



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:59 AM UTC

PDB ID : 3T6V / pdb_00003t6v
Title : Crystal Structure of Laccase from *Steccherinum ochraceum*
Authors : Ferraroni, M.; Briganti, F.; Matera, I.; Kolomytseva, M.; Golovleva, L.; Scoz-
zafava, A.; Chernykh, A.M.
Deposited on : 2011-07-29
Resolution : 2.00 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
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

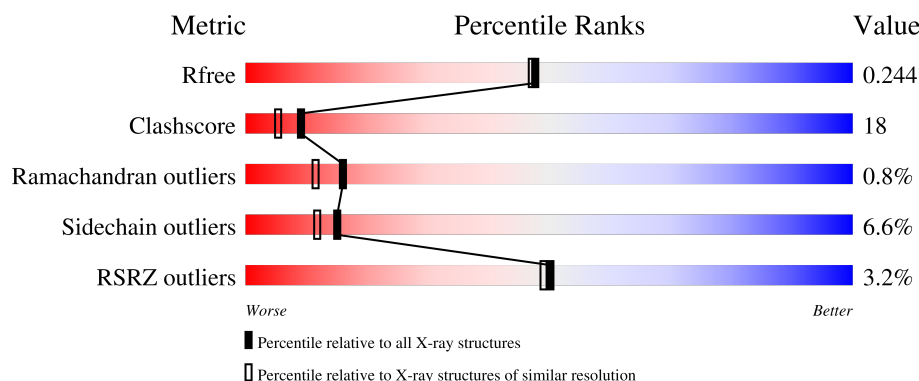
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	495	 2% 74% 22% .
1	B	495	 3% 73% 24% .
1	C	495	 5% 73% 21% 5% .
2	D	2	 100%
2	E	2	 100%

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	H	1	-	-	X	-
4	SO4	C	505	-	-	X	-
4	SO4	C	506	-	-	X	-
5	GOL	A	509	-	-	X	-
5	GOL	B	506	-	X	X	-
5	GOL	C	507	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12647 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 Laccase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	5	0
			3734	2358	625	731	20			
1	B	495	Total	C	N	O	S	0	6	0
			3739	2363	630	728	18			
1	C	495	Total	C	N	O	S	0	3	0
			3731	2356	629	729	17			

- 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	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
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			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Cu	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	Cu	0	0
			4	4		
3	C	4	Total	Cu	0	0
			4	4		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

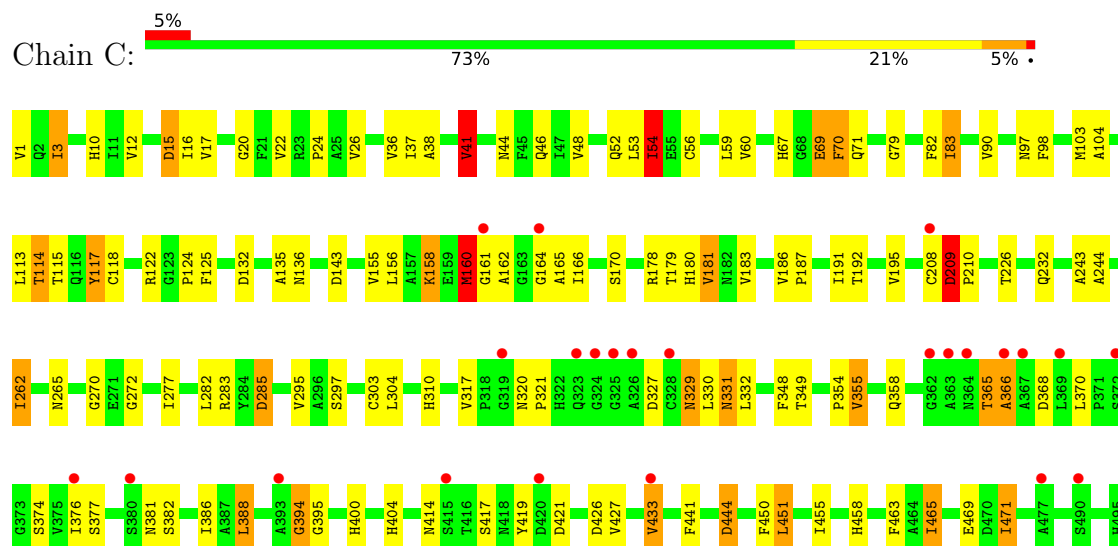


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		

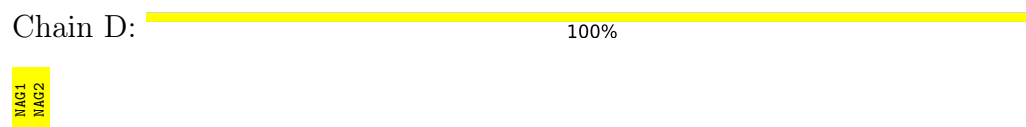
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	478	Total	O	0	0
			478	478		
7	B	376	Total	O	0	0
			376	376		
7	C	340	Total	O	0	0
			340	340		

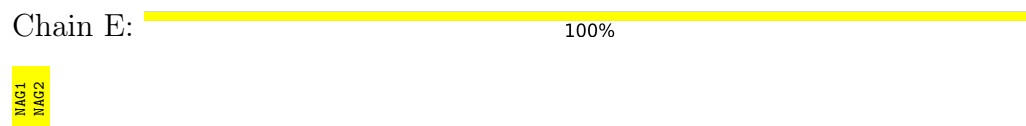
- Molecule 1: Laccase



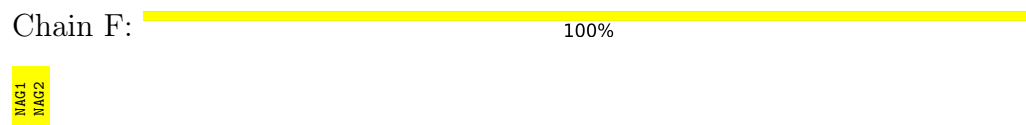
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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

Chain H:



MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.53Å 140.66Å 174.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (30.00-2.00) 98.2 (30.00-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.181 , 0.241 0.186 , 0.244	Depositor DCC
R_{free} test set	6068 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 66.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12647	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CU, NAG, GOL, SO4

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	1.35	7/3857 (0.2%)	1.20	12/5297 (0.2%)
1	B	1.25	7/3865 (0.2%)	1.22	18/5307 (0.3%)
1	C	1.26	6/3850 (0.2%)	1.25	20/5287 (0.4%)
All	All	1.29	20/11572 (0.2%)	1.22	50/15891 (0.3%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	ALA	CA-CB	7.68	1.63	1.52
1	B	293	VAL	CA-CB	6.89	1.63	1.54
1	B	229	VAL	CA-CB	6.78	1.62	1.54
1	C	277	ILE	CA-CB	6.46	1.60	1.54
1	A	7	THR	CA-CB	6.29	1.64	1.53
1	B	168	ALA	CA-CB	6.23	1.63	1.53
1	A	204	VAL	C-O	6.00	1.30	1.24
1	C	282	LEU	N-CA	-5.75	1.39	1.46
1	C	304	LEU	N-CA	-5.71	1.39	1.46
1	A	80	PRO	CA-C	-5.68	1.47	1.52
1	C	295	VAL	CA-CB	5.60	1.64	1.55
1	B	138	TYR	N-CA	5.51	1.52	1.45
1	A	293	VAL	CA-CB	5.46	1.60	1.54
1	B	83	ILE	CA-CB	-5.44	1.50	1.55
1	C	433	VAL	CA-CB	5.39	1.59	1.54
1	A	455	ILE	C-O	5.36	1.29	1.23
1	C	54	ILE	C-O	-5.29	1.17	1.25
1	B	222	THR	CA-CB	5.28	1.59	1.53
1	B	432	GLY	N-CA	5.26	1.50	1.44
1	A	202	ARG	CZ-NH2	5.02	1.40	1.33

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	365	THR	N-CA-C	-9.70	95.73	109.69
1	C	209	ASP	CA-C-N	-7.87	112.23	120.03
1	C	209	ASP	C-N-CA	-7.87	112.23	120.03
1	C	365	THR	CA-C-N	7.72	135.59	121.70
1	C	365	THR	C-N-CA	7.72	135.59	121.70
1	B	3	ILE	N-CA-C	-7.61	96.64	108.44
1	A	83	ILE	N-CA-C	-7.36	104.56	111.48
1	C	232	GLN	N-CA-C	-7.14	101.10	110.53
1	C	160	MET	N-CA-C	-6.64	100.65	110.48
1	A	79	GLY	N-CA-C	6.59	125.78	112.34
1	C	41	VAL	CB-CA-C	-6.45	100.86	111.51
1	B	30	GLY	N-CA-C	6.22	123.91	115.32
1	C	394	GLY	N-CA-C	-6.19	95.34	113.30
1	B	319	GLY	N-CA-C	6.09	122.81	112.22
1	A	394	GLY	N-CA-C	6.05	127.52	113.18
1	C	79	GLY	N-CA-C	5.99	124.55	112.34
1	A	265	ASN	N-CA-CB	5.93	117.70	110.17
1	C	83	ILE	N-CA-C	-5.87	105.96	111.48
1	B	471	ILE	CB-CA-C	-5.84	106.35	114.00
1	C	317	VAL	CB-CA-C	-5.62	101.13	111.36
1	B	220	ASP	CB-CA-C	-5.59	100.78	110.45
1	B	265[A]	ASN	N-CA-CB	-5.49	103.20	110.17
1	B	265[B]	ASN	N-CA-CB	-5.49	103.20	110.17
1	C	70	PHE	N-CA-C	5.46	117.31	111.36
1	C	262	ILE	N-CA-C	-5.44	100.55	108.17
1	B	3	ILE	CA-C-N	5.43	131.48	121.70
1	B	3	ILE	C-N-CA	5.43	131.48	121.70
1	B	41	VAL	CB-CA-C	-5.43	102.55	111.51
1	A	349	THR	CB-CA-C	5.39	118.11	110.02
1	A	226	THR	CB-CA-C	5.37	119.08	110.16
1	A	73	GLY	N-CA-C	-5.35	107.96	114.92
1	C	161	GLY	N-CA-C	-5.34	97.82	113.30
1	B	79	GLY	CA-C-N	-5.33	113.67	120.23
1	B	79	GLY	C-N-CA	-5.33	113.67	120.23
1	C	320	ASN	N-CA-C	5.33	117.66	110.31
1	C	395	GLY	N-CA-C	-5.32	97.88	113.30
1	A	380	SER	N-CA-CB	-5.28	102.56	110.17
1	B	160	MET	N-CA-C	-5.19	104.03	110.41
1	B	480	VAL	CA-C-N	-5.18	114.91	120.03
1	B	480	VAL	C-N-CA	-5.18	114.91	120.03
1	B	474	THR	N-CA-C	5.17	118.04	111.69
1	A	490	SER	CB-CA-C	-5.16	102.56	110.81
1	A	324	GLY	N-CA-C	-5.11	108.56	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	ALA	N-CA-C	5.10	116.69	110.41
1	C	3	ILE	CA-C-N	5.08	130.84	121.70
1	C	3	ILE	C-N-CA	5.08	130.84	121.70
1	C	381	ASN	N-CA-C	5.03	118.55	111.90
1	A	323	GLN	N-CA-C	5.03	117.50	109.96
1	B	3	ILE	CA-C-O	-5.01	116.44	121.45
1	B	135	ALA	N-CA-C	5.00	118.48	112.38

