



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 28, 2025 – 01:53 PM JST

PDB ID : 9KUD / pdb_00009kud
Title : Crystal structure of SARS-CoV-2 JN.1 variant RBD complexed with squirrel ACE2
Authors : Lan, J.; Wang, C.H.
Deposited on : 2024-12-03
Resolution : 3.14 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 Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

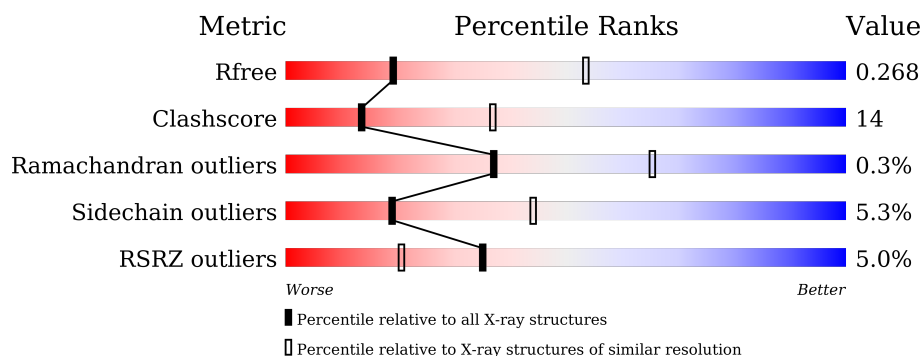
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.14 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}	164625	2149 (3.18-3.10)
Clashscore	180529	2290 (3.18-3.10)
Ramachandran outliers	177936	2178 (3.18-3.10)
Sidechain outliers	177891	2178 (3.18-3.10)
RSRZ outliers	164620	2149 (3.18-3.10)

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	596	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>29%</div> <div>..</div> </div> </div>
1	B	596	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>28%</div> <div>..</div> </div> </div>
2	E	197	<div> <div>7%</div> <div> <div></div> <div>66%</div> <div>30%</div> <div>.</div> </div> </div>
2	F	197	<div> <div>11%</div> <div> <div></div> <div>60%</div> <div>35%</div> <div>..</div> </div> </div>
3	C	4	<div> <div></div> <div> <div></div> <div>75%</div> <div>25%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12990 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 Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	593	Total	C	N	O	S	0	0	0
			4869	3109	819	911	30			
1	B	591	Total	C	N	O	S	0	0	0
			4844	3090	816	908	30			

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	197	Total	C	N	O	S	0	0	0
			1584	1024	268	284	8			
2	F	194	Total	C	N	O	S	0	0	0
			1557	1007	261	281	8			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	332	PRO	ILE	conflict	UNP P0DTC2
E	339	HIS	GLY	variant	UNP P0DTC2
E	356	THR	LYS	conflict	UNP P0DTC2
E	371	PHE	SER	variant	UNP P0DTC2
E	373	PRO	SER	variant	UNP P0DTC2
E	375	PHE	SER	variant	UNP P0DTC2
E	376	ALA	THR	variant	UNP P0DTC2
E	403	LYS	ARG	conflict	UNP P0DTC2
E	405	ASN	ASP	variant	UNP P0DTC2
E	408	SER	ARG	variant	UNP P0DTC2
E	417	ASN	LYS	variant	UNP P0DTC2
E	440	LYS	ASN	variant	UNP P0DTC2
E	445	HIS	VAL	conflict	UNP P0DTC2
E	446	SER	GLY	variant	UNP P0DTC2
E	450	ASP	ASN	conflict	UNP P0DTC2
E	452	TRP	LEU	conflict	UNP P0DTC2

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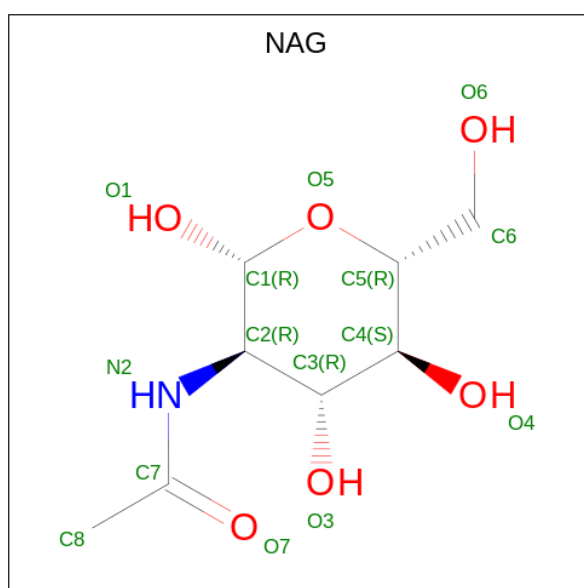
Chain	Residue	Modelled	Actual	Comment	Reference
E	455	SER	LEU	conflict	UNP P0DTC2
E	460	LYS	ASN	variant	UNP P0DTC2
E	477	ASN	SER	variant	UNP P0DTC2
E	478	LYS	THR	variant	UNP P0DTC2
E	481	LYS	ASN	conflict	UNP P0DTC2
E	?	-	VAL	deletion	UNP P0DTC2
E	483	LYS	GLU	variant	UNP P0DTC2
E	485	PRO	PHE	variant	UNP P0DTC2
E	497	ARG	GLN	variant	UNP P0DTC2
E	500	TYR	ASN	variant	UNP P0DTC2
E	504	HIS	TYR	variant	UNP P0DTC2
E	527	HIS	-	expression tag	UNP P0DTC2
E	528	HIS	-	expression tag	UNP P0DTC2
F	332	PRO	ILE	conflict	UNP P0DTC2
F	339	HIS	GLY	variant	UNP P0DTC2
F	356	THR	LYS	conflict	UNP P0DTC2
F	371	PHE	SER	variant	UNP P0DTC2
F	373	PRO	SER	variant	UNP P0DTC2
F	375	PHE	SER	variant	UNP P0DTC2
F	376	ALA	THR	variant	UNP P0DTC2
F	403	LYS	ARG	conflict	UNP P0DTC2
F	405	ASN	ASP	variant	UNP P0DTC2
F	408	SER	ARG	variant	UNP P0DTC2
F	417	ASN	LYS	variant	UNP P0DTC2
F	440	LYS	ASN	variant	UNP P0DTC2
F	445	HIS	VAL	conflict	UNP P0DTC2
F	446	SER	GLY	variant	UNP P0DTC2
F	450	ASP	ASN	conflict	UNP P0DTC2
F	452	TRP	LEU	conflict	UNP P0DTC2
F	455	SER	LEU	conflict	UNP P0DTC2
F	460	LYS	ASN	variant	UNP P0DTC2
F	477	ASN	SER	variant	UNP P0DTC2
F	478	LYS	THR	variant	UNP P0DTC2
F	481	LYS	ASN	conflict	UNP P0DTC2
F	?	-	VAL	deletion	UNP P0DTC2
F	483	LYS	GLU	variant	UNP P0DTC2
F	485	PRO	PHE	variant	UNP P0DTC2
F	497	ARG	GLN	variant	UNP P0DTC2
F	500	TYR	ASN	variant	UNP P0DTC2
F	504	HIS	TYR	variant	UNP P0DTC2
F	527	HIS	-	expression tag	UNP P0DTC2
F	528	HIS	-	expression tag	UNP P0DTC2

