



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:55 AM UTC

PDB ID : 5ANM / pdb_00005anm
Title : Crystal structure of IgE Fc in complex with a neutralizing antibody
Authors : Cohen, E.S.; Dobson, C.L.; Kack, H.; Wang, B.; Sims, D.A.; Lloyd, C.O.; England, E.; Rees, D.G.; Guo, H.; Karagiannis, S.N.; O'Brien, S.; Persdotter, S.; Ekdahl, H.; Butler, R.; Keyes, F.; Oakley, S.; Carlsson, M.; Briend, E.; Wilkinson, T.; Anderson, I.K.; Monk, P.D.; vonWachenfeldt, K.; Eriksson, P.O.; Gould, H.J.; Vaughan, T.J.; May, R.D.
Deposited on : 2015-09-07
Resolution : 2.85 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)

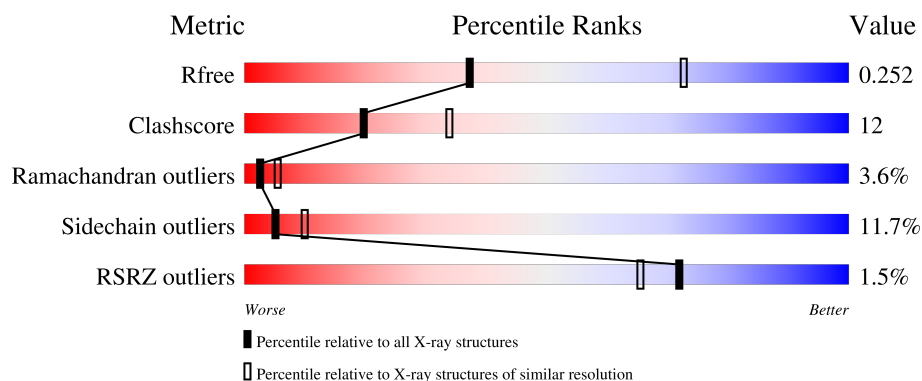
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

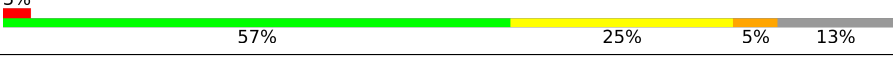
The reported resolution of this entry is 2.85 Å.

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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	217	
1	C	217	
1	L	217	
2	B	229	

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Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	D	229	74% 17% 3% 6%
2	H	229	50% 33% 7% 9%
3	E	242	46% 29% 10% 15%
3	F	242	62% 20% 14% 4%
3	G	242	60% 21% 6% 13%
4	I	6	33% 67%
5	J	5	80% 20%
6	K	6	83% 17%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14788 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 IMMUNOGLOBULIN G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1582	991	262	325	4			
1	C	213	Total	C	N	O	S	0	0	0
			1582	991	262	325	4			
1	L	189	Total	C	N	O	S	0	0	0
			1383	865	228	286	4			

- Molecule 2 is a protein called IMMUNOGLOBULIN G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	220	Total	C	N	O	S	0	0	0
			1673	1068	272	325	8			
2	D	219	Total	C	N	O	S	0	0	0
			1664	1062	270	324	8			
2	H	208	Total	C	N	O	S	0	0	0
			1580	1008	255	309	8			

- Molecule 3 is a protein called IG EPSILON CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	206	Total	C	N	O	S	0	0	0
			1636	1026	301	303	6			
3	F	208	Total	C	N	O	S	0	0	0
			1628	1016	301	305	6			
3	G	211	Total	C	N	O	S	0	0	0
			1665	1042	307	310	6			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	326	ALA	-	expression tag	UNP P01854
E	327	ASP	-	expression tag	UNP P01854

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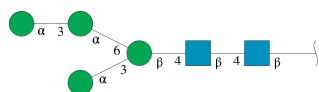
Chain	Residue	Modelled	Actual	Comment	Reference
E	328	PRO	-	expression tag	UNP P01854
E	329	CYS	-	expression tag	UNP P01854
E	548	ASP	-	expression tag	UNP P01854
E	549	TYR	-	expression tag	UNP P01854
E	550	LYS	-	expression tag	UNP P01854
E	551	ASP	-	expression tag	UNP P01854
E	552	ASP	-	expression tag	UNP P01854
E	553	ASP	-	expression tag	UNP P01854
E	554	ASP	-	expression tag	UNP P01854
E	555	LYS	-	expression tag	UNP P01854
E	556	ALA	-	expression tag	UNP P01854
E	557	ALA	-	expression tag	UNP P01854
E	558	HIS	-	expression tag	UNP P01854
E	559	HIS	-	expression tag	UNP P01854
E	560	HIS	-	expression tag	UNP P01854
E	561	HIS	-	expression tag	UNP P01854
E	562	HIS	-	expression tag	UNP P01854
E	563	HIS	-	expression tag	UNP P01854
E	564	HIS	-	expression tag	UNP P01854
E	565	HIS	-	expression tag	UNP P01854
E	566	HIS	-	expression tag	UNP P01854
E	567	HIS	-	expression tag	UNP P01854
F	326	ALA	-	expression tag	UNP P01854
F	327	ASP	-	expression tag	UNP P01854
F	328	PRO	-	expression tag	UNP P01854
F	329	CYS	-	expression tag	UNP P01854
F	548	ASP	-	expression tag	UNP P01854
F	549	TYR	-	expression tag	UNP P01854
F	550	LYS	-	expression tag	UNP P01854
F	551	ASP	-	expression tag	UNP P01854
F	552	ASP	-	expression tag	UNP P01854
F	553	ASP	-	expression tag	UNP P01854
F	554	ASP	-	expression tag	UNP P01854
F	555	LYS	-	expression tag	UNP P01854
F	556	ALA	-	expression tag	UNP P01854
F	557	ALA	-	expression tag	UNP P01854
F	558	HIS	-	expression tag	UNP P01854
F	559	HIS	-	expression tag	UNP P01854
F	560	HIS	-	expression tag	UNP P01854
F	561	HIS	-	expression tag	UNP P01854
F	562	HIS	-	expression tag	UNP P01854
F	563	HIS	-	expression tag	UNP P01854

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Chain	Residue	Modelled	Actual	Comment	Reference
F	564	HIS	-	expression tag	UNP P01854
F	565	HIS	-	expression tag	UNP P01854
F	566	HIS	-	expression tag	UNP P01854
F	567	HIS	-	expression tag	UNP P01854
G	326	ALA	-	expression tag	UNP P01854
G	327	ASP	-	expression tag	UNP P01854
G	328	PRO	-	expression tag	UNP P01854
G	329	CYS	-	expression tag	UNP P01854
G	548	ASP	-	expression tag	UNP P01854
G	549	TYR	-	expression tag	UNP P01854
G	550	LYS	-	expression tag	UNP P01854
G	551	ASP	-	expression tag	UNP P01854
G	552	ASP	-	expression tag	UNP P01854
G	553	ASP	-	expression tag	UNP P01854
G	554	ASP	-	expression tag	UNP P01854
G	555	LYS	-	expression tag	UNP P01854
G	556	ALA	-	expression tag	UNP P01854
G	557	ALA	-	expression tag	UNP P01854
G	558	HIS	-	expression tag	UNP P01854
G	559	HIS	-	expression tag	UNP P01854
G	560	HIS	-	expression tag	UNP P01854
G	561	HIS	-	expression tag	UNP P01854
G	562	HIS	-	expression tag	UNP P01854
G	563	HIS	-	expression tag	UNP P01854
G	564	HIS	-	expression tag	UNP P01854
G	565	HIS	-	expression tag	UNP P01854
G	566	HIS	-	expression tag	UNP P01854
G	567	HIS	-	expression tag	UNP P01854

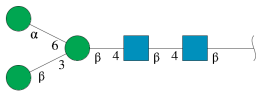
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	6	Total	C	N	O	0	0	0
			72	40	2	30			

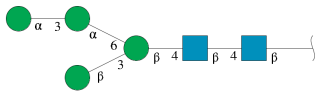
- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

se-(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
5	J	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]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
6	K	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 7 is water.

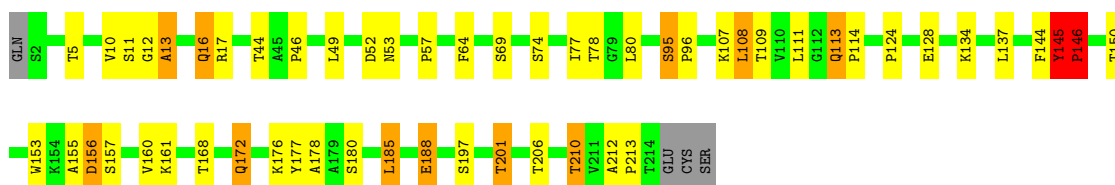
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	14	Total	O	0	0
			14	14		
7	B	60	Total	O	0	0
			60	60		
7	C	16	Total	O	0	0
			16	16		
7	D	60	Total	O	0	0
			60	60		
7	E	6	Total	O	0	0
			6	6		
7	F	10	Total	O	0	0
			10	10		
7	G	22	Total	O	0	0
			22	22		
7	H	2	Total	O	0	0
			2	2		

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.

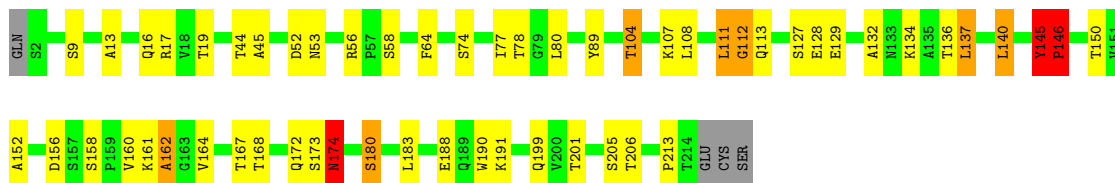
- Molecule 1: IMMUNOGLOBULIN G

Chain A: 



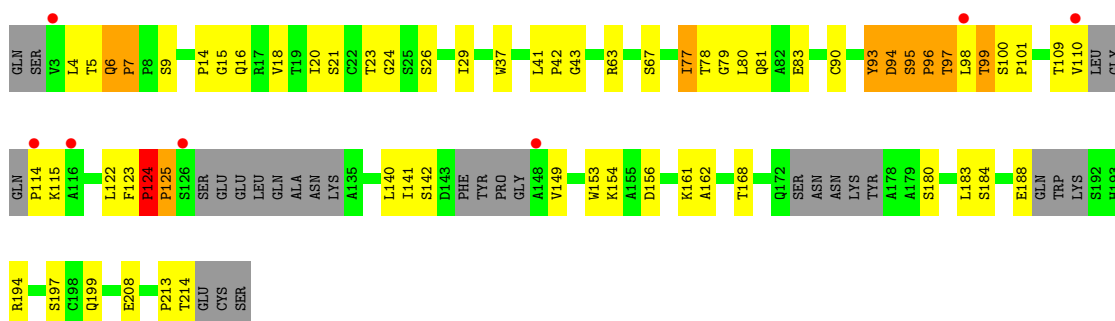
- Molecule 1: IMMUNOGLOBULIN G

Chain C: 



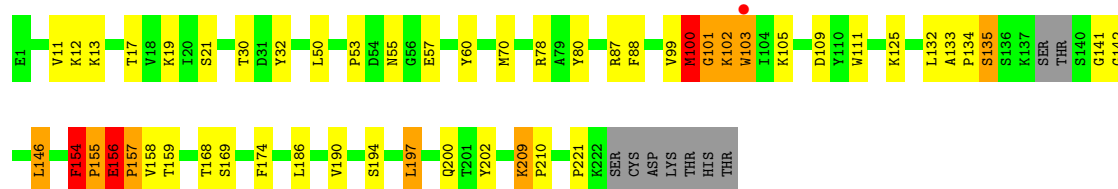
- Molecule 1: IMMUNOGLOBULIN G

Chain L: 