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	3734	0	3504	131	0
1	B	3739	0	3520	143	1
1	C	3731	0	3508	143	1
2	D	28	0	25	0	0
2	E	28	0	25	4	0
2	F	28	0	25	4	0
2	G	28	0	25	2	0
2	H	28	0	25	7	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
4	A	20	0	0	0	0
4	B	5	0	0	0	0
4	C	10	0	0	9	0
5	A	6	0	8	4	0
5	B	30	0	40	9	0
5	C	12	0	16	12	0
6	C	14	0	13	0	0
7	A	478	0	0	32	0
7	B	376	0	0	23	0
7	C	340	0	0	23	0
All	All	12647	0	10734	405	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 (405) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:ASN:ND2	2:H:1:NAG:C1	1.68	1.53
1:B:414:ASN:HD21	2:F:1:NAG:C1	1.18	1.52
1:A:436:ASN:ND2	2:E:1:NAG:C1	1.68	1.51
1:B:414:ASN:ND2	2:F:1:NAG:C1	1.75	1.43
2:H:1:NAG:H3	2:H:1:NAG:C8	1.41	1.42
2:H:1:NAG:H83	2:H:1:NAG:C3	1.73	1.19
1:B:72:LYS:N	5:B:506:GOL:H12	1.59	1.18
1:B:17:VAL:HG12	1:B:22:VAL:CA	1.76	1.15
1:A:161:GLY:HA2	1:A:162:ALA:CB	1.78	1.14
1:B:17:VAL:HG12	1:B:22:VAL:HA	1.26	1.11
2:H:1:NAG:C8	2:H:1:NAG:C3	2.30	1.04
1:A:17:VAL:HG12	1:A:22:VAL:HA	1.34	1.03
1:A:59:LEU:CD1	1:A:114:THR:HG21	1.89	1.03
1:C:53:LEU:O	1:C:90:VAL:HG21	1.60	1.01
1:A:299:VAL:HB	7:A:1042:HOH:O	1.62	1.00
1:B:17:VAL:HG12	1:B:22:VAL:N	1.75	1.00
1:B:17:VAL:CG1	1:B:22:VAL:HA	1.91	1.00
1:C:70:PHE:H	1:C:103:MET:HE1	1.24	0.98
1:A:17:VAL:HG12	1:A:22:VAL:CA	1.92	0.98
1:B:265[A]:ASN:HD21	1:B:272:GLY:H	1.08	0.97
1:C:17:VAL:HG12	1:C:22:VAL:HA	1.46	0.97
1:B:358:GLN:HE22	1:B:370:LEU:H	1.12	0.97
1:A:59:LEU:HD11	1:A:114:THR:HG21	1.46	0.97
1:A:161:GLY:HA2	1:A:162:ALA:HB2	1.46	0.97
1:B:12:VAL:HG22	7:B:901:HOH:O	1.62	0.97
1:C:17:VAL:HG12	1:C:22:VAL:CA	1.94	0.96
1:A:162:ALA:H	1:A:163:GLY:HA2	1.26	0.95
1:C:265[B]:ASN:HD21	1:C:272:GLY:H	1.06	0.95
1:C:12:VAL:HG22	7:C:632:HOH:O	1.65	0.95
1:C:162:ALA:HB2	7:C:891:HOH:O	1.65	0.94
1:A:160:MET:O	1:A:162:ALA:HB2	1.68	0.94
1:B:161:GLY:N	1:B:162:ALA:CB	2.30	0.94
1:A:56[A]:CYS:SG	1:B:52:GLN:NE2	2.39	0.94
1:B:36:VAL:HG22	1:B:124:PRO:HG2	1.47	0.94
1:C:36:VAL:HG22	1:C:124:PRO:HG2	1.47	0.94
1:C:365:THR:HB	1:C:366:ALA:CB	1.97	0.94
1:C:329:ASN:N	1:C:329:ASN:HD22	1.58	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LEU:HD11	1:B:114:THR:HG21	1.48	0.94
1:B:215:SER:C	1:B:216[B]:ILE:HD12	1.92	0.94
1:C:358:GLN:HE22	1:C:370:LEU:H	1.14	0.94
1:A:17:VAL:HG23	5:C:507:GOL:O1	1.68	0.93
1:C:48:VAL:HG23	7:C:714:HOH:O	1.67	0.92
1:B:59:LEU:HD21	1:B:158[B]:LYS:HE3	1.51	0.92
1:C:329:ASN:ND2	1:C:329:ASN:H	1.59	0.92
1:B:59:LEU:CD1	1:B:114:THR:HG21	1.99	0.92
1:B:161:GLY:CA	1:B:162:ALA:HB2	1.99	0.92
5:C:507:GOL:C1	7:C:929:HOH:O	2.17	0.92
1:B:72:LYS:H	5:B:506:GOL:H12	1.15	0.92
1:B:214:PHE:CE2	1:B:216[B]:ILE:HD11	2.04	0.92
1:A:161:GLY:HA2	1:A:162:ALA:HB3	1.50	0.91
1:C:20:GLY:O	5:C:507:GOL:H31	1.71	0.91
1:A:48:VAL:HG23	7:A:692:HOH:O	1.71	0.90
1:C:179:THR:O	1:C:183:VAL:HG22	1.71	0.90
1:A:70:PHE:H	1:A:103:MET:HE1	1.34	0.90
1:B:414:ASN:ND2	2:F:1:NAG:O5	1.83	0.90
1:B:56[A]:CYS:SG	1:C:52:GLN:NE2	2.44	0.90
1:A:451:LEU:HD23	1:A:465:ILE:HD11	1.54	0.89
1:B:17:VAL:CG1	1:B:22:VAL:CA	2.47	0.89
1:A:12:VAL:HG21	7:C:637:HOH:O	1.72	0.89
1:B:179:THR:O	1:B:183:VAL:HG22	1.72	0.89
1:A:195:VAL:HG23	7:A:648:HOH:O	1.74	0.88
1:C:60:VAL:HG21	7:C:801:HOH:O	1.74	0.88
1:A:12:VAL:HG22	7:A:800:HOH:O	1.73	0.88
1:B:161:GLY:N	1:B:162:ALA:HB2	1.89	0.87
1:A:329:ASN:OD1	1:A:329:ASN:N	2.06	0.86
1:A:10:HIS:CD2	1:C:56[A]:CYS:SG	2.69	0.86
1:C:365:THR:HB	1:C:366:ALA:HB2	1.58	0.86
1:A:52:GLN:NE2	1:C:56[A]:CYS:SG	2.48	0.85
1:C:117:TYR:CE1	1:C:208:CYS:SG	2.70	0.84
1:A:183:VAL:HG21	7:A:767:HOH:O	1.76	0.84
1:B:68:GLY:O	1:B:103:MET:HE1	1.78	0.84
7:B:670:HOH:O	1:C:12:VAL:HG21	1.77	0.84
1:C:164:GLY:HA2	1:C:165:ALA:HB3	1.60	0.84
1:B:53:LEU:O	1:B:90:VAL:HG21	1.77	0.83
1:A:113:LEU:HG	1:A:114:THR:HG22	1.60	0.83
1:C:44:ASN:ND2	1:C:46:GLN:HE21	1.76	0.83
1:A:436:ASN:CG	2:E:1:NAG:C1	2.51	0.82
1:C:329:ASN:HD22	1:C:329:ASN:H	0.86	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:VAL:HG23	5:C:507:GOL:HO1	1.41	0.82
1:C:366:ALA:HB1	4:C:506:SO4:S	2.20	0.81
2:H:1:NAG:H3	2:H:1:NAG:H83	0.82	0.81
1:B:265[A]:ASN:ND2	1:B:272:GLY:H	1.78	0.81
1:B:161:GLY:HA3	1:B:162:ALA:HB2	1.62	0.81
1:A:161:GLY:CA	1:A:162:ALA:CB	2.56	0.80
1:B:161:GLY:N	1:B:162:ALA:HB3	1.96	0.79
1:C:366:ALA:HB1	4:C:506:SO4:O2	1.82	0.79
5:C:507:GOL:H11	7:C:929:HOH:O	1.78	0.79
1:A:265:ASN:HD21	1:A:272:GLY:H	1.29	0.79
1:B:72:LYS:H	5:B:506:GOL:C1	1.93	0.79
1:B:391:GLY:HA2	1:B:433:VAL:HG22	1.65	0.79
1:C:17:VAL:HG21	5:C:507:GOL:H2	1.64	0.78
1:A:90:VAL:HG22	7:A:702:HOH:O	1.82	0.78
1:B:3:ILE:O	1:B:37:ILE:HA	1.84	0.78
1:B:113:LEU:HG	1:B:114:THR:HG22	1.64	0.78
2:H:1:NAG:H3	2:H:1:NAG:H82	1.58	0.77
1:A:179:THR:O	1:A:183:VAL:HG22	1.83	0.77
1:A:161:GLY:CA	1:A:162:ALA:HB2	2.14	0.77
7:A:847:HOH:O	1:B:12:VAL:HG21	1.84	0.77
1:C:365:THR:HB	1:C:366:ALA:HB3	1.65	0.77
1:A:17:VAL:CG1	1:A:22:VAL:HA	2.13	0.77
1:C:365:THR:CB	1:C:366:ALA:CB	2.63	0.77
1:B:56[A]:CYS:SG	1:C:10:HIS:CD2	2.79	0.76
1:C:366:ALA:CB	4:C:506:SO4:O2	2.33	0.76
1:B:161:GLY:H	1:B:162:ALA:HB3	1.52	0.75
1:C:332:LEU:HD12	1:C:388:LEU:HD23	1.68	0.75
1:A:391:GLY:HA2	1:A:433:VAL:HG22	1.68	0.75
1:A:95:SER:HB3	7:A:737:HOH:O	1.85	0.74
1:C:310:HIS:HD2	1:C:421:ASP:O	1.70	0.74
1:A:136:ASN:OD1	7:A:1050:HOH:O	2.03	0.74
1:A:59:LEU:HD12	1:A:114:THR:HG21	1.69	0.74
1:C:183:VAL:HG21	7:C:776:HOH:O	1.88	0.74
1:C:70:PHE:N	1:C:103:MET:HE1	2.02	0.73
1:A:60:VAL:HG21	7:A:688:HOH:O	1.88	0.72
1:B:183:VAL:HG21	7:B:668:HOH:O	1.89	0.72
1:A:436:ASN:ND2	2:E:1:NAG:O5	2.22	0.72
1:A:70:PHE:N	1:A:103:MET:HE1	2.04	0.72
1:C:59:LEU:HD11	1:C:114:THR:HG21	1.72	0.72
1:A:165:ALA:HB1	7:A:1076:HOH:O	1.88	0.72
1:C:53:LEU:O	1:C:90:VAL:CG2	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:VAL:HG23	7:A:647:HOH:O	1.91	0.71
1:A:60:VAL:HG23	7:A:660:HOH:O	1.91	0.70
1:C:265[B]:ASN:ND2	1:C:272:GLY:H	1.86	0.70
1:C:365:THR:CB	1:C:366:ALA:HB3	2.21	0.70
1:B:59:LEU:CD1	1:B:114:THR:CG2	2.69	0.70
1:A:10:HIS:NE2	1:C:56[A]:CYS:SG	2.64	0.70
1:B:48:VAL:HG23	7:B:799:HOH:O	1.91	0.69
1:B:60:VAL:HG23	7:B:681:HOH:O	1.92	0.69
1:A:162:ALA:N	1:A:163:GLY:HA2	2.02	0.69
1:C:60:VAL:HG23	7:C:644:HOH:O	1.92	0.69
1:B:70:PHE:CD2	1:B:103:MET:SD	2.85	0.68
1:C:70:PHE:H	1:C:103:MET:CE	2.03	0.68
1:A:117:TYR:CE1	1:A:208[B]:CYS:SG	2.87	0.68
1:B:17:VAL:HG12	1:B:21:PHE:C	2.20	0.67
1:B:17:VAL:HG23	5:B:510:GOL:O2	1.95	0.67
1:A:17:VAL:HG22	4:C:505:SO4:O4	1.95	0.67
1:A:426:ASP:OD1	1:A:427:VAL:HG23	1.95	0.67
1:C:17:VAL:HG22	4:C:505:SO4:O2	1.94	0.67
1:A:331:ASN:HD22	1:A:331:ASN:C	2.03	0.67
1:A:36:VAL:HG22	1:A:124:PRO:HG2	1.77	0.67
1:C:285:ASP:OD1	7:C:868:HOH:O	2.12	0.66
1:C:471:ILE:HG13	7:C:927:HOH:O	1.95	0.66
1:A:41:VAL:CG2	1:A:104:ALA:HB2	2.25	0.66
7:A:649:HOH:O	1:C:155:VAL:HG21	1.95	0.66
1:B:90:VAL:HG22	7:B:679:HOH:O	1.95	0.66
1:A:394:GLY:HA2	7:A:924:HOH:O	1.96	0.66
1:B:340:ASN:ND2	7:B:959:HOH:O	2.29	0.66
1:A:10:HIS:CD2	1:C:56[A]:CYS:HG	2.14	0.65
1:B:70:PHE:HB2	5:B:506:GOL:H2	1.79	0.64
1:C:17:VAL:CG1	1:C:22:VAL:HB	2.26	0.64
1:A:56[A]:CYS:SG	1:B:10:HIS:CD2	2.90	0.64
1:C:374:SER:O	1:C:465:ILE:HG22	1.97	0.64
1:B:214:PHE:HE2	1:B:216[B]:ILE:HD11	1.58	0.64
1:C:444:ASP:HB2	7:C:681:HOH:O	1.97	0.64
1:A:70:PHE:H	1:A:103:MET:CE	2.10	0.63
1:C:365:THR:CB	1:C:366:ALA:HB2	2.27	0.63
1:A:103:MET:HE2	7:A:726:HOH:O	1.96	0.63
1:A:53:LEU:O	1:A:90:VAL:HG21	1.98	0.63
1:A:54:ILE:HG13	7:B:618:HOH:O	1.98	0.63
1:C:366:ALA:HB1	4:C:506:SO4:O3	1.97	0.63
1:A:100:VAL:HG23	1:A:100:VAL:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:VAL:HG23	7:B:921:HOH:O	1.99	0.62
1:B:103:MET:HE3	7:B:841:HOH:O	1.97	0.62
1:C:3:ILE:O	1:C:38:ALA:N	2.33	0.62
1:A:95:SER:CB	7:A:737:HOH:O	2.43	0.62
1:A:400:HIS:HB2	1:A:427:VAL:HG22	1.81	0.62
7:A:626:HOH:O	1:C:54:ILE:HD12	2.00	0.62
1:A:160:MET:HE3	1:A:160:MET:HA	1.82	0.61
1:B:117:TYR:CE1	1:B:208[B]:CYS:SG	2.88	0.61
1:B:162:ALA:HB1	7:B:870:HOH:O	2.00	0.61
1:C:20:GLY:C	5:C:507:GOL:H31	2.25	0.61
1:C:17:VAL:HG23	7:C:688:HOH:O	2.00	0.61
1:A:162:ALA:H	1:A:164:GLY:HA3	1.64	0.61
1:B:195:VAL:HG11	7:B:866:HOH:O	2.00	0.60
1:A:113:LEU:C	1:A:114:THR:HG22	2.27	0.60
1:B:72:LYS:N	5:B:506:GOL:C1	2.51	0.60
1:B:22:VAL:HG23	7:C:607:HOH:O	2.01	0.60
1:A:310:HIS:HE1	7:A:787:HOH:O	1.83	0.60
1:B:155:VAL:HG23	7:B:633:HOH:O	2.01	0.60
1:A:163:GLY:HA3	7:A:965:HOH:O	2.01	0.59
1:B:17:VAL:HG23	1:B:17:VAL:O	2.01	0.59
1:C:17:VAL:HG12	1:C:22:VAL:N	2.17	0.59
1:B:17:VAL:CG1	1:B:22:VAL:N	2.59	0.59
1:C:118:CYS:SG	1:C:208:CYS:HB3	2.42	0.59
1:C:118:CYS:HA	1:C:208:CYS:SG	2.43	0.59
1:B:155:VAL:HG21	7:C:856:HOH:O	2.02	0.59
1:C:243:ALA:O	1:C:244:ALA:HB3	2.03	0.59
1:C:365:THR:O	1:C:368:ASP:HB2	2.02	0.59
1:B:329:ASN:OD1	1:B:329:ASN:N	2.36	0.59
1:C:17:VAL:HG12	1:C:22:VAL:CB	2.32	0.59
1:A:112:HIS:CE1	5:A:509:GOL:H32	2.38	0.59
1:B:22:VAL:CG2	7:C:607:HOH:O	2.50	0.59
1:A:59:LEU:HD12	1:A:114:THR:CG2	2.33	0.58
1:C:400:HIS:HB2	1:C:427:VAL:HG22	1.85	0.58
1:A:155:VAL:HG21	7:B:858:HOH:O	2.03	0.58
1:B:320:ASN:O	1:B:322:HIS:N	2.35	0.58
1:C:90:VAL:HG22	7:C:628:HOH:O	2.03	0.58
1:C:186:VAL:HG23	7:C:756:HOH:O	2.03	0.58