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

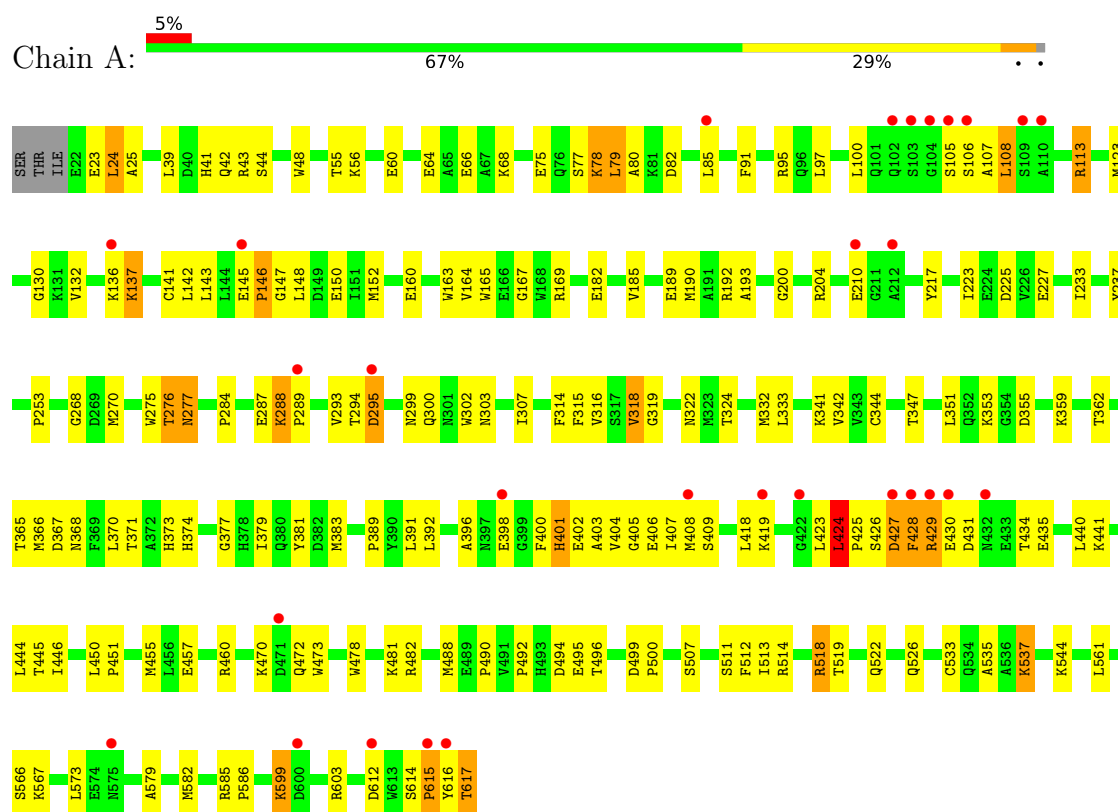
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Zn 1	0	0
5	B	1	Total 1	Zn 1	0	0

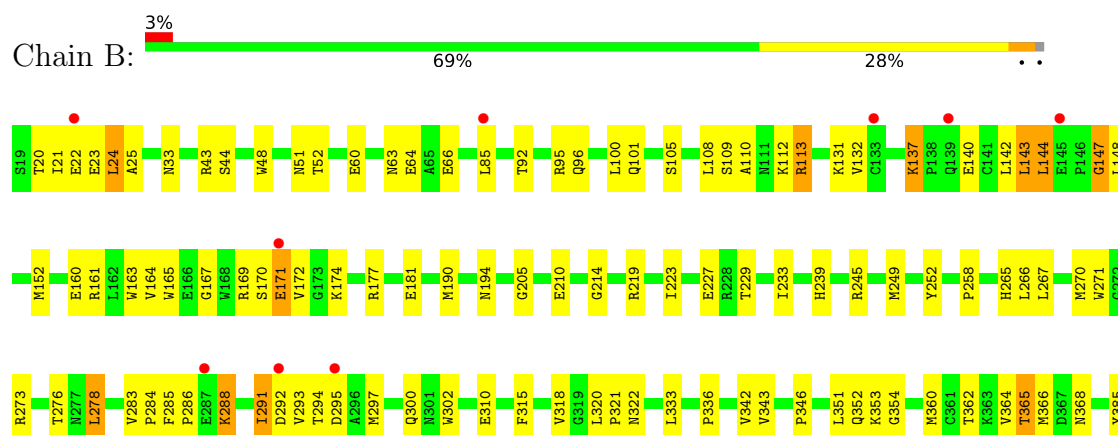
3 Residue-property plots [i](#)

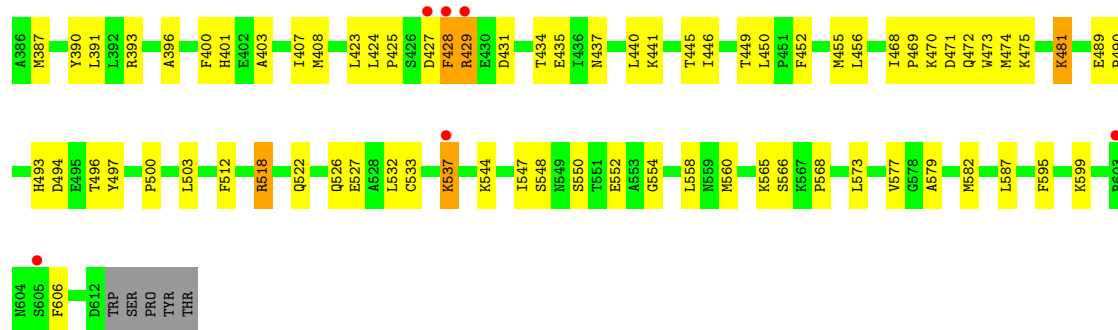
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Angiotensin-converting enzyme

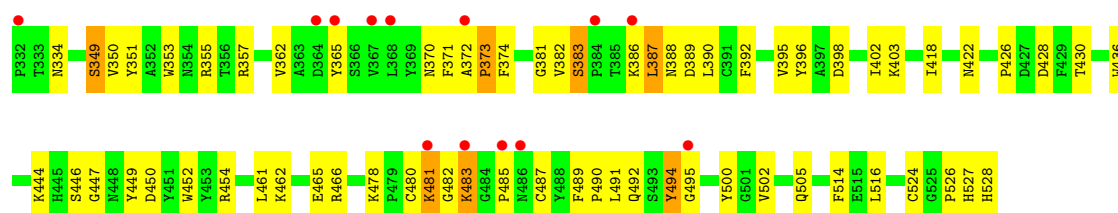


- Molecule 1: Angiotensin-converting enzyme

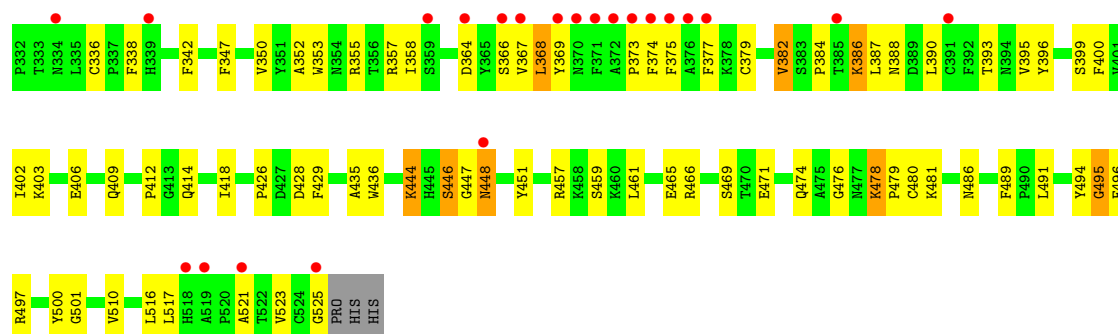




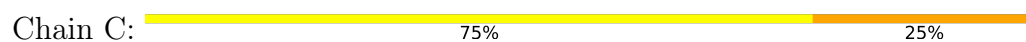
• Molecule 2: Spike protein S1



• Molecule 2: Spike protein S1



• Molecule 3: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	128.67Å 129.16Å 138.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.38 – 3.14 32.38 – 3.14	Depositor EDS
% Data completeness (in resolution range)	99.9 (32.38-3.14) 99.8 (32.38-3.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.19.1_4122: ???)	Depositor
R, R_{free}	0.225 , 0.281 0.228 , 0.268	Depositor DCC
R_{free} test set	2100 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12990	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.62	1/5004 (0.0%)	0.98	6/6788 (0.1%)
1	B	0.57	0/4975	0.89	4/6746 (0.1%)
2	E	0.62	0/1639	1.01	12/2231 (0.5%)
2	F	0.59	0/1609	0.92	4/2189 (0.2%)
All	All	0.60	1/13227 (0.0%)	0.94	26/17954 (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	2
1	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	495	GLU	CA-C	-5.53	1.42	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	LEU	N-CA-C	-12.53	97.62	113.16
2	F	373	PRO	N-CA-C	-9.35	102.53	114.03
2	E	370	ASN	N-CA-C	-7.67	104.02	113.15
2	E	371	PHE	N-CA-C	-7.01	101.95	112.54
2	F	494	TYR	CB-CA-C	-6.59	100.24	110.78
1	B	278	LEU	N-CA-C	-6.57	104.41	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	ILE	N-CA-C	-6.18	105.03	111.58
2	E	494	TYR	CA-CB-CG	6.05	124.79	113.90
1	A	253	PRO	CB-CA-C	-6.00	101.66	111.56
2	E	387	LEU	N-CA-C	-5.79	103.29	110.41
1	A	277	ASN	N-CA-C	-5.71	104.52	113.02
1	B	214	GLY	N-CA-C	-5.61	107.30	114.37
2	E	494	TYR	CA-C-N	-5.55	115.98	120.98
2	E	494	TYR	C-N-CA	-5.55	115.98	120.98
2	F	446	SER	N-CA-C	5.52	119.28	112.54
2	E	495	GLY	CA-C-N	-5.50	115.35	123.05
2	E	495	GLY	C-N-CA	-5.50	115.35	123.05
2	E	495	GLY	N-CA-C	-5.49	102.41	110.97
2	E	450	ASP	N-CA-C	-5.48	106.18	112.92
1	A	141	CYS	CB-CA-C	5.38	118.71	109.51
1	B	194	ASN	N-CA-C	-5.32	106.02	112.88
2	E	495	GLY	CA-C-O	-5.22	115.97	120.30
2	E	389	ASP	N-CA-C	-5.16	106.52	114.16
1	A	318	VAL	N-CA-C	-5.08	106.97	113.22
2	F	495	GLY	CA-C-O	-5.04	117.04	121.58
1	A	424	LEU	N-CA-C	-5.02	104.28	110.31

