



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:38 PM UTC

PDB ID : 3B3Q / pdb_00003b3q
Title : Crystal structure of a synaptic adhesion complex
Authors : Chen, X.; Liu, H.; Shim, A.; Focia, P.; He, X.
Deposited on : 2007-10-22
Resolution : 2.40 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

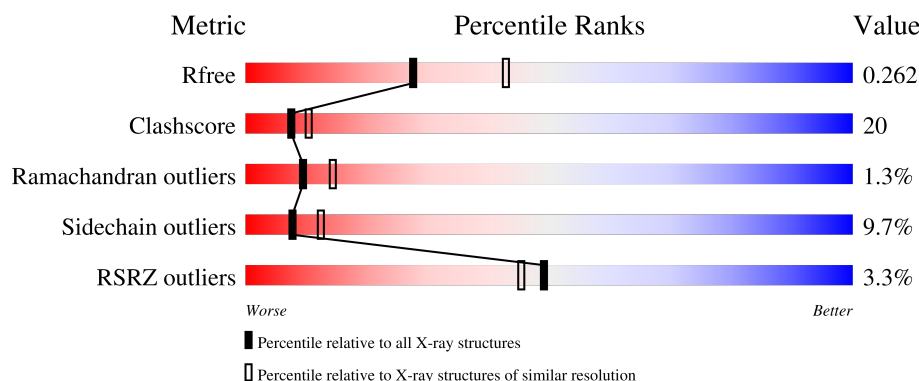
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	577	 2% 60% 29% 7%
1	B	577	 2% 62% 26% 5% 7%
2	E	197	 3% 52% 39% 5% 5%
2	F	197	 9% 49% 43% 5% 5%
3	C	2	 100%

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Mol	Chain	Length	Quality of chain
3	D	2	 100%
3	G	2	 50%50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12952 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 Nlgn1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4219	2710	697	796	16			
1	B	536	Total	C	N	O	S	0	0	0
			4219	2710	697	796	16			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	ALA	-	expression tag	UNP Q4KMN5
A	31	ASP	-	expression tag	UNP Q4KMN5
A	32	PRO	-	expression tag	UNP Q4KMN5
A	33	HIS	-	expression tag	UNP Q4KMN5
A	34	HIS	-	expression tag	UNP Q4KMN5
A	35	HIS	-	expression tag	UNP Q4KMN5
A	36	HIS	-	expression tag	UNP Q4KMN5
A	37	HIS	-	expression tag	UNP Q4KMN5
A	38	HIS	-	expression tag	UNP Q4KMN5
A	39	GLU	-	expression tag	UNP Q4KMN5
A	40	ASN	-	expression tag	UNP Q4KMN5
A	41	LEU	-	expression tag	UNP Q4KMN5
A	42	TYR	-	expression tag	UNP Q4KMN5
A	43	PHE	-	expression tag	UNP Q4KMN5
A	44	GLN	-	expression tag	UNP Q4KMN5
A	45	GLY	-	expression tag	UNP Q4KMN5
A	343	GLN	ASN	engineered mutation	UNP Q4KMN5
B	30	ALA	-	expression tag	UNP Q4KMN5
B	31	ASP	-	expression tag	UNP Q4KMN5
B	32	PRO	-	expression tag	UNP Q4KMN5
B	33	HIS	-	expression tag	UNP Q4KMN5
B	34	HIS	-	expression tag	UNP Q4KMN5
B	35	HIS	-	expression tag	UNP Q4KMN5
B	36	HIS	-	expression tag	UNP Q4KMN5
B	37	HIS	-	expression tag	UNP Q4KMN5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	38	HIS	-	expression tag	UNP Q4KMN5
B	39	GLU	-	expression tag	UNP Q4KMN5
B	40	ASN	-	expression tag	UNP Q4KMN5
B	41	LEU	-	expression tag	UNP Q4KMN5
B	42	TYR	-	expression tag	UNP Q4KMN5
B	43	PHE	-	expression tag	UNP Q4KMN5
B	44	GLN	-	expression tag	UNP Q4KMN5
B	45	GLY	-	expression tag	UNP Q4KMN5
B	343	GLN	ASN	engineered mutation	UNP Q4KMN5

- Molecule 2 is a protein called NRXN1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	187	Total	C	N	O	S	14	0	0
			1431	902	255	273	1			
2	F	187	Total	C	N	O	S	14	0	0
			1431	902	255	273	1			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	73	HIS	-	expression tag	UNP A4FVB9
E	74	SER	-	expression tag	UNP A4FVB9
E	75	ALA	-	expression tag	UNP A4FVB9
E	76	PHE	-	expression tag	UNP A4FVB9
E	77	ALA	-	expression tag	UNP A4FVB9
E	78	ALA	-	expression tag	UNP A4FVB9
E	79	ASP	-	expression tag	UNP A4FVB9
E	80	PRO	-	expression tag	UNP A4FVB9
E	293	HIS	-	expression tag	UNP A4FVB9
E	294	HIS	-	expression tag	UNP A4FVB9
E	295	HIS	-	expression tag	UNP A4FVB9
E	296	HIS	-	expression tag	UNP A4FVB9
E	297	HIS	-	expression tag	UNP A4FVB9
E	298	HIS	-	expression tag	UNP A4FVB9
E	299	HIS	-	expression tag	UNP A4FVB9
F	73	HIS	-	expression tag	UNP A4FVB9
F	74	SER	-	expression tag	UNP A4FVB9
F	75	ALA	-	expression tag	UNP A4FVB9
F	76	PHE	-	expression tag	UNP A4FVB9
F	77	ALA	-	expression tag	UNP A4FVB9
F	78	ALA	-	expression tag	UNP A4FVB9

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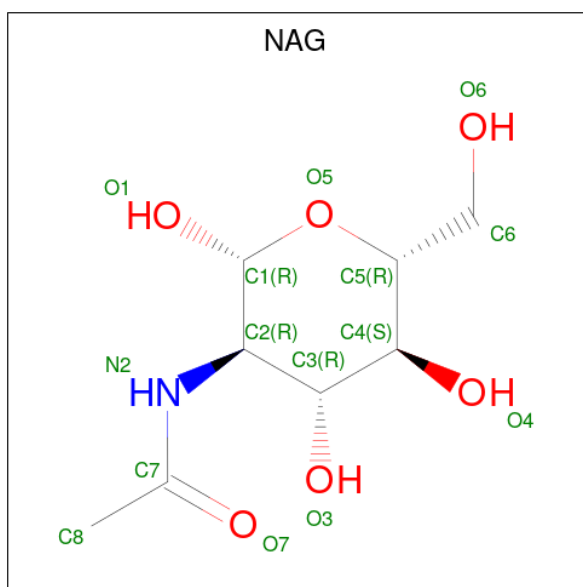
Chain	Residue	Modelled	Actual	Comment	Reference
F	79	ASP	-	expression tag	UNP A4FVB9
F	80	PRO	-	expression tag	UNP A4FVB9
F	293	HIS	-	expression tag	UNP A4FVB9
F	294	HIS	-	insertion	UNP A4FVB9
F	295	HIS	-	expression tag	UNP A4FVB9
F	296	HIS	-	expression tag	UNP A4FVB9
F	297	HIS	-	expression tag	UNP A4FVB9
F	298	HIS	-	expression tag	UNP A4FVB9
F	299	HIS	-	expression tag	UNP A4FVB9

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		

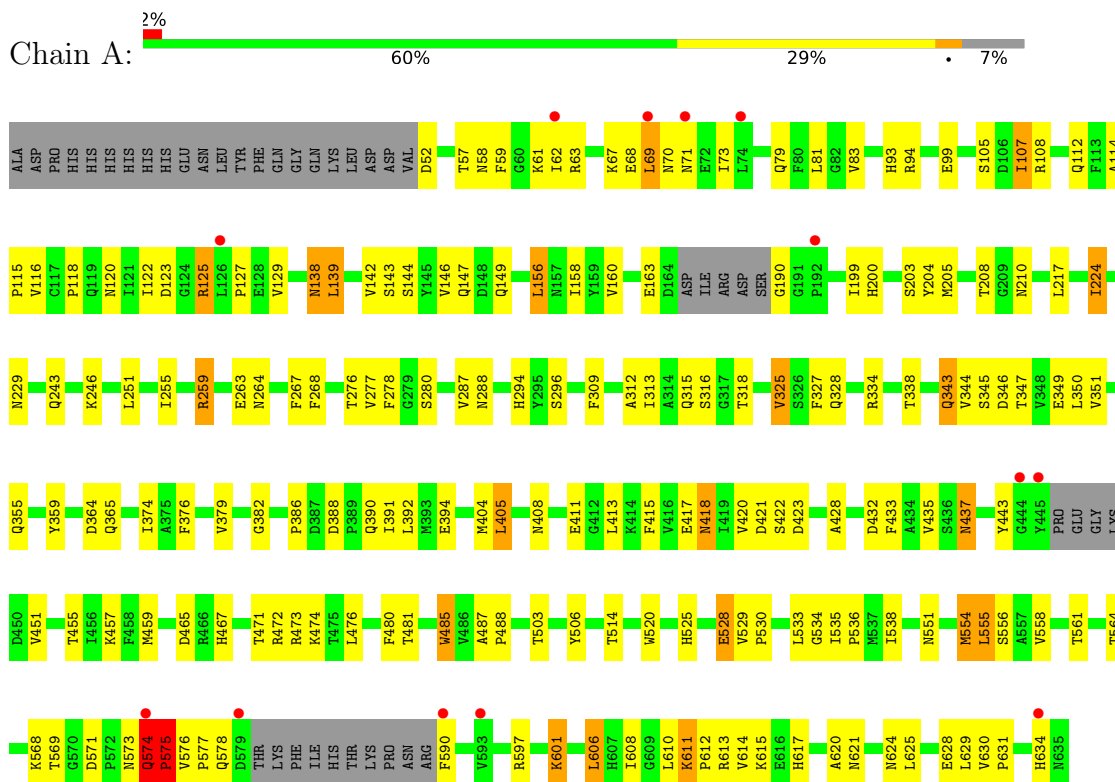
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	536	Total	O	0	0
			536	536		
6	B	598	Total	O	0	0
			598	598		
6	E	230	Total	O	0	0
			230	230		
6	F	188	Total	O	0	0
			188	188		