1:A:30:GLY:N	7:A:800:HOH:O	2.33	0.58
1:C:310:HIS:CD2	1:C:421:ASP:O	2.54	0.58
1:A:17:VAL:CG2	4:C:505:SO4:O4	2.52	0.58
1:A:386:ILE:HD12	1:A:441:PHE:HE1	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ASN:ND2	7:B:908:HOH:O	2.19	0.57
1:A:17:VAL:HG12	1:A:22:VAL:N	2.19	0.57
1:B:426:ASP:OD1	1:B:427:VAL:HG23	2.03	0.57
1:A:176:LEU:HD21	5:C:507:GOL:H32	1.86	0.57
1:B:95:SER:HB3	7:B:908:HOH:O	2.04	0.57
1:C:59:LEU:CD1	1:C:114:THR:HG21	2.34	0.57
1:C:17:VAL:CG1	1:C:22:VAL:HA	2.30	0.56
1:C:41:VAL:HG13	1:C:103:MET:O	2.06	0.56
1:A:56[A]:CYS:HG	1:B:10:HIS:CD2	2.22	0.56
1:B:59:LEU:HD21	1:B:158[A]:LYS:HD2	1.86	0.56
1:B:54:ILE:HD11	7:B:652:HOH:O	2.05	0.56
1:C:181:VAL:HG13	7:C:626:HOH:O	2.06	0.56
1:A:310:HIS:HD2	1:A:421:ASP:O	1.88	0.56
1:B:162:ALA:HB2	1:B:166:ILE:HD11	1.88	0.56
1:C:451:LEU:HB3	1:C:465:ILE:HD12	1.87	0.56
1:B:56[A]:CYS:HG	1:C:10:HIS:CD2	2.23	0.56
1:C:170:SER:HB3	1:C:179:THR:HA	1.88	0.56
1:C:118:CYS:SG	1:C:208:CYS:CB	2.95	0.55
1:A:83:ILE:HD11	1:A:348:PHE:CZ	2.41	0.55
1:C:59:LEU:CD1	1:C:114:THR:CG2	2.85	0.55
1:C:114:THR:OG1	1:C:115:THR:N	2.40	0.55
1:C:59:LEU:HD21	1:C:158[A]:LYS:HD2	1.89	0.55
1:C:117:TYR:CD1	1:C:208:CYS:SG	2.98	0.55
1:A:17:VAL:CG1	1:A:22:VAL:HB	2.36	0.55
1:B:356:LEU:HD23	1:B:484:TRP:CZ2	2.42	0.54
7:A:801:HOH:O	2:E:1:NAG:H81	2.06	0.54
1:B:430:ILE:HA	1:B:437:VAL:HG21	1.87	0.54
1:C:67:HIS:CE1	1:C:244:ALA:HB1	2.42	0.54
1:B:181:VAL:HG13	7:B:783:HOH:O	2.07	0.54
1:B:178:ARG:HG2	1:B:186:VAL:HG22	1.88	0.54
1:A:17:VAL:CG1	1:A:22:VAL:CA	2.75	0.54
1:C:17:VAL:CG1	1:C:22:VAL:CB	2.86	0.54
1:B:358:GLN:HE22	1:B:370:LEU:N	1.95	0.53
5:C:507:GOL:H12	7:C:929:HOH:O	1.98	0.53
1:A:103:MET:CE	7:A:726:HOH:O	2.55	0.53
1:B:56[A]:CYS:SG	1:C:10:HIS:HD2	2.31	0.53
1:B:72:LYS:CA	5:B:506:GOL:H12	2.37	0.53
1:C:366:ALA:HB3	4:C:506:SO4:O2	2.08	0.53
1:C:3:ILE:O	1:C:37:ILE:HA	2.09	0.53
1:C:414:ASN:ND2	2:H:1:NAG:O5	2.38	0.52
1:B:54:ILE:C	1:B:54:ILE:HD12	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:ASN:N	1:C:329:ASN:ND2	2.28	0.52
1:A:113:LEU:C	1:A:114:THR:CG2	2.82	0.52
1:C:365:THR:CA	1:C:366:ALA:HB2	2.39	0.52
1:A:10:HIS:HD2	1:C:56[A]:CYS:SG	2.32	0.52
1:A:41:VAL:HG22	1:A:104:ALA:HB2	1.92	0.52
1:A:59:LEU:CD1	1:A:114:THR:CG2	2.76	0.52
1:A:302:LYS:HD3	7:A:1016:HOH:O	2.08	0.52
1:C:17:VAL:HG21	5:C:507:GOL:C2	2.36	0.52
1:A:180:HIS:CD2	1:A:270:GLY:H	2.27	0.52
1:C:321:PRO:HA	1:C:419:TYR:CG	2.46	0.51
1:B:54:ILE:HD13	7:C:750:HOH:O	2.09	0.51
1:A:265:ASN:ND2	1:A:272:GLY:H	2.04	0.51
1:A:386:ILE:CD1	1:A:441:PHE:HE1	2.23	0.51
1:B:151:ASP:OD2	1:B:208[A]:CYS:HB2	2.11	0.51
1:C:132:ASP:HB3	1:C:135:ALA:HB2	1.93	0.50
1:A:160:MET:C	1:A:162:ALA:HB2	2.33	0.50
1:A:331:ASN:C	1:A:331:ASN:ND2	2.70	0.50
1:B:17:VAL:CG1	1:B:22:VAL:CB	2.90	0.50
1:B:17:VAL:HG13	1:B:22:VAL:HA	1.88	0.50
1:B:44:ASN:ND2	1:B:46:GLN:HE21	2.08	0.50
1:C:36:VAL:HG21	1:C:143:ASP:OD2	2.11	0.50
1:B:180:HIS:CD2	1:B:270:GLY:H	2.28	0.50
1:C:82:PHE:C	1:C:83:ILE:HD13	2.36	0.50
1:C:209:ASP:HA	1:C:455:ILE:HG23	1.93	0.50
1:A:67:HIS:C	1:A:67:HIS:CD2	2.90	0.49
1:B:265[A]:ASN:HD21	1:B:272:GLY:N	1.92	0.49
1:A:69:GLU:HA	1:A:103:MET:HE1	1.95	0.49
1:B:60:VAL:HG22	7:B:689:HOH:O	2.13	0.49
1:C:160:MET:HE2	1:C:166:ILE:HG12	1.95	0.49
1:B:83:ILE:HD11	1:B:348:PHE:HZ	1.76	0.49
1:B:178:ARG:HG2	1:B:186:VAL:CG2	2.42	0.49
1:B:320:ASN:HD22	1:B:322:HIS:CE1	2.30	0.49
1:C:331:ASN:C	1:C:331:ASN:HD22	2.21	0.49
1:B:46:GLN:HA	1:B:97:ASN:HD22	1.78	0.48
1:C:71:GLN:HE22	1:C:98:PHE:CB	2.26	0.48
1:A:191:ILE:HD12	1:A:262:ILE:HD13	1.95	0.48
1:C:426:ASP:OD1	1:C:427:VAL:HG23	2.13	0.48
1:A:17:VAL:CG1	1:A:22:VAL:CB	2.90	0.48
1:B:162:ALA:CB	1:B:166:ILE:HD11	2.43	0.48
1:B:305:ILE:HD11	7:B:948:HOH:O	2.13	0.48
1:B:160:MET:HE3	1:B:160:MET:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ASP:OD2	1:A:22:VAL:HG22	2.13	0.48
1:C:136:ASN:ND2	1:C:136:ASN:H	2.12	0.48
1:C:20:GLY:O	5:C:507:GOL:C3	2.53	0.47
1:B:256:PRO:HB3	7:B:969:HOH:O	2.14	0.47
1:C:59:LEU:HD11	1:C:114:THR:CG2	2.42	0.47
1:C:69:GLU:HA	1:C:103:MET:HE1	1.97	0.47
1:A:225:GLU:HB3	1:A:248:SER:HB2	1.96	0.47
1:A:22:VAL:HG21	1:B:16:ILE:HG22	1.97	0.47
1:B:301:THR:HG22	1:B:302:LYS:HG2	1.96	0.47
1:C:376:ILE:HG22	1:C:377:SER:O	2.15	0.47
1:B:83:ILE:HD11	1:B:348:PHE:CZ	2.50	0.47
1:A:36:VAL:HG23	7:A:969:HOH:O	2.14	0.47
1:A:41:VAL:HG21	1:A:104:ALA:HB2	1.97	0.47
1:A:56[A]:CYS:SG	1:B:10:HIS:HD2	2.38	0.47
1:B:320:ASN:ND2	1:B:322:HIS:CE1	2.83	0.47
1:A:83:ILE:HD11	1:A:348:PHE:HZ	1.79	0.47
1:B:17:VAL:HG22	4:C:505:SO4:O3	2.14	0.47
1:B:36:VAL:HG21	1:B:143:ASP:OD2	2.15	0.47
1:B:176:LEU:HD22	5:B:510:GOL:H12	1.96	0.47
1:C:209:ASP:HB3	1:C:210:PRO:CD	2.45	0.47
1:C:332:LEU:HD12	1:C:388:LEU:CD2	2.41	0.46
1:A:112:HIS:ND1	5:A:509:GOL:H32	2.30	0.46
1:A:181:VAL:HG13	7:A:826:HOH:O	2.14	0.46
1:C:113:LEU:HG	1:C:114:THR:HG22	1.98	0.46
1:A:90:VAL:HG22	1:A:91:GLY:N	2.30	0.46
1:C:83:ILE:HD11	1:C:348:PHE:HZ	1.81	0.46
1:A:16:ILE:HD11	1:A:152:TRP:CH2	2.50	0.46
1:B:354:PRO:O	1:B:355:VAL:C	2.57	0.46
1:A:10:HIS:HE2	1:C:56[A]:CYS:HG	1.52	0.46
1:A:198:ARG:HD3	7:A:977:HOH:O	2.15	0.46
1:B:76:TRP:CE2	1:B:481:PRO:HD3	2.51	0.46
1:C:386:ILE:CD1	1:C:441:PHE:HE1	2.28	0.45
7:A:656:HOH:O	1:C:54:ILE:HG13	2.14	0.45
1:B:216[B]:ILE:HD13	1:B:221:MET:SD	2.57	0.45
1:B:414:ASN:CG	2:F:1:NAG:C1	2.76	0.45
1:B:49:THR:O	1:B:93:SER:HA	2.16	0.45
1:B:404:HIS:NE2	1:B:469:GLU:OE1	2.42	0.45
1:A:182:ASN:HD21	1:B:192:THR:H	1.65	0.45
1:C:83:ILE:HD13	1:C:83:ILE:N	2.31	0.45
1:B:155:VAL:HG22	1:C:1:VAL:HG13	1.98	0.45
1:B:318:PRO:HB2	1:B:383:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:VAL:HG13	1:A:103:MET:O	2.16	0.45
1:C:41:VAL:CG1	1:C:103:MET:O	2.65	0.45
1:A:459:LEU:HD21	5:A:509:GOL:C3	2.47	0.44
1:B:358:GLN:NE2	1:B:370:LEU:H	1.96	0.44
1:C:451:LEU:HD12	1:C:465:ILE:HD11	1.99	0.44
1:A:36:VAL:HG21	1:A:143:ASP:OD2	2.16	0.44
1:B:22:VAL:HG21	1:C:16:ILE:HG22	2.00	0.44
1:C:178:ARG:HG2	1:C:186:VAL:HG22	2.00	0.44
1:A:459:LEU:HD21	5:A:509:GOL:H31	1.99	0.44
1:A:61:ASP:O	1:A:113:LEU:HD23	2.17	0.44
1:C:17:VAL:HG23	1:C:17:VAL:O	2.17	0.44
1:B:181:VAL:HA	5:B:507:GOL:H2	2.00	0.44
1:B:241:ILE:HG23	1:B:241:ILE:O	2.18	0.44
1:B:378:LEU:HD22	1:B:384:ILE:HD12	1.99	0.44
1:B:70:PHE:CE2	1:B:103:MET:SD	3.11	0.43
1:B:161:GLY:H	1:B:162:ALA:CB	2.13	0.43
1:C:191:ILE:HD12	1:C:262:ILE:HD13	1.99	0.43
1:C:243:ALA:O	1:C:244:ALA:CB	2.66	0.43
1:A:160:MET:HA	1:A:160:MET:CE	2.46	0.43
1:A:413:SER:HB2	7:A:979:HOH:O	2.17	0.43
1:B:323:GLN:NE2	2:G:1:NAG:H61	2.33	0.43
1:A:392:ALA:O	1:A:393:ALA:C	2.60	0.43
1:C:191:ILE:HD12	1:C:262:ILE:CD1	2.48	0.43
1:A:394:GLY:HA2	1:A:395:GLY:HA3	1.65	0.43
1:A:111:SER:HB2	1:A:121:LEU:HD13	2.01	0.43
1:C:365:THR:CA	1:C:366:ALA:CB	2.94	0.43
1:B:181:VAL:O	1:B:182:ASN:C	2.62	0.43
1:C:26:VAL:HG13	1:C:53:LEU:HD21	2.00	0.43
1:B:53:LEU:O	1:B:90:VAL:CG2	2.58	0.43
1:C:15:ASP:OD2	1:C:22:VAL:HG22	2.19	0.42
1:A:82:PHE:C	1:A:83:ILE:HD13	2.43	0.42
1:C:331:ASN:C	1:C:331:ASN:ND2	2.77	0.42
1:A:430:ILE:HA	1:A:437:VAL:HG21	2.02	0.42
1:B:386:ILE:CD1	1:B:441:PHE:HE1	2.32	0.42
1:B:70:PHE:CG	1:B:103:MET:SD	3.12	0.42
1:B:400:HIS:HB2	1:B:427:VAL:HG22	2.01	0.42
1:C:209:ASP:HB3	1:C:210:PRO:HD3	2.01	0.42
1:C:354:PRO:O	1:C:355:VAL:C	2.62	0.42
1:B:59:LEU:HD12	1:B:114:THR:CG2	2.49	0.42
1:C:186:VAL:HB	1:C:187:PRO:CD	2.49	0.42
1:A:54:ILE:HD13	7:A:790:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ILE:O	1:B:38:ALA:N	2.52	0.42
1:B:155:VAL:HG22	1:C:1:VAL:CG1	2.50	0.42
1:B:340:ASN:ND2	7:B:965:HOH:O	2.38	0.42
1:B:182:ASN:ND2	1:C:192:THR:OG1	2.53	0.42
1:B:432:GLY:O	1:B:433:VAL:C	2.63	0.41
1:B:389:PRO:HG3	2:G:1:NAG:H82	2.02	0.41
1:C:83:ILE:HD11	1:C:348:PHE:CZ	2.54	0.41
1:C:394:GLY:O	1:C:458:HIS:HE1	2.03	0.41
1:B:162:ALA:H	1:B:164:GLY:HA3	1.85	0.41
1:A:82:PHE:HB3	1:A:351:PRO:HD2	2.03	0.41
1:A:243:ALA:O	1:A:244:ALA:HB3	2.20	0.41
1:A:305:ILE:HD13	7:A:1046:HOH:O	2.20	0.41
1:B:15:ASP:OD2	1:B:22:VAL:HG22	2.20	0.41
1:B:195:VAL:HG12	7:B:693:HOH:O	2.20	0.41
1:C:192:THR:HA	1:C:283:ARG:O	2.21	0.41
1:B:151:ASP:OD1	1:B:151:ASP:N	2.49	0.41
1:A:113:LEU:O	1:A:114:THR:C	2.64	0.41
1:B:191:ILE:HD12	1:B:262:ILE:CD1	2.51	0.41
1:C:37:ILE:O	1:C:125:PHE:HA	2.21	0.41
1:C:404:HIS:NE2	1:C:469:GLU:OE1	2.53	0.41
1:B:414:ASN:OD1	1:B:414:ASN:C	2.64	0.41
1:C:330:LEU:HD23	1:C:330:LEU:HA	1.76	0.41
1:A:19:ASP:HA	1:A:177:GLY:O	2.21	0.40
1:C:179:THR:CG2	1:C:183:VAL:HA	2.51	0.40
1:C:180:HIS:CD2	1:C:270:GLY:H	2.39	0.40
1:C:181:VAL:CG1	7:C:626:HOH:O	2.67	0.40
1:A:30:GLY:HA3	1:C:24:PRO:HG3	2.02	0.40
1:A:115:THR:HA	1:A:456:ASP:OD2	2.20	0.40
1:A:311:PRO:HD3	1:A:423:ILE:HA	2.03	0.40
1:A:413:SER:CB	7:A:979:HOH:O	2.69	0.40
1:B:227:ASP:OD2	1:B:425:ARG:HB2	2.22	0.40
1:B:386:ILE:HD11	1:B:441:PHE:CE1	2.56	0.40
1:C:41:VAL:HG23	7:C:835:HOH:O	2.22	0.40
1:A:17:VAL:HG11	1:A:22:VAL:HB	2.02	0.40
1:B:63:SER:OG	1:B:79:GLY:O	2.33	0.40
1:C:41:VAL:HG13	1:C:104:ALA:HB2	2.03	0.40
1:C:374:SER:C	1:C:465:ILE:HG22	2.46	0.40
1:A:176:LEU:CD2	5:C:507:GOL:H32	2.52	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:B:136:ASN:ND2	1:C:136:ASN:ND2[3_554]	1.85	0.35

