



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:27 AM UTC

PDB ID : 4BTW / pdb_00004btw
Title : Crystal structure of human vascular adhesion protein-1 in complex with pyridazinone inhibitors
Authors : Bligt-Linden, E.; Pihlavisto, M.; Szatmari, I.; Otwinowski, Z.; Smith, D.J.; Lazar, L.; Fulop, F.; Salminen, T.A.
Deposited on : 2013-06-19
Resolution : 2.80 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:

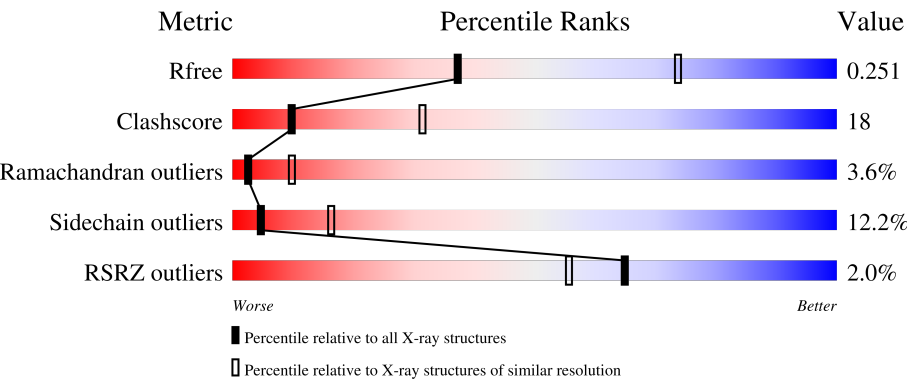
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



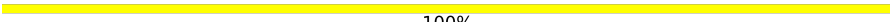
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	737	2% 56%32%8% . .
1	B	737	2% 57%30%8% . .
2	C	3	67%33%
3	D	2	100%

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Mol	Chain	Length	Quality of chain
3	F	2	 100%
4	E	5	 60% 40%

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
7	NAG	A	1770	X	-	-	-
7	NAG	A	1771	X	-	-	-
7	NAG	B	1774	X	-	-	-

2 Entry composition [i](#)

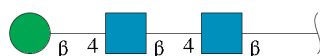
There are 9 unique types of molecules in this entry. The entry contains 11573 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MEMBRANE PRIMARY AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	711	Total	C	N	O	S	0	0	0
			5609	3599	970	1020	20			
1	B	705	Total	C	N	O	S	0	0	0
			5562	3571	959	1012	20			

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



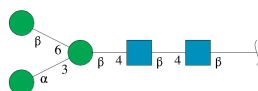
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 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
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	5	Total	C	N	O	0	0	0
			61	34	2	25			

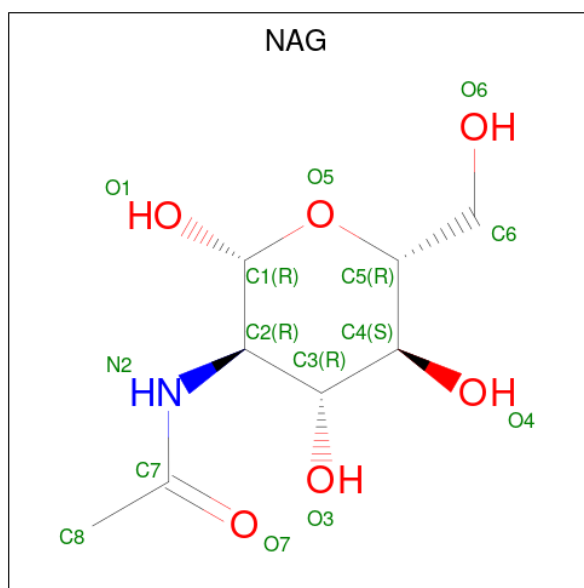
- Molecule 5 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cu	0	0
			1	1		
5	B	1	Total	Cu	0	0
			1	1		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

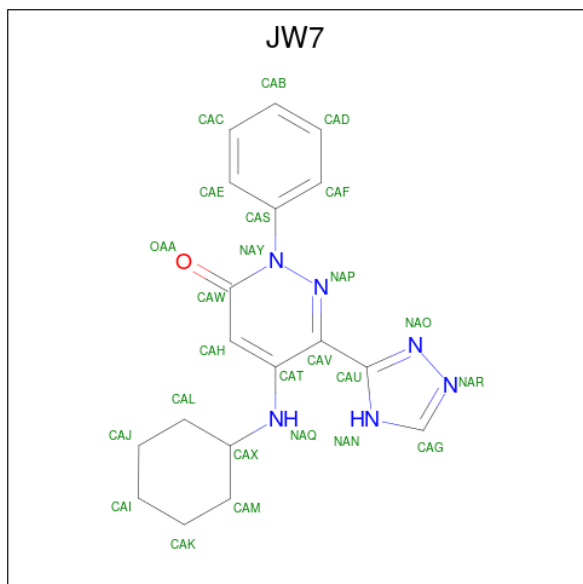
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Ca	0	0
			2	2		
6	B	2	Total	Ca	0	0
			2	2		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 8 is 5-(cyclohexylamino)-2-phenyl-6-(1H-1,2,4-triazol-5-yl)-3(2H)-pyridazinone (CCD ID: JW7) (formula: C₁₈H₂₀N₆O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			25	18	6	1		
8	B	1	Total	C	N	O	0	0
			25	18	6	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	64	Total	O	0	0
			64	64		

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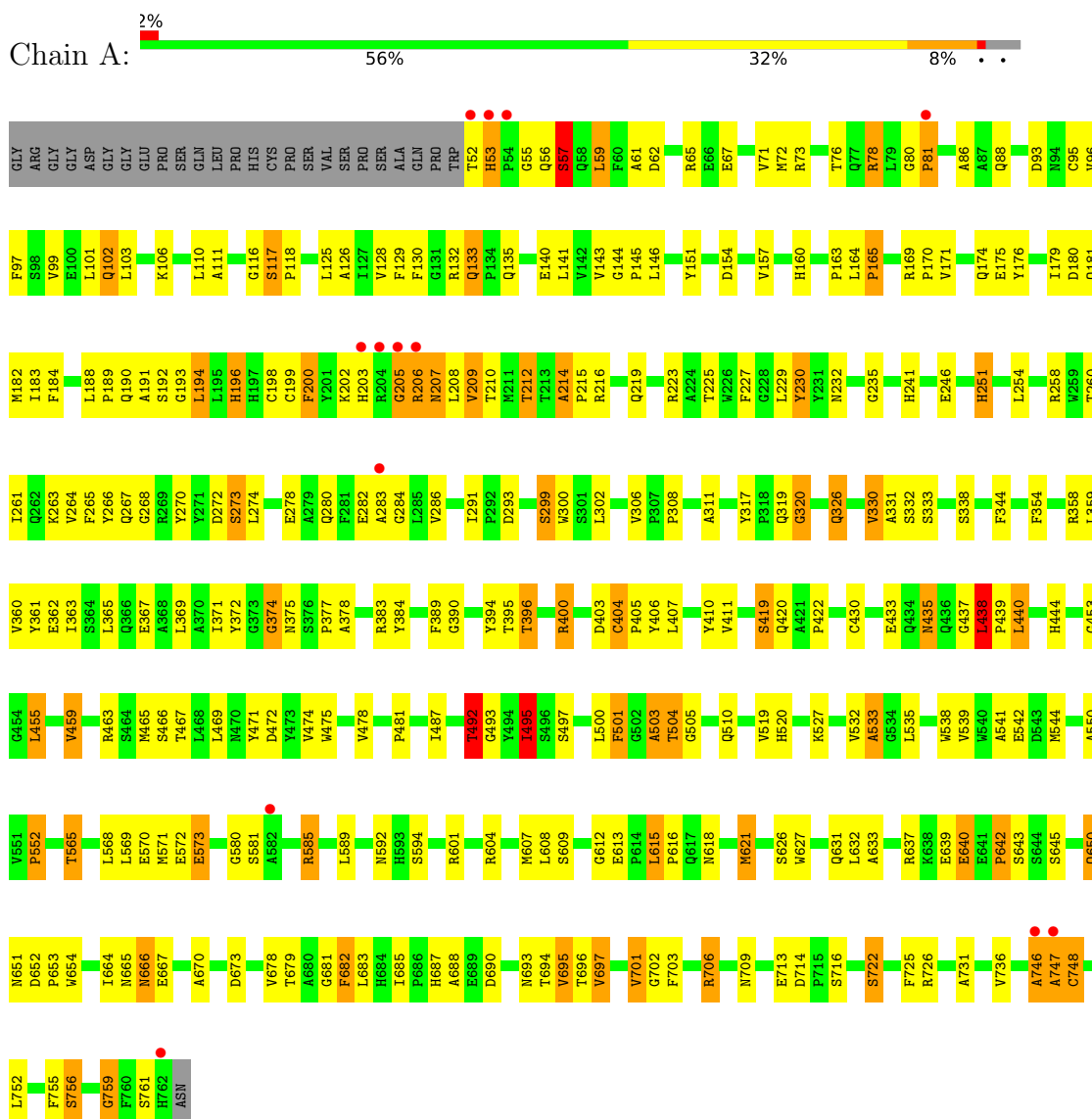
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	42	Total	O	0	0
			42	42		

3 Residue-property plots

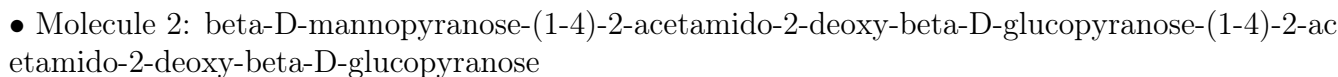
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: MEMBRANE PRIMARY AMINE OXIDASE





NAG1
NAG2
BMA3

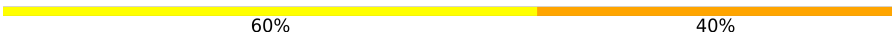
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

NAG1
NAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

NAG1
NAG2

- Molecule 4: α -D-mannopyranose-(1-3)-[β -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain E: 

MAG1
MAG2
BM13
MAM4
BM15

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	226.47Å 226.47Å 219.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.39 – 2.80 49.39 – 2.80	Depositor EDS
% Data completeness (in resolution range)	77.9 (49.39-2.80) 77.9 (49.39-2.80)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.205 , 0.260 0.199 , 0.251	Depositor DCC
R_{free} test set	3176 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11573	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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: CU, JW7, BMA, MAN, NAG, CA, TPQ

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	0.98	2/5774 (0.0%)	1.20	35/7874 (0.4%)
1	B	0.95	5/5724 (0.1%)	1.18	26/7805 (0.3%)
All	All	0.96	7/11498 (0.1%)	1.19	61/15679 (0.4%)

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	A	0	3
1	B	0	4
All	All	0	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	641	GLU	CA-C	7.57	1.62	1.52
1	B	214	ALA	CA-C	-6.46	1.44	1.52
1	B	613	GLU	CA-C	5.75	1.59	1.53
1	A	169	ARG	CA-C	-5.70	1.47	1.53
1	B	373	GLY	N-CA	5.56	1.49	1.44
1	A	503	ALA	CA-C	5.46	1.60	1.52
1	B	641	GLU	C-N	5.27	1.39	1.33

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	ALA	CA-C-N	-9.60	111.01	120.52
1	B	214	ALA	C-N-CA	-9.60	111.01	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	613	GLU	N-CA-C	8.84	120.44	109.57
1	B	685	ILE	CA-C-N	-8.33	111.20	119.78
1	B	685	ILE	C-N-CA	-8.33	111.20	119.78
1	A	501	PHE	N-CA-C	7.99	121.26	107.28
1	A	374	GLY	N-CA-C	7.62	121.77	110.42
1	B	592	ASN	N-CA-C	-7.58	103.02	111.28
1	A	581	SER	N-CA-C	7.08	117.87	107.88
1	A	291	ILE	CB-CA-C	-6.91	102.85	110.52
1	A	404	CYS	N-CA-C	-6.86	101.95	108.13
1	A	62	ASP	N-CA-C	-6.85	101.69	110.53
1	A	682	PHE	N-CA-C	6.83	118.72	107.73
1	B	117	SER	CA-C-N	-6.78	113.39	120.38
1	B	117	SER	C-N-CA	-6.78	113.39	120.38
1	B	301	SER	N-CA-C	6.65	119.52	109.41
1	B	84	VAL	N-CA-C	6.59	119.01	108.85
1	B	372	TYR	N-CA-C	6.58	120.26	110.52
1	B	382	THR	N-CA-C	6.58	120.17	110.30
1	A	117	SER	CA-C-N	-6.53	113.66	120.38
1	A	117	SER	C-N-CA	-6.53	113.66	120.38
1	A	685	ILE	N-CA-C	-6.26	101.95	108.15
1	A	330	VAL	CB-CA-C	-6.11	101.11	110.95
1	A	495	ILE	CB-CA-C	-6.06	101.66	110.63
1	A	673	ASP	CA-C-N	-5.84	113.74	122.74
1	A	673	ASP	C-N-CA	-5.84	113.74	122.74
1	B	691	ILE	CB-CA-C	-5.83	104.13	110.37
1	A	103	LEU	CA-C-N	5.79	123.89	119.66
1	A	103	LEU	C-N-CA	5.79	123.89	119.66
1	B	583	THR	CA-C-N	-5.76	114.63	120.85
1	B	583	THR	C-N-CA	-5.76	114.63	120.85
1	A	615	LEU	N-CA-C	-5.70	102.56	109.57
1	A	440	LEU	N-CA-C	-5.69	105.16	111.36
1	A	592	ASN	N-CA-C	-5.69	104.29	111.11
1	B	153	ARG	CB-CA-C	-5.67	104.40	111.43
1	B	462	VAL	CB-CA-C	-5.66	101.78	110.50
1	A	639	GLU	N-CA-C	-5.66	104.73	111.69
1	B	535	LEU	N-CA-C	5.66	117.45	111.28
1	A	438	LEU	CA-C-N	-5.57	114.23	119.85
1	A	438	LEU	C-N-CA	-5.57	114.23	119.85
1	B	641	GLU	CA-CB-CG	5.56	125.23	114.10
1	A	492	THR	CB-CA-C	-5.54	107.48	114.40
1	A	311	ALA	CA-C-N	-5.47	114.74	120.38
1	A	311	ALA	C-N-CA	-5.47	114.74	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	245	LEU	N-CA-C	5.47	117.64	108.73
1	B	209	VAL	N-CA-C	5.46	114.36	107.70
1	A	736	VAL	CB-CA-C	-5.33	105.10	112.24
1	B	469	LEU	CB-CA-C	-5.31	110.00	117.23
1	A	759	GLY	N-CA-C	5.24	125.59	113.18
1	B	66	GLU	N-CA-C	-5.23	105.49	111.14
1	A	643	SER	CA-C-N	5.19	127.24	120.28
1	A	643	SER	C-N-CA	5.19	127.24	120.28
1	A	492	THR	N-CA-CB	5.16	115.30	108.96
1	A	535	LEU	N-CA-C	5.16	116.59	111.07
1	A	196	HIS	N-CA-C	-5.09	105.92	111.82
1	A	157	VAL	CB-CA-C	-5.08	104.28	112.16
1	B	654	TRP	N-CA-C	-5.07	106.25	112.90
1	B	381	THR	CB-CA-C	-5.07	103.15	110.96
1	A	188	LEU	CA-C-N	-5.03	113.47	119.05
1	A	188	LEU	C-N-CA	-5.03	113.47	119.05
1	B	381	THR	N-CA-C	-5.02	105.50	110.97

