



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:52 PM UTC

PDB ID : 8ZES / pdb_00008zes
Title : Crystal structure of the Wuhan SARS-CoV-2 RBD (333-541) complexed with P2C5 nanobody
Authors : Sluchanko, N.N.; Varfolomeeva, L.A.; Shcheblyakov, D.V.; Logunov, D.Y.; Gintsburg, A.L.; Popov, V.O.; Boyko, K.M.
Deposited on : 2024-05-06
Resolution : 3.70 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

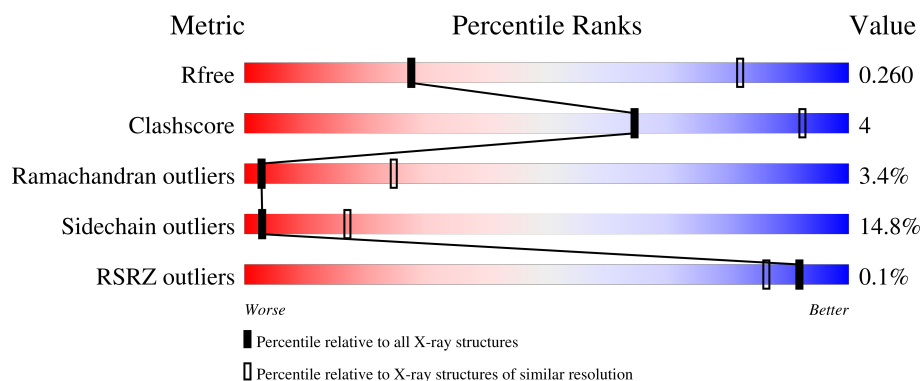
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	221	
1	C	221	
1	D	221	
1	G	221	
1	I	221	

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Mol	Chain	Length	Quality of chain
2	B	146	
2	E	146	
2	F	146	
2	H	146	
2	J	146	
3	K	2	
3	L	2	
3	M	2	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12398 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	194	Total	C	N	O	S	0	0	0
			1530	983	254	285	8			
1	A	194	Total	C	N	O	S	0	0	0
			1528	981	253	286	8			
1	G	193	Total	C	N	O	S	0	0	0
			1520	977	251	284	8			
1	I	194	Total	C	N	O	S	0	0	0
			1531	982	254	287	8			
1	D	195	Total	C	N	O	S	0	0	0
			1540	988	256	288	8			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	542	GLY	-	expression tag	UNP P0DTC2
C	543	SER	-	expression tag	UNP P0DTC2
C	544	HIS	-	expression tag	UNP P0DTC2
C	545	HIS	-	expression tag	UNP P0DTC2
C	546	HIS	-	expression tag	UNP P0DTC2
C	547	HIS	-	expression tag	UNP P0DTC2
C	548	HIS	-	expression tag	UNP P0DTC2
C	549	HIS	-	expression tag	UNP P0DTC2
C	550	HIS	-	expression tag	UNP P0DTC2
C	551	HIS	-	expression tag	UNP P0DTC2
C	552	HIS	-	expression tag	UNP P0DTC2
C	553	HIS	-	expression tag	UNP P0DTC2
A	542	GLY	-	expression tag	UNP P0DTC2
A	543	SER	-	expression tag	UNP P0DTC2
A	544	HIS	-	expression tag	UNP P0DTC2
A	545	HIS	-	expression tag	UNP P0DTC2
A	546	HIS	-	expression tag	UNP P0DTC2
A	547	HIS	-	expression tag	UNP P0DTC2
A	548	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	549	HIS	-	expression tag	UNP P0DTC2
A	550	HIS	-	expression tag	UNP P0DTC2
A	551	HIS	-	expression tag	UNP P0DTC2
A	552	HIS	-	expression tag	UNP P0DTC2
A	553	HIS	-	expression tag	UNP P0DTC2
G	542	GLY	-	expression tag	UNP P0DTC2
G	543	SER	-	expression tag	UNP P0DTC2
G	544	HIS	-	expression tag	UNP P0DTC2
G	545	HIS	-	expression tag	UNP P0DTC2
G	546	HIS	-	expression tag	UNP P0DTC2
G	547	HIS	-	expression tag	UNP P0DTC2
G	548	HIS	-	expression tag	UNP P0DTC2
G	549	HIS	-	expression tag	UNP P0DTC2
G	550	HIS	-	expression tag	UNP P0DTC2
G	551	HIS	-	expression tag	UNP P0DTC2
G	552	HIS	-	expression tag	UNP P0DTC2
G	553	HIS	-	expression tag	UNP P0DTC2
I	542	GLY	-	expression tag	UNP P0DTC2
I	543	SER	-	expression tag	UNP P0DTC2
I	544	HIS	-	expression tag	UNP P0DTC2
I	545	HIS	-	expression tag	UNP P0DTC2
I	546	HIS	-	expression tag	UNP P0DTC2
I	547	HIS	-	expression tag	UNP P0DTC2
I	548	HIS	-	expression tag	UNP P0DTC2
I	549	HIS	-	expression tag	UNP P0DTC2
I	550	HIS	-	expression tag	UNP P0DTC2
I	551	HIS	-	expression tag	UNP P0DTC2
I	552	HIS	-	expression tag	UNP P0DTC2
I	553	HIS	-	expression tag	UNP P0DTC2
D	542	GLY	-	expression tag	UNP P0DTC2
D	543	SER	-	expression tag	UNP P0DTC2
D	544	HIS	-	expression tag	UNP P0DTC2
D	545	HIS	-	expression tag	UNP P0DTC2
D	546	HIS	-	expression tag	UNP P0DTC2
D	547	HIS	-	expression tag	UNP P0DTC2
D	548	HIS	-	expression tag	UNP P0DTC2
D	549	HIS	-	expression tag	UNP P0DTC2
D	550	HIS	-	expression tag	UNP P0DTC2
D	551	HIS	-	expression tag	UNP P0DTC2
D	552	HIS	-	expression tag	UNP P0DTC2
D	553	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Nanobody P2C5.

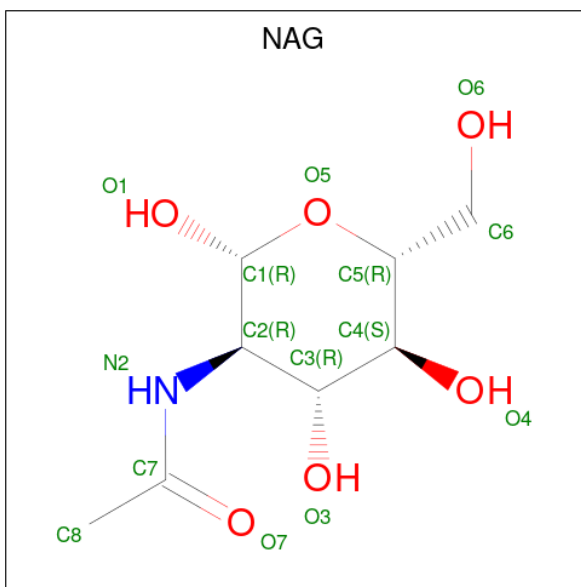
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	121	Total	C	N	O	S	0	0	0
			931	576	158	190	7			
2	B	121	Total	C	N	O	S	0	0	0
			931	576	158	190	7			
2	F	121	Total	C	N	O	S	0	0	0
			931	576	158	190	7			
2	H	120	Total	C	N	O	S	0	0	0
			925	573	157	188	7			
2	J	119	Total	C	N	O	S	0	0	0
			919	570	156	186	7			

- 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	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	M	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).

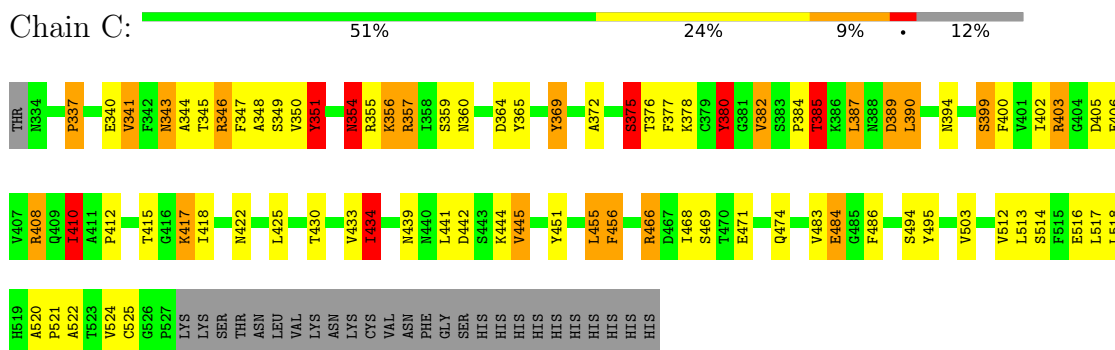


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

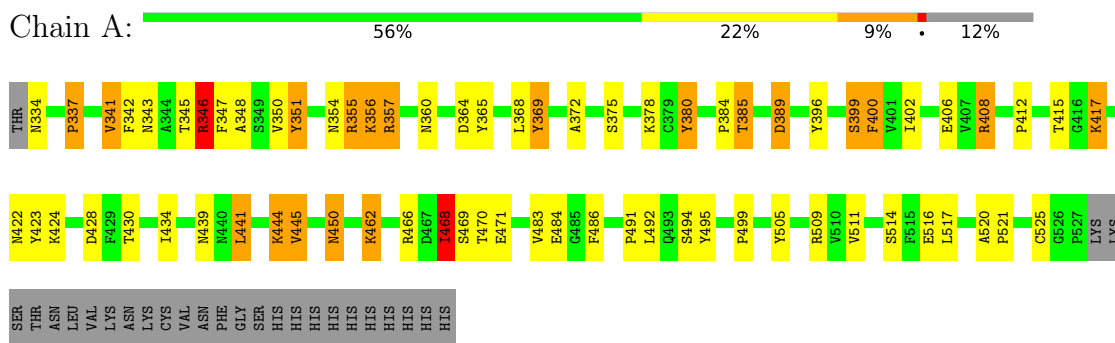
3 Residue-property plots

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.

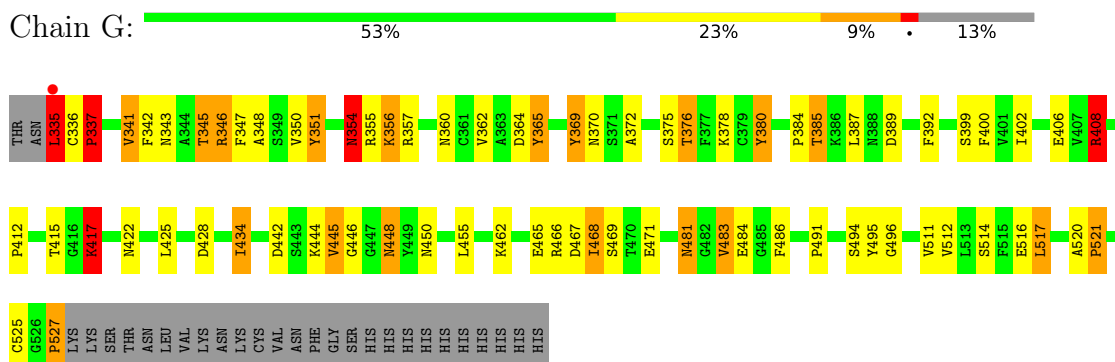
• Molecule 1: Spike protein S1



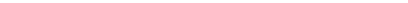
• Molecule 1: Spike protein S1

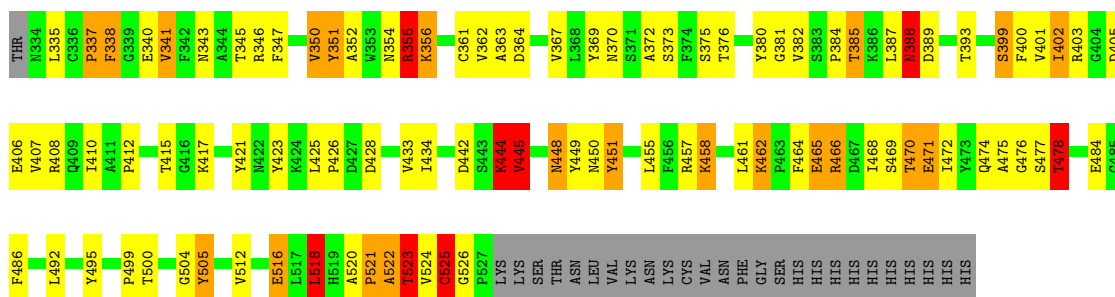


• Molecule 1: Spike protein S1



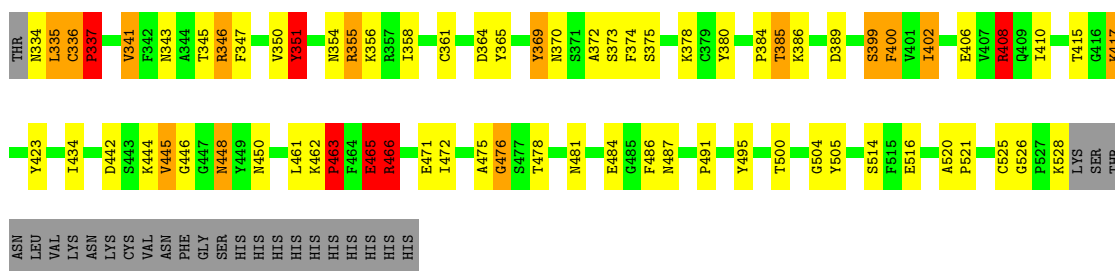
- Molecule 1: Spike protein S1

Chain I: 

