



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 03:42 AM EDT

PDB ID : 8XYE / pdb_00008xye
Title : Crystal structure of SARS-CoV-2 BA.4 RBD and human ACE2
Authors : Lan, J.; Wang, C.H.
Deposited on : 2024-01-19
Resolution : 3.32 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

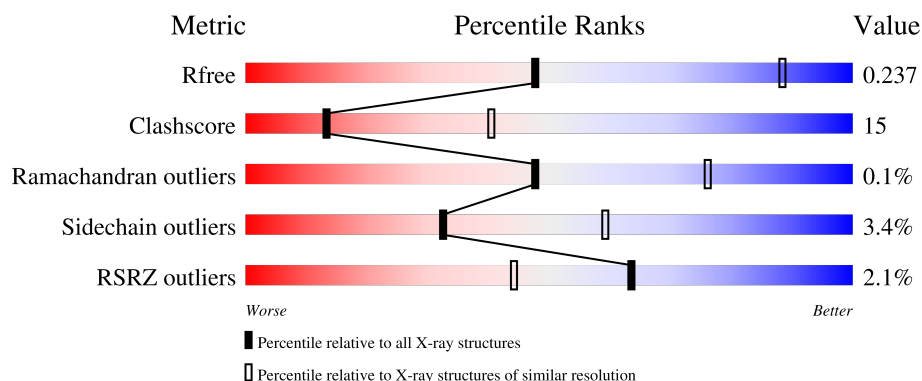
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 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.



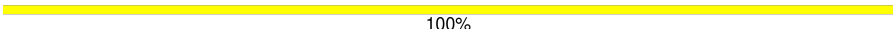
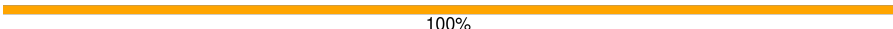
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

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	598	6% 76% 21% .
1	B	598	72% 27% .
2	C	194	6% 46% 49% 5%
2	D	194	6% 54% 42% ..
3	E	3	33% 67%

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Mol	Chain	Length	Quality of chain
3	F	3	 33% 67%
3	G	3	 100%
4	H	2	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13101 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 Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	598	Total	C	N	O	S	0	1	0
			4884	3125	809	921	29			
1	A	597	Total	C	N	O	S	0	1	0
			4876	3121	808	918	29			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	17	ASP	-	expression tag	UNP Q9BYF1
B	18	PRO	-	expression tag	UNP Q9BYF1
A	17	ASP	-	expression tag	UNP Q9BYF1
A	18	PRO	-	expression tag	UNP Q9BYF1

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	194	Total	C	N	O	S	0	0	0
			1549	997	262	282	8			
2	D	194	Total	C	N	O	S	0	0	0
			1549	997	262	282	8			

There are 32 discrepancies between the modelled and reference sequences:

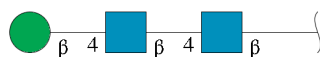
Chain	Residue	Modelled	Actual	Comment	Reference
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	452	ARG	LEU	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	VAL	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
D	339	ASP	GLY	variant	UNP P0DTC2
D	371	PHE	SER	variant	UNP P0DTC2
D	373	PRO	SER	variant	UNP P0DTC2
D	375	PHE	SER	variant	UNP P0DTC2
D	405	ASN	ASP	variant	UNP P0DTC2
D	408	SER	ARG	variant	UNP P0DTC2
D	417	ASN	LYS	variant	UNP P0DTC2
D	440	LYS	ASN	variant	UNP P0DTC2
D	452	ARG	LEU	variant	UNP P0DTC2
D	477	ASN	SER	variant	UNP P0DTC2
D	478	LYS	THR	variant	UNP P0DTC2
D	484	ALA	GLU	variant	UNP P0DTC2
D	486	VAL	PHE	variant	UNP P0DTC2
D	498	ARG	GLN	variant	UNP P0DTC2
D	501	TYR	ASN	variant	UNP P0DTC2
D	505	HIS	TYR	variant	UNP P0DTC2

- Molecule 3 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.



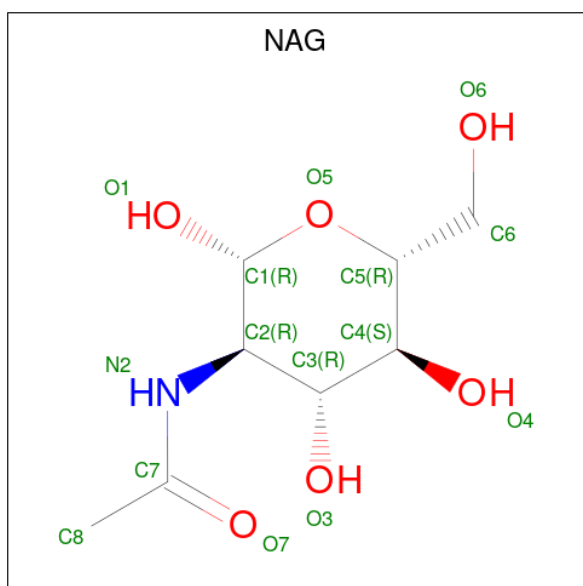
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 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
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

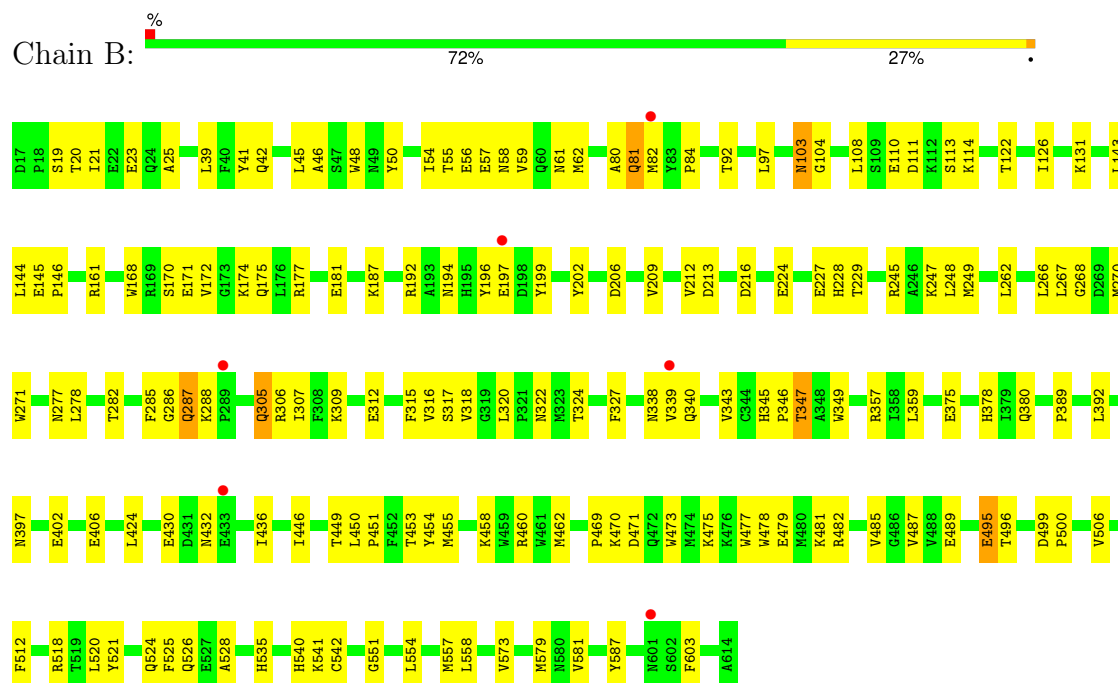


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

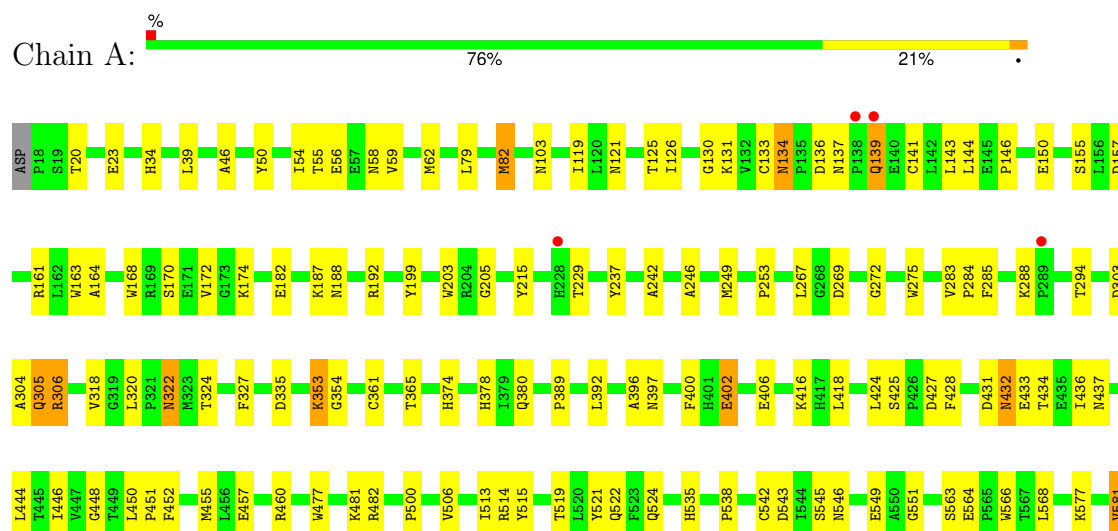
3 Residue-property plots

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: Processed angiotensin-converting enzyme 2