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	CYS	Peptide
1	A	205	GLY	Peptide
1	A	437	GLY	Peptide
1	B	213	THR	Peptide
1	B	214	ALA	Peptide
1	B	512	SER	Peptide
1	B	749	ALA	Peptide

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	5609	0	5351	194	1
1	B	5562	0	5313	222	0
2	C	39	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	28	0	25	0	0
3	F	28	0	25	0	0
4	E	61	0	52	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	28	0	26	0	0
7	B	56	0	52	2	0
8	A	25	0	20	4	0
8	B	25	0	20	6	0
9	A	64	0	0	1	0
9	B	42	0	0	8	0
All	All	11573	0	10918	394	1

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 18.

All (394) 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:367:GLU:OE2	1:A:645:SER:OG	1.75	1.04
1:A:492:THR:HG21	1:B:441:ARG:HA	1.42	1.01
1:B:620:SER:HG	1:B:654:TRP:HD1	1.10	0.91
1:B:620:SER:HG	1:B:654:TRP:CD1	1.87	0.91
1:A:80:GLY:O	1:A:81:PRO:O	1.90	0.90
1:A:495:ILE:HB	9:A:2046:HOH:O	1.70	0.89
8:B:2000:JW7:HAM1	8:B:2000:JW7:HAH	1.59	0.85
1:A:265:PHE:HD2	1:A:270:TYR:CE1	1.95	0.85
1:A:469:LEU:HD21	8:A:2000:JW7:CAD	2.07	0.84
1:A:585:ARG:NH1	1:B:611:ALA:O	2.11	0.83
1:B:500:LEU:HD11	1:B:504:THR:HG21	1.60	0.83
4:E:3:BMA:HO4	4:E:5:BMA:HO2	1.14	0.82
1:A:102:GLN:HE21	1:A:102:GLN:HA	1.45	0.79
1:B:214:ALA:CB	1:B:382:THR:HA	2.12	0.79
1:A:519:VAL:HG13	1:B:562:LEU:HD23	1.63	0.79
1:B:271:TYR:CE2	1:B:277:LEU:HD13	2.18	0.79
1:A:86:ALA:HA	1:A:95:CYS:SG	2.25	0.76
1:A:214:ALA:CB	1:A:215:PRO:HD3	2.16	0.75
1:B:214:ALA:HB2	1:B:382:THR:HA	1.67	0.75
1:B:163:PRO:HB3	4:E:1:NAG:H82	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:THR:O	1:B:383:ARG:HD3	1.87	0.74
1:A:191:ALA:HA	1:A:278:GLU:HG2	1.70	0.73
1:A:472:ASP:OD2	1:B:443:HIS:ND1	2.20	0.72
1:B:407:LEU:HD21	1:B:752:LEU:HD23	1.72	0.72
1:B:251:HIS:HA	1:B:259:TRP:CD1	2.25	0.71
1:B:214:ALA:CB	1:B:215:PRO:CD	2.68	0.71
1:B:214:ALA:CB	1:B:215:PRO:HD2	2.21	0.71
1:A:214:ALA:HB1	1:A:215:PRO:HD3	1.73	0.70
1:B:683:LEU:HD12	1:B:684:HIS:N	2.06	0.70
1:A:191:ALA:HA	1:A:278:GLU:CG	2.22	0.70
8:B:2000:JW7:HAF	8:B:2000:JW7:OAA	1.91	0.69
1:A:130:PHE:HB3	1:A:133:GLN:OE1	1.93	0.69
1:A:212:THR:OG1	1:A:216:ARG:NH2	2.26	0.69
1:B:474:VAL:HB	1:B:490:TYR:HB2	1.74	0.68
1:B:115:ARG:O	1:B:117:SER:N	2.26	0.68
1:B:214:ALA:HB1	1:B:215:PRO:CD	2.24	0.68
1:A:171:VAL:HG13	1:A:175:GLU:HB3	1.77	0.67
1:B:360:VAL:HG12	1:B:530:LEU:HA	1.77	0.66
1:B:525:HIS:CE1	1:B:644:SER:HG	2.13	0.66
1:B:382:THR:C	1:B:383:ARG:HD3	2.21	0.66
1:A:492:THR:HG22	1:A:694:THR:O	1.96	0.65
1:A:544:MET:HE1	1:B:521:THR:CG2	2.27	0.65
1:B:478:VAL:HG22	1:B:486:GLU:HB3	1.78	0.65
1:B:349:ILE:HD11	1:B:363:ILE:HB	1.77	0.65
1:A:440:LEU:HD23	1:A:455:LEU:HD23	1.79	0.65
1:A:640:GLU:C	1:A:642:PRO:HD3	2.22	0.65
1:B:271:TYR:CD2	1:B:277:LEU:HD13	2.31	0.65
1:B:229:LEU:CD1	1:B:245:LEU:HD23	2.28	0.64
1:A:214:ALA:CB	1:A:215:PRO:CD	2.75	0.64
1:B:366:GLN:HG3	1:B:644:SER:HB2	1.80	0.64
1:B:496:SER:O	1:B:518:THR:HG22	1.98	0.64
1:B:214:ALA:HB1	1:B:383:ARG:H	1.63	0.63
1:A:78:ARG:HH11	1:A:78:ARG:HB2	1.63	0.63
1:B:469:LEU:HD21	8:B:2000:JW7:CAC	2.28	0.63
1:B:615:LEU:HD12	1:B:616:PRO:HD2	1.79	0.62
1:A:394:TYR:CE1	8:A:2000:JW7:HAE	2.34	0.62
1:A:544:MET:HE1	1:B:521:THR:HG22	1.79	0.62
1:A:67:GLU:O	1:A:71:VAL:HG23	1.99	0.62
1:B:575:ALA:HB1	1:B:634:VAL:HG23	1.81	0.62
1:B:129:PHE:CZ	1:B:169:ARG:HB2	2.34	0.62
1:A:532:VAL:O	1:A:533:ALA:C	2.42	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ALA:HB3	1:B:215:PRO:HD2	1.81	0.62
1:A:52:THR:OG1	1:A:53:HIS:CD2	2.53	0.61
1:B:683:LEU:HD12	1:B:684:HIS:H	1.66	0.61
1:B:690:ASP:OD1	1:B:694:THR:HG23	1.99	0.61
1:A:369:LEU:HD12	1:A:384:TYR:O	2.01	0.61
1:B:542:GLU:HA	1:B:565:THR:O	2.01	0.60
1:B:419:SER:OG	1:B:420:GLN:N	2.34	0.60
1:B:468:LEU:O	1:B:471:TPQ:H6	2.01	0.60
1:A:344:PHE:HA	1:A:390:GLY:HA2	1.83	0.60
1:A:265:PHE:CD2	1:A:270:TYR:CE1	2.84	0.60
1:B:551:VAL:HG23	1:B:557:HIS:O	2.02	0.60
1:A:246:GLU:OE1	1:A:377:PRO:HD2	2.02	0.59
1:B:187:GLU:O	1:B:274:LEU:HD13	2.01	0.59
1:B:716:SER:O	1:B:719:SER:HB2	2.02	0.59
1:A:495:ILE:HD12	1:A:495:ILE:N	2.17	0.59
1:B:212:THR:HG21	1:B:216:ARG:HH21	1.67	0.59
1:B:738:PRO:HA	1:B:741:CYS:SG	2.42	0.59
1:B:72:MET:HE1	1:B:96:VAL:HG11	1.84	0.59
1:B:175:GLU:O	1:B:179:ILE:HG13	2.02	0.59
1:A:266:TYR:O	1:A:268:GLY:N	2.34	0.58
1:A:205:GLY:O	1:A:207:ASN:N	2.36	0.58
1:A:403:ASP:OD2	1:B:442:ARG:NH1	2.35	0.58
1:A:209:VAL:HG23	1:A:232:ASN:HB2	1.85	0.58
1:B:212:THR:HG21	1:B:216:ARG:NH2	2.19	0.58
1:A:265:PHE:HD2	1:A:270:TYR:HE1	1.48	0.58
1:A:241:HIS:NE2	1:A:299:SER:O	2.35	0.58
1:A:308:PRO:HA	1:B:720:ALA:O	2.04	0.58
1:B:187:GLU:HG3	1:B:274:LEU:HD12	1.86	0.57
1:B:229:LEU:HD13	1:B:245:LEU:HD23	1.87	0.57
1:A:102:GLN:HE21	1:A:102:GLN:CA	2.14	0.57
1:B:213:THR:HB	1:B:382:THR:OG1	2.05	0.57
1:B:214:ALA:HB2	1:B:382:THR:CA	2.35	0.57
1:B:187:GLU:CG	1:B:274:LEU:HD12	2.34	0.57
1:B:383:ARG:HD3	1:B:383:ARG:N	2.19	0.57
1:B:611:ALA:O	1:B:613:GLU:N	2.37	0.57
1:A:59:LEU:HD23	1:A:59:LEU:N	2.20	0.56
1:A:265:PHE:CD2	1:A:270:TYR:HE1	2.23	0.56
1:A:371:ILE:O	1:A:520:HIS:HA	2.04	0.56
1:B:716:SER:O	1:B:719:SER:CB	2.52	0.56
1:A:319:GLN:O	1:A:320:GLY:O	2.23	0.56
1:B:252:LYS:O	1:B:252:LYS:HD3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ARG:H	1:B:206:ARG:HH22	1.54	0.56
1:B:276:GLN:HG3	9:B:2014:HOH:O	2.06	0.56
1:A:372:TYR:CD1	1:A:520:HIS:HB3	2.40	0.55
1:A:403:ASP:HB3	1:A:465:MET:CE	2.36	0.55
1:A:492:THR:CG2	1:B:441:ARG:HA	2.27	0.55
1:B:500:LEU:CD1	1:B:504:THR:HG21	2.34	0.55
1:A:57:SER:HB3	1:A:59:LEU:HD22	1.89	0.55
1:A:493:GLY:O	1:A:693:ASN:HA	2.07	0.55
1:B:72:MET:HE1	1:B:96:VAL:CG1	2.37	0.55
1:A:374:GLY:O	1:B:561:ARG:NH2	2.36	0.55
1:B:204:ARG:H	1:B:206:ARG:NH2	2.05	0.54
1:B:445:SER:HB3	1:B:451:TYR:CE1	2.42	0.54
1:A:214:ALA:HB3	1:A:215:PRO:HD3	1.90	0.54
1:B:214:ALA:HB1	1:B:215:PRO:HD2	1.86	0.54
1:A:440:LEU:HD23	1:A:455:LEU:CD2	2.37	0.54
1:A:607:MET:HE1	1:A:631:GLN:HB3	1.89	0.54
1:A:200:PHE:CD1	1:A:200:PHE:N	2.75	0.54
1:A:214:ALA:O	1:A:215:PRO:C	2.50	0.54
1:A:627:TRP:CE3	1:A:679:THR:HG23	2.43	0.54
1:B:371:ILE:HG12	1:B:383:ARG:HB3	1.90	0.54
8:A:2000:JW7:HAE	8:A:2000:JW7:OAA	2.08	0.53
1:B:623:ARG:HD3	1:B:659:ASP:OD2	2.08	0.53
1:A:332:SER:OG	1:A:333:SER:N	2.42	0.53
1:A:550:ALA:O	1:A:552:PRO:HD3	2.09	0.53
1:A:678:VAL:HG11	1:A:703:PHE:CD2	2.43	0.53
1:B:714:ASP:OD2	1:B:716:SER:OG	2.24	0.53
1:A:171:VAL:HG11	1:A:176:TYR:CE1	2.43	0.53
1:B:640:GLU:C	1:B:642:PRO:HD3	2.34	0.53
1:B:256:PRO:HA	1:B:259:TRP:CE2	2.44	0.52
1:B:445:SER:CB	1:B:451:TYR:CE1	2.92	0.52
1:B:349:ILE:CD1	1:B:363:ILE:HB	2.39	0.52
1:B:275:ALA:O	1:B:276:GLN:C	2.52	0.52
7:B:1774:NAG:H82	7:B:1774:NAG:O3	2.09	0.52
1:A:264:VAL:HG12	1:A:265:PHE:N	2.24	0.52
1:A:182:MET:HE1	1:A:260:THR:N	2.24	0.52
1:A:67:GLU:HB3	1:A:146:LEU:HD22	1.90	0.52
1:A:144:GLY:O	1:A:151:TYR:CD1	2.63	0.52
1:B:366:GLN:CG	1:B:644:SER:HB2	2.39	0.52
1:B:383:ARG:N	1:B:383:ARG:CD	2.72	0.52
1:A:544:MET:SD	1:B:613:GLU:HB3	2.50	0.52
1:A:495:ILE:HD12	1:A:495:ILE:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:PHE:HA	1:B:286:VAL:HB	1.91	0.52
1:B:214:ALA:HB1	1:B:383:ARG:N	2.23	0.52
1:A:453:GLY:HA3	1:B:302:LEU:HD13	1.92	0.51
1:A:219:GLN:O	1:A:654:TRP:CE3	2.63	0.51
1:A:209:VAL:HG13	1:B:448:TYR:CE2	2.46	0.51
1:B:102:GLN:OE1	1:B:125:LEU:HD12	2.11	0.51
1:A:141:LEU:HD23	1:A:154:ASP:HA	1.93	0.51
1:B:223:ARG:HH11	1:B:223:ARG:CG	2.24	0.51
1:A:235:GLY:O	1:B:724:TYR:OH	2.23	0.51
1:A:181:GLN:O	1:A:182:MET:C	2.52	0.51
1:A:106:LYS:HG3	1:A:361:TYR:CZ	2.46	0.51
1:B:352:VAL:HB	1:B:360:VAL:CG2	2.40	0.51
1:A:179:ILE:HD11	1:A:251:HIS:ND1	2.26	0.50
1:B:417:LEU:O	1:B:418:GLU:C	2.54	0.50
1:A:696:THR:HG21	1:B:439:PRO:O	2.11	0.50
1:A:192:SER:O	1:A:196:HIS:CD2	2.64	0.50
1:B:409:THR:O	1:B:430:CYS:HA	2.11	0.50
1:A:539:VAL:HB	1:A:589:LEU:CD2	2.42	0.50
1:A:746:ALA:O	1:A:747:ALA:C	2.55	0.50
1:B:372:TYR:CD1	1:B:520:HIS:HB3	2.47	0.50
1:A:706:ARG:NH2	1:B:699:ASN:OD1	2.45	0.50
1:A:71:VAL:HG13	1:A:143:VAL:HG11	1.94	0.50
1:A:72:MET:HE1	1:A:96:VAL:HG21	1.92	0.50
1:A:652:ASP:N	1:A:653:PRO:HD3	2.26	0.50
1:A:701:VAL:CG1	1:A:702:GLY:N	2.75	0.49
1:A:665:ASN:O	1:A:667:GLU:N	2.46	0.49
1:B:532:VAL:HG21	1:B:589:LEU:O	2.13	0.49
1:A:52:THR:HG1	1:A:53:HIS:CD2	2.30	0.49
1:A:683:LEU:HD13	1:B:544:MET:HE2	1.95	0.49
1:B:266:TYR:O	1:B:268:GLY:N	2.45	0.49
1:A:214:ALA:HB2	1:A:384:TYR:HA	1.94	0.49
4:E:3:BMA:O4	4:E:5:BMA:O2	1.97	0.49
1:A:241:HIS:CE1	1:A:300:TRP:CZ3	3.00	0.49
1:A:272:ASP:O	1:A:273:SER:HB3	2.13	0.49
1:B:266:TYR:O	1:B:267:GLN:C	2.56	0.49
1:B:404:CYS:HB2	1:B:410:TYR:OH	2.12	0.49
1:B:571:MET:O	1:B:573:GLU:N	2.45	0.49
1:B:551:VAL:HG23	1:B:557:HIS:C	2.37	0.49
1:A:59:LEU:HD23	1:A:59:LEU:H	1.77	0.49
1:B:74:PHE:O	1:B:75:LEU:C	2.55	0.49
1:A:568:LEU:HD23	1:A:570:GLU:CG	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:ARG:NH1	1:B:613:GLU:HB2	2.28	0.48
1:A:438:LEU:HD12	1:A:439:PRO:HD2	1.95	0.48
8:B:2000:JW7:OAA	8:B:2000:JW7:CAF	2.61	0.48
1:A:199:CYS:C	1:A:200:PHE:HD1	2.21	0.48
1:A:214:ALA:HB1	1:A:215:PRO:CD	2.42	0.48