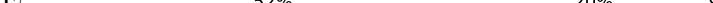


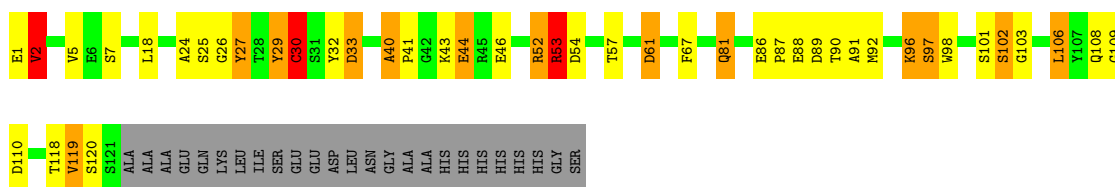
- Molecule 1: Spike protein S1

Chain D:  56% 24% 6% • 12%

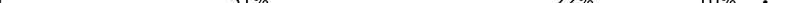


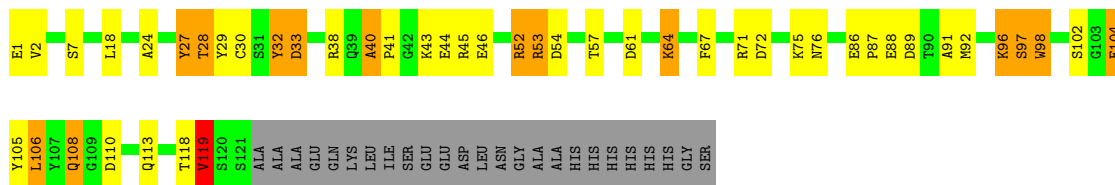
- Molecule 2: Nanobody P2C5

Chain E:  52% 20% 9% • 17%

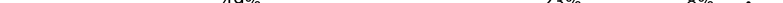


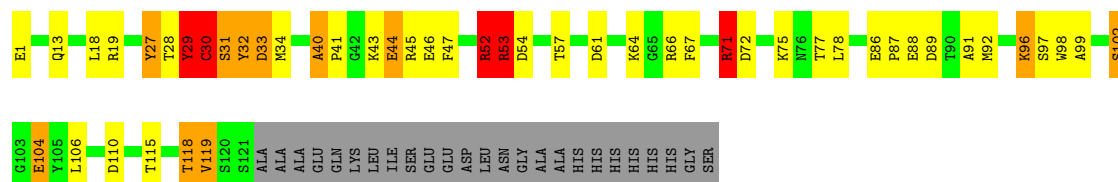
- Molecule 2: Nanobody P2C5

Chain B:  51% 22% 10% 1% 17%

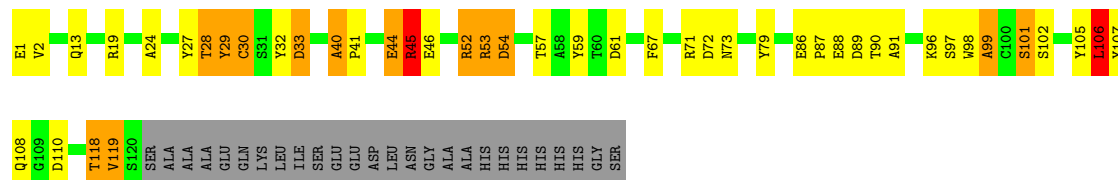


- Molecule 2: Nanobody P2C5

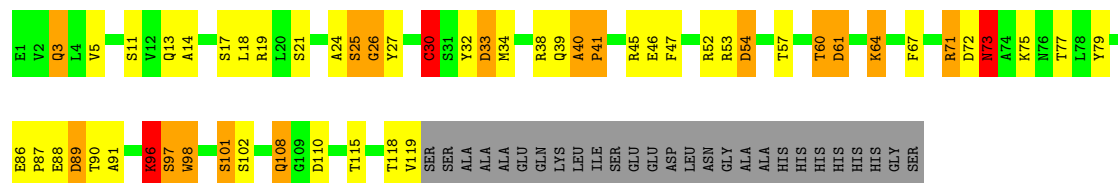
Chain F:  49% 23% 8% 1% 17%



- Molecule 2: Nanobody P2C5



- Molecule 2: Nanobody P2C5



- 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



- Molecule 3: 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	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	126.64Å 194.24Å 264.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.10 – 3.70 74.10 – 3.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (74.10-3.70) 98.9 (74.10-3.70)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.207 , 0.269 0.209 , 0.260	Depositor DCC
R_{free} test set	1792 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	150.3	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 205.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12398	wwPDB-VP
Average B, all atoms (Å ²)	195.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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	1.14	4/1571 (0.3%)	1.99	53/2139 (2.5%)
1	C	1.18	2/1574 (0.1%)	2.09	69/2143 (3.2%)
1	D	1.09	4/1583 (0.3%)	1.98	43/2154 (2.0%)
1	G	1.15	3/1563 (0.2%)	2.06	64/2128 (3.0%)
1	I	1.26	5/1574 (0.3%)	2.19	74/2143 (3.5%)
2	B	1.13	1/950 (0.1%)	2.03	35/1285 (2.7%)
2	E	1.11	0/950	1.93	29/1285 (2.3%)
2	F	1.12	1/950 (0.1%)	2.07	44/1285 (3.4%)
2	H	1.18	2/944 (0.2%)	2.00	33/1277 (2.6%)
2	J	1.13	0/938	2.05	43/1269 (3.4%)
All	All	1.15	22/12597 (0.2%)	2.05	487/17108 (2.8%)

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	8
1	C	0	18
1	D	0	9
1	G	0	11
1	I	0	19
2	B	0	7
2	E	0	16
2	F	0	11
2	H	0	17
2	J	0	16
All	All	0	132

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	514	SER	CA-CB	8.15	1.66	1.53
1	A	399	SER	CA-CB	8.03	1.64	1.53
1	C	399	SER	CA-CB	6.70	1.62	1.53
2	H	45	ARG	NE-CZ	6.58	1.40	1.33
1	D	335	LEU	C-N	6.54	1.41	1.33
2	H	99	ALA	C-O	6.40	1.31	1.23
1	I	399	SER	CA-CB	6.30	1.62	1.53
1	I	524	VAL	C-N	6.29	1.38	1.33
1	D	336	CYS	CA-C	5.92	1.58	1.52
1	D	399	SER	CA-CB	5.76	1.61	1.53
1	I	466	ARG	NE-CZ	5.59	1.39	1.33
1	G	468	ILE	CB-CG1	5.54	1.64	1.53
1	C	468	ILE	C-N	5.47	1.41	1.33
1	I	468	ILE	C-O	5.44	1.30	1.24
1	A	468	ILE	CB-CG1	5.43	1.64	1.53
2	B	102	SER	CA-CB	-5.42	1.47	1.53
1	I	373	SER	CA-CB	5.41	1.62	1.53
1	A	468	ILE	C-N	5.18	1.40	1.33
1	G	408	ARG	NE-CZ	5.06	1.38	1.33
1	A	408	ARG	NE-CZ	5.04	1.38	1.33
1	D	336	CYS	N-CA	5.04	1.52	1.45
2	F	102	SER	CA-CB	5.01	1.61	1.53

