



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 04:36 PM EST

PDB ID : 4WI5
Title : Structural mapping of the human IgG1 binding site for FcRn: hu3S193 Fc mutation H310A
Authors : Farrugia, W.; Burvenich, I.J.G.; Scott, A.M.; Ramsland, P.A.
Deposited on : 2014-09-25
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

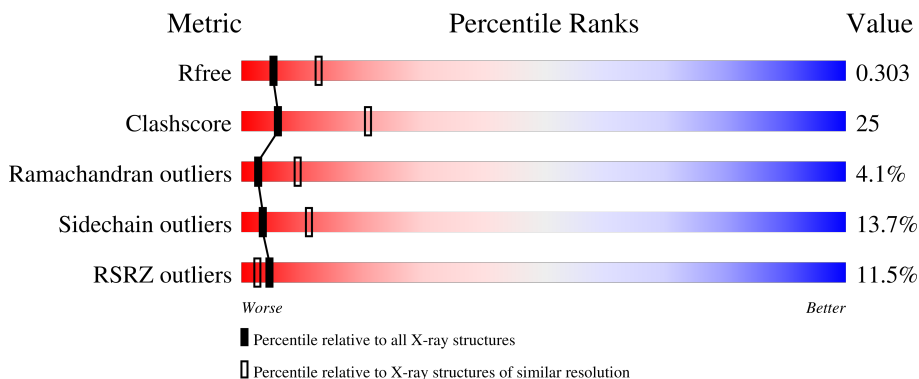
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	208	
1	B	208	
2	C	8	
2	D	8	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3536 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.

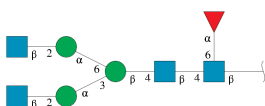
- Molecule 1 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	208	Total 1659	C 1056	N 278	O 319	S 6	0	0	0
1	B	208	Total 1659	C 1056	N 278	O 319	S 6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	ALA	HIS	engineered mutation	UNP P01857
B	310	ALA	HIS	engineered mutation	UNP P01857

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	8	Total 99	C 56	N 4	O 39	0	0	0
2	D	8	Total 99	C 56	N 4	O 39	0	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

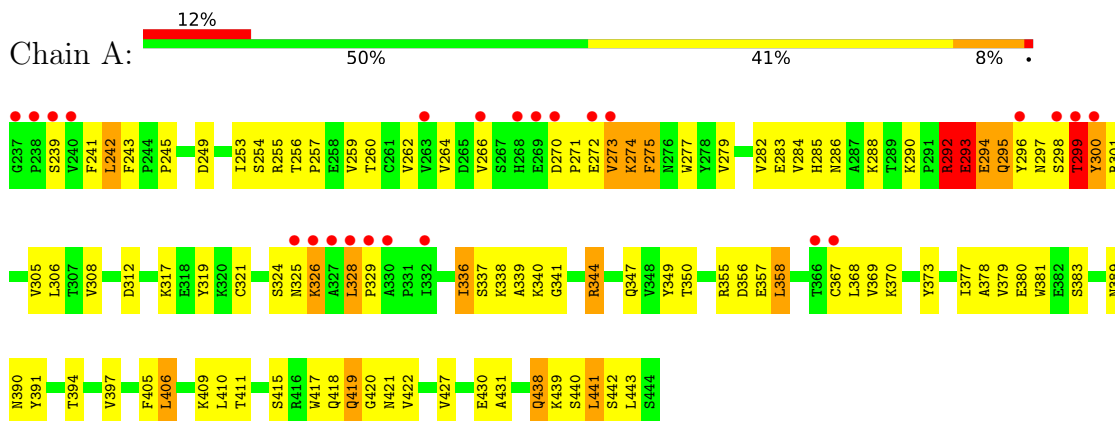
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total O 4 4	0	0
4	B	4	Total O 4 4	0	0

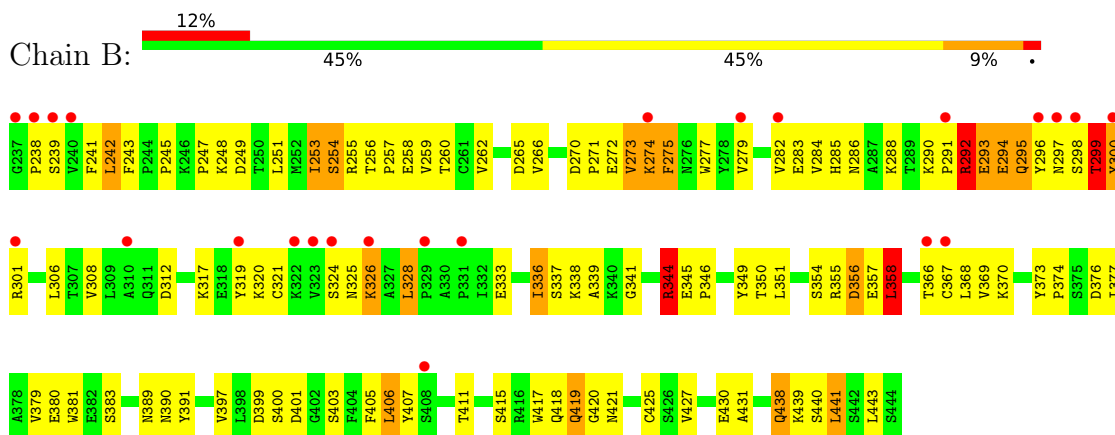
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ig gamma-1 chain C region



- Molecule 1: Ig gamma-1 chain C region



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  25% 12% 62%

MAG1	MAG2	BRG3	MAN4	MAG5	MAG6	MAG7	FUC8
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.00Å 77.48Å 136.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.67 – 2.80 29.67 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.9 (29.67-2.80) 97.0 (29.67-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.80Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.227 , 0.301 0.225 , 0.303	Depositor DCC
R_{free} test set	1300 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	70.8	Xtrriage
Anisotropy	0.517	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 93.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3536	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.06% 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: MAN, BMA, NAG, EDO, FUC