1:B:337:PHE:CE2	1:B:479:PHE:CE2	3.02	0.48
1:A:372:TYR:CE1	1:A:520:HIS:HB3	2.49	0.48
1:B:659:ASP:C	1:B:659:ASP:OD1	2.56	0.48
1:A:97:PHE:CG	1:A:129:PHE:CZ	3.01	0.48
1:A:469:LEU:HD21	8:A:2000:JW7:CAF	2.42	0.48
1:A:573:GLU:OE2	1:A:666:ASN:HA	2.14	0.48
1:B:386:ASP:HB3	1:B:468:LEU:CD1	2.44	0.48
1:B:469:LEU:HD21	8:B:2000:JW7:CAE	2.44	0.48
1:B:497:SER:HB2	1:B:515:THR:HG22	1.95	0.48
1:A:317:TYR:CD1	1:A:317:TYR:N	2.80	0.47
1:B:376:SER:O	1:B:380:MET:HE2	2.14	0.47
1:A:403:ASP:HB3	1:A:465:MET:HE3	1.96	0.47
1:B:214:ALA:HB2	1:B:382:THR:HG23	1.96	0.47
1:B:744:GLN:NE2	9:B:2041:HOH:O	2.47	0.47
1:B:129:PHE:CE1	1:B:169:ARG:HB2	2.49	0.47
1:B:556:GLU:HA	1:B:556:GLU:OE1	2.14	0.47
1:B:571:MET:HB2	1:B:574:GLN:HG3	1.96	0.47
1:B:737:ASN:OD1	1:B:737:ASN:C	2.57	0.47
1:A:65:ARG:NH2	1:A:422:PRO:O	2.48	0.47
1:A:110:LEU:HD22	1:A:358:ARG:NH1	2.29	0.47
1:A:354:PHE:HB2	1:A:359:LEU:HD11	1.96	0.47
1:A:688:ALA:O	1:B:713:GLU:HA	2.14	0.47
1:A:330:VAL:HG12	1:A:331:ALA:N	2.29	0.47
1:A:467:THR:HG21	1:B:444:HIS:O	2.14	0.47
1:A:435:ASN:OD1	1:A:435:ASN:C	2.57	0.47
1:A:601:ARG:HA	1:A:709:ASN:O	2.15	0.47
1:B:132:ARG:O	1:B:133:GLN:HB3	2.14	0.47
1:A:126:ALA:HB3	1:A:141:LEU:HB2	1.96	0.47
1:B:447:LEU:O	1:B:449:SER:N	2.42	0.47
1:B:593:HIS:HE1	7:B:1773:NAG:H82	1.79	0.47
1:B:620:SER:OG	1:B:654:TRP:CD1	2.62	0.47
1:B:486:GLU:HG3	1:B:704:PHE:CE1	2.50	0.47
1:B:258:ARG:NH1	1:B:258:ARG:HB2	2.30	0.47
1:A:278:GLU:OE1	1:A:278:GLU:HA	2.15	0.47
1:A:696:THR:O	1:A:697:VAL:C	2.58	0.47
1:B:463:ARG:HB2	1:B:476:ASP:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:MET:HE2	1:A:474:VAL:HG22	1.97	0.46
1:A:214:ALA:HB3	1:A:215:PRO:CD	2.46	0.46
1:A:282:GLU:C	1:A:284:GLY:H	2.22	0.46
1:A:495:ILE:HD11	1:A:690:ASP:O	2.15	0.46
1:A:544:MET:HE2	1:B:683:LEU:HD13	1.97	0.46
1:A:400:ARG:HG2	1:A:406:TYR:CD1	2.51	0.46
1:B:112:HIS:CD2	1:B:112:HIS:C	2.91	0.46
1:B:191:ALA:HA	1:B:278:GLU:HB2	1.96	0.46
1:B:742:LEU:HA	9:B:2041:HOH:O	2.16	0.46
1:B:91:PRO:HB2	1:B:254:LEU:HA	1.97	0.46
1:A:280:GLN:HB3	1:A:286:VAL:CG2	2.45	0.46
1:A:487:ILE:HG12	1:A:703:PHE:CE1	2.51	0.46
1:B:339:PHE:HA	1:B:349:ILE:HG22	1.97	0.46
1:B:440:LEU:HD12	1:B:440:LEU:O	2.15	0.46
1:A:144:GLY:C	1:A:151:TYR:CE1	2.94	0.46
1:A:695:VAL:HG13	1:B:440:LEU:CD1	2.45	0.46
1:B:381:THR:HG21	9:B:2012:HOH:O	2.16	0.46
1:B:512:SER:HB3	1:B:515:THR:HB	1.98	0.46
1:A:56:GLN:O	1:A:57:SER:C	2.58	0.46
1:A:140:GLU:OE1	1:A:160:HIS:NE2	2.47	0.46
1:B:246:GLU:OE1	1:B:376:SER:HB2	2.16	0.46
1:A:117:SER:HB3	1:A:118:PRO:CD	2.46	0.46
1:A:225:THR:HB	1:A:227:PHE:CE2	2.50	0.46
1:B:217:GLY:C	1:B:218:LEU:HD13	2.41	0.46
1:B:258:ARG:HB2	1:B:258:ARG:HH11	1.81	0.46
1:A:492:THR:HB	1:A:493:GLY:H	1.47	0.45
1:A:683:LEU:HD13	1:B:544:MET:CE	2.46	0.45
1:B:342:GLY:O	1:B:343:ALA:C	2.58	0.45
1:B:382:THR:HG21	1:B:384:TYR:CE1	2.51	0.45
1:B:501:PHE:O	1:B:503:ALA:N	2.48	0.45
1:A:419:SER:OG	1:A:420:GLN:N	2.49	0.45
1:B:212:THR:CG2	1:B:216:ARG:HH21	2.28	0.45
1:B:488:ARG:NH2	1:B:608:LEU:HD22	2.31	0.45
1:B:478:VAL:HG22	1:B:486:GLU:CB	2.46	0.45
1:B:171:VAL:HG13	1:B:175:GLU:HB3	1.98	0.45
1:B:335:TRP:HZ2	1:B:480:HIS:O	1.99	0.45
1:B:195:LEU:HB3	1:B:201:TYR:HB2	1.97	0.45
1:B:394:TYR:HA	9:B:2020:HOH:O	2.16	0.45
1:B:509:ASN:HB2	1:B:686:PRO:O	2.16	0.45
1:A:164:LEU:O	1:A:165:PRO:C	2.60	0.44
1:B:451:TYR:N	1:B:451:TYR:CD1	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ASN:ND2	1:A:501:PHE:O	2.48	0.44
1:A:612:GLY:O	1:A:613:GLU:C	2.59	0.44
1:A:683:LEU:HD22	1:B:544:MET:HE2	1.98	0.44
1:B:508:GLY:HA3	1:B:517:GLY:O	2.16	0.44
1:A:61:ALA:O	1:A:101:LEU:HD22	2.17	0.44
1:B:195:LEU:CB	1:B:201:TYR:HB2	2.47	0.44
1:A:459:VAL:CG1	1:A:478:VAL:CG1	2.95	0.44
1:A:627:TRP:HE3	1:A:679:THR:HG23	1.83	0.44
1:B:225:THR:HB	1:B:227:PHE:CE1	2.52	0.44
1:A:440:LEU:HD22	1:A:481:PRO:HG2	1.99	0.44
1:A:714:ASP:HB2	1:B:689:GLU:O	2.17	0.44
1:B:238:PHE:CD1	1:B:238:PHE:C	2.96	0.44
1:B:474:VAL:O	1:B:489:PHE:HA	2.18	0.44
1:B:716:SER:O	1:B:719:SER:N	2.51	0.44
1:B:212:THR:HG22	1:B:213:THR:N	2.31	0.44
1:B:537:ASN:HA	1:B:590:ALA:O	2.18	0.44
1:A:193:GLY:O	1:A:194:LEU:C	2.59	0.44
1:A:266:TYR:C	1:A:268:GLY:H	2.24	0.44
1:A:407:LEU:HD21	1:A:752:LEU:HD22	1.99	0.44
1:B:187:GLU:CD	1:B:261:ILE:HG13	2.43	0.44
1:B:188:LEU:N	1:B:189:PRO:CD	2.81	0.44
1:A:633:ALA:HB1	1:A:664:ILE:HD11	1.99	0.44
1:B:231:TYR:HE2	1:B:291:ILE:HG22	1.83	0.44
1:B:281:PHE:O	1:B:284:GLY:N	2.47	0.44
1:B:251:HIS:HA	1:B:259:TRP:CG	2.53	0.43
1:A:88:GLN:HA	1:A:174:GLN:HG2	2.00	0.43
1:A:171:VAL:HG11	1:A:176:TYR:CD1	2.54	0.43
1:A:400:ARG:HG2	1:A:406:TYR:CE1	2.54	0.43
1:A:542:GLU:HA	1:A:565:THR:O	2.18	0.43
1:B:183:ILE:HG22	1:B:188:LEU:HG	1.99	0.43
1:B:453:GLY:HA2	1:B:723:ILE:O	2.18	0.43
1:B:650:GLN:HA	1:B:650:GLN:OE1	2.18	0.43
1:B:742:LEU:O	1:B:743:PRO:C	2.61	0.43
1:A:117:SER:HB3	1:A:118:PRO:HD2	2.00	0.43
1:A:410:TYR:C	1:A:411:VAL:HG23	2.43	0.43
1:A:214:ALA:HB1	1:A:383:ARG:O	2.18	0.43
1:A:538:TRP:CD1	1:A:670:ALA:HA	2.53	0.43
1:B:366:GLN:NE2	1:B:527:LYS:HB2	2.34	0.43
1:B:393:LYS:HG3	1:B:417:LEU:HD13	2.01	0.43
1:A:209:VAL:CG2	1:A:232:ASN:HB2	2.48	0.43
1:B:256:PRO:HA	1:B:259:TRP:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:GLU:OE2	1:B:387:GLY:N	2.44	0.43
1:A:344:PHE:HA	1:A:390:GLY:CA	2.48	0.43
1:B:195:LEU:HD12	1:B:201:TYR:CD2	2.54	0.43
1:B:502:GLY:O	1:B:504:THR:N	2.52	0.43
1:A:78:ARG:HB2	1:A:78:ARG:NH1	2.32	0.43
1:A:171:VAL:HG22	1:A:223:ARG:HH21	1.84	0.43
1:B:498:ALA:HB3	1:B:516:LEU:HB3	2.01	0.43
1:A:163:PRO:HB3	2:C:1:NAG:H82	2.01	0.42
1:A:229:LEU:C	1:A:230:TYR:CD1	2.97	0.42
1:A:395:THR:HA	1:A:466:SER:HA	2.01	0.42
1:B:275:ALA:C	1:B:277:LEU:N	2.77	0.42
1:B:571:MET:O	1:B:572:GLU:C	2.62	0.42
1:B:587:LEU:C	1:B:587:LEU:HD23	2.44	0.42
1:B:245:LEU:HD12	1:B:265:PHE:O	2.19	0.42
1:A:395:THR:CG2	1:A:396:THR:N	2.83	0.42
1:A:179:ILE:HG22	1:A:180:ASP:N	2.35	0.42
1:A:306:VAL:HG21	1:B:718:TYR:O	2.19	0.42
1:A:365:LEU:HD21	1:A:475:TRP:CZ2	2.54	0.42
1:A:389:PHE:HB3	1:A:394:TYR:CE2	2.54	0.42
1:B:749:ALA:CB	1:B:750:PRO:CD	2.97	0.42
1:A:612:GLY:HA3	1:B:544:MET:HE1	2.00	0.42
1:A:504:THR:HG22	1:A:505:GLY:N	2.35	0.42
1:B:165:PRO:HD2	1:B:168:ARG:NH1	2.34	0.42
1:B:613:GLU:C	1:B:613:GLU:OE1	2.62	0.42
1:A:403:ASP:O	1:A:404:CYS:SG	2.77	0.42
1:B:696:THR:O	1:B:697:VAL:C	2.62	0.42
1:A:205:GLY:O	1:A:207:ASN:ND2	2.41	0.42
1:B:94:ASN:OD1	1:B:130:PHE:HA	2.20	0.42
1:B:360:VAL:CG1	1:B:530:LEU:HD23	2.50	0.42
1:B:416:LEU:C	1:B:417:LEU:HG	2.45	0.42
1:A:72:MET:HE3	1:A:72:MET:HA	2.02	0.42
1:A:183:ILE:HG22	1:A:184:PHE:N	2.34	0.42
1:A:444:HIS:O	1:B:467:THR:HG21	2.20	0.42
1:A:500:LEU:HD22	1:A:510:GLN:HG3	2.01	0.42
1:A:541:ALA:HB2	1:A:569:LEU:HD11	2.01	0.42
1:B:297:GLY:O	1:B:299:SER:N	2.49	0.42
1:B:198:CYS:HB2	1:B:266:TYR:OH	2.20	0.42
1:B:587:LEU:HD23	1:B:587:LEU:O	2.20	0.41
1:A:182:MET:HE1	1:A:260:THR:C	2.45	0.41
1:A:695:VAL:HG13	1:B:440:LEU:HD12	2.00	0.41
1:A:725:PHE:CD2	1:A:731:ALA:HB2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:PHE:CD1	1:A:756:SER:N	2.88	0.41
1:B:143:VAL:HG12	1:B:144:GLY:N	2.34	0.41
1:A:539:VAL:HB	1:A:589:LEU:HD22	2.02	0.41
1:A:544:MET:HE1	1:B:521:THR:HG21	2.03	0.41
1:B:203:HIS:HA	1:B:204:ARG:HA	1.78	0.41
8:B:2000:JW7:HAM1	8:B:2000:JW7:CAH	2.40	0.41
1:A:93:ASP:HA	1:A:132:ARG:NH2	2.35	0.41
1:A:216:ARG:HE	1:A:225:THR:HG1	1.65	0.41
1:A:319:GLN:C	1:A:320:GLY:O	2.62	0.41
1:B:66:GLU:N	1:B:66:GLU:CD	2.77	0.41
1:B:101:LEU:HD23	1:B:103:LEU:HD23	2.03	0.41
1:B:187:GLU:O	1:B:274:LEU:CD1	2.67	0.41
1:A:405:PRO:O	1:A:410:TYR:OH	2.31	0.41
1:A:615:LEU:HA	1:A:616:PRO:HD2	1.82	0.41
1:B:164:LEU:O	1:B:165:PRO:C	2.63	0.41
1:B:524:ALA:O	1:B:679:THR:HA	2.20	0.41
1:B:633:ALA:O	1:B:677:TRP:N	2.48	0.41
1:A:362:GLU:OE1	1:A:527:LYS:HE2	2.21	0.41
1:B:722:SER:O	1:B:723:ILE:HD13	2.20	0.41
1:A:189:PRO:C	1:A:191:ALA:H	2.29	0.41
1:B:153:ARG:HD2	9:B:2005:HOH:O	2.21	0.41
1:B:352:VAL:HB	1:B:360:VAL:HG23	2.01	0.41
1:B:388:GLY:HA3	1:B:650:GLN:HB2	2.01	0.41
1:B:564:VAL:HG12	1:B:565:THR:N	2.36	0.41
1:A:503:ALA:O	1:A:504:THR:C	2.64	0.41
1:B:501:PHE:O	1:B:501:PHE:CD2	2.74	0.41
1:A:430:CYS:SG	1:A:463:ARG:HB3	2.60	0.41
1:A:571:MET:O	1:A:572:GLU:C	2.64	0.41
1:B:116:GLY:O	1:B:117:SER:C	2.64	0.41
1:B:242:HIS:HD2	1:B:499:PHE:H	1.68	0.41
1:B:497:SER:HB2	1:B:515:THR:CG2	2.51	0.41
1:B:499:PHE:CD1	1:B:500:LEU:N	2.88	0.41
1:B:571:MET:HE2	9:B:2037:HOH:O	2.21	0.41
1:A:110:LEU:O	1:A:111:ALA:C	2.64	0.40
1:A:681:GLY:O	1:A:682:PHE:HB3	2.21	0.40
1:B:492:THR:OG1	1:B:694:THR:O	2.35	0.40
1:B:330:VAL:O	1:B:336:THR:HA	2.21	0.40
1:B:352:VAL:HB	1:B:360:VAL:HG22	2.03	0.40
1:A:383:ARG:HD3	1:A:621:MET:SD	2.62	0.40
1:A:433:GLU:HA	1:A:459:VAL:O	2.20	0.40
1:B:399:THR:HA	9:B:2022:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ILE:O	1:B:425:ILE:HG22	2.20	0.40
1:B:480:HIS:HA	1:B:481:PRO:HD2	1.92	0.40
1:B:215:PRO:HG3	1:B:621:MET:SD	2.61	0.40
1:A:650:GLN:HG3	1:A:651:ASN:OD1	2.22	0.40
1:B:610:PHE:O	1:B:611:ALA:C	2.64	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:GLN:OE1	1:A:326:GLN:OE1[10_665]	1.91	0.29