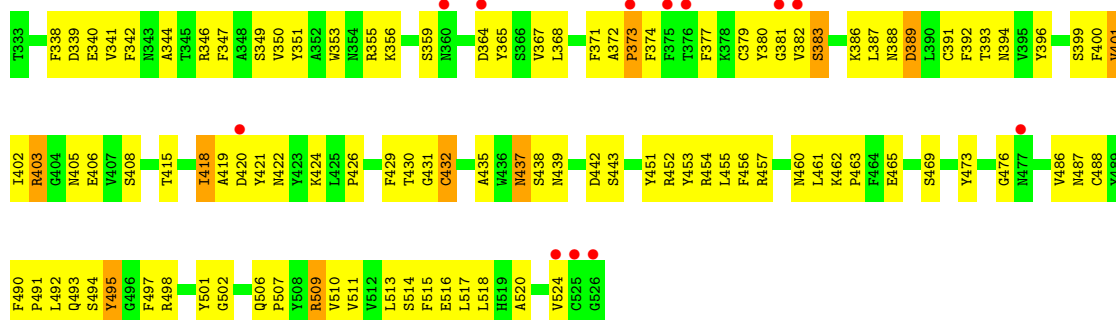


• Molecule 1: Processed angiotensin-converting enzyme 2

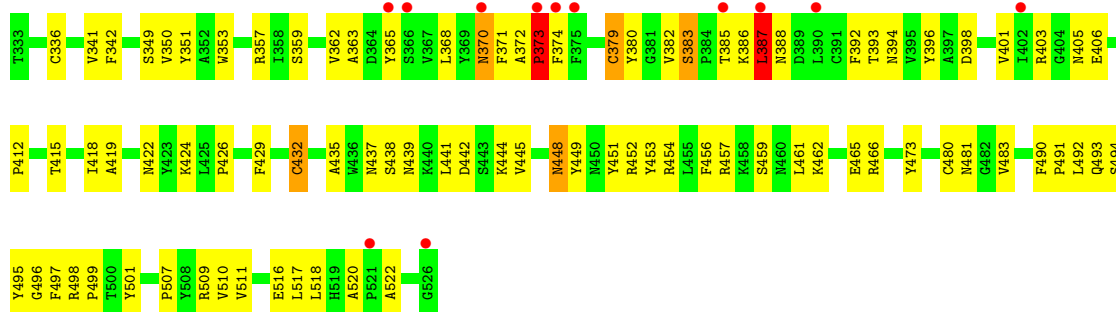




- Molecule 2: Spike protein S1



- Molecule 2: Spike protein S1



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



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

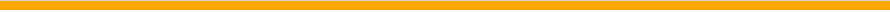


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

MAG1
MAG2
BGA3

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

Chain H:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.47Å 165.82Å 98.98Å 90.00° 102.18° 90.00°	Depositor
Resolution (Å)	31.37 – 3.32 31.37 – 3.32	Depositor EDS
% Data completeness (in resolution range)	98.3 (31.37-3.32) 98.2 (31.37-3.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.31Å)	Xtriage
Refinement program	PHENIX (1.19.1_4122: ???)	Depositor
R, R_{free}	0.191 , 0.242 0.197 , 0.237	Depositor DCC
R_{free} test set	1942 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	78.4	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13101	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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: BMA, NAG

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	0.60	0/5018	0.89	5/6818 (0.1%)
1	B	0.58	0/5026	0.86	4/6830 (0.1%)
2	C	0.72	0/1595	1.10	5/2171 (0.2%)
2	D	0.64	0/1595	0.99	2/2171 (0.1%)
All	All	0.61	0/13234	0.92	16/17990 (0.1%)

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
2	C	0	1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	353	TRP	CA-C-N	-8.16	109.10	122.81
2	C	353	TRP	C-N-CA	-8.16	109.10	122.81
2	C	373	PRO	N-CA-C	-7.88	96.24	112.47
1	B	496	THR	N-CA-C	-7.59	104.00	113.18
2	D	373	PRO	N-CA-CB	-6.42	96.51	103.25
1	A	306	ARG	CA-C-N	-5.75	113.32	120.56
1	A	306	ARG	C-N-CA	-5.75	113.32	120.56
2	D	387	LEU	N-CA-C	-5.46	106.69	113.19
1	B	194	ASN	N-CA-C	-5.40	106.89	112.93
1	B	202	TYR	CA-CB-CG	5.37	123.56	113.90
2	C	509	ARG	CB-CG-CD	5.28	123.43	111.30
1	A	402	GLU	CG-CD-OE2	5.24	130.44	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	GLN	N-CA-C	-5.17	107.00	113.15
1	A	432	ASN	CB-CA-C	-5.12	102.35	110.84
2	C	346	ARG	CG-CD-NE	-5.06	100.86	112.00
1	A	285	PHE	CB-CA-C	5.02	119.27	112.09