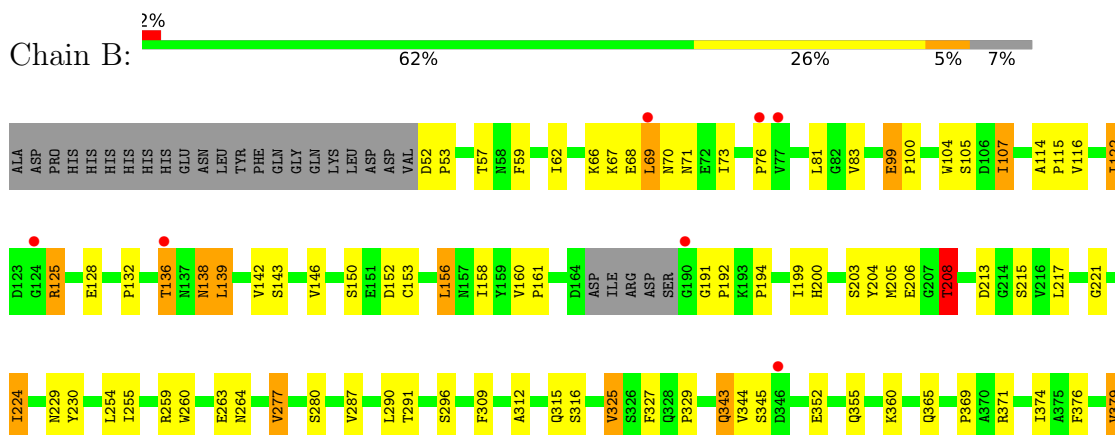
3 Residue-property plots

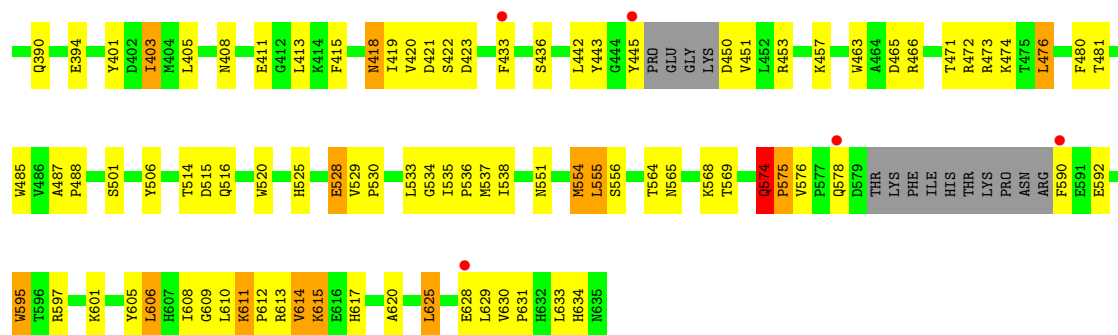
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Nlgn1 protein

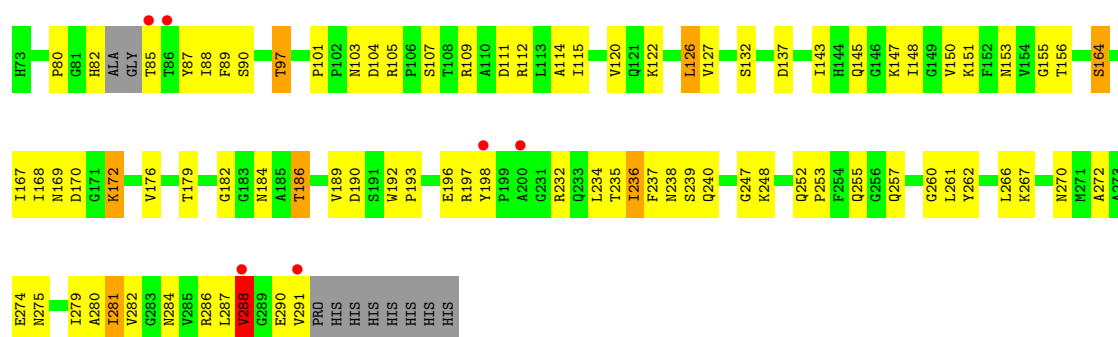


• Molecule 1: Nlgn1 protein

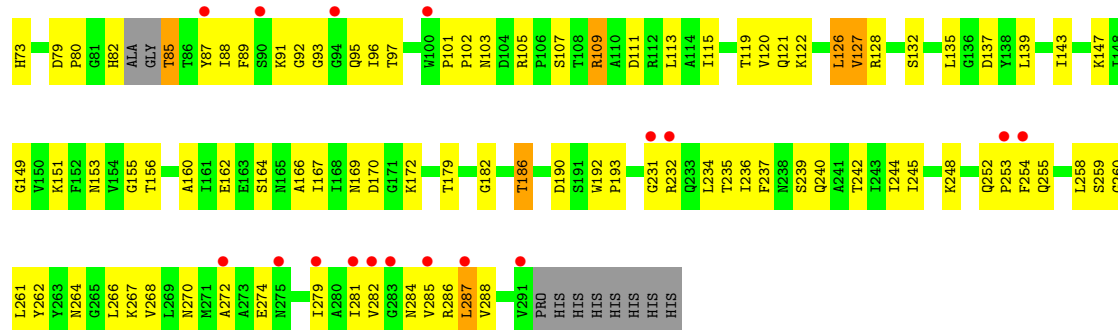




• Molecule 2: NRXN1 protein



• Molecule 2: NRXN1 protein



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



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

Chain D:  100%

MAG1
MAG2

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

Chain G:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.59Å 125.40Å 131.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.64 – 2.40 24.64 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.5 (24.64-2.40) 97.8 (24.64-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.28Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.261 0.242 , 0.262	Depositor DCC
R_{free} test set	4282 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12952	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: CA, 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	0.47	0/4338	0.82	5/5922 (0.1%)
1	B	0.50	0/4338	0.82	6/5922 (0.1%)
2	E	0.45	0/1459	0.80	2/1977 (0.1%)
2	F	0.49	0/1459	0.79	2/1977 (0.1%)
All	All	0.48	0/11594	0.82	15/15798 (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
1	A	0	1
1	B	0	1
2	F	0	1
All	All	0	3

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	GLN	OE1-CD-NE2	-9.81	112.79	122.60
1	B	343	GLN	OE1-CD-NE2	-9.77	112.83	122.60
1	A	73	ILE	N-CA-C	-7.74	106.36	113.71
1	B	73	ILE	N-CA-C	-6.92	107.14	113.71
1	B	574	GLN	CA-C-N	6.88	128.44	119.84
1	B	574	GLN	C-N-CA	6.88	128.44	119.84
1	A	343	GLN	CG-CD-NE2	6.66	126.39	116.40
1	B	343	GLN	CG-CD-NE2	6.66	126.38	116.40
2	F	122	LYS	CA-CB-CG	-6.64	100.83	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	574	GLN	CA-C-N	6.57	128.05	119.84
1	A	574	GLN	C-N-CA	6.57	128.05	119.84
2	F	236	ILE	N-CA-C	6.30	116.92	108.11
2	E	236	ILE	N-CA-C	5.61	115.96	108.11
1	B	208	THR	CB-CA-C	-5.44	100.51	110.62
2	E	122	LYS	CA-CB-CG	-5.18	103.73	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	574	GLN	Peptide
1	B	574	GLN	Peptide
2	F	109	ARG	Mainchain

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	4219	0	4049	154	0
1	B	4219	0	4049	148	1
2	E	1431	0	1406	64	0
2	F	1431	0	1406	79	2
3	C	28	0	25	4	0
3	D	28	0	25	3	0
3	G	28	0	25	2	0
4	A	14	0	13	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	536	0	0	32	1
6	B	598	0	0	40	1
6	E	230	0	0	15	3
6	F	188	0	0	26	2
All	All	12952	0	10998	452	5

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 20.