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	0.78	6/1704 (0.4%)	1.01	12/2322 (0.5%)
1	B	0.73	4/1704 (0.2%)	0.98	11/2322 (0.5%)
All	All	0.75	10/3408 (0.3%)	0.99	23/4644 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	300	TYR	CD2-CE2	-9.20	1.25	1.39
1	A	300	TYR	CB-CG	-8.91	1.38	1.51
1	B	300	TYR	CB-CG	-7.56	1.40	1.51
1	B	300	TYR	CD2-CE2	-7.48	1.28	1.39
1	A	300	TYR	CD1-CE1	-6.92	1.28	1.39
1	A	294	GLU	CB-CG	-6.29	1.40	1.52
1	A	274	LYS	CB-CG	-5.47	1.37	1.52
1	B	274	LYS	CB-CG	-5.44	1.37	1.52
1	B	300	TYR	CD1-CE1	-5.30	1.31	1.39
1	A	344	ARG	CG-CD	-5.15	1.39	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	ARG	NE-CZ-NH1	11.78	126.19	120.30
1	A	344	ARG	NE-CZ-NH1	-11.45	114.58	120.30
1	B	344	ARG	NE-CZ-NH1	-10.09	115.26	120.30
1	B	300	TYR	CA-CB-CG	-9.28	95.76	113.40
1	A	358	LEU	CA-CB-CG	8.53	134.91	115.30
1	A	356	ASP	CB-CA-C	-8.30	93.81	110.40
1	A	300	TYR	CA-CB-CG	-8.25	97.73	113.40
1	A	356	ASP	CB-CG-OD2	-7.93	111.17	118.30
1	A	292	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	B	274	LYS	CB-CA-C	-7.04	96.32	110.40
1	B	292	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	B	358	LEU	CB-CG-CD2	6.59	122.21	111.00
1	B	358	LEU	CB-CG-CD1	-6.55	99.87	111.00
1	A	341	GLY	N-CA-C	-6.45	96.99	113.10
1	B	406	LEU	CA-CB-CG	6.25	129.68	115.30
1	A	356	ASP	CB-CG-OD1	6.14	123.83	118.30
1	B	356	ASP	N-CA-CB	5.88	121.19	110.60
1	B	300	TYR	CB-CA-C	5.72	121.84	110.40
1	A	406	LEU	CA-CB-CG	5.50	127.96	115.30
1	A	293	GLU	OE1-CD-OE2	5.50	129.90	123.30
1	B	341	GLY	N-CA-C	-5.50	99.36	113.10
1	A	358	LEU	N-CA-CB	-5.43	99.54	110.40
1	B	358	LEU	CA-CB-CG	5.43	127.78	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	299	THR	Peptide
1	B	291	PRO	Peptide
1	B	299	THR	Peptide

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	1659	0	1628	85	0
1	B	1659	0	1627	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	99	0	85	11	0
2	D	99	0	85	8	0
3	A	4	0	6	0	0
3	B	8	0	12	1	0
4	A	4	0	0	2	0
4	B	4	0	0	2	0
All	All	3536	0	3443	173	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 25.