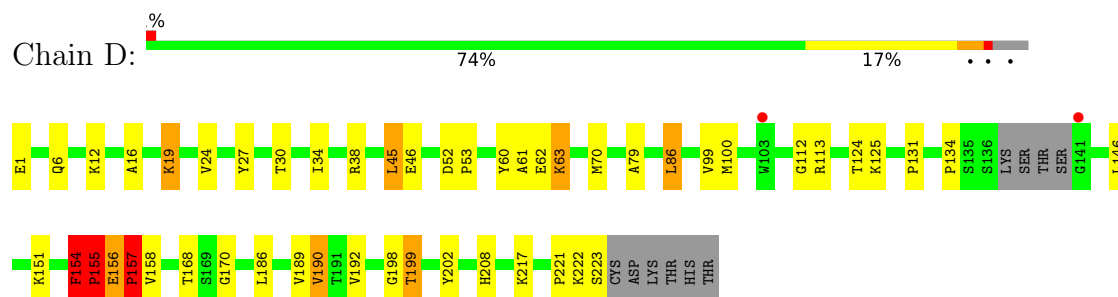


- Molecule 2: IMMUNOGLOBULIN G

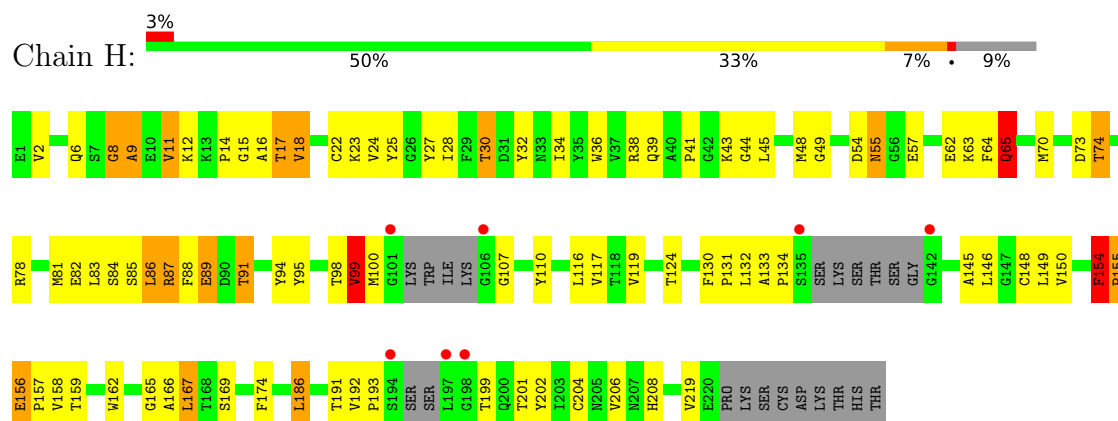
Chain B: 



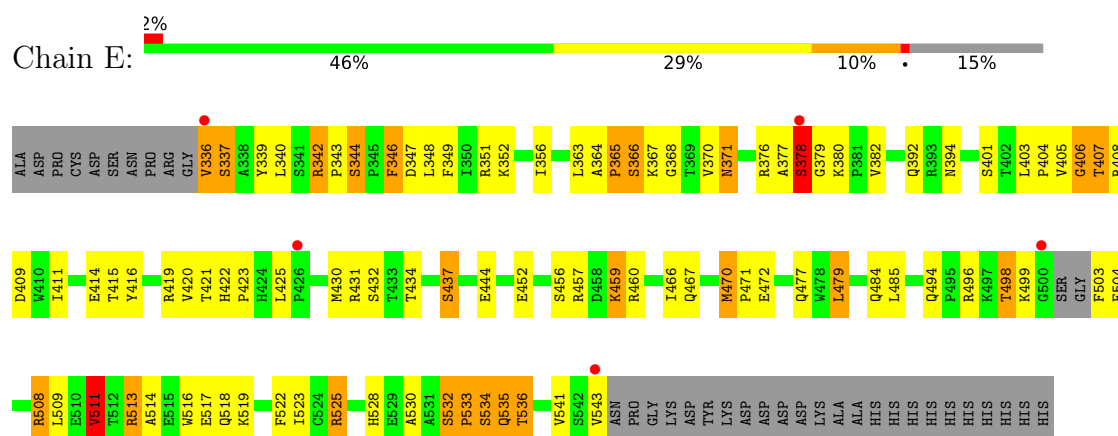
• Molecule 2: IMMUNOGLOBULIN G



• Molecule 2: IMMUNOGLOBULIN G

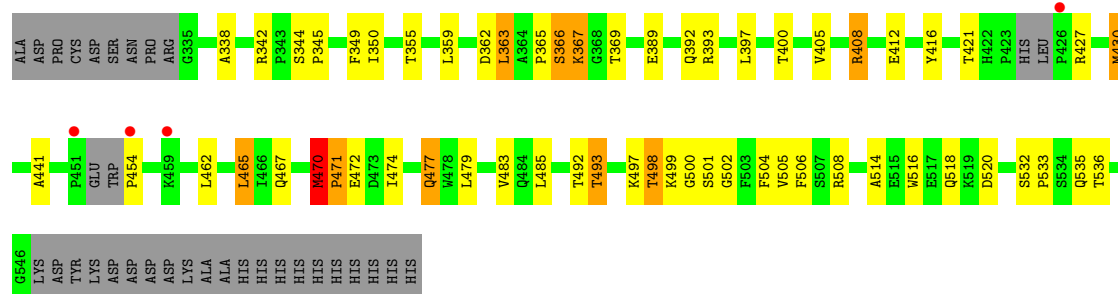


• Molecule 3: IG EPSILON CHAIN C REGION

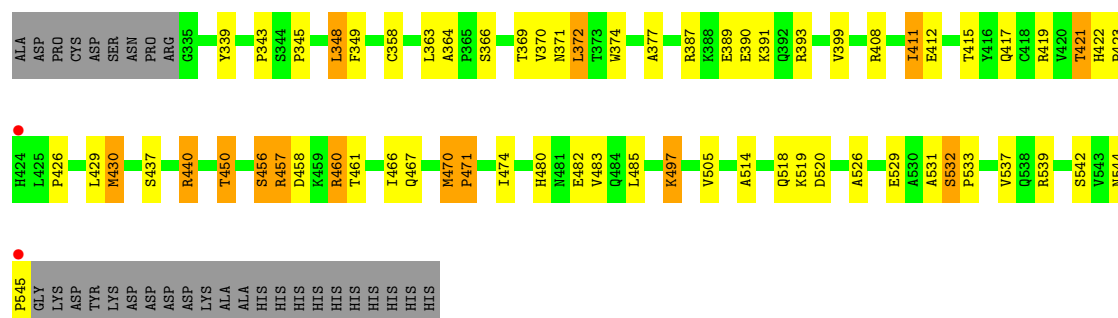


• Molecule 3: IG EPSILON CHAIN C REGION





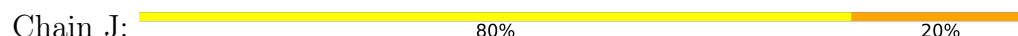
• Molecule 3: IG EPSILON CHAIN C REGION



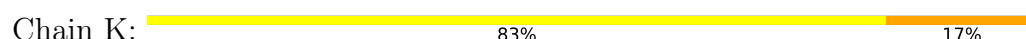
• Molecule 4: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 5: beta-D-mannopyranose-(1-3)-[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



• Molecule 6: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]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 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.96Å 140.96Å 244.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.29 – 2.85 31.29 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.29-2.85) 99.9 (31.29-2.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.196 , 0.260 0.192 , 0.252	Depositor DCC
R_{free} test set	3355 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14788	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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, 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	0.85	0/1623	1.12	7/2222 (0.3%)
1	C	0.83	0/1623	1.20	10/2222 (0.5%)
1	L	0.87	4/1413 (0.3%)	1.16	13/1930 (0.7%)
2	B	1.01	1/1715 (0.1%)	1.36	18/2332 (0.8%)
2	D	1.00	0/1706	1.94	12/2321 (0.5%)
2	H	0.74	1/1617 (0.1%)	1.25	12/2199 (0.5%)
3	E	0.74	0/1677	1.13	10/2282 (0.4%)
3	F	0.85	0/1666	1.39	10/2262 (0.4%)
3	G	0.91	0/1708	1.21	8/2326 (0.3%)
All	All	0.87	6/14748 (0.0%)	1.33	100/20096 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
1	L	0	1
2	B	0	4
2	D	0	1
2	H	0	2
3	E	0	3
3	F	0	1
3	G	0	2
All	All	0	17

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	14	PRO	C-O	11.09	1.38	1.24
1	L	14	PRO	C-N	6.98	1.44	1.33
1	L	124	PRO	CA-C	6.39	1.58	1.52
2	H	98	THR	CA-C	5.31	1.59	1.52
2	B	99	VAL	C-O	-5.22	1.18	1.24
1	L	14	PRO	CA-C	-5.08	1.45	1.52