All (487) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	486	PHE	CA-CB-CG	20.15	133.95	113.80
1	I	341	VAL	N-CA-CB	13.56	125.40	110.62
2	F	32	TYR	N-CA-CB	13.49	133.28	110.49
1	D	465	GLU	CB-CG-CD	13.17	134.99	112.60
1	C	341	VAL	N-CA-CB	12.62	124.38	110.62
2	H	45	ARG	CG-CD-NE	12.35	139.16	112.00
2	J	27	TYR	CB-CA-C	12.26	130.41	111.77
1	G	341	VAL	N-CA-CB	12.08	124.68	110.55
2	B	1	GLU	CB-CG-CD	11.47	132.11	112.60
2	H	44	GLU	CB-CG-CD	11.44	132.05	112.60
1	D	341	VAL	N-CA-CB	11.40	123.88	110.55
2	E	61	ASP	CA-CB-CG	10.74	123.34	112.60
2	F	1	GLU	CB-CG-CD	10.39	130.27	112.60
1	A	341	VAL	N-CA-CB	10.36	123.83	110.57
1	I	408	ARG	CA-CB-CG	10.16	134.42	114.10
1	D	471	GLU	CB-CG-CD	10.13	129.82	112.60
1	A	343	ASN	CA-CB-CG	9.94	122.54	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	ASN	CB-CA-C	9.89	126.54	112.11
2	F	32	TYR	CA-CB-CG	9.64	131.24	113.90
1	I	350	VAL	CB-CA-C	-9.54	99.45	112.24
2	B	27	TYR	N-CA-CB	9.53	126.60	110.49
1	C	343	ASN	CA-CB-CG	9.46	122.06	112.60
2	H	28	THR	CA-C-O	-9.28	109.13	120.54
2	H	33	ASP	CA-CB-CG	9.26	121.86	112.60
1	G	343	ASN	CA-CB-CG	9.19	121.79	112.60
1	A	439	ASN	OD1-CG-ND2	-9.19	113.41	122.60
1	I	343	ASN	CA-CB-CG	9.09	121.69	112.60
1	G	415	THR	CA-CB-OG1	-9.09	95.97	109.60
2	E	52	ARG	CB-CA-C	9.07	126.14	110.45
2	B	105	TYR	CA-C-O	-9.05	110.83	120.42
1	G	337	PRO	N-CA-CB	-9.04	93.75	103.25
1	G	471	GLU	CB-CG-CD	8.95	127.81	112.60
2	H	106	LEU	N-CA-CB	8.94	125.60	110.49
2	B	52	ARG	CB-CA-C	8.87	125.79	110.45
1	D	495	TYR	N-CA-CB	8.87	123.45	110.06
2	J	64	LYS	CG-CD-CE	8.85	131.65	111.30
1	D	343	ASN	CA-CB-CG	8.84	121.44	112.60
2	E	44	GLU	CB-CG-CD	8.81	127.58	112.60
2	J	33	ASP	CA-CB-CG	8.71	121.31	112.60
1	I	522	ALA	CA-C-N	8.71	138.17	121.54
1	I	522	ALA	C-N-CA	8.71	138.17	121.54
2	F	52	ARG	CB-CA-C	8.67	125.45	110.45
2	B	46	GLU	CB-CG-CD	8.67	127.34	112.60
1	C	360	ASN	CB-CA-C	8.63	125.38	112.09
1	G	408	ARG	N-CA-CB	-8.63	95.91	110.49
2	H	52	ARG	CB-CA-C	8.60	126.77	110.51
2	J	88	GLU	N-CA-CB	8.59	122.74	110.12
2	J	52	ARG	CB-CA-C	8.58	126.73	110.51
1	A	469	SER	CB-CA-C	-8.57	99.26	109.80
2	J	3	GLN	CB-CA-C	8.51	124.40	110.78
1	I	338	PHE	CA-CB-CG	8.49	122.29	113.80
1	G	378	LYS	CG-CD-CE	8.46	130.75	111.30
1	C	444	LYS	CA-CB-CG	8.40	130.89	114.10
1	G	514	SER	CB-CA-C	8.35	124.17	109.72
1	A	385	THR	CA-CB-OG1	-8.33	97.10	109.60
2	E	52	ARG	NE-CZ-NH2	8.32	126.69	119.20
2	B	33	ASP	CA-CB-CG	8.27	120.87	112.60
1	G	462	LYS	CB-CG-CD	8.23	130.23	111.30
2	B	44	GLU	CB-CG-CD	8.23	126.59	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	64	LYS	CB-CG-CD	8.17	130.09	111.30
1	I	495	TYR	N-CA-C	8.15	120.24	111.36
1	G	360	ASN	CB-CA-C	8.13	124.61	112.09
1	C	495	TYR	N-CA-C	8.10	120.11	111.28
1	G	385	THR	CA-CB-OG1	-8.10	97.46	109.60
1	I	369	TYR	N-CA-CB	8.09	121.96	110.07
1	C	469	SER	CB-CA-C	-8.09	99.85	109.80
2	J	88	GLU	CB-CA-C	-8.05	97.43	110.79
1	D	385	THR	CA-CB-OG1	-7.99	97.61	109.60
1	I	412	PRO	N-CD-CG	-7.96	91.25	103.20
1	C	385	THR	CA-CB-OG1	-7.96	97.66	109.60
2	J	46	GLU	CB-CG-CD	7.94	126.10	112.60
2	J	67	PHE	CA-CB-CG	7.90	121.70	113.80
1	C	405	ASP	CA-CB-CG	7.89	120.49	112.60
2	J	89	ASP	CA-CB-CG	7.89	120.49	112.60
1	C	474	GLN	CA-CB-CG	7.87	129.85	114.10
2	F	53	ARG	CG-CD-NE	7.87	129.32	112.00
1	I	405	ASP	CA-CB-CG	7.84	120.44	112.60
2	F	33	ASP	CA-CB-CG	7.84	120.44	112.60
2	H	88	GLU	N-CA-CB	7.83	121.81	110.06
2	B	110	ASP	CA-CB-CG	7.80	120.40	112.60
1	C	354	ASN	CA-CB-CG	-7.78	104.82	112.60
1	C	455	LEU	CA-C-O	-7.78	109.39	120.51
1	I	470	THR	CB-CA-C	7.77	125.88	110.42
1	I	518	LEU	CA-C-O	-7.75	112.29	120.89
2	H	88	GLU	CB-CA-C	-7.70	97.59	110.68
1	I	495	TYR	CB-CA-C	-7.63	97.87	110.85
1	D	346	ARG	NE-CZ-NH2	7.62	126.06	119.20
1	G	486	PHE	CA-CB-CG	7.62	121.42	113.80
2	F	88	GLU	CB-CA-C	-7.56	97.82	110.68
2	E	33	ASP	CA-CB-CG	7.54	120.14	112.60
2	F	75	LYS	CB-CG-CD	7.54	128.63	111.30
2	J	115	THR	OG1-CB-CG2	7.51	124.32	109.30
1	D	408	ARG	CB-CG-CD	7.49	128.54	111.30
1	I	345	THR	CA-CB-OG1	-7.48	98.38	109.60
1	D	415	THR	CA-CB-OG1	-7.48	98.38	109.60
1	C	341	VAL	CB-CA-C	-7.47	102.47	111.81
2	E	32	TYR	CA-CB-CG	7.46	127.33	113.90
1	I	415	THR	CA-CB-OG1	-7.46	98.41	109.60
1	C	345	THR	CA-CB-OG1	-7.46	98.42	109.60
1	C	486	PHE	CA-CB-CG	7.45	121.25	113.80
2	H	67	PHE	CA-CB-CG	7.43	121.23	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	376	THR	OG1-CB-CG2	7.42	124.15	109.30
1	I	356	LYS	CB-CG-CD	7.40	128.32	111.30
2	F	88	GLU	N-CA-CB	7.39	121.14	110.06
2	E	110	ASP	CA-CB-CG	7.37	119.97	112.60
2	H	105	TYR	N-CA-CB	7.37	121.61	110.19
2	B	75	LYS	CB-CG-CD	7.37	128.24	111.30
1	A	505	TYR	CA-CB-CG	7.35	127.13	113.90
1	D	346	ARG	CA-CB-CG	7.32	128.74	114.10
2	F	67	PHE	CA-CB-CG	7.30	121.10	113.80
1	C	456	PHE	CB-CA-C	-7.26	95.96	110.42
2	E	67	PHE	CA-CB-CG	7.26	121.06	113.80
1	I	444	LYS	CB-CA-C	7.26	122.84	109.70
1	A	444	LYS	N-CA-CB	7.26	125.03	111.53
2	J	73	ASN	CB-CA-C	7.26	123.90	110.11
1	D	463	PRO	N-CA-CB	-7.25	95.64	103.25
1	C	415	THR	CA-CB-OG1	-7.25	98.73	109.60
1	G	495	TYR	N-CA-CB	7.23	120.98	110.06
2	H	1	GLU	CB-CG-CD	7.23	124.89	112.60
1	G	408	ARG	CA-CB-CG	7.19	128.47	114.10
1	D	495	TYR	CB-CA-C	-7.10	97.53	109.53
1	I	393	THR	OG1-CB-CG2	-7.10	95.10	109.30
1	D	369	TYR	CA-CB-CG	7.09	126.67	113.90
1	A	369	TYR	CA-CB-CG	7.09	126.66	113.90
1	I	376	THR	CB-CA-C	7.08	121.48	109.80
1	C	430	THR	CA-CB-OG1	-7.06	99.01	109.60
1	G	369	TYR	CA-CB-CG	7.05	126.59	113.90
2	F	46	GLU	CB-CG-CD	7.05	124.58	112.60
2	E	29	TYR	N-CA-CB	-7.04	102.47	110.35
2	J	3	GLN	N-CA-CB	-7.04	98.76	110.37
1	I	341	VAL	CB-CA-C	-7.04	103.02	111.81
1	G	341	VAL	CB-CA-C	-7.03	102.97	111.97
2	H	61	ASP	CA-CB-CG	7.03	119.63	112.60
2	H	89	ASP	CA-CB-CG	7.02	119.62	112.60
2	B	67	PHE	CA-CB-CG	6.99	120.79	113.80
1	D	355	ARG	CD-NE-CZ	6.98	134.17	124.40
1	D	444	LYS	CB-CA-C	6.96	122.29	109.70
1	I	462	LYS	CB-CG-CD	6.95	127.29	111.30
1	A	495	TYR	N-CA-CB	6.93	120.53	110.06
2	F	92	MET	CG-SD-CE	6.92	116.12	100.90
2	B	105	TYR	N-CA-CB	6.91	120.38	110.16
1	I	444	LYS	CB-CG-CD	6.88	127.12	111.30
1	G	365	TYR	CA-CB-CG	6.87	126.26	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	ASP	CA-CB-CG	6.84	119.44	112.60
1	D	505	TYR	CA-CB-CG	6.83	126.20	113.90
1	D	365	TYR	CA-CB-CG	6.83	126.19	113.90
1	G	448	ASN	CB-CA-C	6.82	120.49	110.26
2	F	29	TYR	CA-C-N	6.82	133.54	121.75
2	F	29	TYR	C-N-CA	6.82	133.54	121.75
1	G	495	TYR	CB-CA-C	-6.81	98.02	109.53
1	I	445	VAL	N-CA-CB	-6.79	100.03	111.23
1	D	341	VAL	CB-CA-C	-6.77	103.31	111.97
2	E	88	GLU	CB-CA-C	-6.76	99.18	110.68
1	C	495	TYR	CB-CA-C	-6.76	99.57	110.79
1	A	469	SER	CA-C-O	-6.76	114.53	120.88
1	D	448	ASN	CB-CA-C	6.75	120.39	110.26
1	C	369	TYR	N-CA-CB	6.75	119.76	109.98
1	C	471	GLU	CA-C-O	-6.74	113.08	120.36
2	B	88	GLU	CB-CA-C	-6.73	99.24	110.68
1	I	458	LYS	CG-CD-CE	6.70	126.71	111.30
1	I	505	TYR	CA-CB-CG	6.69	125.95	113.90
1	D	336	CYS	O-C-N	-6.69	117.13	121.88
1	A	408	ARG	CA-CB-CG	6.67	127.45	114.10
1	C	456	PHE	N-CA-C	6.62	124.90	110.80
2	B	88	GLU	N-CA-CB	6.62	119.99	110.06
1	A	334	ASN	CB-CA-C	6.62	122.67	110.10
2	J	27	TYR	N-CA-CB	-6.61	98.60	110.82
1	C	434	ILE	CB-CG1-CD1	6.60	127.67	113.80
1	C	484	GLU	CB-CG-CD	6.60	123.81	112.60
1	G	378	LYS	CA-CB-CG	6.59	127.28	114.10
1	A	341	VAL	CB-CA-C	-6.58	103.40	112.02
1	C	417	LYS	CB-CG-CD	6.58	126.42	111.30
1	I	462	LYS	CG-CD-CE	6.57	126.42	111.30
1	G	335	LEU	CB-CA-C	6.57	122.58	110.10
2	E	52	ARG	NH1-CZ-NH2	-6.54	110.79	119.30
2	F	110	ASP	CA-CB-CG	6.54	119.14	112.60
1	G	514	SER	CA-CB-OG	6.54	124.18	111.10
2	F	44	GLU	CB-CG-CD	6.53	123.70	112.60
2	F	89	ASP	CA-CB-CG	6.53	119.13	112.60
1	D	526	GLY	O-C-N	-6.50	115.27	121.77
1	A	495	TYR	CB-CA-C	-6.49	98.57	109.53
1	G	444	LYS	CB-CA-C	6.48	121.44	109.70
1	I	385	THR	CA-CB-CG2	6.47	121.50	110.50
1	C	351	TYR	CB-CA-C	-6.46	98.68	110.63
2	H	46	GLU	CA-CB-CG	6.46	127.01	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	462	LYS	CB-CG-CD	6.45	126.14	111.30
1	C	455	LEU	N-CA-CB	-6.44	99.61	110.49
1	D	351	TYR	CB-CA-C	-6.43	98.73	110.63
2	B	89	ASP	CA-CB-CG	6.43	119.03	112.60
2	E	88	GLU	CB-CG-CD	6.42	123.51	112.60
1	C	469	SER	CA-C-O	-6.40	114.86	120.88
2	B	61	ASP	CA-CB-CG	6.40	119.00	112.60
2	E	61	ASP	CB-CA-C	6.38	122.83	110.46
1	A	471	GLU	CA-C-O	-6.35	113.50	120.36
1	G	354	ASN	OD1-CG-ND2	6.34	128.94	122.60
2	E	92	MET	CG-SD-CE	6.34	114.84	100.90
2	H	106	LEU	CA-C-O	-6.33	111.45	120.51
1	D	466	ARG	CD-NE-CZ	6.33	133.26	124.40
2	J	13	GLN	CA-C-N	6.32	133.61	121.54
2	J	13	GLN	C-N-CA	6.32	133.61	121.54
2	F	64	LYS	CB-CG-CD	6.30	125.79	111.30
1	A	517	LEU	CB-CA-C	6.30	120.20	111.51
1	I	499	PRO	CA-C-N	6.29	129.56	120.38
1	I	499	PRO	C-N-CA	6.29	129.56	120.38
1	A	430	THR	CA-CB-OG1	-6.28	100.18	109.60
1	C	378	LYS	CD-CE-NZ	6.27	131.98	111.90
1	G	351	TYR	N-CA-CB	6.27	119.88	110.22
1	I	448	ASN	CB-CA-C	6.26	119.65	110.26
1	C	365	TYR	CA-CB-CG	6.24	125.14	113.90
1	I	458	LYS	CB-CG-CD	6.23	125.63	111.30
1	G	408	ARG	CG-CD-NE	-6.22	98.31	112.00
1	C	444	LYS	N-CA-CB	6.21	123.09	111.53
1	A	486	PHE	CA-CB-CG	6.21	120.01	113.80
1	I	380	TYR	CA-C-O	-6.21	111.64	120.51
1	I	448	ASN	CA-CB-CG	6.18	118.78	112.60
2	E	88	GLU	N-CA-CB	6.18	119.33	110.06
1	C	369	TYR	CA-CB-CG	6.17	125.00	113.90
2	J	61	ASP	CA-C-N	6.17	128.87	120.54
2	J	61	ASP	C-N-CA	6.17	128.87	120.54
2	J	13	GLN	CB-CG-CD	6.17	123.08	112.60
1	D	336	CYS	N-CA-C	6.17	119.24	108.82
2	F	30	CYS	N-CA-CB	-6.16	101.37	111.66
2	F	71	ARG	CB-CG-CD	6.16	125.47	111.30
2	J	60	THR	OG1-CB-CG2	6.15	121.59	109.30
1	I	376	THR	CA-CB-OG1	-6.14	100.39	109.60
1	D	462	LYS	CA-C-N	6.13	127.50	119.84
1	D	462	LYS	C-N-CA	6.13	127.50	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	471	GLU	N-CA-CB	6.13	120.97	110.68
2	J	45	ARG	CG-CD-NE	6.12	125.47	112.00
2	E	120	SER	N-CA-C	6.11	117.17	108.74
2	B	98	TRP	CB-CG-CD2	-6.11	118.25	126.80
1	G	346	ARG	NE-CZ-NH2	-6.10	113.71	119.20
1	D	369	TYR	N-CA-CB	6.09	118.81	109.98
1	I	403	ARG	CA-CB-CG	6.08	126.25	114.10
2	F	99	ALA	CA-C-O	6.07	128.18	121.56
2	E	96	LYS	CD-CE-NZ	6.07	131.33	111.90
1	C	406	GLU	CB-CG-CD	6.06	122.91	112.60
2	F	43	LYS	CB-CA-C	6.06	119.46	109.70
1	A	444	LYS	CG-CD-CE	6.06	125.23	111.30
2	B	29	TYR	N-CA-CB	-6.06	101.34	110.91
1	C	389	ASP	CA-CB-CG	6.05	118.65	112.60
1	C	521	PRO	N-CA-C	6.05	119.69	111.22
2	F	96	LYS	CD-CE-NZ	6.05	131.25	111.90