All (173) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ARG:HH11	1:A:292:ARG:HG2	1.10	1.14
1:B:266:VAL:HB	1:B:300:TYR:HB3	1.31	1.13
1:A:266:VAL:HB	1:A:300:TYR:HB3	1.30	1.05
1:B:292:ARG:HG2	1:B:292:ARG:HH11	1.29	0.96
1:A:292:ARG:HG3	1:A:300:TYR:CE2	2.04	0.92
1:A:292:ARG:HG3	1:A:300:TYR:HE2	1.36	0.91
1:A:241:PHE:HE2	2:C:2:NAG:H4	1.37	0.90
1:A:292:ARG:HG2	1:A:292:ARG:NH1	1.82	0.89
1:B:292:ARG:HG3	1:B:300:TYR:HE2	1.40	0.86
1:B:292:ARG:HG3	1:B:300:TYR:CE2	2.10	0.86
1:A:241:PHE:CE2	2:C:2:NAG:H4	2.17	0.79
1:B:295:GLN:HG3	1:B:296:TYR:H	1.48	0.78
1:A:292:ARG:CG	1:A:300:TYR:HE2	2.02	0.73
1:A:283:GLU:HG2	1:A:285:HIS:CE1	2.24	0.72
1:B:376:ASP:OD1	4:B:601:HOH:O	2.07	0.72
1:B:283:GLU:HG2	1:B:285:HIS:CE1	2.26	0.71
1:B:299:THR:OG1	1:B:300:TYR:N	2.16	0.71
1:A:295:GLN:HG3	1:A:296:TYR:H	1.56	0.69
1:B:292:ARG:CG	1:B:300:TYR:HE2	2.04	0.69
1:A:338:LYS:NZ	1:A:430:GLU:OE1	2.21	0.69
1:B:370:LYS:NZ	4:B:604:HOH:O	2.22	0.69
1:A:242:LEU:HG	1:A:336:ILE:HG21	1.75	0.68
1:A:295:GLN:OE1	2:C:8:FUC:O2	2.01	0.68
1:B:242:LEU:HG	1:B:336:ILE:HG21	1.75	0.68
1:A:242:LEU:HD12	1:A:243:PHE:H	1.59	0.67
1:B:295:GLN:HG3	1:B:296:TYR:N	2.09	0.66
1:A:273:VAL:HB	1:A:275:PHE:HE1	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:VAL:HG21	1:B:319:TYR:CE1	2.32	0.65
1:B:338:LYS:NZ	1:B:430:GLU:OE1	2.27	0.64
1:B:242:LEU:HD12	1:B:243:PHE:H	1.63	0.64
1:A:308:VAL:HG21	1:A:319:TYR:CE1	2.33	0.63
1:A:301:ARG:NH1	2:C:2:NAG:O7	2.25	0.63
1:B:273:VAL:HB	1:B:275:PHE:HE1	1.62	0.62
1:A:301:ARG:HH12	2:C:2:NAG:C7	2.10	0.62
1:B:379:VAL:O	1:B:380:GLU:HG3	1.99	0.62
1:B:350:THR:H	1:B:439:LYS:HZ3	1.47	0.62
1:A:299:THR:OG1	1:A:300:TYR:N	2.27	0.61
1:A:295:GLN:HG3	1:A:296:TYR:N	2.14	0.61
1:A:390:ASN:ND2	1:A:411:THR:HB	2.15	0.60
2:C:6:MAN:H61	2:C:7:NAG:H82	1.82	0.60
1:A:293:GLU:HG3	1:A:294:GLU:N	2.17	0.59
1:B:292:ARG:HG2	1:B:292:ARG:NH1	2.05	0.59
1:B:241:PHE:HE2	2:D:2:NAG:H4	1.69	0.58
1:B:273:VAL:HG12	1:B:274:LYS:H	1.69	0.58
1:B:338:LYS:HG2	1:B:339:ALA:N	2.19	0.57
1:A:292:ARG:NH1	1:A:292:ARG:CG	2.64	0.57
1:B:312:ASP:HB3	1:B:319:TYR:OH	2.05	0.56
1:B:295:GLN:CG	1:B:296:TYR:H	2.15	0.56
1:A:379:VAL:O	1:A:380:GLU:HG3	2.06	0.56
1:A:350:THR:H	1:A:439:LYS:HZ3	1.54	0.55
1:A:295:GLN:CG	1:A:296:TYR:H	2.19	0.54
1:A:336:ILE:HG12	1:A:337:SER:N	2.23	0.54
1:B:283:GLU:HG2	1:B:285:HIS:HE1	1.73	0.54
1:A:249:ASP:HA	1:A:255:ARG:HD3	1.89	0.54
1:A:338:LYS:HG2	1:A:339:ALA:N	2.23	0.53
1:B:241:PHE:CE2	2:D:2:NAG:H4	2.42	0.53
1:A:273:VAL:HG12	1:A:274:LYS:H	1.72	0.53
1:A:397:VAL:HB	1:A:405:PHE:CE2	2.43	0.53
1:A:357:GLU:HG3	1:B:349:TYR:CZ	2.44	0.53
1:B:277:TRP:O	1:B:283:GLU:HG3	2.08	0.53
1:A:312:ASP:HB3	1:A:319:TYR:OH	2.10	0.52
1:B:397:VAL:HB	1:B:405:PHE:CE2	2.44	0.52
1:A:275:PHE:N	1:A:275:PHE:CD1	2.78	0.51
1:B:248:LYS:HD3	1:B:255:ARG:NH1	2.25	0.51
2:D:1:NAG:O6	2:D:2:NAG:N2	2.44	0.51
1:A:296:TYR:C	1:A:298:SER:H	2.14	0.51
1:B:249:ASP:HA	1:B:255:ARG:HD3	1.93	0.51
1:A:242:LEU:HD12	1:A:243:PHE:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:ASN:ND2	1:B:411:THR:HB	2.26	0.50
1:B:415:SER:O	1:B:419:GLN:HG3	2.10	0.50
1:B:275:PHE:CD1	1:B:275:PHE:N	2.79	0.50
1:B:368:LEU:HD12	1:B:369:VAL:H	1.76	0.50
2:C:2:NAG:O4	2:D:4:MAN:O4	2.27	0.50
1:A:275:PHE:N	1:A:275:PHE:HD1	2.10	0.50
1:A:377:ILE:HG12	1:A:378:ALA:N	2.26	0.49
1:B:257:PRO:HG2	1:B:308:VAL:O	2.12	0.49
1:B:296:TYR:C	1:B:298:SER:H	2.15	0.49
1:A:377:ILE:HD11	1:A:427:VAL:CG1	2.42	0.49
1:A:415:SER:O	1:A:419:GLN:HG3	2.12	0.49
1:B:293:GLU:HG3	1:B:294:GLU:N	2.27	0.49
1:A:390:ASN:HD22	1:A:411:THR:HB	1.78	0.49
1:A:283:GLU:HG2	1:A:285:HIS:HE1	1.74	0.49
1:B:279:VAL:HG23	1:B:284:VAL:HG21	1.95	0.49
1:B:275:PHE:N	1:B:275:PHE:HD1	2.11	0.49
1:A:368:LEU:HD12	1:A:369:VAL:H	1.78	0.48
1:B:274:LYS:HB2	1:B:324:SER:O	2.13	0.48
1:A:370:LYS:HB2	4:A:602:HOH:O	2.14	0.48
2:D:1:NAG:H61	2:D:2:NAG:H82	1.96	0.47
1:B:358:LEU:C	1:B:358:LEU:HD12	2.35	0.47
1:B:286:ASN:HB3	1:B:306:LEU:HD12	1.97	0.47
1:B:336:ILE:HG12	1:B:337:SER:N	2.28	0.47
1:A:262:VAL:HG11	1:A:301:ARG:NH2	2.30	0.47
1:A:308:VAL:HG21	1:A:319:TYR:CZ	2.49	0.47
2:C:1:NAG:H4	2:C:8:FUC:H5	1.95	0.47
1:B:301:ARG:NH2	2:D:2:NAG:O7	2.48	0.47
1:A:292:ARG:O	1:A:300:TYR:OH	2.32	0.47
1:B:438:GLN:O	1:B:438:GLN:HG2	2.15	0.47
1:B:245:PRO:HD3	1:B:259:VAL:HG12	1.96	0.47
1:B:381:TRP:HB2	1:B:391:TYR:CD1	2.50	0.47
1:B:262:VAL:HG11	1:B:301:ARG:NH2	2.30	0.46
1:A:264:VAL:CG2	2:C:1:NAG:H5	2.45	0.46
1:B:325:ASN:OD1	1:B:328:LEU:N	2.48	0.46
1:A:266:VAL:CG1	1:A:271:PRO:HA	2.46	0.46
2:D:7:NAG:O4	2:D:7:NAG:O6	2.33	0.46
1:A:292:ARG:HG3	1:A:300:TYR:CZ	2.50	0.46
1:B:417:TRP:CZ2	1:B:443:LEU:HD13	2.52	0.45
1:A:325:ASN:OD1	1:A:328:LEU:N	2.49	0.45
1:B:294:GLU:HB3	1:B:300:TYR:HE1	1.81	0.45
1:A:350:THR:OG1	1:A:441:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:VAL:HG22	1:A:442:SER:HB3	1.99	0.45
1:B:274:LYS:C	1:B:275:PHE:HD1	2.21	0.45
1:A:245:PRO:HD3	1:A:259:VAL:HG12	1.99	0.45
1:A:391:TYR:HB3	1:A:410:LEU:HD12	1.99	0.45
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.52	0.44
1:B:338:LYS:HG2	1:B:339:ALA:H	1.83	0.44
1:A:270:ASP:OD1	1:A:326:LYS:HG2	2.18	0.44
1:A:277:TRP:O	1:A:283:GLU:HG3	2.16	0.44
1:A:340:LYS:HA	1:A:340:LYS:HD3	1.78	0.44
1:B:351:LEU:HB2	1:B:366:THR:HB	2.00	0.44
1:A:349:TYR:CZ	1:B:357:GLU:HG3	2.52	0.44
1:A:370:LYS:HE3	4:A:602:HOH:O	2.18	0.44
1:A:381:TRP:HB2	1:A:391:TYR:CD1	2.53	0.44
1:A:279:VAL:HG23	1:A:284:VAL:HG21	1.99	0.44
1:B:345:GLU:HA	1:B:346:PRO:HD2	1.84	0.44
1:B:350:THR:OG1	1:B:441:LEU:HB2	2.18	0.44
1:A:249:ASP:HB3	1:A:257:PRO:HB3	2.00	0.44
1:B:292:ARG:CG	1:B:292:ARG:NH1	2.78	0.44
1:B:401:ASP:OD1	1:B:403:SER:OG	2.27	0.44
1:B:317:LYS:HB2	1:B:319:TYR:CE2	2.53	0.43
1:A:274:LYS:HB3	1:A:324:SER:HB3	1.99	0.43
1:A:391:TYR:HB2	1:A:409:LYS:O	2.18	0.43
1:A:274:LYS:HB3	1:A:324:SER:O	2.18	0.43
1:A:279:VAL:O	1:A:282:VAL:HB	2.19	0.43
1:A:283:GLU:CG	1:A:285:HIS:HE1	2.32	0.43
1:B:308:VAL:HG21	1:B:319:TYR:HE1	1.83	0.43
1:A:257:PRO:HG2	1:A:308:VAL:O	2.18	0.43
1:B:443:LEU:HD12	1:B:443:LEU:HA	1.74	0.43
2:C:2:NAG:O3	2:C:6:MAN:H3	2.18	0.43
1:A:264:VAL:HG21	2:C:1:NAG:O4	2.18	0.43
1:A:349:TYR:HB3	1:B:354:SER:CB	2.47	0.43
1:A:438:GLN:HG2	1:A:438:GLN:O	2.19	0.43
1:B:270:ASP:OD1	1:B:326:LYS:HG2	2.18	0.43
1:A:328:LEU:HA	1:A:329:PRO:HD3	1.88	0.43
1:B:247:PRO:O	1:B:251:LEU:HG	2.19	0.43
1:B:266:VAL:CG1	1:B:271:PRO:HA	2.48	0.43
1:B:344:ARG:HH11	1:B:344:ARG:HD2	1.41	0.42
1:A:443:LEU:HD12	1:A:443:LEU:HA	1.80	0.42
1:A:286:ASN:HB3	1:A:306:LEU:HD12	2.02	0.42
1:B:377:ILE:HD11	1:B:427:VAL:CG1	2.50	0.42
1:A:377:ILE:HG12	1:A:378:ALA:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LYS:HB3	1:A:305:VAL:O	2.20	0.42
1:A:294:GLU:HA	1:A:300:TYR:CE1	2.54	0.42
1:A:296:TYR:O	1:A:298:SER:N	2.50	0.42
1:B:242:LEU:HD12	1:B:243:PHE:N	2.31	0.42
1:B:320:LYS:HD3	1:B:333:GLU:OE2	2.20	0.41
1:B:238:PRO:HB3	1:B:265:ASP:O	2.20	0.41
1:B:406:LEU:HD22	3:B:509:EDO:H12	2.02	0.41
1:B:425:CYS:O	1:B:438:GLN:HA	2.20	0.41
1:B:399:ASP:OD1	1:B:400:SER:N	2.51	0.41
1:A:338:LYS:HG2	1:A:339:ALA:H	1.86	0.41
1:A:394:THR:HA	1:B:397:VAL:HG21	2.03	0.41
1:B:253:ILE:HG13	1:B:254:SER:H	1.86	0.41
1:B:308:VAL:HG21	1:B:319:TYR:CZ	2.55	0.41
1:B:243:PHE:HE1	2:D:3:BMA:H62	1.86	0.41
1:B:367:CYS:O	1:B:407:TYR:HA	2.21	0.41
1:B:373:TYR:CG	1:B:374:PRO:HA	2.55	0.41
1:B:296:TYR:O	1:B:298:SER:N	2.51	0.41
1:A:312:ASP:O	1:A:317:LYS:HG2	2.21	0.40
1:A:344:ARG:HB2	1:A:373:TYR:N	2.36	0.40
1:A:417:TRP:CZ2	1:A:443:LEU:HD13	2.55	0.40
1:B:292:ARG:O	1:B:300:TYR:OH	2.39	0.40
1:B:373:TYR:CD2	1:B:374:PRO:HA	2.57	0.40
1:B:312:ASP:O	1:B:317:LYS:HG2	2.21	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	206/208 (99%)	170 (82%)	28 (14%)	8 (4%)	3 10
1	B	206/208 (99%)	171 (83%)	26 (13%)	9 (4%)	2 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	412/416 (99%)	341 (83%)	54 (13%)	17 (4%)	3 9