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	156	GLU	CA-C-N	45.30	176.46	119.84
2	D	156	GLU	C-N-CA	45.30	176.46	119.84
3	F	470	MET	CA-C-N	26.24	152.64	119.84
3	F	470	MET	C-N-CA	26.24	152.64	119.84
2	D	154	PHE	CA-C-N	22.09	147.45	119.84
2	D	154	PHE	C-N-CA	22.09	147.45	119.84
2	H	156	GLU	CA-C-N	17.72	142.00	119.84
2	H	156	GLU	C-N-CA	17.72	142.00	119.84
2	B	156	GLU	CA-C-N	16.73	140.76	119.84
2	B	156	GLU	C-N-CA	16.73	140.76	119.84
3	G	470	MET	CA-C-N	14.06	137.42	119.84
3	G	470	MET	C-N-CA	14.06	137.42	119.84
3	E	337	SER	N-CA-C	13.97	127.60	110.41
2	D	156	GLU	C-N-CD	-12.52	73.67	125.00
1	L	115	LYS	N-CA-C	11.30	123.14	108.34
3	F	470	MET	C-N-CD	-9.80	84.80	125.00
2	B	154	PHE	CA-C-N	9.40	131.59	119.84
2	B	154	PHE	C-N-CA	9.40	131.59	119.84
3	E	470	MET	CA-C-N	9.39	131.58	119.84
3	E	470	MET	C-N-CA	9.39	131.58	119.84
2	D	155	PRO	N-CA-C	-9.37	93.18	112.47
1	C	145	TYR	CA-C-N	9.24	131.39	119.84
1	C	145	TYR	C-N-CA	9.24	131.39	119.84
2	H	98	THR	N-CA-C	9.02	122.57	109.14
2	H	156	GLU	C-N-CD	-8.11	91.74	125.00
1	A	145	TYR	CA-C-N	7.99	129.83	119.84
1	A	145	TYR	C-N-CA	7.99	129.83	119.84
2	D	154	PHE	C-N-CD	-7.94	92.45	125.00
1	L	100	SER	CA-C-N	-7.90	112.53	120.98
1	L	100	SER	C-N-CA	-7.90	112.53	120.98
2	B	157	PRO	N-CA-C	-7.69	96.64	112.47
3	F	470	MET	N-CA-C	7.27	125.63	108.40
2	D	158	VAL	N-CA-C	-7.20	97.73	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	531	ALA	CA-C-N	-7.19	115.12	122.74
3	G	531	ALA	C-N-CA	-7.19	115.12	122.74
2	B	156	GLU	C-N-CD	-6.96	96.45	125.00
2	B	156	GLU	N-CA-C	-6.83	101.19	109.72
2	H	130	PHE	CA-C-N	6.75	128.28	119.84
2	H	130	PHE	C-N-CA	6.75	128.28	119.84
1	L	6	GLN	CA-C-N	6.73	127.31	120.38
1	L	6	GLN	C-N-CA	6.73	127.31	120.38
2	H	154	PHE	CA-C-N	6.68	128.19	119.84
2	H	154	PHE	C-N-CA	6.68	128.19	119.84
1	A	11	SER	N-CA-C	6.63	119.97	109.50
1	L	124	PRO	CA-C-N	6.44	127.89	119.84
1	L	124	PRO	C-N-CA	6.44	127.89	119.84
1	L	14	PRO	CA-C-N	-6.38	114.46	123.08
1	L	14	PRO	C-N-CA	-6.38	114.46	123.08
3	F	467	GLN	N-CA-C	6.38	118.46	108.96
3	G	470	MET	C-N-CD	-6.19	99.62	125.00
2	B	100	MET	CB-CG-SD	-6.13	94.31	112.70
2	D	52	ASP	CA-C-N	6.13	125.75	119.56
2	D	52	ASP	C-N-CA	6.13	125.75	119.56
3	G	437	SER	N-CA-C	6.10	118.20	110.33
3	E	511	VAL	N-CA-C	6.10	116.91	108.12
2	D	157	PRO	CA-N-CD	-6.08	103.48	112.00
1	L	123	PHE	CA-C-N	6.06	126.62	120.38
1	L	123	PHE	C-N-CA	6.06	126.62	120.38
3	F	342	ARG	CA-C-N	-6.03	113.76	119.85
3	F	342	ARG	C-N-CA	-6.03	113.76	119.85
2	B	197	LEU	N-CA-C	6.00	118.59	111.33
2	B	100	MET	CB-CA-C	-5.95	102.42	112.00
2	B	101	GLY	N-CA-C	-5.95	99.08	113.18
1	C	104	THR	N-CA-CB	-5.89	100.54	110.49
2	D	156	GLU	N-CA-C	-5.84	102.53	110.36
2	B	78	ARG	NE-CZ-NH1	-5.82	115.68	121.50
1	C	174	ASN	CA-C-N	-5.82	113.95	122.86
1	C	174	ASN	C-N-CA	-5.82	113.95	122.86
3	E	536	THR	N-CA-C	5.79	117.81	107.80
2	B	99	VAL	N-CA-C	-5.67	99.89	108.17
3	F	430	MET	N-CA-C	5.66	117.72	108.55
1	L	14	PRO	O-C-N	5.61	130.21	122.64
2	H	8	GLY	N-CA-C	5.58	122.33	111.34
1	C	9	SER	N-CA-C	5.55	117.51	109.07
3	E	437	SER	N-CA-C	5.50	117.02	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	109	ASP	N-CA-C	-5.50	106.62	113.55
3	F	470	MET	O-C-N	5.49	126.32	121.32
1	A	212	ALA	CA-C-N	5.42	126.62	119.84
1	A	212	ALA	C-N-CA	5.42	126.62	119.84
1	L	94	ASP	N-CA-C	5.36	117.20	111.36
2	B	133	ALA	N-CA-C	5.35	116.43	109.64
2	H	28	ILE	N-CA-CB	-5.32	105.22	111.60
3	E	342	ARG	CB-CA-C	5.28	116.80	108.88
2	H	169	SER	N-CA-C	5.22	116.67	110.97
1	C	145	TYR	C-N-CD	-5.21	103.66	125.00
3	F	471	PRO	N-CA-C	-5.20	101.76	112.47
2	B	154	PHE	C-N-CD	-5.17	103.78	125.00
1	C	132	ALA	N-CA-C	-5.12	107.00	113.20
3	E	336	VAL	CA-C-N	5.12	130.68	121.06
3	E	336	VAL	C-N-CA	5.12	130.68	121.06
3	G	391	LYS	N-CA-C	-5.09	101.66	109.76
2	H	64	PHE	N-CA-C	-5.09	107.02	113.43
1	A	95	SER	CA-C-N	-5.08	114.43	119.56
1	A	95	SER	C-N-CA	-5.08	114.43	119.56
3	E	470	MET	C-N-CD	-5.07	104.22	125.00
2	B	109	ASP	CA-C-N	5.03	130.08	122.99
2	B	109	ASP	C-N-CA	5.03	130.08	122.99
3	G	467	GLN	N-CA-C	5.01	115.92	108.60
1	C	45	ALA	CA-C-N	-5.00	115.08	120.03
1	C	45	ALA	C-N-CA	-5.00	115.08	120.03

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	TYR	Peptide
2	B	154	PHE	Mainchain,Peptide
2	B	156	GLU	Mainchain,Peptide
1	C	145	TYR	Peptide
1	C	160	VAL	Peptide
2	D	154	PHE	Peptide
3	E	336	VAL	Peptide
3	E	366	SER	Peptide
3	E	470	MET	Peptide
3	F	470	MET	Peptide
3	G	470	MET	Peptide
3	G	532	SER	Peptide

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Mol	Chain	Res	Type	Group
2	H	154	PHE	Peptide
2	H	156	GLU	Peptide
1	L	114	PRO	Peptide

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	1582	0	1528	33	0
1	C	1582	0	1528	27	0
1	L	1383	0	1339	34	0
2	B	1673	0	1642	27	0
2	D	1664	0	1629	29	0
2	H	1580	0	1537	67	0
3	E	1636	0	1622	64	0
3	F	1628	0	1616	33	0
3	G	1665	0	1647	38	0
4	I	72	0	61	0	0
5	J	61	0	52	1	0
6	K	72	0	61	1	0
7	A	14	0	0	0	0
7	B	60	0	0	2	0
7	C	16	0	0	0	0
7	D	60	0	0	2	0
7	E	6	0	0	1	0
7	F	10	0	0	0	0
7	G	22	0	0	0	0
7	H	2	0	0	0	0
All	All	14788	0	14262	332	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 12.