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	498/495 (101%)	476 (96%)	18 (4%)	4 (1%)	16	11
1	B	498/495 (101%)	473 (95%)	20 (4%)	5 (1%)	12	8
1	C	496/495 (100%)	470 (95%)	23 (5%)	3 (1%)	21	17
All	All	1492/1485 (100%)	1419 (95%)	61 (4%)	12 (1%)	16	11

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	ALA
1	B	162	ALA
1	C	209	ASP
1	C	366	ALA
1	A	209	ASP
1	A	394	GLY
1	B	209	ASP
1	B	297	SER
1	C	355	VAL
1	A	59	LEU
1	B	161	GLY
1	B	325	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	410/406 (101%)	385 (94%)	25 (6%)	17	14
1	B	410/406 (101%)	385 (94%)	25 (6%)	17	14
1	C	408/406 (100%)	376 (92%)	32 (8%)	11	8
All	All	1228/1218 (101%)	1146 (93%)	82 (7%)	15	11

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	54	ILE
1	A	69	GLU
1	A	97	ASN
1	A	114	THR
1	A	122	ARG
1	A	156	LEU
1	A	158	LYS
1	A	160	MET
1	A	181	VAL
1	A	226	THR
1	A	285	ASP
1	A	297	SER
1	A	303	CYS
1	A	329	ASN
1	A	331	ASN
1	A	347	SER
1	A	349	THR
1	A	364	ASN
1	A	380	SER
1	A	417	SER
1	A	450	PHE
1	A	460	ASP
1	A	463	PHE
1	A	465	ILE
1	B	15	ASP
1	B	41	VAL
1	B	69	GLU
1	B	158[A]	LYS
1	B	158[B]	LYS
1	B	160	MET

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Mol	Chain	Res	Type
1	B	181	VAL
1	B	195	VAL
1	B	226	THR
1	B	285	ASP
1	B	297	SER
1	B	299	VAL
1	B	301	THR
1	B	303	CYS
1	B	320	ASN
1	B	329	ASN
1	B	349	THR
1	B	372	SER
1	B	380	SER
1	B	382	SER
1	B	417	SER
1	B	450	PHE
1	B	451	LEU
1	B	463	PHE
1	B	465	ILE
1	C	15	ASP
1	C	41	VAL
1	C	54	ILE
1	C	69	GLU
1	C	97	ASN
1	C	114	THR
1	C	117	TYR
1	C	122	ARG
1	C	156	LEU
1	C	158[A]	LYS
1	C	158[B]	LYS
1	C	160	MET
1	C	181	VAL
1	C	195	VAL
1	C	226	THR
1	C	285	ASP
1	C	297	SER
1	C	303	CYS
1	C	327	ASP
1	C	329	ASN
1	C	331	ASN
1	C	349	THR
1	C	382	SER