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	418	GLN
1	A	419	GLN
1	A	421	ASN
1	B	418	GLN
1	B	419	GLN
1	B	421	ASN
1	A	297	ASN
1	B	297	ASN
1	B	431	ALA
1	A	355	ARG
1	B	355	ARG
1	A	431	ALA
1	B	288	LYS
1	B	253	ILE
1	A	253	ILE
1	A	420	GLY
1	B	420	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	193/193 (100%)	168 (87%)	25 (13%)	4 13
1	B	193/193 (100%)	165 (86%)	28 (14%)	3 9
All	All	386/386 (100%)	333 (86%)	53 (14%)	3 11

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	SER

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Mol	Chain	Res	Type
1	A	242	LEU
1	A	254	SER
1	A	256	THR
1	A	260	THR
1	A	272	GLU
1	A	273	VAL
1	A	275	PHE
1	A	290	LYS
1	A	292	ARG
1	A	293	GLU
1	A	295	GLN
1	A	299	THR
1	A	321	CYS
1	A	326	LYS
1	A	328	LEU
1	A	336	ILE
1	A	347	GLN
1	A	358	LEU
1	A	383	SER
1	A	389	ASN
1	A	406	LEU
1	A	438	GLN
1	A	440	SER
1	A	441	LEU
1	B	239	SER
1	B	242	LEU
1	B	254	SER
1	B	256	THR
1	B	258	GLU
1	B	260	THR
1	B	272	GLU
1	B	273	VAL
1	B	275	PHE
1	B	282	VAL
1	B	290	LYS
1	B	292	ARG
1	B	293	GLU
1	B	294	GLU
1	B	295	GLN
1	B	299	THR
1	B	321	CYS
1	B	326	LYS