All (332) 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)
3:G:371:ASN:HB2	3:G:421:THR:HG22	1.33	1.06
2:H:48:MET:HE1	2:H:94:TYR:HD2	1.23	1.02
3:F:514:ALA:HB2	2:H:165:GLY:HA3	1.41	1.01
3:G:371:ASN:HB2	3:G:421:THR:CG2	1.96	0.96
3:E:508:ARG:HH11	3:E:508:ARG:HG3	1.30	0.95
2:H:30:THR:HG22	2:H:54:ASP:HA	1.48	0.92
2:H:43:LYS:HD2	2:H:44:GLY:H	1.38	0.86
2:H:192:VAL:HG22	2:H:193:PRO:HD2	1.56	0.86
2:H:6:GLN:HG2	2:H:22:CYS:HB3	1.59	0.85
2:H:62:GLU:HA	2:H:65:GLN:HG3	1.60	0.84
1:A:155:ALA:O	1:A:156:ASP:HB2	1.76	0.84
2:H:154:PHE:CD2	2:H:155:PRO:HD3	2.12	0.84
1:A:160:VAL:HG23	1:A:161:LYS:H	1.44	0.83
3:E:477:GLN:HG2	3:E:484:GLN:HE22	1.42	0.83
1:A:145:TYR:CD2	1:A:146:PRO:HD3	2.16	0.80
2:H:49:GLY:HA3	2:H:70:MET:HE1	1.62	0.80
3:E:365:PRO:O	3:E:367:LYS:N	2.14	0.79
2:H:88:PHE:O	2:H:91:THR:HG23	1.82	0.79
1:C:161:LYS:HE2	1:C:164:VAL:HB	1.64	0.79
2:H:48:MET:HE1	2:H:94:TYR:CD2	2.14	0.79
3:G:440:ARG:HG2	3:G:440:ARG:HH11	1.47	0.78
3:G:417:GLN:OE1	3:G:430:MET:HE1	1.83	0.78
2:H:150:VAL:HG12	2:H:186:LEU:HD12	1.66	0.77
2:B:134:PRO:HD3	2:B:146:LEU:HB3	1.66	0.76
1:A:145:TYR:CD2	1:A:146:PRO:CD	2.68	0.75
1:A:160:VAL:HG23	1:A:161:LYS:N	2.02	0.74
2:H:150:VAL:CG1	2:H:186:LEU:HD12	2.16	0.74
2:H:99:VAL:O	2:H:100:MET:SD	2.45	0.74
3:F:497:LYS:NZ	3:F:501:SER:HA	2.02	0.73
3:G:387:ARG:NH1	3:G:389:GLU:HG3	2.04	0.72
2:H:30:THR:HG22	2:H:54:ASP:CA	2.20	0.72
3:E:365:PRO:C	3:E:367:LYS:H	1.97	0.72
3:E:367:LYS:HD2	3:E:423:PRO:HB2	1.72	0.71
3:E:525:ARG:HD3	3:E:536:THR:HG23	1.71	0.71
3:E:532:SER:N	3:E:533:PRO:HD2	2.04	0.71
2:H:30:THR:CG2	2:H:54:ASP:HA	2.19	0.71
1:C:145:TYR:CD2	1:C:146:PRO:HD3	2.26	0.71
2:D:38:ARG:NH1	2:D:46:GLU:OE2	2.25	0.69
2:D:100:MET:HB2	3:E:394:ASN:HD22	1.58	0.69
2:B:134:PRO:HD3	2:B:146:LEU:CB	2.24	0.68
1:A:172:GLN:HG3	1:A:176:LYS:O	1.95	0.67
3:G:456:SER:O	3:G:458:ASP:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:344:SER:HB3	3:E:347:ASP:OD2	1.96	0.66
2:H:124:THR:HA	2:H:155:PRO:HD2	1.78	0.65
1:C:167:THR:HG22	1:C:168:THR:O	1.95	0.65
2:H:91:THR:HG22	2:H:119:VAL:H	1.61	0.65
3:G:372:LEU:C	3:G:372:LEU:HD23	2.22	0.65
3:E:508:ARG:HH11	3:E:508:ARG:CG	2.08	0.64
1:L:124:PRO:HB2	1:L:125:PRO:CD	2.26	0.64
3:G:544:ASN:HB3	3:G:545:PRO:HD2	1.78	0.64
3:F:365:PRO:C	3:F:367:LYS:N	2.55	0.63
3:E:415:THR:OG1	3:E:434:THR:CG2	2.46	0.63
3:F:493:THR:HG22	3:F:505:VAL:HA	1.81	0.63
3:E:349:PHE:HB3	3:E:535:GLN:HG3	1.82	0.62
1:L:124:PRO:HB2	1:L:125:PRO:HD2	1.81	0.62
2:H:174:PHE:CE1	1:L:140:LEU:HD23	2.35	0.62
1:L:154:LYS:HD3	1:L:197:SER:HB2	1.82	0.62
1:A:49:LEU:O	1:A:57:PRO:HD2	1.98	0.62
1:A:145:TYR:CE2	1:A:146:PRO:HD3	2.34	0.61
1:L:18:VAL:HG22	1:L:80:LEU:HD11	1.82	0.61
3:F:441:ALA:HB3	3:F:470:MET:HB2	1.82	0.61
2:D:60:TYR:CE1	2:D:70:MET:HE2	2.35	0.61
2:D:100:MET:HA	2:D:100:MET:HE2	1.83	0.60
3:F:365:PRO:C	3:F:367:LYS:H	2.06	0.60
2:B:101:GLY:O	2:B:102:LYS:HB2	2.01	0.60
3:E:430:MET:O	3:E:431:ARG:NH1	2.34	0.60
3:E:508:ARG:HG3	3:E:508:ARG:NH1	2.08	0.59
2:H:91:THR:CG2	2:H:119:VAL:H	2.15	0.59
2:H:49:GLY:CA	2:H:70:MET:HE1	2.31	0.59
2:H:154:PHE:CD2	2:H:155:PRO:CD	2.84	0.59
1:A:52:ASP:O	1:A:53:ASN:HB2	2.03	0.58
3:E:364:ALA:N	3:E:365:PRO:CD	2.67	0.58
3:E:337:SER:HB2	7:E:2001:HOH:O	2.02	0.58
1:L:81:GLN:HB3	1:L:83:GLU:HG2	1.86	0.58
3:F:516:TRP:O	3:F:520:ASP:HB2	2.03	0.58
1:L:94:ASP:C	1:L:96:PRO:HD2	2.28	0.58
1:A:197:SER:OG	1:A:210:THR:HB	2.03	0.58
1:C:167:THR:CG2	1:C:168:THR:O	2.51	0.58
1:A:17:ARG:HG3	1:A:78:THR:HG22	1.84	0.57
3:F:498:THR:HB	3:F:502:GLY:O	2.05	0.57
2:H:11:VAL:O	2:H:11:VAL:HG12	2.03	0.57
1:C:137:LEU:HD22	1:C:183:LEU:HD23	1.87	0.57
1:C:161:LYS:O	1:C:162:ALA:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:432:SER:H	2:H:74:THR:HB	1.70	0.57
3:F:465:LEU:HG	3:F:506:PHE:CE1	2.40	0.56
2:D:34:ILE:HD12	2:D:79:ALA:HB2	1.87	0.56
1:C:167:THR:HB	1:C:180:SER:H	1.69	0.56
2:H:24:VAL:HG11	2:H:27:TYR:CE1	2.39	0.56
3:E:414:GLU:O	3:E:434:THR:HG22	2.06	0.56
2:B:125:LYS:HA	1:C:128:GLU:HG2	1.87	0.56
2:B:102:LYS:HA	7:B:2046:HOH:O	2.07	0.55
3:G:514:ALA:O	3:G:518:GLN:HB2	2.06	0.55
2:D:131:PRO:HD3	2:D:217:LYS:HE2	1.88	0.55
3:E:376:ARG:NH2	3:E:409:ASP:OD2	2.40	0.55
1:C:129:GLU:OE2	2:D:151:LYS:NZ	2.40	0.55
2:D:16:ALA:O	2:D:86:LEU:HB2	2.06	0.55
2:B:50:LEU:C	2:B:50:LEU:HD12	2.31	0.55
1:A:153:TRP:HB2	1:A:160:VAL:CG2	2.37	0.55
3:G:349:PHE:CE1	3:G:411:ILE:HD11	2.42	0.55
1:C:80:LEU:HD11	1:C:108:LEU:HD21	1.89	0.54
2:B:60:TYR:CE2	2:B:70:MET:HE2	2.43	0.54
3:E:365:PRO:C	3:E:367:LYS:N	2.64	0.54
1:L:41:LEU:HB3	1:L:42:PRO:HD3	1.90	0.54
2:H:150:VAL:HG12	2:H:186:LEU:O	2.07	0.54
3:E:534:SER:C	3:E:535:GLN:HG2	2.31	0.54
3:F:497:LYS:HZ2	3:F:501:SER:HA	1.73	0.54
3:G:417:GLN:OE1	3:G:430:MET:CE	2.54	0.54
2:H:8:GLY:O	2:H:9:ALA:O	2.26	0.54
2:H:17:THR:OG1	2:H:84:SER:HA	2.08	0.54
2:H:36:TRP:CG	2:H:81:MET:HE2	2.43	0.54
1:L:94:ASP:O	1:L:96:PRO:HD2	2.08	0.54
3:E:479:LEU:HB2	3:E:523:ILE:HB	1.89	0.53
2:B:101:GLY:O	2:B:102:LYS:CB	2.56	0.53
3:F:408:ARG:O	3:F:412:GLU:HG3	2.08	0.53
3:G:440:ARG:HE	3:G:529:GLU:CD	2.15	0.53
2:H:2:VAL:HB	2:H:110:TYR:CE1	2.43	0.53
3:G:364:ALA:C	3:G:366:SER:H	2.17	0.53
3:G:440:ARG:HH11	3:G:440:ARG:CG	2.19	0.53
3:E:431:ARG:HD2	2:H:74:THR:HG21	1.91	0.53
3:F:393:ARG:HH21	2:H:107:GLY:H	1.56	0.53
2:D:63:LYS:HB3	7:D:2028:HOH:O	2.08	0.52
3:G:387:ARG:HH12	3:G:389:GLU:HG3	1.74	0.52
1:C:13:ALA:O	1:C:16:GLN:HB2	2.10	0.52
3:E:343:PRO:HD3	3:E:356:ILE:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:508:ARG:CG	3:E:508:ARG:NH1	2.69	0.52
3:E:377:ALA:O	3:E:378:SER:HB2	2.10	0.52
1:A:160:VAL:CG2	1:A:161:LYS:H	2.19	0.52
1:C:17:ARG:HG3	1:C:78:THR:HG22	1.91	0.52
3:E:467:GLN:OE1	3:F:508:ARG:NE	2.43	0.52
3:E:430:MET:CG	3:E:431:ARG:N	2.73	0.52
1:L:124:PRO:CB	1:L:125:PRO:CD	2.87	0.52
3:G:339:TYR:CE2	6:K:3:BMA:H3	2.45	0.52
1:L:81:GLN:HB3	1:L:83:GLU:H	1.75	0.52
2:D:24:VAL:HG13	2:D:27:TYR:CE1	2.45	0.51
2:H:32:TYR:CE2	2:H:100:MET:HG3	2.45	0.51
1:L:6:GLN:HE22	1:L:90:CYS:H	1.58	0.51
3:F:366:SER:O	3:F:367:LYS:HG3	2.11	0.51
1:A:128:GLU:HG2	2:D:125:LYS:HA	1.92	0.51
3:G:480:HIS:HE1	3:G:519:LYS:O	1.94	0.51
3:E:496:ARG:HB2	3:E:504:PHE:CE1	2.46	0.51
2:H:15:GLY:O	2:H:85:SER:HA	2.10	0.51
1:C:89:TYR:CD2	2:D:45:LEU:HD22	2.46	0.51
2:H:24:VAL:CG1	2:H:27:TYR:CE1	2.93	0.51
3:F:389:GLU:HG3	3:F:397:LEU:HD11	1.93	0.51
1:L:93:TYR:CE2	1:L:98:LEU:HA	2.45	0.51
1:A:64:PHE:CD1	1:A:77:ILE:HG12	2.46	0.50
3:E:405:VAL:HB	3:E:416:TYR:CZ	2.46	0.50
3:G:544:ASN:O	3:G:545:PRO:C	2.54	0.50
2:D:157:PRO:HD2	2:D:157:PRO:O	2.12	0.50
1:L:4:LEU:HD22	1:L:29:ILE:HD11	1.92	0.50
3:E:351:ARG:O	3:E:352:LYS:HB2	2.11	0.50
2:H:154:PHE:O	2:H:208:HIS:CE1	2.65	0.49
2:D:198:GLY:HA3	3:G:532:SER:HB3	1.94	0.49
3:F:345:PRO:HG2	3:F:474:ILE:HA	1.95	0.49
1:A:46:PRO:HG2	2:B:111:TRP:CZ3	2.48	0.49
1:C:190:TRP:CZ2	1:C:213:PRO:HA	2.47	0.49
1:L:95:SER:HB3	1:L:96:PRO:CD	2.42	0.49
2:H:145:ALA:HB2	2:H:191:THR:HG22	1.93	0.49
3:G:440:ARG:HG2	3:G:440:ARG:NH1	2.20	0.49
1:A:172:GLN:OE1	1:A:178:ALA:HB2	2.13	0.49
3:E:459:LYS:O	3:E:460:ARG:HG3	2.12	0.49
1:L:77:ILE:HD11	1:L:80:LEU:HG	1.92	0.49
3:E:511:VAL:HG21	3:E:522:PHE:CE2	2.48	0.49
1:L:94:ASP:OD2	1:L:99:THR:HG22	2.13	0.49
2:B:134:PRO:HG2	2:B:221:PRO:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:466:ILE:HD13	3:G:526:ALA:HB2	1.94	0.49
2:D:19:LYS:NZ	7:D:2013:HOH:O	2.46	0.48
3:F:392:GLN:OE1	3:F:392:GLN:HA	2.12	0.48
2:D:100:MET:HB2	3:E:394:ASN:ND2	2.26	0.48
2:B:11:VAL:O	2:B:12:LYS:HD3	2.13	0.48
2:H:48:MET:CE	2:H:94:TYR:CD2	2.91	0.48
1:L:24:GLY:HA3	1:L:29:ILE:HD13	1.94	0.48
1:C:152:ALA:O	1:C:199:GLN:HB2	2.13	0.48
3:G:371:ASN:CB	3:G:421:THR:HG22	2.24	0.48
3:G:460:ARG:HA	3:G:460:ARG:HD3	1.59	0.48
2:D:155:PRO:HD2	2:D:208:HIS:NE2	2.28	0.48
2:H:91:THR:HG22	2:H:119:VAL:HB	1.95	0.48
2:B:30:THR:HA	2:B:53:PRO:HB2	1.95	0.48
2:B:135:SER:HB2	7:B:2053:HOH:O	2.12	0.48
2:B:146:LEU:HD22	2:B:190:VAL:CG1	2.43	0.48
3:E:422:HIS:HB3	3:E:425:LEU:HB2	1.96	0.48
2:H:49:GLY:C	2:H:70:MET:HE1	2.39	0.48
1:A:13:ALA:H	1:A:111:LEU:H	1.62	0.48
2:D:134:PRO:HB3	2:D:146:LEU:HB3	1.95	0.48
2:B:55:ASN:CG	2:B:57:GLU:HG3	2.39	0.47
1:A:188:GLU:CD	1:A:188:GLU:H	2.22	0.47
1:C:145:TYR:CD2	1:C:146:PRO:CD	2.97	0.47
3:G:393:ARG:HD3	3:G:393:ARG:C	2.39	0.47
3:G:497:LYS:HB2	3:G:497:LYS:HE3	1.68	0.47
2:H:36:TRP:CB	2:H:81:MET:HE2	2.44	0.47
1:L:41:LEU:HB3	1:L:42:PRO:CD	2.45	0.47
1:C:52:ASP:O	1:C:53:ASN:HB2	2.15	0.47
2:B:105:LYS:HA	2:B:105:LYS:HD3	1.73	0.46
3:E:508:ARG:HD2	3:F:504:PHE:CE1	2.50	0.46
2:H:133:ALA:HB1	2:H:134:PRO:HD2	1.97	0.46
1:L:37:TRP:CZ3	1:L:90:CYS:HB3	2.50	0.46
3:F:349:PHE:CG	3:F:535:GLN:HG2	2.49	0.46
1:C:129:GLU:OE2	1:C:136:THR:OG1	2.32	0.46
1:A:95:SER:N	1:A:96:PRO:CD	2.79	0.46
1:A:137:LEU:HD11	1:A:185:LEU:HD11	1.96	0.46
3:E:376:ARG:HD2	3:E:416:TYR:CE1	2.49	0.46
1:C:64:PHE:CD1	1:C:77:ILE:HG12	2.51	0.46
2:H:192:VAL:HG22	2:H:193:PRO:CD	2.37	0.46
1:L:93:TYR:HE2	1:L:98:LEU:HA	1.81	0.46
3:E:403:LEU:HD12	3:E:404:PRO:HD2	1.98	0.46
3:E:430:MET:HG2	3:E:431:ARG:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:154:PHE:CG	2:H:155:PRO:N	2.84	0.46
2:H:192:VAL:HG21	2:H:202:TYR:CE2	2.51	0.46
3:F:362:ASP:OD2	3:F:365:PRO:HA	2.16	0.45
1:L:15:GLY:C	1:L:79:GLY:HA2	2.41	0.45
1:L:97:THR:O	1:L:98:LEU:HB3	2.16	0.45
2:D:12:LYS:HD2	2:D:12:LYS:HA	1.66	0.45
1:L:96:PRO:O	1:L:97:THR:OG1	2.25	0.45
2:B:209:LYS:N	2:B:210:PRO:CD	2.79	0.45
1:A:113:GLN:HA	1:A:114:PRO:HD3	1.80	0.45
2:D:6:GLN:OE1	2:D:112:GLY:HA3	2.17	0.45
3:E:378:SER:O	3:E:380:LYS:N	2.39	0.45
3:E:514:ALA:HA	3:E:517:GLU:HB2	1.99	0.45
3:F:344:SER:O	3:F:345:PRO:C	2.55	0.45
1:L:154:LYS:HB2	1:L:197:SER:HB2	1.99	0.45
2:H:38:ARG:N	2:H:48:MET:HE2	2.32	0.45
2:H:146:LEU:HD13	2:H:219:VAL:HG21	1.99	0.45
2:H:99:VAL:C	2:H:100:MET:SD	3.00	0.45
1:C:129:GLU:CD	1:C:136:THR:HG1	2.23	0.45
2:H:132:LEU:HD13	2:H:149:LEU:HB2	1.99	0.45
1:A:153:TRP:HB2	1:A:160:VAL:HG21	1.99	0.45
2:B:142:GLY:O	2:B:194:SER:HB3	2.16	0.45
3:F:393:ARG:HD3	3:F:393:ARG:C	2.42	0.45
1:L:154:LYS:HD2	1:L:199:GLN:NE2	2.31	0.45
1:L:99:THR:O	1:L:101:PRO:HD3	2.17	0.45
1:L:153:TRP:CD2	1:L:183:LEU:HD12	2.52	0.45
3:E:479:LEU:HD21	3:E:525:ARG:HB2	1.98	0.44
3:E:499:LYS:N	3:E:499:LYS:HD2	2.33	0.44
3:G:389:GLU:HG2	3:G:399:VAL:HG22	1.98	0.44
3:E:343:PRO:HD3	3:E:356:ILE:CG2	2.47	0.44
3:G:345:PRO:HG2	3:G:474:ILE:HA	1.99	0.44
1:L:161:LYS:O	1:L:162:ALA:HB3	2.17	0.44
3:F:498:THR:HG23	3:F:499:LYS:N	2.32	0.44
2:H:154:PHE:O	2:H:208:HIS:NE2	2.50	0.44
1:L:6:GLN:HA	1:L:7:PRO:HD2	1.76	0.44
3:G:358:CYS:HB2	3:G:374:TRP:CH2	2.52	0.44
3:E:364:ALA:N	3:E:365:PRO:HD2	2.32	0.44
3:E:528:HIS:CD2	3:E:530:ALA:H	2.36	0.44
3:E:532:SER:N	3:E:533:PRO:CD	2.76	0.44
3:F:363:LEU:HD22	5:J:1:NAG:H83	2.00	0.44
2:B:100:MET:H	2:B:100:MET:HG2	1.05	0.44
1:C:173:SER:C	1:C:174:ASN:O	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:440:ARG:CZ	3:G:471:PRO:HG3	2.48	0.44
3:G:450:THR:HB	3:G:461:THR:O	2.18	0.44
1:L:6:GLN:NE2	1:L:90:CYS:SG	2.91	0.43
1:A:13:ALA:O	1:A:16:GLN:HB2	2.18	0.43
1:A:144:PHE:CE1	1:A:177:TYR:HB2	2.53	0.43
2:D:190:VAL:HG22	2:D:192:VAL:HG13	1.99	0.43
2:H:39:GLN:O	2:H:39:GLN:HG2	2.18	0.43
3:E:525:ARG:HH11	3:E:536:THR:HG21	1.82	0.43
2:D:192:VAL:HG11	2:D:202:TYR:CE1	2.54	0.43
3:E:472:GLU:OE1	2:H:78:ARG:NH2	2.51	0.43
2:H:6:GLN:OE1	2:H:95:TYR:HA	2.18	0.43
2:H:43:LYS:CD	2:H:44:GLY:H	2.20	0.43
2:B:87:ARG:O	2:B:88:PHE:C	2.60	0.43
2:D:30:THR:HA	2:D:53:PRO:HB2	2.01	0.43
1:L:37:TRP:CH2	1:L:90:CYS:HB3	2.54	0.43
1:A:12:GLY:HA3	1:A:80:LEU:CD2	2.49	0.42
1:A:124:PRO:HA	1:A:137:LEU:HD23	2.00	0.42
2:B:103:TRP:HA	2:B:103:TRP:CE3	2.53	0.42
3:E:444:GLU:OE2	3:F:454:PRO:HG2	2.18	0.42
3:E:525:ARG:HD3	3:E:536:THR:CG2	2.44	0.42
1:C:111:LEU:O	1:C:112:GLY:C	2.63	0.42
3:E:415:THR:OG1	3:E:434:THR:HG21	2.20	0.42
2:B:200:GLN:HG2	2:B:202:TYR:CZ	2.54	0.42
3:E:364:ALA:O	3:E:365:PRO:C	2.61	0.42
3:F:405:VAL:HG12	3:F:416:TYR:CE2	2.55	0.42
3:F:493:THR:HG22	3:F:505:VAL:CA	2.48	0.42
2:H:73:ASP:C	2:H:73:ASP:OD1	2.63	0.42
3:E:342:ARG:NH2	3:E:434:THR:O	2.44	0.42
2:D:124:THR:HA	2:D:154:PHE:O	2.19	0.42
3:E:406:GLY:C	3:E:408:ARG:N	2.77	0.42
1:C:161:LYS:O	1:C:162:ALA:CB	2.66	0.42
3:E:498:THR:HG23	3:E:503:PHE:N	2.33	0.42
3:F:338:ALA:HA	3:F:359:LEU:O	2.20	0.42
2:H:18:VAL:O	2:H:82:GLU:HA	2.18	0.42
1:C:188:GLU:CD	1:C:188:GLU:H	2.28	0.42
3:E:430:MET:HB3	2:H:55:ASN:HA	2.02	0.42
3:G:387:ARG:HH12	3:G:389:GLU:CG	2.33	0.42
2:B:32:TYR:CE1	2:B:101:GLY:O	2.73	0.42
2:B:174:PHE:CD1	2:B:174:PHE:N	2.88	0.42
3:E:431:ARG:CD	2:H:74:THR:HG21	2.49	0.42
2:H:23:LYS:HD3	2:H:25:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:192:VAL:HG21	2:H:202:TYR:HE2	1.84	0.42
1:A:108:LEU:HD13	1:A:109:THR:N	2.36	0.41
2:B:19:LYS:HE2	2:B:80:TYR:CG	2.54	0.41
2:D:24:VAL:CG1	2:D:27:TYR:CE1	3.03	0.41
3:E:343:PRO:HB2	3:E:348:LEU:HD11	2.02	0.41
3:F:477:GLN:H	3:F:477:GLN:HG2	1.75	0.41
2:H:12:LYS:HB3	2:H:86:LEU:HD23	2.02	0.41
2:H:134:PRO:HB3	2:H:146:LEU:HB3	2.01	0.41
3:G:345:PRO:HG2	3:G:474:ILE:CA	2.50	0.41
3:E:479:LEU:CD1	3:E:484:GLN:HA	2.51	0.41
3:E:513:ARG:HD3	3:E:516:TRP:CE2	2.55	0.41
3:F:350:ILE:HD13	3:F:350:ILE:N	2.36	0.41
3:G:520:ASP:O	3:G:542:SER:OG	2.29	0.41
2:H:162:TRP:HB2	2:H:167:LEU:HB3	2.03	0.41
2:D:170:GLY:O	2:D:190:VAL:HA	2.20	0.41
3:G:377:ALA:HB2	3:G:415:THR:HB	2.03	0.41
3:G:408:ARG:O	3:G:412:GLU:HG3	2.21	0.41
2:H:55:ASN:OD1	2:H:57:GLU:HB2	2.21	0.41
2:B:55:ASN:OD1	2:B:57:GLU:HG3	2.21	0.41
3:E:466:ILE:O	3:E:504:PHE:HA	2.19	0.41
3:F:493:THR:CG2	3:F:506:PHE:H	2.33	0.41
1:L:94:ASP:O	1:L:95:SER:CB	2.69	0.41
1:A:153:TRP:HB2	1:A:160:VAL:HG22	2.01	0.41
1:C:140:LEU:HD13	2:D:189:VAL:HG21	2.03	0.41
3:E:371:ASN:O	3:E:420:VAL:HA	2.20	0.41
3:G:544:ASN:CB	3:G:545:PRO:HD2	2.48	0.41
2:H:14:PRO:HA	2:H:86:LEU:O	2.21	0.41
1:L:63:ARG:CG	1:L:78:THR:O	2.69	0.41
1:A:12:GLY:O	1:A:13:ALA:HB3	2.21	0.41
2:B:154:PHE:CG	2:B:155:PRO:N	2.89	0.41
1:C:201:THR:HG23	1:C:206:THR:OG1	2.20	0.41
3:F:349:PHE:C	3:F:350:ILE:HD13	2.46	0.41
1:A:201:THR:OG1	1:A:206:THR:OG1	2.38	0.40
1:C:172:GLN:O	1:C:174:ASN:O	2.38	0.40
2:H:87:ARG:NH2	2:H:89:GLU:OE1	2.54	0.40
2:D:154:PHE:CD1	2:D:154:PHE:C	2.99	0.40
3:E:344:SER:O	3:E:346:PHE:N	2.51	0.40
3:F:465:LEU:HD23	3:F:465:LEU:HA	1.94	0.40
3:G:343:PRO:HB2	3:G:348:LEU:HD22	2.02	0.40
1:A:160:VAL:CG2	1:A:161:LYS:N	2.73	0.40
2:D:61:ALA:O	2:D:62:GLU:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LYS:O	1:A:161:LYS:HG2	2.22	0.40
3:G:371:ASN:HB2	3:G:421:THR:HG21	1.91	0.40
2:H:150:VAL:CG1	2:H:186:LEU:CD1	2.96	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	211/217 (97%)	189 (90%)	16 (8%)	6 (3%)	4	9
1	C	211/217 (97%)	189 (90%)	15 (7%)	7 (3%)	3	7
1	L	177/217 (82%)	146 (82%)	21 (12%)	10 (6%)	1	2
2	B	216/229 (94%)	204 (94%)	7 (3%)	5 (2%)	5	11
2	D	215/229 (94%)	200 (93%)	12 (6%)	3 (1%)	9	19
2	H	200/229 (87%)	174 (87%)	16 (8%)	10 (5%)	1	2
3	E	202/242 (84%)	175 (87%)	14 (7%)	13 (6%)	1	1
3	F	202/242 (84%)	181 (90%)	16 (8%)	5 (2%)	4	10
3	G	209/242 (86%)	191 (91%)	10 (5%)	8 (4%)	2	5
All	All	1843/2064 (89%)	1649 (90%)	127 (7%)	67 (4%)	2	5

