



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:29 AM UTC

PDB ID : 2V5S / pdb_00002v5s
Title : Structural basis for Dscam isoform specificity
Authors : Meijers, R.; Puettmann-Holgado, R.; Skiniotis, G.; Liu, J.-H.; Walz, T.;
Schmucker, D.; Wang, J.-H.
Deposited on : 2007-07-09
Resolution : 2.30 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

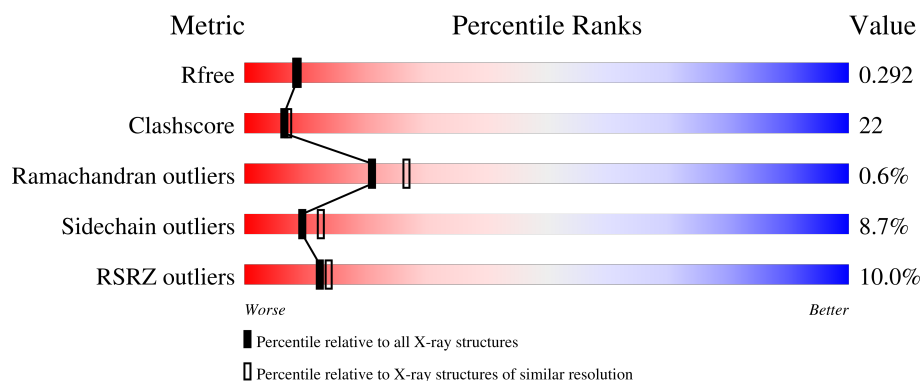
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	394	10% 64% 29% 5% ••
1	B	394	10% 67% 26% 5% •
2	C	2	50% 50%
2	D	2	100%
2	E	2	50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	2	 100%

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	F	1	X	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6627 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 DSCAM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	19	0
			3110	1962	538	597	13			
1	B	394	Total	C	N	O	S	0	21	0
			3159	1994	545	607	13			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	expression tag	UNP Q9NBA1
A	-4	TYR	-	expression tag	UNP Q9NBA1
A	-3	PHE	-	expression tag	UNP Q9NBA1
A	-2	GLN	-	expression tag	UNP Q9NBA1
A	-1	GLY	-	expression tag	UNP Q9NBA1
A	0	ASP	-	expression tag	UNP Q9NBA1
A	207	ILE	VAL	variant	UNP Q9NBA1
A	211	ALA	PRO	variant	UNP Q9NBA1
A	213	ARG	LYS	variant	UNP Q9NBA1
A	214	THR	ILE	variant	UNP Q9NBA1
A	215	PRO	ASN	variant	UNP Q9NBA1
A	216	ALA	THR	variant	UNP Q9NBA1
A	218	VAL	THR	variant	UNP Q9NBA1
A	219	GLN	TYR	variant	UNP Q9NBA1
A	222	LEU	ASN	variant	UNP Q9NBA1
A	223	GLU	ILE	variant	UNP Q9NBA1
A	224	LEU	VAL	variant	UNP Q9NBA1
A	225	MET	GLU	variant	UNP Q9NBA1
A	226	VAL	SER	variant	UNP Q9NBA1
A	227	ALA	MET	variant	UNP Q9NBA1
A	228	HIS	ALA	variant	UNP Q9NBA1
A	229	THR	SER	variant	UNP Q9NBA1
A	230	ILE	THR	variant	UNP Q9NBA1
A	231	SER	ALA	variant	UNP Q9NBA1
A	232	LEU	ILE	variant	UNP Q9NBA1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	239	PHE	TYR	variant	UNP Q9NBA1
B	-5	ALA	-	expression tag	UNP Q9NBA1
B	-4	TYR	-	expression tag	UNP Q9NBA1
B	-3	PHE	-	expression tag	UNP Q9NBA1
B	-2	GLN	-	expression tag	UNP Q9NBA1
B	-1	GLY	-	expression tag	UNP Q9NBA1
B	0	ASP	-	expression tag	UNP Q9NBA1
B	207	ILE	VAL	variant	UNP Q9NBA1
B	211	ALA	PRO	variant	UNP Q9NBA1
B	213	ARG	LYS	variant	UNP Q9NBA1
B	214	THR	ILE	variant	UNP Q9NBA1
B	215	PRO	ASN	variant	UNP Q9NBA1
B	216	ALA	THR	variant	UNP Q9NBA1
B	218	VAL	THR	variant	UNP Q9NBA1
B	219	GLN	TYR	variant	UNP Q9NBA1
B	222	LEU	ASN	variant	UNP Q9NBA1
B	223	GLU	ILE	variant	UNP Q9NBA1
B	224	LEU	VAL	variant	UNP Q9NBA1
B	225	MET	GLU	variant	UNP Q9NBA1
B	226	VAL	SER	variant	UNP Q9NBA1
B	227	ALA	MET	variant	UNP Q9NBA1
B	228	HIS	ALA	variant	UNP Q9NBA1
B	229	THR	SER	variant	UNP Q9NBA1
B	230	ILE	THR	variant	UNP Q9NBA1
B	231	SER	ALA	variant	UNP Q9NBA1
B	232	LEU	ILE	variant	UNP Q9NBA1
B	239	PHE	TYR	variant	UNP Q9NBA1

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

Continued on next page...

Continued from previous page...

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

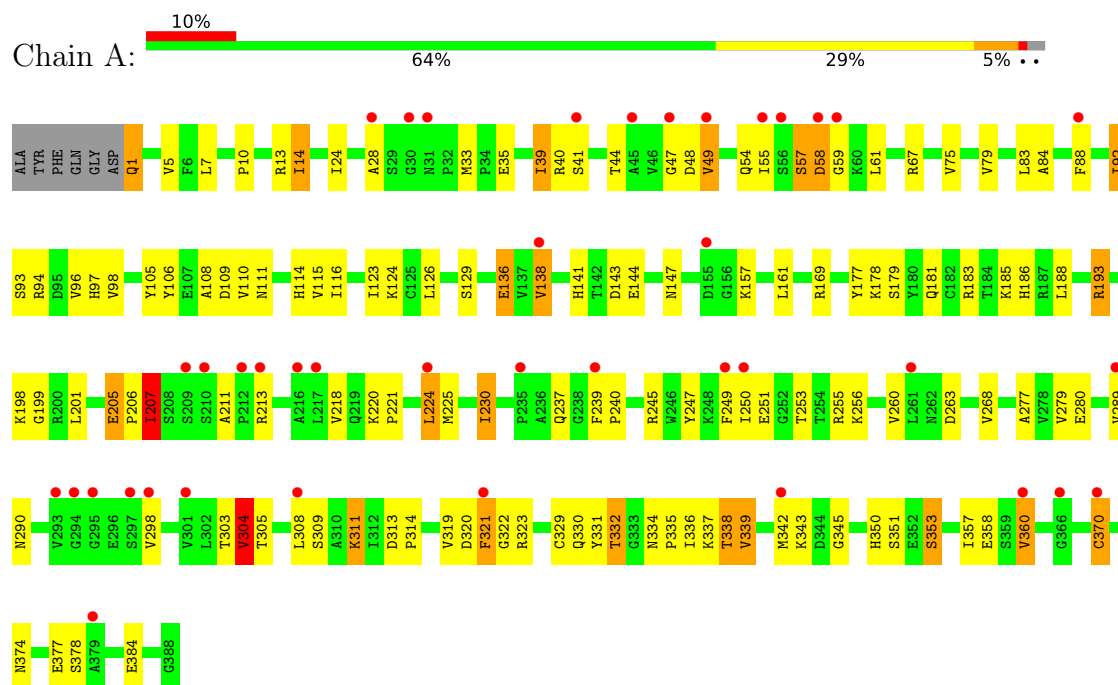
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	119	Total	O	0	0
			119	119		
3	B	127	Total	O	0	0
			127	127		

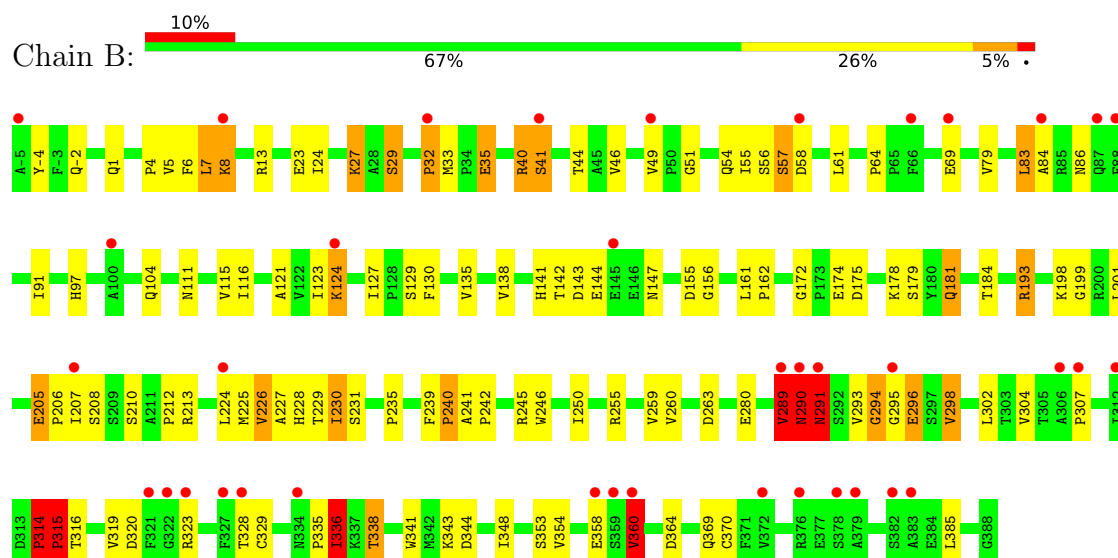
3 Residue-property plots

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: DSCAM



• Molecule 1: DSCAM



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

Chain C:  50% 50%

MAG1
MAG2

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

Chain D:  100%

MAG1
MAG2

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

Chain E:  50% 50%

MAG1
MAG2

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

Chain F:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	99.77Å 166.84Å 125.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.30 19.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.6 (19.99-2.30) 95.4 (19.99-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.28Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.227 , 0.287 0.235 , 0.292	Depositor DCC
R_{free} test set	2269 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 69.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6627	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.8332e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.56	1/3243 (0.0%)	1.38	32/4394 (0.7%)
1	B	0.56	2/3299 (0.1%)	1.45	28/4470 (0.6%)
All	All	0.56	3/6542 (0.0%)	1.42	60/8864 (0.7%)