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Mol	Chain	Res	Type
1	B	328	LEU
1	B	336	ILE
1	B	344	ARG
1	B	356	ASP
1	B	358	LEU
1	B	383	SER
1	B	389	ASN
1	B	438	GLN
1	B	440	SER
1	B	441	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	295	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

16 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	C	1	1,2	14,14,15	0.82	1 (7%)	17,19,21	2.15	6 (35%)
2	NAG	C	2	2	14,14,15	0.76	1 (7%)	17,19,21	1.53	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	C	3	2	11,11,12	0.69	0	15,15,17	1.68	3 (20%)
2	MAN	C	4	2	11,11,12	0.57	0	15,15,17	1.22	2 (13%)
2	NAG	C	5	2	14,14,15	0.54	0	17,19,21	1.37	4 (23%)
2	MAN	C	6	2	11,11,12	0.71	0	15,15,17	1.86	4 (26%)
2	NAG	C	7	2	14,14,15	0.47	0	17,19,21	2.08	4 (23%)
2	FUC	C	8	2	10,10,11	0.90	1 (10%)	14,14,16	1.05	0
2	NAG	D	1	1,2	14,14,15	0.36	0	17,19,21	1.63	3 (17%)
2	NAG	D	2	2	14,14,15	0.69	0	17,19,21	1.72	4 (23%)
2	BMA	D	3	2	11,11,12	0.81	0	15,15,17	1.30	1 (6%)
2	MAN	D	4	2	11,11,12	0.58	0	15,15,17	1.24	2 (13%)
2	NAG	D	5	2	14,14,15	0.49	0	17,19,21	0.73	0
2	MAN	D	6	2	11,11,12	0.67	0	15,15,17	0.76	0
2	NAG	D	7	2	14,14,15	0.44	0	17,19,21	1.34	1 (5%)
2	FUC	D	8	2	10,10,11	0.71	0	14,14,16	1.40	4 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	NAG	C	5	2	-	4/6/23/26	0/1/1/1
2	MAN	C	6	2	-	2/2/19/22	0/1/1/1
2	NAG	C	7	2	-	3/6/23/26	0/1/1/1
2	FUC	C	8	2	-	-	0/1/1/1
2	NAG	D	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	1/2/19/22	0/1/1/1
2	NAG	D	5	2	-	3/6/23/26	0/1/1/1
2	MAN	D	6	2	-	2/2/19/22	0/1/1/1
2	NAG	D	7	2	-	4/6/23/26	0/1/1/1
2	FUC	D	8	2	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	C1-C2	2.27	1.55	1.52
2	C	2	NAG	O5-C1	-2.04	1.40	1.43
2	C	8	FUC	O5-C1	-2.03	1.40	1.43

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-O5-C5	4.87	118.80	112.19
2	D	2	NAG	C1-O5-C5	-4.61	105.95	112.19
2	C	6	MAN	O2-C2-C1	4.45	118.26	109.15
2	D	7	NAG	C1-O5-C5	4.43	118.20	112.19
2	C	7	NAG	C2-N2-C7	-4.08	117.09	122.90
2	C	3	BMA	C1-C2-C3	4.04	114.64	109.67
2	C	7	NAG	C4-C3-C2	-4.02	105.12	111.02
2	C	7	NAG	O5-C1-C2	-3.95	105.06	111.29
2	C	1	NAG	O5-C5-C6	3.92	113.35	107.20
2	C	1	NAG	C4-C3-C2	3.85	116.67	111.02
2	C	1	NAG	C1-O5-C5	3.72	117.23	112.19
2	C	7	NAG	C1-O5-C5	3.59	117.05	112.19
2	C	2	NAG	C2-N2-C7	-3.47	117.96	122.90
2	C	3	BMA	O3-C3-C2	-2.99	104.28	109.99
2	C	6	MAN	O5-C5-C6	2.89	111.73	107.20
2	D	2	NAG	C6-C5-C4	2.77	119.50	113.00
2	D	4	MAN	O5-C5-C6	2.77	111.55	107.20
2	C	1	NAG	C3-C4-C5	2.77	115.17	110.24
2	C	5	NAG	C3-C4-C5	2.75	115.15	110.24
2	C	5	NAG	C1-O5-C5	2.75	115.92	112.19
2	D	4	MAN	O2-C2-C1	2.69	114.65	109.15
2	C	5	NAG	O5-C1-C2	-2.54	107.27	111.29
2	C	2	NAG	O5-C1-C2	-2.49	107.36	111.29
2	D	3	BMA	C1-C2-C3	2.48	112.71	109.67
2	C	2	NAG	C4-C3-C2	2.47	114.64	111.02
2	D	2	NAG	C2-N2-C7	-2.46	119.39	122.90
2	C	6	MAN	C1-O5-C5	-2.45	108.88	112.19
2	D	8	FUC	O5-C5-C4	2.44	113.89	109.52
2	D	8	FUC	C1-O5-C5	2.42	118.27	112.78
2	C	4	MAN	C1-O5-C5	2.40	115.45	112.19
2	D	2	NAG	O4-C4-C5	2.40	115.25	109.30
2	C	1	NAG	O5-C5-C4	2.39	116.63	110.83
2	D	8	FUC	C1-C2-C3	2.30	112.50	109.67
2	C	2	NAG	C3-C4-C5	2.29	114.32	110.24
2	C	4	MAN	C6-C5-C4	-2.28	107.67	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	BMA	O5-C5-C6	2.22	110.69	107.20
2	D	1	NAG	O5-C1-C2	-2.20	107.81	111.29
2	C	6	MAN	O2-C2-C3	-2.16	105.81	110.14
2	D	1	NAG	O5-C5-C4	2.14	116.03	110.83
2	C	5	NAG	O5-C5-C6	2.10	110.49	107.20
2	C	1	NAG	O7-C7-C8	-2.08	118.20	122.06
2	D	8	FUC	C3-C4-C5	2.03	112.94	109.77
2	C	2	NAG	O4-C4-C5	2.01	114.28	109.30