All (452) 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:F:147:LYS:HD3	2:F:164:SER:HA	1.22	1.18
1:A:334:ARG:HG3	1:A:344:VAL:CG2	1.86	1.04
2:E:147:LYS:HD3	2:E:164:SER:HA	1.43	1.00
1:A:334:ARG:HG3	1:A:344:VAL:HG21	1.40	0.99
3:G:1:NAG:H62	3:G:2:NAG:H2	1.45	0.96
3:C:1:NAG:H3	3:C:2:NAG:H61	1.45	0.95
1:A:613:ARG:HD3	6:A:691:HOH:O	1.71	0.91
2:F:248:LYS:HB2	6:F:719:HOH:O	1.70	0.90
1:A:67:LYS:HE3	6:A:930:HOH:O	1.74	0.88
2:E:291:VAL:HB	6:E:482:HOH:O	1.75	0.86
1:B:355:GLN:HG3	6:B:875:HOH:O	1.73	0.86
1:A:112:GLN:NE2	6:A:876:HOH:O	2.06	0.85
2:F:192:TRP:HB3	2:F:193:PRO:HD2	1.58	0.85
1:A:574:GLN:HB3	1:A:575:PRO:HD2	1.56	0.84
2:F:127:VAL:HG21	2:F:261:LEU:HD11	1.59	0.84
1:A:52:ASP:N	6:A:1055:HOH:O	2.10	0.84
3:G:1:NAG:C6	3:G:2:NAG:H2	2.07	0.84
1:B:450:ASP:HB2	6:B:707:HOH:O	1.76	0.84
2:F:287:LEU:HD12	6:F:795:HOH:O	1.78	0.84
1:B:574:GLN:HB3	1:B:575:PRO:HD2	1.60	0.83
1:A:418:ASN:HD22	1:A:418:ASN:H	1.26	0.82
1:A:574:GLN:HB3	1:A:575:PRO:CD	2.09	0.82
2:F:135:LEU:HA	6:F:759:HOH:O	1.78	0.82
1:A:473:ARG:NH2	1:A:520:TRP:HB2	1.93	0.81
1:A:108:ARG:HG3	6:A:836:HOH:O	1.80	0.81
1:A:199:ILE:CD1	1:A:277:VAL:HG13	2.10	0.81
2:E:115:ILE:HD13	2:E:261:LEU:HD12	1.62	0.81
1:A:190:GLY:HA3	6:A:941:HOH:O	1.80	0.80
1:A:208:THR:HG23	1:A:229:ASN:OD1	1.81	0.80
1:A:421:ASP:O	1:A:423:ASP:N	2.15	0.80
2:F:164:SER:HB2	6:F:761:HOH:O	1.82	0.79
1:B:421:ASP:O	1:B:423:ASP:N	2.16	0.78
2:F:166:ALA:HB3	2:F:192:TRP:CZ3	2.18	0.78
1:B:205:MET:HE1	1:B:376:PHE:HB2	1.67	0.77
2:F:170:ASP:OD1	2:F:172:LYS:HG2	1.85	0.77
1:B:466:ARG:HG2	6:B:693:HOH:O	1.84	0.77
1:A:577:PRO:HB3	6:A:1068:HOH:O	1.86	0.76
1:B:418:ASN:H	1:B:418:ASN:HD22	1.33	0.75
2:F:286:ARG:HG2	6:F:795:HOH:O	1.85	0.74
1:A:334:ARG:CG	1:A:344:VAL:HG21	2.15	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:80:PRO:O	2:F:260:GLY:HA3	1.85	0.74
2:F:179:THR:HB	2:F:186:THR:HB	1.70	0.74
1:A:611:LYS:H	1:A:611:LYS:HD2	1.53	0.73
2:E:192:TRP:HB3	2:E:193:PRO:HD2	1.69	0.73
1:B:146:VAL:HG12	1:B:146:VAL:O	1.89	0.73
1:B:481:THR:HA	1:B:485:TRP:HD1	1.54	0.72
1:B:125:ARG:HG3	6:B:1216:HOH:O	1.89	0.72
1:A:564:THR:O	1:A:568:LYS:HG3	1.88	0.72
2:F:160:ALA:HA	6:F:802:HOH:O	1.89	0.72
1:A:569:THR:HG21	1:A:575:PRO:HD2	1.72	0.72
1:A:421:ASP:C	1:A:423:ASP:H	1.97	0.72
2:E:184:ASN:HB3	6:E:373:HOH:O	1.88	0.72
2:E:275:ASN:HB3	6:E:343:HOH:O	1.88	0.72
2:F:89:PHE:O	2:F:255:GLN:HA	1.90	0.72
2:F:92:GLY:HA2	6:F:721:HOH:O	1.89	0.72
1:A:116:VAL:HG21	1:A:146:VAL:HG13	1.71	0.71
1:B:597:ARG:NH2	6:B:869:HOH:O	2.22	0.71
1:B:139:LEU:O	1:B:143:SER:OG	2.07	0.71
1:A:578:GLN:HB3	6:A:974:HOH:O	1.89	0.71
1:B:565:ASN:OD1	6:B:669:HOH:O	2.08	0.71
2:F:287:LEU:HD21	6:F:835:HOH:O	1.91	0.70
1:B:125:ARG:HB3	6:B:1216:HOH:O	1.91	0.70
1:B:208:THR:HG22	1:B:229:ASN:OD1	1.92	0.70
1:A:259:ARG:HG3	1:A:259:ARG:HH11	1.57	0.69
1:B:421:ASP:C	1:B:423:ASP:H	2.00	0.69
1:A:443:TYR:CD2	1:A:634:HIS:HE1	2.10	0.69
1:A:481:THR:HA	1:A:485:TRP:HD1	1.57	0.69
1:A:328:GLN:NE2	6:A:671:HOH:O	2.24	0.69
1:A:437:ASN:HB3	6:A:640:HOH:O	1.92	0.69
1:B:574:GLN:HB3	1:B:575:PRO:CD	2.21	0.69
1:A:334:ARG:HD3	6:A:966:HOH:O	1.92	0.68
1:B:481:THR:HA	1:B:485:TRP:CD1	2.28	0.68
2:F:147:LYS:CD	2:F:164:SER:HA	2.14	0.68
1:B:355:GLN:HB3	6:B:967:HOH:O	1.93	0.68
1:B:613:ARG:HD2	6:B:671:HOH:O	1.94	0.67
1:A:481:THR:HA	1:A:485:TRP:CD1	2.29	0.67
2:F:267:LYS:HE3	6:F:718:HOH:O	1.93	0.67
1:A:93:HIS:HB3	6:A:669:HOH:O	1.94	0.67
2:E:88:ILE:HD13	2:E:257:GLN:HG2	1.77	0.67
1:A:199:ILE:HD11	1:A:277:VAL:HG13	1.76	0.67
1:A:208:THR:CG2	1:A:229:ASN:OD1	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:ASN:HD22	1:B:418:ASN:N	1.90	0.67
2:F:244:ILE:O	2:F:244:ILE:HG22	1.95	0.67
1:A:577:PRO:HD2	6:A:1126:HOH:O	1.94	0.66
1:A:127:PRO:HG3	6:A:1011:HOH:O	1.94	0.66
1:B:255:ILE:HD11	1:B:290:LEU:HD22	1.78	0.66
2:F:270:ASN:O	2:F:274:GLU:HG2	1.96	0.66
1:B:457:LYS:NZ	6:B:953:HOH:O	2.28	0.66
2:F:272:ALA:CB	2:F:279:ILE:HG21	2.25	0.66
2:F:85:THR:O	2:F:85:THR:OG1	2.11	0.66
3:C:1:NAG:H83	3:C:2:NAG:H61	1.78	0.66
1:B:146:VAL:O	1:B:146:VAL:CG1	2.44	0.65
1:A:471:THR:HA	1:A:474:LYS:HD2	1.77	0.65
1:A:597:ARG:HD3	6:A:665:HOH:O	1.96	0.65
1:B:132:PRO:O	1:B:136:THR:HG23	1.97	0.65
1:B:125:ARG:CG	6:B:1216:HOH:O	2.43	0.65
1:B:360:LYS:HE3	6:B:933:HOH:O	1.95	0.65
2:E:238:ASN:ND2	6:E:311:HOH:O	2.19	0.65
1:A:70:ASN:HB2	1:A:538:ILE:HG23	1.79	0.65
1:B:191:GLY:HA3	6:B:965:HOH:O	1.96	0.65
2:E:281:ILE:HD12	2:E:281:ILE:H	1.62	0.65
2:F:93:GLY:HA3	6:F:805:HOH:O	1.97	0.64
1:A:146:VAL:HG12	1:A:146:VAL:O	1.97	0.64
1:A:205:MET:HE1	1:A:376:PHE:HB2	1.79	0.64
1:B:634:HIS:HB2	6:B:1005:HOH:O	1.97	0.64
1:A:125:ARG:HA	6:A:706:HOH:O	1.96	0.64
1:A:139:LEU:HA	1:A:142:VAL:HB	1.80	0.63
1:A:315:GLN:HG2	1:A:506:TYR:OH	1.98	0.63
1:B:408:ASN:HD21	1:B:528:GLU:HG3	1.62	0.63
1:A:487:ALA:HB3	1:A:488:PRO:HD3	1.79	0.63
1:B:569:THR:HG21	1:B:575:PRO:HD2	1.81	0.63
1:A:277:VAL:HG12	1:A:287:VAL:HG22	1.80	0.63
1:B:125:ARG:CB	6:B:1216:HOH:O	2.44	0.62
2:E:290:GLU:HG2	6:E:324:HOH:O	1.98	0.62
1:B:564:THR:O	1:B:568:LYS:HG3	1.99	0.62
1:B:70:ASN:HB2	1:B:538:ILE:HG23	1.82	0.62
1:A:125:ARG:HD3	6:A:922:HOH:O	1.99	0.61
1:A:139:LEU:HD12	1:A:139:LEU:H	1.66	0.61
1:A:535:ILE:N	1:A:536:PRO:CD	2.63	0.61
2:E:182:GLY:HA2	2:E:235:THR:HA	1.81	0.61
2:F:155:GLY:HA3	2:F:234:LEU:HD12	1.83	0.61
1:A:597:ARG:HH11	1:A:597:ARG:HG3	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ARG:HB3	6:A:1011:HOH:O	2.01	0.60
1:B:208:THR:CG2	1:B:229:ASN:OD1	2.50	0.60
2:F:182:GLY:HA2	2:F:235:THR:HA	1.81	0.60
2:F:87:TYR:HD2	2:F:285:VAL:HG12	1.67	0.60
1:B:535:ILE:N	1:B:536:PRO:CD	2.64	0.59
1:B:592:GLU:HG3	6:B:1153:HOH:O	2.02	0.59
2:E:90:SER:HB2	2:E:284:ASN:OD1	2.03	0.59
1:B:122:ILE:HD11	6:B:745:HOH:O	2.00	0.59
2:E:120:VAL:HG22	6:E:303:HOH:O	2.03	0.59
1:B:568:LYS:CE	6:B:669:HOH:O	2.50	0.58
2:F:149:GLY:HA3	2:F:162:GLU:HG3	1.85	0.58
1:A:138:ASN:N	1:A:138:ASN:HD22	2.01	0.58
1:B:203:SER:O	1:B:204:TYR:HB2	2.03	0.58
2:E:115:ILE:CG2	2:E:176:VAL:CG1	2.82	0.58
2:F:192:TRP:H	2:F:192:TRP:CD1	2.20	0.58
1:A:467:HIS:HD2	6:A:699:HOH:O	1.85	0.58
1:A:57:THR:HA	1:A:267:PHE:CD1	2.39	0.58
2:E:80:PRO:O	2:E:260:GLY:HA3	2.03	0.58
1:A:455:THR:O	1:A:459:MET:HG2	2.04	0.58
2:F:281:ILE:H	2:F:281:ILE:HD12	1.69	0.58
1:B:199:ILE:HD12	1:B:277:VAL:HG13	1.85	0.57
1:A:243:GLN:HG3	1:A:246:LYS:HE2	1.87	0.57
2:E:115:ILE:HG23	2:E:176:VAL:HG12	1.85	0.57
2:E:155:GLY:HA3	2:E:234:LEU:HD12	1.86	0.57
1:A:634:HIS:HB3	6:A:681:HOH:O	2.04	0.57
2:F:272:ALA:HB2	2:F:279:ILE:HG21	1.87	0.57
1:A:139:LEU:H	1:A:139:LEU:CD1	2.17	0.57
2:F:151:LYS:HB2	6:F:802:HOH:O	2.03	0.57
1:A:415:PHE:CD1	1:A:480:PHE:HB2	2.39	0.56
1:B:609:GLY:O	1:B:612:PRO:HD3	2.06	0.56
