



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:36 PM UTC

PDB ID : 3QCW / pdb_00003qcw
Title : Structure of neuexin 1 alpha (domains LNS1-LNS6), no splice inserts
Authors : Rudenko, G.
Deposited on : 2011-01-17
Resolution : 2.65 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

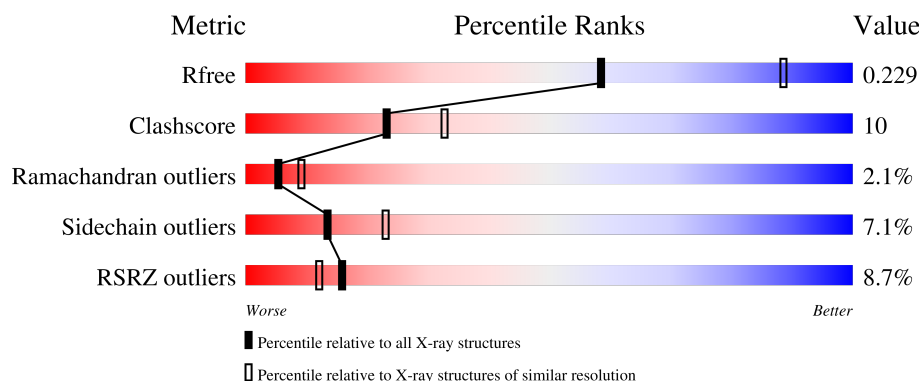
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	1245	7% 58% 18% • 19%
1	B	1245	7% 59% 18% • 19%
2	C	2	100%
2	D	2	100%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 15440 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 Neurexin-1-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1003	Total	C	N	O	S	0	0	0
			7692	4835	1326	1489	42			
1	B	1003	Total	C	N	O	S	0	0	0
			7692	4835	1326	1489	42			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	210	GLN	ASN	engineered mutation	UNP Q28146
A	612	GLU	GLN	SEE REMARK 999	UNP Q28146
A	1112	PHE	ILE	SEE REMARK 999	UNP Q28146
B	210	GLN	ASN	engineered mutation	UNP Q28146
B	612	GLU	GLN	SEE REMARK 999	UNP Q28146
B	1112	PHE	ILE	SEE REMARK 999	UNP Q28146

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

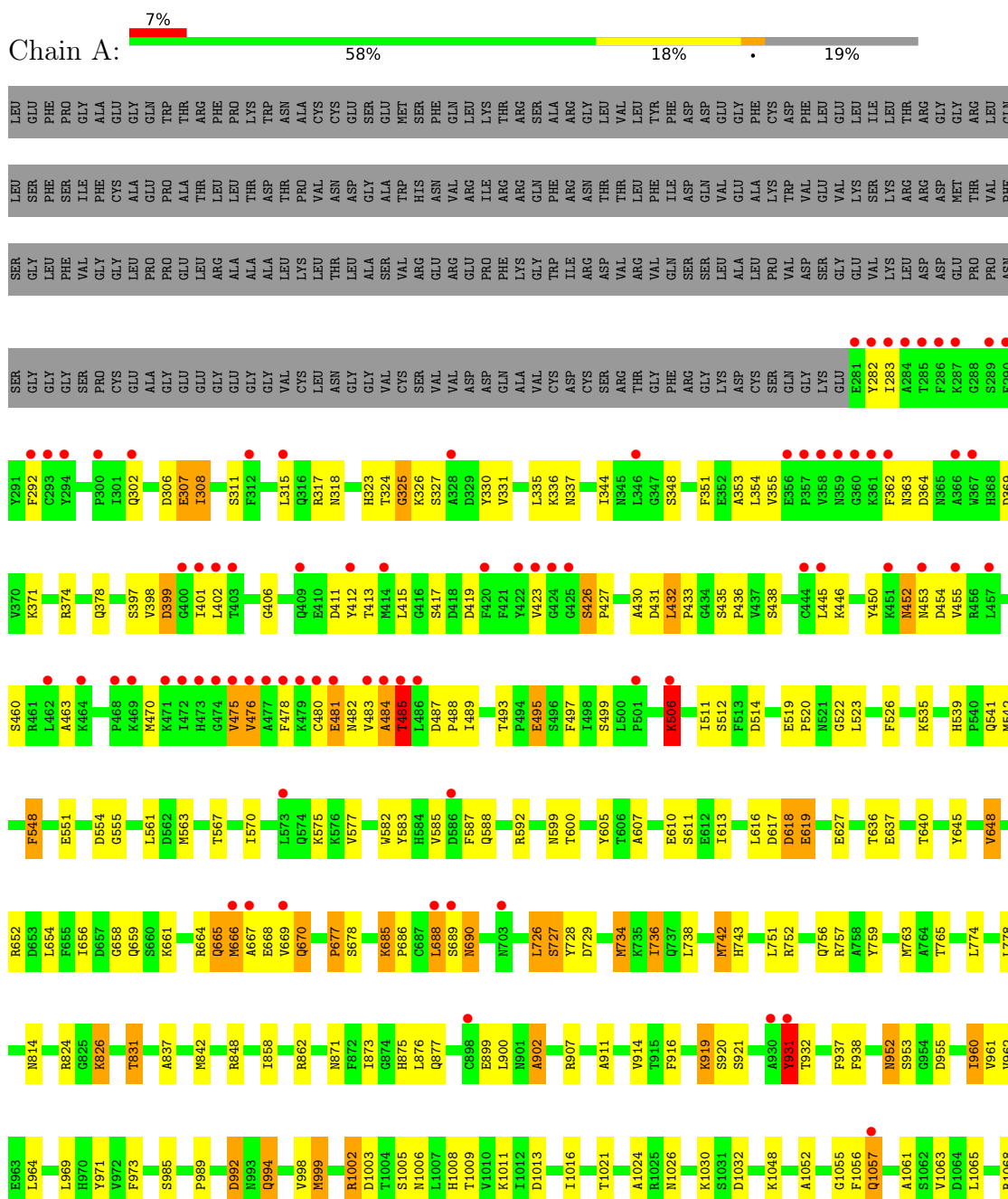


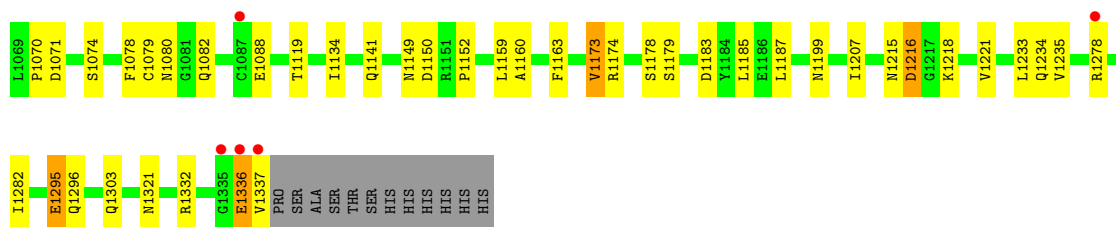
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

3 Residue-property plots

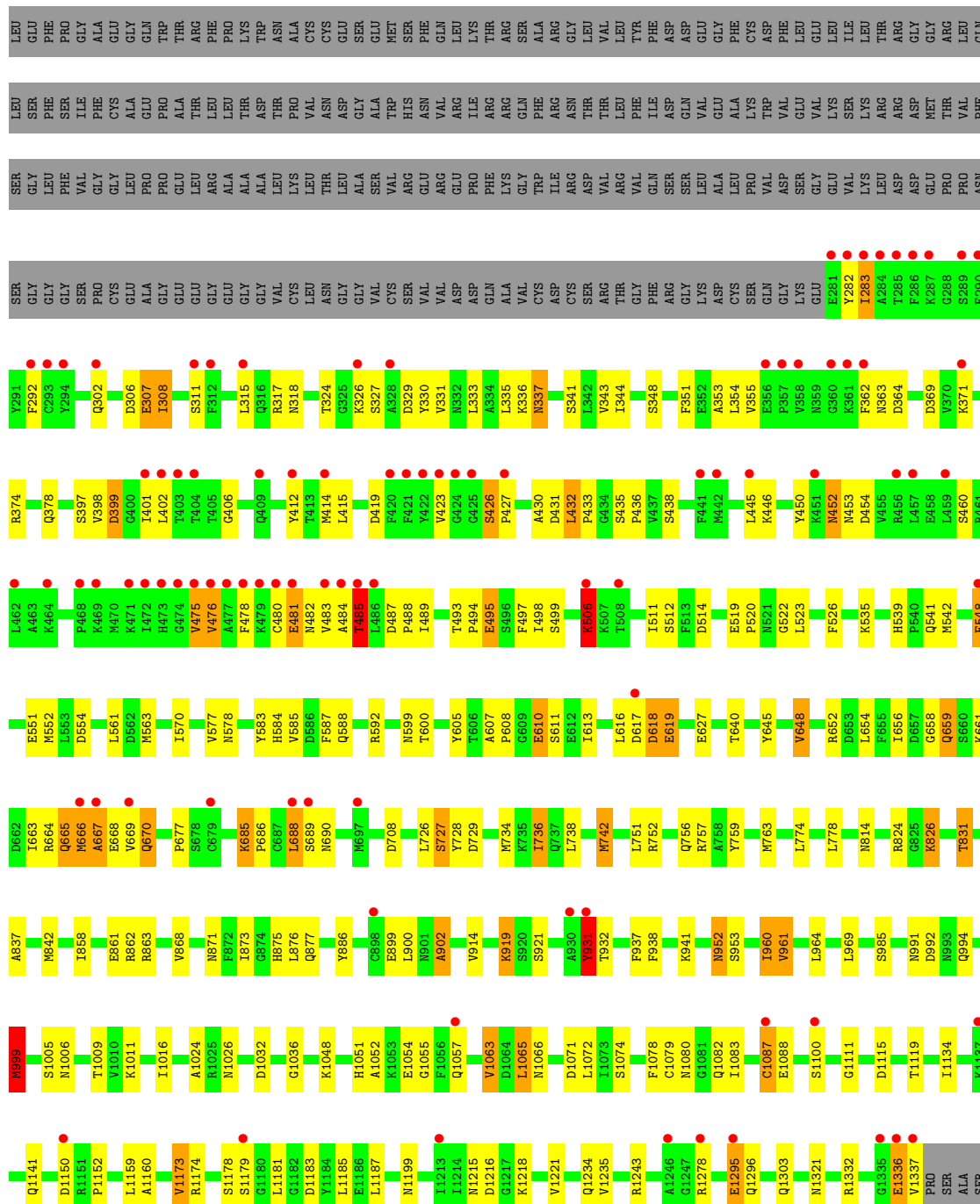
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Neurexin-1-alpha