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	495	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	4876	0	4649	99	0
1	B	4884	0	4650	104	0
2	C	1549	0	1472	99	0
2	D	1549	0	1472	77	0
3	E	39	0	34	0	0
3	F	39	0	34	3	0
3	G	39	0	34	0	0
4	H	28	0	25	1	0
5	A	42	0	39	1	0
5	B	56	0	52	0	0
All	All	13101	0	12461	378	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (378) 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)
2:D:453:TYR:CD2	2:D:495:TYR:HE1	1.85	0.95
1:A:378:HIS:NE2	1:A:402:GLU:OE2	2.02	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:393:THR:HG21	2:C:518:LEU:HD23	1.53	0.89
2:D:442:ASP:OD1	2:D:451:TYR:OH	1.93	0.86
2:D:453:TYR:CD2	2:D:495:TYR:CE1	2.65	0.85
2:C:340:GLU:O	2:C:344:ALA:HB2	1.81	0.81
2:D:495:TYR:HD2	2:D:497:PHE:CZ	1.98	0.81
2:C:453:TYR:CD2	2:C:495:TYR:HE1	2.00	0.79
2:C:453:TYR:HD2	2:C:495:TYR:CE1	2.02	0.77
2:C:453:TYR:CD2	2:C:495:TYR:CE1	2.72	0.77
1:A:134:ASN:HD21	1:A:137:ASN:HB3	1.51	0.75
2:C:392:PHE:HD1	2:C:517:LEU:HB2	1.50	0.75
2:C:495:TYR:HD2	2:C:497:PHE:CZ	2.04	0.74
2:D:349:SER:HB2	2:D:452:ARG:H	1.54	0.73
2:D:359:SER:OG	2:D:394:ASN:OD1	2.07	0.71
1:A:374:HIS:HE2	1:A:402:GLU:CD	1.98	0.71
1:A:134:ASN:ND2	1:A:137:ASN:HB3	2.06	0.71
2:C:342:PHE:HE1	2:C:511:VAL:HG11	1.56	0.69
1:B:57:GLU:O	1:B:61:ASN:ND2	2.24	0.69
2:D:365:TYR:CD1	2:D:387:LEU:HD12	2.28	0.69
1:A:524:GLN:HG2	1:A:583:PRO:HG2	1.74	0.68
2:C:420:ASP:HB2	2:C:460:ASN:OD1	1.93	0.67
2:C:419:ALA:O	2:C:424:LYS:HB2	1.95	0.67
2:C:371:PHE:C	2:C:373:PRO:HD3	2.20	0.67
1:B:224:GLU:HB3	1:B:228[A]:HIS:CE1	2.30	0.66
2:C:365:TYR:HE1	2:C:388:ASN:HA	1.60	0.66
1:B:168:TRP:CZ3	1:B:172:VAL:HG21	2.30	0.66
1:A:187:LYS:HD2	1:A:199:TYR:CZ	2.30	0.66
1:B:21:ILE:HG21	1:B:84:PRO:HD2	1.78	0.66
1:A:131:LYS:HB3	1:A:143:LEU:HD23	1.78	0.66
2:D:422:ASN:HD21	2:D:453:TYR:HB2	1.59	0.65
1:B:50:TYR:CE1	1:B:54:ILE:HG23	2.32	0.65
2:C:381:GLY:HA3	2:C:430:THR:HA	1.78	0.65
1:B:20:THR:N	1:B:23:GLU:OE1	2.22	0.65
2:C:365:TYR:CE1	2:C:387:LEU:HG	2.32	0.64
2:D:448:ASN:HD21	2:D:451:TYR:HD1	1.42	0.64
1:B:458:LYS:HG2	1:B:462:MET:HE2	1.80	0.64
2:C:453:TYR:HD2	2:C:495:TYR:HE1	1.40	0.64
3:F:2:NAG:H4	3:F:3:BMA:O2	1.97	0.63
1:B:131:LYS:HB3	1:B:143:LEU:HD23	1.79	0.63
2:C:453:TYR:CE1	2:C:493:GLN:HB3	2.32	0.63
2:D:453:TYR:CE1	2:D:493:GLN:HB3	2.33	0.63
2:C:365:TYR:CD1	2:C:387:LEU:HG	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:426:PRO:HD2	2:C:429:PHE:HD1	1.63	0.62
2:D:373:PRO:HD2	2:D:374:PHE:CD2	2.34	0.62
1:B:50:TYR:CE1	1:B:59:VAL:HG22	2.35	0.62
2:C:401:VAL:HG11	2:C:451:TYR:CD2	2.34	0.62
1:B:268:GLY:O	1:B:277:ASN:ND2	2.29	0.62
1:B:406:GLU:HG3	1:B:518:ARG:HH11	1.65	0.62
2:D:452:ARG:HG2	2:D:494:SER:HB3	1.80	0.62
1:A:564:GLU:HB3	1:A:568:LEU:HD23	1.82	0.62
2:C:456:PHE:HB3	2:C:473:TYR:CD2	2.35	0.61
2:C:435:ALA:HB2	2:C:510:VAL:HG12	1.81	0.61
2:C:377:PHE:HE1	2:C:432:CYS:SG	2.24	0.61
1:A:460:ARG:HH21	1:A:506:VAL:HA	1.66	0.61
2:C:392:PHE:CD1	2:C:517:LEU:HB2	2.34	0.60
2:D:456:PHE:HB3	2:D:473:TYR:CD2	2.36	0.60
2:C:403:ARG:HH21	2:C:405:ASN:CG	2.09	0.60
2:D:418:ILE:HG13	2:D:422:ASN:HD22	1.67	0.60
1:B:320:LEU:HD13	1:B:380:GLN:HG2	1.83	0.60
1:B:458:LYS:HZ2	1:B:462:MET:HE2	1.65	0.60
2:C:421:TYR:CD1	2:C:457:ARG:HB3	2.37	0.59
2:D:453:TYR:HD2	2:D:495:TYR:CE1	2.15	0.59
1:A:396:ALA:HB1	1:A:566:TRP:HA	1.85	0.59
2:D:383:SER:O	2:D:387:LEU:HD23	2.02	0.59
1:A:121:ASN:O	1:A:125:THR:HG23	2.03	0.59
1:A:374:HIS:CE1	1:A:402:GLU:OE1	2.55	0.59
1:B:111:ASP:HA	1:B:114:LYS:HE3	1.83	0.58
1:A:229:THR:HB	1:A:581:VAL:HG13	1.85	0.58
2:D:368:LEU:HA	2:D:371:PHE:CD1	2.38	0.58
1:A:50:TYR:HE1	1:A:54:ILE:HG23	1.69	0.58
1:B:287:GLN:HE21	1:B:287:GLN:HA	1.67	0.58
1:B:247:LYS:HB2	1:B:282:THR:HG22	1.86	0.58
2:C:502:GLY:O	2:C:506:GLN:HG3	2.04	0.58
2:C:368:LEU:HA	2:C:371:PHE:CE1	2.40	0.57
1:B:312:GLU:OE2	1:B:322:ASN:HB2	2.04	0.57
2:D:415:THR:O	2:D:415:THR:OG1	2.22	0.57
2:C:387:LEU:HD11	2:C:515:PHE:CZ	2.41	0.56
1:A:549:GLU:H	1:A:549:GLU:CD	2.13	0.56
1:B:177:ARG:HH22	1:B:495:GLU:HG3	1.70	0.56
1:A:170:SER:O	1:A:174:LYS:HD2	2.06	0.56
1:B:187:LYS:HD2	1:B:199:TYR:CZ	2.41	0.56
1:B:229:THR:HB	1:B:581:VAL:HG13	1.88	0.56
2:C:437:ASN:HD22	2:C:439:ASN:H	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:372:ALA:N	2:D:373:PRO:HD3	2.21	0.55
2:D:349:SER:CB	2:D:452:ARG:H	2.19	0.55
2:D:435:ALA:HB2	2:D:510:VAL:HG12	1.89	0.55
1:A:137:ASN:OD1	1:A:139:GLN:HB2	2.07	0.55
1:B:482:ARG:HH21	1:B:489:GLU:CD	2.15	0.55
1:A:50:TYR:CE1	1:A:54:ILE:HG23	2.42	0.55
1:A:133:CYS:HA	1:A:141:CYS:HA	1.89	0.55
2:C:443:SER:HB3	2:C:507:PRO:HG3	1.89	0.54
2:D:415:THR:HG22	2:D:424:LYS:NZ	2.21	0.54
1:A:389:PRO:HG2	1:A:392:LEU:HD12	1.89	0.54
1:A:581:VAL:O	1:A:582:ARG:C	2.50	0.54
1:B:55:THR:O	1:B:56:GLU:C	2.49	0.54
2:C:438:SER:OG	2:C:507:PRO:HB2	2.08	0.54
2:C:372:ALA:C	2:C:374:PHE:H	2.16	0.54
1:A:168:TRP:CZ3	1:A:172:VAL:HG21	2.42	0.54
1:A:374:HIS:NE2	1:A:402:GLU:OE1	2.41	0.54
1:B:55:THR:O	1:B:58:ASN:N	2.40	0.54
2:C:396:TYR:HB2	2:C:514:SER:HB3	1.89	0.54
2:D:380:TYR:CD2	2:D:412:PRO:HD3	2.43	0.54
1:B:245:ARG:NH2	1:B:603:PHE:O	2.41	0.54
1:B:285:PHE:HE2	1:B:436:ILE:HB	1.73	0.54
1:B:81:GLN:HB3	3:F:2:NAG:H81	1.90	0.53
2:C:442:ASP:OD1	2:C:451:TYR:OH	2.25	0.53
2:C:393:THR:HG22	2:C:517:LEU:HA	1.89	0.53
1:B:469:PRO:HB2	1:B:471:ASP:OD1	2.08	0.53
2:C:359:SER:OG	2:C:394:ASN:OD1	2.22	0.53
2:D:350:VAL:HG11	2:D:418:ILE:HD11	1.89	0.53
2:D:351:TYR:CZ	2:D:492:LEU:HD21	2.43	0.53
2:D:392:PHE:HA	2:D:517:LEU:HD13	1.91	0.53
2:D:349:SER:HB3	2:D:451:TYR:HA	1.90	0.53
1:B:450:LEU:HB2	1:B:451:PRO:HD3	1.91	0.53
2:C:387:LEU:CD1	2:C:515:PHE:CE2	2.92	0.53
2:D:498:ARG:HB2	2:D:501:TYR:CE1	2.44	0.53
2:D:462:LYS:O	2:D:465:GLU:HB2	2.09	0.52
1:B:145:GLU:OE2	1:B:146:PRO:HB3	2.09	0.52
2:D:379:CYS:HA	2:D:432:CYS:HA	1.91	0.52
2:C:438:SER:OG	2:C:442:ASP:HB2	2.10	0.52
2:C:476:GLY:H	2:C:487:ASN:HB3	1.74	0.52
2:D:393:THR:HG22	2:D:517:LEU:HA	1.92	0.52
1:A:246:ALA:HA	1:A:249:MET:HE2	1.91	0.52
1:A:582:ARG:O	1:A:583:PRO:C	2.51	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:476:GLY:N	2:C:487:ASN:HB3	2.25	0.52
2:C:502:GLY:HA3	1:A:354:GLY:HA3	1.92	0.52
1:B:477:TRP:CE3	1:B:500:PRO:HG3	2.46	0.51
1:A:55:THR:O	1:A:56:GLU:C	2.53	0.51
2:C:373:PRO:HD2	2:C:374:PHE:CD1	2.45	0.51
2:C:497:PHE:CD1	2:C:507:PRO:HD3	2.46	0.51
2:D:481:ASN:N	2:D:483:VAL:HG23	2.25	0.51
1:A:242:ALA:HB3	1:A:599:ASN:ND2	2.26	0.51
1:A:335:ASP:HB2	1:A:361:CYS:HB3	1.93	0.51
1:A:582:ARG:HB3	1:A:583:PRO:HD3	1.91	0.51
2:D:461:LEU:HD22	2:D:465:GLU:HB3	1.93	0.50
1:A:144:LEU:HD22	1:A:168:TRP:CZ2	2.46	0.50
1:B:248:LEU:HD12	1:B:262:LEU:HD22	1.93	0.50
2:C:393:THR:OG1	2:C:520:ALA:HB3	2.11	0.50
1:B:318:VAL:O	1:B:551:GLY:HA3	2.12	0.50
1:B:324:THR:OG1	1:B:327:PHE:N	2.39	0.50
1:A:452:PHE:CE2	1:A:481:LYS:NZ	2.80	0.50
1:B:557:MET:HE2	1:B:573:VAL:HG21	1.94	0.50
2:D:441:LEU:HD11	2:D:509:ARG:NH1	2.27	0.50
2:D:449:TYR:OH	2:D:498:ARG:NH2	2.44	0.50
1:A:55:THR:O	1:A:58:ASN:N	2.44	0.50
1:B:270:MET:HB3	1:B:271:TRP:CZ3	2.47	0.50
1:B:525:PHE:O	1:B:526:GLN:C	2.54	0.50
2:C:501:TYR:CE2	1:A:353:LYS:HD3	2.47	0.50
2:D:370:ASN:C	2:D:372:ALA:N	2.69	0.50
2:D:393:THR:HA	2:D:522:ALA:HA	1.94	0.50
1:B:144:LEU:HD22	1:B:168:TRP:CZ2	2.46	0.49
2:C:415:THR:O	2:C:415:THR:OG1	2.30	0.49
2:D:351:TYR:CE2	2:D:492:LEU:HD21	2.47	0.49
1:A:20:THR:OG1	1:A:23:GLU:HG3	2.12	0.49
1:B:460:ARG:NH2	1:B:506:VAL:HA	2.27	0.49
1:B:108:LEU:HB2	1:B:113:SER:OG	2.11	0.49
1:A:477:TRP:CE3	1:A:500:PRO:HG3	2.47	0.49
2:C:387:LEU:HD12	2:C:387:LEU:O	2.12	0.49
1:A:519:THR:O	1:A:522:GLN:HG2	2.13	0.49
1:B:554:LEU:HG	1:B:558:LEU:HD11	1.94	0.48
1:B:192:ARG:NH1	1:B:197:GLU:O	2.46	0.48
1:B:347:THR:HB	1:B:349:TRP:NE1	2.28	0.48
2:D:393:THR:CG2	2:D:516:GLU:HG3	2.42	0.48
1:B:25:ALA:HB1	1:B:97:LEU:HD11	1.95	0.48
1:B:177:ARG:O	1:B:181:GLU:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:349:SER:HB3	2:C:451:TYR:HA	1.94	0.48
2:C:460:ASN:N	2:C:460:ASN:HD22	2.11	0.48
2:C:351:TYR:CD2	2:C:492:LEU:HD21	2.49	0.48
2:C:418:ILE:O	2:C:422:ASN:N	2.44	0.48
2:C:442:ASP:OD2	2:C:509:ARG:NE	2.45	0.48
2:C:452:ARG:HG2	2:C:494:SER:HB3	1.96	0.48
2:D:357:ARG:HG3	2:D:396:TYR:HE1	1.77	0.48
1:A:119:ILE:HD11	1:A:182:GLU:CD	2.38	0.48
1:A:402:GLU:O	1:A:406:GLU:HG2	2.14	0.48
1:B:161:ARG:HE	1:B:266:LEU:HD23	1.79	0.48
2:C:338:PHE:O	2:C:339:ASP:C	2.57	0.48
2:C:355:ARG:C	2:C:356:LYS:HD2	2.39	0.48
1:B:375:GLU:O	1:B:378:HIS:HB2	2.14	0.48
1:B:424:LEU:HD12	1:B:424:LEU:HA	1.69	0.48
2:C:365:TYR:CZ	2:C:387:LEU:HG	2.49	0.48
2:D:392:PHE:HD1	2:D:517:LEU:HB2	1.79	0.48
1:A:46:ALA:HB1	1:A:62:MET:HA	1.95	0.48
1:A:188:ASN:O	1:A:192:ARG:HG3	2.14	0.48
2:C:461:LEU:HD22	2:C:465:GLU:HB3	1.95	0.47
2:D:373:PRO:HD2	2:D:374:PHE:CG	2.50	0.47