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ARG	Sidechain
1	A	603	ARG	Sidechain
1	B	113	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4869	0	4672	131	0
1	B	4844	0	4659	128	0
2	E	1584	0	1494	51	0
2	F	1557	0	1474	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	50	0	43	1	0
4	A	42	0	39	0	0
4	E	28	0	26	0	0
4	F	14	0	13	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	12990	0	12420	367	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (367) 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:488:MET:HE1	1:A:614:SER:HA	1.28	1.12
2:F:448:ASN:HB3	2:F:496:PHE:HB2	1.26	1.12
1:A:189:GLU:HG2	1:A:192:ARG:NH2	1.68	1.08
2:F:478:LYS:HE2	2:F:486:ASN:HB2	1.31	1.04
1:B:293:VAL:HG21	1:B:423:LEU:HB3	1.41	1.03
1:A:165:TRP:HA	1:A:270:MET:HE1	1.47	0.96
1:B:429:ARG:NE	1:B:431:ASP:HB3	1.81	0.95
1:A:425:PRO:HG2	1:A:429:ARG:NH1	1.83	0.93
1:A:189:GLU:HG2	1:A:192:ARG:HH22	1.36	0.90
1:B:165:TRP:HA	1:B:270:MET:HE1	1.51	0.89
1:B:429:ARG:HE	1:B:431:ASP:HB3	1.39	0.87
1:A:145:GLU:HB3	1:A:344:CYS:HB2	1.59	0.85
1:B:169:ARG:HH12	1:B:270:MET:HE2	1.42	0.84
1:A:169:ARG:HH12	1:A:270:MET:HE2	1.42	0.84
1:B:333:LEU:O	1:B:362:THR:HG22	1.78	0.83
1:B:518:ARG:HD3	1:B:522:GLN:HE21	1.43	0.83
2:E:392:PHE:CD1	2:E:516:LEU:HD13	2.13	0.82
1:A:419:LYS:NZ	1:A:425:PRO:HD2	1.95	0.82
1:A:107:ALA:HB3	1:A:190:MET:HG2	1.62	0.82
1:A:419:LYS:HZ3	1:A:425:PRO:HD2	1.46	0.81
2:F:448:ASN:HD21	2:F:451:TYR:HD2	1.27	0.80
1:A:425:PRO:HG2	1:A:429:ARG:HH12	1.49	0.78
1:A:492:PRO:HD3	1:A:617:THR:HB	1.66	0.78
1:A:217:TYR:OH	1:A:225:ASP:OD2	2.03	0.77
1:B:95:ARG:NH1	1:B:566:SER:O	2.19	0.76
1:B:400:PHE:CE2	1:B:560:MET:HE1	2.21	0.76
2:F:367:VAL:HG23	2:F:368:LEU:HD22	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:392:PHE:HD1	2:E:516:LEU:HD13	1.49	0.74
1:B:267:LEU:HA	1:B:278:LEU:HD11	1.70	0.73
1:B:293:VAL:CG2	1:B:423:LEU:HB3	2.16	0.73
1:B:353:LYS:HD2	2:F:500:TYR:HE1	1.54	0.72
1:B:468:ILE:HG22	1:B:473:TRP:HD1	1.54	0.72
1:A:107:ALA:HB1	1:A:193:ALA:HB3	1.73	0.71
2:E:452:TRP:HA	2:E:492:GLN:O	1.91	0.71
1:A:333:LEU:O	1:A:362:THR:HG22	1.90	0.71
2:F:393:THR:HA	2:F:521:ALA:HA	1.73	0.70
1:A:189:GLU:HG2	1:A:192:ARG:HH21	1.58	0.69
2:E:390:LEU:HB3	2:E:392:PHE:CE2	2.28	0.68
2:F:412:PRO:HG3	2:F:429:PHE:HB3	1.75	0.68
1:A:189:GLU:CG	1:A:192:ARG:NH2	2.53	0.68
2:F:448:ASN:ND2	2:F:451:TYR:HD2	1.92	0.68
2:F:366:SER:HA	2:F:369:TYR:CZ	2.29	0.68
1:A:189:GLU:CG	1:A:192:ARG:HH22	2.05	0.67
2:F:374:PHE:HA	2:F:436:TRP:HB3	1.76	0.67
1:B:160:GLU:HA	1:B:163:TRP:CD1	2.30	0.67
2:F:353:TRP:O	2:F:466:ARG:NH1	2.29	0.66
1:A:353:LYS:HB3	2:E:500:TYR:HD1	1.60	0.66
1:A:268:GLY:HA2	1:A:277:ASN:HB2	1.78	0.66
1:A:130:GLY:O	1:A:143:LEU:HD23	1.97	0.65
2:E:392:PHE:CD1	2:E:516:LEU:CD1	2.80	0.63
2:F:379:CYS:HB3	2:F:382:VAL:HG23	1.79	0.63
1:A:300:GLN:HB3	1:A:302:TRP:CD1	2.34	0.63
2:E:392:PHE:HD1	2:E:516:LEU:CD1	2.11	0.63
1:A:457:GLU:HG3	1:A:513:ILE:HB	1.81	0.63
1:A:585:ARG:HB3	1:A:586:PRO:HD3	1.81	0.63
1:A:494:ASP:OD1	1:A:496:THR:HG22	1.99	0.62
1:B:474:MET:HE1	1:B:500:PRO:HD2	1.81	0.62
1:B:132:VAL:HG12	1:B:148:LEU:HD11	1.81	0.62
1:B:336:PRO:HG2	1:B:342:VAL:HG21	1.82	0.62
2:E:390:LEU:HD13	2:E:392:PHE:HE2	1.65	0.62
2:E:483:LYS:HG2	2:E:489:PHE:HB2	1.81	0.61
2:F:409:GLN:HA	2:F:414:GLN:HG2	1.83	0.61
2:F:444:LYS:HE3	2:F:448:ASN:HA	1.82	0.61
1:A:367:ASP:O	1:A:371:THR:HG23	2.02	0.60
1:B:165:TRP:HA	1:B:270:MET:CE	2.29	0.60
1:B:400:PHE:HE2	1:B:560:MET:HE1	1.64	0.60
2:F:457:ARG:NH1	2:F:459:SER:O	2.34	0.59
2:F:364:ASP:O	2:F:367:VAL:HG22	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:ARG:HA	1:B:452:PHE:CD2	2.37	0.59
1:B:48:TRP:CE2	1:B:52:THR:HG21	2.37	0.59
1:B:353:LYS:HD2	2:F:500:TYR:CE1	2.37	0.59
1:B:472:GLN:HG2	1:B:475:LYS:HD3	1.84	0.59
1:B:494:ASP:OD1	1:B:496:THR:HG22	2.03	0.59
2:F:474:GLN:HB2	2:F:480:CYS:SG	2.42	0.59
2:F:355:ARG:HD3	2:F:396:TYR:CD1	2.38	0.58
1:A:488:MET:HE2	1:A:615:PRO:HD3	1.85	0.58
2:E:381:GLY:HA3	2:E:430:THR:HG22	1.84	0.58
1:A:276:THR:OG1	1:A:445:THR:HG22	2.03	0.58
1:A:404:VAL:HA	1:A:407:ILE:HD12	1.84	0.58
2:E:372:ALA:O	2:E:374:PHE:N	2.36	0.58
1:B:144:LEU:HA	1:B:148:LEU:HB2	1.85	0.58