1	G	406	GLU	CB-CG-CD	6.04	122.86	112.60
1	G	417	LYS	CA-CB-CG	6.02	126.14	114.10
2	H	32	TYR	CA-CB-CG	6.00	124.71	113.90
1	I	369	TYR	CA-CB-CG	6.00	124.69	113.90
1	I	523	THR	N-CA-CB	5.99	120.62	110.49
1	C	415	THR	N-CA-CB	-5.99	101.27	111.69
1	I	406	GLU	CB-CG-CD	5.99	122.78	112.60
1	I	355	ARG	NH1-CZ-NH2	-5.97	111.54	119.30
1	G	356	LYS	CA-CB-CG	5.96	126.02	114.10
2	H	61	ASP	CA-C-O	-5.96	113.37	120.10
1	C	516	GLU	CB-CA-C	-5.95	96.35	109.56
1	I	337	PRO	N-CA-CB	-5.95	97.01	103.25
1	I	500	THR	CA-CB-CG2	5.95	120.61	110.50
1	G	369	TYR	N-CA-CB	5.93	118.58	109.98
1	A	428	ASP	CA-CB-CG	5.93	118.53	112.60
2	H	110	ASP	CA-CB-CG	5.93	118.53	112.60
2	B	105	TYR	N-CA-C	-5.93	104.90	111.36
1	D	491	PRO	N-CA-C	5.93	121.31	114.20
1	A	365	TYR	CA-CB-CG	5.90	124.52	113.90
2	J	110	ASP	CA-CB-CG	5.90	118.50	112.60
2	B	92	MET	CG-SD-CE	5.89	113.86	100.90
1	D	442	ASP	CA-CB-CG	5.89	118.49	112.60
1	A	415	THR	CA-CB-OG1	-5.89	100.77	109.60
1	C	483	VAL	N-CA-CB	5.88	119.29	111.64
1	G	514	SER	N-CA-CB	-5.88	101.33	110.57
1	G	376	THR	CA-CB-OG1	5.88	118.42	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	13	GLN	CB-CA-C	-5.87	101.03	109.84
1	G	355	ARG	NH1-CZ-NH2	-5.87	111.67	119.30
1	C	378	LYS	CA-CB-CG	5.86	125.83	114.10
1	A	471	GLU	N-CA-CB	5.85	120.51	110.68
2	B	28	THR	OG1-CB-CG2	5.85	121.00	109.30
2	B	45	ARG	CG-CD-NE	5.84	124.86	112.00
1	A	346	ARG	NE-CZ-NH1	5.84	127.34	121.50
2	B	96	LYS	CD-CE-NZ	5.83	130.55	111.90
1	I	455	LEU	N-CA-CB	-5.82	100.91	110.40
1	A	417	LYS	N-CA-CB	5.82	120.32	110.49
1	C	503	VAL	CA-C-N	5.80	126.38	120.00
1	C	503	VAL	C-N-CA	5.80	126.38	120.00
2	E	89	ASP	CA-CB-CG	5.80	118.40	112.60
1	C	474	GLN	N-CA-CB	5.79	118.98	110.35
1	A	417	LYS	CD-CE-NZ	5.79	130.44	111.90
1	G	376	THR	OG1-CB-CG2	-5.79	97.72	109.30
1	C	410	ILE	CA-C-O	5.79	128.01	120.78
2	J	13	GLN	CB-CA-C	5.79	121.54	109.68
1	D	400	PHE	N-CA-C	5.79	116.04	107.88
2	J	90	THR	CA-CB-OG1	-5.78	100.93	109.60
1	C	408	ARG	CB-CA-C	5.78	121.92	110.42
2	E	43	LYS	CB-CA-C	5.78	119.00	109.70
1	I	403	ARG	N-CA-CB	5.77	118.47	110.17
2	E	46	GLU	CG-CD-OE1	5.76	131.65	118.40
2	E	81	GLN	OE1-CD-NE2	-5.76	116.84	122.60
2	J	32	TYR	CA-CB-CG	5.75	124.26	113.90
1	I	525	CYS	CA-C-O	-5.75	113.83	121.47
1	A	355	ARG	NH1-CZ-NH2	-5.74	111.84	119.30
2	H	27	TYR	N-CA-CB	-5.74	100.46	111.53
2	F	97	SER	CA-C-O	-5.71	114.53	121.05
1	C	466	ARG	CD-NE-CZ	5.71	132.39	124.40
2	E	102	SER	N-CA-CB	5.71	120.13	110.49
1	C	340	GLU	CA-C-O	-5.71	114.37	120.42
2	B	28	THR	CA-CB-OG1	-5.70	101.05	109.60
2	F	71	ARG	CG-CD-NE	5.69	124.52	112.00
1	C	417	LYS	N-CA-CB	5.68	120.09	110.49
1	G	469	SER	CB-CA-C	-5.68	99.11	110.42
1	I	465	GLU	CB-CA-C	5.68	119.13	109.53
1	I	351	TYR	N-CA-CB	5.68	118.97	110.22
2	E	27	TYR	CB-CA-C	5.68	124.69	113.45
1	G	376	THR	CA-CB-CG2	5.67	120.15	110.50
1	G	467	ASP	O-C-N	5.67	130.19	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	97	SER	CA-C-O	-5.67	114.59	121.05
2	F	28	THR	OG1-CB-CG2	5.66	120.62	109.30
1	G	351	TYR	CB-CA-C	-5.65	100.17	110.63
2	B	97	SER	CA-C-O	-5.65	114.61	121.05
2	J	77	THR	CA-CB-OG1	-5.64	101.14	109.60
2	B	104	GLU	CB-CG-CD	-5.63	103.03	112.60
1	D	408	ARG	CD-NE-CZ	5.63	132.28	124.40
2	J	61	ASP	CB-CA-C	-5.63	101.11	110.68
1	C	356	LYS	CB-CG-CD	5.62	124.24	111.30
1	I	462	LYS	CB-CA-C	5.62	119.62	109.45
1	G	491	PRO	N-CA-C	5.60	120.92	114.20
1	I	351	TYR	CB-CA-C	-5.60	100.26	110.63
1	G	442	ASP	CA-CB-CG	5.60	118.20	112.60
1	D	351	TYR	N-CA-CB	5.59	118.83	110.22
1	D	335	LEU	CA-C-O	-5.59	112.51	120.51
1	I	384	PRO	N-CA-C	5.59	121.19	113.98
2	H	29	TYR	N-CA-CB	-5.59	104.09	110.35
2	J	96	LYS	CD-CE-NZ	5.59	129.78	111.90
1	C	451	TYR	N-CA-CB	5.58	119.72	110.63
2	H	1	GLU	CB-CA-C	5.58	120.69	110.10
1	A	364	ASP	CA-CB-CG	5.57	118.17	112.60
1	G	448	ASN	CA-CB-CG	5.57	118.17	112.60
1	A	439	ASN	CB-CG-ND2	5.56	124.74	116.40
1	G	481	ASN	CA-CB-CG	5.55	118.15	112.60
1	A	378	LYS	CA-CB-CG	5.54	125.18	114.10
1	D	406	GLU	CB-CG-CD	5.54	122.02	112.60
1	I	369	TYR	N-CA-C	-5.54	104.10	111.24
2	B	53	ARG	CB-CA-C	5.53	119.96	110.79
2	J	97	SER	CA-C-O	-5.53	114.75	121.05
1	G	335	LEU	O-C-N	-5.52	114.16	123.00
1	I	442	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	406	GLU	CB-CG-CD	5.51	121.97	112.60
1	G	471	GLU	CA-C-N	5.51	128.00	120.35
1	G	471	GLU	C-N-CA	5.51	128.00	120.35
1	D	337	PRO	N-CA-CB	-5.50	97.47	103.25
1	G	364	ASP	CA-CB-CG	5.50	118.10	112.60
1	G	517	LEU	CB-CA-C	5.49	121.34	110.42
1	G	428	ASP	CA-CB-CG	5.49	118.09	112.60
1	I	523	THR	CA-C-O	-5.48	112.67	120.51
1	I	478	THR	CA-CB-OG1	5.48	117.82	109.60
1	I	393	THR	CA-CB-OG1	5.47	117.81	109.60
1	C	357	ARG	CB-CG-CD	5.47	123.87	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	98	TRP	CB-CG-CD2	-5.45	119.17	126.80
1	G	345	THR	CA-C-O	-5.45	112.89	119.27
1	I	370	ASN	N-CA-C	5.43	119.45	113.21
2	B	43	LYS	CB-CA-C	5.42	118.43	109.70
2	J	71	ARG	CB-CG-CD	5.42	123.77	111.30
1	A	417	LYS	CB-CG-CD	5.41	123.75	111.30
2	F	72	ASP	CA-CB-CG	5.41	118.01	112.60
1	I	340	GLU	CA-C-O	-5.41	114.68	120.42
2	H	98	TRP	CB-CG-CD2	-5.41	119.22	126.80
2	E	2	VAL	N-CA-CB	5.41	120.15	111.23
1	D	448	ASN	CA-CB-CG	5.41	118.01	112.60
2	H	118	THR	CA-CB-OG1	5.39	117.69	109.60
1	A	499	PRO	CA-C-N	5.39	131.83	121.54
1	A	499	PRO	C-N-CA	5.39	131.83	121.54
2	F	44	GLU	CG-CD-OE1	-5.39	106.00	118.40
1	C	466	ARG	CA-CB-CG	5.37	124.84	114.10
2	H	27	TYR	CB-CA-C	5.37	122.65	111.97
2	J	54	ASP	CA-CB-CG	5.37	117.97	112.60
2	H	72	ASP	CA-CB-CG	5.36	117.96	112.60
2	H	79	TYR	CB-CA-C	5.36	119.00	109.72
2	J	39	GLN	N-CA-CB	-5.36	101.85	110.69
1	I	428	ASP	CA-CB-CG	5.35	117.95	112.60
2	F	77	THR	CA-CB-OG1	-5.35	101.58	109.60
1	C	390	LEU	CB-CG-CD1	5.35	126.74	110.70
1	A	334	ASN	CA-C-N	5.35	129.33	120.94
1	A	334	ASN	C-N-CA	5.35	129.33	120.94
1	A	345	THR	CA-CB-OG1	-5.34	101.59	109.60
1	D	486	PHE	CA-CB-CG	5.33	119.13	113.80
2	F	44	GLU	CB-CA-C	5.33	121.03	110.42
1	C	364	ASP	CA-CB-CG	5.33	117.93	112.60
1	G	465	GLU	CB-CA-C	5.32	118.53	109.53
1	I	457	ARG	CA-C-N	5.31	127.40	120.28
1	I	457	ARG	C-N-CA	5.31	127.40	120.28
2	E	61	ASP	CA-C-N	5.31	127.71	120.54
2	E	61	ASP	C-N-CA	5.31	127.71	120.54
1	D	423	TYR	N-CA-CB	-5.31	102.62	110.90
1	C	380	TYR	CA-CB-CG	5.30	123.44	113.90
2	E	97	SER	CA-C-O	-5.30	115.01	121.05
2	F	115	THR	OG1-CB-CG2	5.29	119.89	109.30
2	J	34	MET	CG-SD-CE	5.29	112.54	100.90
2	H	28	THR	O-C-N	5.29	129.60	123.41
2	F	61	ASP	CA-C-N	5.28	128.74	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	61	ASP	C-N-CA	5.28	128.74	120.82
1	A	351	TYR	CB-CA-C	-5.28	100.87	110.63
1	C	387	LEU	CA-C-O	-5.27	114.30	120.20
2	F	104	GLU	N-CA-CB	5.27	119.39	110.49
1	G	527	PRO	N-CA-C	5.27	125.27	112.10
1	G	362	VAL	N-CA-CB	5.26	117.31	110.99
2	H	108	GLN	N-CA-C	-5.26	103.74	110.53
1	A	356	LYS	CA-CB-CG	5.26	124.61	114.10
1	G	483	VAL	N-CA-CB	5.25	118.47	111.64
1	A	423	TYR	N-CA-CB	-5.25	102.22	110.77
2	F	47	PHE	CA-C-O	-5.24	114.78	120.81
1	C	517	LEU	CB-CA-C	5.24	119.66	111.70
1	A	351	TYR	N-CA-CB	5.24	118.28	110.22
1	G	469	SER	CA-C-O	-5.23	113.03	120.51
1	D	364	ASP	CA-CB-CG	5.23	117.83	112.60
2	B	38	ARG	N-CA-CB	-5.23	102.59	111.69
1	C	439	ASN	OD1-CG-ND2	-5.23	117.37	122.60
2	B	32	TYR	CA-CB-CG	5.22	123.30	113.90
1	G	408	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	G	471	GLU	CG-CD-OE1	5.20	130.37	118.40
2	J	47	PHE	CA-C-O	-5.20	114.83	120.81
2	F	118	THR	CA-CB-OG1	5.20	117.39	109.60
1	I	466	ARG	CA-CB-CG	5.19	124.48	114.10
1	G	455	LEU	N-CA-CB	-5.18	101.96	110.40
2	J	75	LYS	CB-CA-C	5.17	120.80	109.99
2	F	45	ARG	CG-CD-NE	5.17	123.37	112.00
2	F	98	TRP	CB-CG-CD2	-5.17	119.57	126.80
1	C	345	THR	CA-CB-CG2	5.16	119.27	110.50
1	C	382	VAL	CA-CB-CG1	5.16	119.17	110.40
1	A	417	LYS	CB-CA-C	-5.15	100.17	110.42
2	F	1	GLU	CB-CA-C	5.15	119.88	110.10
1	C	351	TYR	N-CA-CB	5.15	118.15	110.22
1	G	376	THR	CB-CA-C	5.15	118.29	109.80
2	J	64	LYS	CD-CE-NZ	5.14	128.36	111.90
2	E	90	THR	CA-CB-OG1	-5.14	101.90	109.60
1	C	522	ALA	CA-C-O	-5.13	115.54	121.19
1	C	422	ASN	O-C-N	5.13	129.42	122.59
1	I	340	GLU	CB-CA-C	5.13	119.58	110.85
2	F	44	GLU	CA-CB-CG	5.13	124.36	114.10
2	J	79	TYR	CB-CA-C	5.12	118.59	109.72
1	I	370	ASN	CB-CA-C	-5.12	101.65	110.72
1	I	421	TYR	O-C-N	-5.11	116.17	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	72	ASP	CA-CB-CG	5.11	117.71	112.60
2	B	76	ASN	OD1-CG-ND2	-5.10	117.50	122.60
1	D	504	GLY	CA-C-O	-5.10	115.25	120.66
1	G	422	ASN	O-C-N	5.09	129.37	122.59
1	C	405	ASP	CB-CA-C	5.09	120.05	110.63
2	J	41	PRO	CA-C-O	-5.09	115.92	121.27
1	D	463	PRO	CA-N-CD	-5.09	104.87	112.00
2	H	54	ASP	CA-CB-CG	5.09	117.69	112.60
1	C	344	ALA	CA-C-N	5.09	127.36	120.44
1	C	344	ALA	C-N-CA	5.09	127.36	120.44
1	C	357	ARG	CG-CD-NE	-5.08	100.82	112.00
1	C	516	GLU	N-CA-CB	-5.08	102.07	111.53
2	B	1	GLU	CB-CA-C	5.08	119.76	110.10
2	F	66	ARG	CD-NE-CZ	5.08	131.52	124.40
2	F	86	GLU	CB-CG-CD	5.08	121.24	112.60
1	C	442	ASP	CA-CB-CG	5.08	117.68	112.60
1	I	408	ARG	CD-NE-CZ	5.08	131.51	124.40
1	A	369	TYR	N-CA-CB	5.08	117.34	109.98
1	G	336	CYS	N-CA-C	5.08	121.03	109.81
1	I	451	TYR	N-CA-CB	5.07	118.90	110.63
2	E	98	TRP	CB-CG-CD2	-5.07	119.71	126.80
1	A	422	ASN	O-C-N	5.06	129.32	122.59
2	J	52	ARG	N-CA-CB	-5.06	102.72	110.42
1	D	370	ASN	CB-CA-C	5.06	118.18	111.14
1	I	340	GLU	CB-CG-CD	5.06	121.20	112.60
1	I	423	TYR	N-CA-CB	-5.06	102.25	110.59
1	A	424	LYS	CG-CD-CE	5.05	122.93	111.30
1	A	491	PRO	N-CA-C	5.05	120.26	114.20
2	H	90	THR	CA-CB-OG1	-5.05	102.03	109.60
1	I	350	VAL	N-CA-CB	5.05	118.99	110.56
1	G	521	PRO	CA-C-N	5.03	127.98	120.90
1	G	521	PRO	C-N-CA	5.03	127.98	120.90
1	A	483	VAL	N-CA-CB	5.02	118.16	111.64
2	B	30	CYS	CA-C-N	5.02	129.82	122.85
2	B	30	CYS	C-N-CA	5.02	129.82	122.85
2	F	1	GLU	CA-C-N	5.01	129.57	123.10
2	F	1	GLU	C-N-CA	5.01	129.57	123.10
1	A	400	PHE	N-CA-C	5.01	114.95	107.88
1	G	345	THR	N-CA-CB	5.01	118.26	110.44
1	I	400	PHE	N-CA-C	5.01	115.14	108.38
1	I	504	GLY	CA-C-O	-5.01	115.35	120.66
1	D	481	ASN	CA-CB-CG	5.01	117.61	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	72	ASP	CA-CB-CG	5.01	117.61	112.60
2	H	73	ASN	CB-CA-C	-5.01	99.76	110.32
1	A	343	ASN	CA-C-N	5.00	130.67	122.81
1	A	343	ASN	C-N-CA	5.00	130.67	122.81
1	I	451	TYR	CE1-CZ-OH	5.00	134.91	119.90
1	C	394	ASN	CB-CG-ND2	5.00	123.90	116.40
2	J	25	SER	CA-C-N	5.00	131.21	121.41
2	J	25	SER	C-N-CA	5.00	131.21	121.41