2:C:393:THR:CG2	2:C:516:GLU:HG3	2.44	0.47
2:C:462:LYS:O	2:C:465:GLU:HB2	2.14	0.47
1:A:249:MET:O	1:A:253:PRO:HA	2.14	0.47
2:C:460:ASN:HD22	2:C:460:ASN:H	1.63	0.47
1:A:460:ARG:NH2	1:A:506:VAL:HA	2.28	0.47
1:B:287:GLN:HE21	1:B:287:GLN:CA	2.27	0.47
1:B:288:LYS:HA	1:B:288:LYS:HD3	1.64	0.47
1:B:103:ASN:O	1:B:104:GLY:C	2.58	0.47
1:B:111:ASP:HA	1:B:114:LYS:CE	2.45	0.47
1:B:453:THR:HG23	1:B:512:PHE:CD2	2.50	0.47
2:C:406:GLU:HG3	2:C:418:ILE:HG12	1.95	0.47
2:C:454:ARG:NH2	2:C:469:SER:O	2.34	0.47
2:D:426:PRO:HD2	2:D:429:PHE:HD2	1.80	0.47
2:D:438:SER:OG	2:D:507:PRO:HB2	2.15	0.47
1:A:126:ILE:O	1:A:130:GLY:N	2.41	0.47
1:A:452:PHE:HE2	1:A:481:LYS:NZ	2.12	0.47
1:B:19:SER:HA	1:B:23:GLU:OE1	2.14	0.46
1:B:192:ARG:HA	1:B:196:TYR:O	2.15	0.46
2:C:431:GLY:HA3	2:C:513:LEU:O	2.15	0.46
2:C:453:TYR:OH	1:A:34:HIS:CD2	2.68	0.46
2:C:351:TYR:CE2	2:C:492:LEU:HD21	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:426:PRO:HD2	2:C:429:PHE:CD1	2.46	0.46
2:D:439:ASN:HD21	2:D:499:PRO:HA	1.79	0.46
2:D:457:ARG:NH1	2:D:459:SER:O	2.45	0.46
1:A:50:TYR:CE1	1:A:59:VAL:HG22	2.51	0.46
1:B:206:ASP:OD2	1:B:397:ASN:HB2	2.16	0.46
1:B:286:GLY:O	1:B:287:GLN:C	2.59	0.46
1:B:41:TYR:HE2	1:B:45:LEU:HD22	1.80	0.46
2:C:371:PHE:HB3	2:C:373:PRO:HD3	1.97	0.46
2:C:498:ARG:HB2	2:C:501:TYR:CE1	2.51	0.46
1:B:80:ALA:C	1:B:82:MET:H	2.23	0.46
2:C:422:ASN:HD21	2:C:453:TYR:HB2	1.80	0.46
2:C:342:PHE:CE1	2:C:511:VAL:HG11	2.45	0.46
2:D:353:TRP:NE1	2:D:466:ARG:HG3	2.30	0.46
2:C:350:VAL:HA	2:C:400:PHE:HB2	1.97	0.45
1:A:303:ASP:O	1:A:304:ALA:C	2.59	0.45
1:A:452:PHE:HE2	1:A:481:LYS:HZ3	1.62	0.45
2:C:403:ARG:HG2	2:C:495:TYR:CE2	2.50	0.45
2:D:403:ARG:HH21	2:D:405:ASN:HB2	1.81	0.45
2:D:490:PHE:CD1	2:D:491:PRO:HD2	2.52	0.45
2:D:497:PHE:CE2	2:D:507:PRO:HB3	2.51	0.45
1:B:39:LEU:O	1:B:42:GLN:HB2	2.17	0.45
2:C:338:PHE:O	2:C:341:VAL:N	2.48	0.45
1:A:79:LEU:O	1:A:82:MET:HG3	2.15	0.45
1:B:389:PRO:HG2	1:B:392:LEU:HD12	1.97	0.45
1:B:521:TYR:O	1:B:524:GLN:N	2.49	0.45
2:D:438:SER:O	2:D:439:ASN:C	2.59	0.45
1:B:346:PRO:HA	1:B:359:LEU:O	2.17	0.45
1:A:482:ARG:HD3	1:A:608:THR:O	2.17	0.45
1:A:535:HIS:HE1	1:A:538:PRO:O	2.00	0.45
2:C:401:VAL:HG11	2:C:451:TYR:HD2	1.79	0.45
2:C:391:CYS:HA	2:C:524:VAL:O	2.16	0.45
1:A:322:ASN:ND2	5:A:703:NAG:O7	2.44	0.45
1:A:397:ASN:ND2	1:A:400:PHE:HE1	2.15	0.45
1:A:433:GLU:O	1:A:434:THR:C	2.59	0.45
4:H:1:NAG:H61	4:H:2:NAG:C7	2.46	0.45
1:B:446:ILE:O	1:B:449:THR:HG22	2.17	0.45
1:B:520:LEU:O	1:B:524:GLN:HG3	2.17	0.45
2:C:453:TYR:CE1	2:C:455:LEU:HB3	2.52	0.45
2:D:481:ASN:H	2:D:483:VAL:HG23	1.82	0.45
1:A:418:LEU:HD23	1:A:418:LEU:HA	1.76	0.45
1:B:20:THR:OG1	1:B:23:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:GLU:O	1:B:114:LYS:HG3	2.17	0.45
2:C:347:PHE:CE2	2:C:399:SER:HB2	2.51	0.45
2:D:403:ARG:HE	2:D:403:ARG:HB2	1.57	0.44
2:C:403:ARG:HG3	2:C:406:GLU:OE1	2.17	0.44
2:C:486:VAL:O	2:C:488:CYS:SG	2.75	0.44
1:A:431:ASP:O	1:A:432:ASN:C	2.60	0.44
1:B:267:LEU:HA	1:B:278:LEU:HD11	1.98	0.44
2:D:495:TYR:CD2	2:D:497:PHE:CZ	2.91	0.44
1:A:137:ASN:C	1:A:139:GLN:H	2.25	0.44
1:A:237:TYR:CD1	1:A:451:PRO:HG2	2.52	0.44
1:A:397:ASN:ND2	1:A:521:TYR:OH	2.51	0.44
2:C:373:PRO:HD2	2:C:374:PHE:CE1	2.52	0.44
1:A:416:LYS:HD2	1:A:543:ASP:HB3	1.99	0.44
1:B:347:THR:CB	1:B:349:TRP:HE1	2.31	0.44
2:D:415:THR:HG22	2:D:424:LYS:HZ3	1.82	0.44
1:A:20:THR:HG23	1:A:23:GLU:OE1	2.17	0.44
1:B:306:ARG:O	1:B:307:ILE:C	2.61	0.44
1:A:545:SER:O	1:A:546:ASN:HB2	2.17	0.44
1:B:97:LEU:HA	1:B:97:LEU:HD23	1.59	0.44
1:B:177:ARG:NH2	1:B:495:GLU:HG3	2.33	0.44
1:A:288:LYS:HE3	1:A:433:GLU:CG	2.48	0.44
1:A:320:LEU:HD13	1:A:380:GLN:HG2	2.00	0.44
1:B:430:GLU:OE1	1:B:541:LYS:NZ	2.51	0.44
2:D:368:LEU:HA	2:D:371:PHE:CE1	2.53	0.44
1:B:209:VAL:HG12	1:B:216:ASP:HA	2.00	0.43
2:C:342:PHE:CE2	2:C:368:LEU:HD21	2.53	0.43
1:B:48:TRP:CH2	1:B:357:ARG:HB3	2.53	0.43
1:B:345:HIS:O	1:B:346:PRO:C	2.60	0.43
2:C:387:LEU:HD11	2:C:515:PHE:CE2	2.52	0.43
2:D:419:ALA:O	2:D:424:LYS:HB2	2.18	0.43
2:D:495:TYR:HD2	2:D:497:PHE:CE2	2.36	0.43
1:A:155:SER:O	1:A:161:ARG:HD2	2.18	0.43
1:A:237:TYR:CE1	1:A:451:PRO:HG2	2.53	0.43
1:A:187:LYS:HD2	1:A:199:TYR:CE1	2.53	0.43
1:A:305:GLN:O	1:A:306:ARG:C	2.62	0.43
1:A:514:ARG:HG2	1:A:515:TYR:N	2.32	0.43
1:A:433:GLU:O	1:A:436:ILE:N	2.52	0.43
1:B:406:GLU:HG3	1:B:518:ARG:NH1	2.31	0.43
2:C:372:ALA:N	2:C:373:PRO:HD3	2.34	0.43
2:D:422:ASN:OD1	2:D:454:ARG:HB2	2.19	0.43
1:B:378:HIS:NE2	1:B:402:GLU:OE2	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:ARG:HH21	1:B:506:VAL:HA	1.83	0.43
1:B:122:THR:O	1:B:126:ILE:HG13	2.18	0.43
2:C:380:TYR:O	2:C:431:GLY:O	2.37	0.43
2:C:420:ASP:O	2:C:460:ASN:HA	2.19	0.43
1:B:247:LYS:CB	1:B:282:THR:HG22	2.49	0.43
2:D:444:LYS:O	2:D:444:LYS:HG3	2.19	0.43
1:B:81:GLN:CB	3:F:2:NAG:H81	2.49	0.42
1:B:227:GLU:HG2	1:B:454:TYR:OH	2.19	0.42
1:A:215:TYR:CE1	1:A:577:LYS:HE2	2.54	0.42
1:B:315:PHE:O	1:B:318:VAL:HG22	2.19	0.42
1:B:320:LEU:HB3	1:B:380:GLN:OE1	2.19	0.42
2:C:401:VAL:CG1	2:C:451:TYR:HD2	2.32	0.42
2:D:350:VAL:HG22	2:D:422:ASN:HB3	2.01	0.42
2:D:386:LYS:C	2:D:388:ASN:N	2.74	0.42
2:C:368:LEU:O	2:C:368:LEU:HD23	2.20	0.42
2:C:383:SER:O	2:C:387:LEU:N	2.49	0.42
1:A:275:TRP:O	1:A:444:LEU:HB3	2.19	0.42
1:B:525:PHE:O	1:B:528:ALA:N	2.52	0.42
2:C:387:LEU:HD13	2:C:515:PHE:CE2	2.54	0.42
1:A:134:ASN:OD1	1:A:136:ASP:N	2.53	0.42
1:A:294:THR:HG23	1:A:365:THR:HA	2.01	0.42
1:B:475:LYS:HE2	1:B:479:GLU:OE2	2.20	0.42
2:C:365:TYR:CD1	2:C:388:ASN:OD1	2.73	0.42
2:C:386:LYS:HA	2:C:389:ASP:OD2	2.20	0.42
2:D:342:PHE:CE1	2:D:511:VAL:HG21	2.55	0.42
2:D:461:LEU:HA	2:D:461:LEU:HD23	1.55	0.42
1:B:41:TYR:CE2	1:B:45:LEU:HD22	2.54	0.42
2:C:473:TYR:O	2:C:488:CYS:HA	2.20	0.42
2:D:341:VAL:HG12	2:D:342:PHE:HD1	1.83	0.42
1:A:267:LEU:HA	1:A:267:LEU:HD23	1.85	0.42
1:B:170:SER:O	1:B:174:LYS:HD2	2.20	0.42
1:B:316:VAL:HA	1:B:320:LEU:O	2.20	0.42
1:A:448:GLY:O	1:A:451:PRO:HD2	2.20	0.42
2:D:442:ASP:OD1	2:D:451:TYR:CZ	2.71	0.41
1:A:592:PHE:CZ	1:A:596:LYS:HD2	2.55	0.41
2:D:336:CYS:HB2	2:D:363:ALA:HA	2.01	0.41
1:A:318:VAL:O	1:A:551:GLY:HA3	2.20	0.41
2:C:382:VAL:HG22	2:C:383:SER:H	1.85	0.41
2:D:398:ASP:O	2:D:511:VAL:HA	2.21	0.41
2:D:452:ARG:HD2	2:D:492:LEU:HD23	2.01	0.41
1:A:457:GLU:HG2	1:A:513:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:368:LEU:HA	2:C:371:PHE:CD1	2.55	0.41
2:D:353:TRP:O	2:D:466:ARG:NE	2.51	0.41
1:A:455:MET:HE2	1:A:481:LYS:HD3	2.01	0.41
1:B:144:LEU:HB2	1:B:168:TRP:CH2	2.56	0.41
1:B:171:GLU:O	1:B:175:GLN:HG3	2.20	0.41
2:D:373:PRO:CD	2:D:374:PHE:CE2	3.03	0.41
2:D:386:LYS:C	2:D:388:ASN:H	2.28	0.41
1:A:269:ASP:OD1	1:A:272:GLY:N	2.54	0.41
1:A:450:LEU:HB2	1:A:451:PRO:HD3	2.03	0.41
2:C:403:ARG:HA	2:C:506:GLN:O	2.21	0.41
1:A:249:MET:HE2	1:A:249:MET:HB3	1.93	0.41
1:B:114:LYS:HE3	1:B:114:LYS:HB2	1.99	0.41
1:B:249:MET:HE2	1:B:249:MET:HB3	1.91	0.41
1:B:455:MET:HE2	1:B:481:LYS:HG2	2.03	0.41
1:B:470:LYS:HA	1:B:473:TRP:CD1	2.56	0.41
1:B:485:VAL:HG12	1:B:487:VAL:HG23	2.03	0.41
2:D:387:LEU:H	2:D:387:LEU:HG	1.72	0.41
2:D:336:CYS:N	2:D:362:VAL:O	2.54	0.41
1:A:163:TRP:O	1:A:164:ALA:C	2.62	0.41
1:A:535:HIS:NE2	1:A:542:CYS:HA	2.36	0.41
1:B:478:TRP:CD2	1:B:489:GLU:HB3	2.56	0.41
2:C:364:ASP:OD1	2:C:367:VAL:HG12	2.21	0.41
2:C:462:LYS:O	2:C:463:PRO:C	2.64	0.41
1:A:39:LEU:HD23	1:A:39:LEU:HA	1.54	0.41
1:A:157:ASP:O	1:A:161:ARG:HG3	2.20	0.41
1:A:324:THR:O	1:A:327:PHE:HB3	2.21	0.41
1:A:392:LEU:HD13	1:A:563:SER:HA	2.03	0.41
1:B:46:ALA:HB1	1:B:62:MET:HA	2.01	0.41
1:B:305:GLN:O	1:B:309:LYS:HG2	2.21	0.41
1:B:535:HIS:CE1	1:B:542:CYS:HA	2.56	0.41
2:C:490:PHE:CD1	2:C:491:PRO:HD2	2.55	0.41
2:D:393:THR:OG1	2:D:520:ALA:HB3	2.21	0.41
1:B:499:ASP:O	1:B:500:PRO:C	2.63	0.40
1:A:427:ASP:O	1:A:428:PHE:C	2.64	0.40
1:B:267:LEU:HA	1:B:267:LEU:HD23	1.79	0.40
1:A:146:PRO:O	1:A:150:GLU:HB2	2.20	0.40
1:A:284:PRO:HD2	1:A:437:ASN:OD1	2.21	0.40
1:A:425:SER:C	1:A:427:ASP:H	2.28	0.40
1:A:446:ILE:O	1:A:450:LEU:HG	2.22	0.40
1:B:212:VAL:O	1:B:213:ASP:C	2.64	0.40
2:C:422:ASN:ND2	2:C:453:TYR:HB2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:449:TYR:CE1	2:D:496:GLY:HA2	2.56	0.40
1:A:203:TRP:C	1:A:205:GLY:N	2.80	0.40
1:A:424:LEU:HD12	1:A:424:LEU:HA	1.62	0.40
2:D:480:CYS:SG	2:D:483:VAL:HB	2.61	0.40
1:B:540:HIS:HA	1:B:587:TYR:CE2	2.57	0.40
1:A:203:TRP:C	1:A:205:GLY:H	2.30	0.40
1:A:425:SER:C	1:A:427:ASP:N	2.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	596/598 (100%)	568 (95%)	28 (5%)	0	100	100
1	B	597/598 (100%)	563 (94%)	34 (6%)	0	100	100
2	C	192/194 (99%)	172 (90%)	20 (10%)	0	100	100
2	D	192/194 (99%)	166 (86%)	25 (13%)	1 (0%)	24	56
All	All	1577/1584 (100%)	1469 (93%)	107 (7%)	1 (0%)	48	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	373	PRO