1:B:425:PRO:HG2	1:B:428:PHE:HB3	1.86	0.57
1:B:318:VAL:O	1:B:554:GLY:HA3	2.05	0.57
1:A:189:GLU:HA	1:A:192:ARG:NH2	2.19	0.57
1:A:353:LYS:HG3	2:E:500:TYR:HE1	1.69	0.57
1:B:144:LEU:HA	1:B:148:LEU:HD12	1.87	0.57
1:A:511:SER:HB3	1:A:514:ARG:HH21	1.70	0.56
1:A:43:ARG:HD2	1:A:66:GLU:OE1	2.04	0.56
1:B:353:LYS:HB3	2:F:500:TYR:CD1	2.41	0.56
1:A:288:LYS:HD3	1:A:434:THR:HG23	1.87	0.56
2:F:393:THR:HG23	2:F:516:LEU:HA	1.87	0.56
1:B:407:ILE:HD11	1:B:522:GLN:HA	1.88	0.55
1:A:289:PRO:HB3	1:A:429:ARG:HH11	1.72	0.55
2:F:448:ASN:N	2:F:496:PHE:H	2.05	0.55
1:B:435:GLU:OE2	1:B:544:LYS:HD3	2.06	0.55
2:E:365:TYR:CD1	2:E:387:LEU:HB3	2.41	0.55
1:B:43:ARG:NH1	1:B:66:GLU:OE2	2.39	0.54
1:A:160:GLU:HA	1:A:163:TRP:CD1	2.41	0.54
1:A:374:HIS:CE1	1:A:402:GLU:OE1	2.59	0.54
1:A:60:GLU:O	1:A:64:GLU:HG3	2.07	0.54
1:A:457:GLU:HG2	1:A:512:PHE:HB3	1.90	0.54
1:B:92:THR:O	1:B:96:GLN:HG3	2.08	0.54
2:F:448:ASN:O	2:F:495:GLY:HA2	2.08	0.54
2:F:412:PRO:HG3	2:F:429:PHE:CB	2.38	0.54
1:A:374:HIS:HD1	1:A:406:GLU:HG2	1.72	0.54
1:A:293:VAL:HG21	1:A:423:LEU:HB3	1.88	0.53
1:A:332:MET:SD	1:A:342:VAL:HG11	2.48	0.53
1:A:460:ARG:NH2	1:A:512:PHE:HB2	2.23	0.53
1:A:142:LEU:HD21	1:A:147:GLY:HA3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:HD22	1:A:164:VAL:HG13	1.90	0.53
1:B:169:ARG:NH1	1:B:270:MET:HE2	2.16	0.53
1:B:174:LYS:HG2	1:B:496:THR:O	2.09	0.53
1:B:320:LEU:HB3	1:B:321:PRO:HD2	1.90	0.53
2:E:461:LEU:HD22	2:E:465:GLU:HB3	1.90	0.53
2:E:483:LYS:CG	2:E:489:PHE:HB2	2.39	0.53
1:B:131:LYS:HA	1:B:142:LEU:O	2.09	0.53
2:E:524:CYS:HB3	2:E:528:HIS:NE2	2.23	0.53
2:F:369:TYR:CG	2:F:384:PRO:HB3	2.43	0.53
2:E:334:ASN:O	2:E:362:VAL:HG12	2.09	0.53
2:E:388:ASN:HA	2:E:526:PRO:HD2	1.90	0.53
2:F:388:ASN:O	2:F:525:GLY:HA3	2.09	0.53
1:B:85:LEU:HD23	1:B:101:GLN:NE2	2.24	0.53
1:A:425:PRO:HB2	1:A:427:ASP:OD1	2.09	0.53
1:B:283:VAL:HG13	1:B:286:PRO:HG3	1.90	0.53
2:F:350:VAL:HG21	2:F:402:ILE:HD13	1.89	0.53
2:F:497:ARG:HB2	2:F:500:TYR:CE2	2.44	0.52
1:B:142:LEU:HD21	1:B:147:GLY:HA3	1.90	0.52
1:A:270:MET:O	1:A:270:MET:HG3	2.09	0.52
1:B:171:GLU:HG3	1:B:172:VAL:HG13	1.92	0.52
2:E:387:LEU:O	2:E:388:ASN:HB2	2.09	0.52
1:A:147:GLY:O	1:A:150:GLU:HB2	2.10	0.52
1:A:470:LYS:HA	1:A:473:TRP:CD1	2.45	0.52
1:A:289:PRO:HG2	1:A:434:THR:HG21	1.92	0.52
2:E:365:TYR:CG	2:E:387:LEU:HB3	2.45	0.52
2:E:382:VAL:HG21	2:E:514:PHE:CE2	2.45	0.51
1:B:142:LEU:HD23	1:B:143:LEU:N	2.25	0.51
1:B:400:PHE:CD2	1:B:560:MET:HE1	2.46	0.51
2:F:374:PHE:HA	2:F:436:TRP:CB	2.41	0.51
1:A:353:LYS:HG3	2:E:500:TYR:CE1	2.44	0.51
1:B:152:MET:HE2	1:B:164:VAL:HB	1.93	0.51
2:F:497:ARG:HB2	2:F:500:TYR:CD2	2.46	0.51
1:B:161:ARG:NH2	1:B:267:LEU:O	2.44	0.51
2:F:358:ILE:HB	2:F:395:VAL:HB	1.93	0.51
1:B:526:GLN:HG3	1:B:533:CYS:SG	2.51	0.51
2:E:403:LYS:HG3	2:E:494:TYR:CE1	2.46	0.51
2:E:527:HIS:O	2:E:528:HIS:C	2.52	0.51
1:A:284:PRO:HD3	1:A:440:LEU:HD22	1.93	0.50
1:B:320:LEU:HD22	1:B:558:LEU:HD22	1.93	0.50
1:B:425:PRO:HB2	1:B:427:ASP:H	1.76	0.50
1:B:284:PRO:HD3	1:B:440:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:PRO:HA	1:A:615:PRO:HG2	1.94	0.50
2:E:426:PRO:HB2	2:E:428:ASP:OD1	2.12	0.50
1:A:95:ARG:NH1	1:A:566:SER:O	2.45	0.50
1:B:205:GLY:HA2	1:B:219:ARG:HG2	1.94	0.49
2:F:444:LYS:HG2	2:F:447:GLY:H	1.76	0.49
2:F:469:SER:HB3	2:F:471:GLU:HG3	1.93	0.49
1:B:346:PRO:HB3	1:B:360:MET:HE2	1.95	0.49
2:E:485:PRO:C	2:E:487:CYS:N	2.68	0.49
2:F:399:SER:HB3	2:F:510:VAL:HG22	1.94	0.49
2:F:448:ASN:ND2	2:F:496:PHE:HD2	2.11	0.49
1:B:110:ALA:HA	1:B:113:ARG:HB2	1.93	0.49
1:B:352:GLN:OE1	1:B:393:ARG:NH1	2.45	0.49
2:E:353:TRP:O	2:E:466:ARG:NH1	2.45	0.49
1:B:297:MET:HB3	1:B:364:VAL:CG1	2.43	0.49
2:F:393:THR:HG21	2:F:517:LEU:H	1.77	0.49
1:A:41:HIS:HE1	1:A:355:ASP:OD2	1.95	0.49
1:A:324:THR:HG23	1:A:383:MET:HE2	1.95	0.48
1:A:478:TRP:HA	1:A:481:LYS:HB2	1.94	0.48
1:B:252:TYR:CE2	1:B:266:LEU:HD22	2.48	0.48
1:A:23:GLU:C	1:A:25:ALA:H	2.21	0.48
1:A:233:ILE:HG21	1:A:450:LEU:HD12	1.95	0.48
1:A:428:PHE:CE1	1:A:430:GLU:HB3	2.48	0.48
1:B:85:LEU:HD23	1:B:101:GLN:HE21	1.79	0.48
1:A:499:ASP:N	1:A:500:PRO:HD2	2.28	0.48
2:F:367:VAL:CG2	2:F:368:LEU:HD22	2.38	0.48
1:A:316:VAL:O	1:A:319:GLY:N	2.45	0.48