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	4
1	B	0	7
All	All	0	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	109	ASP	C-N	-8.58	1.23	1.33
1	B	-2	GLN	CD-OE1	7.50	1.37	1.23
1	B	-2	GLN	CD-NE2	5.36	1.44	1.33

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	MET	N-CA-C	-15.89	86.58	109.62
1	B	336	ILE	N-CA-C	12.72	125.16	108.12
1	B	290	ASN	N-CA-C	11.03	125.39	108.96
1	B	314	PRO	CA-C-N	10.62	133.11	119.84
1	B	314	PRO	C-N-CA	10.62	133.11	119.84
1	B	-4	TYR	N-CA-C	8.60	121.44	108.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	VAL	N-CA-C	8.07	126.12	109.34
1	A	138	VAL	N-CA-C	-7.73	105.23	112.96
1	B	40	ARG	N-CA-C	-7.55	99.35	110.52
1	A	138	VAL	CB-CA-C	7.49	117.65	111.06
1	A	108	ALA	O-C-N	-7.18	114.83	123.16
1	B	289[A]	VAL	N-CA-C	7.14	119.10	108.46
1	B	294	GLY	O-C-N	-7.08	117.15	123.88
1	B	208	SER	N-CA-C	-7.01	99.18	110.32
1	A	48	ASP	N-CA-C	-6.97	98.38	109.59
1	B	207	ILE	CB-CA-C	-6.66	103.89	111.55
1	B	293	VAL	N-CA-C	6.17	118.12	111.58
1	A	49	VAL	N-CA-C	-6.16	102.05	108.15
1	B	64	PRO	O-C-N	6.16	124.14	121.31
1	A	338	THR	N-CA-C	6.10	118.34	109.07
1	A	322	GLY	N-CA-C	-6.00	98.97	113.18
1	B	24	ILE	CB-CA-C	-5.93	101.67	110.33
1	A	339	VAL	CB-CA-C	-5.79	101.88	110.33
1	A	205[A]	GLU	CA-C-N	-5.78	113.23	120.51
1	A	205[A]	GLU	C-N-CA	-5.78	113.23	120.51
1	A	205[B]	GLU	CA-C-N	-5.78	113.23	120.51
1	A	205[B]	GLU	C-N-CA	-5.78	113.23	120.51
1	B	338	THR	N-CA-C	5.77	118.05	108.99
1	B	64	PRO	CA-C-O	-5.68	116.81	120.90
1	B	144[A]	GLU	N-CA-C	-5.68	106.24	112.72
1	B	144[B]	GLU	N-CA-C	-5.68	106.24	112.72
1	A	183	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	A	161	LEU	CA-C-N	5.67	125.78	119.32
1	A	161	LEU	C-N-CA	5.67	125.78	119.32
1	A	211	ALA	CA-C-N	5.66	125.67	119.90
1	A	211	ALA	C-N-CA	5.66	125.67	119.90
1	A	207	ILE	CB-CA-C	-5.62	105.08	111.55
1	B	193	ARG	CB-CA-C	-5.58	98.46	110.45
1	B	111	ASN	N-CA-C	5.46	118.41	110.17
1	A	377	GLU	N-CA-C	5.45	116.81	108.52
1	A	105	TYR	N-CA-C	5.45	118.37	110.42
1	A	75	VAL	CB-CA-C	-5.44	105.29	111.55
1	A	321	PHE	N-CA-C	-5.43	103.36	110.53
1	A	357	ILE	N-CA-C	-5.38	100.67	108.36
1	B	161	LEU	CA-C-N	-5.36	114.10	119.56
1	B	161	LEU	C-N-CA	-5.36	114.10	119.56
1	A	311	LYS	N-CA-C	-5.36	99.54	108.32
1	B	360	VAL	N-CA-C	5.32	115.86	108.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ARG	CB-CG-CD	-5.27	99.18	111.30
1	B	246	TRP	N-CA-C	5.26	117.54	109.07
1	B	127	ILE	CA-C-N	5.22	126.37	119.84
1	B	127	ILE	C-N-CA	5.22	126.37	119.84
1	A	138	VAL	N-CA-CB	-5.16	102.43	112.75
1	A	353	SER	N-CA-CB	-5.10	101.64	110.32
1	B	230[A]	ILE	CB-CA-C	-5.06	102.71	110.50
1	B	230[B]	ILE	CB-CA-C	-5.06	102.71	110.50
1	A	177	TYR	N-CA-C	-5.05	105.39	112.25
1	A	370	CYS	N-CA-C	-5.03	101.51	109.76
1	A	205[A]	GLU	CB-CA-C	-5.02	104.31	110.08
1	A	205[B]	GLU	CB-CA-C	-5.02	104.31	110.08

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	THR	Peptide
1	A	321	PHE	Peptide
1	A	41	SER	Peptide
1	A	59	GLY	Peptide
1	B	155	ASP	Peptide
1	B	240	PRO	Peptide
1	B	290	ASN	Mainchain
1	B	314	PRO	Peptide
1	B	32	PRO	Peptide
1	B	335	PRO	Peptide
1	B	41	SER	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3110	0	3089	123	2
1	B	3159	0	3123	148	2
2	C	28	0	25	2	0
2	D	28	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	28	0	25	1	0
2	F	28	0	25	32	0
3	A	119	0	0	27	1
3	B	127	0	0	20	0
All	All	6627	0	6312	275	3

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 22.