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	5	NAG	C8-C7-N2-C2
2	D	5	NAG	O7-C7-N2-C2
2	D	7	NAG	C8-C7-N2-C2
2	D	7	NAG	O7-C7-N2-C2
2	C	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	C	5	NAG	C8-C7-N2-C2
2	C	5	NAG	O7-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	6	MAN	O5-C5-C6-O6
2	D	7	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	C	5	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	7	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	D	6	MAN	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	C	5	NAG	O5-C5-C6-O6
2	C	6	MAN	C4-C5-C6-O6
2	D	4	MAN	O5-C5-C6-O6
2	C	7	NAG	C8-C7-N2-C2
2	C	6	MAN	O5-C5-C6-O6
2	C	7	NAG	O5-C5-C6-O6

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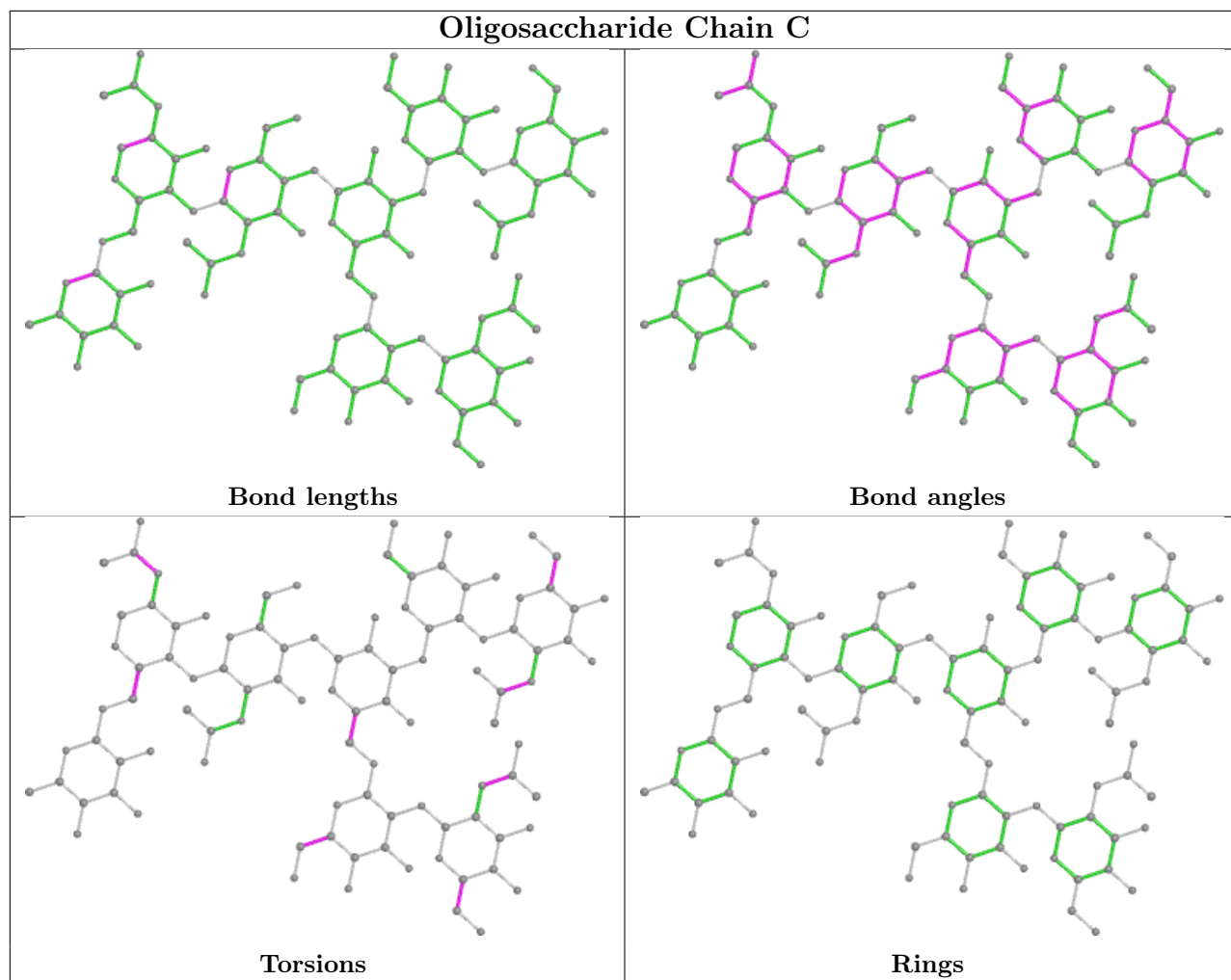
Mol	Chain	Res	Type	Atoms
2	D	5	NAG	O5-C5-C6-O6
2	C	7	NAG	O7-C7-N2-C2