2:E:395:VAL:HG22	2:E:514:PHE:HD1	1.78	0.48
1:B:249:MET:SD	1:B:258:PRO:HG3	2.53	0.48
1:A:44:SER:HB3	1:A:351:LEU:HG	1.96	0.48
1:A:123:MET:HE3	1:A:507:SER:O	2.13	0.48
2:F:448:ASN:HB3	2:F:496:PHE:CB	2.19	0.48
1:A:488:MET:CE	1:A:615:PRO:HD3	2.43	0.47
1:B:354:GLY:HA3	2:F:501:GLY:HA3	1.96	0.47
2:E:374:PHE:CD1	2:E:436:TRP:HB3	2.48	0.47
1:A:275:TRP:HB2	1:A:444:LEU:O	2.14	0.47
2:E:357:ARG:HG3	2:E:396:TYR:CE1	2.49	0.47
1:B:132:VAL:HG21	1:B:167:GLY:HA3	1.96	0.47
1:B:100:LEU:HB2	1:B:391:LEU:HD11	1.97	0.47
2:F:350:VAL:HA	2:F:400:PHE:HB2	1.96	0.47
2:E:383:SER:OG	2:E:386:LYS:HG3	2.15	0.47
1:B:44:SER:HB3	1:B:351:LEU:HG	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:369:TYR:CD2	2:F:384:PRO:HB3	2.50	0.47
2:F:409:GLN:HA	2:F:414:GLN:CG	2.43	0.47
1:A:80:ALA:C	1:A:82:ASP:H	2.23	0.47
2:F:478:LYS:O	2:F:479:PRO:C	2.58	0.47
1:A:314:PHE:CE2	1:A:408:MET:HB3	2.49	0.46
1:B:223:ILE:O	1:B:227:GLU:HG3	2.15	0.46
1:A:294:THR:HG23	1:A:365:THR:HA	1.96	0.46
1:A:615:PRO:C	1:A:617:THR:H	2.23	0.46
1:B:252:TYR:CZ	1:B:266:LEU:HD22	2.50	0.46
1:B:233:ILE:HD11	1:B:587:LEU:HD22	1.97	0.46
2:F:366:SER:HA	2:F:369:TYR:CE2	2.51	0.46
1:A:567:LYS:HA	1:A:567:LYS:HD3	1.71	0.46
1:B:441:LYS:HE3	1:B:441:LYS:HB3	1.70	0.46
1:A:315:PHE:O	1:A:318:VAL:HG22	2.16	0.46
1:B:167:GLY:O	1:B:171:GLU:HB3	2.15	0.46
1:B:233:ILE:HG21	1:B:450:LEU:HD12	1.98	0.46
1:A:518:ARG:O	1:A:522:GLN:HG3	2.16	0.46
1:A:377:GLY:HA3	1:A:405:GLY:HA2	1.96	0.46
1:A:425:PRO:O	1:A:426:SER:HB3	2.15	0.46
1:B:302:TRP:CH2	1:B:310:GLU:HG3	2.50	0.46
1:B:552:GLU:H	1:B:552:GLU:CD	2.23	0.46
1:A:366:MET:HE1	1:A:441:LYS:NZ	2.30	0.46
1:B:565:LYS:O	1:B:565:LYS:HG3	2.16	0.46
1:B:23:GLU:C	1:B:25:ALA:N	2.73	0.45
1:B:429:ARG:CZ	1:B:429:ARG:HB2	2.45	0.45
2:E:355:ARG:NE	2:E:398:ASP:OD1	2.40	0.45
2:F:352:ALA:O	2:F:353:TRP:C	2.58	0.45
1:A:182:GLU:O	1:A:185:VAL:HG22	2.16	0.45
1:B:276:THR:HG23	1:B:445:THR:HG22	1.98	0.45
2:E:390:LEU:HB3	2:E:392:PHE:HE2	1.79	0.45
1:A:75:GLU:O	1:A:79:LEU:HB2	2.17	0.45
1:B:142:LEU:HD23	1:B:143:LEU:H	1.81	0.45
1:A:446:ILE:HG23	1:A:519:THR:CG2	2.46	0.45
1:B:577:VAL:HG23	1:B:579:ALA:H	1.82	0.45
2:E:462:LYS:H	2:E:465:GLU:CD	2.25	0.45
1:A:145:GLU:HB2	1:A:146:PRO:HD3	1.98	0.45
1:B:315:PHE:CE1	1:B:408:MET:HG3	2.52	0.45
1:A:341:LYS:HD3	1:A:341:LYS:HA	1.75	0.45
1:A:353:LYS:CB	2:E:500:TYR:HD1	2.29	0.44
1:A:268:GLY:CA	1:A:277:ASN:HB2	2.46	0.44
2:F:375:PHE:N	2:F:435:ALA:O	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:402:ILE:HG23	2:F:403:LYS:O	2.17	0.44
1:A:366:MET:HE1	1:A:441:LYS:CE	2.47	0.44
1:B:456:LEU:HD11	1:B:503:LEU:HD23	2.00	0.44
1:B:60:GLU:HA	1:B:63:ASN:HD22	1.83	0.44
1:B:239:HIS:NE2	1:B:599:LYS:HG2	2.32	0.44
2:E:374:PHE:HD1	2:E:436:TRP:HB3	1.83	0.44
1:A:223:ILE:O	1:A:227:GLU:HG3	2.17	0.44
1:A:455:MET:HE2	1:A:481:LYS:HD3	1.98	0.44
1:B:547:ILE:O	1:B:550:SER:HB3	2.18	0.44
1:A:169:ARG:NH1	1:A:270:MET:HE2	2.22	0.44
2:F:444:LYS:CE	2:F:448:ASN:HA	2.46	0.44
1:A:599:LYS:HB2	1:A:599:LYS:HE2	1.71	0.44
2:E:365:TYR:CD2	2:E:387:LEU:HD13	2.52	0.44
1:B:285:PHE:HB2	1:B:437:ASN:HD21	1.82	0.44
1:B:300:GLN:HB2	1:B:302:TRP:CD1	2.52	0.44
2:E:349:SER:HB3	2:E:351:TYR:CE1	2.53	0.44
2:E:481:LYS:HG3	2:E:482:GLY:N	2.33	0.44
1:B:431:ASP:OD1	1:B:434:THR:HG23	2.17	0.43
2:E:402:ILE:HD11	2:E:418:ILE:HG13	2.00	0.43
2:F:338:PHE:O	2:F:342:PHE:HD1	2.00	0.43
1:A:100:LEU:HD12	1:A:391:LEU:HD11	2.00	0.43
1:A:535:ALA:C	1:A:537:LYS:H	2.25	0.43
2:E:349:SER:O	2:E:350:VAL:C	2.60	0.43
1:A:276:THR:HG23	1:A:445:THR:CG2	2.48	0.43
1:A:293:VAL:CG2	1:A:423:LEU:HB3	2.48	0.43
1:A:347:THR:OG1	1:A:359:LYS:HE3	2.18	0.43
1:A:404:VAL:HG21	1:A:561:LEU:HD21	2.00	0.43
1:B:368:ASN:HD22	1:B:368:ASN:HA	1.59	0.43
2:E:383:SER:O	2:E:386:LYS:N	2.37	0.43
2:E:454:ARG:HA	2:E:491:LEU:HD23	2.01	0.43
1:A:39:LEU:HA	1:A:42:GLN:HG3	2.00	0.43
1:B:265:HIS:ND1	1:B:490:PRO:HG3	2.34	0.43
1:B:294:THR:HG23	1:B:365:THR:HA	2.00	0.43
1:B:407:ILE:CD1	1:B:522:GLN:HA	2.47	0.43
1:A:455:MET:HE3	1:A:455:MET:HB3	1.84	0.43
1:B:288:LYS:HD2	1:B:288:LYS:HA	1.62	0.43
2:F:347:PHE:CE2	2:F:399:SER:HB2	2.53	0.43
2:F:357:ARG:HE	2:F:357:ARG:HB3	1.63	0.43
1:A:80:ALA:C	1:A:82:ASP:N	2.75	0.43
1:A:132:VAL:HG21	1:A:167:GLY:HA3	2.00	0.43