Molecule 1: Neurexin-1-alpha



THR
SER
HIS
HIS
HIS
HIS
HIS
HIS

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

Chain C:  100%

NAG1
NAG2

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

Chain D:  100%

NAG1
NAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.95Å 114.54Å 159.58Å 90.61° 90.87° 92.18°	Depositor
Resolution (Å)	30.00 – 2.65 30.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-2.65) 98.4 (30.00-2.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 2.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.208 , 0.230 0.208 , 0.229	Depositor DCC
R_{free} test set	6451 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.126 for h,-k,-l 0.008 for -h,k,-l 0.011 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15440	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: 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	1.03	15/7846 (0.2%)	1.10	21/10637 (0.2%)
1	B	1.00	11/7846 (0.1%)	1.09	15/10637 (0.1%)
All	All	1.01	26/15692 (0.2%)	1.10	36/21274 (0.2%)

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	3
1	B	0	2
All	All	0	5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1057	GLN	CG-CD	9.23	1.75	1.52
1	B	1057	GLN	CG-CD	7.79	1.71	1.52
1	A	902	ALA	CA-CB	-6.76	1.42	1.53
1	B	902	ALA	CA-CB	-6.75	1.42	1.53
1	A	962	VAL	CA-CB	-6.55	1.46	1.54
1	A	1056	PHE	C-O	6.54	1.31	1.23
1	A	1052	ALA	CA-CB	-6.34	1.43	1.53
1	A	1065	LEU	CA-C	-6.16	1.46	1.53
1	A	1061	ALA	CA-C	-6.10	1.45	1.52
1	A	911	ALA	CA-CB	-6.07	1.44	1.53
1	B	919	LYS	C-O	5.96	1.30	1.24
1	A	919	LYS	C-O	5.85	1.30	1.24
1	B	1087	CYS	CA-C	5.78	1.60	1.53
1	B	1065	LEU	CA-C	-5.69	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1083	ILE	CA-CB	-5.66	1.47	1.54
1	A	998	VAL	CA-CB	-5.59	1.47	1.54
1	A	989	PRO	C-O	-5.58	1.16	1.23
1	B	1079	CYS	CB-SG	-5.42	1.63	1.81
1	B	1083	ILE	C-O	-5.32	1.18	1.24
1	A	1079	CYS	CB-SG	-5.31	1.63	1.81
1	A	1063	VAL	C-O	-5.20	1.18	1.23
1	B	868	VAL	C-O	-5.17	1.20	1.24
1	A	1009	THR	CA-C	-5.15	1.46	1.52
1	B	1063	VAL	C-O	-5.13	1.18	1.23
1	A	992	ASP	CB-CG	5.11	1.64	1.52
1	B	1036	GLY	C-O	5.05	1.31	1.24

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	LYS	N-CA-C	8.27	115.56	108.78
1	B	326	LYS	N-CA-C	7.90	115.26	108.78
1	A	485	THR	N-CA-C	7.75	127.31	110.80
1	B	478	PHE	N-CA-C	7.03	119.87	110.88
1	B	485	THR	N-CA-C	6.73	125.14	110.80
1	B	1119	THR	N-CA-C	-6.49	100.86	110.46
1	A	1119	THR	CA-C-N	-6.49	110.64	122.38
1	A	1119	THR	C-N-CA	-6.49	110.64	122.38
1	A	685	LYS	CA-C-N	6.43	126.66	119.32
1	A	685	LYS	C-N-CA	6.43	126.66	119.32
1	A	478	PHE	N-CA-C	6.39	120.39	111.56
1	B	1111	GLY	N-CA-C	-6.02	105.47	111.85
1	A	1119	THR	N-CA-C	-6.01	101.56	110.46
1	B	685	LYS	CA-C-N	6.00	126.16	119.32
1	B	685	LYS	C-N-CA	6.00	126.16	119.32
1	B	1032	ASP	N-CA-C	-5.92	102.72	110.53
1	A	1002	ARG	N-CA-C	-5.90	98.47	108.26
1	A	920	SER	N-CA-C	5.87	119.54	112.38
1	B	1119	THR	CA-C-N	-5.86	111.77	122.38
1	B	1119	THR	C-N-CA	-5.86	111.77	122.38
1	A	1032	ASP	N-CA-C	-5.65	103.08	110.53
1	A	426	SER	N-CA-C	5.61	113.06	108.07
1	A	325	GLY	N-CA-C	5.41	118.35	112.29
1	B	1100	SER	N-CA-C	5.41	119.85	112.88
1	A	1013	ASP	CA-C-N	-5.32	114.14	122.65
1	A	1013	ASP	C-N-CA	-5.32	114.14	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	999	MET	CG-SD-CE	5.29	112.55	100.90
1	A	484	ALA	N-CA-C	5.26	122.00	110.80
1	A	765	THR	N-CA-C	-5.20	101.79	110.17
1	A	1079	CYS	N-CA-CB	-5.17	101.84	110.99
1	A	1282	ILE	N-CA-C	5.16	115.39	108.17
1	B	426	SER	N-CA-C	5.11	112.61	108.07
1	B	667	ALA	N-CA-C	-5.10	105.37	112.30
1	B	484	ALA	N-CA-C	5.04	121.54	110.80
1	A	690	ASN	CA-C-N	-5.03	115.09	120.47
1	A	690	ASN	C-N-CA	-5.03	115.09	120.47