1:A:606:LEU:CD1	1:A:608:ILE:HG12	2.35	0.56
2:F:91:LYS:O	2:F:284:ASN:ND2	2.39	0.56
1:B:200:HIS:HA	6:B:868:HOH:O	2.04	0.56
1:B:128:GLU:CD	6:B:1010:HOH:O	2.48	0.56
1:B:625:LEU:HD22	1:B:630:VAL:HG23	1.87	0.56
1:A:208:THR:HG22	1:A:210:ASN:H	1.71	0.56
2:E:127:VAL:HG21	2:E:261:LEU:HD11	1.87	0.56
1:B:418:ASN:H	1:B:418:ASN:ND2	2.02	0.56
2:F:248:LYS:HA	2:F:253:PRO:HG3	1.88	0.56
1:B:471:THR:HA	1:B:474:LYS:HD2	1.88	0.56
1:A:259:ARG:HG3	6:A:1058:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:112:ARG:NH1	2:E:179:THR:HG23	2.20	0.55
1:B:516:GLN:NE2	6:B:1046:HOH:O	2.39	0.55
2:E:179:THR:HB	2:E:186:THR:HB	1.88	0.55
2:F:245:ILE:HD11	2:F:268:VAL:HG11	1.88	0.55
1:A:200:HIS:HE1	6:A:639:HOH:O	1.90	0.55
1:B:473:ARG:NH2	1:B:520:TRP:HB2	2.21	0.55
1:A:617:HIS:HB3	1:A:620:ALA:HB2	1.88	0.55
2:F:82:HIS:H	2:F:259:SER:HB3	1.72	0.55
2:F:192:TRP:CD1	2:F:192:TRP:N	2.72	0.54
1:A:421:ASP:C	1:A:423:ASP:N	2.64	0.54
1:A:578:GLN:HB2	1:A:590:PHE:HB2	1.87	0.54
1:A:465:ASP:HB2	6:A:938:HOH:O	2.07	0.54
1:B:68:GLU:HG2	1:B:76:PRO:HB3	1.90	0.54
1:A:597:ARG:CD	6:A:665:HOH:O	2.54	0.54
1:A:428:ALA:HB2	1:A:472:ARG:NH1	2.22	0.54
1:A:83:VAL:HB	1:A:156:LEU:HD23	1.89	0.54
2:F:248:LYS:HD2	6:F:805:HOH:O	2.07	0.54
1:B:259:ARG:HG3	1:B:259:ARG:HH11	1.72	0.54
1:B:578:GLN:HB2	1:B:590:PHE:HB2	1.89	0.54
1:B:611:LYS:HE3	6:B:1007:HOH:O	2.08	0.54
2:F:151:LYS:CB	6:F:802:HOH:O	2.54	0.54
1:A:443:TYR:CD2	1:A:634:HIS:CE1	2.94	0.53
2:F:102:PRO:HG3	2:F:105:ARG:HH21	1.71	0.53
2:E:145:GLN:NE2	6:E:416:HOH:O	2.41	0.53
1:A:146:VAL:HG12	1:A:149:GLN:HE21	1.73	0.53
2:E:120:VAL:HA	2:E:169:ASN:O	2.08	0.53
1:B:116:VAL:HG12	1:B:208:THR:CG2	2.39	0.53
1:B:116:VAL:HG12	1:B:208:THR:HG21	1.91	0.53
1:B:485:TRP:CZ3	1:B:525:HIS:CE1	2.96	0.53
2:F:160:ALA:CB	6:F:802:HOH:O	2.57	0.53
1:A:418:ASN:HD22	1:A:418:ASN:N	2.01	0.53
1:A:473:ARG:HH22	1:A:520:TRP:HB2	1.72	0.53
1:B:277:VAL:CG1	1:B:287:VAL:HG22	2.39	0.53
2:E:112:ARG:HG3	6:E:341:HOH:O	2.09	0.53
1:A:388:ASP:HB3	1:A:391:ILE:HG12	1.90	0.53
1:A:443:TYR:HD2	1:A:634:HIS:HE1	1.56	0.52
2:F:166:ALA:HB3	2:F:192:TRP:HZ3	1.70	0.52
1:B:534:GLY:HA2	1:B:556:SER:OG	2.09	0.52
1:B:612:PRO:HB3	6:B:714:HOH:O	2.09	0.52
1:A:551:ASN:O	1:A:554:MET:HG3	2.10	0.52
2:F:160:ALA:HB1	6:F:822:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ASN:HD21	1:A:528:GLU:HG3	1.73	0.52
1:A:411:GLU:HB2	1:A:481:THR:HG23	1.91	0.52
1:A:163:GLU:HG3	6:A:1044:HOH:O	2.09	0.52
1:B:630:VAL:N	1:B:631:PRO:CD	2.72	0.52
2:E:97:THR:HG22	2:E:280:ALA:HB3	1.92	0.52
1:A:83:VAL:HB	1:A:156:LEU:CD2	2.41	0.51
2:F:242:THR:HG21	6:F:780:HOH:O	2.09	0.51
1:A:208:THR:HG21	1:A:210:ASN:CG	2.35	0.51
1:B:514:THR:HG22	1:B:515:ASP:N	2.25	0.51
1:B:401:TYR:HB2	1:B:403:ILE:HD11	1.91	0.51
2:E:101:PRO:HG2	2:E:104:ASP:HB3	1.93	0.50
2:E:179:THR:HG22	6:E:312:HOH:O	2.11	0.50
1:B:606:LEU:HD12	1:B:608:ILE:HG12	1.93	0.50
2:E:192:TRP:CD1	2:E:192:TRP:N	2.75	0.50
3:C:1:NAG:H83	3:C:2:NAG:C6	2.41	0.50
1:A:473:ARG:NE	1:A:520:TRP:CE3	2.80	0.50
1:B:139:LEU:HA	1:B:142:VAL:HB	1.92	0.50
1:A:390:GLN:O	1:A:394:GLU:HB2	2.10	0.50
1:B:568:LYS:HE2	6:B:669:HOH:O	2.09	0.50
2:E:286:ARG:NH2	6:E:386:HOH:O	2.44	0.50
2:F:137:ASP:HA	2:F:153:ASN:O	2.11	0.50
1:B:371:ARG:HG3	6:B:1136:HOH:O	2.11	0.50
1:B:466:ARG:NH1	6:B:693:HOH:O	2.45	0.50
1:A:94:ARG:O	1:A:355:GLN:NE2	2.44	0.50
1:A:554:MET:HG3	1:A:555:LEU:N	2.26	0.50
2:F:127:VAL:CG2	2:F:261:LEU:HD11	2.37	0.50
1:A:69:LEU:C	1:A:71:ASN:H	2.20	0.49
1:B:442:LEU:HD12	6:B:716:HOH:O	2.12	0.49
1:B:260:TRP:O	1:B:264:ASN:HB2	2.13	0.49
1:B:568:LYS:HE3	6:B:669:HOH:O	2.11	0.49
1:B:421:ASP:C	1:B:423:ASP:N	2.66	0.49
2:E:97:THR:CG2	2:E:97:THR:O	2.61	0.49
1:A:473:ARG:HG3	1:A:474:LYS:N	2.28	0.49
2:F:286:ARG:CG	6:F:795:HOH:O	2.52	0.49
1:A:138:ASN:HD22	1:A:138:ASN:H	1.60	0.49
1:B:418:ASN:HB3	6:B:807:HOH:O	2.12	0.49
1:B:614:VAL:HG12	6:B:788:HOH:O	2.12	0.49
1:B:83:VAL:HB	1:B:156:LEU:HD23	1.93	0.49
2:E:197:ARG:NH1	6:E:434:HOH:O	2.36	0.49
2:E:89:PHE:O	2:E:255:GLN:HA	2.13	0.49
2:F:87:TYR:HD2	2:F:285:VAL:CG1	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:286:ARG:HB2	6:E:447:HOH:O	2.10	0.49
2:F:254:PHE:CE2	2:F:258:LEU:HD21	2.48	0.49
2:E:168:ILE:CG2	2:E:189:VAL:HG11	2.43	0.49
2:F:101:PRO:HB2	2:F:103:ASN:OD1	2.11	0.49
2:F:147:LYS:HG2	2:F:166:ALA:O	2.13	0.49
2:E:114:ALA:HB3	2:E:262:TYR:HB3	1.95	0.48
2:E:272:ALA:CB	2:E:279:ILE:HG21	2.42	0.48
2:F:95:GLN:HG3	6:F:719:HOH:O	2.13	0.48
3:C:1:NAG:H3	3:C:2:NAG:C6	2.32	0.48
1:A:325:VAL:HG22	1:A:327:PHE:CZ	2.48	0.48
1:A:160:VAL:HG13	1:A:224:ILE:CD1	2.43	0.48
2:E:192:TRP:HB3	2:E:193:PRO:CD	2.41	0.48
1:B:287:VAL:CG1	1:B:312:ALA:HB1	2.43	0.48
1:B:296:SER:HB2	1:B:309:PHE:CE1	2.49	0.48
2:E:115:ILE:HG22	2:E:176:VAL:HG13	1.96	0.48
1:A:57:THR:C	1:A:59:PHE:H	2.22	0.48
1:B:371:ARG:CZ	6:B:1160:HOH:O	2.61	0.48
1:A:199:ILE:CD1	1:A:277:VAL:CG1	2.86	0.48
1:B:199:ILE:CD1	1:B:277:VAL:HG13	2.44	0.48
1:B:445:TYR:CD1	1:B:445:TYR:C	2.92	0.48
2:F:252:GLN:N	2:F:253:PRO:HD3	2.29	0.48
1:A:160:VAL:HG13	1:A:224:ILE:HD13	1.96	0.47
2:E:101:PRO:HB2	2:E:103:ASN:OD1	2.14	0.47
1:B:221:GLY:O	1:B:568:LYS:NZ	2.47	0.47
1:A:57:THR:HA	1:A:267:PHE:HD1	1.77	0.47
1:A:114:ALA:HB1	1:A:115:PRO:HD2	1.95	0.47
1:B:514:THR:HG22	1:B:515:ASP:H	1.79	0.47
1:B:617:HIS:HB3	1:B:620:ALA:HB2	1.96	0.47
2:E:192:TRP:CD1	2:E:192:TRP:H	2.32	0.47
2:E:252:GLN:N	2:E:253:PRO:HD3	2.29	0.47
1:A:118:PRO:HB3	1:A:359:TYR:CE1	2.49	0.47
1:A:343:GLN:HB2	6:A:932:HOH:O	2.15	0.47
1:A:443:TYR:HD2	1:A:634:HIS:CE1	2.32	0.47
1:B:465:ASP:N	1:B:465:ASP:OD2	2.46	0.47
1:B:277:VAL:HG12	1:B:287:VAL:HG22	1.96	0.47
1:B:329:PRO:HG3	1:B:379:VAL:HG21	1.95	0.47
1:A:287:VAL:CG1	1:A:312:ALA:HB1	2.45	0.47
1:B:69:LEU:C	1:B:71:ASN:H	2.22	0.47
1:B:554:MET:HE1	6:B:771:HOH:O	2.13	0.47
6:B:1235:HOH:O	3:D:2:NAG:H81	2.15	0.47
2:E:126:LEU:N	2:E:126:LEU:HD23	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ARG:HG3	1:A:259:ARG:NH1	2.27	0.47
1:B:83:VAL:HB	1:B:156:LEU:CD2	2.45	0.47
1:B:99:GLU:HG3	1:B:100:PRO:CD	2.44	0.47
1:B:473:ARG:HG3	1:B:474:LYS:N	2.30	0.47
1:B:487:ALA:N	1:B:488:PRO:CD	2.78	0.47
2:F:82:HIS:C	6:F:840:HOH:O	2.58	0.47
2:F:121:GLN:OE1	2:F:255:GLN:N	2.40	0.47
1:A:144:SER:HA	1:A:147:GLN:HG2	1.97	0.47
1:B:371:ARG:NH2	6:B:1160:HOH:O	2.48	0.47
2:E:143:ILE:HG12	2:E:148:ILE:HD12	1.97	0.47
2:F:113:LEU:HD11	2:F:261:LEU:HD21	1.97	0.47
2:E:234:LEU:HD23	6:E:404:HOH:O	2.15	0.47
1:A:613:ARG:CD	6:A:691:HOH:O	2.43	0.46
1:A:529:VAL:N	1:A:530:PRO:HD2	2.29	0.46
1:A:68:GLU:HA	6:A:646:HOH:O	2.15	0.46
1:A:350:LEU:C	1:A:350:LEU:HD23	2.40	0.46
1:A:259:ARG:NH1	1:A:259:ARG:CG	2.79	0.46
1:A:386:PRO:HG2	1:A:392:LEU:HD11	1.97	0.46
2:E:137:ASP:HA	2:E:153:ASN:O	2.16	0.46