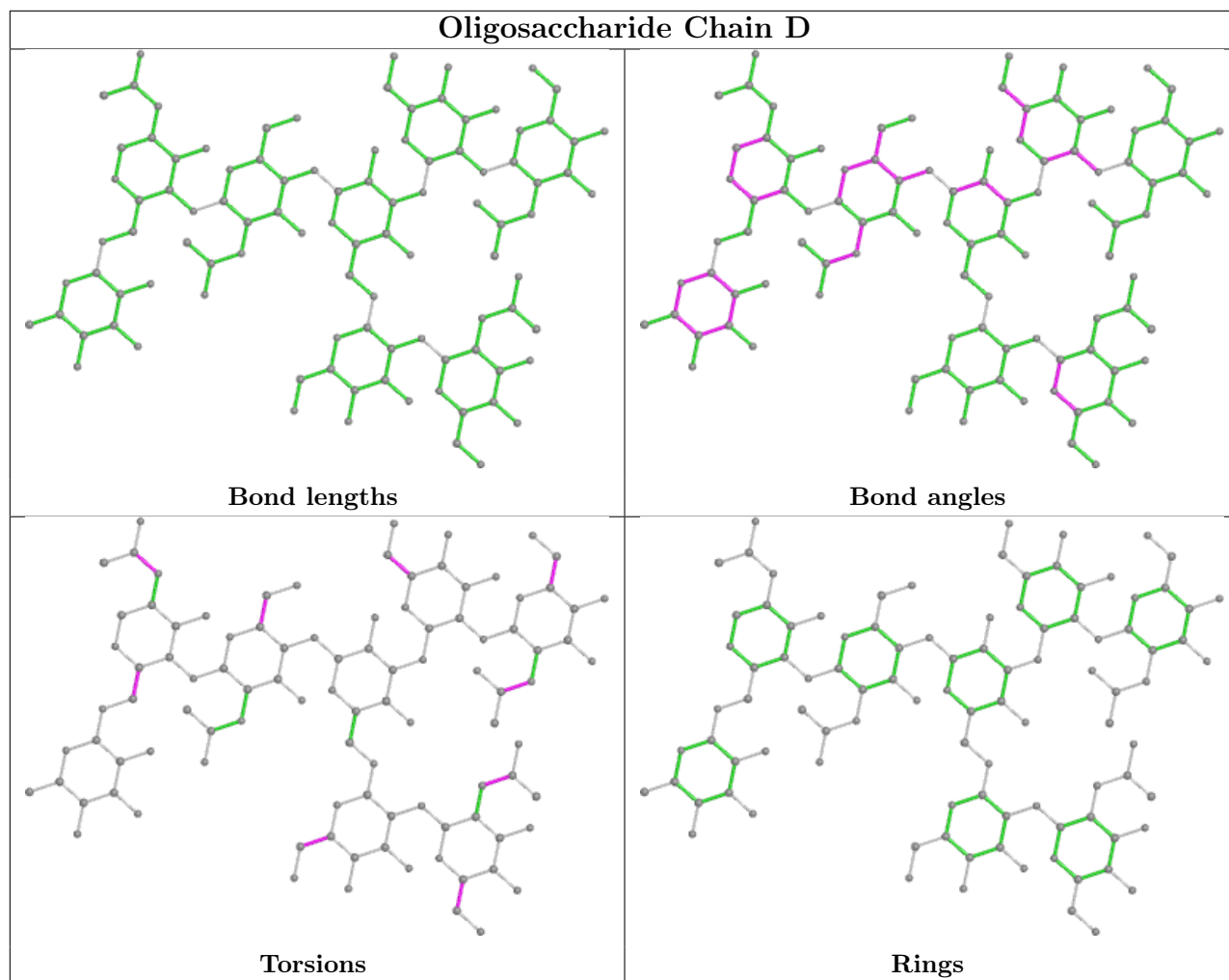
There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	7	NAG	1	0
2	C	8	FUC	2	0
2	C	1	NAG	3	0
2	C	2	NAG	6	0
2	D	1	NAG	2	0
2	D	4	MAN	1	0
2	D	2	NAG	5	0
2	D	3	BMA	1	0
2	D	7	NAG	1	0
2	C	6	MAN	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](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	B	510	-	3,3,3	0.50	0	2,2,2	0.40	0
3	EDO	A	509	-	3,3,3	0.62	0	2,2,2	0.19	0
3	EDO	B	509	-	3,3,3	0.59	0	2,2,2	0.41	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	EDO	B	510	-	-	1/1/1/1	-
3	EDO	A	509	-	-	0/1/1/1	-
3	EDO	B	509	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	510	EDO	O1-C1-C2-O2
3	B	509	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	509	EDO	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	208/208 (100%)	0.44	24 (11%) 4 2	49, 107, 211, 295	0
1	B	208/208 (100%)	0.54	24 (11%) 4 2	47, 108, 213, 293	0
All	All	416/416 (100%)	0.49	48 (11%) 4 2	47, 107, 213, 295	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	239	SER	7.9
1	A	269	GLU	6.8
1	B	238	PRO	6.5
1	A	239	SER	6.2
1	A	330	ALA	6.0
1	A	329	PRO	5.5
1	A	263	VAL	5.5
1	A	332	ILE	5.3
1	B	237	GLY	4.0
1	A	325	ASN	4.0
1	A	266	VAL	3.9
1	B	300	TYR	3.8
1	B	324	SER	3.8
1	A	237	GLY	3.7
1	B	326	LYS	3.7
1	B	298	SER	3.6
1	A	240	VAL	3.6
1	B	329	PRO	3.6
1	A	328	LEU	3.5
1	B	367	CYS	3.5
1	A	268	HIS	3.5
1	A	327	ALA	3.4
1	A	296	TYR	3.3
1	A	300	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	272	GLU	3.2
1	A	273	VAL	3.2
1	B	319	TYR	3.1
1	B	366	THR	2.9
1	B	310	ALA	2.9
1	B	297	ASN	2.8
1	B	323	VAL	2.8
1	B	322	LYS	2.8
1	A	238	PRO	2.8
1	B	331	PRO	2.7
1	A	366	THR	2.7
1	A	326	LYS	2.5
1	B	291	PRO	2.5
1	A	298	SER	2.5
1	B	408	SER	2.4
1	A	270	ASP	2.4
1	B	279	VAL	2.4
1	B	282	VAL	2.4
1	A	367	CYS	2.3
1	B	296	TYR	2.2
1	B	274	LYS	2.2
1	B	240	VAL	2.2
1	A	299	THR	2.1
1	B	301	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FUC	D	8	10/11	0.70	0.23	98,185,210,240	0
2	NAG	C	5	14/15	0.72	0.38	111,185,203,203	0
2	NAG	D	2	14/15	0.73	0.29	166,201,222,233	0
2	FUC	C	8	10/11	0.74	0.36	159,199,214,217	0