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	528/528 (100%)	517 (98%)	11 (2%)	47	66
1	B	529/528 (100%)	516 (98%)	13 (2%)	42	64
2	C	167/167 (100%)	157 (94%)	10 (6%)	17	46
2	D	167/167 (100%)	154 (92%)	13 (8%)	11	37
All	All	1391/1390 (100%)	1344 (97%)	47 (3%)	32	59

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	92	THR
1	B	103	ASN
1	B	287	GLN
1	B	305	GLN
1	B	317	SER
1	B	338	ASN
1	B	339	VAL
1	B	340	GLN
1	B	343	VAL
1	B	347	THR
1	B	432	ASN
1	B	495	GLU
1	B	579	MET
2	C	379	CYS
2	C	383	SER
2	C	389	ASP
2	C	401	VAL
2	C	402	ILE
2	C	403	ARG
2	C	408	SER
2	C	418	ILE
2	C	432	CYS
2	C	437	ASN
2	D	370	ASN
2	D	379	CYS
2	D	382	VAL
2	D	383	SER
2	D	385	THR
2	D	387	LEU
2	D	401	VAL

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Mol	Chain	Res	Type
2	D	406	GLU
2	D	432	CYS
2	D	437	ASN
2	D	445	VAL
2	D	448	ASN
2	D	518	LEU
1	A	82	MET
1	A	103	ASN
1	A	134	ASN
1	A	139	GLN
1	A	283	VAL
1	A	305	GLN
1	A	322	ASN
1	A	353	LYS
1	A	581	VAL
1	A	582	ARG
1	A	583	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	24	GLN
1	B	76	GLN
1	B	89	GLN
1	B	194	ASN
1	B	287	GLN
1	B	338	ASN
1	B	556	ASN
1	B	572	ASN
2	C	360	ASN
2	C	437	ASN
2	C	460	ASN
2	C	474	GLN
2	C	506	GLN
2	D	474	GLN
1	A	76	GLN
1	A	89	GLN
1	A	96	GLN
1	A	330	ASN
1	A	380	GLN
1	A	535	HIS
1	A	599	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