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Mol	Chain	Res	Type
1	C	388	LEU
1	C	417	SER
1	C	433	VAL
1	C	444	ASP
1	C	450	PHE
1	C	451	LEU
1	C	463	PHE
1	C	465	ILE
1	C	471	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	40	ASN
1	A	44	ASN
1	A	52	GLN
1	A	71	GLN
1	A	92	ASN
1	A	97	ASN
1	A	136	ASN
1	A	180	HIS
1	A	182	ASN
1	A	232	GLN
1	A	265	ASN
1	A	310	HIS
1	A	320	ASN
1	A	364	ASN
1	A	486	ASN
1	B	40	ASN
1	B	44	ASN
1	B	52	GLN
1	B	92	ASN
1	B	97	ASN
1	B	116	GLN
1	B	131	ASN
1	B	136	ASN
1	B	180	HIS
1	B	182	ASN
1	B	252	ASN
1	B	320	ASN
1	B	322	HIS

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Mol	Chain	Res	Type
1	B	358	GLN
1	B	364	ASN
1	B	486	ASN
1	B	495	HIS
1	C	2	GLN
1	C	44	ASN
1	C	52	GLN
1	C	71	GLN
1	C	92	ASN
1	C	131	ASN
1	C	136	ASN
1	C	180	HIS
1	C	232	GLN
1	C	240	GLN
1	C	300	HIS
1	C	310	HIS
1	C	320	ASN
1	C	329	ASN
1	C	340	ASN
1	C	358	GLN
1	C	486	ASN
1	C	495	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	D	1	1,2	14,14,15	0.64	0	17,19,21	1.28	2 (11%)
2	NAG	D	2	2	14,14,15	0.63	0	17,19,21	1.27	2 (11%)
2	NAG	E	1	2	14,14,15	0.57	0	17,19,21	0.99	0
2	NAG	E	2	2	14,14,15	0.71	0	17,19,21	3.46	6 (35%)
2	NAG	F	1	2	14,14,15	0.60	0	17,19,21	1.03	0
2	NAG	F	2	2	14,14,15	0.43	0	17,19,21	1.80	4 (23%)
2	NAG	G	1	1,2	14,14,15	0.71	0	17,19,21	2.56	5 (29%)
2	NAG	G	2	2	14,14,15	0.65	0	17,19,21	2.00	3 (17%)
2	NAG	H	1	2	14,14,15	0.55	0	17,19,21	1.50	5 (29%)
2	NAG	H	2	2	14,14,15	0.62	0	17,19,21	1.00	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
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	5/6/23/26	0/1/1/1
2	NAG	F	1	2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	NAG	H	1	2	-	5/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C4-C3-C2	-9.38	97.27	111.02
2	E	2	NAG	O5-C1-C2	-6.62	101.05	111.29
2	G	1	NAG	C4-C3-C2	-6.39	101.66	111.02
2	G	1	NAG	C2-N2-C7	5.93	130.84	122.90
2	G	2	NAG	O5-C1-C2	-5.60	102.62	111.29
2	E	2	NAG	C1-C2-N2	4.56	117.61	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C1-O5-C5	4.48	118.19	112.19
2	G	2	NAG	C3-C4-C5	4.30	118.03	110.23
2	F	2	NAG	C1-O5-C5	4.01	117.56	112.19
2	G	1	NAG	O5-C1-C2	-3.84	105.34	111.29
2	F	2	NAG	C2-N2-C7	-3.54	118.15	122.90
2	F	2	NAG	C6-C5-C4	-3.38	104.72	113.02
2	D	1	NAG	C1-O5-C5	3.24	116.53	112.19
2	H	1	NAG	C4-C3-C2	3.24	115.77	111.02
2	E	2	NAG	O5-C5-C4	3.19	118.60	110.83
2	G	2	NAG	C4-C3-C2	3.04	115.47	111.02
2	D	2	NAG	C1-O5-C5	2.83	115.97	112.19
2	G	1	NAG	O7-C7-N2	-2.65	117.30	121.98
2	D	2	NAG	C2-N2-C7	-2.58	119.44	122.90
2	G	1	NAG	C8-C7-N2	2.46	120.19	116.12
2	E	2	NAG	C2-N2-C7	2.43	126.15	122.90
2	D	1	NAG	O3-C3-C2	-2.26	104.71	109.40
2	H	1	NAG	O5-C1-C2	-2.25	107.81	111.29
2	F	2	NAG	C1-C2-N2	2.20	113.90	110.43
2	H	2	NAG	C3-C4-C5	-2.13	106.37	110.23
2	H	1	NAG	O3-C3-C4	-2.13	105.35	110.38
2	H	1	NAG	C6-C5-C4	-2.05	107.98	113.02
2	H	1	NAG	C2-N2-C7	-2.05	120.15	122.90

There are no chirality outliers.

All (25) torsion outliers are listed below:

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

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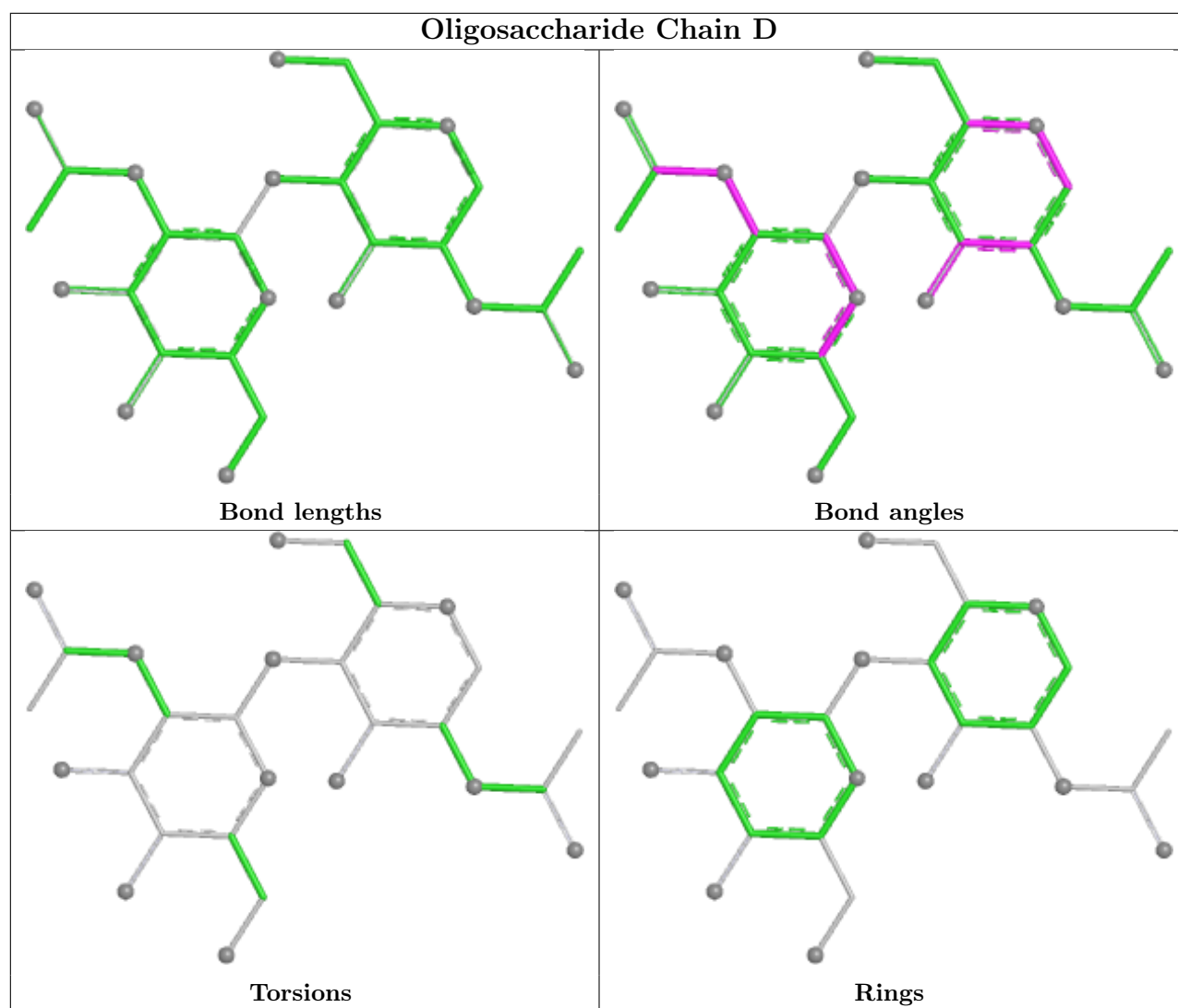
Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	H	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C3-C2-N2-C7
2	H	1	NAG	O5-C5-C6-O6

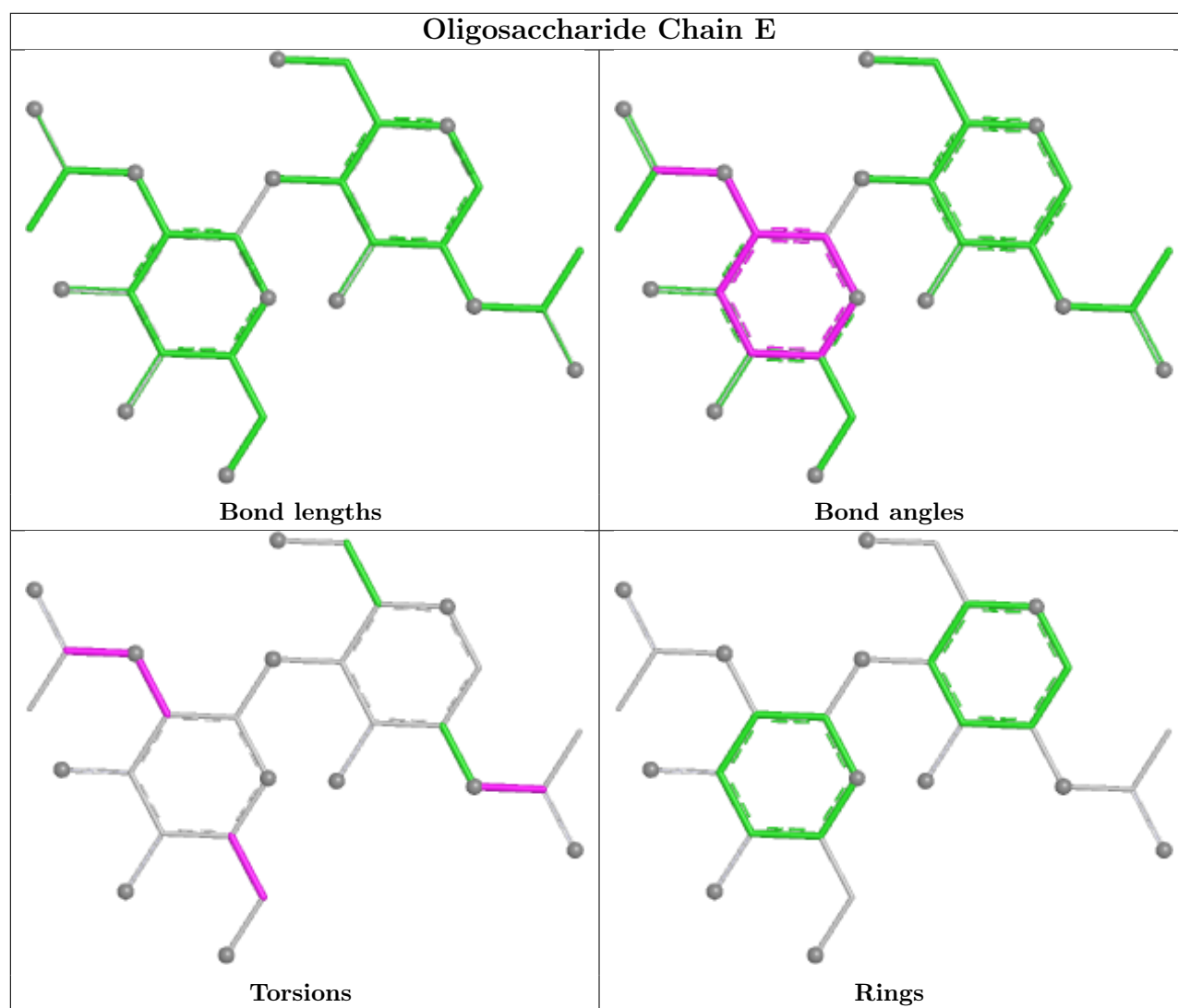
There are no ring outliers.