There are no chirality outliers.

All (132) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	348	ALA	Peptide
1	A	355	ARG	Peptide
1	A	356	LYS	Peptide
1	A	357	ARG	Sidechain
1	A	372	ALA	Peptide
1	A	466	ARG	Sidechain
1	A	470	THR	Peptide
1	A	525	CYS	Peptide
2	B	119	VAL	Peptide
2	B	2	VAL	Peptide
2	B	24	ALA	Peptide
2	B	40	ALA	Peptide
2	B	41	PRO	Peptide
2	B	52	ARG	Sidechain
2	B	57	THR	Peptide
1	C	343	ASN	Mainchain
1	C	346	ARG	Sidechain
1	C	348	ALA	Peptide
1	C	351	TYR	Sidechain
1	C	354	ASN	Sidechain
1	C	355	ARG	Peptide
1	C	356	LYS	Peptide
1	C	357	ARG	Sidechain
1	C	372	ALA	Peptide
1	C	385	THR	Peptide
1	C	390	LEU	Peptide
1	C	403	ARG	Sidechain
1	C	408	ARG	Sidechain
1	C	466	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	518	LEU	Mainchain,Peptide
1	C	520	ALA	Peptide
1	C	525	CYS	Peptide
1	D	346	ARG	Sidechain
1	D	355	ARG	Peptide
1	D	356	LYS	Peptide
1	D	372	ALA	Peptide
1	D	408	ARG	Sidechain
1	D	446	GLY	Peptide
1	D	466	ARG	Sidechain
1	D	476	GLY	Peptide
1	D	525	CYS	Peptide
2	E	101	SER	Peptide
2	E	103	GLY	Peptide
2	E	106	LEU	Mainchain
2	E	109	GLY	Mainchain
2	E	2	VAL	Peptide
2	E	24	ALA	Peptide
2	E	25	SER	Peptide
2	E	26	GLY	Peptide
2	E	29	TYR	Peptide
2	E	30	CYS	Peptide
2	E	40	ALA	Peptide
2	E	41	PRO	Peptide
2	E	52	ARG	Sidechain
2	E	53	ARG	Sidechain
2	E	57	THR	Peptide
2	E	81	GLN	Sidechain
2	F	19	ARG	Sidechain
2	F	27	TYR	Peptide
2	F	29	TYR	Mainchain,Peptide
2	F	30	CYS	Peptide
2	F	40	ALA	Peptide
2	F	41	PRO	Peptide
2	F	52	ARG	Sidechain
2	F	53	ARG	Sidechain
2	F	57	THR	Peptide
2	F	71	ARG	Sidechain
1	G	335	LEU	Peptide
1	G	346	ARG	Sidechain
1	G	348	ALA	Peptide
1	G	356	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	G	357	ARG	Sidechain
1	G	372	ALA	Peptide
1	G	408	ARG	Sidechain
1	G	446	GLY	Peptide
1	G	466	ARG	Sidechain
1	G	496	GLY	Mainchain
1	G	525	CYS	Peptide
2	H	101	SER	Peptide
2	H	102	SER	Peptide
2	H	106	LEU	Mainchain
2	H	19	ARG	Sidechain
2	H	2	VAL	Peptide
2	H	24	ALA	Peptide
2	H	28	THR	Mainchain,Peptide
2	H	29	TYR	Peptide
2	H	30	CYS	Peptide
2	H	40	ALA	Peptide
2	H	41	PRO	Peptide
2	H	45	ARG	Sidechain
2	H	52	ARG	Sidechain
2	H	53	ARG	Sidechain
2	H	57	THR	Peptide
2	H	99	ALA	Peptide
1	I	346	ARG	Sidechain
1	I	355	ARG	Peptide,Sidechain
1	I	356	LYS	Peptide
1	I	372	ALA	Peptide
1	I	381	GLY	Peptide
1	I	385	THR	Peptide
1	I	388	ASN	Peptide
1	I	449	TYR	Peptide
1	I	466	ARG	Sidechain
1	I	469	SER	Peptide
1	I	471	GLU	Peptide
1	I	476	GLY	Peptide
1	I	516	GLU	Peptide
1	I	518	LEU	Peptide
1	I	521	PRO	Peptide
1	I	522	ALA	Peptide
1	I	525	CYS	Peptide
1	I	526	GLY	Peptide
2	J	101	SER	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
2	J	11	SER	Peptide
2	J	17	SER	Peptide
2	J	19	ARG	Sidechain
2	J	24	ALA	Peptide
2	J	25	SER	Peptide
2	J	26	GLY	Peptide
2	J	30	CYS	Peptide
2	J	38	ARG	Sidechain
2	J	40	ALA	Peptide
2	J	41	PRO	Peptide
2	J	53	ARG	Sidechain
2	J	57	THR	Peptide
2	J	71	ARG	Sidechain
2	J	73	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	1528	0	1443	12	0
1	C	1530	0	1444	11	0
1	D	1540	0	1460	11	0
1	G	1520	0	1437	16	0
1	I	1531	0	1446	26	0
2	B	931	0	864	5	0
2	E	931	0	864	3	0
2	F	931	0	864	5	0
2	H	925	0	859	6	0
2	J	919	0	854	6	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
4	A	14	0	13	0	0
4	D	14	0	13	0	0
All	All	12398	0	11636	94	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 4.

All (94) 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:I:361:CYS:SG	1:I:362:VAL:N	2.45	0.90
1:I:382:VAL:HG11	1:I:387:LEU:HD23	1.61	0.81
1:C:380:TYR:CE2	1:C:412:PRO:HD2	2.25	0.71
1:A:380:TYR:CE2	1:A:412:PRO:HD2	2.24	0.71
1:I:401:VAL:HG11	1:I:451:TYR:CD2	2.27	0.70
1:G:380:TYR:CE2	1:G:412:PRO:HD2	2.27	0.70
1:C:350:VAL:HG23	1:C:400:PHE:CD2	2.29	0.68
2:H:101:SER:HB2	2:H:106:LEU:HA	1.79	0.65
1:G:350:VAL:HG23	1:G:400:PHE:CD2	2.33	0.64
1:G:392:PHE:HA	1:G:517:LEU:HD13	1.83	0.61
1:I:387:LEU:O	1:I:388:ASN:HB2	2.02	0.59
1:A:346:ARG:HH22	1:A:450:ASN:HB3	1.70	0.56
1:C:382:VAL:CG1	1:C:387:LEU:HD23	2.36	0.55
1:G:342:PHE:CE1	1:G:511:VAL:HG21	2.42	0.55
1:A:468:ILE:HG22	1:A:468:ILE:O	2.07	0.54
2:J:87:PRO:HA	2:J:119:VAL:HB	1.90	0.53
1:G:520:ALA:HB1	1:G:521:PRO:HD2	1.91	0.53
1:A:350:VAL:HG23	1:A:400:PHE:CD1	2.44	0.53
1:A:342:PHE:CE1	1:A:511:VAL:HG21	2.44	0.52
2:J:30:CYS:SG	2:J:101:SER:O	2.67	0.52
1:A:492:LEU:HD12	2:B:98:TRP:CZ3	2.45	0.52
1:I:362:VAL:O	1:I:525:CYS:O	2.28	0.52
1:D:402:ILE:HD13	1:D:410:ILE:HD11	1.91	0.52
1:G:342:PHE:CZ	1:G:511:VAL:HG11	2.45	0.51
2:F:34:MET:HE2	2:F:78:LEU:CD2	2.42	0.50
1:G:354:ASN:HA	2:H:106:LEU:HD12	1.93	0.50
1:I:477:SER:O	1:I:478:THR:HG23	2.11	0.50
2:F:31:SER:CB	2:F:53:ARG:HD2	2.42	0.50
2:H:101:SER:HB2	2:H:106:LEU:HD23	1.94	0.50
1:G:434:ILE:N	1:G:434:ILE:HD12	2.27	0.49
1:I:492:LEU:HD12	2:J:98:TRP:CZ3	2.48	0.49
2:B:27:TYR:O	2:B:28:THR:OG1	2.27	0.48
2:E:53:ARG:NH2	1:D:374:PHE:O	2.45	0.48
1:D:434:ILE:HD12	1:D:434:ILE:N	2.29	0.48
1:D:476:GLY:HA3	1:D:478:THR:HG22	1.95	0.48
1:G:483:VAL:HA	2:H:59:TYR:O	2.13	0.48
1:A:441:LEU:HD12	1:A:509:ARG:NH2	2.29	0.48
1:I:426:PRO:HD3	1:I:464:PHE:CE1	2.49	0.47
1:I:364:ASP:HA	1:I:388:ASN:OD1	2.13	0.47
1:I:434:ILE:HD12	1:I:434:ILE:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:52:ARG:O	2:F:71:ARG:NH2	2.47	0.47
1:I:387:LEU:O	1:I:388:ASN:CB	2.63	0.47
2:E:96:LYS:HE2	2:E:97:SER:O	2.15	0.47
1:A:434:ILE:HD12	1:A:434:ILE:N	2.30	0.47
1:G:380:TYR:CE2	1:G:412:PRO:CD	2.96	0.47
2:B:87:PRO:HA	2:B:119:VAL:HB	1.96	0.47
1:G:468:ILE:HG22	1:G:468:ILE:O	2.14	0.46
1:I:444:LYS:HA	1:I:444:LYS:CE	2.45	0.46
1:I:382:VAL:CG1	1:I:387:LEU:HD23	2.40	0.46
1:D:350:VAL:HG23	1:D:400:PHE:CD1	2.51	0.46
1:D:520:ALA:HB1	1:D:521:PRO:CD	2.46	0.46
2:B:96:LYS:HE2	2:B:97:SER:O	2.16	0.46
1:I:335:LEU:HA	1:I:362:VAL:HG22	1.97	0.46
2:H:87:PRO:HA	2:H:119:VAL:HB	1.98	0.45
1:D:475:ALA:HB3	1:D:487:ASN:HA	1.98	0.45
1:I:410:ILE:HG22	1:I:433:VAL:HG11	1.99	0.45
1:I:461:LEU:HD22	1:I:465:GLU:HG2	1.98	0.45
1:I:520:ALA:HB1	1:I:521:PRO:CD	2.47	0.45
1:D:369:TYR:CE2	1:D:384:PRO:O	2.70	0.45
1:C:377:PHE:CE2	1:C:434:ILE:HD11	2.52	0.45
1:D:461:LEU:HD22	1:D:465:GLU:HG2	1.98	0.44
2:F:87:PRO:HA	2:F:119:VAL:HB	1.99	0.44
1:G:468:ILE:O	1:G:468:ILE:CG2	2.66	0.44
1:G:369:TYR:CE2	1:G:384:PRO:O	2.71	0.44
1:D:335:LEU:O	1:D:361:CYS:HB2	2.18	0.44
1:A:520:ALA:HB1	1:A:521:PRO:CD	2.48	0.43
2:E:87:PRO:HA	2:E:119:VAL:HB	2.01	0.43
1:G:365:TYR:CD1	1:G:387:LEU:HD13	2.54	0.43
1:I:355:ARG:NH2	1:I:464:PHE:CD2	2.87	0.43
1:C:369:TYR:CE2	1:C:384:PRO:O	2.72	0.43
1:I:474:GLN:O	1:I:474:GLN:HG3	2.19	0.43
1:I:484:GLU:O	2:J:61:ASP:HB2	2.18	0.42
2:B:108:GLN:OE1	2:B:108:GLN:HA	2.18	0.42
1:I:352:ALA:O	2:J:108:GLN:NE2	2.52	0.42
1:C:350:VAL:HG23	1:C:400:PHE:CE2	2.54	0.42
1:C:425:LEU:HD21	1:C:512:VAL:HG11	2.02	0.42
1:I:410:ILE:HG22	1:I:433:VAL:CG1	2.49	0.42
1:I:444:LYS:HE2	1:I:445:VAL:HG22	2.02	0.42
1:A:369:TYR:CE2	1:A:384:PRO:O	2.73	0.42
1:A:380:TYR:CE2	1:A:412:PRO:CD	3.00	0.42
1:I:477:SER:C	1:I:478:THR:HG23	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:VAL:HG13	1:C:387:LEU:HD23	2.02	0.42
2:F:34:MET:HE2	2:F:78:LEU:HD23	2.02	0.42
1:C:375:SER:OG	1:C:376:THR:N	2.53	0.41
2:J:96:LYS:HE2	2:J:97:SER:O	2.20	0.41
1:D:351:TYR:O	1:D:466:ARG:HG3	2.20	0.41
1:A:357:ARG:HG3	1:A:396:TYR:CE1	2.55	0.41
1:C:410:ILE:HD11	1:C:418:ILE:HG21	2.03	0.41
1:I:402:ILE:HD11	1:I:407:VAL:HG12	2.03	0.41
1:G:520:ALA:HB1	1:G:521:PRO:CD	2.50	0.40
1:C:410:ILE:HG22	1:C:433:VAL:HG11	2.04	0.40
1:I:425:LEU:HD21	1:I:512:VAL:HG11	2.02	0.40
1:G:425:LEU:HD21	1:G:512:VAL:HG11	2.04	0.40
2:H:101:SER:CB	2:H:106:LEU:HA	2.49	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	192/221 (87%)	160 (83%)	29 (15%)	3 (2%)	7	35
1	C	192/221 (87%)	163 (85%)	24 (12%)	5 (3%)	4	28
1	D	193/221 (87%)	162 (84%)	25 (13%)	6 (3%)	3	26
1	G	191/221 (86%)	161 (84%)	25 (13%)	5 (3%)	4	28
1	I	192/221 (87%)	153 (80%)	29 (15%)	10 (5%)	1	17
2	B	119/146 (82%)	107 (90%)	8 (7%)	4 (3%)	3	25
2	E	119/146 (82%)	105 (88%)	9 (8%)	5 (4%)	2	20
2	F	119/146 (82%)	102 (86%)	11 (9%)	6 (5%)	1	17
2	H	118/146 (81%)	105 (89%)	9 (8%)	4 (3%)	3	25
2	J	117/146 (80%)	104 (89%)	8 (7%)	5 (4%)	2	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1552/1835 (85%)	1322 (85%)	177 (11%)	53 (3%)	3	25