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1078	PHE	Peptide
1	A	1215	ASN	Peptide
1	A	484	ALA	Peptide
1	B	1078	PHE	Peptide
1	B	1215	ASN	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	7692	0	7454	154	1
1	B	7692	0	7454	158	1
2	C	28	0	25	0	0
2	D	28	0	25	0	0
All	All	15440	0	14958	312	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (312) 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:1057:GLN:CD	1:A:1057:GLN:CG	1.75	1.54
1:A:931:TYR:HD1	1:A:932:THR:H	1.12	0.93
1:B:931:TYR:HD1	1:B:932:THR:H	1.16	0.93
1:B:667:ALA:HA	1:B:670:GLN:HB2	1.54	0.89
1:A:667:ALA:HA	1:A:670:GLN:HB2	1.56	0.85
1:A:618:ASP:HB3	1:A:619:GLU:OE2	1.86	0.76
1:A:519:GLU:HG3	1:A:648:VAL:HG22	1.70	0.74
1:B:302:GLN:HA	1:B:415:LEU:O	1.89	0.73
1:A:688:LEU:C	1:A:690:ASN:N	2.45	0.72
1:A:302:GLN:HA	1:A:415:LEU:O	1.89	0.72
1:B:618:ASP:HB3	1:B:619:GLU:OE2	1.90	0.71
1:B:519:GLU:HG3	1:B:648:VAL:HG22	1.71	0.71
1:B:763:MET:HE1	1:B:774:LEU:HD23	1.70	0.71
1:B:688:LEU:C	1:B:690:ASN:N	2.46	0.71
1:A:599:ASN:O	1:A:600:THR:HB	1.90	0.70
1:B:599:ASN:O	1:B:600:THR:HB	1.90	0.70
1:B:306:ASP:OD2	1:B:374:ARG:HB3	1.93	0.68
1:A:763:MET:HE1	1:A:774:LEU:HD23	1.74	0.68
1:B:1141:GLN:HE22	1:B:1295:GLU:HG2	1.57	0.68
1:B:727:SER:HB2	1:B:875:HIS:CD2	2.30	0.67
1:B:668:GLU:C	1:B:670:GLN:H	2.03	0.67
1:A:1141:GLN:HE22	1:A:1295:GLU:HG2	1.58	0.67
1:A:369:ASP:HB2	1:A:399:ASP:HA	1.77	0.66
1:A:282:TYR:HB3	1:A:460:SER:HB3	1.79	0.65
1:B:688:LEU:C	1:B:688:LEU:HD12	2.21	0.65
1:A:688:LEU:C	1:A:690:ASN:H	2.05	0.65
1:A:668:GLU:C	1:A:670:GLN:H	2.06	0.64
1:A:751:LEU:HD12	1:A:751:LEU:C	2.23	0.64
1:B:369:ASP:HB2	1:B:399:ASP:HA	1.79	0.64
1:B:282:TYR:HB3	1:B:460:SER:HB3	1.80	0.63
1:A:1216:ASP:OD2	1:A:1218:LYS:HB2	1.99	0.63
1:A:306:ASP:OD2	1:A:374:ARG:HB3	1.98	0.63
1:B:292:PHE:HB2	1:B:423:VAL:HB	1.80	0.63
1:B:688:LEU:C	1:B:690:ASN:H	2.06	0.62
1:B:488:PRO:HB3	1:B:652:ARG:HB3	1.81	0.62
1:A:292:PHE:HB2	1:A:423:VAL:HB	1.82	0.61
1:A:308:ILE:CD1	1:A:450:TYR:HD1	2.13	0.61
1:A:727:SER:HB2	1:A:875:HIS:CD2	2.35	0.61
1:A:452:ASN:ND2	1:A:454:ASP:H	1.99	0.60
1:B:1216:ASP:OD2	1:B:1218:LYS:HB2	2.01	0.60
1:B:1024:ALA:O	1:B:1026:ASN:ND2	2.35	0.60
1:B:430:ALA:HB2	1:B:438:SER:CB	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1159:LEU:HD23	1:B:1160:ALA:N	2.18	0.59
1:A:488:PRO:HB3	1:A:652:ARG:HB3	1.83	0.59
1:B:452:ASN:ND2	1:B:454:ASP:H	2.01	0.59
1:A:430:ALA:HB2	1:A:438:SER:CB	2.31	0.59
1:A:1159:LEU:HD23	1:A:1160:ALA:N	2.18	0.59
1:A:426:SER:HB2	1:A:427:PRO:HD2	1.85	0.59
1:A:688:LEU:C	1:A:688:LEU:HD12	2.28	0.58
1:B:308:ILE:CD1	1:B:450:TYR:HD1	2.16	0.58
1:A:751:LEU:HD12	1:A:751:LEU:O	2.03	0.58
1:A:511:ILE:HD12	1:A:656:ILE:HD13	1.85	0.57
1:A:511:ILE:CG2	1:A:587:PHE:HB3	2.34	0.57
1:A:1011:LYS:HG3	1:A:1016:ILE:HG13	1.87	0.57
1:B:493:THR:HB	1:B:495:GLU:OE2	2.05	0.57
1:A:1024:ALA:O	1:A:1026:ASN:ND2	2.38	0.56
1:A:539:HIS:HB2	1:A:542:MET:HE2	1.87	0.56
1:B:688:LEU:HD12	1:B:688:LEU:O	2.06	0.56
1:B:726:LEU:HD22	1:B:902:ALA:HB3	1.88	0.56
1:B:511:ILE:CG2	1:B:587:PHE:HB3	2.35	0.56
1:B:563:MET:CE	1:B:607:ALA:HB3	2.36	0.56
1:B:426:SER:HB2	1:B:427:PRO:HD2	1.87	0.56
1:B:570:ILE:HD11	1:B:605:TYR:HB2	1.88	0.56
1:B:432:LEU:HD12	1:B:435:SER:HB2	1.88	0.55
1:B:331:VAL:HG23	1:B:344:ILE:HG12	1.89	0.55
1:A:563:MET:CE	1:A:607:ALA:HB3	2.37	0.55
1:B:511:ILE:HD12	1:B:656:ILE:HD13	1.88	0.55
1:A:1071:ASP:OD2	1:A:1074:SER:HB2	2.07	0.55
1:A:738:LEU:HD22	1:A:742:MET:HG2	1.89	0.55
1:A:331:VAL:HG23	1:A:344:ILE:HG12	1.90	0.54
1:B:992:ASP:OD2	1:B:994:GLN:NE2	2.41	0.54
1:A:336:LYS:HD2	1:A:436:PRO:HB2	1.89	0.54
1:A:548:PHE:HB2	1:A:561:LEU:HD12	1.90	0.54
1:A:599:ASN:O	1:A:600:THR:CB	2.55	0.53
1:B:539:HIS:HB2	1:B:542:MET:HE2	1.90	0.53
1:B:1005:SER:O	1:B:1006:ASN:HB2	2.08	0.53
1:B:336:LYS:HD2	1:B:436:PRO:HB2	1.90	0.53
1:B:523:LEU:HB2	1:B:640:THR:OG1	2.08	0.53
1:A:493:THR:HB	1:A:495:GLU:OE2	2.09	0.53
1:B:599:ASN:O	1:B:600:THR:CB	2.56	0.53
1:A:475:VAL:O	1:A:476:VAL:HB	2.08	0.53
1:A:432:LEU:HD12	1:A:435:SER:HB2	1.91	0.53
1:B:738:LEU:HD22	1:B:742:MET:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1011:LYS:HG3	1:B:1016:ILE:HG13	1.90	0.53
1:B:475:VAL:O	1:B:476:VAL:HB	2.09	0.52
1:A:1183:ASP:HA	1:A:1199:ASN:O	2.09	0.52
1:B:548:PHE:HB2	1:B:561:LEU:HD12	1.92	0.52
1:B:751:LEU:C	1:B:751:LEU:HD12	2.34	0.52
1:B:551:GLU:OE1	1:B:640:THR:HG23	2.10	0.52
1:B:1159:LEU:HD23	1:B:1159:LEU:C	2.35	0.52
1:B:315:LEU:HD13	1:B:485:THR:HG23	1.92	0.52
1:A:751:LEU:C	1:A:751:LEU:CD1	2.83	0.52
1:B:324:THR:HG22	1:B:331:VAL:HG12	1.91	0.52
1:A:1150:ASP:O	1:A:1152:PRO:HD3	2.10	0.51
1:A:728:TYR:CE2	1:A:876:LEU:HD12	2.44	0.51
1:B:523:LEU:HD11	1:B:526:PHE:HB2	1.91	0.51
1:B:1278:ARG:HB3	1:B:1278:ARG:CZ	2.40	0.51
1:A:738:LEU:H	1:A:738:LEU:HD12	1.76	0.51
1:A:311:SER:HB2	1:A:446:LYS:HE2	1.93	0.50
1:B:931:TYR:CD1	1:B:932:THR:HG22	2.46	0.50
1:A:1278:ARG:HB3	1:A:1278:ARG:CZ	2.42	0.50
1:A:592:ARG:HH21	1:A:610:GLU:HA	1.77	0.50
1:B:668:GLU:C	1:B:670:GLN:N	2.69	0.50
1:B:654:LEU:HB3	1:B:661:LYS:HB2	1.93	0.49
1:B:665:GLN:O	1:B:666:MET:C	2.55	0.49
1:A:315:LEU:HD13	1:A:485:THR:HG23	1.94	0.49
1:A:1159:LEU:HD23	1:A:1159:LEU:C	2.36	0.49
1:B:919:LYS:HG2	1:B:1055:GLY:O	2.12	0.49
1:B:438:SER:O	1:B:658:GLY:HA3	2.12	0.49
1:A:523:LEU:HD11	1:A:526:PHE:HB2	1.93	0.49
1:B:756:GLN:HG3	1:B:814:ASN:OD1	2.12	0.49
1:A:522:GLY:HA2	1:A:645:TYR:O	2.12	0.49
1:B:736:ILE:HD11	1:B:886:TYR:HB3	1.94	0.49
1:A:318:ASN:HA	1:A:335:LEU:O	2.12	0.49
1:A:351:PHE:CE1	1:A:406:GLY:HA3	2.48	0.48
1:A:307:GLU:C	1:A:308:ILE:HD13	2.38	0.48
1:A:315:LEU:O	1:A:363:ASN:HB2	2.13	0.48
1:B:311:SER:HB2	1:B:446:LYS:HE2	1.95	0.48
1:B:1071:ASP:OD2	1:B:1074:SER:HB2	2.12	0.48
1:B:726:LEU:HD22	1:B:902:ALA:CB	2.43	0.48
1:B:728:TYR:CE2	1:B:876:LEU:HD12	2.47	0.48
1:B:522:GLY:HA2	1:B:645:TYR:O	2.14	0.48
1:A:726:LEU:HD22	1:A:902:ALA:HB3	1.96	0.48
1:A:757:ARG:HD2	1:A:873:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:PHE:CE1	1:A:398:VAL:HG11	2.48	0.48
1:B:317:ARG:HG2	1:B:337:ASN:HA	1.96	0.48
1:B:362:PHE:CE1	1:B:398:VAL:HG11	2.48	0.48
1:A:324:THR:HG22	1:A:331:VAL:HG12	1.94	0.48
1:A:523:LEU:HB2	1:A:640:THR:OG1	2.13	0.48
1:B:324:THR:HG22	1:B:331:VAL:CG1	2.44	0.48
1:B:738:LEU:HD12	1:B:738:LEU:H	1.79	0.48
1:B:826:LYS:HA	1:B:842:MET:HE2	1.96	0.48
1:B:514:ASP:HA	1:B:583:TYR:O	2.14	0.47
1:B:1174:ARG:HD3	1:B:1296:GLN:HE21	1.79	0.47
1:A:362:PHE:CZ	1:A:398:VAL:HG11	2.49	0.47
1:A:542:MET:HE2	1:A:542:MET:HB3	1.76	0.47
1:A:1174:ARG:HD3	1:A:1296:GLN:HE21	1.79	0.47
1:B:318:ASN:HA	1:B:335:LEU:O	2.13	0.47
1:B:665:GLN:N	1:B:668:GLU:CB	2.78	0.47
1:B:1150:ASP:O	1:B:1152:PRO:HD3	2.13	0.47
1:B:592:ARG:HH21	1:B:610:GLU:HA	1.79	0.47
1:B:759:TYR:HA	1:B:778:LEU:O	2.15	0.47
1:B:831:THR:HB	1:B:837:ALA:HA	1.96	0.47
1:A:431:ASP:O	1:A:432:LEU:C	2.58	0.47
1:A:511:ILE:HG23	1:A:587:PHE:HB3	1.96	0.47
1:A:665:GLN:O	1:A:666:MET:C	2.57	0.47
1:B:511:ILE:HG22	1:B:587:PHE:HB3	1.96	0.47
1:A:497:PHE:CD1	1:A:497:PHE:C	2.93	0.47
1:A:668:GLU:C	1:A:670:GLN:N	2.72	0.47
1:A:577:VAL:O	1:A:583:TYR:HE1	1.98	0.47
1:B:430:ALA:HB2	1:B:438:SER:HB3	1.96	0.47
1:B:960:ILE:HG12	1:B:961:VAL:N	2.30	0.47