11 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
3	NAG	E	1	1,3	14,14,15	0.69	1 (7%)	17,19,21	0.58	0
3	NAG	E	2	3	14,14,15	0.52	0	17,19,21	0.67	0
3	BMA	E	3	3	11,11,12	3.21	8 (72%)	15,15,17	1.60	3 (20%)
3	NAG	F	1	1,3	14,14,15	1.15	1 (7%)	17,19,21	1.08	2 (11%)
3	NAG	F	2	3	14,14,15	0.83	1 (7%)	17,19,21	1.18	1 (5%)
3	BMA	F	3	3	11,11,12	3.72	9 (81%)	15,15,17	1.90	5 (33%)
3	NAG	G	1	1,3	14,14,15	0.98	1 (7%)	17,19,21	0.56	0
3	NAG	G	2	3	14,14,15	0.62	0	17,19,21	0.97	1 (5%)
3	BMA	G	3	3	11,11,12	2.72	8 (72%)	15,15,17	1.41	2 (13%)
4	NAG	H	1	1,4	14,14,15	1.14	1 (7%)	17,19,21	0.90	1 (5%)
4	NAG	H	2	4	14,14,15	0.91	1 (7%)	17,19,21	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	1/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	3/6/23/26	0/1/1/1
3	BMA	G	3	3	-	1/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	4/6/23/26	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3	BMA	O5-C1	6.73	1.55	1.43
3	E	3	BMA	C4-C3	4.96	1.65	1.52
3	F	3	BMA	O5-C5	4.90	1.53	1.43
3	F	3	BMA	C4-C5	4.53	1.62	1.53
3	F	3	BMA	C1-C2	4.51	1.63	1.52
3	E	3	BMA	C1-C2	4.21	1.62	1.52
3	E	3	BMA	O5-C1	4.13	1.50	1.43
3	F	1	NAG	C1-C2	3.98	1.57	1.52
3	G	3	BMA	C4-C3	3.89	1.62	1.52
4	H	1	NAG	O5-C1	3.85	1.50	1.43
3	G	3	BMA	C1-C2	3.83	1.61	1.52
3	E	3	BMA	C4-C5	3.81	1.61	1.53
3	G	3	BMA	O3-C3	3.48	1.51	1.43
3	G	1	NAG	O5-C1	-3.48	1.37	1.43
3	G	3	BMA	C4-C5	3.44	1.60	1.53
3	F	3	BMA	C4-C3	3.44	1.61	1.52
3	E	3	BMA	O3-C3	3.39	1.51	1.43
3	G	3	BMA	C2-C3	3.23	1.57	1.52
3	E	3	BMA	O4-C4	2.92	1.50	1.43
3	E	3	BMA	O5-C5	2.89	1.49	1.43
4	H	2	NAG	O5-C1	2.87	1.48	1.43
3	F	3	BMA	O2-C2	2.86	1.49	1.43
3	F	3	BMA	C6-C5	2.82	1.61	1.51
3	F	3	BMA	O4-C4	2.76	1.49	1.43
3	F	3	BMA	O3-C3	2.58	1.49	1.43
3	E	3	BMA	C6-C5	2.56	1.60	1.51
3	E	1	NAG	O5-C1	2.43	1.47	1.43
3	G	3	BMA	O4-C4	2.38	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	NAG	C1-C2	2.36	1.55	1.52
3	G	3	BMA	O2-C2	2.23	1.48	1.43
3	G	3	BMA	O5-C1	2.08	1.47	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3	BMA	O5-C5-C6	3.69	114.84	107.66
3	E	3	BMA	C1-O5-C5	3.60	117.02	112.19
3	F	2	NAG	O4-C4-C3	-3.15	102.95	110.38
3	E	3	BMA	O3-C3-C4	3.03	117.52	110.38
3	G	3	BMA	C1-O5-C5	2.70	115.81	112.19
3	F	3	BMA	O2-C2-C1	2.69	115.39	109.22
3	G	3	BMA	C1-C2-C3	2.58	113.41	109.64
4	H	1	NAG	O3-C3-C2	-2.31	104.60	109.40
3	F	1	NAG	C2-N2-C7	2.29	125.97	122.90
3	F	1	NAG	O3-C3-C2	-2.29	104.64	109.40
3	F	3	BMA	O4-C4-C3	2.21	115.58	110.38
3	G	2	NAG	C1-C2-N2	2.17	113.85	110.43
3	E	3	BMA	O4-C4-C3	2.15	115.44	110.38
3	F	3	BMA	C2-C3-C4	-2.13	107.12	110.86
3	F	3	BMA	O5-C1-C2	2.00	115.56	110.79

There are no chirality outliers.

All (14) torsion outliers are listed below:

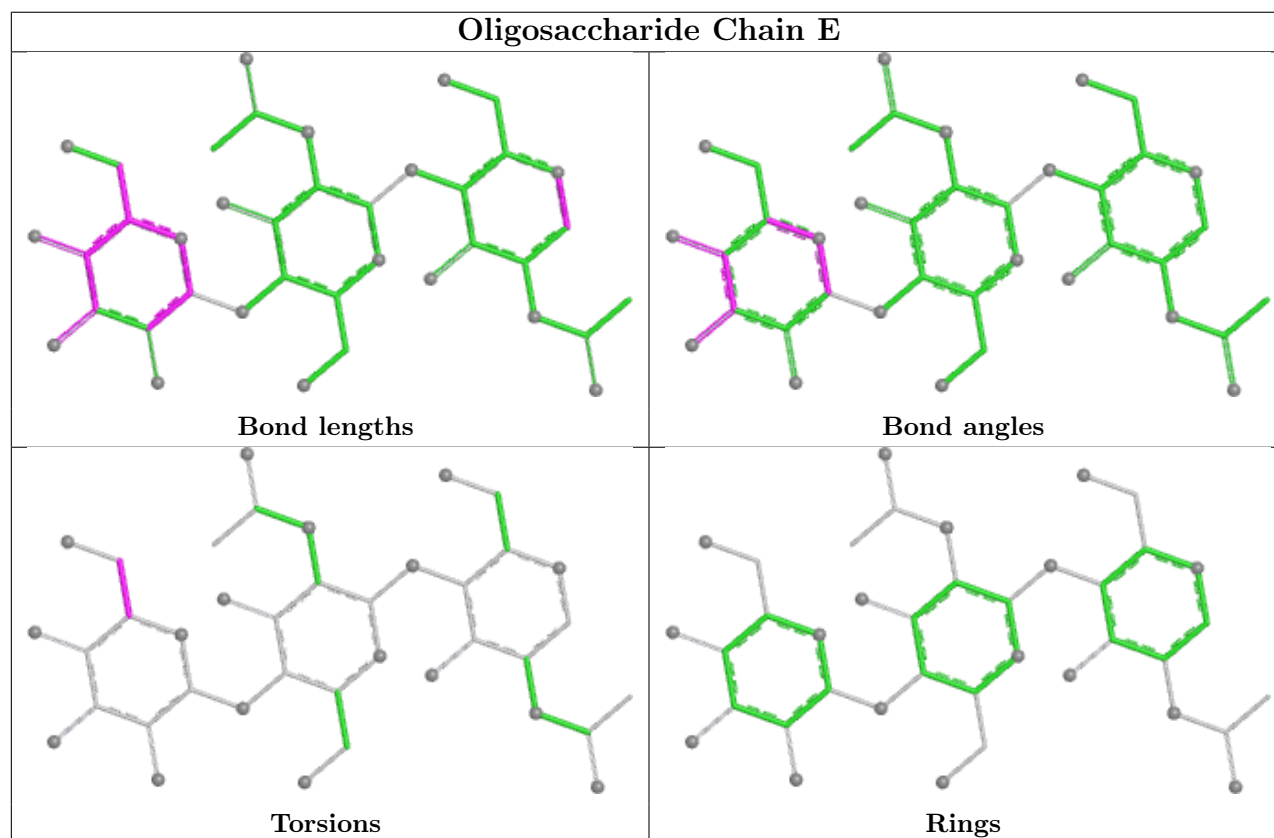
Mol	Chain	Res	Type	Atoms
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
3	G	1	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6

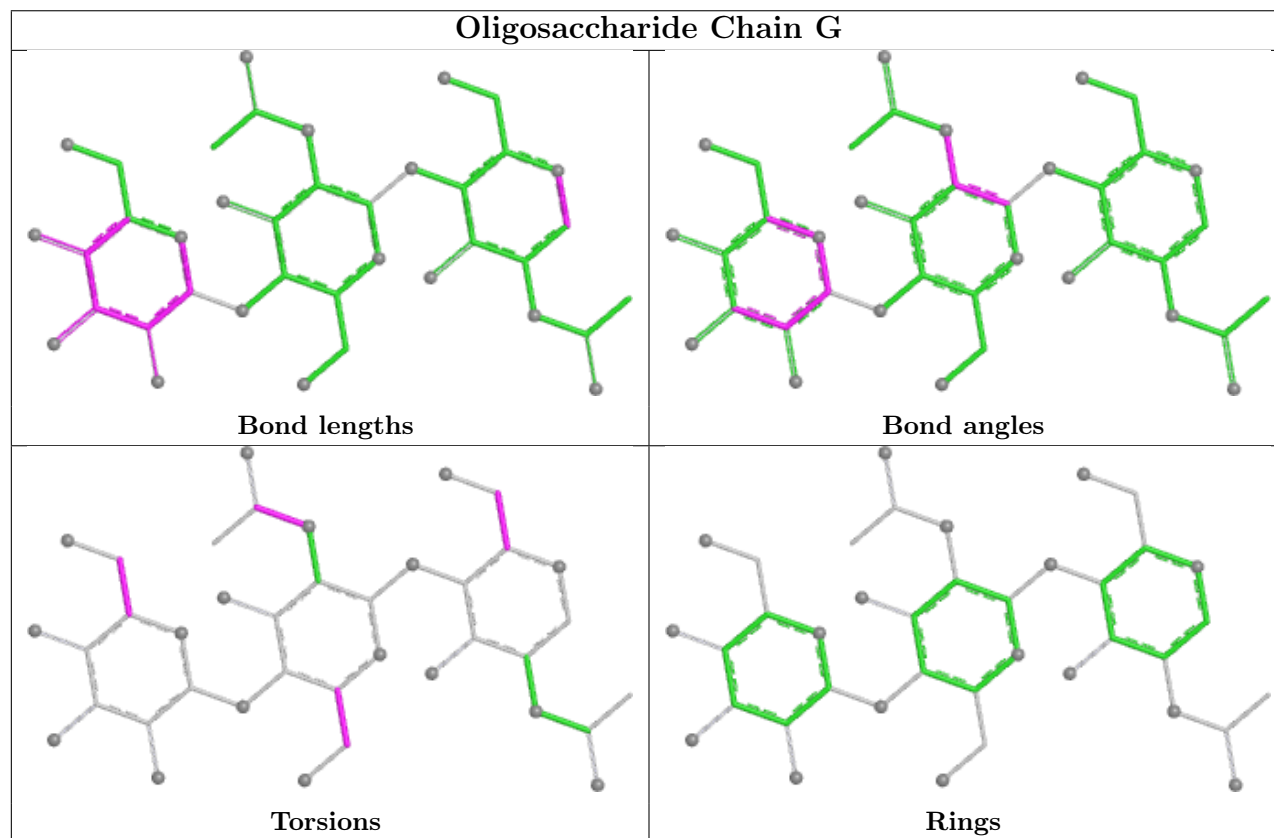
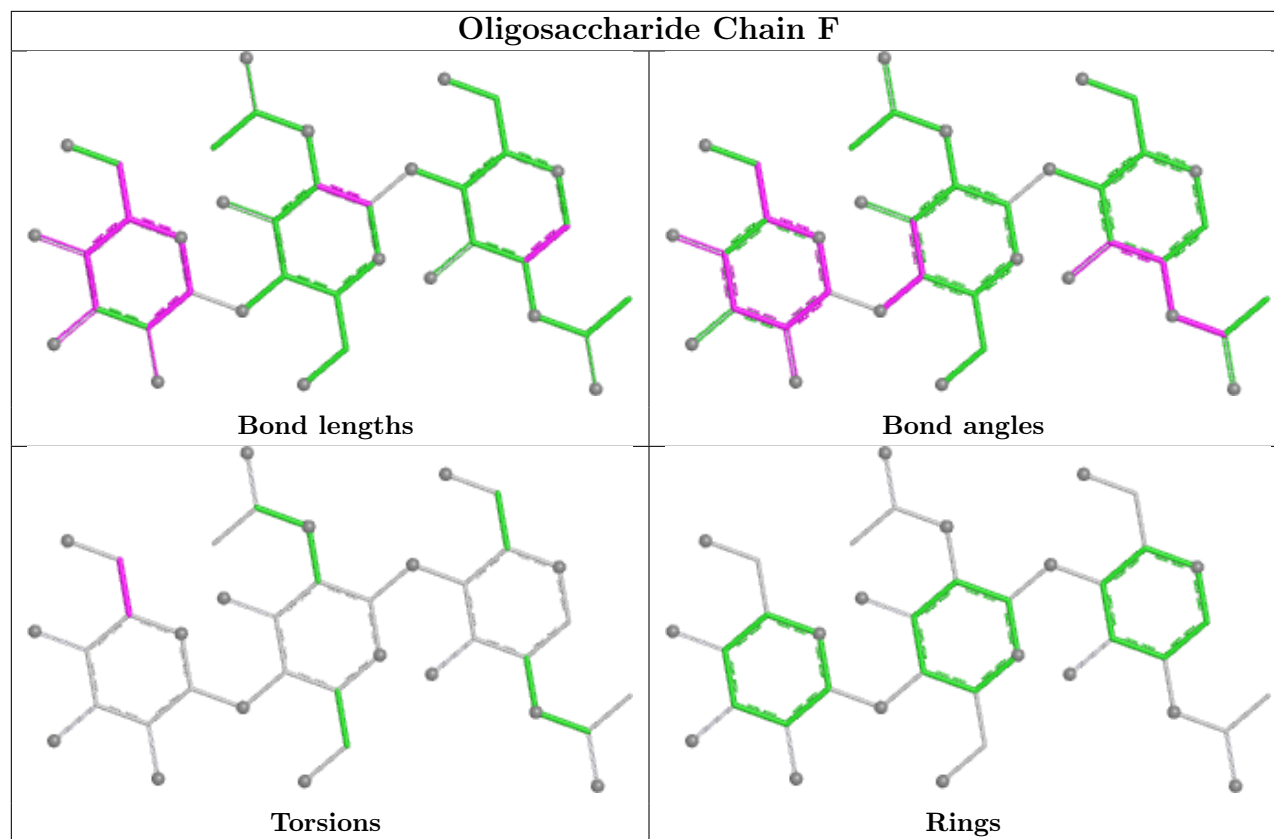
There are no ring outliers.