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	708/737 (96%)	599 (85%)	82 (12%)	27 (4%)	2	9
1	B	702/737 (95%)	607 (86%)	71 (10%)	24 (3%)	3	11
All	All	1410/1474 (96%)	1206 (86%)	153 (11%)	51 (4%)	2	10

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	PRO
1	A	116	GLY
1	A	206	ARG
1	A	214	ALA
1	A	267	GLN
1	A	504	THR
1	A	697	VAL
1	A	747	ALA

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Mol	Chain	Res	Type
1	B	214	ALA
1	B	267	GLN
1	B	502	GLY
1	B	744	GLN
1	B	747	ALA
1	B	749	ALA
1	A	57	SER
1	A	273	SER
1	A	283	ALA
1	A	320	GLY
1	A	378	ALA
1	A	580	GLY
1	A	666	ASN
1	A	748	CYS
1	A	759	GLY
1	B	116	GLY
1	B	280	GLN
1	B	418	GLU
1	B	448	TYR
1	B	503	ALA
1	B	572	GLU
1	B	612	GLY
1	A	274	LEU
1	B	513	GLU
1	B	740	ALA
1	A	190	GLN
1	A	533	ALA
1	A	722	SER
1	A	746	ALA
1	B	117	SER
1	B	405	PRO
1	B	618	ASN
1	B	628	GLU
1	A	165	PRO
1	B	170	PRO
1	B	481	PRO
1	B	750	PRO
1	A	438	LEU
1	A	642	PRO
1	B	133	GLN
1	B	641	GLU
1	A	55	GLY

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Mol	Chain	Res	Type
1	A	145	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	590/610 (97%)	519 (88%)	71 (12%)	5	17
1	B	585/610 (96%)	513 (88%)	72 (12%)	4	16
All	All	1175/1220 (96%)	1032 (88%)	143 (12%)	5	16

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	57	SER
1	A	59	LEU
1	A	73	ARG
1	A	76	THR
1	A	78	ARG
1	A	99	VAL
1	A	102	GLN
1	A	125	LEU
1	A	128	VAL
1	A	133	GLN
1	A	135	GLN
1	A	170	PRO
1	A	194	LEU
1	A	200	PHE
1	A	202	LYS
1	A	203	HIS
1	A	206	ARG
1	A	207	ASN
1	A	208	LEU
1	A	209	VAL
1	A	210	THR

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Mol	Chain	Res	Type
1	A	212	THR
1	A	230	TYR
1	A	251	HIS
1	A	254	LEU
1	A	258	ARG
1	A	261	ILE
1	A	263	LYS
1	A	293	ASP
1	A	299	SER
1	A	302	LEU
1	A	326	GLN
1	A	338	SER
1	A	360	VAL
1	A	363	ILE
1	A	396	THR
1	A	400	ARG
1	A	419	SER
1	A	435	ASN
1	A	455	LEU
1	A	459	VAL
1	A	492	THR
1	A	495	ILE
1	A	497	SER
1	A	552	PRO
1	A	565	THR
1	A	573	GLU
1	A	585	ARG
1	A	594	SER
1	A	604	ARG
1	A	608	LEU
1	A	609	SER
1	A	618	ASN
1	A	621	MET
1	A	626	SER
1	A	632	LEU
1	A	637	ARG
1	A	640	GLU
1	A	650	GLN
1	A	687	HIS
1	A	695	VAL
1	A	701	VAL
1	A	706	ARG

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Mol	Chain	Res	Type
1	A	713	GLU
1	A	716	SER
1	A	722	SER
1	A	726	ARG
1	A	748	CYS
1	A	756	SER
1	A	761	SER
1	B	83	LEU
1	B	84	VAL
1	B	125	LEU
1	B	152	MET
1	B	157	VAL
1	B	179	ILE
1	B	187	GLU
1	B	190	GLN
1	B	198	CYS
1	B	199	CYS
1	B	204	ARG
1	B	206	ARG
1	B	207	ASN
1	B	208	LEU
1	B	209	VAL
1	B	210	THR
1	B	218	LEU
1	B	223	ARG
1	B	243	VAL
1	B	251	HIS
1	B	252	LYS
1	B	258	ARG
1	B	260	THR
1	B	261	ILE
1	B	273	SER
1	B	276	GLN
1	B	280	GLN
1	B	286	VAL
1	B	319	GLN
1	B	345	SER
1	B	358	ARG
1	B	376	SER
1	B	381	THR
1	B	383	ARG
1	B	391	MET

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Mol	Chain	Res	Type
1	B	405	PRO
1	B	409	THR
1	B	419	SER
1	B	425	ILE
1	B	438	LEU
1	B	440	LEU
1	B	442	ARG
1	B	455	LEU
1	B	458	THR
1	B	478	VAL
1	B	489	PHE
1	B	539	VAL
1	B	544	MET
1	B	545	VAL
1	B	567	LYS
1	B	568	LEU
1	B	570	GLU
1	B	583	THR
1	B	596	LYS
1	B	608	LEU
1	B	613	GLU
1	B	626	SER
1	B	634	VAL
1	B	637	ARG
1	B	640	GLU
1	B	644	SER
1	B	645	SER
1	B	646	SER
1	B	650	GLN
1	B	659	ASP
1	B	661	SER
1	B	668	THR
1	B	687	HIS
1	B	694	THR
1	B	713	GLU
1	B	735	GLU
1	B	742	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS

