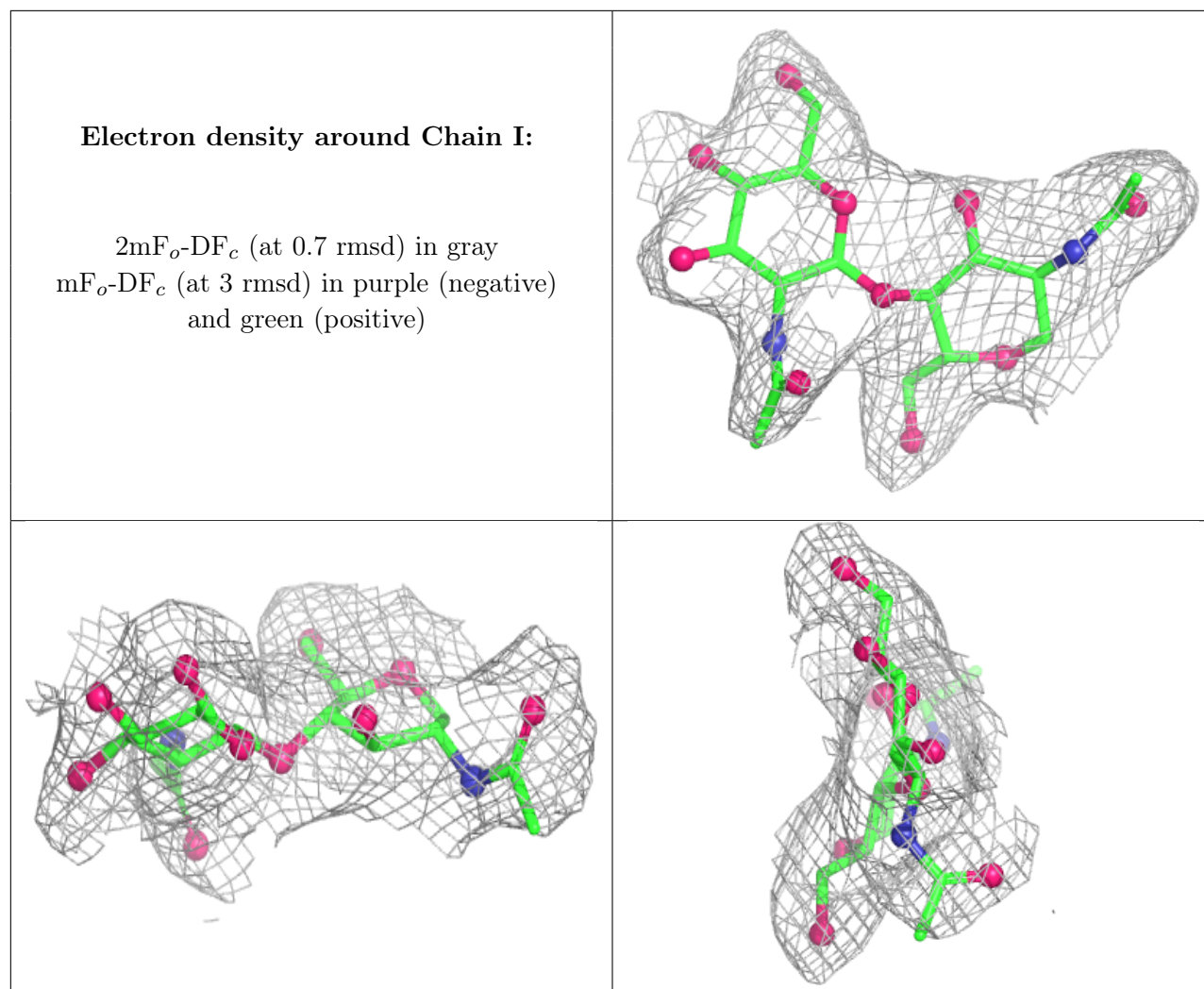
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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)





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.