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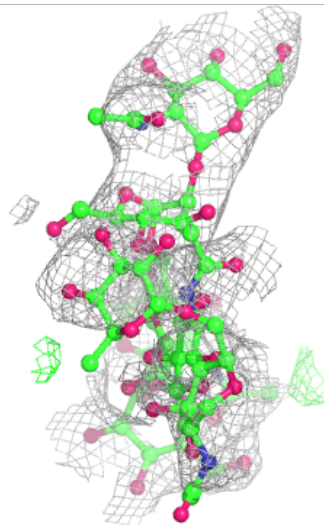
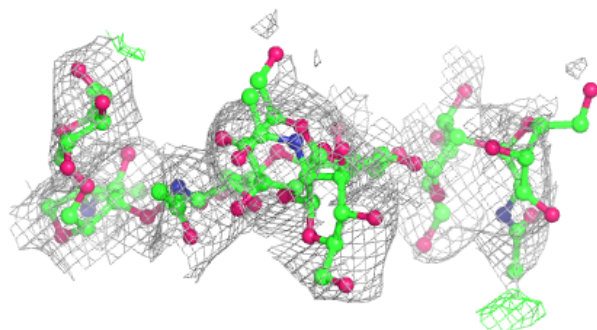
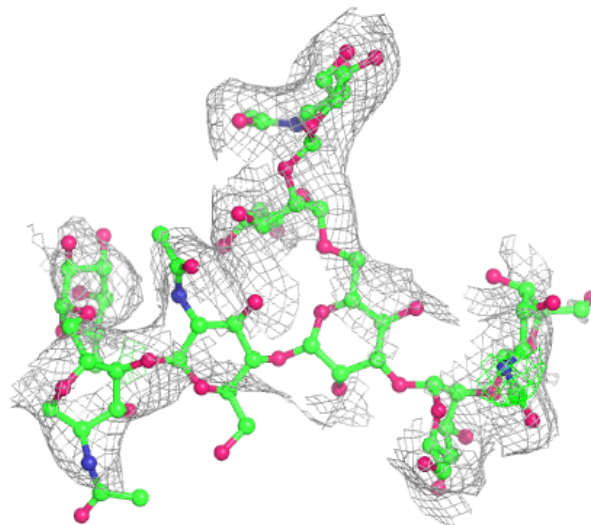
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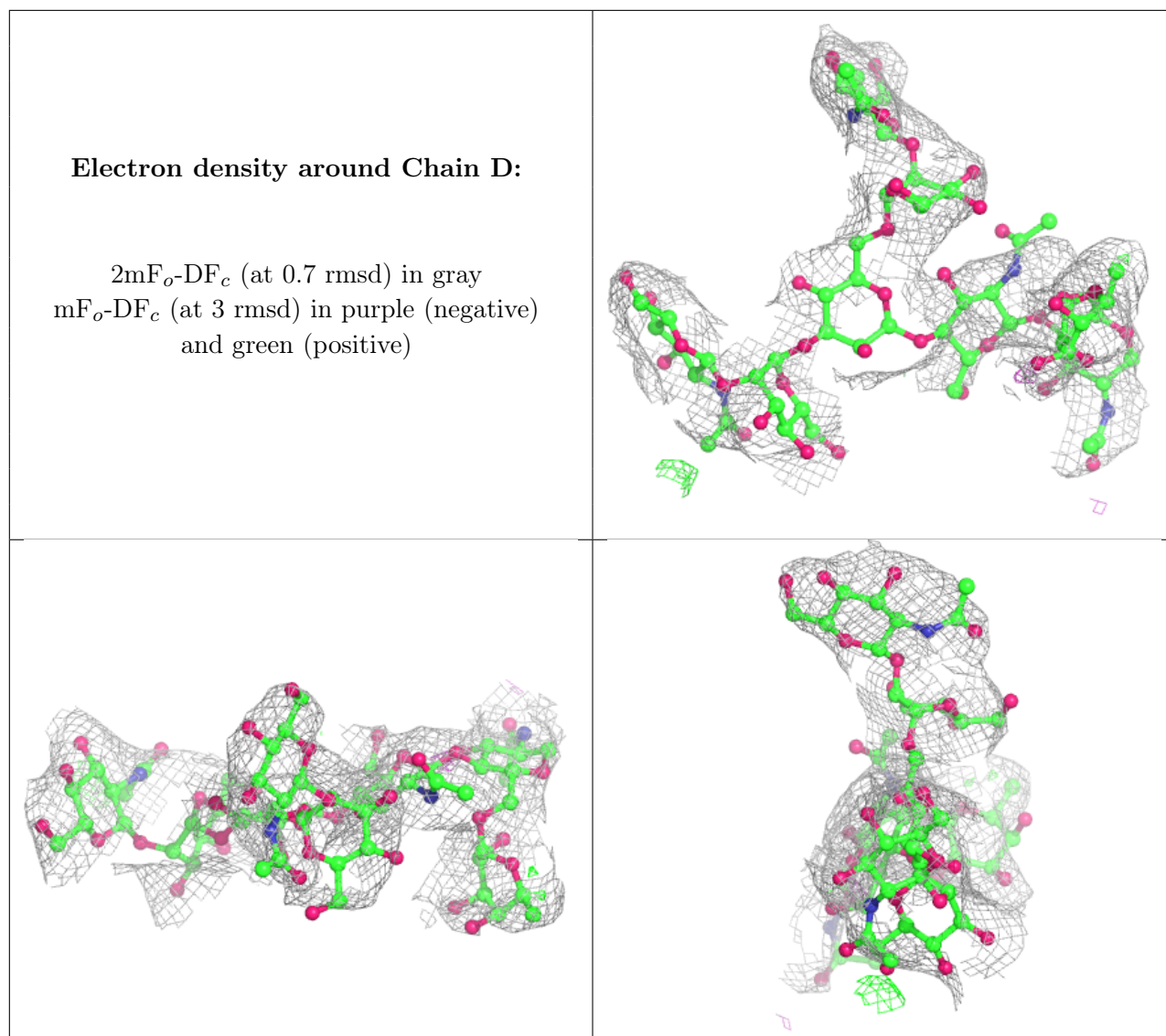
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	D	1	14/15	0.76	0.28	192,205,229,254	0
2	BMA	C	3	11/12	0.78	0.11	153,184,202,210	0
2	BMA	D	3	11/12	0.81	0.12	153,163,168,173	0
2	NAG	C	2	14/15	0.81	0.28	146,200,219,221	0
2	NAG	C	1	14/15	0.83	0.25	129,186,217,226	0
2	MAN	C	4	11/12	0.84	0.12	130,157,195,202	0
2	NAG	D	5	14/15	0.85	0.14	147,181,204,204	0
2	MAN	C	6	11/12	0.88	0.20	155,171,184,188	0
2	NAG	D	7	14/15	0.88	0.23	98,153,170,173	0
2	MAN	D	4	11/12	0.88	0.16	93,161,181,206	0
2	NAG	C	7	14/15	0.89	0.17	85,130,155,162	0
2	MAN	D	6	11/12	0.90	0.18	114,153,164,176	0

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

Electron density around Chain C:

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





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
3	EDO	B	510	4/4	0.80	0.27	113,142,146,150	0
3	EDO	A	509	4/4	0.85	0.84	97,102,116,121	0
3	EDO	B	509	4/4	0.87	0.27	53,66,78,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.