All (275) 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:B:291[B]:ASN:ND2	1:B:294:GLY:O	1.75	1.20
1:B:294:GLY:O	2:F:1:NAG:C1	1.91	1.19
1:B:291[A]:ASN:ND2	1:B:294:GLY:O	1.76	1.17
1:A:106:TYR:O	3:A:2019:HOH:O	1.62	1.16
3:B:2110:HOH:O	2:F:1:NAG:H82	1.48	1.13
1:A:224:LEU:HD22	1:A:230[A]:ILE:HD11	1.23	1.12
1:A:298:VAL:HG23	3:A:2092:HOH:O	1.48	1.11
1:B:225[B]:MET:HE1	1:B:307:PRO:HD3	1.34	1.07
1:B:295:GLY:HA3	2:F:1:NAG:C5	1.88	1.03
1:A:224:LEU:HD22	1:A:230[A]:ILE:CD1	1.92	1.00
1:B:295:GLY:HA3	2:F:1:NAG:C6	1.93	0.97
1:B:143[A]:ASP:OD2	1:B:179:SER:HB3	1.65	0.95
1:A:44:THR:HG22	3:A:2005:HOH:O	1.66	0.94
1:B:295:GLY:HA3	2:F:1:NAG:O5	1.67	0.92
1:B:295:GLY:CA	2:F:1:NAG:C6	2.48	0.92
1:B:295:GLY:C	2:F:1:NAG:H61	1.96	0.90
1:B:295:GLY:HA3	2:F:1:NAG:H61	1.54	0.90
1:B:295:GLY:CA	2:F:1:NAG:H61	2.02	0.90
1:B:224:LEU:HD22	1:B:230[A]:ILE:CG1	2.03	0.89
1:B:298:VAL:HG12	3:B:2114:HOH:O	1.71	0.88
1:B:206:PRO:CB	3:B:2074:HOH:O	2.21	0.88
1:B:224:LEU:HD22	1:B:230[B]:ILE:CG1	2.04	0.88
1:A:61:LEU:HD12	3:A:2010:HOH:O	1.76	0.86
1:A:350:HIS:ND1	3:A:2103:HOH:O	2.08	0.86
1:A:54:GLN:O	3:A:2010:HOH:O	1.94	0.85
1:A:224:LEU:HD13	1:A:230[B]:ILE:HG12	1.56	0.85
1:A:116:ILE:HG23	1:A:206:PRO:HG3	1.57	0.84
1:B:294:GLY:O	2:F:1:NAG:O5	1.95	0.83
1:B:130:PHE:HA	3:B:2037:HOH:O	1.78	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1:NAG:O6	2:F:2:NAG:N2	2.12	0.83
1:A:343:LYS:HG2	3:A:2108:HOH:O	1.79	0.82
1:B:4:PRO:HA	1:B:29:SER:O	1.80	0.80
1:A:250:ILE:HD12	1:A:255:ARG:HB2	1.64	0.80
1:B:295:GLY:CA	2:F:1:NAG:O5	2.29	0.80
1:A:141:HIS:HD2	1:A:147:ASN:HD22	1.29	0.79
1:B:225[B]:MET:HE1	1:B:307:PRO:CD	2.13	0.79
1:B:290:ASN:HA	1:B:291[A]:ASN:ND2	1.99	0.78
1:A:141:HIS:CD2	1:A:147:ASN:HD22	2.02	0.78
2:F:2:NAG:O3	2:F:2:NAG:O7	2.01	0.78
1:A:67:ARG:HA	2:C:1:NAG:H83	1.65	0.76
1:B:40:ARG:HB2	3:B:2015:HOH:O	1.84	0.76
1:A:323:ARG:O	1:A:360:VAL:HG12	1.86	0.75
1:A:44:THR:CG2	3:A:2005:HOH:O	2.27	0.75
1:B:290:ASN:HA	1:B:291[B]:ASN:ND2	2.00	0.75
1:B:290:ASN:CG	2:F:1:NAG:H5	2.13	0.73
1:B:116:ILE:HG23	1:B:206:PRO:HG3	1.70	0.73
1:B:7:LEU:HD21	1:B:29:SER:CB	2.18	0.73
1:A:250:ILE:O	1:A:253:THR:OG1	2.06	0.73
1:B:206:PRO:CA	3:B:2074:HOH:O	2.36	0.72
1:A:129:SER:O	1:B:213:ARG:HD3	1.89	0.72
1:A:116:ILE:H	1:A:237:GLN:NE2	1.88	0.72
1:B:7:LEU:HD21	1:B:29:SER:HB2	1.70	0.72
3:A:2116:HOH:O	2:C:1:NAG:H81	1.90	0.71
1:B:294:GLY:C	2:F:1:NAG:O5	2.32	0.71
1:A:224:LEU:HD13	1:A:230[A]:ILE:HD13	1.72	0.71
1:B:323:ARG:O	1:B:360:VAL:HG12	1.91	0.70
1:B:290:ASN:HA	2:F:1:NAG:C1	2.22	0.69
1:A:342:MET:HE2	1:A:345:GLY:O	1.92	0.69
1:A:224:LEU:HD13	1:A:230[A]:ILE:CG1	2.23	0.69
1:A:143[A]:ASP:OD2	1:A:179:SER:HB3	1.93	0.68
1:A:224:LEU:CD2	1:A:230[A]:ILE:HD11	2.14	0.68
1:B:224:LEU:HD22	1:B:230[A]:ILE:HD11	1.75	0.68
1:B:40:ARG:HG3	1:B:46:VAL:HG12	1.73	0.68
1:B:123:ILE:HD11	1:B:201:LEU:HD21	1.75	0.68
1:B:13[A]:ARG:HD2	3:B:2008:HOH:O	1.94	0.68
1:B:343:LYS:NZ	1:B:344:ASP:OD2	2.28	0.67
1:B:212:PRO:HD3	1:B:291[A]:ASN:CG	2.20	0.67
1:B:212:PRO:HD3	1:B:291[B]:ASN:CG	2.20	0.67
1:B:295:GLY:CA	2:F:1:NAG:C5	2.69	0.66
1:B:224:LEU:HD22	1:B:230[A]:ILE:CD1	2.25	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ASN:OD1	2:F:1:NAG:H5	1.94	0.66
1:B:245[A]:ARG:HD2	3:B:2092:HOH:O	1.94	0.66
1:A:124[A]:LYS:HD2	1:A:126:LEU:HD23	1.76	0.66
1:A:116:ILE:HG23	1:A:206:PRO:CG	2.25	0.65
1:A:250:ILE:HB	1:A:253:THR:OG1	1.97	0.65
1:B:291[A]:ASN:CG	1:B:294:GLY:O	2.39	0.65
1:A:224:LEU:HD13	1:A:230[A]:ILE:CD1	2.26	0.65
1:B:226:VAL:O	1:B:227:ALA:HB3	1.97	0.64
1:B:225[B]:MET:CE	1:B:307:PRO:HD3	2.22	0.64
1:A:308:LEU:HA	1:A:332:THR:O	1.98	0.63
1:B:294:GLY:C	2:F:1:NAG:C1	2.70	0.63
2:F:2:NAG:O3	2:F:2:NAG:C7	2.44	0.63
1:A:79:VAL:HG22	1:A:97:HIS:ND1	2.14	0.63
1:B:130:PHE:CA	3:B:2037:HOH:O	2.38	0.63
1:A:224:LEU:CD2	1:A:230[A]:ILE:CD1	2.75	0.62
1:A:342:MET:CE	1:A:345:GLY:O	2.47	0.62
1:A:250:ILE:HD12	1:A:255:ARG:CB	2.29	0.62
1:A:28:ALA:O	1:A:33:MET:HE3	1.99	0.62
1:B:224:LEU:HD22	1:B:230[B]:ILE:HG12	1.82	0.62
1:A:92:ILE:HG22	1:A:93:SER:O	2.00	0.62
1:B:239:PHE:HA	1:B:240:PRO:C	2.24	0.62
1:B:83:LEU:HD23	1:B:84:ALA:N	2.15	0.61
1:A:129:SER:O	1:B:213:ARG:CD	2.48	0.61
1:A:141:HIS:HD2	1:A:147:ASN:ND2	1.95	0.61
1:B:328:THR:HG23	1:B:354:VAL:HG22	1.82	0.61
1:A:144[A]:GLU:OE1	1:A:178[A]:LYS:HE2	2.00	0.61
1:B:295:GLY:C	2:F:1:NAG:C6	2.71	0.61
1:B:245[A]:ARG:CD	3:B:2092:HOH:O	2.48	0.61
1:A:343:LYS:CG	3:A:2108:HOH:O	2.43	0.61
1:A:342:MET:HE2	1:A:345:GLY:C	2.26	0.60
1:A:225[B]:MET:HG3	3:A:2080:HOH:O	2.00	0.60
1:A:111:ASN:ND2	1:A:126:LEU:HD12	2.17	0.60
1:B:116:ILE:HG23	1:B:206:PRO:CG	2.31	0.60
1:A:320:ASP:O	1:A:360:VAL:HG13	2.03	0.59
1:A:54:GLN:C	3:A:2010:HOH:O	2.42	0.59
1:B:290:ASN:CG	2:F:1:NAG:C5	2.76	0.59
1:A:245[B]:ARG:HG2	1:A:247:TYR:CZ	2.38	0.58
1:B:341:TRP:CB	1:B:348:ILE:HD11	2.33	0.58
1:B:341:TRP:HB2	1:B:348:ILE:HD11	1.85	0.58
1:A:186:HIS:CE1	1:A:188:LEU:HB2	2.39	0.58
1:A:224:LEU:HD13	1:A:230[A]:ILE:HG12	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:CYS:CB	1:B:370:CYS:HG	2.17	0.57
1:B:193:ARG:HD2	3:B:2024:HOH:O	2.04	0.57
1:B:295:GLY:N	2:F:1:NAG:O5	2.38	0.57
1:B:32:PRO:O	1:B:86:ASN:ND2	2.30	0.57
1:A:178[A]:LYS:NZ	3:A:2056:HOH:O	2.37	0.57
1:B:115:VAL:HG11	1:B:121:ALA:HB2	1.85	0.57
1:A:1:GLN:NE2	1:A:88:PHE:HB2	2.20	0.57
1:B:83:LEU:HD23	1:B:83:LEU:C	2.30	0.57
1:A:13[A]:ARG:HD2	1:A:97:HIS:HB2	1.87	0.57
1:A:305:THR:HG22	1:A:335:PRO:HD3	1.88	0.56
1:B:296:GLU:N	2:F:1:NAG:H61	2.21	0.56
1:A:207:ILE:N	1:A:207:ILE:HD13	2.20	0.56
1:B:83:LEU:C	1:B:83:LEU:CD2	2.78	0.56
1:B:206:PRO:HB3	3:B:2074:HOH:O	1.96	0.56
1:B:224:LEU:HD22	1:B:230[B]:ILE:HG13	1.85	0.56
1:A:88:PHE:CE2	1:A:384:GLU:HG3	2.41	0.55
1:B:51:GLY:H	1:B:54:GLN:HE21	1.54	0.55
1:B:224:LEU:HD22	1:B:230[A]:ILE:HG12	1.83	0.55
1:A:10:PRO:HB2	1:A:96:VAL:HG21	1.89	0.55
1:A:110:VAL:HG12	1:A:199:GLY:HA3	1.89	0.55
1:A:213:ARG:CD	1:B:129:SER:O	2.55	0.55
1:A:335:PRO:O	1:A:374:ASN:HB3	2.07	0.55
1:A:218:VAL:HG12	3:A:2075:HOH:O	2.05	0.55
1:B:245[B]:ARG:NH1	1:B:259:VAL:O	2.39	0.55
1:B:224:LEU:HD22	1:B:230[B]:ILE:HD11	1.88	0.55
1:B:319:VAL:HG12	1:B:360:VAL:HG11	1.89	0.55