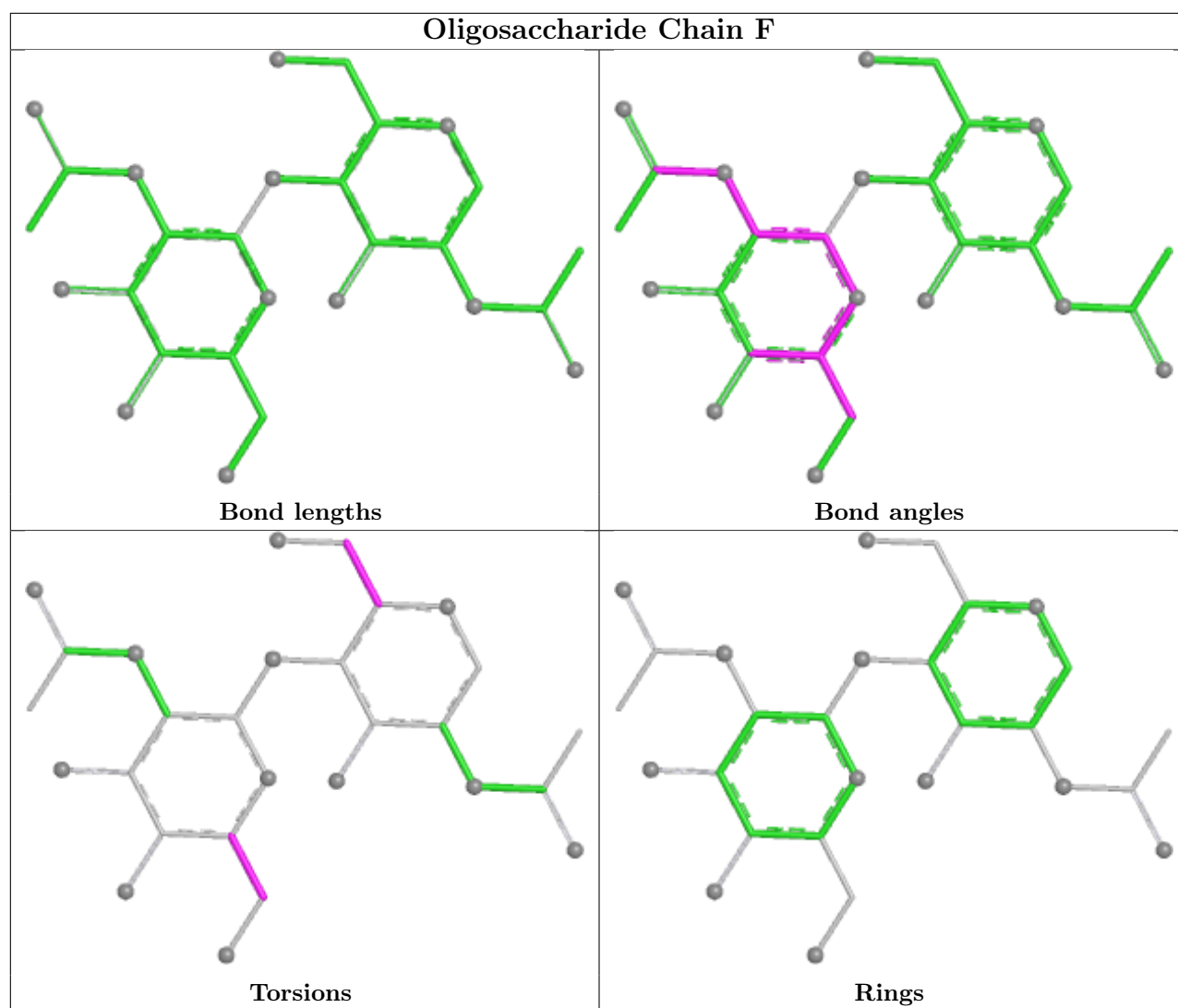
4 monomers are involved in 17 short contacts:

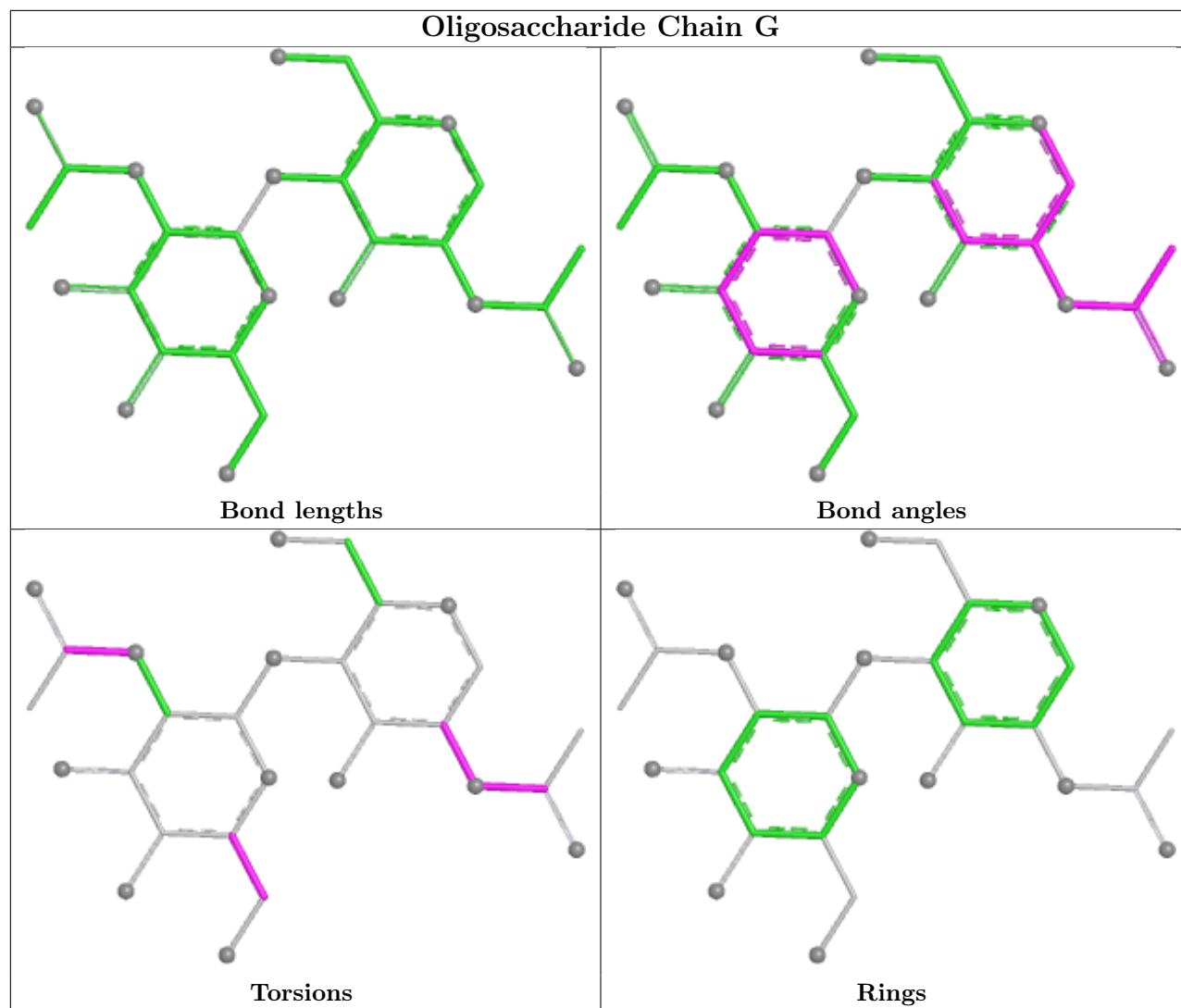
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAG	4	0
2	H	1	NAG	7	0
2	E	1	NAG	4	0
2	G	1	NAG	2	0

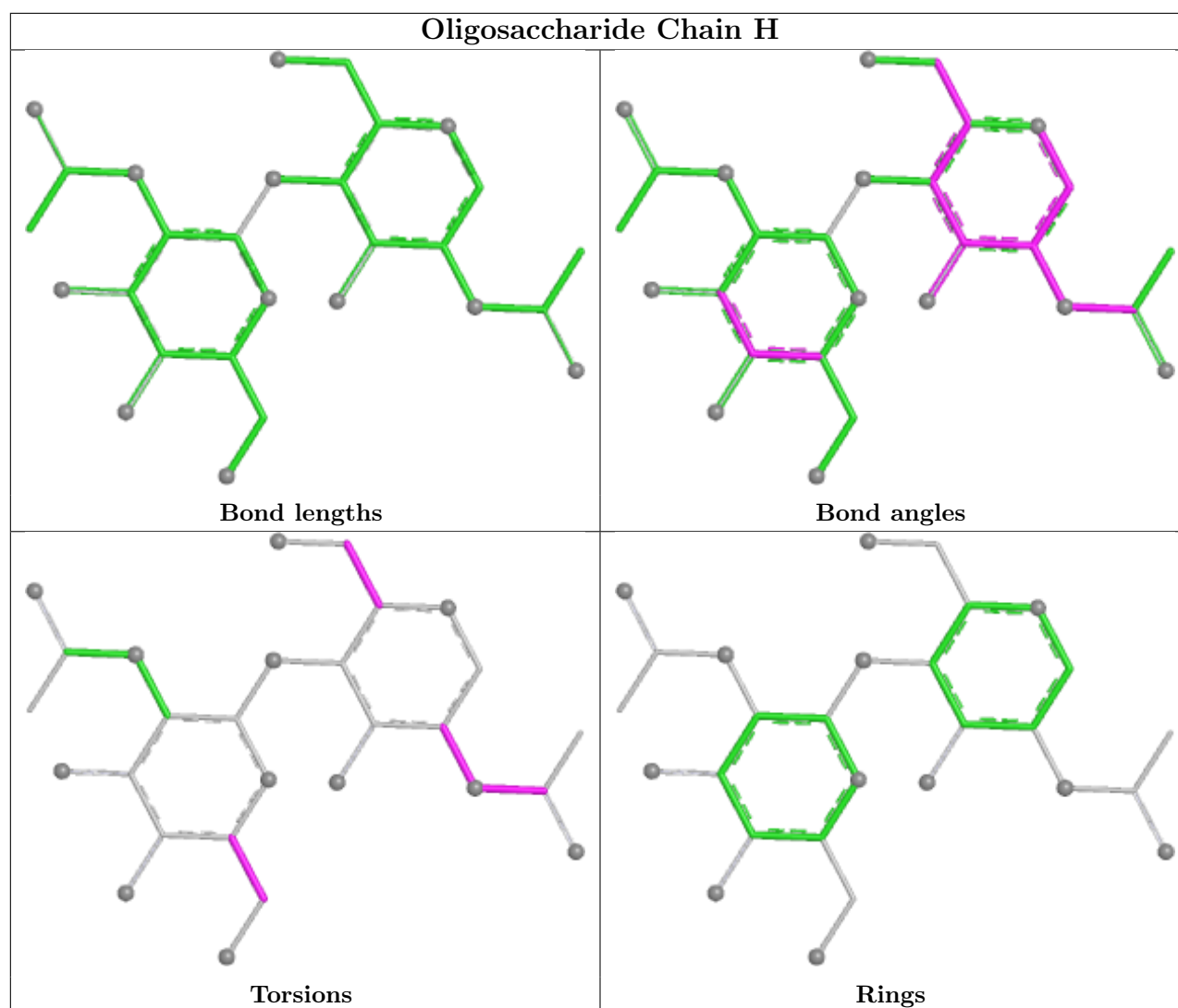
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 12 are monoatomic - leaving 16 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	$\# Z > 2$
4	SO4	B	505	-	4,4,4	0.44	0	6,6,6	0.74	0
4	SO4	A	507	-	4,4,4	0.67	0	6,6,6	0.81	0
5	GOL	B	510	-	5,5,5	0.49	0	5,5,5	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	B	506	-	5,5,5	0.78	0	5,5,5	1.95	3 (60%)
5	GOL	B	508	-	5,5,5	0.19	0	5,5,5	0.64	0
5	GOL	B	509	-	5,5,5	0.89	0	5,5,5	1.41	1 (20%)
4	SO4	A	505	-	4,4,4	0.49	0	6,6,6	0.75	0
4	SO4	C	506	-	4,4,4	0.31	0	6,6,6	0.36	0
5	GOL	C	507	-	5,5,5	0.34	0	5,5,5	1.58	1 (20%)
4	SO4	A	508	-	4,4,4	0.21	0	6,6,6	0.61	0
4	SO4	C	505	-	4,4,4	0.31	0	6,6,6	0.64	0
5	GOL	C	508	-	5,5,5	0.49	0	5,5,5	1.68	1 (20%)
5	GOL	A	509	-	5,5,5	0.48	0	5,5,5	0.69	0
5	GOL	B	507	-	5,5,5	0.73	0	5,5,5	0.96	0
4	SO4	A	506	-	4,4,4	0.36	0	6,6,6	0.55	0
6	NAG	C	510	1	14,14,15	2.30	2 (14%)	17,19,21	2.24	4 (23%)