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	445	VAL
1	C	456	PHE
2	E	40	ALA
1	A	445	VAL
2	B	40	ALA
2	F	31	SER
2	F	32	TYR
2	F	40	ALA
1	G	445	VAL
2	H	40	ALA
1	I	445	VAL
2	J	14	ALA
2	J	26	GLY
2	J	40	ALA
2	J	102	SER
1	D	445	VAL
1	D	463	PRO
1	C	375	SER
2	E	102	SER
1	A	375	SER
2	F	104	GLU
1	G	375	SER
1	G	417	LYS
2	H	106	LEU
2	H	107	TYR
1	I	363	ALA
1	I	375	SER
1	I	388	ASN
1	I	417	LYS
1	I	470	THR
1	I	523	THR
1	D	375	SER
1	D	417	LYS
2	E	2	VAL
2	E	91	ALA
2	B	91	ALA
2	F	91	ALA

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Mol	Chain	Res	Type
2	F	102	SER
2	H	91	ALA
2	J	91	ALA
1	D	408	ARG
1	C	337	PRO
1	C	455	LEU
2	E	30	CYS
1	A	337	PRO
2	B	104	GLU
1	I	478	THR
1	D	337	PRO
2	B	106	LEU
1	G	408	ARG
1	I	475	ALA
1	G	337	PRO
1	I	471	GLU

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	165/193 (86%)	141 (86%)	24 (14%)	3	17
1	C	165/193 (86%)	140 (85%)	25 (15%)	3	16
1	D	167/193 (86%)	138 (83%)	29 (17%)	2	12
1	G	164/193 (85%)	140 (85%)	24 (15%)	3	17
1	I	166/193 (86%)	144 (87%)	22 (13%)	4	20
2	B	98/117 (84%)	84 (86%)	14 (14%)	3	18
2	E	98/117 (84%)	82 (84%)	16 (16%)	2	14
2	F	98/117 (84%)	84 (86%)	14 (14%)	3	18
2	H	97/117 (83%)	85 (88%)	12 (12%)	4	22
2	J	96/117 (82%)	81 (84%)	15 (16%)	2	15
All	All	1314/1550 (85%)	1119 (85%)	195 (15%)	3	17

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	337	PRO
1	C	341	VAL
1	C	346	ARG
1	C	347	PHE
1	C	349	SER
1	C	351	TYR
1	C	354	ASN
1	C	359	SER
1	C	375	SER
1	C	380	TYR
1	C	385	THR
1	C	389	ASP
1	C	399	SER
1	C	402	ILE
1	C	403	ARG
1	C	410	ILE
1	C	417	LYS
1	C	434	ILE
1	C	441	LEU
1	C	445	VAL
1	C	484	GLU
1	C	494	SER
1	C	513	LEU
1	C	514	SER
1	C	524	VAL
2	E	1	GLU
2	E	5	VAL
2	E	7	SER
2	E	18	LEU
2	E	27	TYR
2	E	30	CYS
2	E	33	ASP
2	E	44	GLU
2	E	53	ARG
2	E	54	ASP
2	E	61	ASP
2	E	86	GLU
2	E	106	LEU
2	E	108	GLN
2	E	118	THR
2	E	119	VAL
1	A	337	PRO

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Mol	Chain	Res	Type
1	A	341	VAL
1	A	346	ARG
1	A	347	PHE
1	A	351	TYR
1	A	354	ASN
1	A	368	LEU
1	A	380	TYR
1	A	385	THR
1	A	389	ASP
1	A	399	SER
1	A	402	ILE
1	A	408	ARG
1	A	417	LYS
1	A	441	LEU
1	A	444	LYS
1	A	445	VAL
1	A	450	ASN
1	A	462	LYS
1	A	468	ILE
1	A	484	GLU
1	A	494	SER
1	A	514	SER
1	A	516	GLU
2	B	7	SER
2	B	18	LEU
2	B	32	TYR
2	B	33	ASP
2	B	53	ARG
2	B	54	ASP
2	B	64	LYS
2	B	71	ARG
2	B	86	GLU
2	B	106	LEU
2	B	108	GLN
2	B	113	GLN
2	B	118	THR
2	B	119	VAL
2	F	13	GLN
2	F	18	LEU
2	F	27	TYR
2	F	29	TYR
2	F	30	CYS

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Mol	Chain	Res	Type
2	F	33	ASP
2	F	44	GLU
2	F	53	ARG
2	F	54	ASP
2	F	71	ARG
2	F	96	LYS
2	F	106	LEU
2	F	118	THR
2	F	119	VAL
1	G	335	LEU
1	G	337	PRO
1	G	341	VAL
1	G	345	THR
1	G	347	PHE
1	G	351	TYR
1	G	354	ASN
1	G	370	ASN
1	G	376	THR
1	G	380	TYR
1	G	385	THR
1	G	389	ASP
1	G	399	SER
1	G	402	ILE
1	G	417	LYS
1	G	434	ILE
1	G	445	VAL
1	G	448	ASN
1	G	450	ASN
1	G	481	ASN
1	G	484	GLU
1	G	494	SER
1	G	516	GLU
1	G	527	PRO
2	H	30	CYS
2	H	33	ASP
2	H	44	GLU
2	H	45	ARG
2	H	53	ARG
2	H	54	ASP
2	H	71	ARG
2	H	86	GLU
2	H	96	LYS

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Mol	Chain	Res	Type
2	H	106	LEU
2	H	118	THR
2	H	119	VAL
1	I	337	PRO
1	I	338	PHE
1	I	341	VAL
1	I	347	PHE
1	I	350	VAL
1	I	351	TYR
1	I	354	ASN
1	I	367	VAL
1	I	389	ASP
1	I	399	SER
1	I	402	ILE
1	I	444	LYS
1	I	448	ASN
1	I	450	ASN
1	I	458	LYS
1	I	462	LYS
1	I	472	ILE
1	I	478	THR
1	I	505	TYR
1	I	516	GLU
1	I	518	LEU
1	I	523	THR
2	J	3	GLN
2	J	5	VAL
2	J	18	LEU
2	J	21	SER
2	J	30	CYS
2	J	33	ASP
2	J	54	ASP
2	J	60	THR
2	J	64	LYS
2	J	73	ASN
2	J	86	GLU
2	J	89	ASP
2	J	96	LYS
2	J	108	GLN
2	J	118	THR
1	D	334	ASN
1	D	336	CYS

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Mol	Chain	Res	Type
1	D	337	PRO
1	D	341	VAL
1	D	345	THR
1	D	347	PHE
1	D	351	TYR
1	D	354	ASN
1	D	358	ILE
1	D	373	SER
1	D	378	LYS
1	D	380	TYR
1	D	385	THR
1	D	386	LYS
1	D	389	ASP
1	D	399	SER
1	D	402	ILE
1	D	417	LYS
1	D	445	VAL
1	D	448	ASN
1	D	450	ASN
1	D	463	PRO
1	D	465	GLU
1	D	472	ILE
1	D	484	GLU
1	D	500	THR
1	D	514	SER
1	D	516	GLU
1	D	528	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	437	ASN
1	C	474	GLN
1	C	506	GLN
1	A	437	ASN
1	A	506	GLN
1	G	414	GLN
1	G	437	ASN
1	G	439	ASN
1	G	481	ASN
1	G	498	GLN
1	G	506	GLN

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Mol	Chain	Res	Type
2	H	73	ASN
2	H	76	ASN
1	I	394	ASN
1	I	437	ASN
1	I	439	ASN
1	I	481	ASN
1	I	498	GLN
1	I	506	GLN
2	J	76	ASN
2	J	108	GLN
1	D	370	ASN
1	D	437	ASN
1	D	439	ASN
1	D	498	GLN
1	D	506	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 ⓘ

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	K	1	3	14,14,15	2.48	4 (28%)	17,19,21	4.33	6 (35%)
3	NAG	K	2	3	14,14,15	2.33	4 (28%)	17,19,21	4.49	10 (58%)
3	NAG	L	1	1,3	14,14,15	1.86	2 (14%)	17,19,21	3.75	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	L	2	3	14,14,15	1.33	2 (14%)	17,19,21	2.06	5 (29%)
3	NAG	M	1	1,3	14,14,15	0.76	0	17,19,21	2.75	10 (58%)
3	NAG	M	2	3	14,14,15	0.82	0	17,19,21	2.02	2 (11%)

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	K	1	3	-	3/6/23/26	0/1/1/1
3	NAG	K	2	3	-	5/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	L	2	3	-	6/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	6/6/23/26	0/1/1/1
3	NAG	M	2	3	-	1/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	2	NAG	C1-C2	7.57	1.62	1.52
3	K	1	NAG	O4-C4	7.33	1.61	1.43
3	L	1	NAG	O4-C4	4.90	1.55	1.43
3	L	2	NAG	C1-C2	3.98	1.57	1.52
3	K	1	NAG	O5-C5	2.49	1.48	1.43
3	K	1	NAG	C1-C2	2.33	1.55	1.52
3	K	2	NAG	C2-N2	2.31	1.50	1.46
3	K	2	NAG	C3-C2	2.23	1.57	1.52
3	K	1	NAG	C3-C2	2.19	1.57	1.52
3	L	1	NAG	C2-N2	2.06	1.49	1.46
3	L	2	NAG	C3-C2	2.04	1.56	1.52
3	K	2	NAG	C7-N2	2.03	1.40	1.34