1:A:317:ARG:HG2	1:A:337:ASN:HA	1.97	0.46
1:A:430:ALA:HB2	1:A:438:SER:HB3	1.95	0.46
1:A:688:LEU:HD12	1:A:688:LEU:O	2.15	0.46
1:B:362:PHE:CZ	1:B:398:VAL:HG11	2.51	0.46
1:B:964:LEU:HD12	1:B:964:LEU:HA	1.76	0.46
1:A:756:GLN:HG3	1:A:814:ASN:OD1	2.15	0.46
1:A:324:THR:HG22	1:A:331:VAL:CG1	2.45	0.46
1:A:665:GLN:N	1:A:668:GLU:CB	2.79	0.46
1:A:306:ASP:CG	1:A:374:ARG:HH11	2.24	0.46
1:B:315:LEU:O	1:B:363:ASN:HB2	2.16	0.46
1:B:613:ILE:N	1:B:613:ILE:HD12	2.30	0.46
1:B:751:LEU:HD12	1:B:751:LEU:O	2.15	0.46
1:A:734:MET:HE3	1:A:736:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:964:LEU:HD12	1:A:964:LEU:HA	1.74	0.46
1:A:992:ASP:OD2	1:A:994:GLN:NE2	2.49	0.46
1:B:999:MET:HE1	1:B:1009:THR:CG2	2.46	0.46
1:B:307:GLU:C	1:B:308:ILE:HD13	2.41	0.46
1:B:520:PRO:HB2	1:B:554:ASP:HA	1.98	0.45
1:A:514:ASP:HA	1:A:583:TYR:O	2.15	0.45
1:B:330:TYR:HE1	1:B:343:VAL:HG12	1.82	0.45
1:A:636:THR:HG22	1:A:743:HIS:O	2.16	0.45
1:A:919:LYS:HG2	1:A:1055:GLY:O	2.17	0.45
1:B:431:ASP:O	1:B:432:LEU:C	2.60	0.45
1:A:308:ILE:HD12	1:A:450:TYR:HD1	1.81	0.45
1:A:506:LYS:NZ	1:A:506:LYS:HB2	2.32	0.45
1:A:570:ILE:HD11	1:A:605:TYR:HB2	1.98	0.45
1:A:582:TRP:CZ3	1:A:652:ARG:HG2	2.52	0.45
1:A:613:ILE:HD12	1:A:613:ILE:N	2.31	0.45
1:A:480:CYS:SG	1:A:481:GLU:N	2.83	0.45
1:A:656:ILE:HG12	1:A:661:LYS:HG3	1.99	0.45
1:B:570:ILE:CD1	1:B:605:TYR:HB3	2.47	0.45
1:A:519:GLU:CG	1:A:648:VAL:HG22	2.45	0.45
1:B:1173:VAL:HG13	1:B:1187:LEU:HB3	1.99	0.45
1:B:487:ASP:HB2	1:B:664:ARG:CB	2.47	0.45
1:A:551:GLU:OE1	1:A:640:THR:HG23	2.17	0.44
1:A:999:MET:HE2	1:A:1011:LYS:HB2	1.98	0.44
1:B:306:ASP:CG	1:B:374:ARG:HH11	2.25	0.44
1:B:430:ALA:HB2	1:B:438:SER:HB2	1.98	0.44
1:B:563:MET:HE3	1:B:563:MET:HB2	1.84	0.44
1:B:570:ILE:HD13	1:B:605:TYR:HB3	1.99	0.44
1:A:831:THR:HB	1:A:837:ALA:HA	1.98	0.44
1:A:931:TYR:CD1	1:A:932:THR:HG22	2.52	0.44
1:A:1005:SER:O	1:A:1006:ASN:HB2	2.17	0.44
1:B:351:PHE:CE1	1:B:406:GLY:HA3	2.52	0.44
1:B:362:PHE:C	1:B:364:ASP:H	2.25	0.44
1:B:1332:ARG:HG2	1:B:1332:ARG:HH11	1.82	0.44
1:B:371:LYS:HB3	1:B:397:SER:HB3	1.99	0.44
1:B:480:CYS:SG	1:B:481:GLU:N	2.83	0.44
1:A:567:THR:OG1	1:A:637:GLU:HG2	2.17	0.44
1:A:520:PRO:HB2	1:A:554:ASP:HA	2.00	0.44
1:B:498:ILE:HD12	1:B:667:ALA:HB3	1.99	0.44
1:B:999:MET:HE2	1:B:1011:LYS:HB2	2.00	0.44
1:B:1243:ARG:HA	1:B:1243:ARG:HD3	1.83	0.44
1:A:430:ALA:HB2	1:A:438:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ILE:HG22	1:A:587:PHE:HB3	1.98	0.44
1:A:311:SER:HB2	1:A:446:LYS:HB3	1.99	0.44
1:B:353:ALA:C	1:B:354:LEU:HD12	2.42	0.44
1:B:497:PHE:CD1	1:B:497:PHE:C	2.96	0.43
1:B:511:ILE:HG23	1:B:587:PHE:HB3	1.99	0.43
1:A:362:PHE:C	1:A:364:ASP:H	2.25	0.43
1:B:353:ALA:O	1:B:354:LEU:HD12	2.18	0.43
1:A:374:ARG:NH2	1:A:413:THR:O	2.51	0.43
1:A:432:LEU:HA	1:A:433:PRO:HD3	1.82	0.43
1:A:438:SER:O	1:A:658:GLY:CA	2.66	0.43
1:A:353:ALA:C	1:A:354:LEU:HD12	2.43	0.43
1:A:1163:PHE:HA	1:A:1303:GLN:O	2.18	0.43
1:B:941:LYS:HE3	1:B:1087:CYS:SG	2.59	0.43
1:A:487:ASP:HB2	1:A:664:ARG:CB	2.49	0.43
1:A:512:SER:HA	1:A:585:VAL:O	2.18	0.43
1:A:937:PHE:O	1:A:938:PHE:HB3	2.18	0.43
1:A:955:ASP:OD1	1:A:1030:LYS:HG3	2.19	0.43
1:A:1332:ARG:HG2	1:A:1332:ARG:HH11	1.83	0.43
1:B:919:LYS:HZ2	1:B:1054:GLU:CD	2.26	0.43
1:B:991:ASN:OD1	1:B:991:ASN:N	2.49	0.43
1:A:426:SER:CB	1:A:427:PRO:HD2	2.49	0.43
1:A:759:TYR:HA	1:A:778:LEU:O	2.19	0.43
1:B:685:LYS:HA	1:B:686:PRO:HD2	1.82	0.43
1:B:861:GLU:CD	1:B:863:ARG:HH21	2.27	0.43
1:B:1134:ILE:HG12	1:B:1303:GLN:HG2	1.99	0.43
1:A:371:LYS:HB3	1:A:397:SER:HB3	2.01	0.43
1:A:685:LYS:HA	1:A:686:PRO:HD2	1.79	0.43
1:B:563:MET:HE1	1:B:607:ALA:HB3	2.00	0.43
1:A:542:MET:SD	1:A:848:ARG:HD3	2.59	0.42
1:A:331:VAL:HG13	1:A:331:VAL:O	2.19	0.42
1:A:563:MET:HE1	1:A:607:ALA:HB3	2.01	0.42
1:A:858:ILE:HG12	1:A:871:ASN:CG	2.44	0.42
1:A:973:PHE:HZ	1:A:1021:THR:HG21	1.84	0.42
1:B:282:TYR:CB	1:B:460:SER:HB3	2.46	0.42
1:A:729:ASP:C	1:A:729:ASP:OD1	2.60	0.42
1:A:1134:ILE:HG12	1:A:1303:GLN:HG2	2.01	0.42
1:B:432:LEU:HA	1:B:433:PRO:HD3	1.83	0.42
1:B:1183:ASP:HA	1:B:1199:ASN:O	2.19	0.42
1:A:282:TYR:CB	1:A:460:SER:HB3	2.47	0.42
1:A:1002:ARG:HG2	1:A:1002:ARG:HH11	1.85	0.42
1:A:1173:VAL:HG13	1:A:1187:LEU:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1207:ILE:HD13	1:A:1233:LEU:HB2	2.00	0.42
1:B:329:ASP:OD1	1:B:414:MET:O	2.37	0.42
1:B:506:LYS:HB2	1:B:506:LYS:NZ	2.34	0.42
1:B:570:ILE:HD11	1:B:605:TYR:CB	2.49	0.42
1:B:570:ILE:CD1	1:B:605:TYR:CB	2.97	0.42
1:A:563:MET:HE3	1:A:563:MET:HB2	1.87	0.42
1:A:688:LEU:O	1:A:690:ASN:N	2.52	0.42
1:A:916:PHE:CD2	1:A:916:PHE:N	2.88	0.42
1:B:577:VAL:O	1:B:583:TYR:HE1	2.02	0.42
1:A:374:ARG:HA	1:A:378:GLN:O	2.20	0.42
1:A:677:PRO:HB2	1:A:678:SER:H	1.74	0.42
1:A:398:VAL:HB	1:A:402:LEU:HB3	2.02	0.42
1:A:931:TYR:CD1	1:A:932:THR:N	2.75	0.42
1:B:311:SER:HB2	1:B:446:LYS:HB3	2.01	0.42
1:B:656:ILE:HG12	1:B:661:LYS:HG3	2.01	0.42
1:B:752:ARG:NH1	1:B:877:GLN:OE1	2.52	0.42
1:B:1051:HIS:O	1:B:1052:ALA:C	2.63	0.42
1:B:952:ASN:HD22	1:B:953:SER:N	2.18	0.41
1:A:960:ILE:HG12	1:A:961:VAL:N	2.35	0.41
1:B:348:SER:HB2	1:B:412:TYR:HB2	2.01	0.41
1:B:435:SER:HA	1:B:436:PRO:HD3	1.91	0.41
1:A:353:ALA:O	1:A:354:LEU:HD12	2.20	0.41
1:B:751:LEU:C	1:B:751:LEU:CD1	2.93	0.41
1:B:708:ASP:OD1	1:B:708:ASP:C	2.64	0.41
1:A:323:HIS:CD2	1:A:323:HIS:C	2.97	0.41
1:B:426:SER:CB	1:B:427:PRO:HD2	2.51	0.41
1:B:1115:ASP:OD1	1:B:1115:ASP:C	2.64	0.41
1:A:971:TYR:HH	1:A:1008:HIS:CE1	2.38	0.41
1:A:1068:ARG:O	1:A:1070:PRO:HD3	2.20	0.41
1:B:333:LEU:HD12	1:B:341:SER:O	2.21	0.41
1:B:663:ILE:H	1:B:663:ILE:HG13	1.71	0.41
1:B:1063:VAL:HG21	1:B:1072:LEU:HD11	2.01	0.41
1:A:463:ALA:HB2	1:A:470:MET:HE3	2.03	0.41
1:A:555:GLY:O	1:A:577:VAL:HG22	2.21	0.41
1:A:654:LEU:HB3	1:A:661:LYS:HB2	2.02	0.41
1:A:921:SER:HA	1:A:1080:ASN:O	2.21	0.41
1:B:438:SER:O	1:B:658:GLY:CA	2.69	0.41
1:B:757:ARG:HD2	1:B:873:ILE:HD12	2.02	0.41
1:B:858:ILE:HG12	1:B:871:ASN:CG	2.46	0.41
1:B:283:ILE:HG12	1:B:446:LYS:HG3	2.03	0.41
1:B:398:VAL:HB	1:B:402:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:921:SER:HA	1:B:1080:ASN:O	2.21	0.41
1:A:325:GLY:HA2	1:A:417:SER:HB2	2.02	0.40
1:A:330:TYR:CD2	1:A:433:PRO:HB2	2.56	0.40
1:A:752:ARG:NH1	1:A:877:GLN:OE1	2.53	0.40
1:A:952:ASN:HD22	1:A:953:SER:N	2.19	0.40
1:B:512:SER:HA	1:B:585:VAL:O	2.21	0.40
1:B:514:ASP:OD1	1:B:584:HIS:ND1	2.54	0.40
1:B:607:ALA:HA	1:B:608:PRO:HD3	1.91	0.40
1:B:1065:LEU:O	1:B:1066:ASN:C	2.62	0.40
1:B:331:VAL:O	1:B:331:VAL:HG13	2.22	0.40
1:B:659:GLN:HE21	1:B:659:GLN:HB3	1.71	0.40
1:B:729:ASP:OD1	1:B:729:ASP:C	2.63	0.40
1:B:937:PHE:O	1:B:938:PHE:HB3	2.21	0.40
1:A:348:SER:HB2	1:A:412:TYR:HB2	2.03	0.40
1:A:734:MET:CE	1:A:736:ILE:HD12	2.52	0.40
1:A:826:LYS:HA	1:A:842:MET:HE2	2.04	0.40
1:B:552:MET:HE1	1:B:578:ASN:HB3	2.03	0.40
1:B:688:LEU:O	1:B:690:ASN:N	2.53	0.40
1:A:1003:ASP:OD1	1:A:1003:ASP:C	2.64	0.40
1:A:1030:LYS:HA	1:A:1030:LYS:HD3	1.86	0.40
1:B:374:ARG:HA	1:B:378:GLN:O	2.22	0.40
1:B:494:PRO:HA	1:B:648:VAL:HG12	2.04	0.40
1:B:587:PHE:C	1:B:587:PHE:CD1	2.97	0.40
1:B:665:GLN:H	1:B:668:GLU:CB	2.35	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ASP:OD2	1:B:652:ARG:NH2[1_464]	2.15	0.05