1:B:423:LEU:O	1:B:424:LEU:HD23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:PHE:O	1:B:428:PHE:CG	2.70	0.43
1:B:456:LEU:HD13	1:B:512:PHE:CE2	2.54	0.43
1:B:245:ARG:NH2	1:B:606:PHE:O	2.52	0.43
1:B:21:ILE:HG13	1:B:23:GLU:H	1.84	0.43
1:B:22:GLU:C	1:B:24:LEU:H	2.26	0.43
1:B:470:LYS:HA	1:B:473:TRP:CD1	2.54	0.43
1:B:573:LEU:HG	1:B:577:VAL:HG22	2.01	0.43
2:E:350:VAL:HG22	2:E:422:ASN:HB3	2.01	0.43
2:E:372:ALA:O	2:E:373:PRO:C	2.61	0.43
1:A:419:LYS:HA	1:A:424:LEU:HB2	2.00	0.42
1:B:33:ASN:OD1	1:B:390:TYR:HB3	2.19	0.42
1:B:20:THR:HG21	2:F:476:GLY:HA2	2.01	0.42
1:B:105:SER:HA	1:B:190:MET:HG3	2.01	0.42
1:B:366:MET:HE1	1:B:441:LYS:HD3	2.01	0.42
1:B:548:SER:C	1:B:550:SER:H	2.26	0.42
1:B:177:ARG:O	1:B:181:GLU:HG3	2.18	0.42
1:A:78:LYS:HE3	1:A:78:LYS:HB3	1.33	0.42
1:A:237:TYR:CD2	1:A:451:PRO:HG2	2.55	0.42
1:A:368:ASN:HD22	1:A:368:ASN:HA	1.60	0.42
1:A:582:MET:HE3	1:A:582:MET:HB2	1.87	0.42
1:A:615:PRO:HD2	1:A:617:THR:C	2.45	0.42
2:F:384:PRO:C	2:F:386:LYS:H	2.27	0.42
2:F:412:PRO:CG	2:F:429:PHE:HB3	2.48	0.42
1:B:429:ARG:CZ	1:B:431:ASP:HB3	2.48	0.42
1:A:108:LEU:HD12	1:A:108:LEU:HA	1.70	0.42
1:A:132:VAL:HG12	1:A:148:LEU:HD11	2.01	0.42
1:B:229:THR:HG21	1:B:582:MET:HE3	2.02	0.42
2:F:368:LEU:HD13	2:F:368:LEU:HA	1.91	0.42
2:F:406:GLU:HG2	2:F:418:ILE:HG12	2.02	0.42
2:F:461:LEU:HD22	2:F:465:GLU:HG2	2.01	0.42
1:A:97:LEU:HD23	1:A:97:LEU:HA	1.86	0.42
1:B:595:PHE:CE2	1:B:599:LYS:HE2	2.54	0.42
2:F:387:LEU:HD23	2:F:390:LEU:HD12	2.02	0.42
1:B:285:PHE:HB2	1:B:437:ASN:ND2	2.35	0.42
2:F:386:LYS:HZ2	2:F:386:LYS:HG3	1.69	0.42
1:A:573:LEU:HD12	1:A:573:LEU:HA	1.92	0.41
1:A:615:PRO:O	1:A:616:TYR:HB3	2.20	0.41
1:B:276:THR:OG1	1:B:445:THR:HG22	2.19	0.41
1:B:493:HIS:CD2	1:B:497:TYR:CZ	3.08	0.41
1:A:48:TRP:CZ3	1:A:359:LYS:HB2	2.55	0.41
1:A:446:ILE:HG23	1:A:519:THR:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:ILE:O	1:B:449:THR:HG22	2.20	0.41
1:A:68:LYS:HA	1:A:68:LYS:HD3	1.91	0.41
1:A:137:LYS:HE2	1:A:137:LYS:HB2	1.60	0.41
1:A:381:TYR:HB3	1:A:401:HIS:CE1	2.56	0.41
1:B:23:GLU:C	1:B:25:ALA:H	2.27	0.41
1:B:537:LYS:HB2	1:B:537:LYS:HE3	1.82	0.41
1:B:294:THR:HA	1:B:297:MET:HE3	2.01	0.41
2:E:489:PHE:CD1	2:E:490:PRO:HD2	2.55	0.41
1:A:152:MET:HE2	1:A:164:VAL:HB	2.01	0.41
1:A:403:ALA:O	1:A:407:ILE:HG13	2.20	0.41
1:A:441:LYS:HB3	1:A:441:LYS:HE3	1.81	0.41
1:B:403:ALA:O	1:B:407:ILE:HG12	2.21	0.41
1:B:60:GLU:O	1:B:64:GLU:HG3	2.21	0.41
1:A:396:ALA:HB3	1:A:400:PHE:CD2	2.56	0.41
1:A:435:GLU:OE2	1:A:544:LYS:HD3	2.20	0.41
1:B:469:PRO:HB2	1:B:471:ASP:OD1	2.20	0.41
1:B:526:GLN:O	1:B:533:CYS:N	2.49	0.41
2:E:502:VAL:HA	2:E:505:GLN:NE2	2.35	0.41
1:B:396:ALA:HB3	1:B:400:PHE:CD2	2.56	0.41
2:E:447:GLY:HA3	2:E:449:TYR:CE2	2.55	0.41
2:F:426:PRO:HB2	2:F:428:ASP:OD1	2.20	0.41
2:F:489:PHE:HE1	2:F:491:LEU:HB2	1.86	0.41
1:A:303:ASN:O	1:A:307:ILE:HG13	2.21	0.41
1:A:389:PRO:HG2	1:A:392:LEU:HD12	2.02	0.41
1:A:482:ARG:NH2	1:A:488:MET:HE3	2.35	0.41
1:A:535:ALA:C	1:A:537:LYS:N	2.79	0.41
1:B:455:MET:SD	1:B:481:LYS:HG2	2.60	0.41
2:E:349:SER:OG	2:E:452:TRP:N	2.51	0.41
2:E:485:PRO:O	2:E:487:CYS:HB2	2.20	0.41
2:F:366:SER:H	2:F:388:ASN:HD21	1.69	0.41
3:C:1:NAG:H83	3:C:1:NAG:H3	2.02	0.41
1:A:55:THR:HG22	1:A:56:LYS:N	2.36	0.41
1:B:51:ASN:OD1	1:B:343:VAL:HG11	2.20	0.41
2:F:402:ILE:HG13	2:F:406:GLU:OE1	2.21	0.41
1:A:370:LEU:O	1:A:373:HIS:HB2	2.21	0.40
2:E:349:SER:HB3	2:E:351:TYR:CD1	2.56	0.40
2:F:336:CYS:SG	2:F:523:VAL:HG13	2.60	0.40
2:F:368:LEU:HB3	2:F:377:PHE:CZ	2.56	0.40
1:A:200:GLY:O	1:A:204:ARG:HG3	2.21	0.40
1:A:526:GLN:O	1:A:533:CYS:N	2.54	0.40
1:B:22:GLU:C	1:B:24:LEU:N	2.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LYS:HE2	1:B:496:THR:HG23	2.02	0.40
1:A:105:SER:C	1:A:107:ALA:N	2.78	0.40
1:A:294:THR:O	1:A:295:ASP:C	2.64	0.40
1:A:573:LEU:HB3	1:A:579:ALA:O	2.21	0.40
1:B:137:LYS:O	1:B:140:GLU:HB2	2.21	0.40
1:B:21:ILE:C	1:B:23:GLU:N	2.80	0.40
1:B:108:LEU:O	1:B:109:SER:C	2.63	0.40
1:B:284:PRO:HB2	1:B:285:PHE:CD2	2.56	0.40
1:B:489:GLU:OE1	1:B:489:GLU:N	2.40	0.40
1:A:379:ILE:CG2	1:A:383:MET:HE3	2.51	0.40
1:B:95:ARG:NH2	1:B:568:PRO:HD3	2.37	0.40
1:B:468:ILE:HG22	1:B:473:TRP:CD1	2.44	0.40