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	1	NAG	C1-O5-C5	12.62	129.10	112.19
3	K	2	NAG	C1-C2-N2	12.53	130.19	110.43
3	L	1	NAG	C2-N2-C7	9.51	135.65	122.90
3	L	1	NAG	C1-O5-C5	8.53	123.61	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	1	NAG	C2-N2-C7	8.52	134.31	122.90
3	K	2	NAG	C2-N2-C7	7.05	132.35	122.90
3	K	2	NAG	C1-O5-C5	6.93	121.47	112.19
3	M	2	NAG	C2-N2-C7	6.02	130.97	122.90
3	K	1	NAG	C4-C3-C2	5.71	119.38	111.02
3	K	2	NAG	O3-C3-C2	5.56	120.95	109.40
3	M	1	NAG	C1-O5-C5	5.54	119.61	112.19
3	M	1	NAG	C1-C2-N2	4.84	118.06	110.43
3	L	1	NAG	C4-C3-C2	4.70	117.91	111.02
3	K	1	NAG	O4-C4-C3	4.25	120.39	110.38
3	L	2	NAG	C2-N2-C7	4.12	128.43	122.90
3	K	1	NAG	O3-C3-C2	-3.88	101.34	109.40
3	M	1	NAG	O5-C1-C2	-3.86	105.31	111.29
3	L	1	NAG	C1-C2-N2	3.83	116.47	110.43
3	K	2	NAG	O5-C1-C2	-3.72	105.53	111.29
3	L	1	NAG	O3-C3-C2	-3.65	101.82	109.40
3	L	2	NAG	O5-C1-C2	-3.48	105.91	111.29
3	L	2	NAG	O3-C3-C2	3.37	116.41	109.40
3	K	1	NAG	O5-C5-C4	3.36	119.00	110.83
3	L	2	NAG	C1-C2-N2	3.34	115.69	110.43
3	M	2	NAG	O3-C3-C2	3.34	116.33	109.40
3	M	1	NAG	C2-N2-C7	-3.10	118.75	122.90
3	K	2	NAG	O5-C5-C6	-3.03	101.77	107.66
3	M	1	NAG	O3-C3-C2	-2.99	103.19	109.40
3	K	2	NAG	O7-C7-C8	-2.86	116.97	122.05
3	L	1	NAG	O5-C5-C4	2.85	117.77	110.83
3	M	1	NAG	O7-C7-C8	2.77	126.99	122.05
3	L	2	NAG	C1-O5-C5	2.68	115.77	112.19
3	M	1	NAG	C3-C4-C5	2.67	115.08	110.23
3	K	2	NAG	C6-C5-C4	2.49	119.14	113.02
3	K	2	NAG	C8-C7-N2	2.49	120.25	116.12
3	M	1	NAG	O6-C6-C5	2.45	119.67	111.33
3	M	1	NAG	O3-C3-C4	2.42	116.09	110.38
3	M	1	NAG	O5-C5-C6	-2.42	102.96	107.66
3	L	1	NAG	O4-C4-C3	2.08	115.28	110.38
3	K	2	NAG	O4-C4-C5	2.06	114.40	109.32

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	1	NAG	C8-C7-N2-C2

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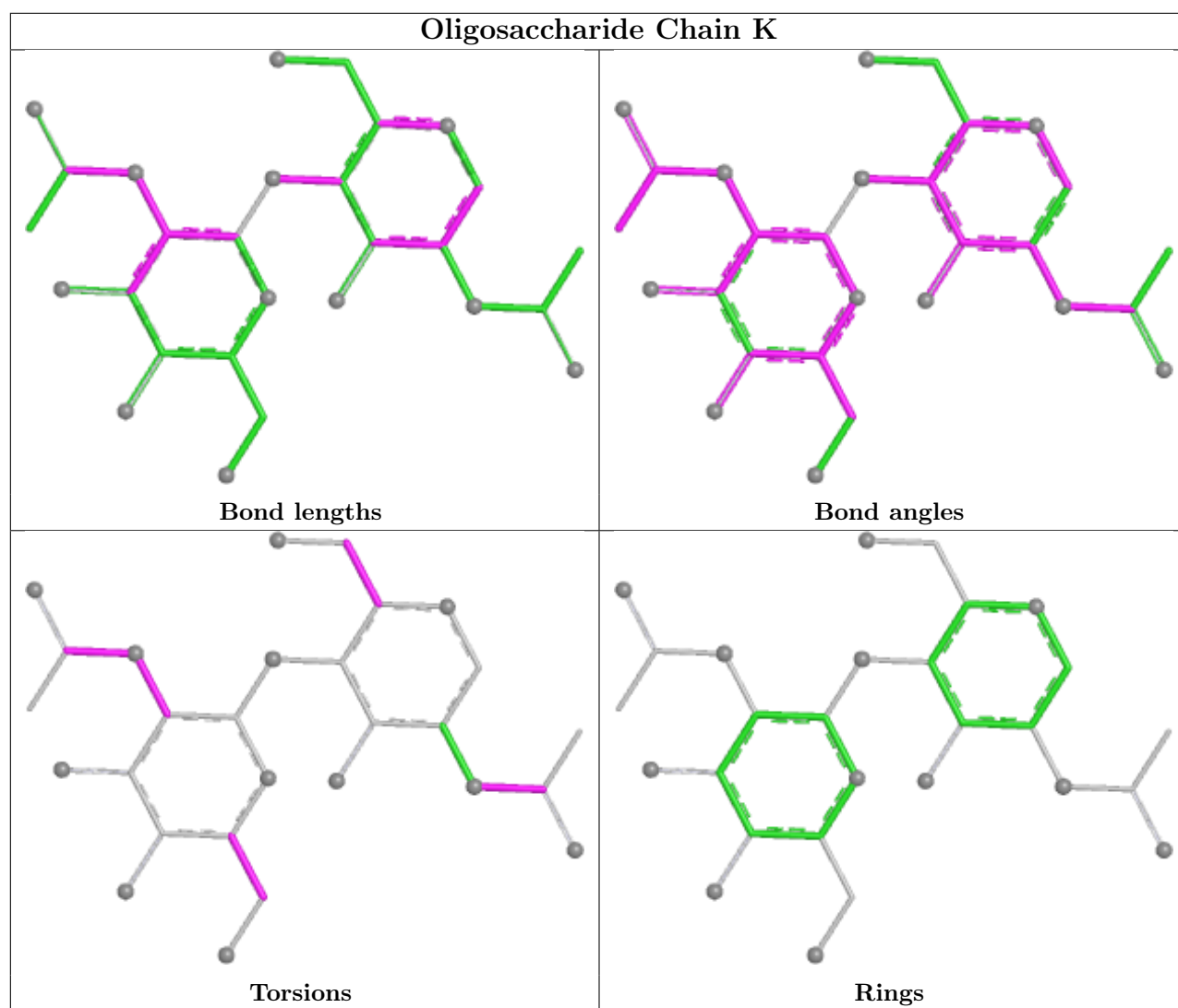
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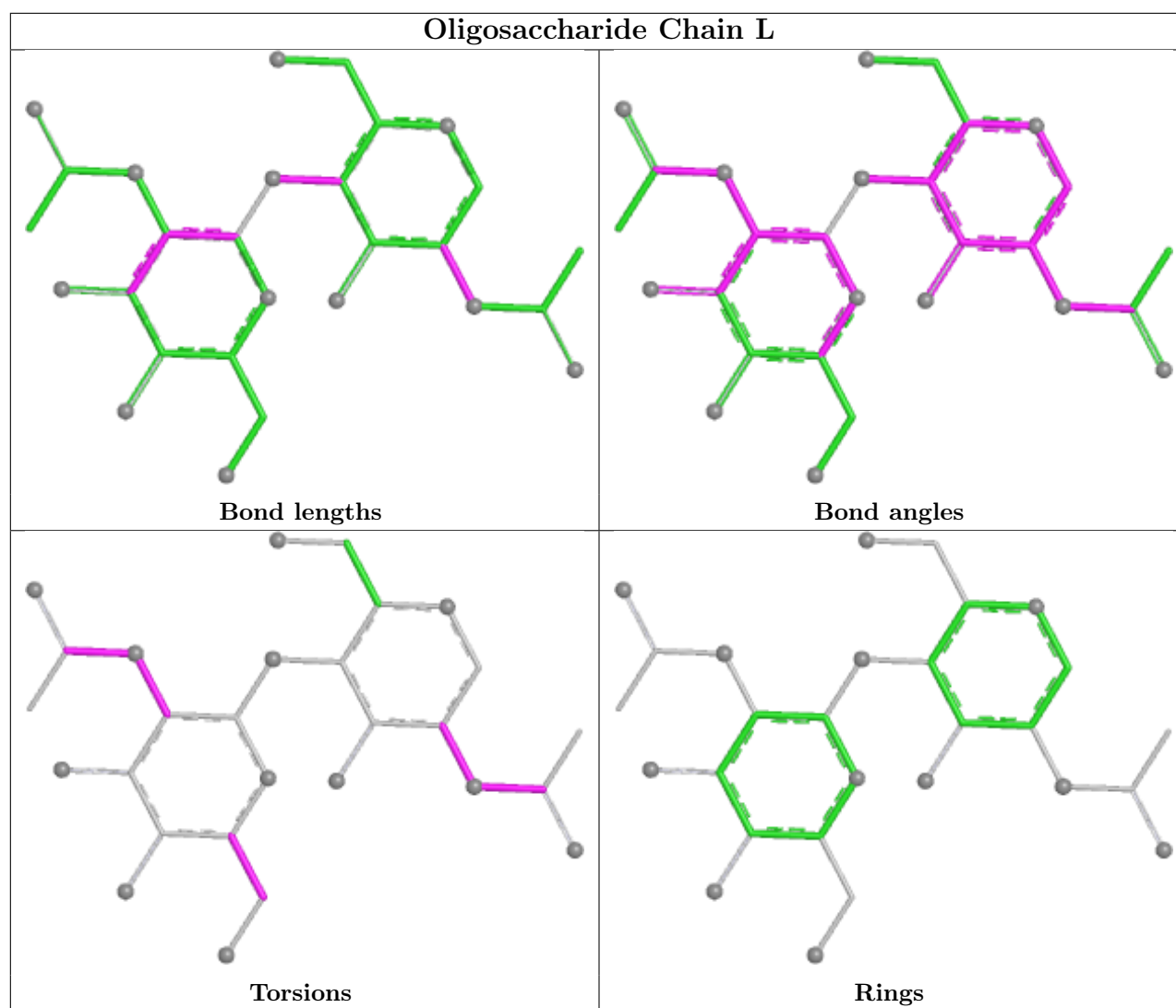
Mol	Chain	Res	Type	Atoms
3	K	1	NAG	O7-C7-N2-C2
3	K	2	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
3	L	1	NAG	C1-C2-N2-C7
3	L	1	NAG	C8-C7-N2-C2
3	L	1	NAG	O7-C7-N2-C2
3	M	1	NAG	C1-C2-N2-C7
3	M	1	NAG	C8-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2
3	M	1	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	L	2	NAG	C8-C7-N2-C2
3	L	2	NAG	C4-C5-C6-O6
3	L	2	NAG	O7-C7-N2-C2
3	L	2	NAG	C1-C2-N2-C7
3	M	2	NAG	C4-C5-C6-O6
3	L	2	NAG	C3-C2-N2-C7
3	K	2	NAG	C4-C5-C6-O6
3	K	2	NAG	C3-C2-N2-C7
3	M	1	NAG	C3-C2-N2-C7
3	K	1	NAG	C4-C5-C6-O6

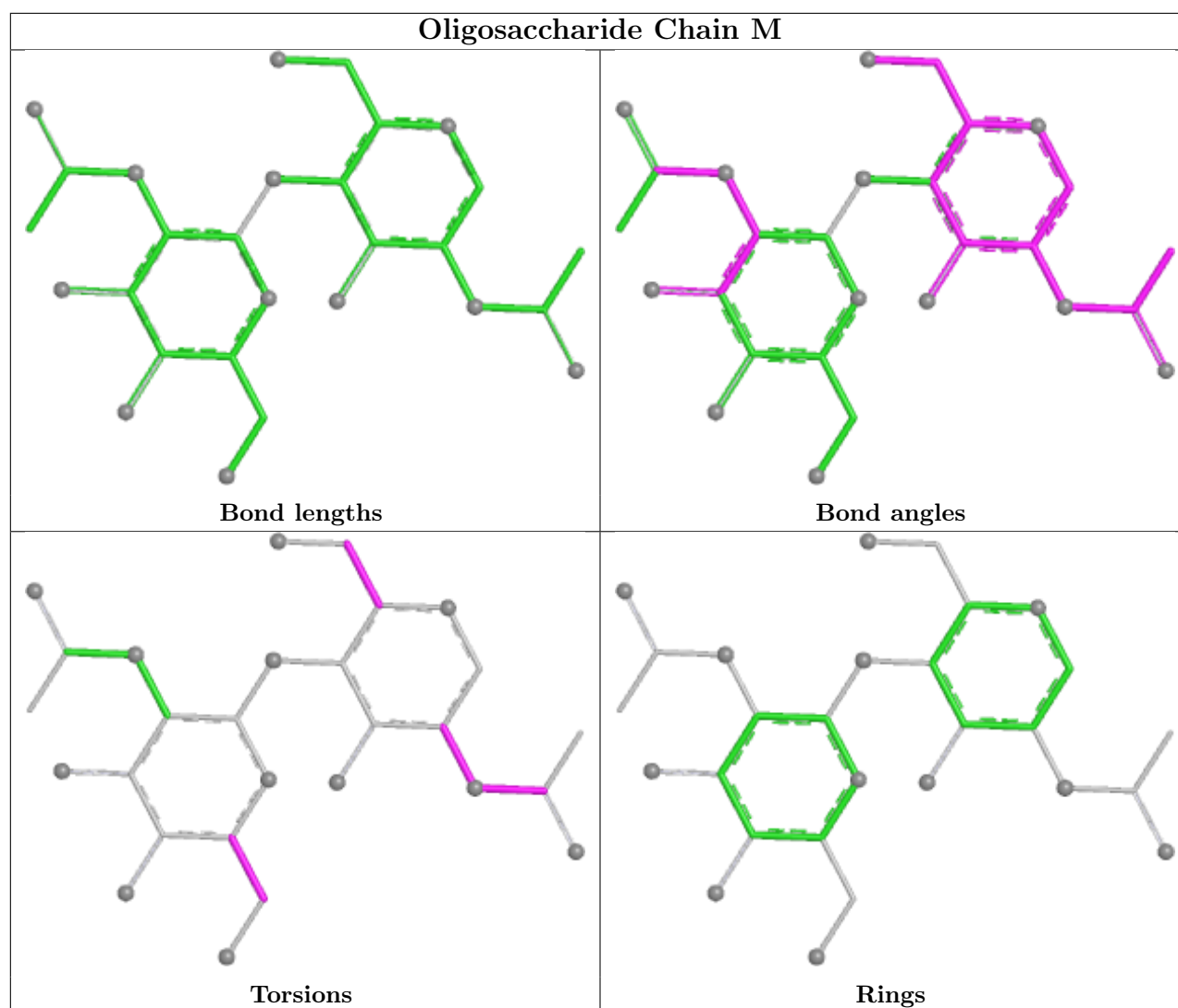
There are no ring outliers.