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
5	GOL	B	510	-	-	0/4/4/4	-
5	GOL	B	509	-	-	0/4/4/4	-
5	GOL	B	508	-	-	2/4/4/4	-
5	GOL	B	506	-	-	3/4/4/4	-
5	GOL	C	507	-	-	4/4/4/4	-
5	GOL	C	508	-	-	1/4/4/4	-
5	GOL	B	507	-	-	3/4/4/4	-
5	GOL	A	509	-	-	4/4/4/4	-
6	NAG	C	510	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)
6	C	510	NAG	O7-C7	7.90	1.40	1.23
6	C	510	NAG	C7-N2	2.53	1.42	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	510	NAG	C1-O5-C5	6.55	120.96	112.19
6	C	510	NAG	C3-C4-C5	-3.58	103.73	110.23
6	C	510	NAG	C2-N2-C7	3.32	127.34	122.90
5	C	508	GOL	C3-C2-C1	-3.07	100.54	111.80
5	C	507	GOL	O1-C1-C2	-3.03	96.73	110.38
5	B	509	GOL	O2-C2-C1	2.72	120.44	109.18
5	B	506	GOL	O1-C1-C2	2.45	121.41	110.38
5	B	506	GOL	O2-C2-C3	2.37	119.01	109.18
6	C	510	NAG	C6-C5-C4	-2.06	107.97	113.02
5	B	506	GOL	O2-C2-C1	2.01	117.49	109.18

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	509	GOL	O1-C1-C2-C3
5	A	509	GOL	C1-C2-C3-O3
5	B	507	GOL	O1-C1-C2-C3
5	C	507	GOL	O1-C1-C2-C3
5	A	509	GOL	O1-C1-C2-O2
5	C	507	GOL	O1-C1-C2-O2
6	C	510	NAG	O5-C5-C6-O6
5	B	506	GOL	O1-C1-C2-C3
5	B	508	GOL	C1-C2-C3-O3
5	C	507	GOL	C1-C2-C3-O3
5	A	509	GOL	O2-C2-C3-O3
5	B	506	GOL	O2-C2-C3-O3
5	B	507	GOL	O1-C1-C2-O2
5	C	507	GOL	O2-C2-C3-O3
5	B	507	GOL	O2-C2-C3-O3
5	B	508	GOL	O2-C2-C3-O3
5	C	508	GOL	O2-C2-C3-O3
6	C	510	NAG	C4-C5-C6-O6
5	B	506	GOL	C1-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	510	GOL	2	0
5	B	506	GOL	6	0
4	C	506	SO4	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	507	GOL	12	0
4	C	505	SO4	4	0
5	A	509	GOL	4	0
5	B	507	GOL	1	0

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	495/495 (100%)	-0.49	10 (2%) 65 64	9, 19, 33, 46	5 (1%)
1	B	495/495 (100%)	-0.19	14 (2%) 55 54	9, 23, 45, 56	5 (1%)
1	C	495/495 (100%)	0.03	24 (4%) 35 34	11, 26, 47, 62	3 (0%)
All	All	1485/1485 (100%)	-0.21	48 (3%) 50 49	9, 23, 43, 62	13 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	415	SER	5.1
1	C	161	GLY	4.6
1	C	363	ALA	4.5
1	C	323	GLN	4.0
1	B	328	CYS	3.7
1	B	162	ALA	3.7
1	C	208	CYS	3.6
1	C	372	SER	3.6
1	C	164	GLY	3.5
1	C	324	GLY	3.4
1	A	161	GLY	3.3
1	B	415	SER	3.3
1	B	161	GLY	3.2
1	C	367	ALA	3.0
1	C	328	CYS	2.8
1	C	325	GLY	2.8
1	B	442	CYS	2.7
1	A	162	ALA	2.7
1	C	369	LEU	2.7
1	A	43	ASP	2.6
1	C	326	ALA	2.6
1	A	415	SER	2.6
1	A	394	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	393	ALA	2.5
1	C	362	GLY	2.5
1	B	323	GLN	2.5
1	C	490	SER	2.4
1	B	367	ALA	2.4
1	B	393	ALA	2.4
1	B	331	ASN	2.4
1	C	366	ALA	2.4
1	A	331	ASN	2.3
1	A	303	CYS	2.3
1	C	477	ALA	2.3
1	A	420	ASP	2.3
1	C	380	SER	2.3
1	B	490	SER	2.3
1	C	376	ILE	2.2
1	B	136	ASN	2.2
1	A	170	SER	2.2
1	B	322	HIS	2.1
1	C	433	VAL	2.1
1	A	329	ASN	2.1
1	C	420	ASP	2.1
1	B	163	GLY	2.1
1	B	320	ASN	2.0
1	C	319	GLY	2.0
1	C	364	ASN	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 ⓘ

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

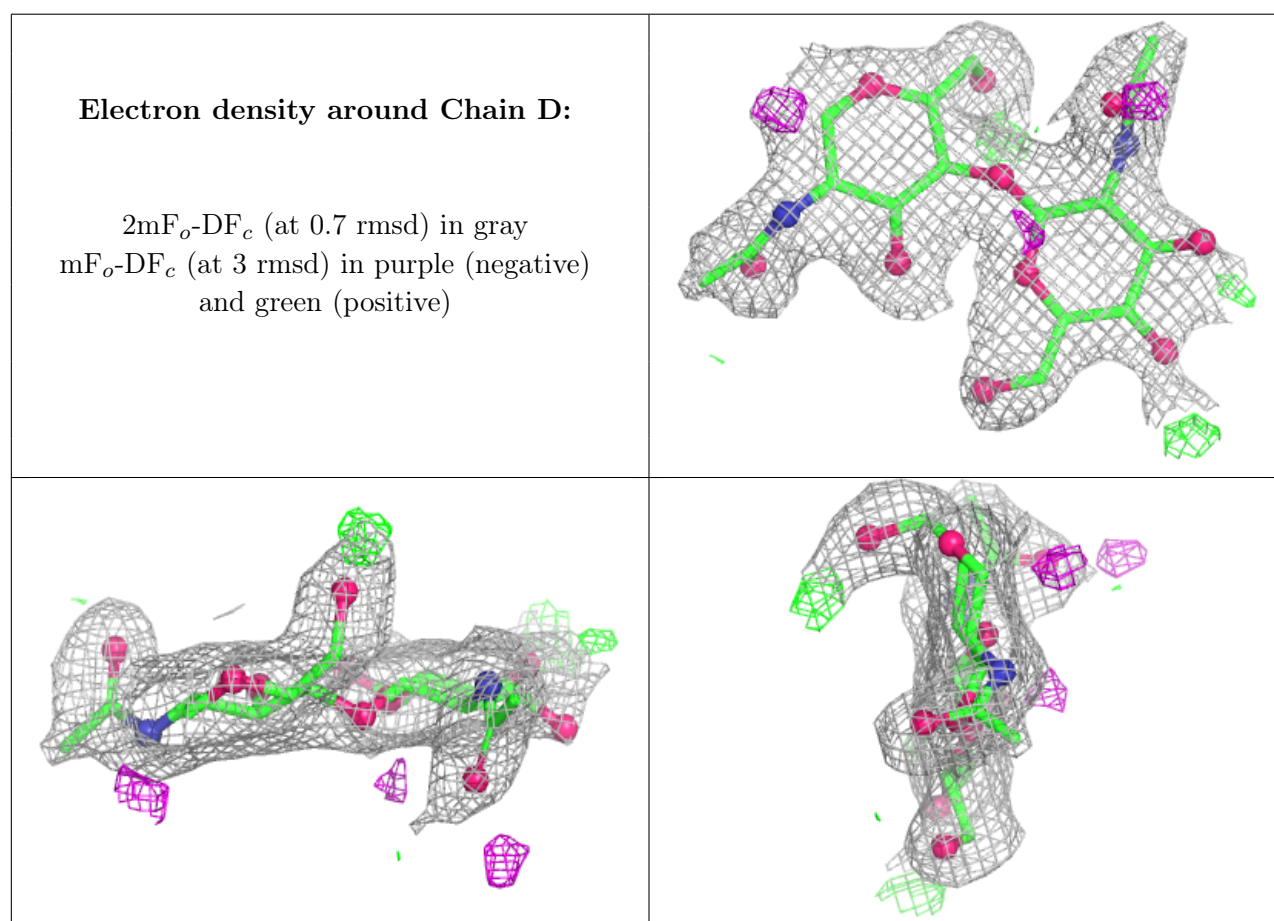
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	G	2	14/15	0.63	0.17	63,77,91,95	0
2	NAG	F	2	14/15	0.66	0.17	61,66,72,73	0
2	NAG	E	2	14/15	0.66	0.16	47,54,58,61	0

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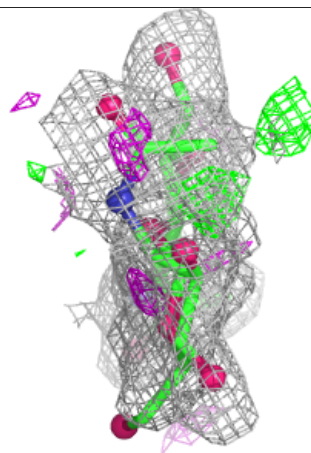
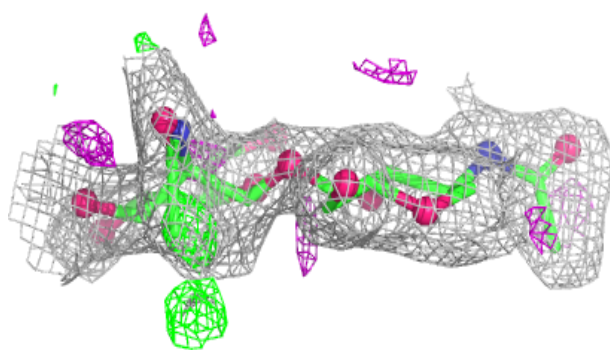
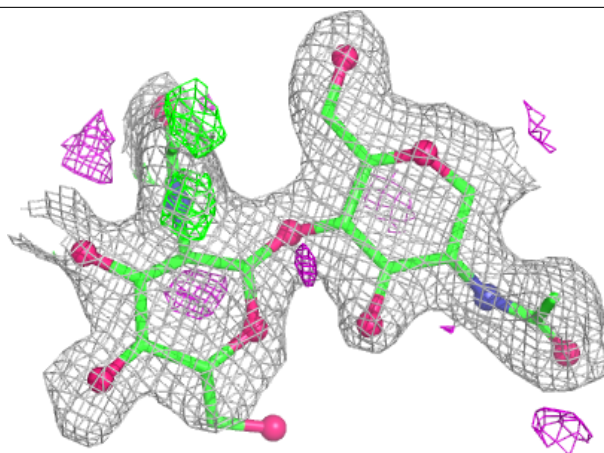
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	H	2	14/15	0.75	0.14	60,68,72,75	0
2	NAG	H	1	14/15	0.77	0.16	66,68,72,85	0
2	NAG	D	2	14/15	0.78	0.12	47,52,58,60	0
2	NAG	F	1	14/15	0.78	0.14	48,59,63,64	0
2	NAG	G	1	14/15	0.79	0.13	45,56,61,68	0
2	NAG	E	1	14/15	0.89	0.09	28,36,42,45	0
2	NAG	D	1	14/15	0.94	0.08	29,33,37,42	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.