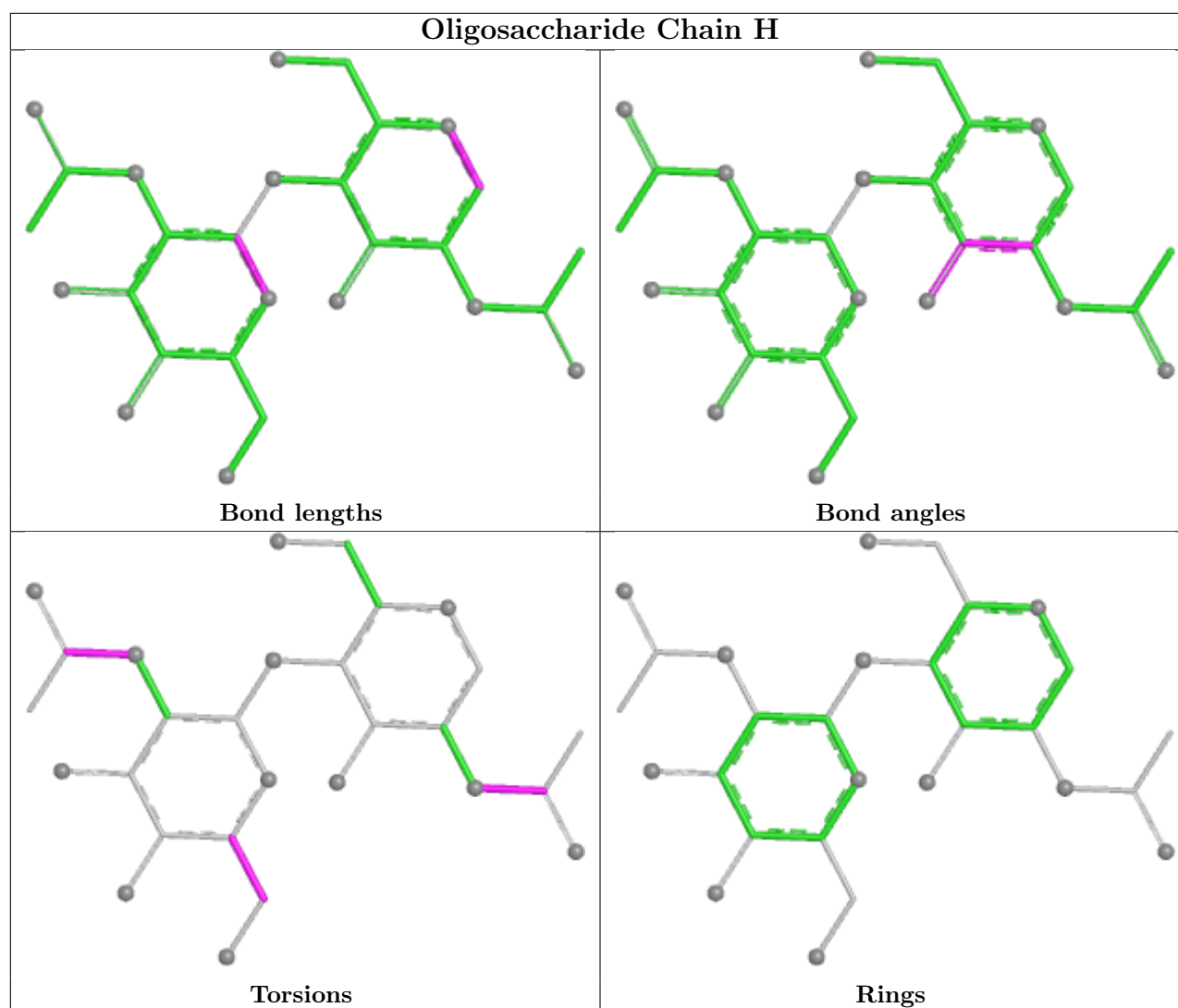
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	3	BMA	1	0
4	H	1	NAG	1	0
4	H	2	NAG	1	0
3	F	2	NAG	3	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](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	B	701	1	14,14,15	1.55	1 (7%)	17,19,21	1.75	1 (5%)
5	NAG	B	704	1	14,14,15	1.25	1 (7%)	17,19,21	0.90	0
5	NAG	B	703	1	14,14,15	1.38	1 (7%)	17,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	703	1	14,14,15	1.93	2 (14%)	17,19,21	0.83	1 (5%)
5	NAG	A	701	1	14,14,15	2.10	2 (14%)	17,19,21	1.19	1 (5%)
5	NAG	B	702	1	14,14,15	1.61	1 (7%)	17,19,21	1.40	4 (23%)
5	NAG	A	702	1	14,14,15	1.40	2 (14%)	17,19,21	1.12	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
5	NAG	B	701	1	-	1/6/23/26	0/1/1/1
5	NAG	B	704	1	-	3/6/23/26	0/1/1/1
5	NAG	B	703	1	-	1/6/23/26	0/1/1/1
5	NAG	A	703	1	-	2/6/23/26	0/1/1/1
5	NAG	A	701	1	-	2/6/23/26	0/1/1/1
5	NAG	B	702	1	-	3/6/23/26	0/1/1/1
5	NAG	A	702	1	-	3/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	701	NAG	O5-C1	7.49	1.56	1.43
5	A	703	NAG	O5-C1	6.09	1.53	1.43
5	B	702	NAG	O5-C1	5.47	1.52	1.43
5	B	701	NAG	O5-C1	5.39	1.52	1.43
5	B	703	NAG	O5-C1	4.81	1.51	1.43
5	B	704	NAG	O5-C1	4.03	1.50	1.43
5	A	702	NAG	O5-C1	3.96	1.50	1.43
5	A	703	NAG	C1-C2	3.47	1.57	1.52
5	A	702	NAG	C1-C2	3.08	1.56	1.52
5	A	701	NAG	C1-C2	2.08	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	701	NAG	C1-O5-C5	6.40	120.76	112.19
5	A	701	NAG	C1-O5-C5	3.79	117.27	112.19
5	A	702	NAG	C1-O5-C5	3.72	117.18	112.19
5	B	702	NAG	C1-O5-C5	3.53	116.91	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	702	NAG	C2-N2-C7	2.39	126.11	122.90
5	B	702	NAG	C1-C2-N2	2.08	113.71	110.43
5	B	702	NAG	O6-C6-C5	2.01	118.19	111.33
5	A	703	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	701	NAG	C1-C2-N2-C7
5	A	702	NAG	O5-C5-C6-O6
5	A	703	NAG	O5-C5-C6-O6
5	B	704	NAG	C8-C7-N2-C2
5	B	704	NAG	O7-C7-N2-C2
5	A	701	NAG	C8-C7-N2-C2
5	A	701	NAG	O7-C7-N2-C2
5	A	703	NAG	C4-C5-C6-O6
5	A	702	NAG	C4-C5-C6-O6
5	B	702	NAG	O5-C5-C6-O6
5	B	703	NAG	O5-C5-C6-O6
5	B	702	NAG	C1-C2-N2-C7
5	B	702	NAG	C3-C2-N2-C7
5	A	702	NAG	C3-C2-N2-C7
5	B	704	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	703	NAG	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	597/598 (99%)	-0.31	4 (0%)	84 70	43, 68, 114, 247	1 (0%)
1	B	598/598 (100%)	-0.13	6 (1%)	79 63	47, 80, 134, 184	1 (0%)
2	C	194/194 (100%)	0.37	12 (6%)	26 18	47, 76, 162, 237	0
2	D	194/194 (100%)	0.44	12 (6%)	26 18	61, 90, 189, 260	0
All	All	1583/1584 (99%)	-0.07	34 (2%)	63 44	43, 76, 150, 260	2 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	365	TYR	4.8
1	A	138	PRO	4.1
1	A	228[A]	HIS	3.7
2	C	375	PHE	3.3
2	D	366	SER	3.1
1	B	601	ASN	3.1
2	D	375	PHE	3.1
2	D	373	PRO	3.1
2	C	381	GLY	3.0
2	C	477	ASN	3.0
2	C	376	THR	3.0
2	C	420	ASP	2.9
2	D	526	GLY	2.9
2	D	387	LEU	2.8
2	D	521	PRO	2.8
2	C	382	VAL	2.7
1	A	139	GLN	2.6
1	B	82	MET	2.5
2	D	390	LEU	2.5
2	D	402	ILE	2.4
2	C	360	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	373	PRO	2.3
1	A	289	PRO	2.3
2	C	525	CYS	2.3
2	C	524	VAL	2.3
1	B	289	PRO	2.2
2	D	374	PHE	2.2
1	B	433	GLU	2.2
2	C	364	ASP	2.1
1	B	339	VAL	2.1
2	C	526	GLY	2.1
2	D	370	ASN	2.1
2	D	385	THR	2.1
1	B	197	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