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	1001/1245 (80%)	910 (91%)	70 (7%)	21 (2%)	5	9
1	B	1001/1245 (80%)	913 (91%)	67 (7%)	21 (2%)	5	9
All	All	2002/2490 (80%)	1823 (91%)	137 (7%)	42 (2%)	5	9

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	SER
1	A	506	LYS
1	A	666	MET
1	A	669	VAL
1	A	677	PRO
1	A	1179	SER
1	A	1336	GLU
1	B	327	SER
1	B	485	THR
1	B	506	LYS
1	B	665	GLN
1	B	666	MET
1	B	669	VAL
1	B	677	PRO
1	B	1179	SER
1	B	1336	GLU
1	A	475	VAL
1	A	476	VAL
1	A	483	VAL
1	A	485	THR
1	A	665	GLN
1	A	689	SER
1	A	1048	LYS
1	B	401	ILE
1	B	475	VAL
1	B	476	VAL
1	B	483	VAL
1	B	689	SER
1	B	1048	LYS
1	A	401	ILE
1	A	481	GLU
1	A	618	ASP
1	A	931	TYR
1	B	481	GLU

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Mol	Chain	Res	Type
1	B	618	ASP
1	A	399	ASP
1	A	453	ASN
1	A	1216	ASP
1	B	399	ASP
1	B	453	ASN
1	B	931	TYR
1	B	337	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	834/1058 (79%)	773 (93%)	61 (7%)	13	22
1	B	834/1058 (79%)	776 (93%)	58 (7%)	14	24
All	All	1668/2116 (79%)	1549 (93%)	119 (7%)	13	23

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	283	ILE
1	A	307	GLU
1	A	308	ILE
1	A	355	VAL
1	A	419	ASP
1	A	432	LEU
1	A	445	LEU
1	A	452	ASN
1	A	455	VAL
1	A	482	ASN
1	A	489	ILE
1	A	495	GLU
1	A	499	SER
1	A	506	LYS
1	A	535	LYS