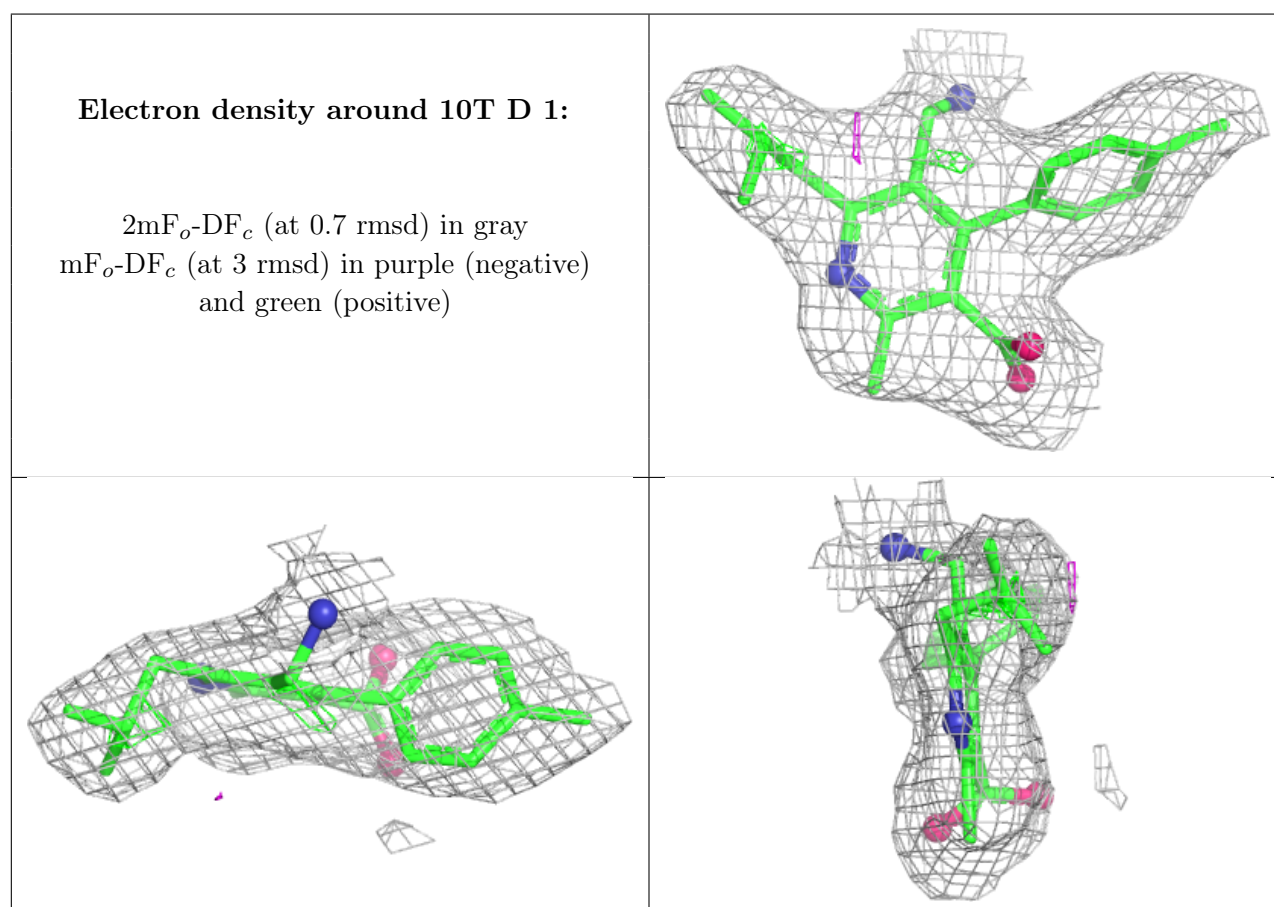
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	B	851	14/15	0.62	0.15	78,79,80,80	0
4	NAG	B	2191	14/15	0.67	0.15	57,59,60,61	0
4	NAG	A	1501	14/15	0.71	0.14	67,70,70,71	0
4	NAG	C	2811	14/15	0.73	0.13	63,66,67,68	0
4	NAG	D	1501	14/15	0.74	0.13	65,69,70,70	0
4	NAG	D	2811	14/15	0.75	0.13	67,69,70,70	0
4	NAG	C	1501	14/15	0.76	0.13	59,63,64,65	0
4	NAG	A	3211	14/15	0.78	0.12	58,61,62,62	0
4	NAG	B	1501	14/15	0.83	0.11	60,63,66,67	0

Continued on next page...

Continued from previous page...

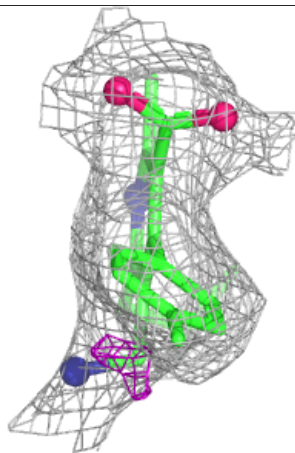
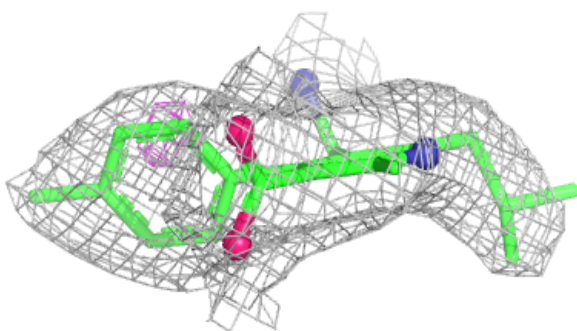
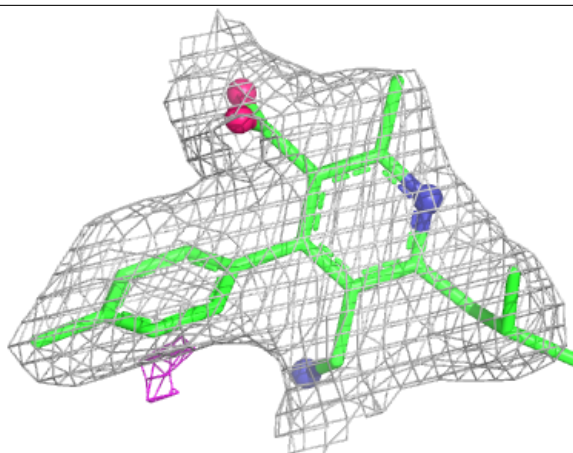
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	B	2811	14/15	0.87	0.10	59,62,64,64	0
3	10T	D	1	23/23	0.92	0.18	46,51,51,53	0
3	10T	C	1	23/23	0.93	0.12	42,44,46,48	0
3	10T	A	1	23/23	0.93	0.14	44,49,50,50	0
3	10T	B	1	23/23	0.93	0.14	46,47,49,51	0

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.