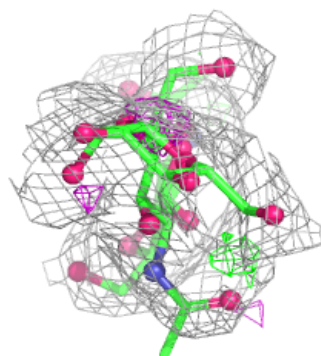
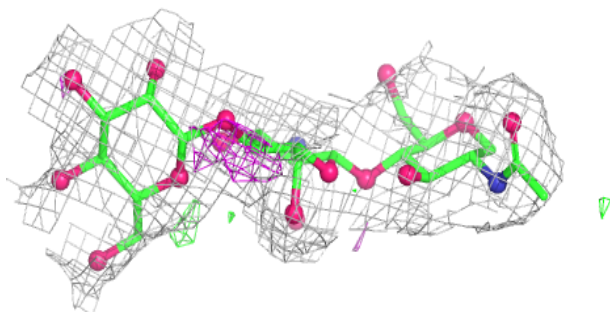
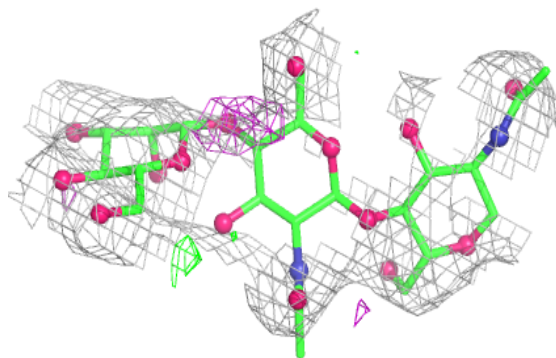
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	F	3	11/12	0.47	0.14	88,95,106,107	0
3	NAG	G	2	14/15	0.58	0.14	102,108,114,114	0
3	BMA	E	3	11/12	0.59	0.11	89,94,103,105	0
3	BMA	G	3	11/12	0.59	0.10	97,106,110,111	0
4	NAG	H	2	14/15	0.70	0.12	88,94,105,106	0
3	NAG	G	1	14/15	0.74	0.14	88,97,106,107	0
3	NAG	E	2	14/15	0.75	0.12	86,98,107,108	0
3	NAG	F	2	14/15	0.79	0.17	103,107,116,117	0
3	NAG	F	1	14/15	0.81	0.17	92,103,124,128	0
4	NAG	H	1	14/15	0.84	0.09	77,83,89,89	0
3	NAG	E	1	14/15	0.90	0.09	73,82,90,94	0

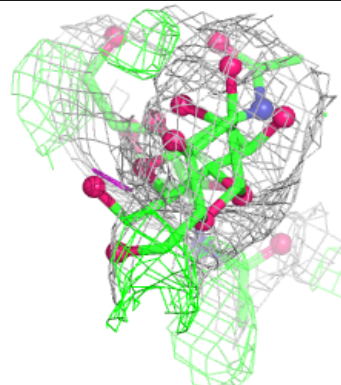
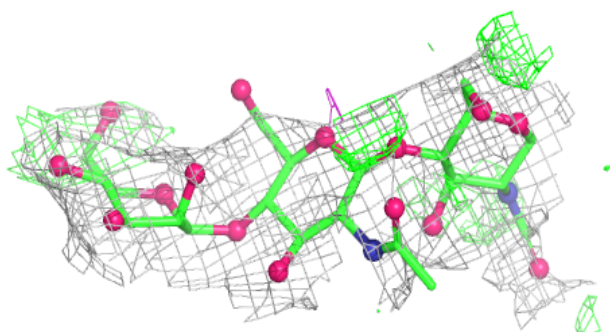
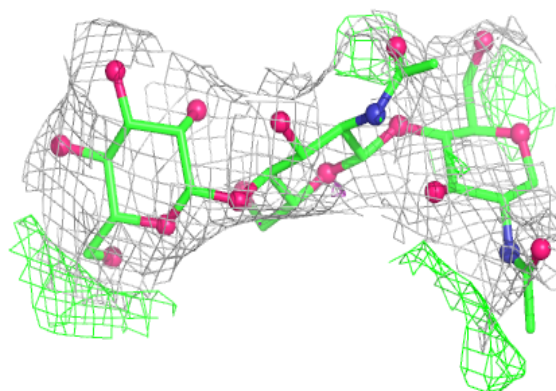
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

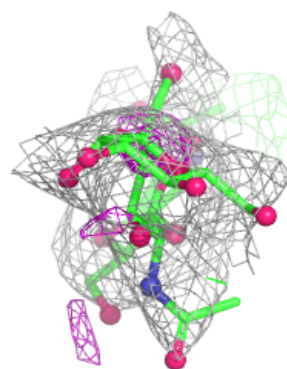
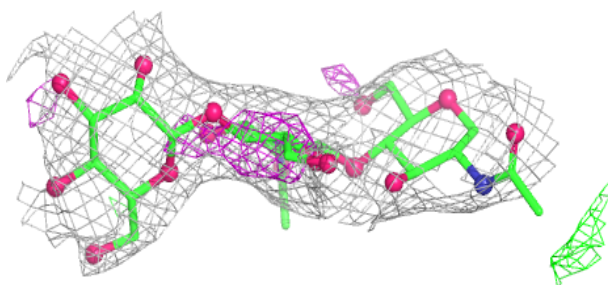
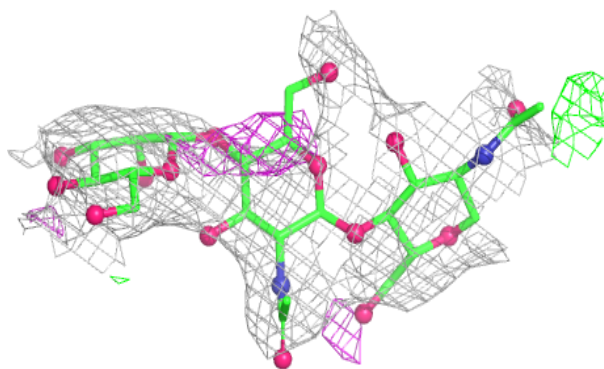
**Electron density around Chain F:**

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

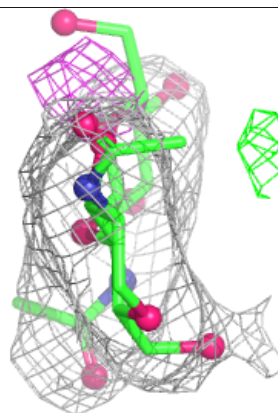
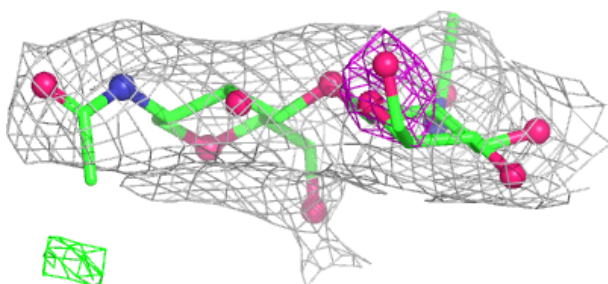
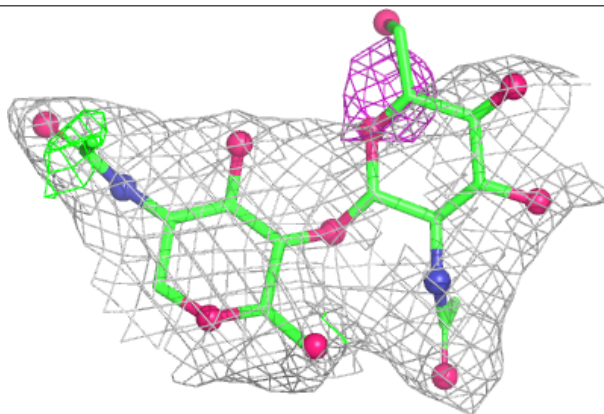


Electron density around Chain G:

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

**Electron density around Chain H:**

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



6.4 Ligands [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
5	NAG	B	702	14/15	0.60	0.15	91,116,126,127	0
5	NAG	B	701	14/15	0.64	0.15	137,146,156,158	0
5	NAG	A	701	14/15	0.64	0.14	102,107,115,117	0
5	NAG	B	703	14/15	0.73	0.12	116,132,144,146	0
5	NAG	A	703	14/15	0.75	0.14	89,109,115,116	0
5	NAG	A	702	14/15	0.77	0.13	109,115,120,122	0
5	NAG	B	704	14/15	0.81	0.08	96,106,110,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.