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Mol	Chain	Res	Type
1	A	541	GLN
1	A	548	PHE
1	A	575	LYS
1	A	588	GLN
1	A	611	SER
1	A	616	LEU
1	A	617	ASP
1	A	619	GLU
1	A	627	GLU
1	A	648	VAL
1	A	659	GLN
1	A	670	GLN
1	A	688	LEU
1	A	726	LEU
1	A	727	SER
1	A	734	MET
1	A	736	ILE
1	A	742	MET
1	A	824	ARG
1	A	826	LYS
1	A	831	THR
1	A	862	ARG
1	A	899	GLU
1	A	900	LEU
1	A	907	ARG
1	A	914	VAL
1	A	931	TYR
1	A	952	ASN
1	A	960	ILE
1	A	969	LEU
1	A	985	SER
1	A	994	GLN
1	A	999	MET
1	A	1082	GLN
1	A	1088	GLU
1	A	1149	ASN
1	A	1173	VAL
1	A	1178	SER
1	A	1185	LEU
1	A	1221	VAL
1	A	1234	GLN
1	A	1235	VAL

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Mol	Chain	Res	Type
1	A	1295	GLU
1	A	1321	ASN
1	A	1336	GLU
1	A	1337	VAL
1	B	283	ILE
1	B	307	GLU
1	B	308	ILE
1	B	355	VAL
1	B	419	ASP
1	B	432	LEU
1	B	445	LEU
1	B	452	ASN
1	B	482	ASN
1	B	489	ILE
1	B	495	GLU
1	B	499	SER
1	B	506	LYS
1	B	535	LYS
1	B	541	GLN
1	B	548	PHE
1	B	588	GLN
1	B	610	GLU
1	B	611	SER
1	B	616	LEU
1	B	617	ASP
1	B	619	GLU
1	B	627	GLU
1	B	648	VAL
1	B	659	GLN
1	B	670	GLN
1	B	688	LEU
1	B	727	SER
1	B	734	MET
1	B	736	ILE
1	B	742	MET
1	B	824	ARG
1	B	826	LYS
1	B	831	THR
1	B	862	ARG
1	B	899	GLU
1	B	900	LEU
1	B	914	VAL

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Mol	Chain	Res	Type
1	B	931	TYR
1	B	952	ASN
1	B	960	ILE
1	B	961	VAL
1	B	969	LEU
1	B	985	SER
1	B	999	MET
1	B	1082	GLN
1	B	1088	GLU
1	B	1173	VAL
1	B	1178	SER
1	B	1181	LEU
1	B	1185	LEU
1	B	1221	VAL
1	B	1234	GLN
1	B	1235	VAL
1	B	1295	GLU
1	B	1321	ASN
1	B	1336	GLU
1	B	1337	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	332	ASN
1	A	452	ASN
1	A	482	ASN
1	A	659	GLN
1	A	810	ASN
1	A	853	ASN
1	A	892	ASN
1	A	935	HIS
1	A	952	ASN
1	A	1057	GLN
1	A	1321	ASN
1	B	332	ASN
1	B	439	ASN
1	B	452	ASN
1	B	482	ASN
1	B	756	GLN
1	B	810	ASN
1	B	814	ASN

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Mol	Chain	Res	Type
1	B	853	ASN
1	B	892	ASN
1	B	935	HIS
1	B	952	ASN
1	B	1057	GLN
1	B	1108	GLN
1	B	1141	GLN
1	B	1188	HIS
1	B	1321	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

4 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	2,1	14,14,15	0.78	0	17,19,21	2.23	6 (35%)
2	NAG	C	2	2	14,14,15	0.76	1 (7%)	17,19,21	1.95	4 (23%)
2	NAG	D	1	2,1	14,14,15	0.74	0	17,19,21	2.26	6 (35%)
2	NAG	D	2	2	14,14,15	0.76	1 (7%)	17,19,21	1.95	4 (23%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	C1-C2	2.33	1.55	1.52
2	D	2	NAG	C1-C2	2.06	1.55	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-O5-C5	6.00	120.23	112.19
2	C	1	NAG	C1-O5-C5	5.31	119.31	112.19
2	C	2	NAG	O5-C5-C6	4.81	117.03	107.66
2	D	2	NAG	O5-C5-C6	4.70	116.82	107.66
2	C	2	NAG	C2-N2-C7	-4.40	117.01	122.90
2	D	2	NAG	C2-N2-C7	-4.23	117.23	122.90
2	C	1	NAG	O7-C7-C8	-3.57	115.69	122.05
2	D	1	NAG	O7-C7-C8	-3.57	115.70	122.05
2	C	1	NAG	C2-N2-C7	3.50	127.59	122.90
2	D	2	NAG	C3-C4-C5	-2.90	104.97	110.23
2	C	2	NAG	C3-C4-C5	-2.82	105.13	110.23
2	D	1	NAG	C2-N2-C7	2.66	126.46	122.90
2	D	1	NAG	C4-C3-C2	2.51	114.69	111.02
2	C	1	NAG	C4-C3-C2	2.47	114.64	111.02
2	D	1	NAG	O7-C7-N2	2.17	125.81	121.98
2	C	1	NAG	O7-C7-N2	2.15	125.78	121.98
2	D	2	NAG	O5-C1-C2	2.14	114.61	111.29
2	C	1	NAG	O6-C6-C5	2.10	118.50	111.33
2	D	1	NAG	O6-C6-C5	2.08	118.40	111.33
2	C	2	NAG	O5-C1-C2	2.07	114.50	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6