1:A:62:ILE:HD11	1:A:268:PHE:CZ	2.51	0.46
1:A:62:ILE:HD11	1:A:268:PHE:HZ	1.80	0.46
1:B:213:ASP:OD1	1:B:215:SER:HB2	2.16	0.46
1:B:605:TYR:CZ	1:B:615:LYS:HB2	2.51	0.46
1:B:114:ALA:HB1	1:B:115:PRO:HD2	1.98	0.46
2:F:107:SER:HA	2:F:237:PHE:O	2.16	0.46
1:B:287:VAL:O	1:B:291:THR:HG23	2.16	0.46
2:E:115:ILE:CG2	2:E:176:VAL:HG13	2.46	0.46
1:B:611:LYS:H	1:B:611:LYS:HD2	1.81	0.46
1:A:325:VAL:HG22	1:A:327:PHE:CE1	2.51	0.46
1:A:606:LEU:HD13	1:A:608:ILE:HG12	1.97	0.46
3:D:1:NAG:O4	3:D:2:NAG:H62	2.16	0.46
1:A:79:GLN:HB2	1:A:81:LEU:HD11	1.99	0.45
2:E:247:GLY:N	6:E:438:HOH:O	2.49	0.45
2:F:120:VAL:HA	2:F:169:ASN:O	2.16	0.45
2:F:73:HIS:HB2	6:F:774:HOH:O	2.16	0.45
2:F:169:ASN:C	6:F:793:HOH:O	2.59	0.45
1:A:203:SER:O	1:A:204:TYR:HB2	2.16	0.45
1:B:390:GLN:O	1:B:394:GLU:HB2	2.17	0.45
1:B:107:ILE:HG12	6:B:926:HOH:O	2.16	0.45
2:F:79:ASP:OD1	2:F:80:PRO:HD2	2.17	0.45
1:A:143:SER:HB3	1:A:147:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:LYS:HD2	1:A:611:LYS:N	2.26	0.45
1:B:57:THR:C	1:B:59:PHE:H	2.24	0.45
2:F:85:THR:N	6:F:746:HOH:O	2.50	0.45
1:B:634:HIS:CD2	6:B:741:HOH:O	2.70	0.45
2:E:105:ARG:HB3	2:E:240:GLN:O	2.17	0.45
2:F:102:PRO:HA	2:F:105:ARG:HE	1.82	0.45
2:F:192:TRP:HB3	2:F:193:PRO:CD	2.38	0.45
1:A:382:GLY:HA2	1:A:386:PRO:HA	1.99	0.45
1:A:575:PRO:O	1:A:576:VAL:C	2.59	0.45
1:B:436:SER:OG	1:B:453:ARG:HD2	2.17	0.45
1:B:575:PRO:O	1:B:576:VAL:C	2.60	0.45
2:F:128:ARG:HA	2:F:139:LEU:O	2.17	0.45
2:F:95:GLN:CG	6:F:719:HOH:O	2.65	0.44
1:A:561:THR:HB	1:A:578:GLN:HE22	1.82	0.44
2:E:87:TYR:O	2:E:257:GLN:HA	2.16	0.44
2:E:148:ILE:HB	2:E:168:ILE:HG12	1.99	0.44
2:E:168:ILE:HG21	2:E:189:VAL:HG11	2.00	0.44
2:F:102:PRO:HA	2:F:105:ARG:NE	2.32	0.44
1:B:515:ASP:N	1:B:515:ASP:OD1	2.47	0.44
1:B:408:ASN:ND2	1:B:528:GLU:HG3	2.32	0.44
1:B:411:GLU:HB2	1:B:481:THR:HG23	2.00	0.44
1:B:259:ARG:HG3	1:B:259:ARG:NH1	2.31	0.44
1:A:503:THR:H	1:A:597:ARG:NH1	2.15	0.44
1:A:624:ASN:HB3	1:A:628:GLU:OE2	2.18	0.44
1:B:138:ASN:N	1:B:138:ASN:HD22	2.15	0.44
1:B:139:LEU:H	1:B:139:LEU:CD1	2.30	0.44
1:B:443:TYR:CD2	1:B:634:HIS:HE1	2.36	0.44
1:A:597:ARG:HG3	1:A:597:ARG:NH1	2.33	0.44
1:B:160:VAL:HG13	1:B:224:ILE:HD13	1.99	0.44
1:A:62:ILE:HG22	1:A:108:ARG:HB3	1.99	0.43
1:A:280:SER:HA	1:A:315:GLN:O	2.18	0.43
1:A:405:LEU:N	1:A:405:LEU:CD2	2.81	0.43
1:B:369:PRO:HD2	6:B:1012:HOH:O	2.18	0.43
1:A:296:SER:HB2	1:A:309:PHE:CE1	2.53	0.43
2:E:270:ASN:O	2:E:274:GLU:HG2	2.18	0.43
2:F:248:LYS:HG3	2:F:253:PRO:HG3	2.00	0.43
1:B:316:SER:OG	1:B:411:GLU:OE2	2.28	0.43
2:F:262:TYR:HA	2:F:266:LEU:O	2.18	0.43
1:A:61:LYS:HE2	6:A:1164:HOH:O	2.17	0.43
2:F:105:ARG:HB3	2:F:240:GLN:O	2.18	0.43
1:A:344:VAL:HG22	1:A:344:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:ASP:OD2	1:A:573:ASN:HB2	2.18	0.43
1:B:259:ARG:O	1:B:263:GLU:HG2	2.19	0.43
2:E:85:THR:OG1	2:E:87:TYR:HE1	2.01	0.43
2:E:107:SER:HA	2:E:237:PHE:O	2.18	0.43
1:B:415:PHE:CD1	1:B:480:PHE:HB2	2.54	0.43
1:A:349:GLU:CD	6:A:932:HOH:O	2.62	0.43
1:A:590:PHE:CZ	1:A:612:PRO:HG3	2.53	0.43
1:B:62:ILE:HG23	1:B:104:TRP:HZ2	1.84	0.43
1:B:514:THR:HG22	1:B:515:ASP:OD1	2.19	0.43
1:A:125:ARG:HA	1:A:125:ARG:NE	2.34	0.43
1:A:125:ARG:HA	1:A:125:ARG:HE	1.84	0.43
1:A:485:TRP:CZ3	1:A:525:HIS:CE1	3.07	0.43
1:A:601:LYS:HD3	6:A:867:HOH:O	2.18	0.43
1:B:325:VAL:HG22	1:B:327:PHE:CZ	2.54	0.43
1:A:120:ASN:ND2	1:A:364:ASP:OD1	2.52	0.43
1:A:143:SER:C	1:A:147:GLN:HE21	2.27	0.43
1:A:288:ASN:HD22	1:A:318:THR:HA	1.84	0.43
1:A:433:PHE:O	1:A:437:ASN:CG	2.61	0.43
1:B:551:ASN:O	1:B:554:MET:HG3	2.19	0.43
1:B:194:PRO:HG2	1:B:568:LYS:HG2	2.01	0.42
2:E:82:HIS:CD2	6:E:365:HOH:O	2.71	0.42
2:F:87:TYR:CD2	2:F:96:ILE:HD11	2.54	0.42
1:A:554:MET:HG3	1:A:555:LEU:H	1.85	0.42
1:B:360:LYS:HG3	6:B:933:HOH:O	2.20	0.42
1:B:472:ARG:O	1:B:476:LEU:HB2	2.19	0.42
1:B:485:TRP:C	1:B:488:PRO:HD2	2.44	0.42
1:B:255:ILE:CD1	1:B:290:LEU:HD22	2.49	0.42
2:E:80:PRO:HA	2:E:267:LYS:NZ	2.34	0.42
1:A:263:GLU:HG3	1:A:264:ASN:ND2	2.34	0.42
1:A:554:MET:O	1:A:558:VAL:HG23	2.20	0.42
1:B:555:LEU:HD23	1:B:555:LEU:HA	1.82	0.42
2:E:170:ASP:OD1	2:E:172:LYS:HG2	2.19	0.42
1:A:63:ARG:NH2	1:A:107:ILE:HD12	2.34	0.42
2:E:196:GLU:OE1	2:E:198:TYR:HE1	2.01	0.42
1:A:347:THR:O	1:A:351:VAL:HG23	2.20	0.42
2:E:111:ASP:O	2:E:112:ARG:HD3	2.20	0.42
2:F:119:THR:HB	2:F:254:PHE:HE1	1.85	0.42
1:A:432:ASP:HA	1:A:457:LYS:HE2	2.01	0.42
1:A:630:VAL:N	1:A:631:PRO:CD	2.83	0.42
1:B:199:ILE:HG12	1:B:254:LEU:HD22	2.01	0.42
1:B:315:GLN:O	1:B:316:SER:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LEU:O	1:A:255:ILE:HG12	2.19	0.41
1:A:288:ASN:ND2	1:A:318:THR:HA	2.35	0.41
1:B:152:ASP:OD1	1:B:152:ASP:C	2.63	0.41
1:B:401:TYR:O	1:B:501:SER:HB3	2.20	0.41
2:F:97:THR:HB	6:F:803:HOH:O	2.19	0.41
2:F:170:ASP:OD2	2:F:172:LYS:HD3	2.20	0.41
1:A:315:GLN:O	1:A:316:SER:C	2.64	0.41
1:B:66:LYS:HG2	1:B:67:LYS:N	2.36	0.41
1:B:99:GLU:HG3	1:B:100:PRO:HD2	2.00	0.41
1:B:506:TYR:HB3	1:B:595:TRP:CZ2	2.55	0.41
1:B:203:SER:O	1:B:204:TYR:CB	2.68	0.41
1:B:191:GLY:HA2	1:B:192:PRO:HD3	1.96	0.41
2:E:148:ILE:HG21	2:E:189:VAL:HG22	2.02	0.41
2:F:170:ASP:CG	2:F:172:LYS:HG2	2.45	0.41
2:E:115:ILE:CG2	2:E:176:VAL:HG12	2.45	0.41
2:E:288:VAL:O	2:E:288:VAL:HG12	2.19	0.41
2:F:231:GLY:HA3	6:F:735:HOH:O	2.19	0.41
1:A:294:HIS:CE1	2:E:236:ILE:HD11	2.55	0.41
1:B:160:VAL:HA	1:B:161:PRO:HD3	1.94	0.41
1:B:230:TYR:CD1	1:B:254:LEU:HD21	2.56	0.41
2:F:111:ASP:HA	2:F:264:ASN:OD1	2.20	0.41
1:B:52:ASP:HA	1:B:53:PRO:HD3	1.92	0.41
1:A:534:GLY:HA2	1:A:556:SER:OG	2.20	0.41
1:B:280:SER:HA	1:B:315:GLN:O	2.21	0.41
1:B:352:GLU:HA	6:B:875:HOH:O	2.21	0.41
1:B:554:MET:HG3	1:B:555:LEU:N	2.35	0.41
1:B:554:MET:CE	6:B:771:HOH:O	2.68	0.41
2:F:126:LEU:HD21	2:F:143:ILE:HG13	2.01	0.41
1:B:125:ARG:NE	1:B:125:ARG:HA	2.36	0.41
2:E:150:VAL:CG1	2:E:151:LYS:N	2.84	0.41
2:F:192:TRP:N	2:F:192:TRP:HD1	2.16	0.41
1:A:313:ILE:HA	1:A:404:MET:O	2.21	0.40
2:F:169:ASN:ND2	6:F:807:HOH:O	2.45	0.40
1:A:590:PHE:HA	6:A:1000:HOH:O	2.21	0.40
1:B:445:TYR:C	1:B:445:TYR:HD1	2.29	0.40
2:E:248:LYS:HA	2:E:253:PRO:HG3	2.02	0.40
1:A:435:VAL:HG11	1:A:457:LYS:HG3	2.04	0.40
1:A:628:GLU:OE2	1:B:463:TRP:CZ2	2.75	0.40
1:B:150:SER:O	1:B:153:CYS:HB3	2.20	0.40
1:B:419:ILE:HG22	1:B:419:ILE:O	2.21	0.40
1:B:529:VAL:N	1:B:530:PRO:HD2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:TYR:CE1	1:B:615:LYS:HB2	2.57	0.40
3:D:1:NAG:H3	3:D:1:NAG:H83	2.04	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:GLN:OE1	6:F:749:HOH:O[4_455]	1.64	0.56
6:A:912:HOH:O	6:F:764:HOH:O[4_445]	1.77	0.43
6:B:1124:HOH:O	6:E:499:HOH:O[4_545]	1.84	0.36
2:F:172:LYS:NZ	6:E:335:HOH:O[2_555]	2.10	0.10
2:F:172:LYS:CE	6:E:335:HOH:O[2_555]	2.16	0.04