1:B:7:LEU:HD21	1:B:29:SER:HB3	1.88	0.54
1:A:124[B]:LYS:HB2	1:A:124[B]:LYS:NZ	2.22	0.54
1:A:358[B]:GLU:CD	1:A:358[B]:GLU:H	2.13	0.54
1:B:55:ILE:CD1	1:B:61:LEU:CD1	2.86	0.54
1:B:141:HIS:ND1	1:B:147:ASN:ND2	2.54	0.54
1:B:7:LEU:CD2	1:B:29:SER:CB	2.85	0.54
1:A:250:ILE:HD13	1:A:255:ARG:NH1	2.23	0.53
1:B:178[A]:LYS:HD2	3:B:2059:HOH:O	2.08	0.53
1:B:224:LEU:HD22	1:B:230[B]:ILE:CD1	2.35	0.53
1:B:142:THR:HG21	1:B:178[B]:LYS:HE2	1.91	0.53
1:A:10:PRO:HB2	1:A:96:VAL:CG2	2.38	0.53
1:A:55:ILE:HD13	3:A:2007:HOH:O	2.09	0.53
1:A:329:CYS:HG	1:A:370:CYS:HG	1.54	0.53
1:B:55:ILE:HD11	1:B:61:LEU:CD1	2.39	0.53
1:A:224:LEU:CD1	1:A:230[A]:ILE:HG12	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:PHE:CD2	1:B:91:ILE:HD12	2.43	0.52
1:B:35:GLU:O	1:B:84:ALA:HA	2.09	0.52
1:B:320:ASP:O	1:B:360:VAL:CG1	2.57	0.52
1:B:290:ASN:CA	2:F:1:NAG:C1	2.87	0.52
1:A:337:LYS:HG2	1:A:338:THR:HG23	1.92	0.52
1:B:174:GLU:OE1	1:B:174:GLU:N	2.39	0.52
1:A:224:LEU:HD22	1:A:230[A]:ILE:CG1	2.38	0.51
1:A:245[B]:ARG:CZ	3:A:2085:HOH:O	2.58	0.51
1:B:358[B]:GLU:H	1:B:358[B]:GLU:CD	2.17	0.51
1:A:224:LEU:O	1:A:304:VAL:HA	2.11	0.51
1:A:186:HIS:HE1	1:A:188:LEU:HB2	1.76	0.51
1:B:242:PRO:HA	1:B:290:ASN:O	2.10	0.51
1:B:44:THR:HB	3:B:2015:HOH:O	2.11	0.51
1:A:14:ILE:HG12	1:A:24:ILE:HD11	1.93	0.51
1:A:213:ARG:HD2	1:B:129:SER:O	2.10	0.50
1:A:279:VAL:HG13	1:A:334:ASN:ND2	2.26	0.50
1:B:8:LYS:HB2	1:B:27:LYS:HB2	1.94	0.50
1:B:123:ILE:HD11	1:B:201:LEU:CD2	2.41	0.50
1:B:7:LEU:CD2	1:B:29:SER:HB3	2.42	0.50
1:A:230[B]:ILE:HD11	1:A:277:ALA:HB2	1.93	0.50
1:B:206:PRO:HA	3:B:2074:HOH:O	2.07	0.50
1:A:39:ILE:HD12	1:A:40:ARG:O	2.12	0.49
1:A:106:TYR:C	3:A:2019:HOH:O	2.30	0.49
1:A:224:LEU:CD1	1:A:230[B]:ILE:HG12	2.36	0.49
1:A:193:ARG:CD	3:A:2019:HOH:O	2.61	0.49
1:A:224:LEU:HD22	1:A:230[B]:ILE:CG1	2.43	0.49
1:B:280:GLU:HA	3:B:2107:HOH:O	2.12	0.49
1:B:295:GLY:CA	2:F:1:NAG:H62	2.41	0.48
1:B:290:ASN:CG	2:F:1:NAG:H83	2.38	0.48
2:F:2:NAG:C7	2:F:2:NAG:HO3	2.21	0.48
2:E:1:NAG:O3	2:E:1:NAG:H82	2.13	0.48
1:B:124[B]:LYS:HB2	1:B:124[B]:LYS:HE3	1.43	0.48
1:B:212:PRO:HD3	1:B:291[B]:ASN:OD1	2.13	0.47
1:B:291[A]:ASN:OD1	1:B:294:GLY:N	2.35	0.47
1:B:79:VAL:HG22	1:B:97:HIS:ND1	2.30	0.47
1:B:225[B]:MET:HE3	1:B:226:VAL:HG12	1.96	0.47
1:A:14:ILE:HG23	1:A:14:ILE:O	2.15	0.47
1:B:341:TRP:HA	1:B:369:GLN:O	2.14	0.47
1:A:116:ILE:H	1:A:237:GLN:HE22	1.58	0.47
1:A:206:PRO:CA	3:A:2068:HOH:O	2.63	0.47
1:A:220:LYS:HB2	1:A:221:PRO:CD	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:HD22	1:A:230[B]:ILE:HG12	1.95	0.47
1:A:245[B]:ARG:NH2	3:A:2085:HOH:O	2.48	0.47
1:A:329:CYS:SG	1:A:370:CYS:CB	3.03	0.47
1:A:304:VAL:O	1:A:334:ASN:ND2	2.37	0.47
1:B:40:ARG:HD2	3:B:2015:HOH:O	2.14	0.47
1:B:212:PRO:HD2	1:B:295:GLY:HA2	1.97	0.46
1:B:290:ASN:CA	1:B:291[A]:ASN:ND2	2.74	0.46
1:A:309:SER:O	1:A:331:TYR:HA	2.16	0.46
1:A:94:ARG:HB2	1:A:378:SER:OG	2.16	0.46
1:B:224:LEU:HD21	1:B:228:HIS:HB2	1.97	0.46
1:A:249:PHE:HA	1:A:256:LYS:HA	1.97	0.46
1:B:179:SER:HA	1:B:199:GLY:O	2.15	0.46
1:B:336:ILE:N	1:B:336:ILE:HD13	2.31	0.46
1:A:206:PRO:HA	3:A:2068:HOH:O	2.16	0.46
1:A:178[B]:LYS:HE3	3:A:2057:HOH:O	2.16	0.46
1:B:235:PRO:HA	3:B:2087:HOH:O	2.16	0.46
1:B:57:SER:HA	1:B:58:ASP:HA	1.58	0.45
1:A:136[A]:GLU:HB2	3:A:2034:HOH:O	2.16	0.45
1:A:319:VAL:HG12	1:A:360:VAL:HG11	1.98	0.45
1:A:169[B]:ARG:HH21	1:A:268:VAL:HG13	1.81	0.45
1:A:329:CYS:HG	1:A:370:CYS:CB	2.29	0.45
1:A:339:VAL:HG13	1:A:370:CYS:SG	2.57	0.45
1:B:290:ASN:CA	1:B:291[B]:ASN:ND2	2.76	0.45
1:B:162:PRO:HG2	1:B:231:SER:HB3	1.99	0.45
1:A:206:PRO:C	1:A:207:ILE:HD13	2.41	0.45
1:A:224:LEU:CD1	1:A:230[A]:ILE:HD13	2.44	0.45
1:A:260:VAL:HG12	3:A:2088:HOH:O	2.16	0.44
1:B:242:PRO:CA	1:B:290:ASN:O	2.65	0.44
1:B:69[B]:GLU:CD	3:B:2018:HOH:O	2.59	0.44
1:B:290:ASN:OD1	2:F:1:NAG:C5	2.64	0.44
1:B:172:GLY:O	1:B:175:ASP:HB2	2.18	0.44
1:B:290:ASN:C	1:B:291[A]:ASN:ND2	2.75	0.44
1:A:114:HIS:C	1:A:115:VAL:HG13	2.43	0.43
1:B:135:VAL:CG1	1:B:184:THR:HB	2.48	0.43
1:B:230[B]:ILE:HD13	1:B:302:LEU:HD21	2.00	0.43
1:A:123:ILE:HD11	1:A:201:LEU:HD21	2.01	0.43
1:A:313:ASP:HB2	1:A:330:GLN:HE22	1.83	0.43
1:B:224:LEU:HD22	1:B:230[A]:ILE:HG13	1.87	0.43
1:B:212:PRO:HD3	1:B:291[A]:ASN:OD1	2.15	0.43
1:B:250:ILE:HD12	1:B:255:ARG:NH1	2.33	0.43
1:A:313:ASP:HA	1:A:314:PRO:HA	1.74	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:ARG:HA	1:B:323:ARG:HD2	1.90	0.43
1:A:313:ASP:CB	1:A:330:GLN:HE22	2.31	0.43
1:A:138:VAL:HG21	1:A:185:LYS:HB2	2.01	0.43
1:A:224:LEU:CB	1:A:230[A]:ILE:HD13	2.48	0.43
1:A:336:ILE:HG23	1:A:336:ILE:HD12	1.69	0.43
1:B:205[A]:GLU:HG2	3:B:2073:HOH:O	2.19	0.43
1:B:225[B]:MET:HE1	1:B:307:PRO:CG	2.49	0.43
1:B:290:ASN:C	1:B:291[B]:ASN:ND2	2.76	0.42
1:B:55:ILE:HD12	1:B:55:ILE:N	2.34	0.42
1:B:226:VAL:O	1:B:227:ALA:CB	2.63	0.42
1:B:364:ASP:O	1:B:385:LEU:HD23	2.20	0.42
1:B:40:ARG:CG	1:B:46:VAL:HG12	2.48	0.42
1:B:225[A]:MET:HE3	1:B:228:HIS:NE2	2.35	0.42
1:B:230[A]:ILE:HD13	1:B:302:LEU:HD21	2.01	0.42
1:A:136[A]:GLU:CB	3:A:2034:HOH:O	2.68	0.41
1:B:295:GLY:N	2:F:1:NAG:H62	2.35	0.41
1:B:224:LEU:O	1:B:304:VAL:HA	2.19	0.41
1:A:57:SER:HA	1:A:58:ASP:HA	1.74	0.41
1:A:35:GLU:O	1:A:84:ALA:HA	2.20	0.41
1:B:242:PRO:HB2	1:B:289[A]:VAL:HG23	2.02	0.41
1:B:314:PRO:HA	1:B:315:PRO:HD2	1.68	0.41
1:A:47:GLY:C	3:A:2007:HOH:O	2.64	0.41
1:A:245[B]:ARG:HG2	1:A:247:TYR:CE2	2.56	0.41
1:A:351:SER:HB3	3:A:2101:HOH:O	2.20	0.41
1:B:115:VAL:HG11	1:B:121:ALA:CB	2.49	0.41
1:A:239:PHE:HA	1:A:240:PRO:C	2.45	0.40
1:A:279:VAL:HA	1:A:304:VAL:HB	2.04	0.40
1:A:329:CYS:CB	1:A:370:CYS:HG	2.34	0.40
1:B:295:GLY:N	2:F:1:NAG:C6	2.84	0.40
1:A:10:PRO:CB	1:A:96:VAL:HG21	2.50	0.40
1:B:13[A]:ARG:CD	1:B:97:HIS:HB2	2.51	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LYS:NZ	1:B:181:GLN:OE1[3_655]	1.98	0.22
3:A:2064:HOH:O	3:A:2064:HOH:O[3_655]	1.99	0.21
1:A:181:GLN:NE2	1:B:198:LYS:NZ[3_655]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	404/394 (102%)	382 (95%)	21 (5%)	1 (0%)	43	55
1	B	411/394 (104%)	386 (94%)	20 (5%)	5 (1%)	10	12
All	All	815/788 (103%)	768 (94%)	41 (5%)	6 (1%)	21	23