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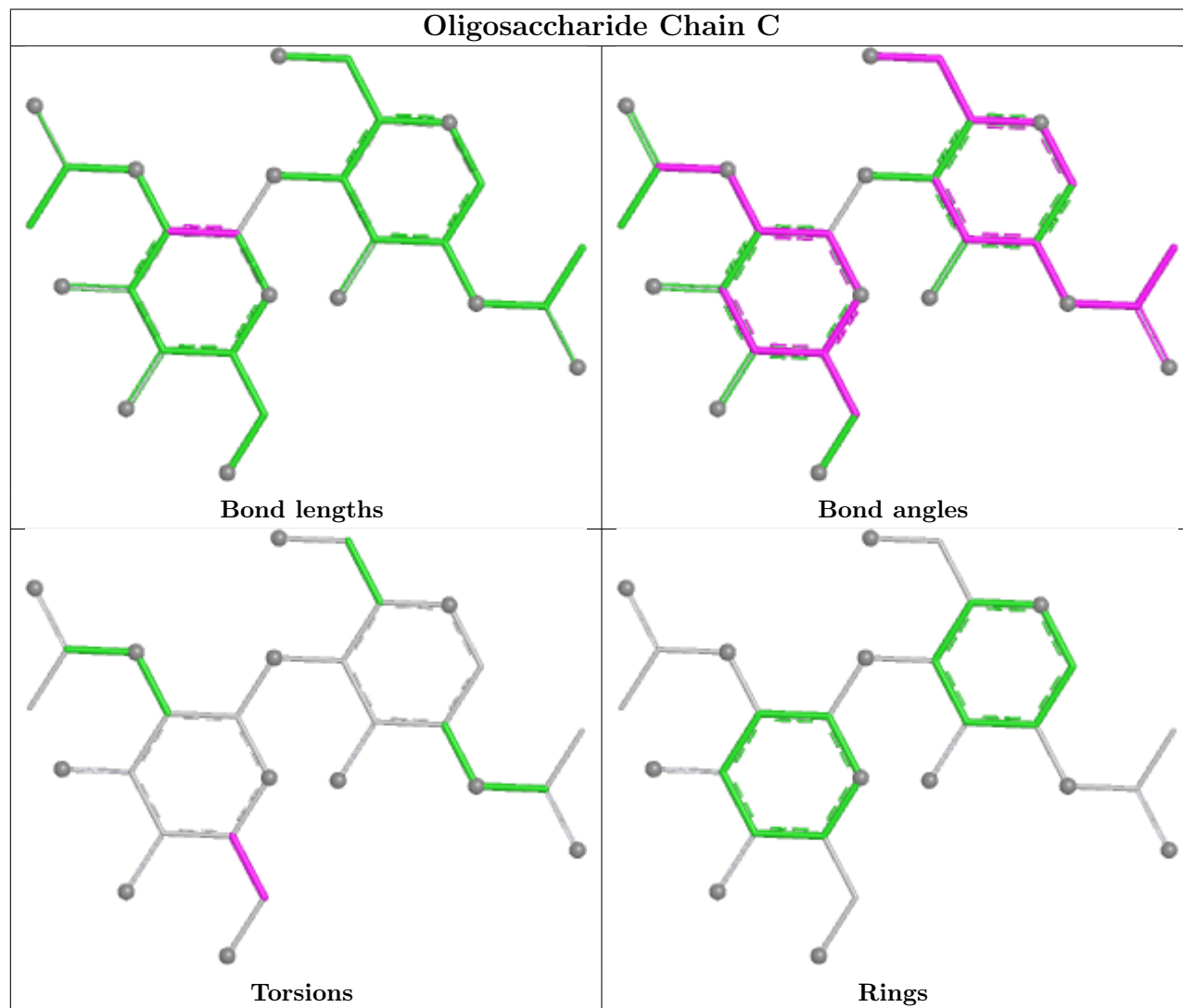
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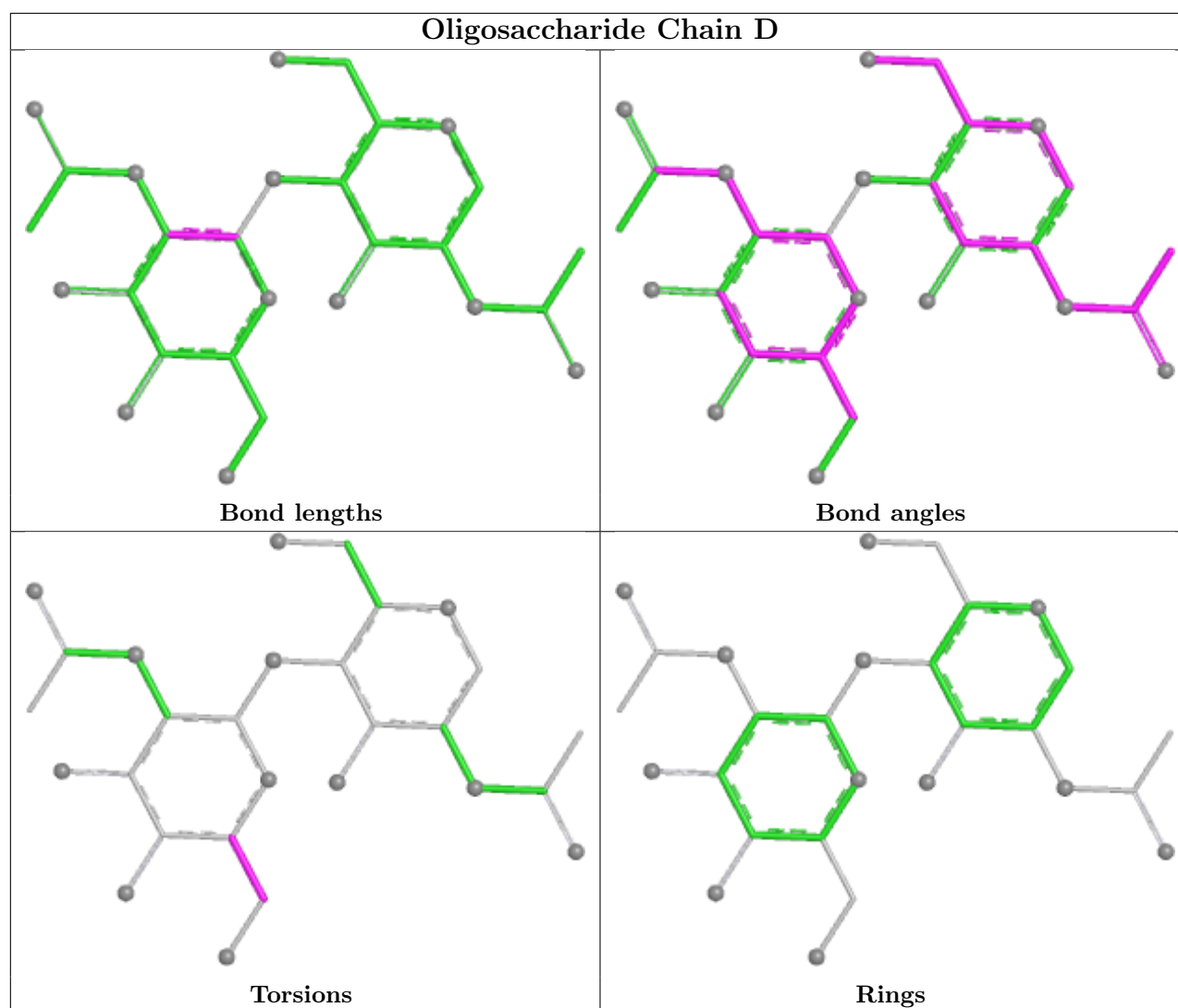
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	1002/1245 (80%)	0.26	83 (8%) 17 12	9, 61, 127, 181	0
1	B	1003/1245 (80%)	0.32	92 (9%) 14 11	9, 64, 131, 190	0
All	All	2005/2490 (80%)	0.29	175 (8%) 16 12	9, 62, 128, 190	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1337	VAL	9.3
1	B	483	VAL	8.7
1	B	484	ALA	8.0
1	A	484	ALA	7.6
1	A	483	VAL	7.5
1	B	481	GLU	5.9
1	A	667	ALA	5.8
1	A	1337	VAL	5.7
1	B	476	VAL	5.7
1	A	669	VAL	5.6
1	A	475	VAL	5.6
1	B	669	VAL	5.4
1	B	472	ILE	5.3
1	B	1336	GLU	5.3
1	A	476	VAL	5.3
1	B	667	ALA	5.1
1	B	401	ILE	5.1
1	B	451	LYS	4.9
1	B	475	VAL	4.9
1	B	485	THR	4.8
1	A	468	PRO	4.8
1	A	462	LEU	4.7
1	B	290	GLU	4.5
1	B	402	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	472	ILE	4.3
1	A	284	ALA	4.3
1	A	302	GLN	4.3
1	A	290	GLU	4.2
1	A	445	LEU	4.2
1	A	414	MET	4.1
1	A	451	LYS	4.1
1	B	462	LEU	4.1
1	B	412	TYR	4.1
1	A	402	LEU	4.1
1	B	357	PRO	4.1
1	A	412	TYR	4.0
1	A	931	TYR	4.0
1	B	478	PHE	3.9
1	B	293	CYS	3.9
1	B	287	LYS	3.8
1	A	1336	GLU	3.6
1	B	688	LEU	3.6
1	B	414	MET	3.6
1	B	420	PHE	3.6
1	B	468	PRO	3.5
1	A	287	LYS	3.5
1	A	473	HIS	3.5
1	B	473	HIS	3.5
1	A	1335	GLY	3.5
1	B	356	GLU	3.5
1	B	931	TYR	3.5
1	B	464	LYS	3.4
1	B	1335	GLY	3.4
1	A	689	SER	3.4
1	B	1278	ARG	3.3
1	A	480	CYS	3.3
1	A	898	CYS	3.3
1	B	284	ALA	3.3
1	B	898	CYS	3.2
1	B	302	GLN	3.2
1	B	477	ALA	3.2
1	B	358	VAL	3.2
1	B	930	ALA	3.2
1	A	401	ILE	3.2
1	A	420	PHE	3.2
1	A	481	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	485	THR	3.2
1	A	358	VAL	3.1
1	A	289	SER	3.1
1	A	478	PHE	3.0
1	B	445	LEU	3.0
1	B	1057	GLN	3.0
1	A	688	LEU	3.0
1	B	311	SER	3.0
1	A	469	LYS	3.0
1	B	286	PHE	3.0
1	A	286	PHE	2.9
1	A	423	VAL	2.9
1	B	471	LYS	2.9
1	A	403	THR	2.8
1	A	357	PRO	2.8
1	B	689	SER	2.8
1	A	283	ILE	2.7
1	B	457	LEU	2.7
1	A	474	GLY	2.7
1	A	477	ALA	2.7
1	A	425	GLY	2.7
1	B	469	LYS	2.7
1	A	356	GLU	2.7
1	A	292	PHE	2.7
1	A	930	ALA	2.7
1	A	444	CYS	2.7
1	A	506	LYS	2.7
1	B	285	THR	2.7
1	B	282	TYR	2.6
1	A	457	LEU	2.6
1	A	409	GLN	2.6
1	A	464	LYS	2.6
1	B	442	MET	2.6
1	B	361	LYS	2.6
1	B	1295	GLU	2.6
1	A	424	GLY	2.6
1	A	453	ASN	2.6
1	A	328	ALA	2.6
1	A	1057	GLN	2.6
1	B	459	LEU	2.5
1	A	479	LYS	2.5
1	A	300	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	359	ASN	2.5
1	B	403	THR	2.5
1	A	281	GLU	2.5
1	A	455	VAL	2.5
1	B	292	PHE	2.5
1	B	1213	ILE	2.4
1	B	312	PHE	2.4
1	A	293	CYS	2.4
1	B	422	TYR	2.4
1	B	506	LYS	2.4
1	A	282	TYR	2.4
1	A	294	TYR	2.4
1	B	697	MET	2.4
1	A	360	GLY	2.3
1	B	294	TYR	2.3
1	B	474	GLY	2.3
1	A	361	LYS	2.3
1	B	424	GLY	2.3
1	A	471	LYS	2.3
1	B	283	ILE	2.2
1	B	1137	LYS	2.2
1	A	285	THR	2.2
1	B	289	SER	2.2
1	B	486	LEU	2.2
1	A	312	PHE	2.2
1	B	328	ALA	2.2
1	B	480	CYS	2.2
1	B	409	GLN	2.2
1	B	315	LEU	2.2
1	B	1100	SER	2.2
1	A	362	PHE	2.2
1	A	366	ALA	2.2
1	B	1087	CYS	2.2
1	A	586	ASP	2.2
1	B	1150	ASP	2.2
1	B	548	PHE	2.2
1	A	367	TRP	2.1
1	A	1278	ARG	2.1
1	A	501	PRO	2.1
1	A	422	TYR	2.1
1	B	421	PHE	2.1
1	B	508	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	315	LEU	2.1
1	B	1246	ALA	2.1
1	B	326	LYS	2.1
1	A	666	MET	2.1
1	B	666	MET	2.1
1	B	679	CYS	2.1
1	A	400	GLY	2.1
1	B	281	GLU	2.1
1	B	371	LYS	2.1
1	A	1087	CYS	2.1
1	B	360	GLY	2.1
1	B	425	GLY	2.1
1	B	362	PHE	2.1
1	B	479	LYS	2.0
1	B	404	THR	2.0
1	A	346	LEU	2.0
1	A	486	LEU	2.0
1	A	703	ASN	2.0
1	B	423	VAL	2.0
1	B	441	PHE	2.0
1	B	617	ASP	2.0
1	B	1179	SER	2.0
1	B	427	PRO	2.0
1	A	573	LEU	2.0
1	B	456	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

