



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:41 PM UTC

PDB ID : 4GRW / pdb_00004grw
Title : Structure of a complex of human IL-23 with 3 Nanobodies (Llama vHHs)
Authors : Desmyter, A.; Spinelli, S.; Button, C.; Saunders, M.; de Haard, H.; Rommelaere, H.; Union, A.; Cambillau, C.
Deposited on : 2012-08-27
Resolution : 2.55 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:

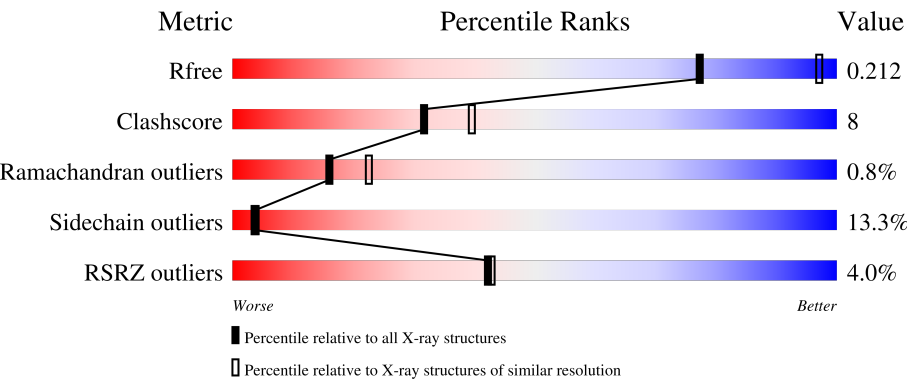
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	189	5% 52%11%5%•31%
1	C	189	2% 62%5%•32%
2	B	328	3% 69%17%••11%
2	D	328	3% 70%15%••11%
3	E	125	80%17%•

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Mol	Chain	Length	Quality of chain
3	G	125	% 79% 18% .
4	F	126	7% 70% 25% . . .
4	J	126	15% 59% 29% 6% . .
5	H	123	% 76% 17% 7%
5	I	123	% 74% 20% 6% .
6	K	5	80% 20%
6	L	5	40% 60%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13131 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 Interleukin-23 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	0	0
			1010	647	181	177	5			
1	C	129	Total	C	N	O	S	0	0	0
			1002	643	179	175	5			

- Molecule 2 is a protein called Interleukin-12 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	293	Total	C	N	O	S	0	0	0
			2331	1478	382	459	12			
2	D	292	Total	C	N	O	S	0	0	0
			2319	1467	379	461	12			

- Molecule 3 is a protein called Nanobody 124C4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	125	Total	C	N	O	S	0	0	0
			938	586	161	187	4			
3	G	125	Total	C	N	O	S	0	0	0
			937	586	161	186	4			

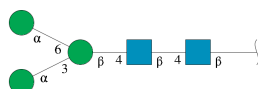
- Molecule 4 is a protein called Nanobody 37D5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	125	Total	C	N	O	S	0	0	0
			954	596	161	192	5			
4	J	122	Total	C	N	O	S	0	0	0
			932	583	158	186	5			

- Molecule 5 is a protein called Nanobody 22E11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	123	Total	C	N	O	S	0	0	0
			938	585	168	182	3			
5	I	123	Total	C	N	O	S	0	0	0
			938	585	168	182	3			

- Molecule 6 is an oligosaccharide called alpha-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.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	K	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	L	5	Total	C	N	O	0	0	0
			61	34	2	25			

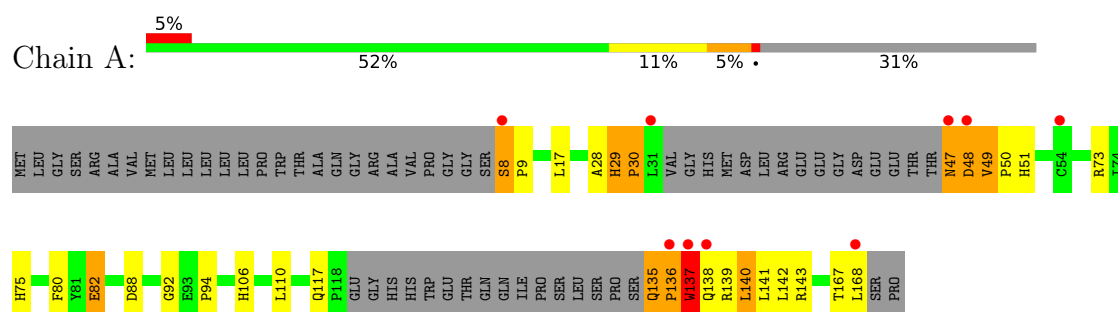
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	24	Total	O	0	0
			24	24		
7	B	143	Total	O	0	0
			143	143		
7	C	48	Total	O	0	0
			48	48		
7	D	187	Total	O	0	0
			187	187		
7	E	67	Total	O	0	0
			67	67		
7	F	38	Total	O	0	0
			38	38		
7	G	57	Total	O	0	0
			57	57		
7	H	50	Total	O	0	0
			50	50		
7	I	73	Total	O	0	0
			73	73		
7	J	23	Total	O	0	0
			23	23		