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
1	A	146	PRO
1	A	213	PRO
2	B	155	PRO
2	B	157	PRO

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Mol	Chain	Res	Type
1	C	113	GLN
1	C	146	PRO
1	C	174	ASN
2	D	155	PRO
2	D	157	PRO
3	E	365	PRO
3	E	366	SER
3	E	471	PRO
3	F	471	PRO
3	G	422	HIS
3	G	423	PRO
3	G	471	PRO
3	G	533	PRO
2	H	9	ALA
2	H	63	LYS
2	H	65	GLN
2	H	155	PRO
2	H	157	PRO
1	L	95	SER
1	C	111	LEU
1	C	112	GLY
3	E	368	GLY
3	E	379	GLY
3	E	407	THR
3	F	533	PRO
3	G	457	ARG
2	H	166	ALA
1	L	97	THR
1	A	157	SER
2	B	102	LYS
2	B	141	GLY
2	D	199	THR
3	E	456	SER
3	E	459	LYS
3	E	533	PRO
3	G	426	PRO
3	G	482	GLU
2	H	16	ALA
1	A	13	ALA
1	C	156	ASP
3	E	346	PHE
3	E	378	SER

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Mol	Chain	Res	Type
2	H	41	PRO
1	L	43	GLY
1	L	124	PRO
1	L	125	PRO
1	L	156	ASP
1	A	156	ASP
2	B	135	SER
1	C	162	ALA
3	F	366	SER
2	H	99	VAL
1	L	7	PRO
1	L	26	SER
1	L	96	PRO
3	F	472	GLU
3	G	456	SER
3	E	406	GLY
3	F	500	GLY
2	H	131	PRO
1	L	213	PRO
3	E	532	SER

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	179/183 (98%)	161 (90%)	18 (10%)	7	15
1	C	179/183 (98%)	162 (90%)	17 (10%)	8	17
1	L	158/183 (86%)	135 (85%)	23 (15%)	3	5
2	B	184/193 (95%)	169 (92%)	15 (8%)	10	23
2	D	183/193 (95%)	168 (92%)	15 (8%)	10	23
2	H	173/193 (90%)	147 (85%)	26 (15%)	3	5
3	E	183/213 (86%)	151 (82%)	32 (18%)	2	3
3	F	182/213 (85%)	161 (88%)	21 (12%)	5	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	186/213 (87%)	165 (89%)	21 (11%)	5	11
All	All	1607/1767 (91%)	1419 (88%)	188 (12%)	5	10