There are no symmetry-related clashes.

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	591/596 (99%)	541 (92%)	48 (8%)	2 (0%)	37	65
1	B	589/596 (99%)	553 (94%)	34 (6%)	2 (0%)	37	65
2	E	195/197 (99%)	174 (89%)	20 (10%)	1 (0%)	25	55
2	F	192/197 (98%)	171 (89%)	21 (11%)	0	100	100
All	All	1567/1586 (99%)	1439 (92%)	123 (8%)	5 (0%)	37	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	PRO
1	B	144	LEU
2	E	373	PRO

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Mol	Chain	Res	Type
1	A	615	PRO
1	B	147	GLY

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	523/526 (99%)	490 (94%)	33 (6%)	15	39
1	B	521/526 (99%)	497 (95%)	24 (5%)	23	49
2	E	171/171 (100%)	163 (95%)	8 (5%)	22	49
2	F	168/171 (98%)	160 (95%)	8 (5%)	21	48
All	All	1383/1394 (99%)	1310 (95%)	73 (5%)	19	44

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	77	SER
1	A	78	LYS
1	A	79	LEU
1	A	85	LEU
1	A	91	PHE
1	A	106	SER
1	A	108	LEU
1	A	113	ARG
1	A	136	LYS
1	A	137	LYS
1	A	210	GLU
1	A	276	THR
1	A	287	GLU
1	A	288	LYS
1	A	295	ASP
1	A	299	ASN
1	A	322	ASN
1	A	398	GLU

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Mol	Chain	Res	Type
1	A	401	HIS
1	A	409	SER
1	A	418	LEU
1	A	424	LEU
1	A	427	ASP
1	A	428	PHE
1	A	429	ARG
1	A	431	ASP
1	A	472	GLN
1	A	518	ARG
1	A	537	LYS
1	A	599	LYS
1	A	612	ASP
1	A	617	THR
1	B	24	LEU
1	B	112	LYS
1	B	137	LYS
1	B	143	LEU
1	B	170	SER
1	B	171	GLU
1	B	210	GLU
1	B	271	TRP
1	B	288	LYS
1	B	291	ILE
1	B	292	ASP
1	B	295	ASP
1	B	322	ASN
1	B	365	THR
1	B	385	TYR
1	B	387	MET
1	B	401	HIS
1	B	428	PHE
1	B	429	ARG
1	B	481	LYS
1	B	518	ARG
1	B	527	GLU
1	B	532	LEU
1	B	537	LYS
2	E	349	SER
2	E	383	SER
2	E	444	LYS
2	E	446	SER

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Mol	Chain	Res	Type
2	E	478	LYS
2	E	480	CYS
2	E	481	LYS
2	E	483	LYS
2	F	368	LEU
2	F	382	VAL
2	F	386	LYS
2	F	444	LYS
2	F	446	SER
2	F	448	ASN
2	F	478	LYS
2	F	481	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	76	GLN
1	A	194	ASN
1	A	330	ASN
1	A	417	HIS
1	A	543	HIS
1	A	610	ASN
1	B	42	GLN
1	B	115	GLN
1	B	121	ASN
1	B	175	GLN
1	B	522	GLN
1	B	555	GLN
2	E	474	GLN
2	E	486	ASN
2	F	370	ASN
2	F	394	ASN
2	F	405	ASN
2	F	448	ASN
2	F	474	GLN

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$
3	NAG	C	1	3,1	14,14,15	0.49	0	17,19,21	1.48	2 (11%)
3	NAG	C	2	3	14,14,15	0.34	0	17,19,21	0.87	1 (5%)
3	BMA	C	3	3	11,11,12	1.12	0	15,15,17	0.97	1 (6%)
3	MAN	C	4	3	11,11,12	1.50	2 (18%)	15,15,17	1.18	1 (6%)

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	3,1	-	5/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	1/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	MAN	C4-C5	3.03	1.59	1.53
3	C	4	MAN	O5-C5	2.80	1.49	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C2-N2-C7	4.45	129.24	122.90
3	C	4	MAN	O2-C2-C3	-3.96	102.20	110.14
3	C	2	NAG	C1-O5-C5	3.02	116.29	112.19
3	C	1	NAG	C1-C2-N2	2.25	114.34	110.49
3	C	3	BMA	O2-C2-C3	-2.08	105.98	110.14

There are no chirality outliers.

All (9) torsion outliers are listed below:

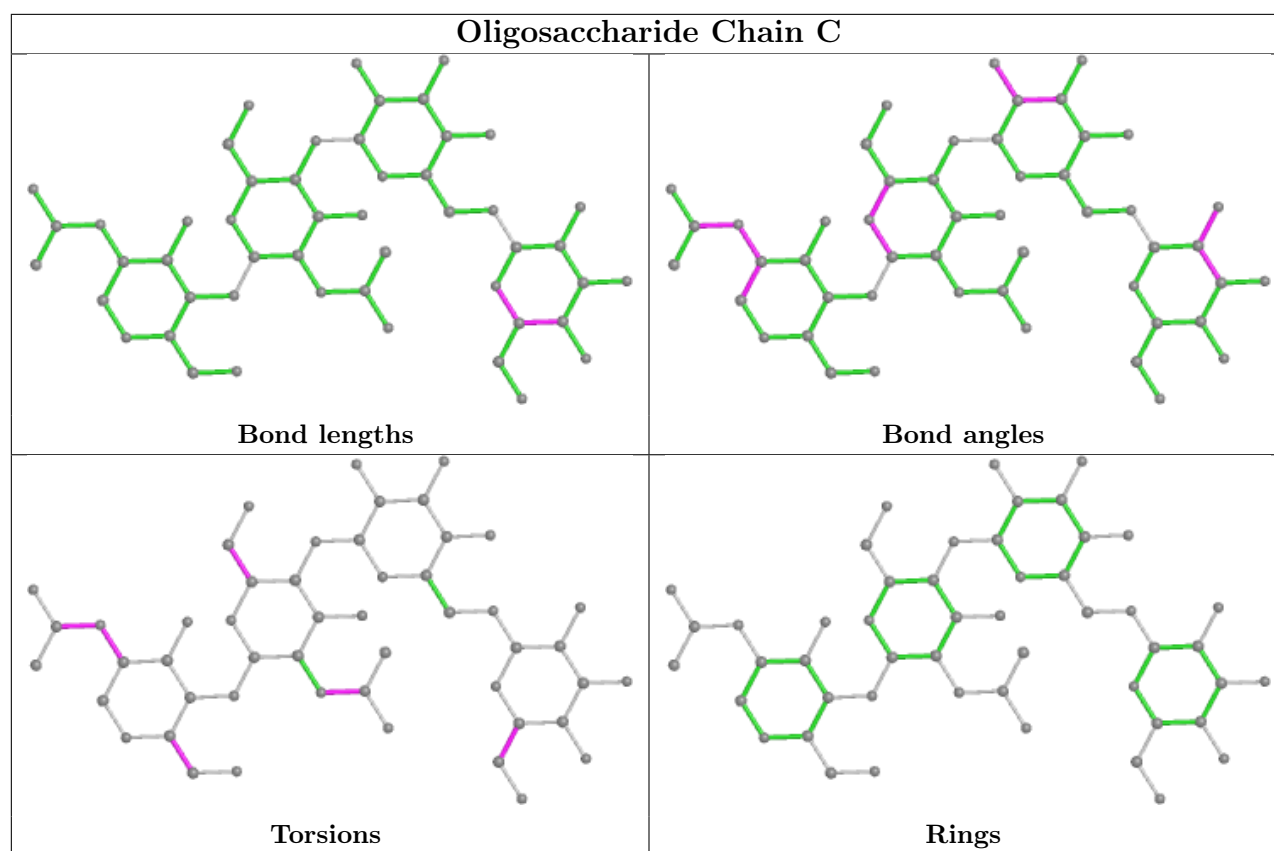
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	C	4	MAN	O5-C5-C6-O6
3	C	1	NAG	C3-C2-N2-C7
3	C	2	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	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](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	703	1	14,14,15	0.48	0	17,19,21	0.42	0
4	NAG	E	602	2	14,14,15	1.04	1 (7%)	17,19,21	0.71	0
4	NAG	F	601	2	14,14,15	1.06	1 (7%)	17,19,21	1.05	1 (5%)
4	NAG	A	701	1	14,14,15	0.43	0	17,19,21	0.90	1 (5%)
4	NAG	E	601	2	14,14,15	0.42	0	17,19,21	0.48	0
4	NAG	A	702	1	14,14,15	0.42	0	17,19,21	0.40	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
4	NAG	A	703	1	-	4/6/23/26	0/1/1/1
4	NAG	E	602	2	-	1/6/23/26	0/1/1/1
4	NAG	F	601	2	-	4/6/23/26	0/1/1/1
4	NAG	A	701	1	-	4/6/23/26	0/1/1/1
4	NAG	E	601	2	-	3/6/23/26	0/1/1/1
4	NAG	A	702	1	-	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)
4	F	601	NAG	O5-C1	3.59	1.49	1.43
4	E	602	NAG	O5-C1	3.53	1.49	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	601	NAG	C1-O5-C5	3.44	116.85	112.19
4	A	701	NAG	O5-C1-C2	2.96	115.96	111.29