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	528/577 (92%)	480 (91%)	44 (8%)	4 (1%)	16	25
1	B	528/577 (92%)	484 (92%)	40 (8%)	4 (1%)	16	25
2	E	183/197 (93%)	166 (91%)	12 (7%)	5 (3%)	4	4
2	F	183/197 (93%)	162 (88%)	16 (9%)	5 (3%)	4	4
All	All	1422/1548 (92%)	1292 (91%)	112 (8%)	18 (1%)	9	14

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	345	SER
1	A	422	SER
1	A	575	PRO
1	B	345	SER

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Mol	Chain	Res	Type
1	B	422	SER
1	B	575	PRO
2	E	156	THR
2	E	239	SER
2	F	156	THR
2	F	239	SER
1	B	595	TRP
2	E	132	SER
1	A	58	ASN
2	F	190	ASP
2	F	132	SER
2	E	190	ASP
2	E	288	VAL
2	F	288	VAL

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	458/496 (92%)	410 (90%)	48 (10%)	6	10
1	B	458/496 (92%)	412 (90%)	46 (10%)	7	11
2	E	150/158 (95%)	137 (91%)	13 (9%)	9	16
2	F	150/158 (95%)	139 (93%)	11 (7%)	13	22
All	All	1216/1308 (93%)	1098 (90%)	118 (10%)	8	12

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	99	GLU
1	A	105	SER
1	A	107	ILE
1	A	122	ILE
1	A	123	ASP
1	A	125	ARG

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Mol	Chain	Res	Type
1	A	129	VAL
1	A	138	ASN
1	A	139	LEU
1	A	156	LEU
1	A	158	ILE
1	A	217	LEU
1	A	224	ILE
1	A	259	ARG
1	A	276	THR
1	A	278	PHE
1	A	325	VAL
1	A	338	THR
1	A	346	ASP
1	A	365	GLN
1	A	374	ILE
1	A	379	VAL
1	A	405	LEU
1	A	413	LEU
1	A	417	GLU
1	A	418	ASN
1	A	420	VAL
1	A	437	ASN
1	A	451	VAL
1	A	476	LEU
1	A	485	TRP
1	A	514	THR
1	A	528	GLU
1	A	533	LEU
1	A	554	MET
1	A	555	LEU
1	A	574	GLN
1	A	575	PRO
1	A	601	LYS
1	A	606	LEU
1	A	610	LEU
1	A	611	LYS
1	A	614	VAL
1	A	615	LYS
1	A	621	ASN
1	A	625	LEU
1	A	629	LEU
1	B	69	LEU

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Mol	Chain	Res	Type
1	B	81	LEU
1	B	99	GLU
1	B	105	SER
1	B	107	ILE
1	B	122	ILE
1	B	125	ARG
1	B	136	THR
1	B	138	ASN
1	B	139	LEU
1	B	156	LEU
1	B	158	ILE
1	B	206	GLU
1	B	208	THR
1	B	217	LEU
1	B	224	ILE
1	B	277	VAL
1	B	325	VAL
1	B	344	VAL
1	B	365	GLN
1	B	374	ILE
1	B	379	VAL
1	B	403	ILE
1	B	405	LEU
1	B	413	LEU
1	B	418	ASN
1	B	420	VAL
1	B	433	PHE
1	B	451	VAL
1	B	476	LEU
1	B	528	GLU
1	B	533	LEU
1	B	537	MET
1	B	554	MET
1	B	555	LEU
1	B	574	GLN
1	B	601	LYS
1	B	606	LEU
1	B	610	LEU
1	B	611	LYS
1	B	614	VAL
1	B	615	LYS
1	B	625	LEU

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Mol	Chain	Res	Type
1	B	628	GLU
1	B	629	LEU
1	B	633	LEU
2	E	97	THR
2	E	109	ARG
2	E	126	LEU
2	E	164	SER
2	E	167	ILE
2	E	172	LYS
2	E	186	THR
2	E	232	ARG
2	E	266	LEU
2	E	281	ILE
2	E	282	VAL
2	E	287	LEU
2	E	288	VAL
2	F	85	THR
2	F	88	ILE
2	F	109	ARG
2	F	115	ILE
2	F	126	LEU
2	F	127	VAL
2	F	167	ILE
2	F	186	THR
2	F	232	ARG
2	F	282	VAL
2	F	287	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	138	ASN
1	A	147	GLN
1	A	328	GLN
1	A	418	ASN
1	A	467	HIS
1	A	496	HIS
1	A	511	HIS
1	A	516	GLN
1	A	634	HIS
1	B	138	ASN

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Mol	Chain	Res	Type
1	B	200	HIS
1	B	288	ASN
1	B	294	HIS
1	B	418	ASN
1	B	437	ASN
1	B	634	HIS
2	E	153	ASN
2	F	284	ASN

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](#)

6 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	C	1	1,3	14,14,15	0.77	0	17,19,21	1.51	2 (11%)
3	NAG	C	2	3	14,14,15	0.68	0	17,19,21	0.89	1 (5%)
3	NAG	D	1	1,3	14,14,15	0.69	0	17,19,21	1.26	3 (17%)
3	NAG	D	2	3	14,14,15	0.75	0	17,19,21	0.96	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.93	1 (7%)	17,19,21	0.96	0
3	NAG	G	2	3	14,14,15	0.85	0	17,19,21	0.80	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	C	1	1,3	-	5/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	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)
3	G	1	NAG	C1-C2	2.80	1.56	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C4-C3-C2	4.40	117.46	111.02
3	D	1	NAG	C4-C3-C2	3.44	116.06	111.02
3	C	1	NAG	C3-C4-C5	2.56	114.88	110.23
3	D	1	NAG	C3-C4-C5	2.50	114.76	110.23
3	D	1	NAG	C2-N2-C7	-2.47	119.59	122.90
3	C	2	NAG	C2-N2-C7	-2.23	119.91	122.90
3	D	2	NAG	C2-N2-C7	-2.14	120.04	122.90

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2

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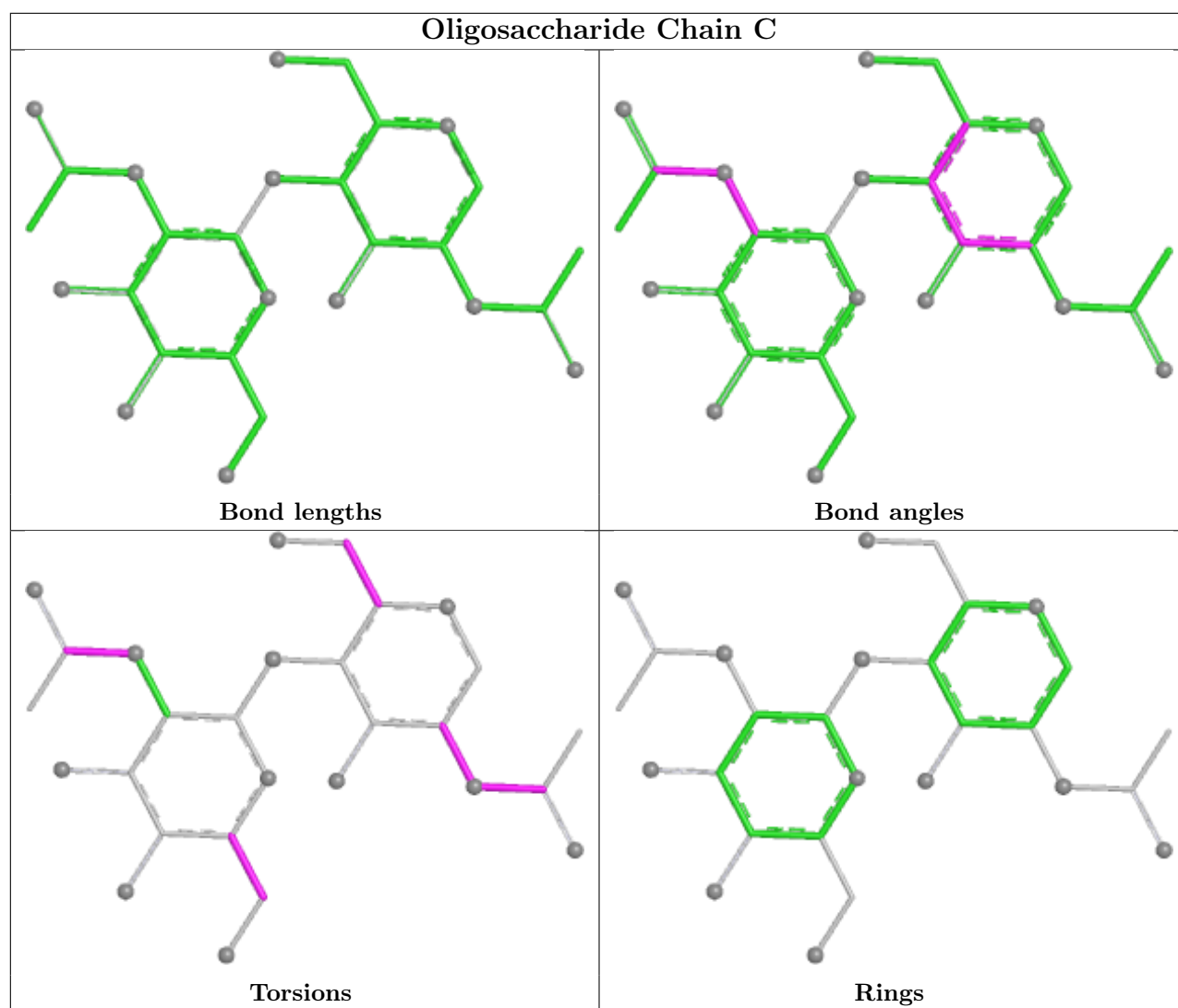
Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O7-C7-N2-C2
3	C	1	NAG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C3-C2-N2-C7
3	D	1	NAG	C3-C2-N2-C7