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Mol	Chain	Res	Type
1	A	197	HIS
1	A	219	GLN
1	A	250	ASN
1	B	112	HIS
1	B	207	ASN
1	B	219	GLN
1	B	294	ASN
1	B	375	ASN
1	B	537	ASN
1	B	563	GLN
1	B	593	HIS
1	B	744	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	TPQ	A	471	1	13,14,15	1.49	2 (15%)	13,19,21	1.59	2 (15%)
1	TPQ	B	471	1	13,14,15	1.44	2 (15%)	13,19,21	1.53	2 (15%)

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
1	TPQ	A	471	1	-	0/5/22/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPQ	B	471	1	-	2/5/22/24	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	TPQ	C3-C4	3.00	1.41	1.36
1	A	471	TPQ	C6-C1	2.81	1.41	1.34
1	B	471	TPQ	C6-C1	2.69	1.41	1.34
1	B	471	TPQ	C3-C4	2.31	1.40	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	471	TPQ	C6-C1-C2	3.82	121.38	118.66
1	A	471	TPQ	O5-C5-C4	3.67	125.22	119.43
1	A	471	TPQ	C6-C1-C2	2.97	120.77	118.66
1	B	471	TPQ	O5-C5-C4	2.43	123.27	119.43

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	471	TPQ	N-CA-CB-C1
1	B	471	TPQ	C-CA-CB-C1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	471	TPQ	1	0

5.5 Carbohydrates [i](#)

12 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	C	1	1,2	14,14,15	0.74	0	17,19,21	1.58	4 (23%)
2	NAG	C	2	2	14,14,15	0.80	1 (7%)	17,19,21	1.63	4 (23%)
2	BMA	C	3	2	11,11,12	0.63	0	15,15,17	1.28	2 (13%)
3	NAG	D	1	3,1	14,14,15	0.61	0	17,19,21	1.54	3 (17%)
3	NAG	D	2	3	14,14,15	0.82	1 (7%)	17,19,21	1.36	2 (11%)
4	NAG	E	1	1,4	14,14,15	0.58	0	17,19,21	1.14	0
4	NAG	E	2	4	14,14,15	0.47	0	17,19,21	1.79	4 (23%)
4	BMA	E	3	4	11,11,12	0.77	0	15,15,17	2.04	2 (13%)
4	MAN	E	4	4	11,11,12	0.53	0	15,15,17	2.51	3 (20%)
4	BMA	E	5	4	11,11,12	0.67	0	15,15,17	2.13	6 (40%)
3	NAG	F	1	3,1	14,14,15	0.84	0	17,19,21	2.17	5 (29%)
3	NAG	F	2	3	14,14,15	0.67	0	17,19,21	1.54	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	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	1/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	BMA	E	5	4	-	0/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	NAG	C1-C2	2.16	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	O5-C1	-2.01	1.40	1.43

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	4	MAN	C1-O5-C5	8.45	123.50	112.19
3	F	1	NAG	C2-N2-C7	5.73	130.58	122.90
4	E	3	BMA	C3-C4-C5	5.21	119.68	110.23
4	E	5	BMA	C1-O5-C5	4.67	118.44	112.19
4	E	3	BMA	O4-C4-C3	-4.63	99.46	110.38
4	E	2	NAG	C2-N2-C7	-4.36	117.06	122.90
4	E	5	BMA	C1-C2-C3	4.29	115.89	109.64
3	F	1	NAG	C1-C2-N2	-4.19	103.84	110.43
4	E	2	NAG	C1-O5-C5	3.70	117.14	112.19
3	D	1	NAG	C1-C2-N2	-3.58	104.79	110.43
2	C	1	NAG	O3-C3-C2	3.48	116.64	109.40
2	C	2	NAG	O4-C4-C3	-3.46	102.22	110.38
2	C	2	NAG	O4-C4-C5	3.26	117.35	109.32
3	F	2	NAG	C1-C2-N2	3.19	115.46	110.43
3	D	2	NAG	C1-O5-C5	3.07	116.31	112.19
2	C	1	NAG	C1-C2-N2	-2.98	105.73	110.43
3	F	1	NAG	O7-C7-N2	2.97	127.23	121.98
3	F	1	NAG	O5-C1-C2	-2.96	106.71	111.29
3	D	1	NAG	C4-C3-C2	-2.85	106.83	111.02
2	C	1	NAG	O4-C4-C3	-2.85	103.66	110.38
4	E	4	MAN	C3-C4-C5	2.81	115.33	110.23
2	C	2	NAG	O5-C1-C2	-2.81	106.95	111.29
3	D	1	NAG	O3-C3-C2	2.78	115.18	109.40
3	F	2	NAG	O7-C7-C8	-2.62	117.38	122.05
4	E	4	MAN	O5-C5-C4	2.62	117.21	110.83
4	E	5	BMA	O2-C2-C3	-2.60	104.77	110.15
4	E	2	NAG	O5-C5-C6	2.49	112.51	107.66
4	E	5	BMA	C3-C4-C5	2.36	114.51	110.23
3	F	1	NAG	O7-C7-C8	-2.33	117.90	122.05
3	D	2	NAG	O7-C7-C8	-2.30	117.95	122.05
3	F	2	NAG	C1-O5-C5	2.27	115.23	112.19
4	E	2	NAG	C1-C2-N2	-2.27	106.86	110.43
2	C	2	NAG	O7-C7-C8	-2.25	118.04	122.05
2	C	1	NAG	C1-O5-C5	2.20	115.14	112.19
4	E	5	BMA	O5-C5-C6	2.07	111.69	107.66
2	C	3	BMA	O4-C4-C3	-2.05	105.55	110.38
2	C	3	BMA	O5-C5-C6	2.04	111.63	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5	BMA	O2-C2-C1	2.01	113.83	109.22

There are no chirality outliers.

All (15) torsion outliers are listed below:

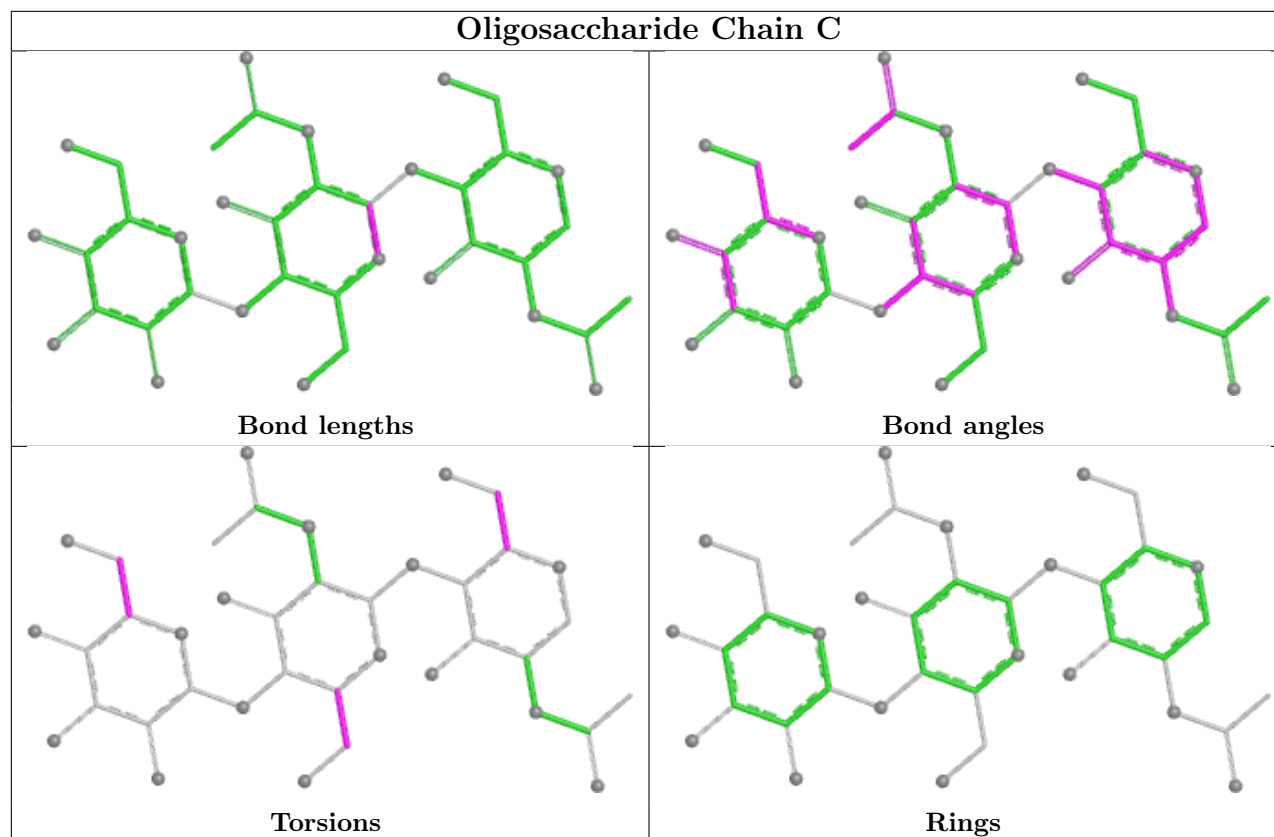
Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C3-C2-N2-C7
3	F	1	NAG	C3-C2-N2-C7
2	C	3	BMA	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6

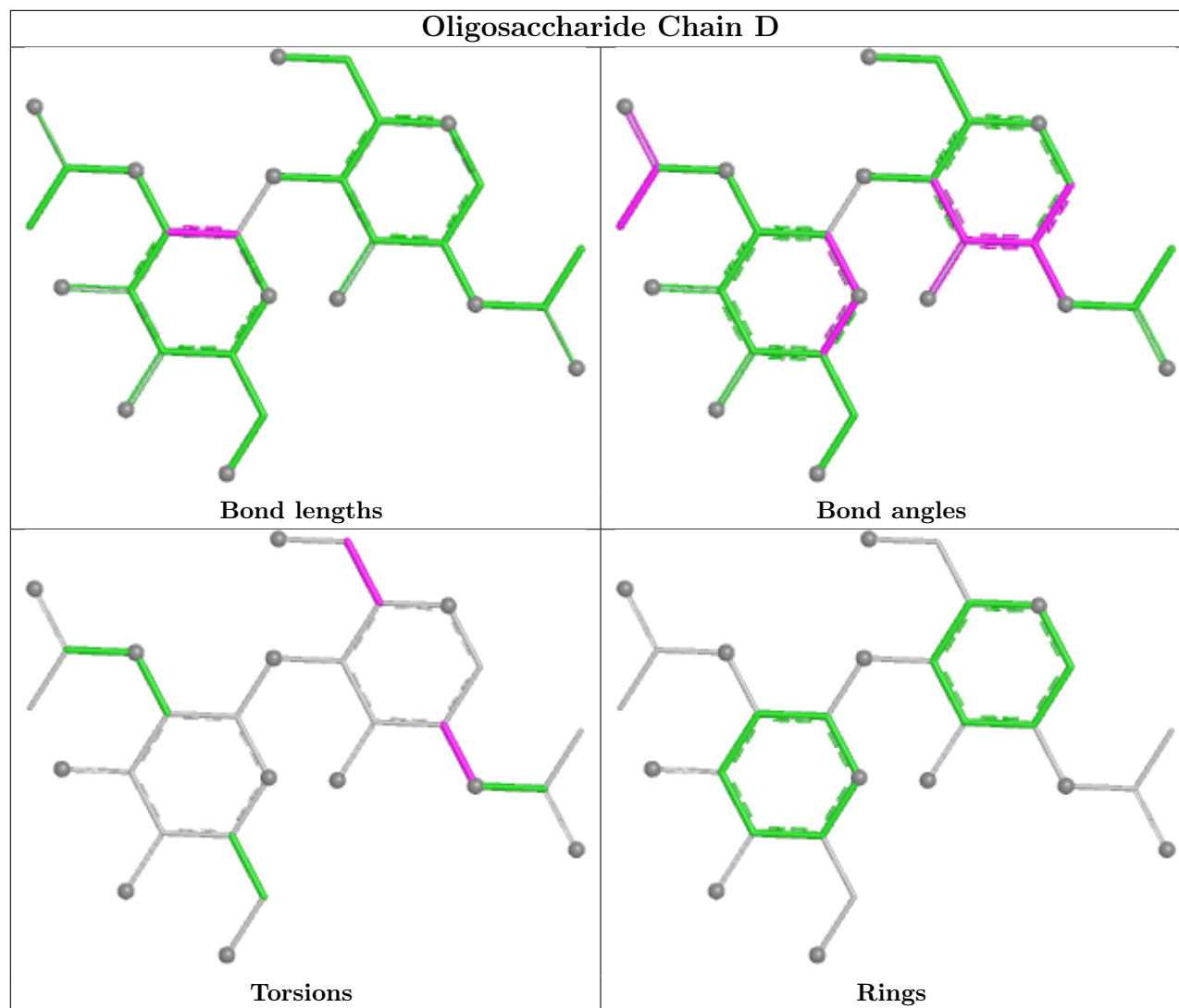
There are no ring outliers.