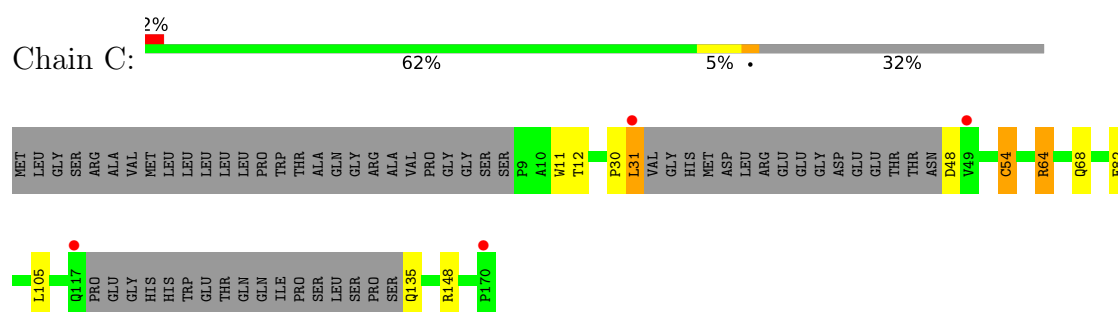
3 Residue-property plots [i](#)

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.

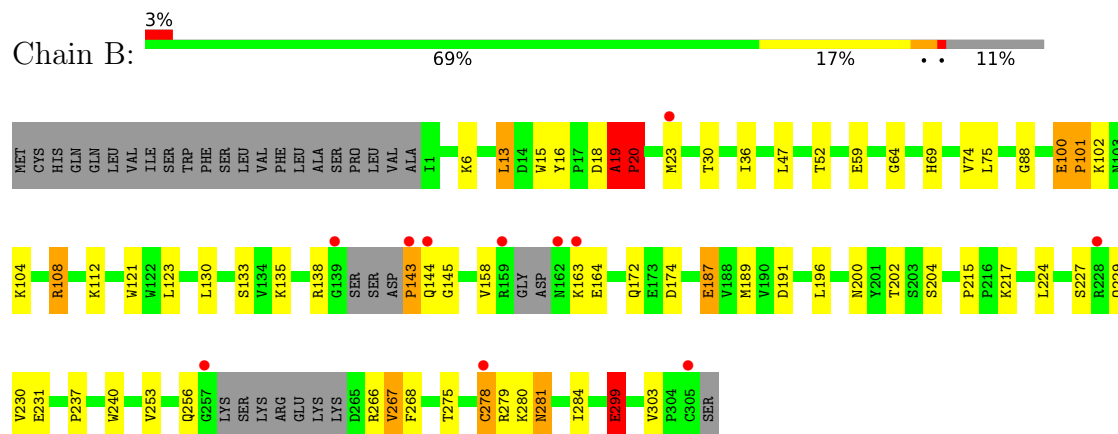
- Molecule 1: Interleukin-23 subunit alpha



- Molecule 1: Interleukin-23 subunit alpha

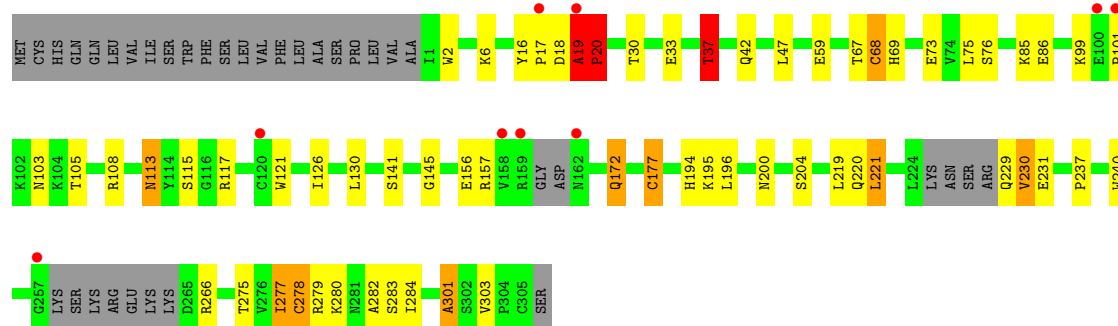


- Molecule 2: Interleukin-12 subunit beta



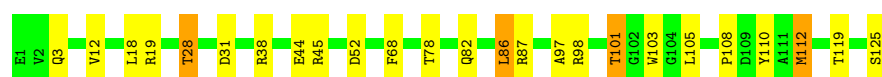
- Molecule 2: Interleukin-12 subunit beta

Chain D: 



• Molecule 3: Nanobody 124C4

Chain E: 