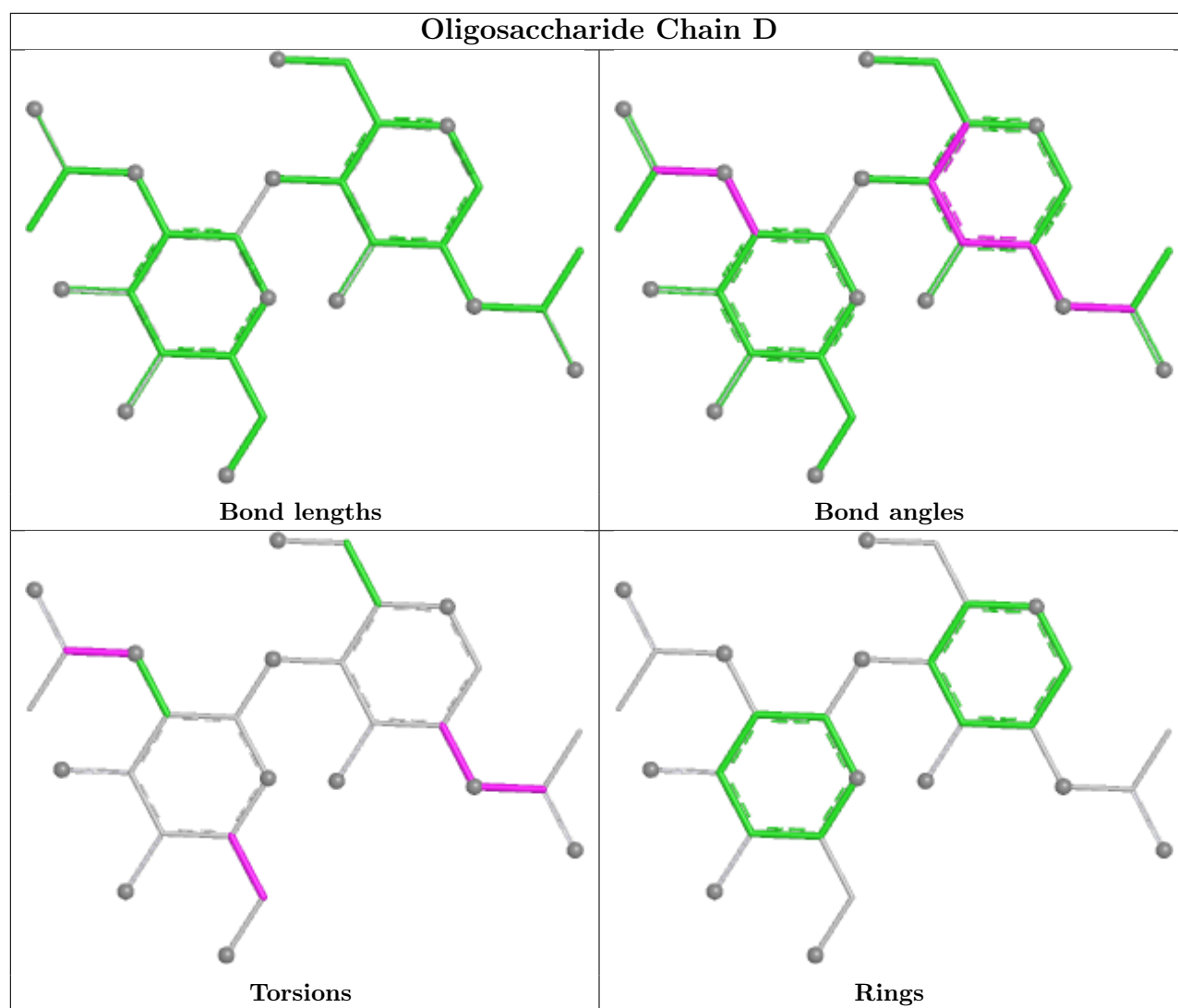
There are no ring outliers.

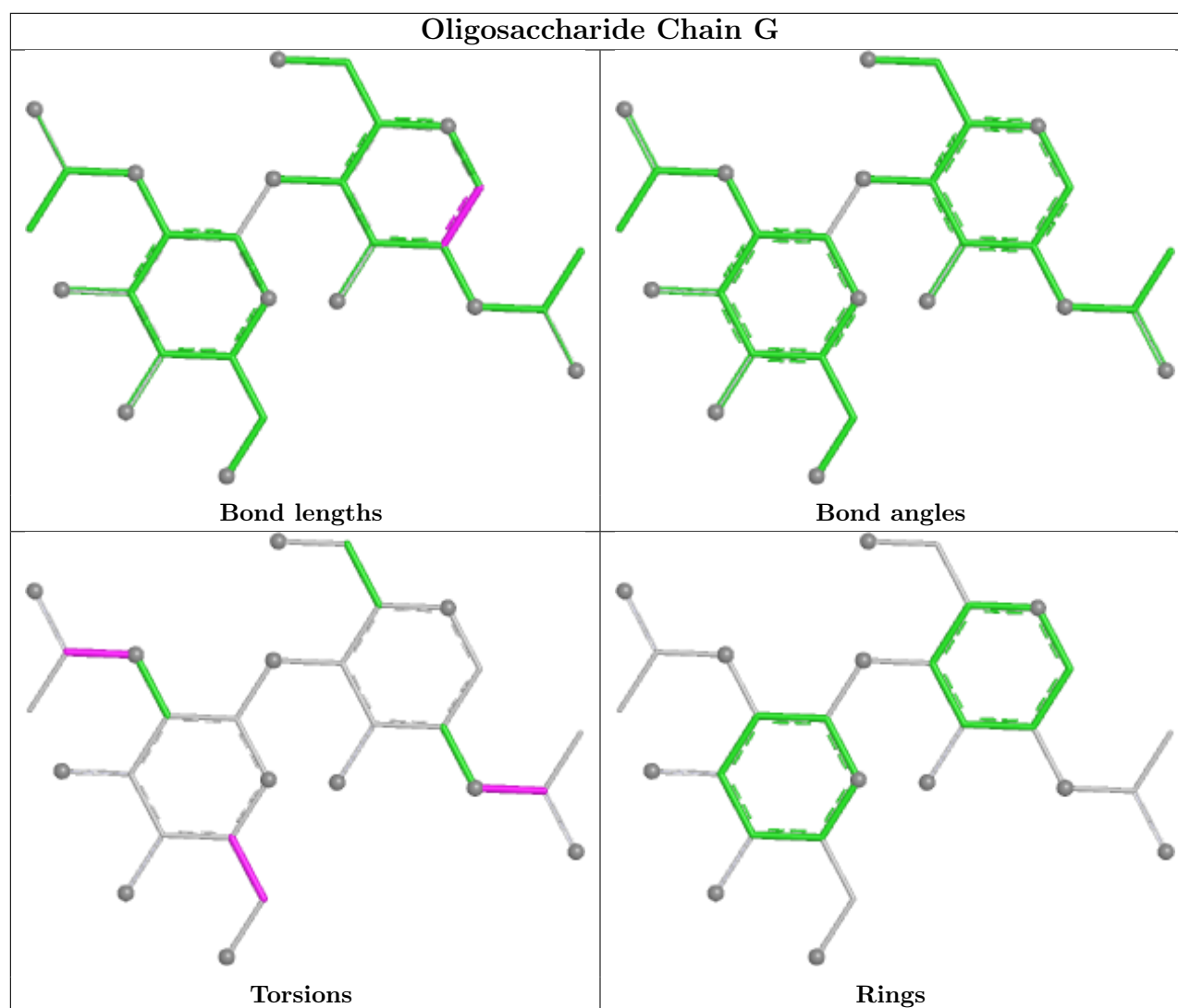
6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	NAG	4	0
3	C	1	NAG	4	0
3	D	1	NAG	2	0
3	G	2	NAG	2	0
3	D	2	NAG	2	0
3	G	1	NAG	2	0

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







5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	636	1	14,14,15	0.75	0	17,19,21	1.40	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	636	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	636	NAG	C4-C3-C2	-3.96	105.22	111.02
4	A	636	NAG	C2-N2-C7	-2.58	119.45	122.90
4	A	636	NAG	C3-C4-C5	-2.09	106.45	110.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	636	NAG	C8-C7-N2-C2
4	A	636	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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	536/577 (92%)	0.11	13 (2%) 59 55	30, 54, 95, 146	0
1	B	536/577 (92%)	0.03	12 (2%) 62 58	27, 50, 97, 146	0
2	E	187/197 (94%)	0.21	6 (3%) 50 46	18, 60, 100, 137	3 (1%)
2	F	187/197 (94%)	0.78	17 (9%) 15 12	22, 71, 104, 139	3 (1%)
All	All	1446/1548 (93%)	0.18	48 (3%) 49 45	18, 56, 101, 146	6 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	291	VAL	4.5
2	E	85	THR	4.1
1	A	590	PHE	3.7
2	F	285	VAL	3.4
2	F	94	GLY	3.3
1	A	444	GLY	3.3
2	F	287	LEU	3.2
1	A	74	LEU	3.1
1	B	433	PHE	3.1
2	F	291	VAL	3.1
2	E	200	ALA	3.0
1	B	590	PHE	2.9
1	B	578	GLN	2.8
1	B	136	THR	2.7
1	B	346	ASP	2.7
2	F	232	ARG	2.6
2	E	288	VAL	2.6
2	F	87	TYR	2.6
1	B	69	LEU	2.5
1	A	69	LEU	2.5
2	F	254	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	275	ASN	2.5
2	F	253	PRO	2.4
1	A	574	GLN	2.3
1	A	62	ILE	2.3
1	B	77	VAL	2.3
1	A	445	TYR	2.3
2	E	198	TYR	2.2
2	F	281	ILE	2.2
1	B	628	GLU	2.2
2	F	272	ALA	2.2
1	B	124	GLY	2.2
1	B	190	GLY	2.2
1	B	76	PRO	2.2
1	A	126	LEU	2.1
2	F	283	GLY	2.1
1	A	579	ASP	2.1
2	F	279	ILE	2.1
2	F	282	VAL	2.1
2	E	86	THR	2.1
1	B	445	TYR	2.1
2	F	90	SER	2.1
1	A	634	HIS	2.1
1	A	71	ASN	2.0
1	A	192	PRO	2.0
1	A	593	VAL	2.0
2	F	231	GLY	2.0
2	F	100	TRP	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.