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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	601	-	14,14,15	1.82	3 (21%)	17,19,21	2.67	7 (41%)
4	NAG	D	601	1	14,14,15	1.29	2 (14%)	17,19,21	2.89	6 (35%)

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	601	-	-	4/6/23/26	0/1/1/1
4	NAG	D	601	1	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	NAG	C1-C2	4.40	1.58	1.52
4	A	601	NAG	O5-C5	2.91	1.49	1.43
4	A	601	NAG	C3-C2	2.73	1.58	1.52
4	D	601	NAG	C3-C2	2.32	1.57	1.52
4	D	601	NAG	C1-C2	2.15	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	601	NAG	C1-O5-C5	7.03	121.60	112.19
4	A	601	NAG	C1-O5-C5	6.57	120.99	112.19
4	A	601	NAG	O3-C3-C2	6.56	123.02	109.40
4	D	601	NAG	C2-N2-C7	6.02	130.97	122.90
4	D	601	NAG	C4-C3-C2	3.96	116.83	111.02
4	D	601	NAG	C1-C2-N2	-3.64	104.69	110.43
4	D	601	NAG	O4-C4-C5	2.92	116.52	109.32
4	D	601	NAG	O3-C3-C4	-2.48	104.54	110.38
4	A	601	NAG	O6-C6-C5	2.34	119.31	111.33
4	A	601	NAG	O7-C7-N2	-2.28	117.94	121.98
4	A	601	NAG	C2-N2-C7	2.25	125.92	122.90
4	A	601	NAG	O5-C1-C2	-2.24	107.82	111.29
4	A	601	NAG	O5-C5-C4	2.15	116.05	110.83

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
4	D	601	NAG	O5-C5-C6-O6
4	D	601	NAG	C4-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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	194/221 (87%)	-0.95	0	100 100	108, 191, 268, 314	0
1	C	194/221 (87%)	-0.81	0	100 100	126, 200, 265, 299	0
1	D	195/221 (88%)	-0.94	0	100 100	120, 190, 253, 284	0
1	G	193/221 (87%)	-0.97	1 (0%)	87 69	130, 195, 266, 329	0
1	I	194/221 (87%)	-0.90	0	100 100	108, 191, 245, 285	0
2	B	121/146 (82%)	-0.92	0	100 100	147, 196, 244, 302	0
2	E	121/146 (82%)	-1.01	0	100 100	150, 208, 252, 293	0
2	F	121/146 (82%)	-1.06	0	100 100	133, 181, 228, 255	0
2	H	120/146 (82%)	-0.92	0	100 100	133, 190, 235, 255	0
2	J	119/146 (81%)	-0.97	0	100 100	140, 199, 248, 277	0
All	All	1572/1835 (85%)	-0.94	1 (0%)	92 86	108, 195, 254, 329	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	335	LEU	2.5

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

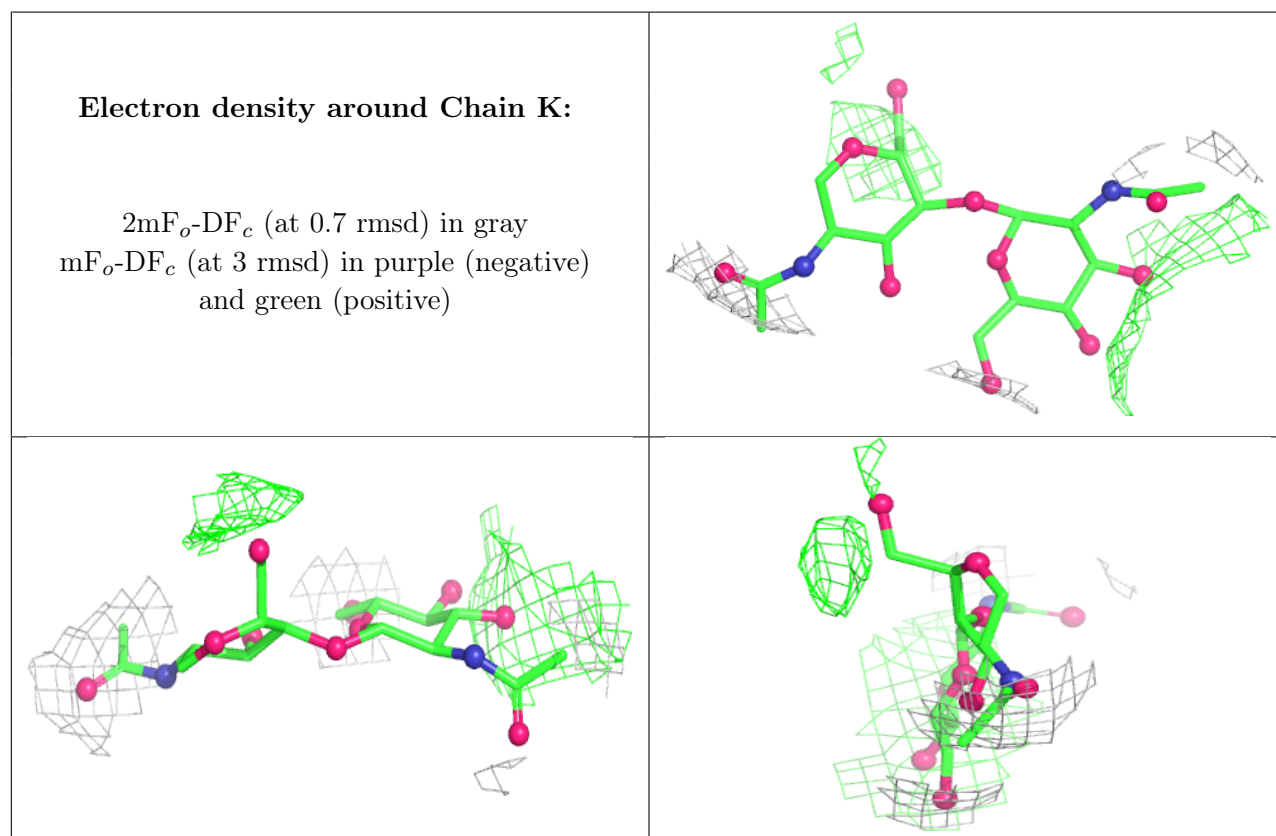
There are no non-standard protein/DNA/RNA residues in this entry.

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.

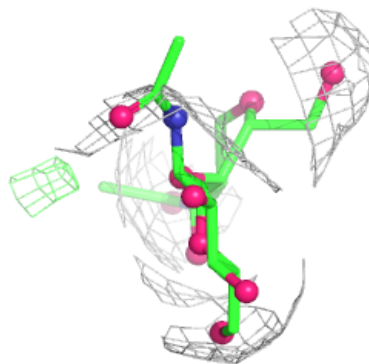
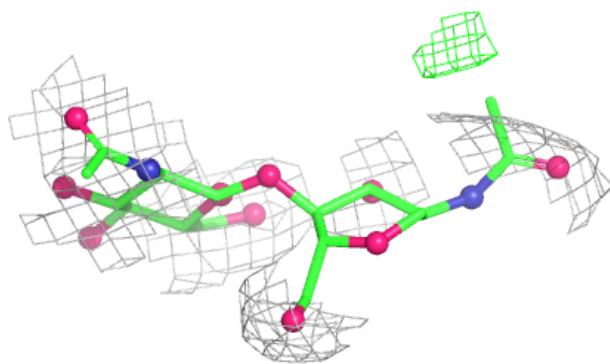
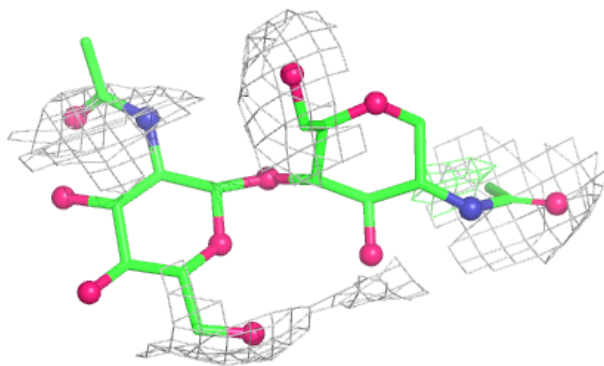
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	M	2	14/15	0.60	0.08	161,292,339,373	0
3	NAG	K	2	14/15	0.71	0.07	151,267,342,348	0
3	NAG	L	2	14/15	0.78	0.07	135,256,330,342	0
3	NAG	L	1	14/15	0.93	0.05	118,180,228,241	0
3	NAG	M	1	14/15	0.94	0.04	118,210,251,254	0
3	NAG	K	1	14/15	0.96	0.04	137,213,244,256	0

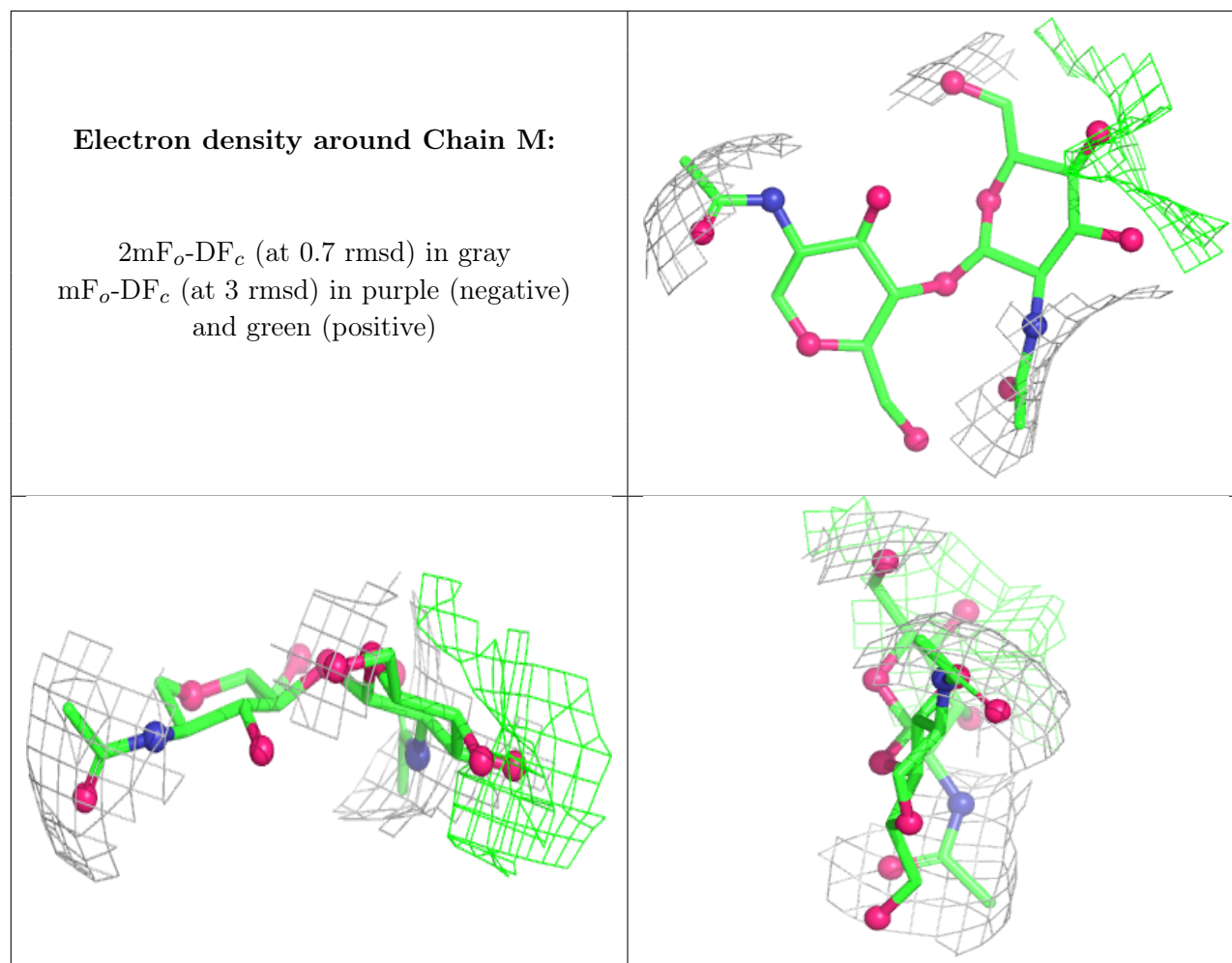
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain L:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	601	14/15	0.91	0.07	145,224,264,268	0
4	NAG	D	601	14/15	0.92	0.06	116,180,245,254	0

6.5 Other polymers [i](#)

There are no such residues in this entry.