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	VAL
1	B	315	PRO
1	B	156	GLY
1	B	241	ALA
1	B	291[A]	ASN
1	B	291[B]	ASN

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	350/336 (104%)	320 (91%)	30 (9%)	10	13
1	B	355/336 (106%)	318 (90%)	37 (10%)	7	8
All	All	705/672 (105%)	638 (90%)	67 (10%)	9	10

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	5	VAL
1	A	7	LEU
1	A	14	ILE
1	A	39	ILE
1	A	49	VAL
1	A	57	SER
1	A	58	ASP
1	A	83	LEU
1	A	92	ILE
1	A	98	VAL
1	A	136[A]	GLU
1	A	136[B]	GLU
1	A	205[A]	GLU
1	A	205[B]	GLU
1	A	207	ILE
1	A	224	LEU
1	A	230[A]	ILE
1	A	230[B]	ILE
1	A	251	GLU
1	A	263[A]	ASP
1	A	263[B]	ASP
1	A	280	GLU
1	A	289[A]	VAL
1	A	290	ASN
1	A	304	VAL
1	A	311	LYS
1	A	332	THR
1	A	353	SER
1	A	360	VAL
1	B	1	GLN
1	B	5	VAL
1	B	7	LEU
1	B	8	LYS
1	B	23[A]	GLU
1	B	23[B]	GLU
1	B	27	LYS
1	B	29	SER
1	B	35	GLU
1	B	41	SER
1	B	49	VAL
1	B	56	SER
1	B	57	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	83	LEU
1	B	124[A]	LYS
1	B	124[B]	LYS
1	B	138	VAL
1	B	181	GLN
1	B	205[A]	GLU
1	B	205[B]	GLU
1	B	210	SER
1	B	226	VAL
1	B	260	VAL
1	B	263[A]	ASP
1	B	263[B]	ASP
1	B	289[A]	VAL
1	B	290	ASN
1	B	291[A]	ASN
1	B	291[B]	ASN
1	B	296	GLU
1	B	298	VAL
1	B	315	PRO
1	B	316	THR
1	B	336	ILE
1	B	338	THR
1	B	353	SER
1	B	360	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	12	ASN
1	A	54	GLN
1	A	87	GLN
1	A	111	ASN
1	A	141	HIS
1	A	181	GLN
1	A	228	HIS
1	A	237	GLN
1	A	330	GLN
1	B	54	GLN
1	B	73	GLN
1	B	87	GLN
1	B	147	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	350	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 ⓘ

8 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	0.53	0	17,19,21	1.85	5 (29%)
2	NAG	C	2	2	14,14,15	0.61	0	17,19,21	1.27	2 (11%)
2	NAG	D	1	1,2	14,14,15	0.49	0	17,19,21	1.94	4 (23%)
2	NAG	D	2	2	14,14,15	0.52	0	17,19,21	1.54	2 (11%)
2	NAG	E	1	1,2	14,14,15	0.52	0	17,19,21	1.54	2 (11%)
2	NAG	E	2	2	14,14,15	0.51	0	17,19,21	1.25	2 (11%)
2	NAG	F	1	1,2	14,14,15	1.09	1 (7%)	17,19,21	5.74	13 (76%)
2	NAG	F	2	2	14,14,15	0.66	0	17,19,21	2.78	5 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	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	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	NAG	F	1	1,2	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	C1-C2	3.29	1.56	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C1-O5-C5	14.66	131.83	112.19
2	F	1	NAG	C4-C3-C2	8.41	123.35	111.02
2	F	1	NAG	O5-C5-C6	8.05	123.33	107.66
2	F	2	NAG	C1-C2-N2	7.69	122.55	110.43
2	F	1	NAG	O5-C1-C2	-6.84	100.71	111.29
2	F	1	NAG	O4-C4-C3	6.71	126.19	110.38
2	F	1	NAG	C6-C5-C4	-6.09	98.07	113.02
2	F	2	NAG	O5-C1-C2	-5.18	103.27	111.29
2	F	1	NAG	C2-N2-C7	4.87	129.43	122.90
2	E	1	NAG	O5-C1-C2	-4.32	104.61	111.29
2	D	1	NAG	C1-O5-C5	4.20	117.81	112.19
2	F	1	NAG	C1-C2-N2	3.99	116.73	110.43
2	F	1	NAG	O7-C7-C8	-3.99	114.95	122.05
2	C	1	NAG	C1-O5-C5	3.81	117.29	112.19
2	C	1	NAG	O5-C1-C2	-3.38	106.07	111.29
2	C	1	NAG	C3-C4-C5	-3.35	104.16	110.23
2	D	1	NAG	O3-C3-C4	-3.33	102.52	110.38
2	F	2	NAG	O7-C7-C8	-3.30	116.17	122.05
2	D	1	NAG	C3-C4-C5	3.19	116.01	110.23
2	D	2	NAG	C1-C2-N2	3.14	115.38	110.43
2	F	2	NAG	O3-C3-C2	3.12	115.88	109.40
2	C	1	NAG	C2-N2-C7	3.01	126.94	122.90
2	F	2	NAG	C1-O5-C5	2.90	116.08	112.19
2	D	2	NAG	C4-C3-C2	-2.60	107.20	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C8-C7-N2	2.58	120.39	116.12
2	C	2	NAG	C1-O5-C5	2.55	115.60	112.19
2	D	1	NAG	O5-C5-C4	2.49	116.89	110.83
2	F	1	NAG	O5-C5-C4	2.32	116.47	110.83
2	C	2	NAG	C1-C2-N2	2.32	114.08	110.43
2	F	1	NAG	O3-C3-C4	-2.31	104.92	110.38
2	E	2	NAG	C1-C2-N2	2.25	113.97	110.43
2	E	1	NAG	C8-C7-N2	2.23	119.82	116.12
2	C	1	NAG	O5-C5-C4	2.13	116.00	110.83
2	E	2	NAG	O4-C4-C5	2.12	114.56	109.32
2	F	1	NAG	O6-C6-C5	2.09	118.44	111.33

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	1	NAG	C1

All (22) torsion outliers are listed below:

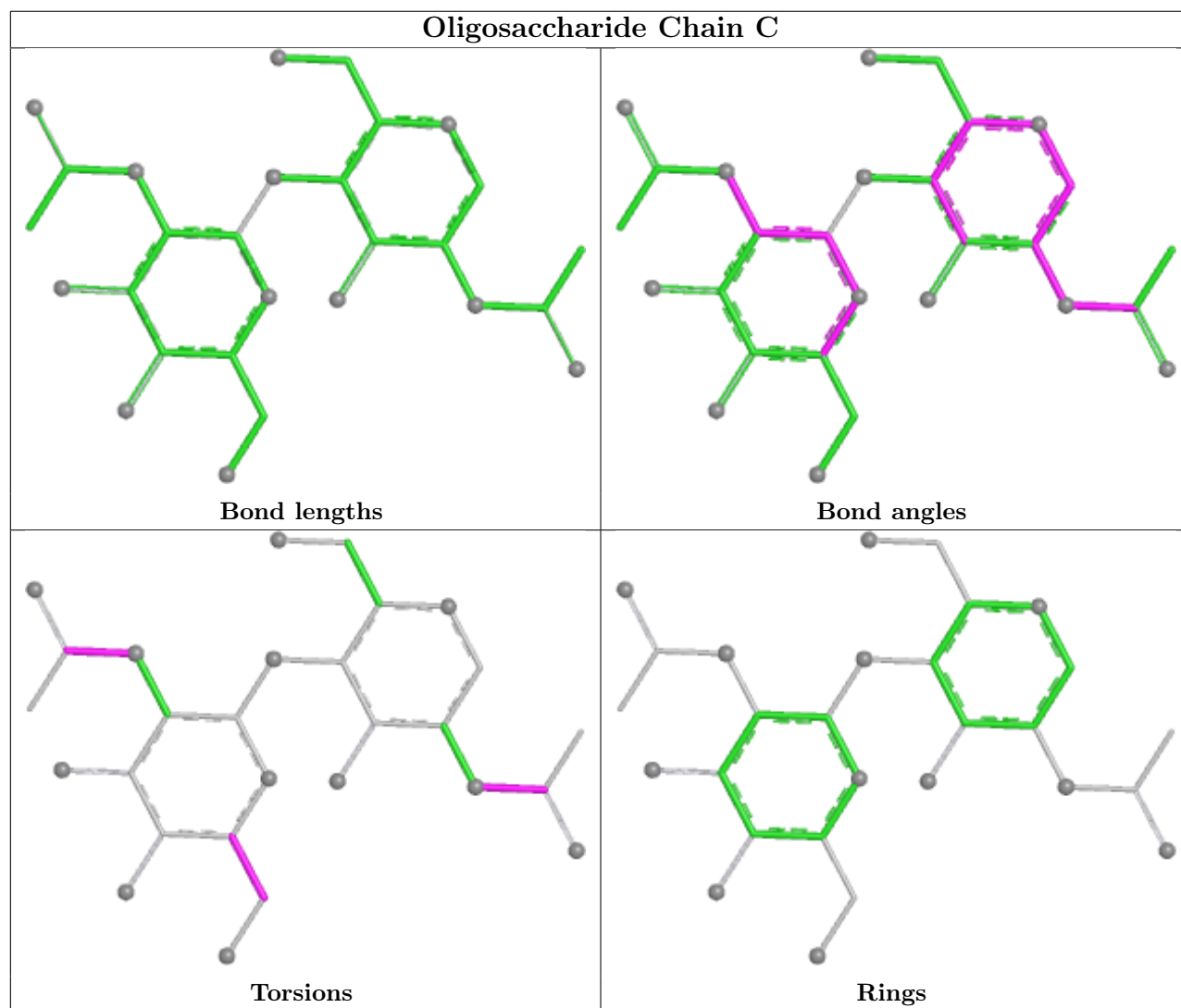
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C3-C2-N2-C7
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C3-C2-N2-C7
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2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

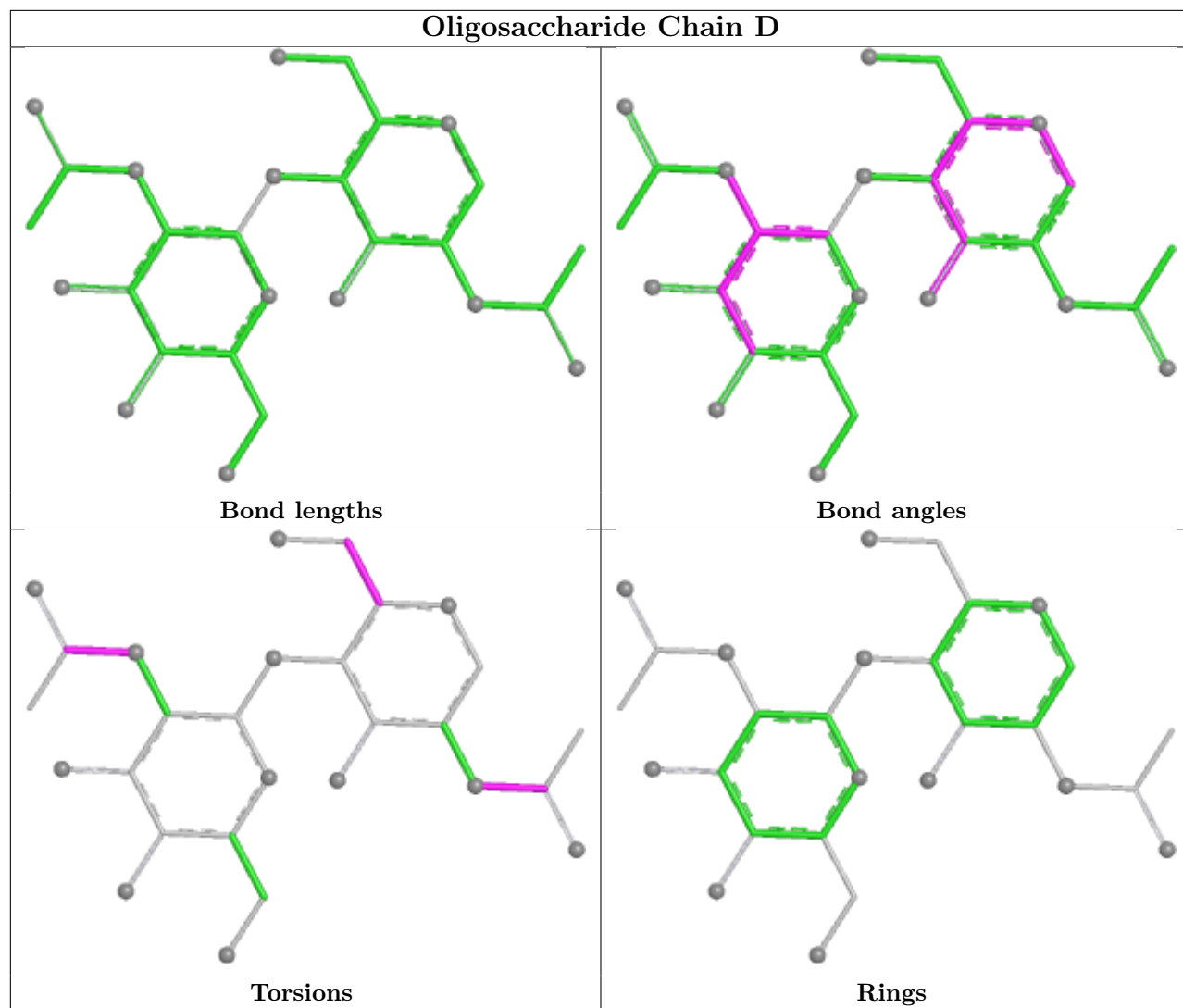
There are no ring outliers.

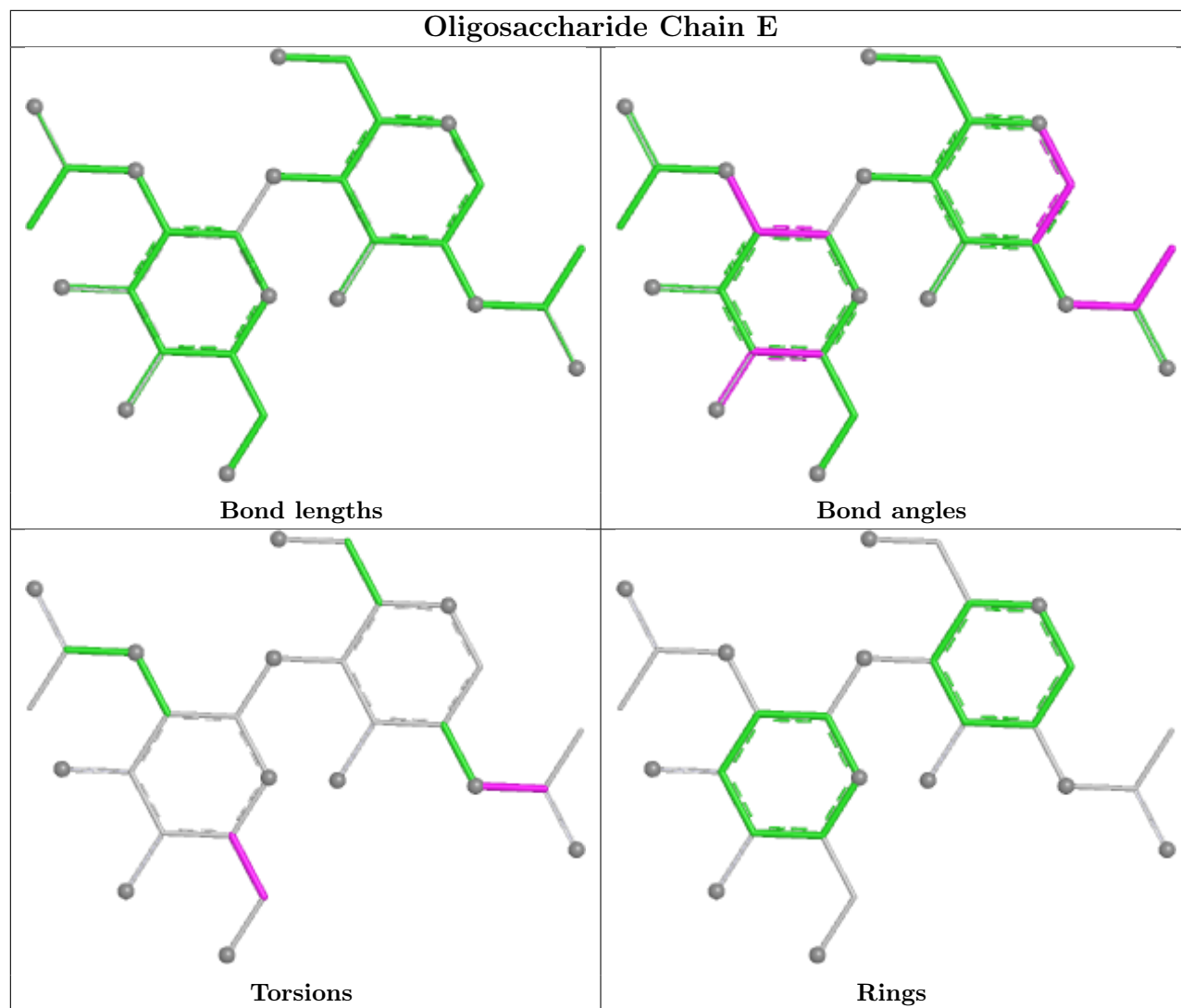
4 monomers are involved in 35 short contacts:

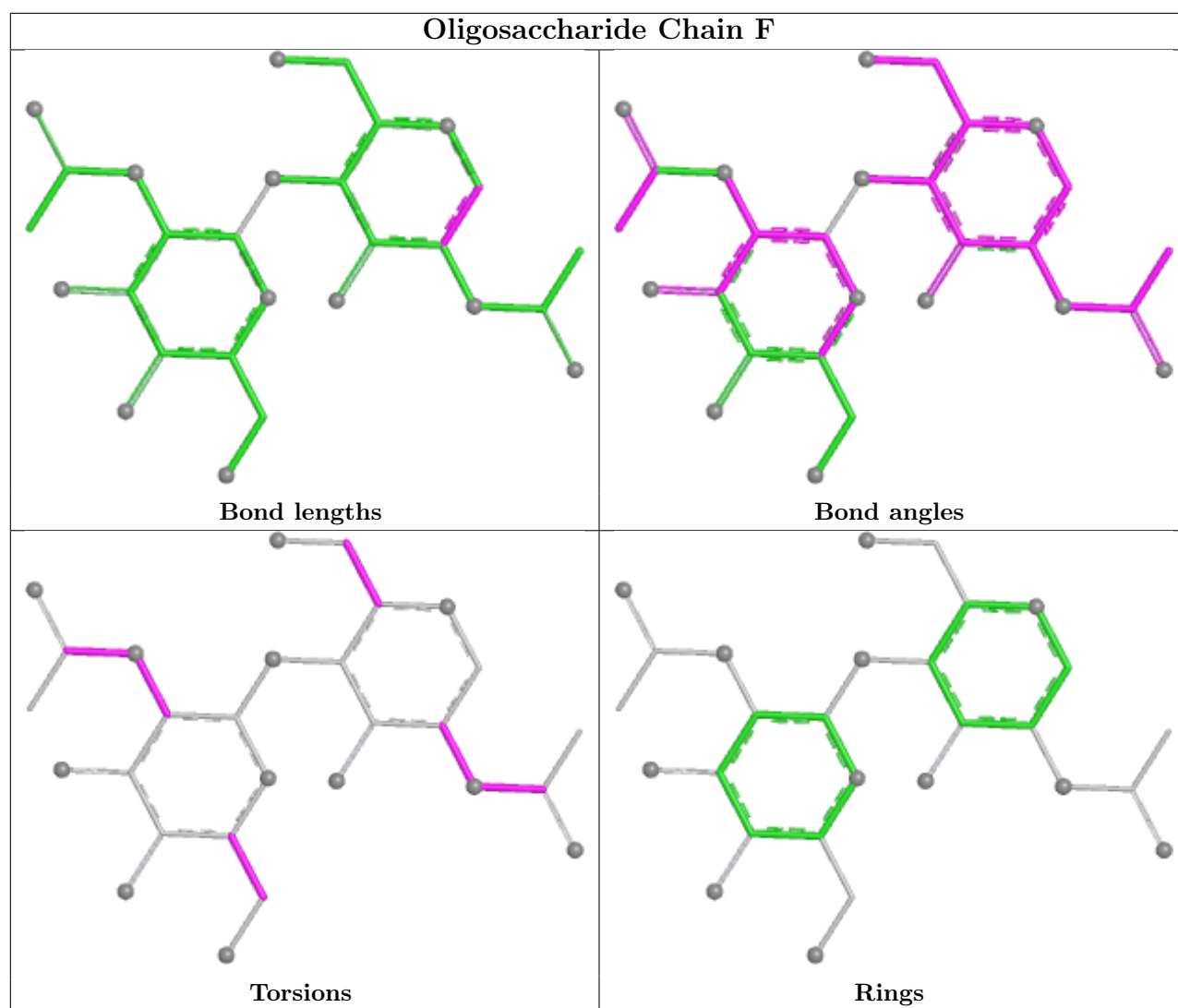
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	NAG	4	0
2	F	1	NAG	29	0
2	C	1	NAG	2	0
2	E	1	NAG	1	0

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









5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	388/394 (98%)	1.06	40 (10%)	12 13	32, 64, 71, 81	24 (6%)
1	B	394/394 (100%)	0.99	38 (9%)	13 15	32, 64, 72, 82	22 (5%)
All	All	782/788 (99%)	1.03	78 (9%)	12 14	32, 64, 72, 82	46 (5%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	55	ILE	10.2
1	A	56	SER	7.5
1	B	-5	ALA	5.7
1	A	289[A]	VAL	5.1
1	B	145[A]	GLU	4.8
1	B	289[A]	VAL	4.3
1	A	41	SER	4.2
1	A	59	GLY	4.0
1	A	58	ASP	3.9
1	A	30	GLY	3.3
1	B	358[A]	GLU	3.3
1	B	307	PRO	3.2
1	B	360	VAL	3.2
1	A	31	ASN	3.2
1	A	88	PHE	3.1
1	A	216	ALA	3.1
1	B	290	ASN	3.0
1	B	87	GLN	3.0
1	A	213	ARG	3.0
1	A	209	SER	3.0
1	A	239	PHE	2.9
1	B	41	SER	2.9
1	B	224	LEU	2.9
1	B	88	PHE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	291[A]	ASN	2.8
1	A	370	CYS	2.8
1	A	28	ALA	2.7
1	B	327	PHE	2.7
1	A	47	GLY	2.7
1	A	297	SER	2.7
1	A	249	PHE	2.7
1	B	58	ASP	2.7
1	A	212	PRO	2.7
1	B	100	ALA	2.6
1	A	366	GLY	2.6
1	B	382	SER	2.6
1	B	321	PHE	2.6
1	A	293	VAL	2.6
1	B	306	ALA	2.6
1	A	360	VAL	2.6
1	B	376	ARG	2.5
1	A	308	LEU	2.5
1	A	49	VAL	2.5
1	B	124[A]	LYS	2.5
1	B	312	ILE	2.4
1	A	298	VAL	2.4
1	A	301	VAL	2.4
1	B	49	VAL	2.4
1	B	32	PRO	2.3
1	A	45	ALA	2.3
1	B	379	ALA	2.3
1	B	383	ALA	2.3
1	A	342	MET	2.3
1	A	235	PRO	2.3
1	B	84	ALA	2.3
1	B	69[A]	GLU	2.3
1	B	323	ARG	2.2
1	B	372	VAL	2.2
1	A	321	PHE	2.2
1	A	379	ALA	2.2
1	B	207	ILE	2.1
1	A	155	ASP	2.1
1	A	295	GLY	2.1
1	A	224	LEU	2.1
1	B	8	LYS	2.1
1	B	66	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	210	SER	2.1
1	B	328	THR	2.1
1	A	138	VAL	2.1
1	B	378	SER	2.1
1	A	250	ILE	2.1
1	B	334	ASN	2.1
1	B	359	SER	2.0
1	A	217	LEU	2.0
1	A	294	GLY	2.0
1	B	295	GLY	2.0
1	B	322	GLY	2.0
1	A	261	LEU	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 ⓘ

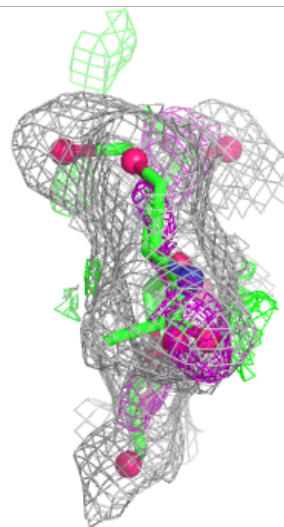
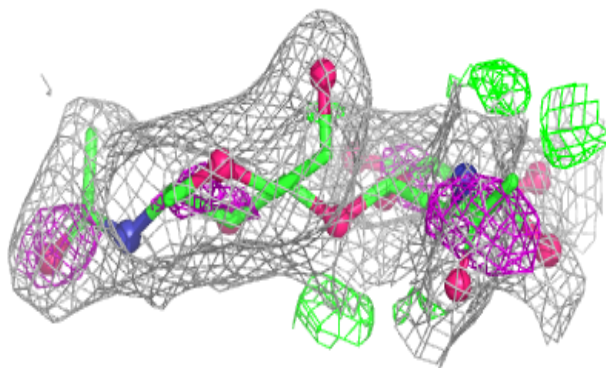
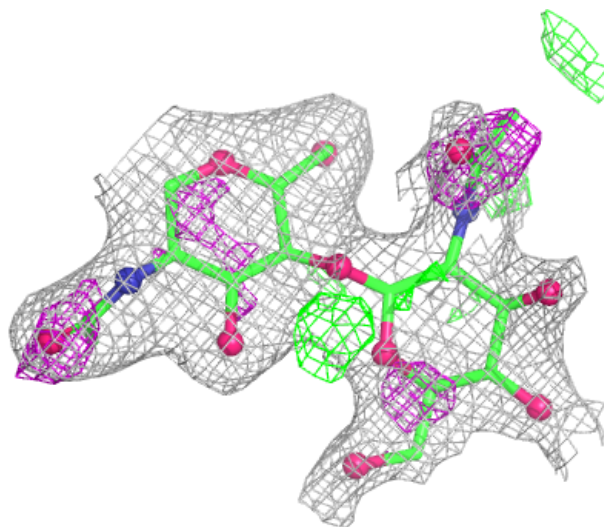
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	F	2	14/15	0.26	0.23	119,122,129,129	0
2	NAG	D	2	14/15	0.32	0.23	93,96,97,98	0
2	NAG	F	1	14/15	0.33	0.32	96,107,112,114	0
2	NAG	C	2	14/15	0.50	0.20	88,94,96,97	0
2	NAG	E	2	14/15	0.51	0.19	71,81,85,86	0
2	NAG	D	1	14/15	0.58	0.19	77,82,85,89	0
2	NAG	E	1	14/15	0.86	0.13	52,62,67,74	0
2	NAG	C	1	14/15	0.89	0.12	56,63,70,78	0