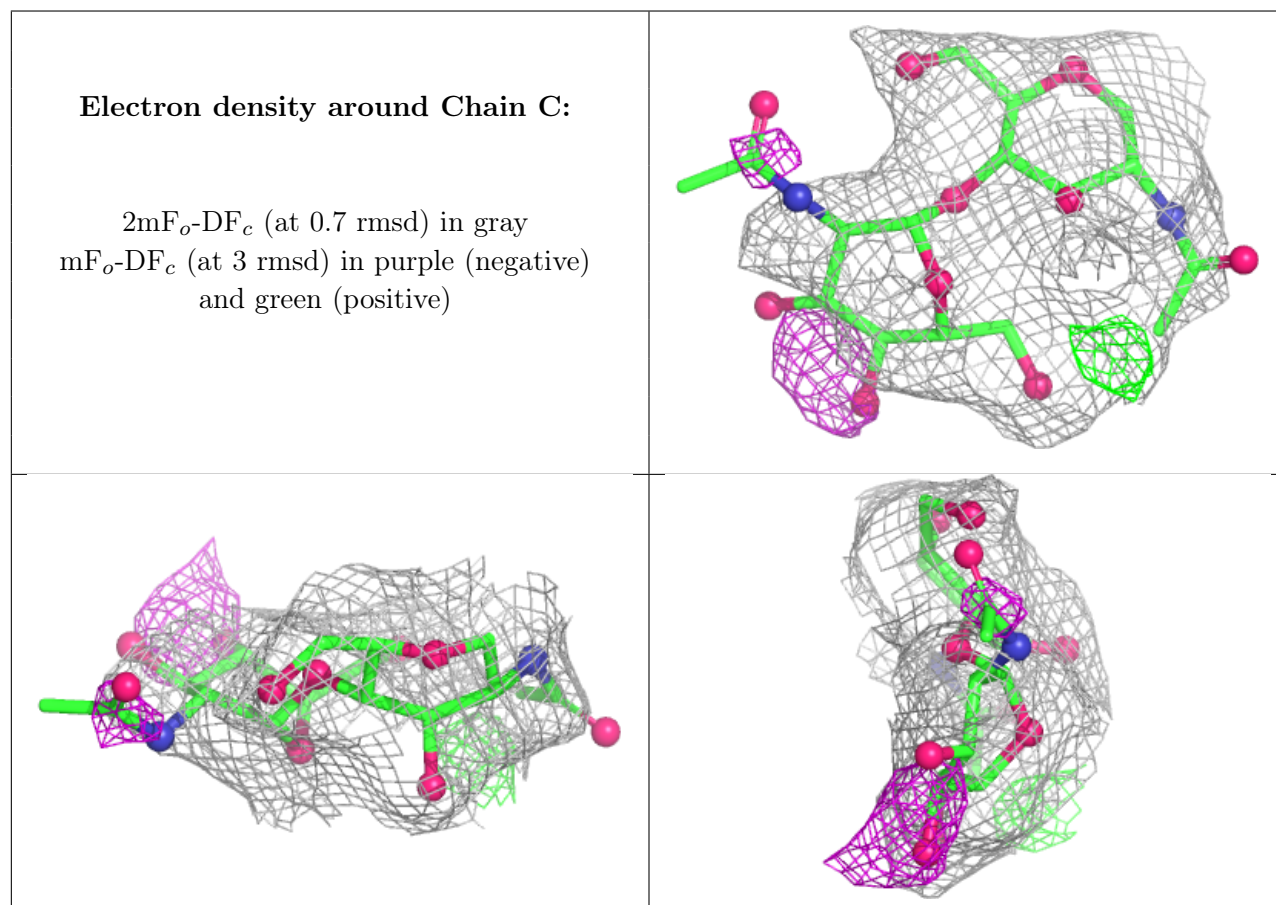
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	C	1	14/15	-	-	96,98,100,101	0

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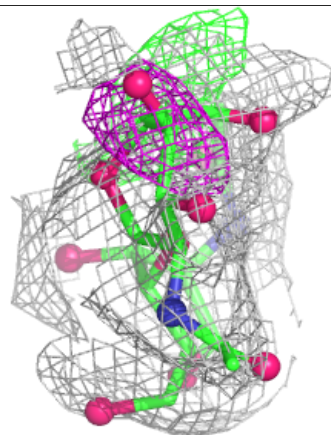
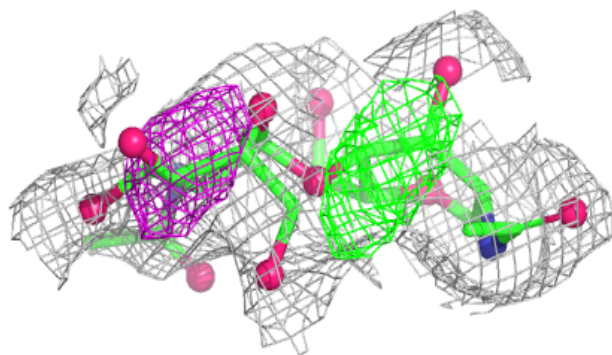
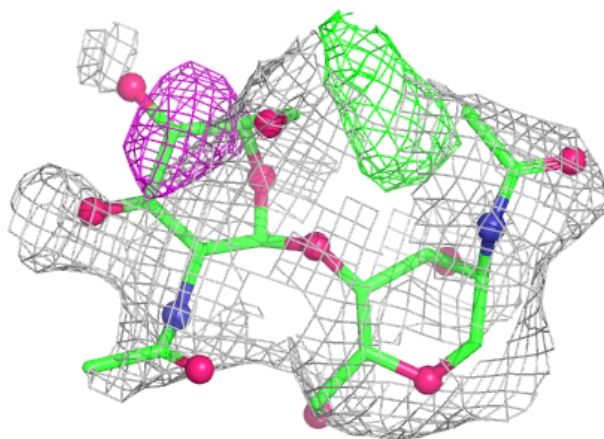
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	C	2	14/15	-	-	100,102,106,108	0
3	NAG	D	1	14/15	-	-	93,97,98,99	0
3	NAG	D	2	14/15	-	-	99,100,102,103	0
3	NAG	G	2	14/15	-0.02	0.18	111,113,113,113	0
3	NAG	G	1	14/15	0.18	0.17	103,106,108,109	0

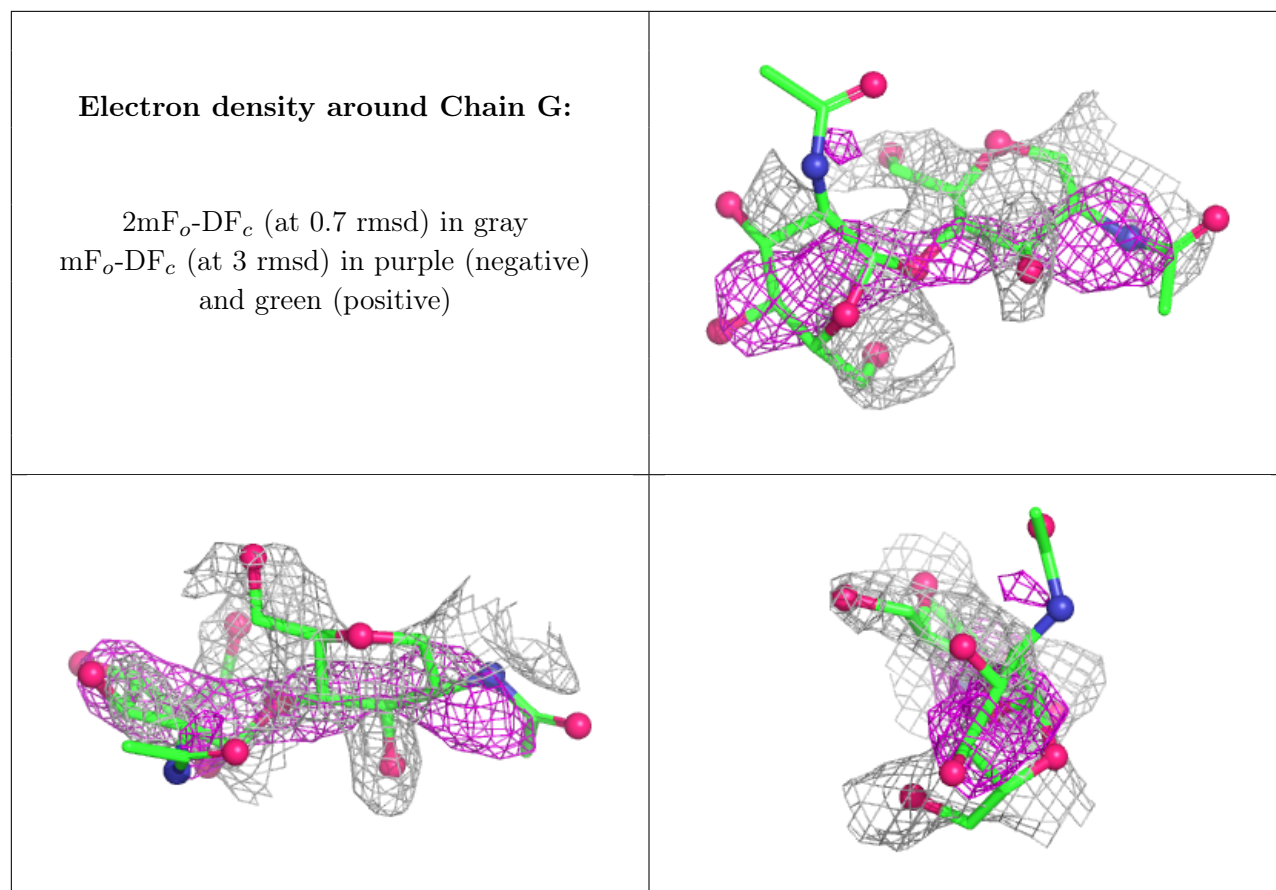
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain D:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
4	NAG	A	636	14/15	0.39	0.17	98,102,105,107	0
5	CA	F	2	1/1	0.74	0.14	33,33,33,33	1
5	CA	E	1	1/1	0.76	0.25	30,30,30,30	1

6.5 Other polymers [i](#)

There are no such residues in this entry.