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	10	VAL
1	A	16	GLN
1	A	44	THR
1	A	69	SER
1	A	74	SER
1	A	107	LYS
1	A	108	LEU
1	A	134	LYS
1	A	146	PRO
1	A	150	THR
1	A	168	THR
1	A	172	GLN
1	A	180	SER
1	A	185	LEU
1	A	188	GLU
1	A	201	THR
1	A	210	THR
2	B	13	LYS
2	B	17	THR
2	B	21	SER
2	B	100	MET
2	B	103	TRP
2	B	132	LEU
2	B	146	LEU
2	B	156	GLU
2	B	158	VAL
2	B	159	THR
2	B	168	THR
2	B	169	SER
2	B	186	LEU
2	B	197	LEU
2	B	209	LYS
1	C	19	THR
1	C	44	THR
1	C	56	ARG

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Mol	Chain	Res	Type
1	C	58	SER
1	C	74	SER
1	C	104	THR
1	C	107	LYS
1	C	127	SER
1	C	134	LYS
1	C	137	LEU
1	C	140	LEU
1	C	146	PRO
1	C	150	THR
1	C	158	SER
1	C	180	SER
1	C	191	LYS
1	C	205	SER
2	D	1	GLU
2	D	19	LYS
2	D	45	LEU
2	D	63	LYS
2	D	86	LEU
2	D	99	VAL
2	D	113	ARG
2	D	156	GLU
2	D	168	THR
2	D	186	LEU
2	D	190	VAL
2	D	199	THR
2	D	221	PRO
2	D	222	LYS
2	D	223	SER
3	E	339	TYR
3	E	340	LEU
3	E	344	SER
3	E	363	LEU
3	E	370	VAL
3	E	371	ASN
3	E	378	SER
3	E	382	VAL
3	E	392	GLN
3	E	401	SER
3	E	407	THR
3	E	411	ILE
3	E	419	ARG

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Mol	Chain	Res	Type
3	E	421	THR
3	E	437	SER
3	E	452	GLU
3	E	457	ARG
3	E	479	LEU
3	E	485	LEU
3	E	494	GLN
3	E	498	THR
3	E	508	ARG
3	E	509	LEU
3	E	511	VAL
3	E	513	ARG
3	E	518	GLN
3	E	519	LYS
3	E	525	ARG
3	E	534	SER
3	E	535	GLN
3	E	541	VAL
3	E	543	VAL
3	F	355	THR
3	F	363	LEU
3	F	367	LYS
3	F	369	THR
3	F	400	THR
3	F	408	ARG
3	F	421	THR
3	F	427	ARG
3	F	430	MET
3	F	462	LEU
3	F	465	LEU
3	F	477	GLN
3	F	479	LEU
3	F	483	VAL
3	F	485	LEU
3	F	492	THR
3	F	493	THR
3	F	498	THR
3	F	518	GLN
3	F	532	SER
3	F	536	THR
3	G	348	LEU
3	G	363	LEU

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Mol	Chain	Res	Type
3	G	369	THR
3	G	370	VAL
3	G	372	LEU
3	G	390	GLU
3	G	411	ILE
3	G	419	ARG
3	G	421	THR
3	G	429	LEU
3	G	430	MET
3	G	440	ARG
3	G	450	THR
3	G	457	ARG
3	G	460	ARG
3	G	483	VAL
3	G	485	LEU
3	G	497	LYS
3	G	505	VAL
3	G	537	VAL
3	G	539	ARG
2	H	11	VAL
2	H	17	THR
2	H	18	VAL
2	H	30	THR
2	H	34	ILE
2	H	45	LEU
2	H	55	ASN
2	H	65	GLN
2	H	74	THR
2	H	83	LEU
2	H	86	LEU
2	H	87	ARG
2	H	89	GLU
2	H	91	THR
2	H	99	VAL
2	H	116	LEU
2	H	117	VAL
2	H	148	CYS
2	H	158	VAL
2	H	159	THR
2	H	167	LEU
2	H	186	LEU
2	H	199	THR

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Mol	Chain	Res	Type
2	H	201	THR
2	H	204	CYS
2	H	206	VAL
1	L	5	THR
1	L	9	SER
1	L	16	GLN
1	L	20	ILE
1	L	21	SER
1	L	23	THR
1	L	67	SER
1	L	77	ILE
1	L	93	TYR
1	L	99	THR
1	L	109	THR
1	L	110	VAL
1	L	122	LEU
1	L	141	ILE
1	L	142	SER
1	L	149	VAL
1	L	168	THR
1	L	180	SER
1	L	184	SER
1	L	188	GLU
1	L	194	ARG
1	L	208	GLU
1	L	214	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	81	GLN
1	A	199	GLN
2	B	65	GLN
2	B	179	GLN
2	B	207	ASN
1	C	55	ASN
2	D	172	HIS
2	D	200	GLN
3	E	383	ASN
3	E	392	GLN
3	E	417	GLN

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Mol	Chain	Res	Type
3	E	484	GLN
3	E	535	GLN
3	E	538	GLN
3	F	422	HIS
3	G	468	ASN
3	G	481	ASN
3	G	535	GLN
3	G	544	ASN
2	H	172	HIS
1	L	6	GLN
1	L	199	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 ⓘ

17 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	$\# Z > 2$
4	NAG	I	1	4,3	14,14,15	0.84	0	17,19,21	1.06	0
4	NAG	I	2	4	14,14,15	0.70	0	17,19,21	1.46	3 (17%)
4	BMA	I	3	4	11,11,12	0.73	0	15,15,17	1.61	5 (33%)
4	MAN	I	4	4	11,11,12	0.69	0	15,15,17	1.52	3 (20%)
4	MAN	I	5	4	11,11,12	0.59	0	15,15,17	0.84	0
4	MAN	I	6	4	11,11,12	0.86	0	15,15,17	1.66	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	J	1	3,5	14,14,15	0.98	0	17,19,21	1.40	2 (11%)
5	NAG	J	2	5	14,14,15	0.84	1 (7%)	17,19,21	2.69	9 (52%)
5	BMA	J	3	5	11,11,12	0.83	0	15,15,17	1.53	2 (13%)
5	BMA	J	4	5	11,11,12	0.99	1 (9%)	15,15,17	1.66	4 (26%)
5	MAN	J	5	5	11,11,12	0.96	1 (9%)	15,15,17	1.57	3 (20%)
6	NAG	K	1	6,3	14,14,15	1.35	2 (14%)	17,19,21	2.20	4 (23%)
6	NAG	K	2	6	14,14,15	0.86	1 (7%)	17,19,21	2.13	4 (23%)
6	BMA	K	3	6	11,11,12	1.10	0	15,15,17	2.40	5 (33%)
6	MAN	K	4	6	11,11,12	0.70	0	15,15,17	2.78	4 (26%)
6	MAN	K	5	6	11,11,12	0.81	0	15,15,17	2.79	5 (33%)
6	BMA	K	6	6	11,11,12	0.59	0	15,15,17	1.51	2 (13%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	1	NAG	O5-C1	-3.59	1.37	1.43
5	J	4	BMA	C2-C3	2.43	1.56	1.52
6	K	2	NAG	O5-C1	-2.41	1.39	1.43
6	K	1	NAG	O5-C5	-2.30	1.39	1.43
5	J	5	MAN	C2-C3	2.23	1.55	1.52
5	J	2	NAG	C2-N2	-2.21	1.42	1.46

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	5	MAN	C1-C2-C3	-8.87	96.73	109.64
6	K	4	MAN	C1-O5-C5	7.94	122.83	112.19
6	K	2	NAG	O5-C1-C2	-7.06	100.37	111.29
6	K	3	BMA	O3-C3-C2	5.55	121.37	110.05
5	J	2	NAG	C2-N2-C7	5.28	129.97	122.90
6	K	4	MAN	C1-C2-C3	-5.23	102.03	109.64
6	K	1	NAG	C1-C2-N2	-4.89	102.73	110.43
5	J	2	NAG	C1-O5-C5	4.87	118.71	112.19
6	K	3	BMA	C3-C4-C5	-4.30	102.44	110.23
6	K	1	NAG	C3-C4-C5	-4.21	102.60	110.23
5	J	4	BMA	C1-C2-C3	4.19	115.74	109.64
6	K	6	BMA	C3-C4-C5	4.04	117.56	110.23
4	I	6	MAN	C3-C4-C5	4.02	117.52	110.23
5	J	2	NAG	O5-C1-C2	-3.80	105.40	111.29
4	I	2	NAG	C1-O5-C5	3.74	117.20	112.19
5	J	5	MAN	C1-C2-C3	3.66	114.97	109.64
6	K	1	NAG	C6-C5-C4	3.62	121.91	113.02
5	J	2	NAG	C1-C2-N2	3.62	116.13	110.43
6	K	3	BMA	O5-C5-C6	3.46	114.39	107.66
4	I	6	MAN	C2-C3-C4	3.40	116.84	110.86
5	J	2	NAG	C8-C7-N2	3.25	121.50	116.12
4	I	3	BMA	C1-O5-C5	3.20	116.47	112.19
6	K	5	MAN	C1-O5-C5	-3.19	107.91	112.19
5	J	3	BMA	C1-O5-C5	3.15	116.41	112.19
6	K	3	BMA	C1-O5-C5	-3.10	108.04	112.19
4	I	4	MAN	C1-C2-C3	3.02	114.04	109.64
5	J	1	NAG	O5-C1-C2	-3.02	106.62	111.29
5	J	3	BMA	C1-C2-C3	3.01	114.03	109.64
4	I	4	MAN	C2-C3-C4	2.98	116.10	110.86
5	J	2	NAG	O7-C7-N2	-2.95	116.77	121.98
6	K	1	NAG	O5-C1-C2	-2.74	107.06	111.29
5	J	2	NAG	O4-C4-C3	-2.73	103.93	110.38
4	I	2	NAG	O4-C4-C3	-2.72	103.96	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	5	MAN	O2-C2-C3	2.70	115.75	110.15
4	I	3	BMA	O3-C3-C4	-2.67	104.07	110.38
5	J	5	MAN	C2-C3-C4	2.61	115.44	110.86
6	K	2	NAG	O7-C7-N2	2.51	126.41	121.98
6	K	4	MAN	O5-C5-C4	2.49	116.89	110.83
4	I	4	MAN	C1-O5-C5	2.48	115.51	112.19
5	J	4	BMA	O5-C5-C6	2.47	112.48	107.66
5	J	2	NAG	C3-C4-C5	-2.43	105.83	110.23
6	K	4	MAN	O3-C3-C4	2.43	116.10	110.38
4	I	3	BMA	C1-C2-C3	2.39	113.12	109.64
6	K	2	NAG	O7-C7-C8	-2.35	117.87	122.05
5	J	1	NAG	C3-C4-C5	-2.33	106.02	110.23
6	K	5	MAN	O5-C5-C6	2.25	112.03	107.66
5	J	4	BMA	O5-C5-C4	-2.24	105.38	110.83
6	K	2	NAG	O5-C5-C6	2.22	111.98	107.66
5	J	2	NAG	O4-C4-C5	2.18	114.69	109.32
5	J	5	MAN	O5-C5-C6	2.17	111.89	107.66
5	J	4	BMA	C2-C3-C4	2.16	114.67	110.86
6	K	3	BMA	O5-C5-C4	-2.12	105.68	110.83
4	I	3	BMA	O4-C4-C5	2.10	114.50	109.32
4	I	6	MAN	O2-C2-C3	2.09	114.47	110.15
4	I	2	NAG	O7-C7-C8	-2.08	118.36	122.05
6	K	5	MAN	C6-C5-C4	2.06	118.08	113.02
6	K	6	BMA	C2-C3-C4	2.04	114.45	110.86
4	I	3	BMA	O4-C4-C3	-2.01	105.64	110.38