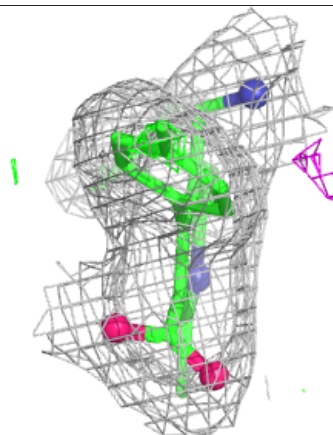
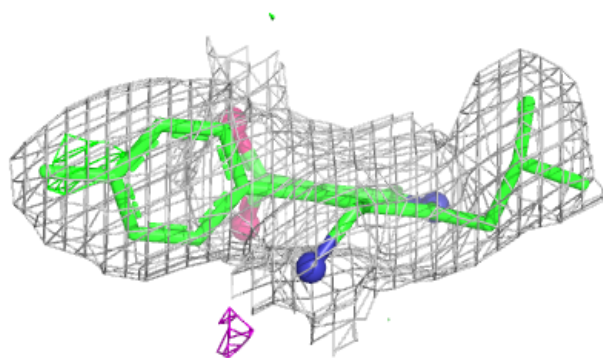
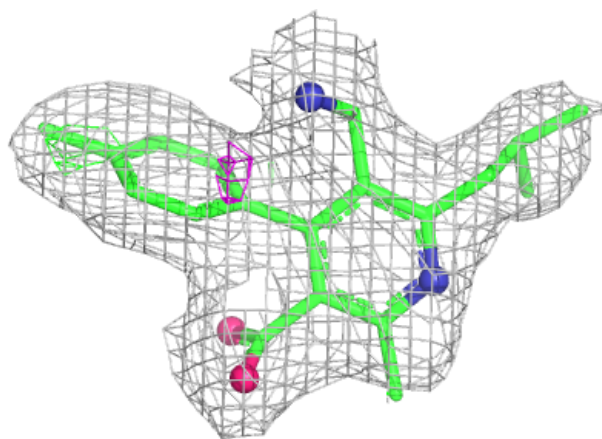
Electron density around 10T C 1:

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



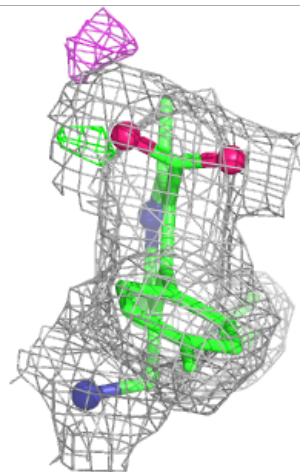
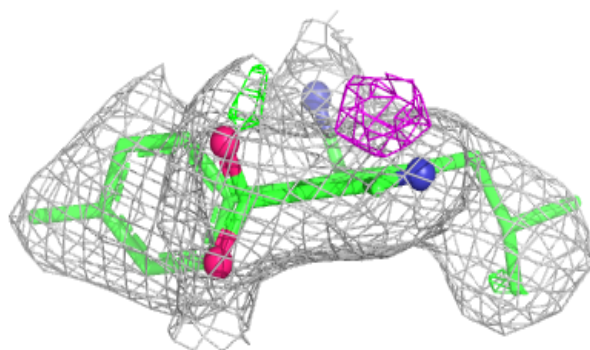
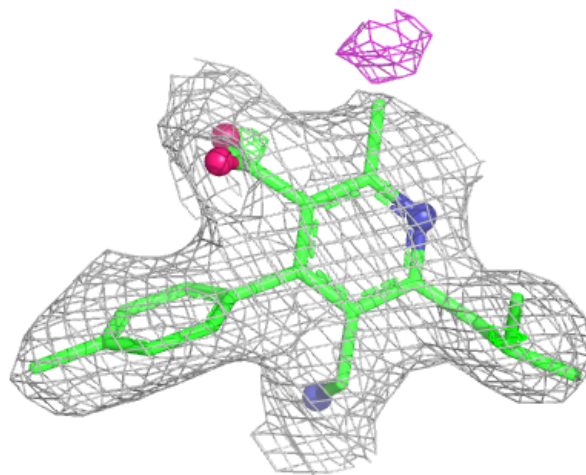
Electron density around 10T A 1:

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



Electron density around 10T B 1:

$2mF_o-DF_c$ (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.