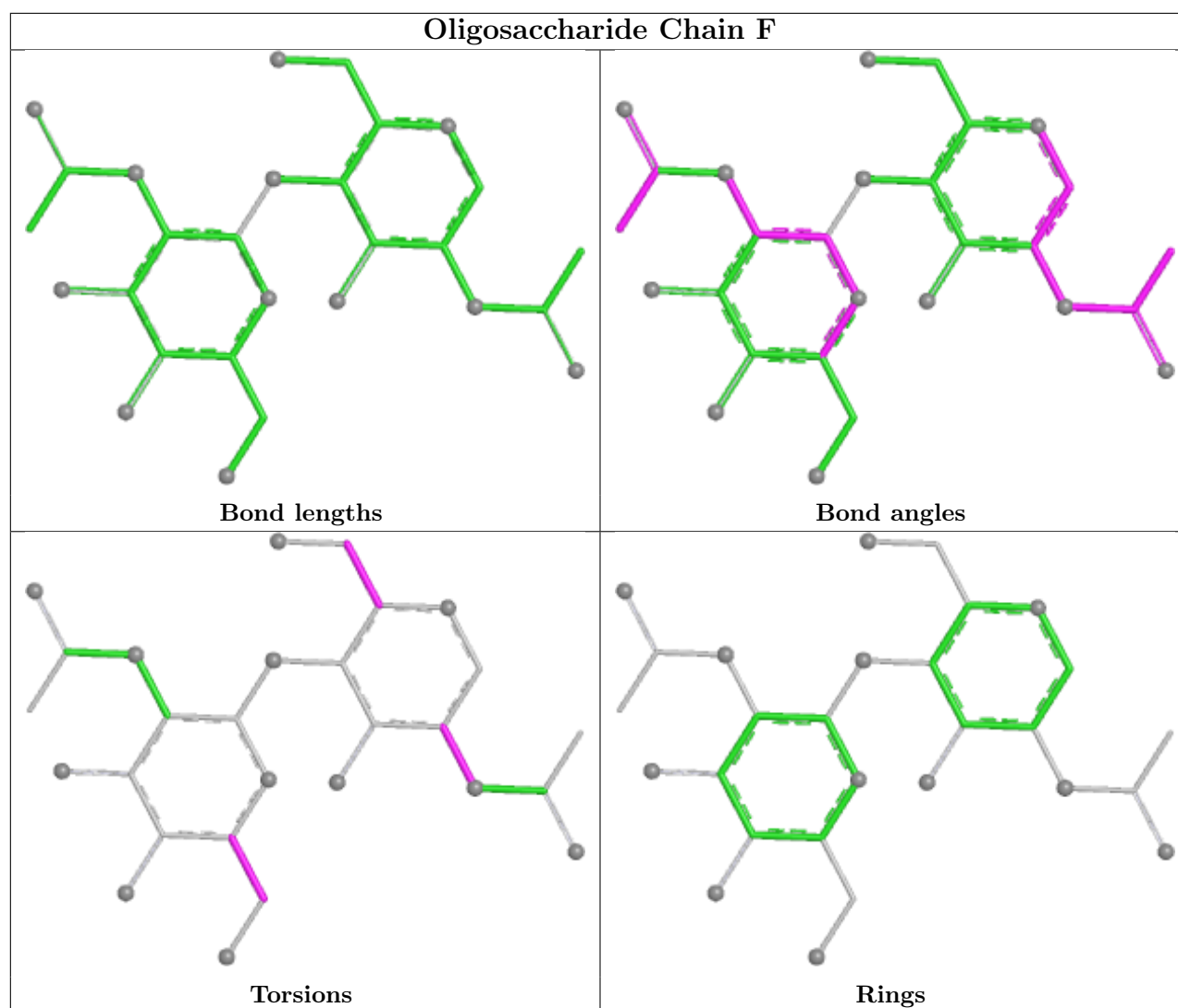
4 monomers are involved in 4 short contacts:

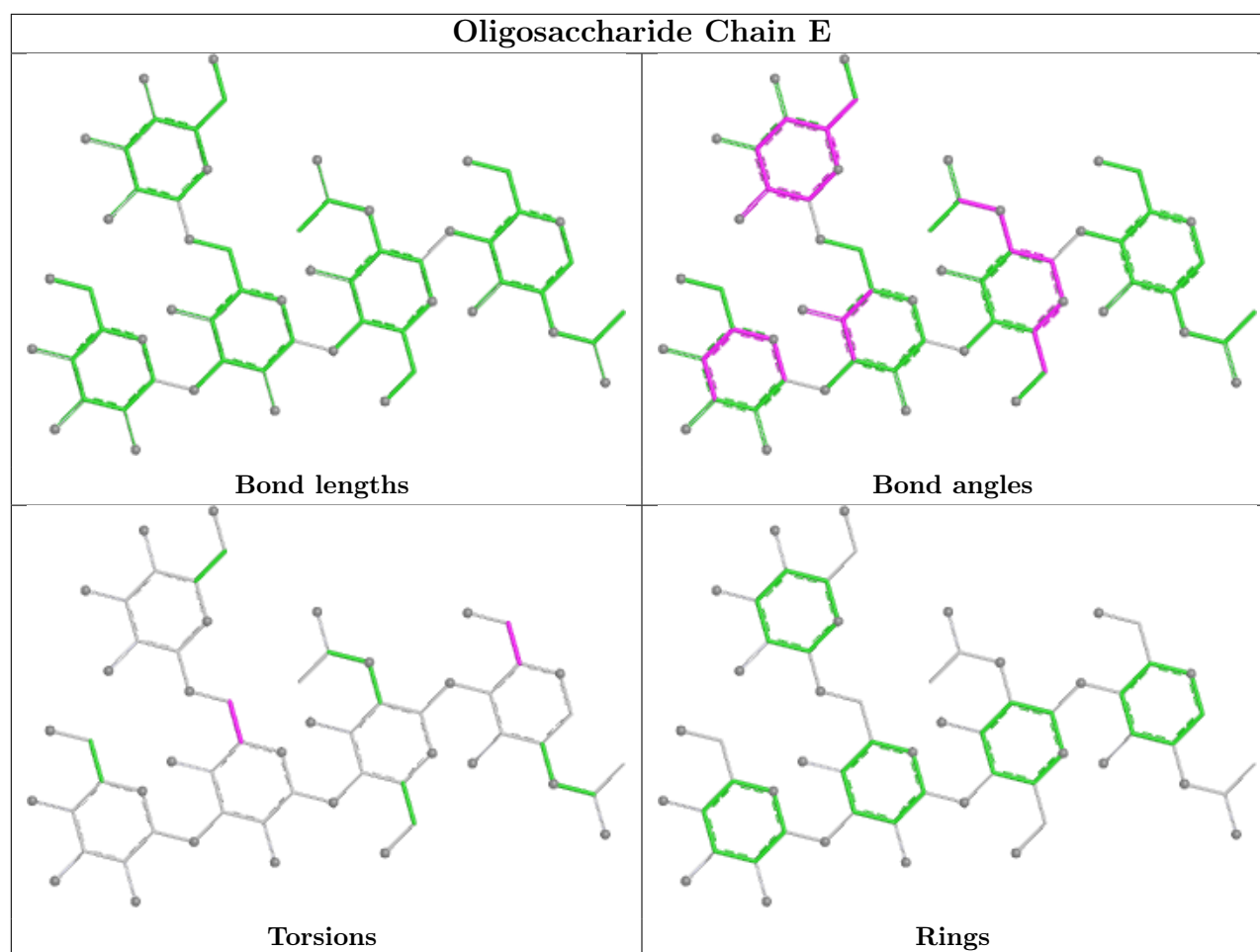
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
4	E	3	BMA	2	0
4	E	1	NAG	1	0
4	E	5	BMA	2	0

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](#)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

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	$\# Z > 2$
7	NAG	B	1774	1	14,14,15	1.55	1 (7%)	17,19,21	2.67	6 (35%)
8	JW7	B	2000	-	28,28,28	2.12	4 (14%)	34,38,38	2.08	13 (38%)
7	NAG	A	1770	1	14,14,15	1.22	2 (14%)	17,19,21	2.15	5 (29%)
7	NAG	A	1771	1	14,14,15	1.89	3 (21%)	17,19,21	3.44	8 (47%)
8	JW7	A	2000	-	28,28,28	1.94	6 (21%)	34,38,38	2.17	10 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	B	1775	1	14,14,15	0.73	0	17,19,21	1.43	2 (11%)
7	NAG	B	1772	-	14,14,15	0.79	1 (7%)	17,19,21	1.49	2 (11%)
7	NAG	B	1773	1	14,14,15	1.06	1 (7%)	17,19,21	2.85	5 (29%)

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
7	NAG	B	1774	1	1/1/5/7	4/6/23/26	0/1/1/1
8	JW7	B	2000	-	-	5/8/20/20	0/4/4/4
7	NAG	A	1770	1	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	A	1771	1	1/1/5/7	1/6/23/26	0/1/1/1
8	JW7	A	2000	-	-	4/8/20/20	0/4/4/4
7	NAG	B	1775	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1772	-	-	1/6/23/26	0/1/1/1
7	NAG	B	1773	1	-	2/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	2000	JW7	OAA-CAW	6.43	1.37	1.23
8	A	2000	JW7	OAA-CAW	6.21	1.36	1.23
8	B	2000	JW7	CAS-NAY	-5.42	1.33	1.43
8	B	2000	JW7	CAV-CAU	-5.27	1.39	1.46
7	A	1771	NAG	C1-C2	5.26	1.59	1.52
7	B	1774	NAG	C1-C2	4.90	1.59	1.52
8	A	2000	JW7	CAS-NAY	-4.54	1.34	1.43
8	A	2000	JW7	CAV-CAU	-4.52	1.40	1.46
7	B	1773	NAG	C1-C2	3.21	1.56	1.52
7	A	1771	NAG	C2-N2	3.15	1.51	1.46
8	B	2000	JW7	CAW-NAY	-3.05	1.34	1.41
7	A	1771	NAG	C3-C2	2.64	1.58	1.52
8	A	2000	JW7	CAW-NAY	-2.41	1.35	1.41
7	A	1770	NAG	C4-C5	2.31	1.57	1.53
7	A	1770	NAG	C1-C2	2.29	1.55	1.52
8	A	2000	JW7	CAH-CAT	2.15	1.40	1.36
8	A	2000	JW7	CAT-CAV	-2.15	1.39	1.43
7	B	1772	NAG	C1-C2	2.09	1.55	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1773	NAG	C1-O5-C5	8.55	123.64	112.19
7	A	1771	NAG	C2-N2-C7	6.83	132.06	122.90
7	B	1774	NAG	C1-O5-C5	6.51	120.91	112.19
7	A	1771	NAG	O5-C1-C2	-6.24	101.64	111.29
8	A	2000	JW7	CAH-CAT-NAQ	-6.09	120.95	125.78
7	A	1770	NAG	C1-O5-C5	5.64	119.74	112.19
7	A	1771	NAG	C1-C2-N2	5.59	119.24	110.43
7	B	1774	NAG	C2-N2-C7	4.81	129.34	122.90
7	A	1771	NAG	C1-O5-C5	4.79	118.61	112.19
8	B	2000	JW7	CAH-CAW-NAY	4.50	119.56	111.90
7	A	1771	NAG	C4-C3-C2	4.22	117.20	111.02
8	A	2000	JW7	CAH-CAW-NAY	4.16	118.97	111.90
7	B	1773	NAG	C1-C2-N2	4.13	116.95	110.43
7	B	1775	NAG	C1-O5-C5	4.12	117.71	112.19
8	A	2000	JW7	OAA-CAW-CAH	-4.10	115.50	125.61
7	B	1774	NAG	C8-C7-N2	4.05	122.83	116.12
7	B	1773	NAG	O7-C7-C8	-3.95	115.02	122.05
7	A	1771	NAG	O7-C7-C8	-3.95	115.02	122.05
7	B	1772	NAG	O5-C5-C6	3.89	115.23	107.66
8	B	2000	JW7	CAG-NAN-CAU	3.88	110.56	106.25
8	A	2000	JW7	OAA-CAW-NAY	3.87	125.53	119.78
8	B	2000	JW7	CAM-CAX-NAQ	3.66	117.88	110.57
8	B	2000	JW7	CAM-CAX-CAL	-3.58	104.62	110.80
8	B	2000	JW7	CAI-CAJ-CAL	3.57	118.77	111.42
7	B	1774	NAG	C1-C2-N2	3.48	115.92	110.43
8	A	2000	JW7	CAG-NAN-CAU	3.48	110.11	106.25
7	A	1770	NAG	O4-C4-C5	3.43	117.78	109.32
8	A	2000	JW7	CAT-CAV-NAP	-3.41	117.92	125.56
7	B	1774	NAG	O7-C7-C8	-3.35	116.09	122.05
7	B	1773	NAG	O5-C1-C2	-3.30	106.19	111.29
8	B	2000	JW7	CAH-CAT-NAQ	-3.14	123.29	125.78
8	B	2000	JW7	CAH-CAT-CAV	-3.06	116.29	119.81
7	A	1770	NAG	C1-C2-N2	2.94	115.07	110.43
7	A	1771	NAG	O3-C3-C2	2.90	115.42	109.40
8	A	2000	JW7	NAN-CAU-NAO	-2.89	105.96	111.74
8	B	2000	JW7	OAA-CAW-CAH	-2.88	118.51	125.61
8	B	2000	JW7	CAF-CAS-NAY	2.77	123.89	119.72
8	A	2000	JW7	CAV-NAP-NAY	2.56	124.28	118.85
8	A	2000	JW7	CAE-CAS-NAY	2.39	123.33	119.72
7	B	1773	NAG	C8-C7-N2	2.38	120.06	116.12
7	A	1770	NAG	O7-C7-C8	-2.34	117.88	122.05
7	A	1771	NAG	O7-C7-N2	2.28	126.01	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1775	NAG	O4-C4-C5	2.20	114.74	109.32
8	B	2000	JW7	CAT-CAV-NAP	-2.14	120.76	125.56
8	B	2000	JW7	CAJ-CAL-CAX	2.13	114.92	111.09
8	B	2000	JW7	NAN-CAU-NAO	-2.12	107.49	111.74
8	B	2000	JW7	CAV-CAU-NAO	2.07	128.09	124.87
7	B	1772	NAG	O5-C1-C2	2.04	114.45	111.29
8	A	2000	JW7	CAW-NAY-NAP	-2.02	118.30	123.86
7	B	1774	NAG	C3-C4-C5	2.02	113.90	110.23
7	A	1770	NAG	O3-C3-C2	2.02	113.59	109.40