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	1	NAG	C4-C5-C6-O6
6	K	4	MAN	C4-C5-C6-O6
6	K	6	BMA	O5-C5-C6-O6
6	K	4	MAN	O5-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
5	J	4	BMA	O5-C5-C6-O6
6	K	5	MAN	C4-C5-C6-O6
4	I	3	BMA	O5-C5-C6-O6
5	J	4	BMA	C4-C5-C6-O6
6	K	5	MAN	O5-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
5	J	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	J	2	NAG	O7-C7-N2-C2
5	J	3	BMA	O5-C5-C6-O6
4	I	3	BMA	C4-C5-C6-O6
5	J	3	BMA	C4-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
6	K	6	BMA	C4-C5-C6-O6

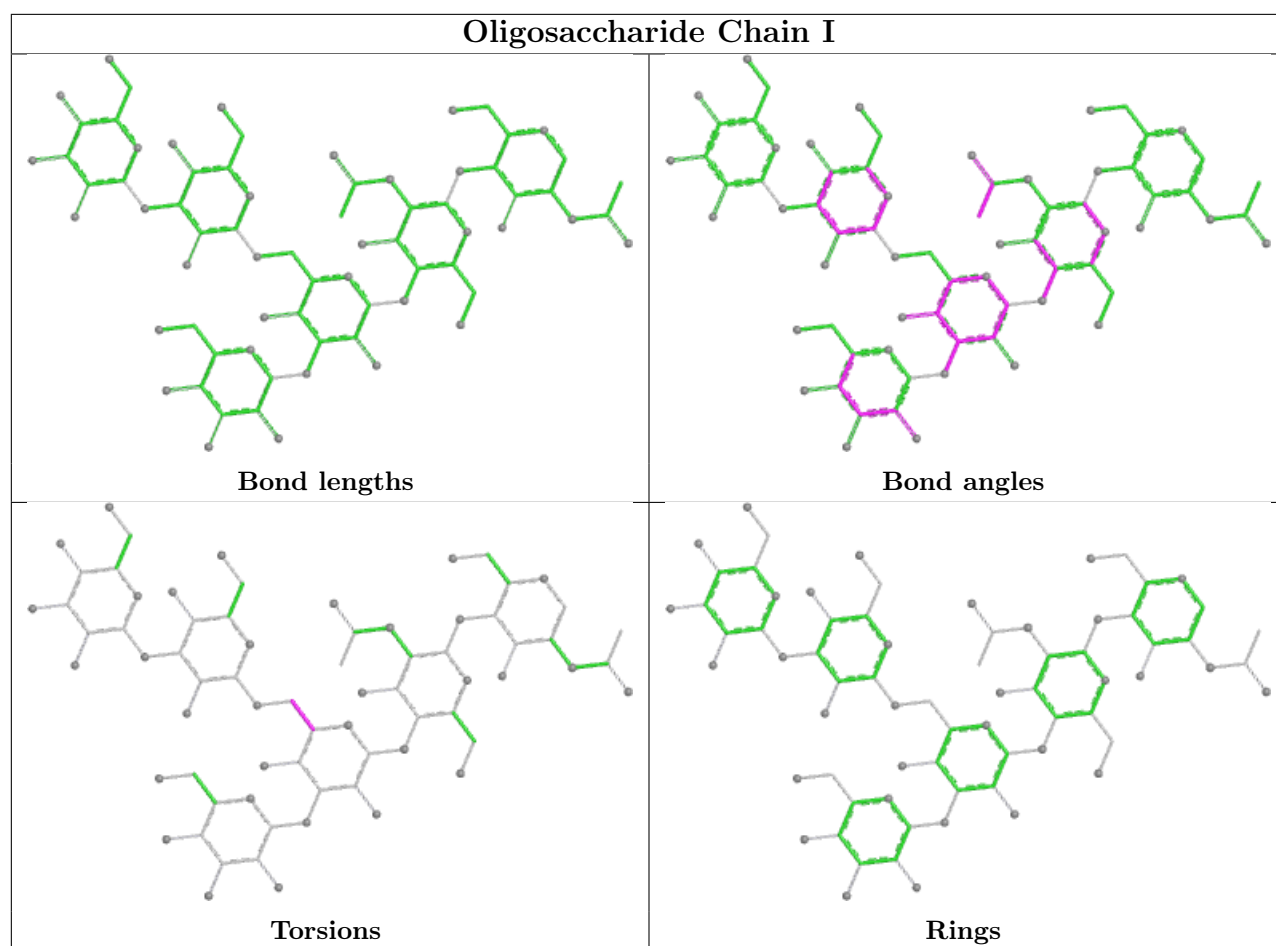
All (1) ring outliers are listed below:

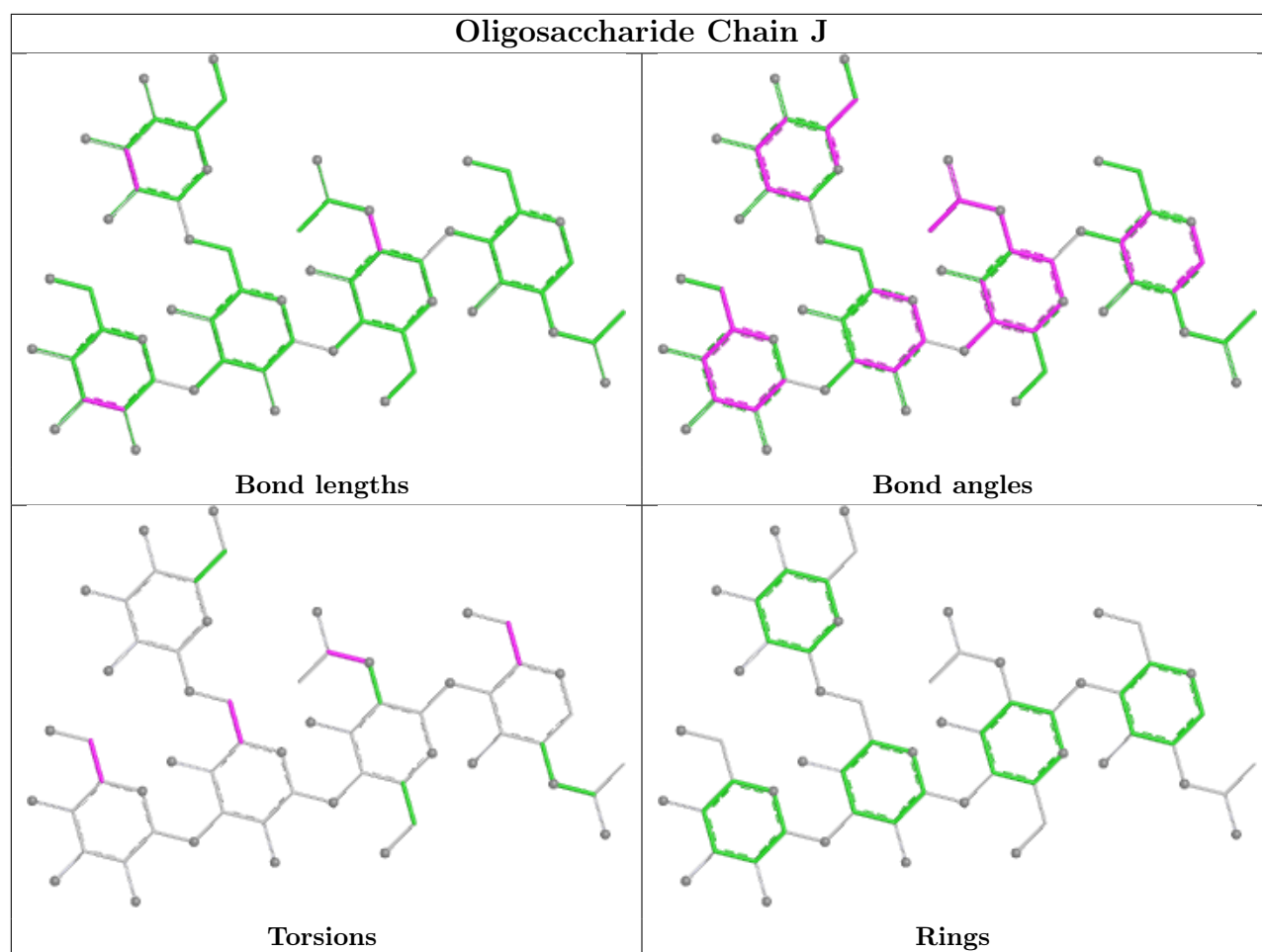
Mol	Chain	Res	Type	Atoms
6	K	5	MAN	C1-C2-C3-C4-C5-O5

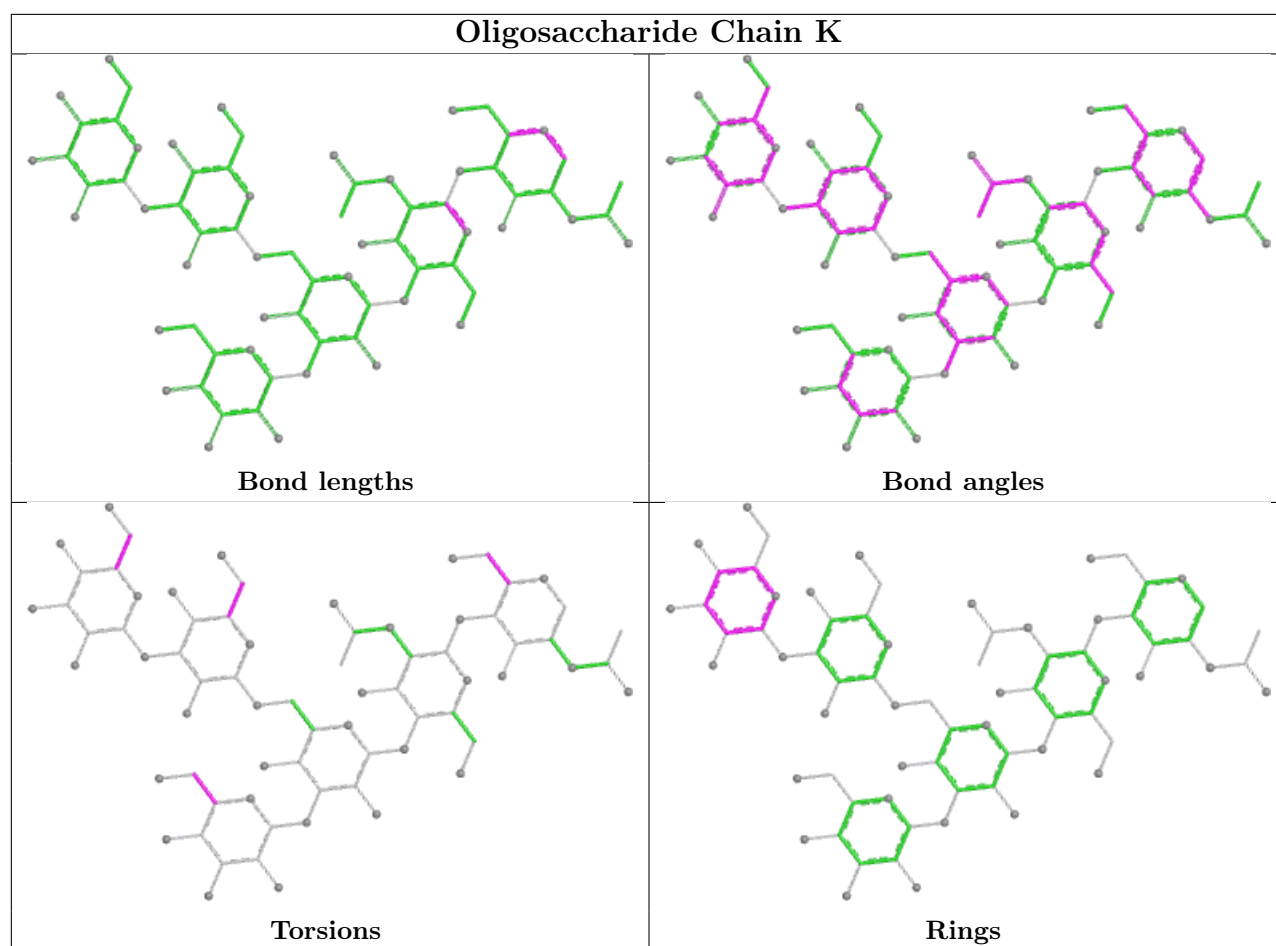
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	3	BMA	1	0
5	J	1	NAG	1	0