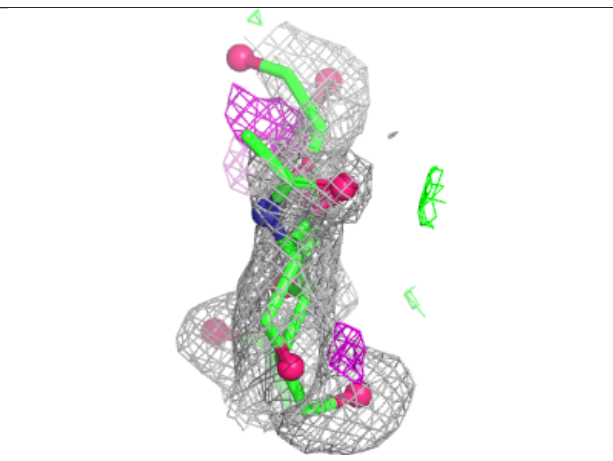
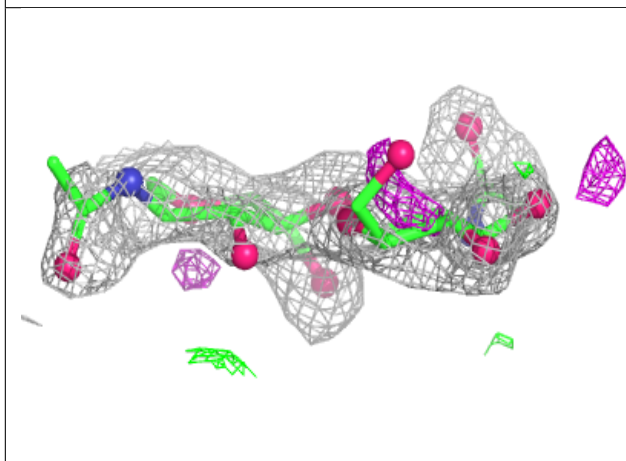
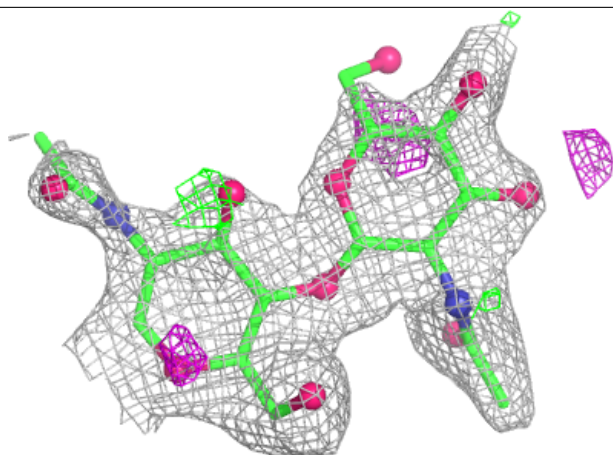
Electron density around Chain E:

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



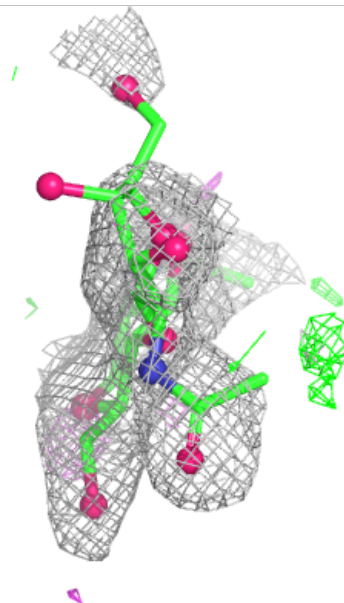
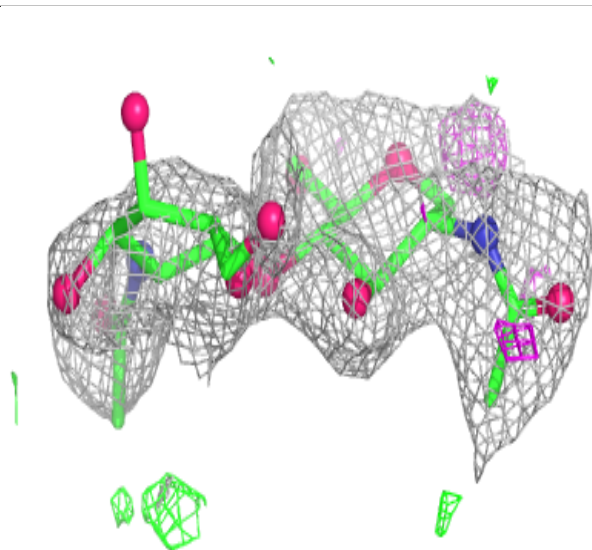
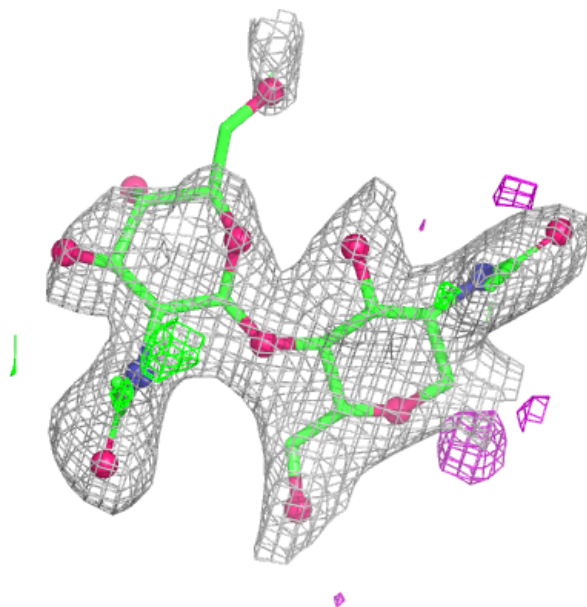
Electron density around Chain F:

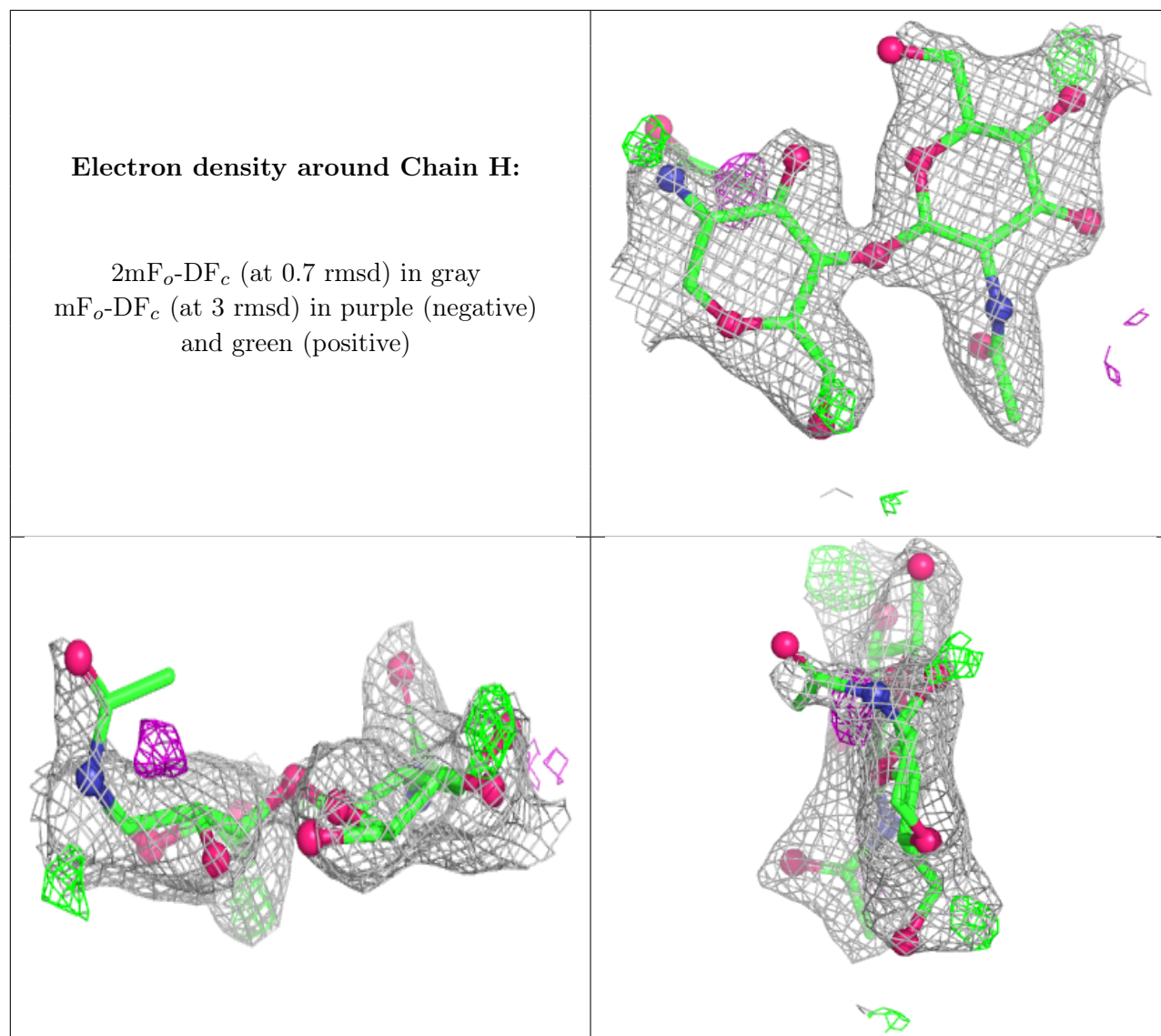
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

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





6.4 Ligands [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	SO4	C	506	5/5	0.54	0.23	46,47,49,49	5
6	NAG	C	510	14/15	0.80	0.14	54,60,62,62	0
5	GOL	A	509	6/6	0.82	0.17	32,48,50,53	0
5	GOL	B	509	6/6	0.85	0.12	20,26,32,40	0
4	SO4	B	505	5/5	0.85	0.14	29,31,32,33	5
5	GOL	C	508	6/6	0.86	0.12	34,38,41,46	0
5	GOL	B	506	6/6	0.88	0.13	22,32,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	B	508	6/6	0.90	0.12	46,52,53,55	0
4	SO4	A	506	5/5	0.91	0.11	60,60,61,61	0
5	GOL	C	507	6/6	0.94	0.15	26,34,41,47	0
4	SO4	A	508	5/5	0.95	0.14	19,22,23,26	5
5	GOL	B	507	6/6	0.95	0.07	23,30,34,35	0
5	GOL	B	510	6/6	0.95	0.08	23,28,30,30	0
4	SO4	A	505	5/5	0.97	0.10	31,36,40,41	0
3	CU	C	503	1/1	0.99	0.03	26,26,26,26	0
4	SO4	C	505	5/5	0.99	0.05	21,26,28,29	0
4	SO4	A	507	5/5	0.99	0.05	19,22,26,28	0
3	CU	C	501	1/1	0.99	0.04	31,31,31,31	0
3	CU	A	501	1/1	1.00	0.01	19,19,19,19	0
3	CU	C	502	1/1	1.00	0.02	22,22,22,22	0
3	CU	A	502	1/1	1.00	0.01	15,15,15,15	0
3	CU	C	504	1/1	1.00	0.05	28,28,28,28	0
3	CU	A	503	1/1	1.00	0.01	19,19,19,19	0
3	CU	A	504	1/1	1.00	0.02	18,18,18,18	0
3	CU	B	501	1/1	1.00	0.02	20,20,20,20	0
3	CU	B	502	1/1	1.00	0.01	19,19,19,19	0
3	CU	B	503	1/1	1.00	0.01	23,23,23,23	0
3	CU	B	504	1/1	1.00	0.03	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.