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	1770	NAG	C1
7	A	1771	NAG	C1
7	B	1774	NAG	C1

All (21) torsion outliers are listed below:

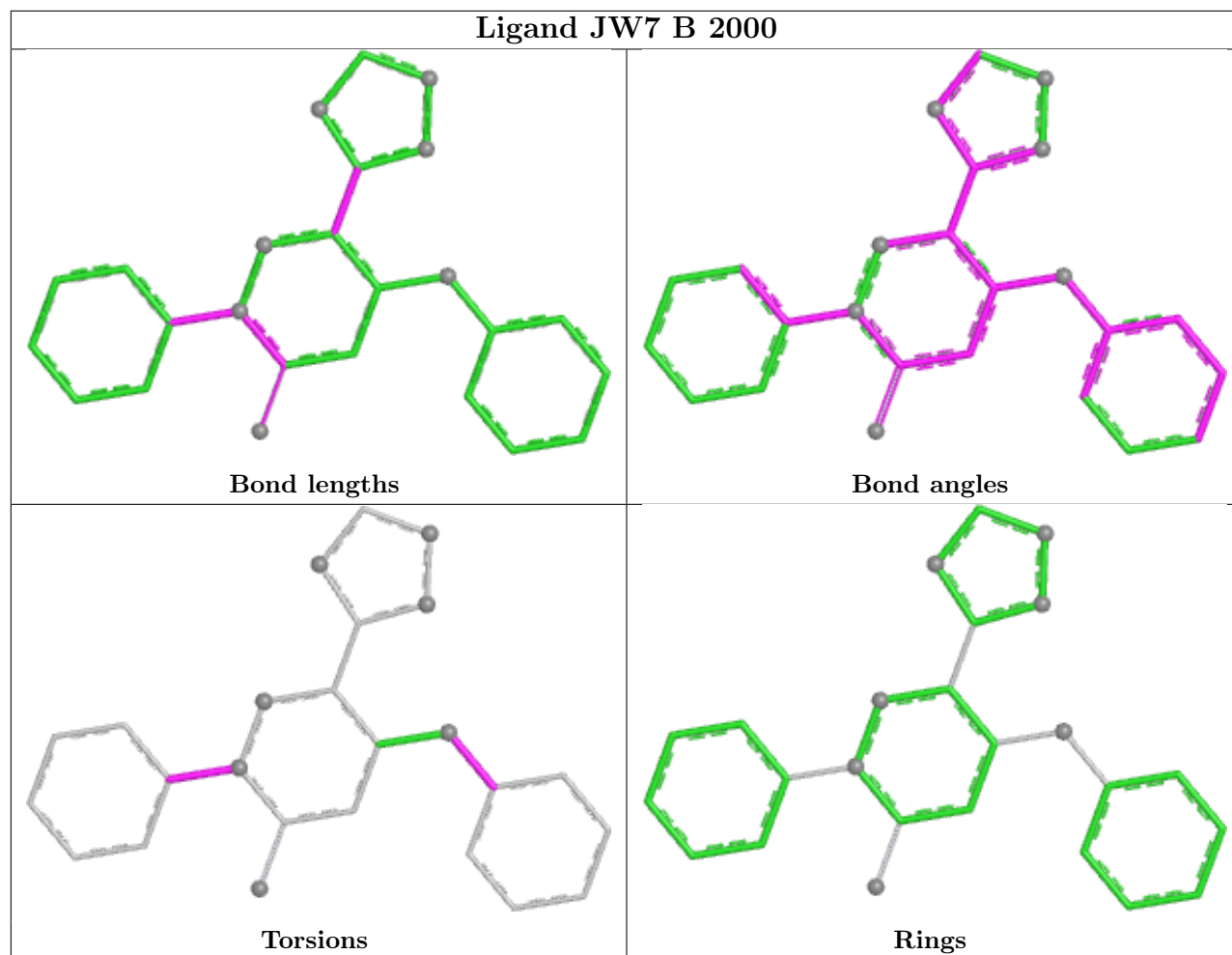
Mol	Chain	Res	Type	Atoms
7	A	1770	NAG	C4-C5-C6-O6
8	A	2000	JW7	CAE-CAS-NAY-CAW
8	A	2000	JW7	CAF-CAS-NAY-CAW
8	B	2000	JW7	CAE-CAS-NAY-CAW
8	B	2000	JW7	CAF-CAS-NAY-CAW
7	A	1770	NAG	O5-C5-C6-O6
7	B	1774	NAG	C8-C7-N2-C2
7	B	1774	NAG	O7-C7-N2-C2
7	B	1772	NAG	O5-C5-C6-O6
7	B	1773	NAG	O5-C5-C6-O6
8	B	2000	JW7	CAF-CAS-NAY-NAP
7	B	1774	NAG	O5-C5-C6-O6
8	A	2000	JW7	CAE-CAS-NAY-NAP
7	B	1775	NAG	C4-C5-C6-O6
8	A	2000	JW7	CAF-CAS-NAY-NAP
8	B	2000	JW7	CAE-CAS-NAY-NAP
7	B	1773	NAG	C4-C5-C6-O6
7	A	1771	NAG	O5-C5-C6-O6
7	B	1774	NAG	C4-C5-C6-O6
8	B	2000	JW7	CAM-CAX-NAQ-CAT
7	B	1775	NAG	O5-C5-C6-O6

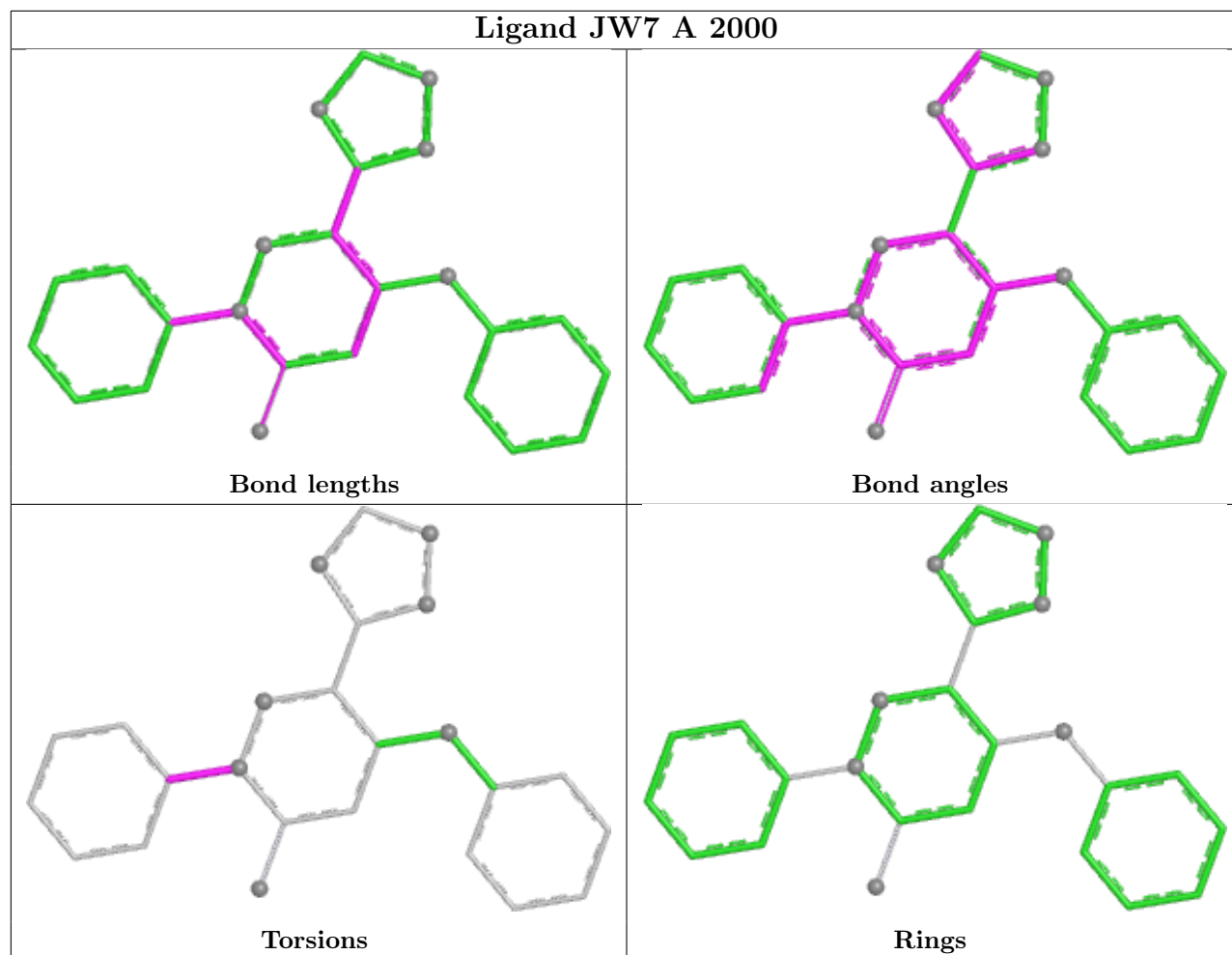
There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1774	NAG	1	0
8	B	2000	JW7	6	0
8	A	2000	JW7	4	0
7	B	1773	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 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	710/737 (96%)	-0.32	13 (1%) 67 58	39, 58, 82, 138	0
1	B	704/737 (95%)	-0.22	15 (2%) 63 54	38, 59, 91, 153	0
All	All	1414/1474 (95%)	-0.27	28 (1%) 65 56	38, 59, 86, 153	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	747	ALA	5.3
1	B	57	SER	5.0
1	B	746	ALA	4.2
1	B	747	ALA	3.8
1	A	54	PRO	3.5
1	A	206	ARG	3.5
1	B	742	LEU	3.4
1	B	745	ALA	3.4
1	A	53	HIS	3.3
1	B	761	SER	3.0
1	A	52	THR	2.9
1	B	381	THR	2.8
1	A	203	HIS	2.8
1	B	205	GLY	2.8
1	B	204	ARG	2.7
1	A	762	HIS	2.5
1	B	375	ASN	2.4
1	B	285	LEU	2.4
1	A	283	ALA	2.3
1	B	58	GLN	2.3
1	A	582	ALA	2.3
1	A	81	PRO	2.3
1	B	202	LYS	2.3
1	B	743	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	204	ARG	2.2
1	B	612	GLY	2.1
1	A	746	ALA	2.0
1	A	205	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TPQ	A	471	14/15	0.96	0.07	43,48,52,54	0
1	TPQ	B	471	14/15	0.96	0.07	44,53,56,59	0

6.3 Carbohydrates [i](#)

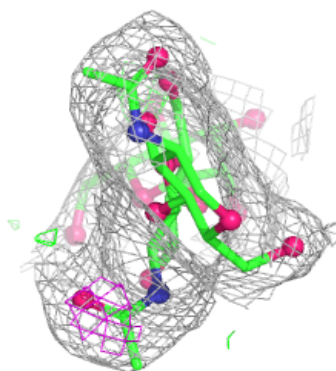
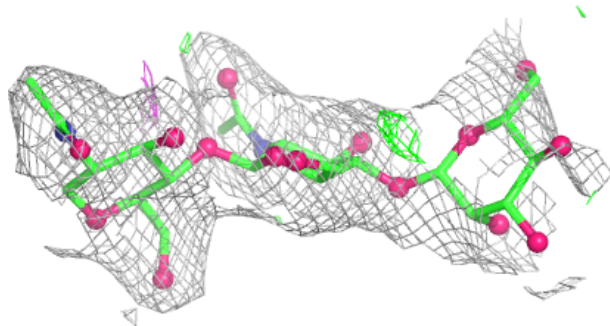
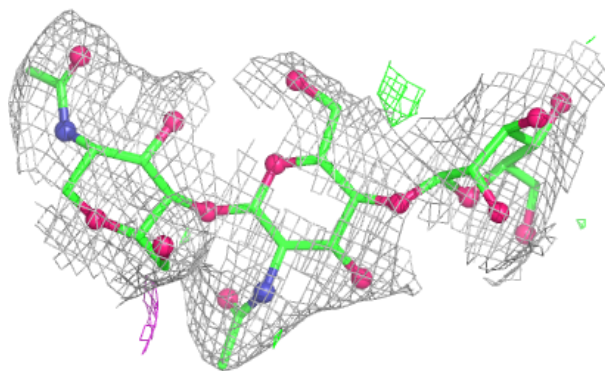
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	E	5	11/12	0.57	0.16	116,140,161,163	0
4	BMA	E	3	11/12	0.73	0.13	116,126,135,160	0
3	NAG	F	2	14/15	0.74	0.17	105,119,128,130	0
2	BMA	C	3	11/12	0.76	0.11	110,116,124,128	0
4	MAN	E	4	11/12	0.78	0.09	112,126,141,142	0
4	NAG	E	2	14/15	0.81	0.14	67,101,115,119	0
3	NAG	D	2	14/15	0.90	0.13	91,112,124,126	0
3	NAG	F	1	14/15	0.94	0.10	70,86,93,104	0
2	NAG	C	2	14/15	0.94	0.07	63,76,95,112	0
2	NAG	C	1	14/15	0.96	0.06	65,71,75,77	0
4	NAG	E	1	14/15	0.96	0.07	49,56,59,66	0
3	NAG	D	1	14/15	0.96	0.08	72,83,99,101	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.