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







5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	213/217 (98%)	-0.54	0	100	100	30, 56, 83, 105	0
1	C	213/217 (98%)	-0.55	0	100	100	31, 56, 90, 108	0
1	L	189/217 (87%)	0.67	7 (3%)	45	35	79, 118, 147, 158	0
2	B	220/229 (96%)	-0.77	1 (0%)	87	85	25, 35, 92, 148	0
2	D	219/229 (95%)	-0.82	2 (0%)	81	76	25, 37, 69, 110	0
2	H	208/229 (90%)	0.19	7 (3%)	48	38	60, 89, 127, 157	0
3	E	206/242 (85%)	0.21	5 (2%)	59	51	54, 92, 137, 165	0
3	F	208/242 (85%)	-0.21	4 (1%)	66	59	31, 67, 126, 153	0
3	G	211/242 (87%)	-0.46	2 (0%)	81	76	28, 47, 98, 161	0
All	All	1887/2064 (91%)	-0.27	28 (1%)	72	65	25, 62, 131, 165	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	543	VAL	6.6
2	H	101	GLY	5.2
2	H	197	LEU	4.6
2	D	103	TRP	4.4
1	L	126	SER	3.9
2	H	142	GLY	3.7
3	F	454	PRO	3.6
1	L	114	PRO	3.5
1	L	110	VAL	3.3
3	F	426	PRO	3.2
3	F	451	PRO	3.2
1	L	98	LEU	3.2
1	L	3	VAL	2.9
2	B	103	TRP	2.8
1	L	148	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	106	GLY	2.7
3	E	378	SER	2.7
2	H	194	SER	2.7
2	H	135	SER	2.4
3	E	336	VAL	2.3
3	G	424	HIS	2.2
1	L	116	ALA	2.2
3	E	426	PRO	2.2
3	G	545	PRO	2.1
3	E	500	GLY	2.1
2	D	141	GLY	2.1
2	H	198	GLY	2.0
3	F	459	LYS	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.

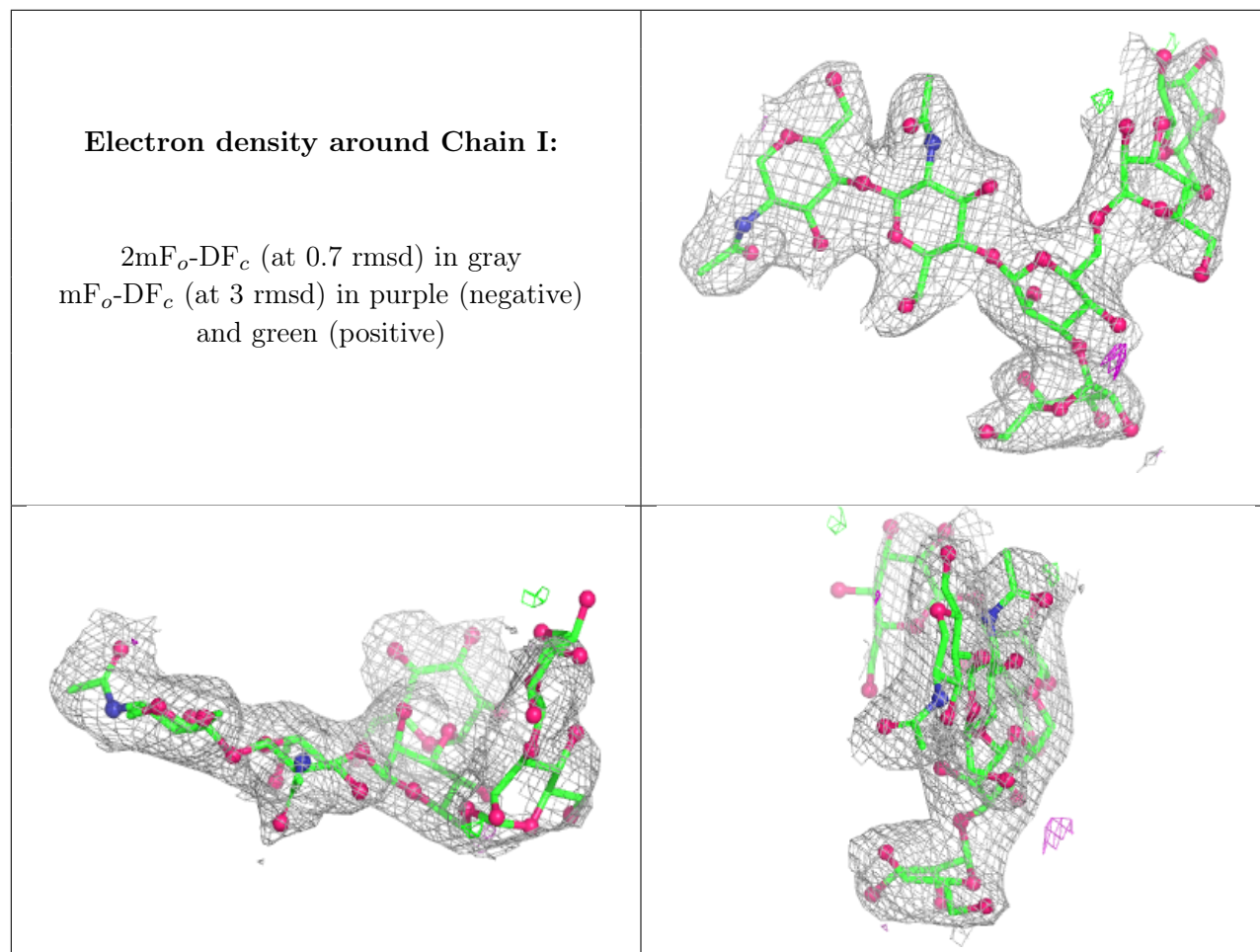
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	I	1	14/15	-	-	47,50,54,55	0
4	NAG	I	2	14/15	-	-	59,62,69,71	0
4	BMA	I	3	11/12	-	-	74,85,96,107	0
4	MAN	I	4	11/12	-	-	101,117,126,143	0
4	MAN	I	5	11/12	-	-	141,147,150,151	0
4	MAN	I	6	11/12	-	-	89,103,107,109	0
5	MAN	J	5	11/12	0.54	0.14	91,95,102,106	0
6	MAN	K	5	11/12	0.74	0.12	83,100,111,119	0
5	BMA	J	3	11/12	0.90	0.08	64,72,81,87	0
5	BMA	J	4	11/12	-	-	85,103,107,114	0
6	NAG	K	2	14/15	0.92	0.08	37,41,44,46	0
6	NAG	K	1	14/15	0.92	0.08	34,37,38,39	0
6	BMA	K	3	11/12	0.94	0.07	51,57,70,76	0
5	NAG	J	2	14/15	0.96	0.06	56,63,68,70	0
6	MAN	K	4	11/12	-	-	81,83,94,97	0

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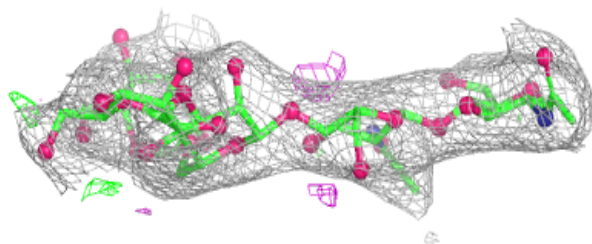
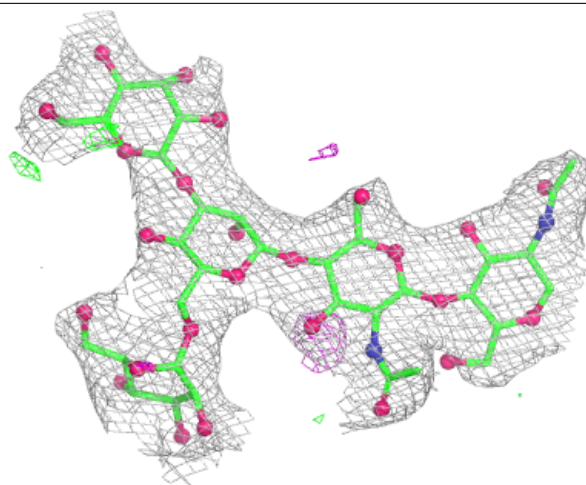
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	J	1	14/15	0.97	0.06	60,62,68,76	0
6	BMA	K	6	11/12	-	-	99,111,121,134	0

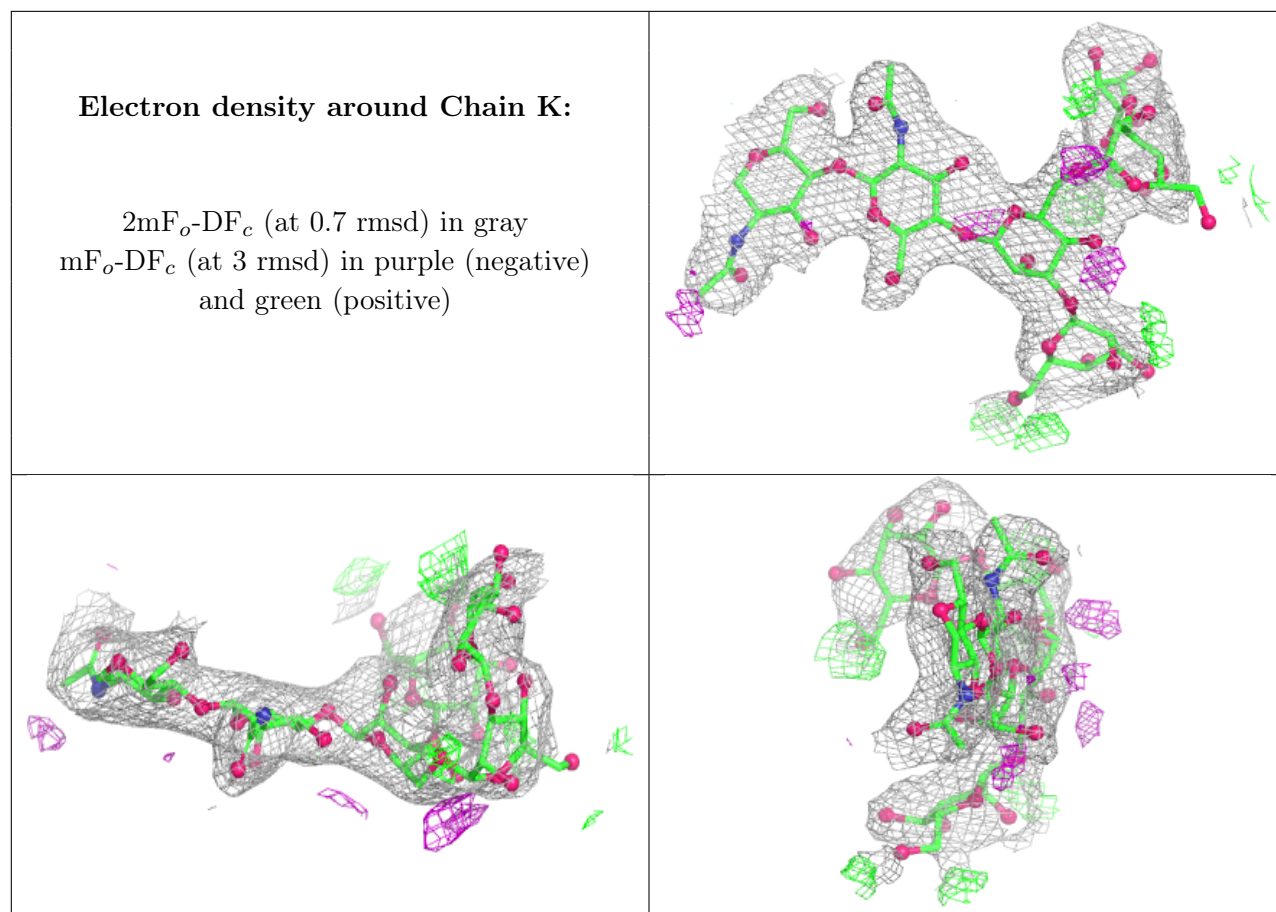
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain J:

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.