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

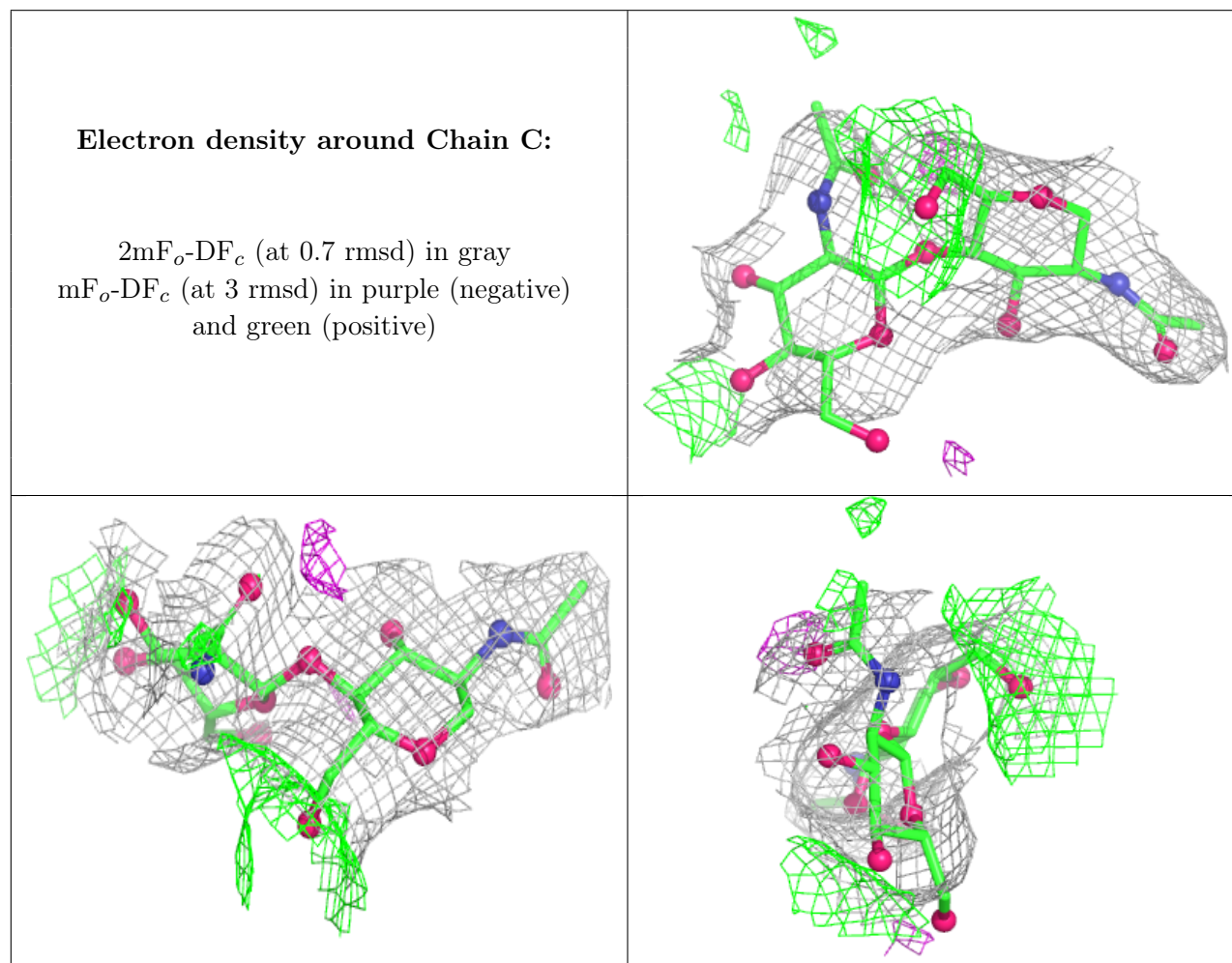
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	D	2	14/15	0.70	0.17	79,91,99,102	0
2	NAG	C	2	14/15	0.74	0.17	77,89,96,100	0
2	NAG	C	1	14/15	0.82	0.12	60,76,81,84	0

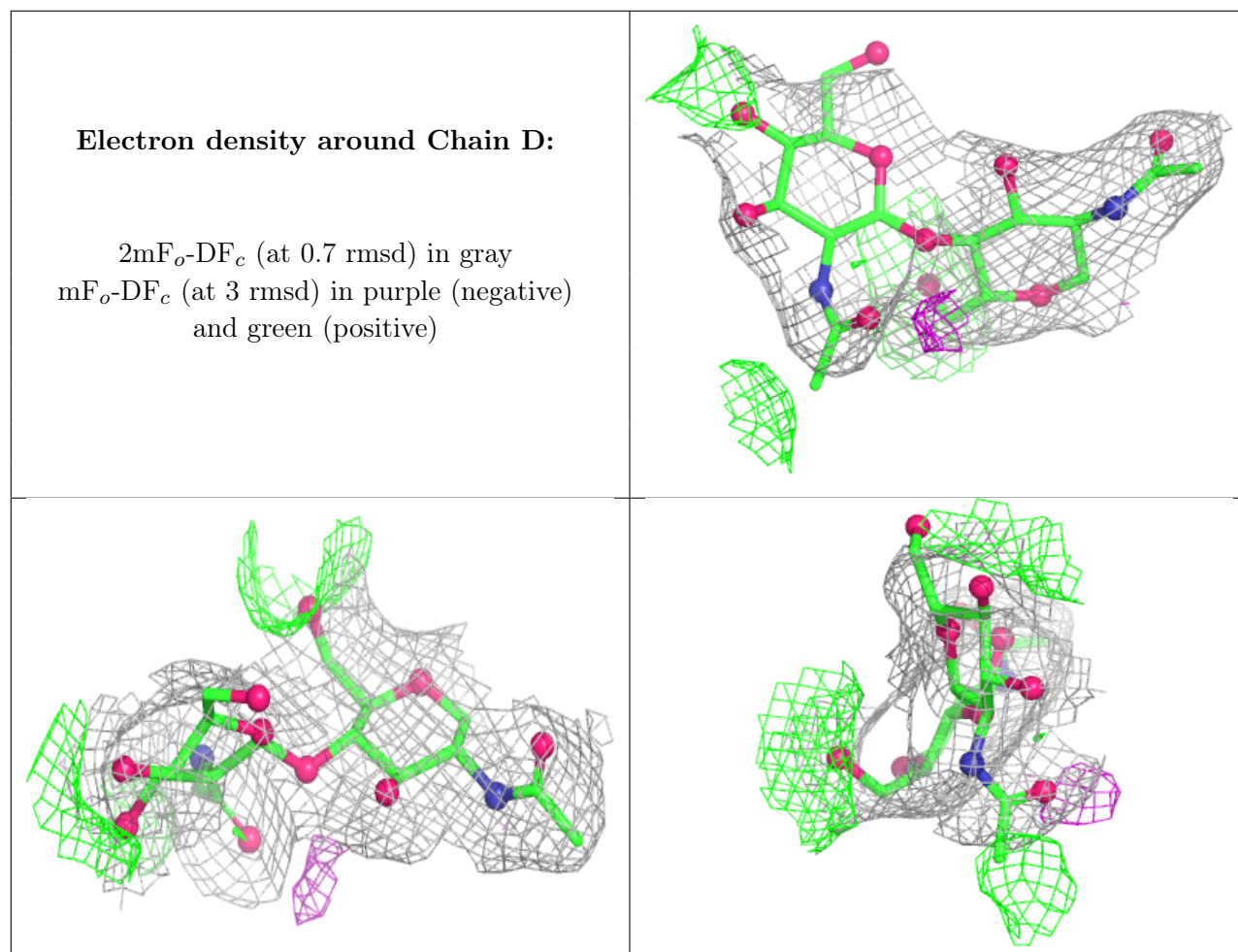
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	D	1	14/15	0.83	0.12	59,76,83,85	0

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.





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.