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

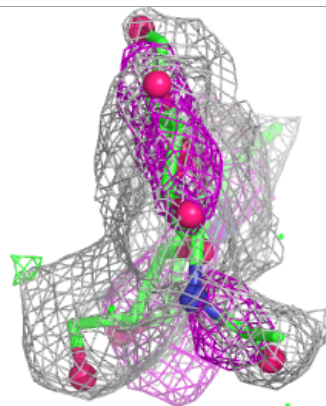
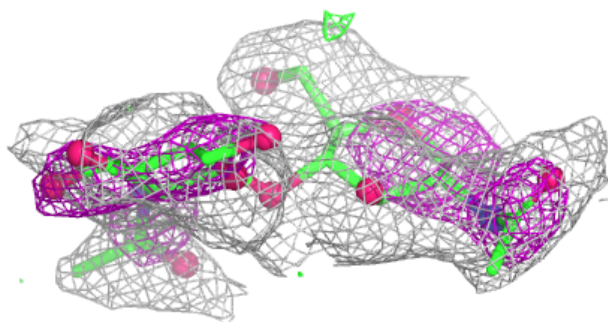
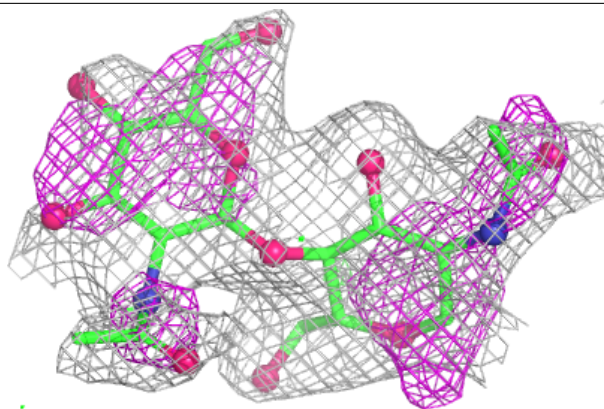
Electron density around Chain C:

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

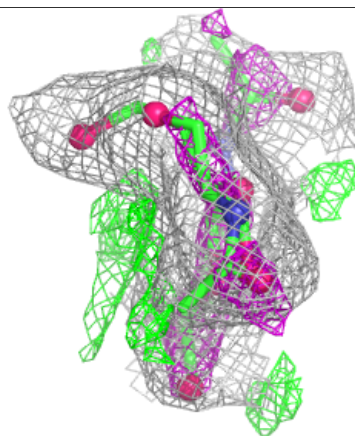
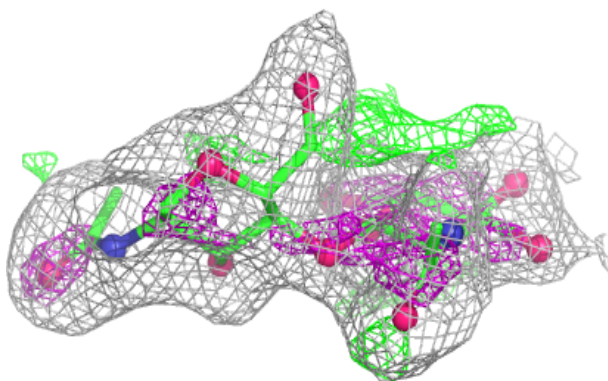
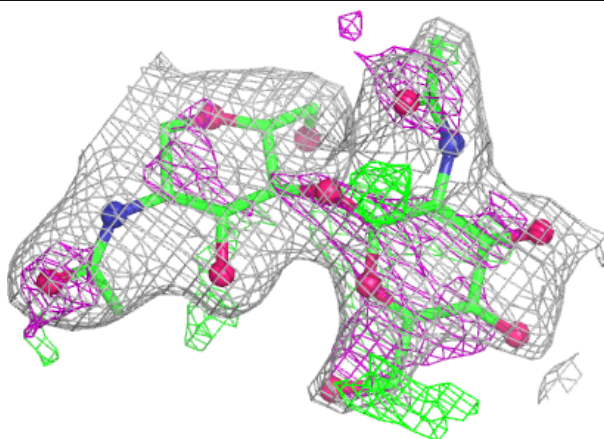


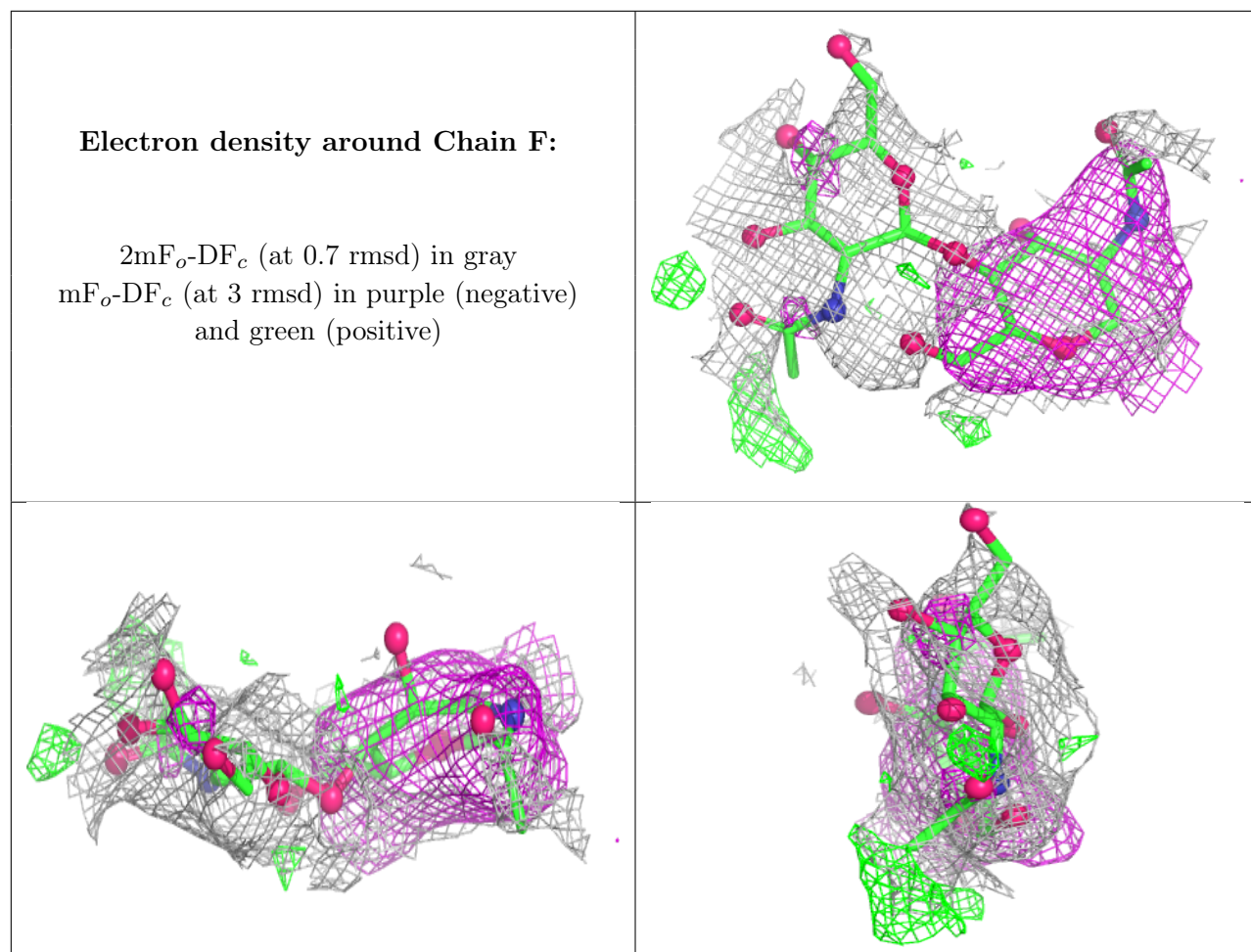
Electron density around Chain D:

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

**Electron density around Chain E:**

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.