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	NAG	C8-C7-N2-C2
4	A	701	NAG	O7-C7-N2-C2
4	E	601	NAG	C8-C7-N2-C2
4	E	601	NAG	O7-C7-N2-C2
4	A	701	NAG	O5-C5-C6-O6
4	A	702	NAG	C8-C7-N2-C2
4	A	702	NAG	O7-C7-N2-C2
4	A	701	NAG	C4-C5-C6-O6
4	A	703	NAG	C8-C7-N2-C2
4	A	703	NAG	O7-C7-N2-C2
4	F	601	NAG	C8-C7-N2-C2
4	F	601	NAG	O7-C7-N2-C2
4	F	601	NAG	O5-C5-C6-O6
4	A	703	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	E	601	NAG	O5-C5-C6-O6
4	E	602	NAG	O5-C5-C6-O6
4	F	601	NAG	C4-C5-C6-O6
4	A	703	NAG	O5-C5-C6-O6

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	593/596 (99%)	0.06	29 (4%)	36 21	14, 31, 60, 98	0
1	B	591/596 (99%)	-0.03	15 (2%)	58 40	15, 31, 58, 94	0
2	E	197/197 (100%)	0.06	13 (6%)	26 16	12, 25, 44, 64	0
2	F	194/197 (98%)	0.54	22 (11%)	11 7	21, 42, 66, 80	0
All	All	1575/1586 (99%)	0.08	79 (5%)	35 21	12, 31, 61, 98	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	376	ALA	8.3
1	A	145	GLU	6.8
1	A	430	GLU	6.0
1	B	292	ASP	5.8
1	A	105	SER	5.6
1	B	22	GLU	5.6
1	A	429	ARG	5.4
2	F	448	ASN	5.3
1	B	429	ARG	5.0
2	F	374	PHE	5.0
1	B	428	PHE	4.9
2	F	373	PRO	4.9
2	F	367	VAL	4.9
2	F	366	SER	4.9
1	A	408	MET	4.8
1	A	102	GLN	4.8
2	E	495	GLY	4.5
1	A	106	SER	4.4
2	F	375	PHE	4.4
1	B	427	ASP	4.3
2	F	371	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	171	GLU	4.0
1	A	428	PHE	3.9
2	F	359	SER	3.8
1	B	537	LYS	3.8
1	A	575	ASN	3.8
2	F	370	ASN	3.8
1	A	432	ASN	3.7
2	F	525	GLY	3.7
1	A	471	ASP	3.7
1	B	145	GLU	3.6
2	F	377	PHE	3.5
2	E	384	PRO	3.5
1	A	419	LYS	3.5
2	F	519	ALA	3.4
1	A	615	PRO	3.4
2	E	386	LYS	3.4
2	F	518	HIS	3.4
2	E	486	ASN	3.3
1	A	427	ASP	3.3
2	E	364	ASP	3.2
2	E	368	LEU	3.2
1	A	289	PRO	3.1
2	F	369	TYR	3.1
1	A	103	SER	3.1
2	E	372	ALA	3.1
2	E	365	TYR	3.0
2	F	385	THR	3.0
1	A	612	ASP	2.9
1	B	295	ASP	2.8
1	A	136	LYS	2.8
2	F	391	CYS	2.7
1	B	85	LEU	2.7
2	E	483	LYS	2.6
1	A	295	ASP	2.6
2	F	372	ALA	2.6
1	A	104	GLY	2.6
1	A	422	GLY	2.6
1	B	287	GLU	2.6
1	B	603	ARG	2.6
2	E	367	VAL	2.6
1	A	109	SER	2.5
1	A	600	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	485	PRO	2.5
1	A	85	LEU	2.4
2	F	364	ASP	2.4
2	F	339	HIS	2.4
1	B	605	SER	2.4
2	E	332	PRO	2.3
1	A	210	GLU	2.3
1	A	212	ALA	2.3
1	A	398	GLU	2.2
2	E	481	LYS	2.2
1	A	616	TYR	2.2
2	F	334	ASN	2.1
1	B	139	GLN	2.0
1	A	110	ALA	2.0
1	B	133	CYS	2.0
2	F	521	ALA	2.0

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

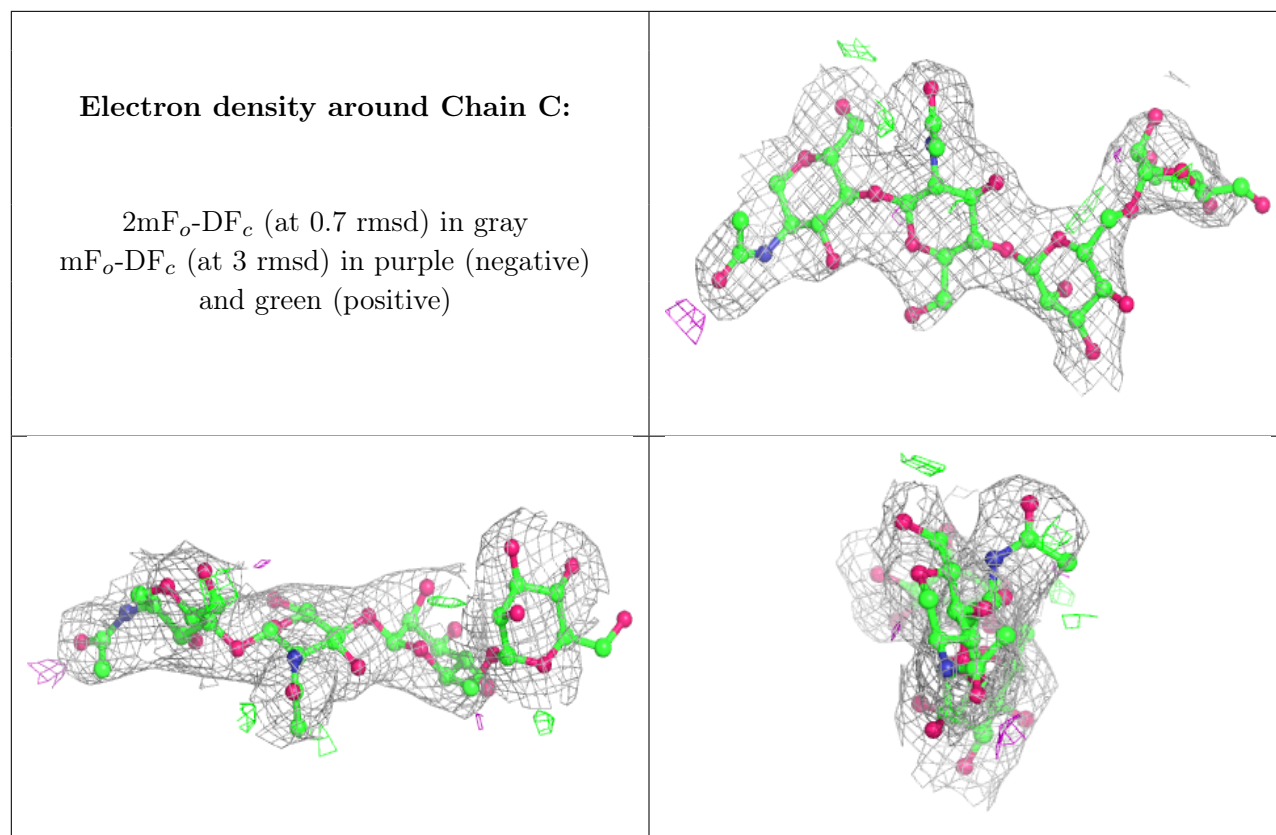
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	1	14/15	-	-	24,30,36,37	0
3	NAG	C	2	14/15	-	-	18,33,45,47	0
3	BMA	C	3	11/12	-	-	45,58,61,62	0
3	MAN	C	4	11/12	-	-	30,45,56,57	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](#)

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(\AA^2)	Q<0.9
4	NAG	E	602	14/15	0.63	0.13	60,72,82,82	0
4	NAG	E	601	14/15	0.65	0.15	38,59,71,71	0
4	NAG	A	702	14/15	0.66	0.15	64,72,78,87	0
4	NAG	F	601	14/15	0.73	0.13	49,62,71,72	0
4	NAG	A	703	14/15	0.77	0.16	62,70,75,77	0
4	NAG	A	701	14/15	0.82	0.13	44,52,59,66	0
5	ZN	B	701	1/1	0.89	0.08	30,30,30,30	0
5	ZN	A	704	1/1	0.92	0.06	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.