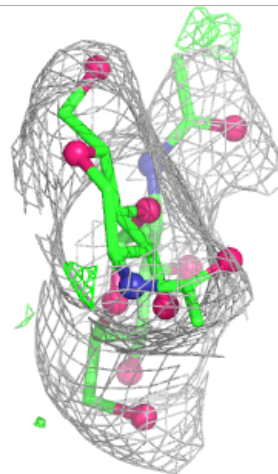
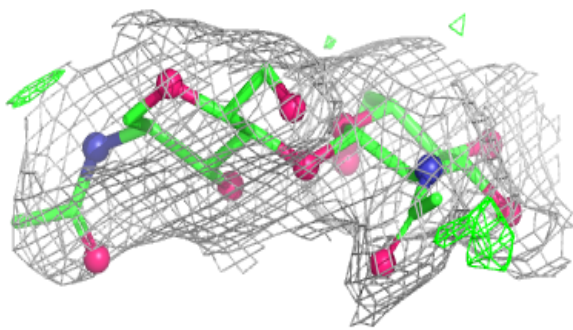
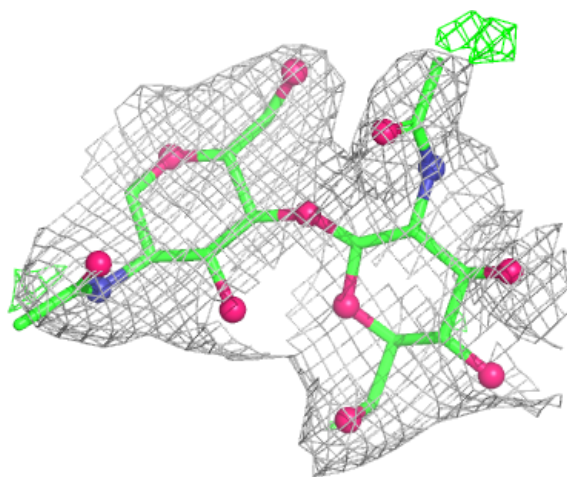
Electron density around Chain C:

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



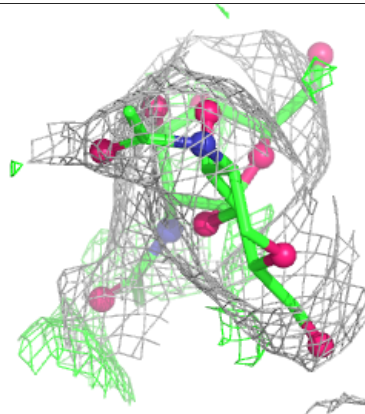
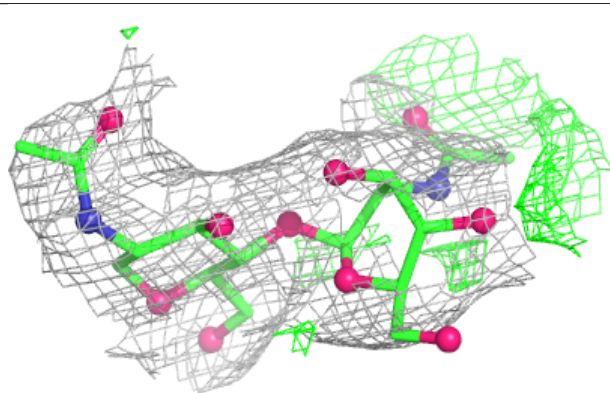
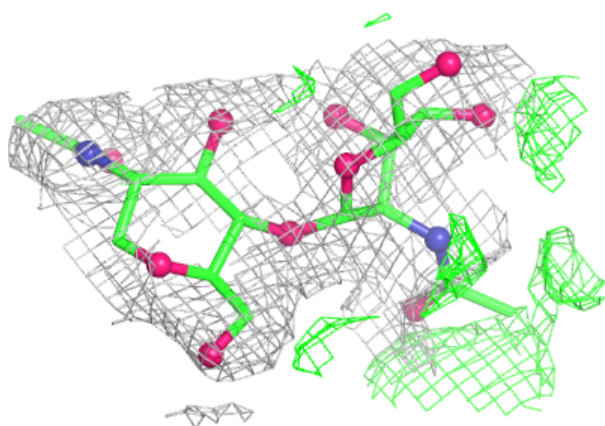
Electron density around Chain D:

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

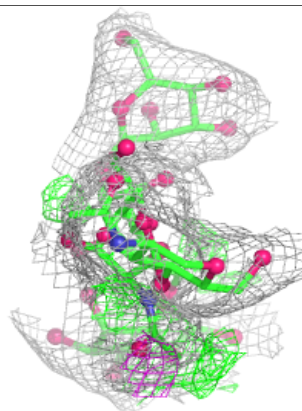
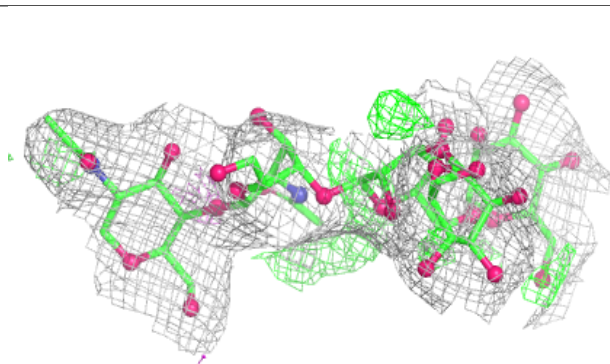
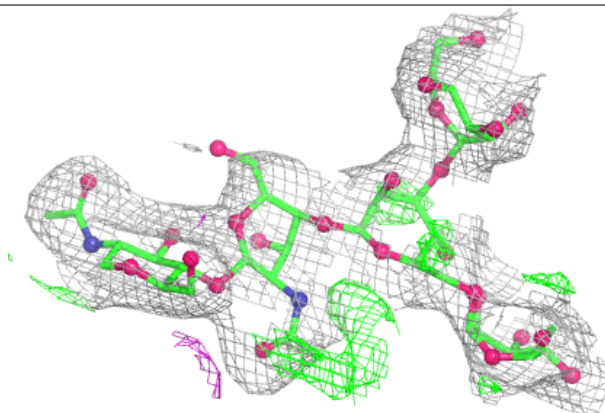


Electron density around Chain F:

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

**Electron density around Chain E:**

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



6.4 Ligands

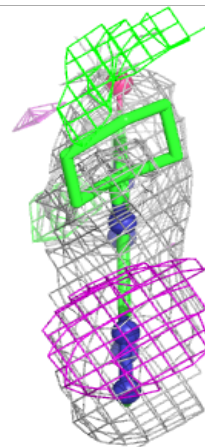
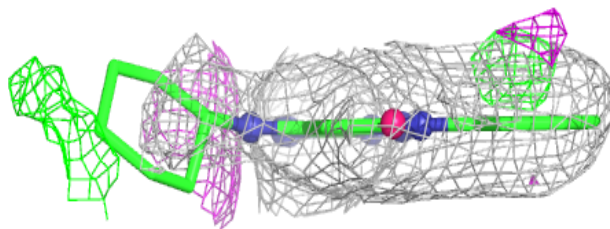
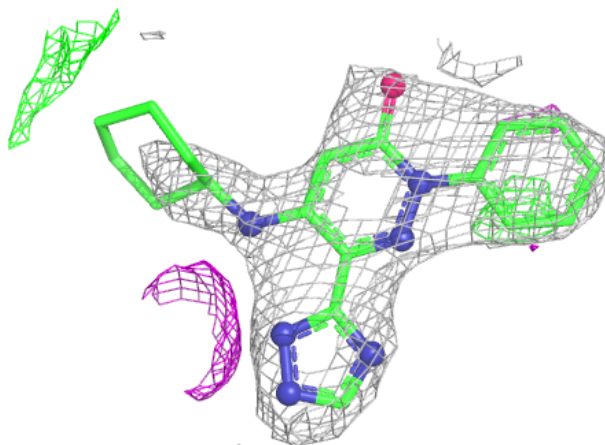
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

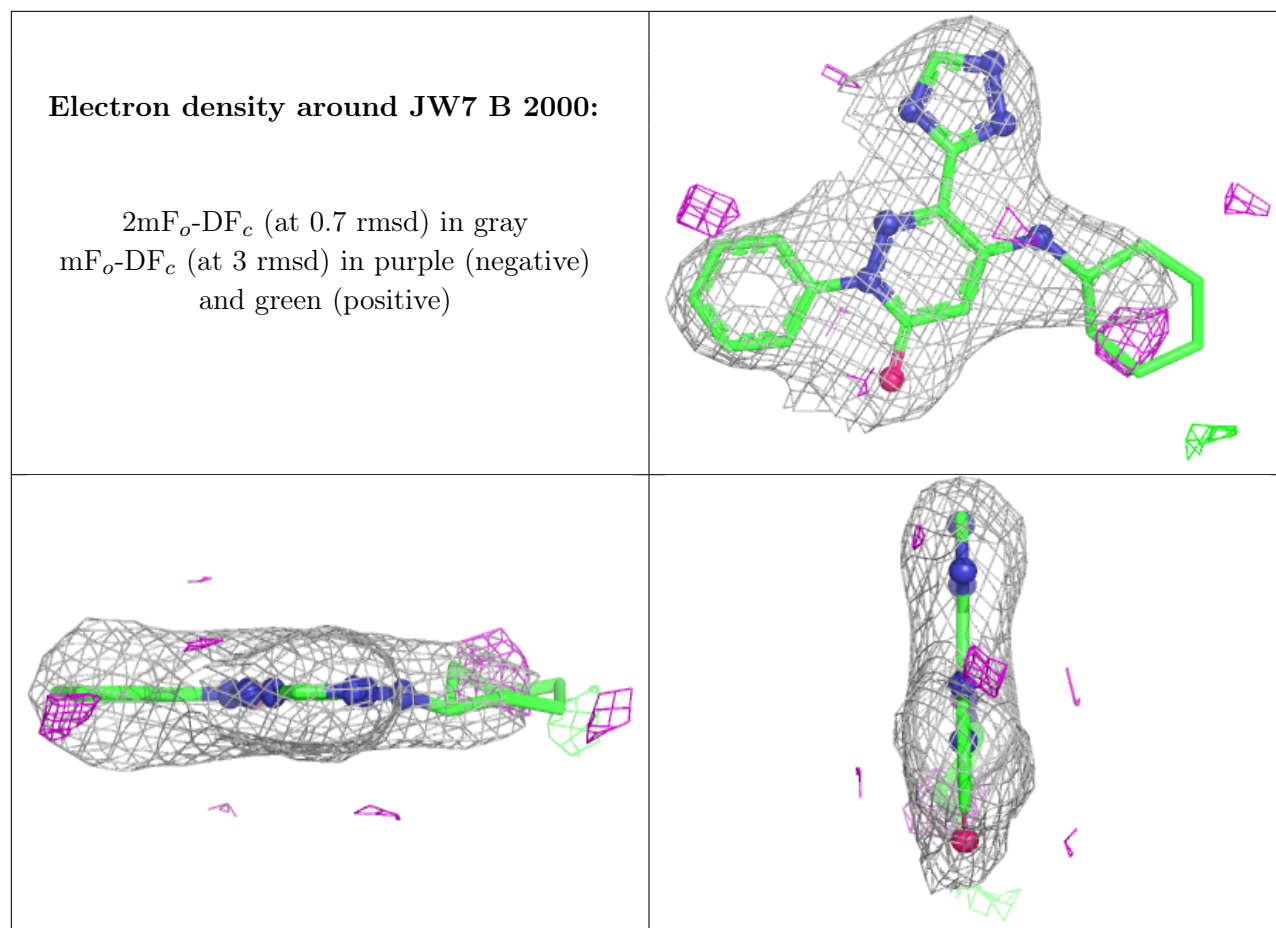
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	B	1774	14/15	0.45	0.17	94,121,135,136	0
7	NAG	A	1771	14/15	0.66	0.14	77,97,104,105	0
7	NAG	B	1772	14/15	0.67	0.16	103,132,140,141	0
7	NAG	B	1775	14/15	0.74	0.13	72,97,107,109	0
7	NAG	A	1770	14/15	0.75	0.15	74,93,115,115	0
7	NAG	B	1773	14/15	0.84	0.13	87,129,136,136	0
8	JW7	A	2000	25/25	0.92	0.19	65,90,143,148	0
6	CA	A	1764	1/1	0.94	0.07	59,59,59,59	0
8	JW7	B	2000	25/25	0.95	0.11	46,54,97,99	0
6	CA	A	1763	1/1	0.98	0.04	51,51,51,51	0
6	CA	B	1764	1/1	0.98	0.07	60,60,60,60	0
6	CA	B	1763	1/1	0.99	0.02	51,51,51,51	0
5	CU	A	1762	1/1	1.00	0.07	54,54,54,54	0
5	CU	B	1762	1/1	1.00	0.02	54,54,54,54	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 JW7 A 2000:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.