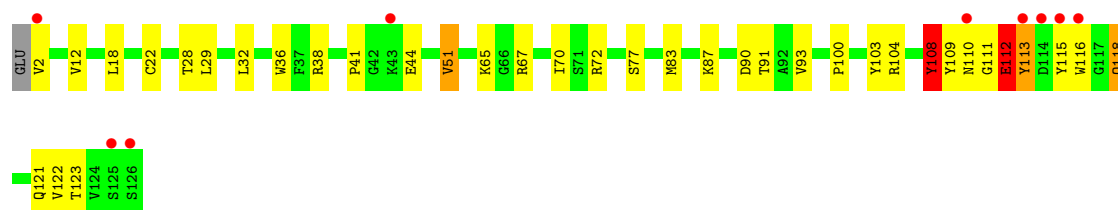
• Molecule 3: Nanobody 124C4

Chain G: 



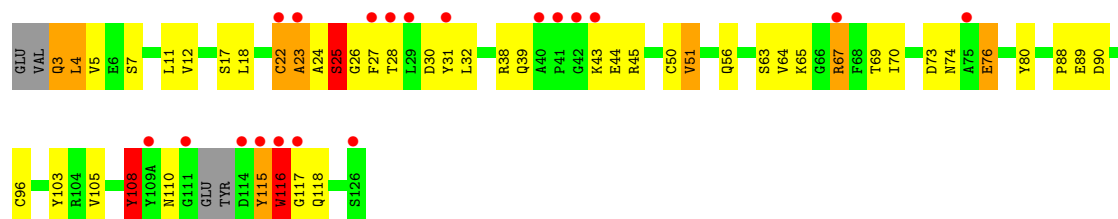
• Molecule 4: Nanobody 37D5

Chain F: 

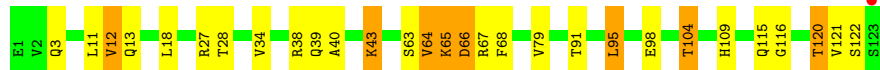
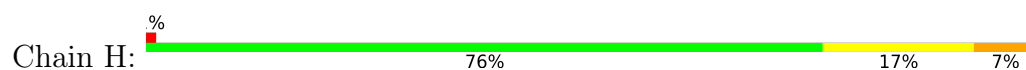


• Molecule 4: Nanobody 37D5

Chain J: 



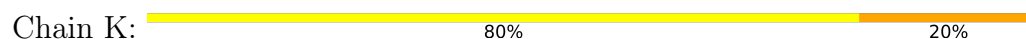
• Molecule 5: Nanobody 22E11



- Molecule 5: Nanobody 22E11



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.27Å 135.14Å 139.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.83 – 2.55 43.83 – 2.55	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.83-2.55) 99.8 (43.83-2.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.54Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.183 , 0.218 (Not available) , 0.212	Depositor DCC
R_{free} test set	1940 reflections (3.06%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13131	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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	0.88	1/1034 (0.1%)	1.45	9/1405 (0.6%)
1	C	0.83	0/1026	1.41	4/1393 (0.3%)
2	B	0.77	0/2387	1.15	7/3241 (0.2%)
2	D	0.77	1/2375 (0.0%)	1.15	7/3228 (0.2%)
3	E	0.90	1/958 (0.1%)	1.22	5/1300 (0.4%)
3	G	0.86	1/957 (0.1%)	1.26	6/1299 (0.5%)
4	F	0.80	1/975 (0.1%)	1.14	2/1323 (0.2%)
4	J	0.80	0/952	1.24	7/1290 (0.5%)
5	H	0.86	0/960	1.12	0/1302
5	I	0.77	0/960	1.09	2/1302 (0.2%)
All	All	0.81	5/12584 (0.0%)	1.21	49/17083 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	B	0	1
4	F	0	2
4	J	0	7
5	H	0	2
5	I	0	1
All	All	0	16

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	108	MET	SD-CE	-9.90	1.54	1.79
3	E	112	MET	SD-CE	-9.59	1.55	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	HIS	C-N	5.99	1.40	1.33
2	D	20	PRO	N-CD	5.53	1.55	1.47
4	F	108	TYR	CA-C	-5.25	1.46	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ARG	N-CA-C	-8.84	101.81	112.59
4	J	110	ASN	CA-C-N	8.24	136.53	121.70
4	J	110	ASN	C-N-CA	8.24	136.53	121.70
2	B	19	ALA	C-N-CD	8.17	138.58	120.60
4	F	108	TYR	N-CA-C	-7.46	97.58	109.59
5	I	18	LEU	N-CA-C	7.08	118.84	108.86
1	A	29	HIS	CA-C-N	-6.69	113.62	120.85
1	A	29	HIS	C-N-CA	-6.69	113.62	120.85
2	D	67	THR	CA-C-N	6.59	131.49	122.19
2	D	67	THR	C-N-CA	6.59	131.49	122.19
2	D	266	ARG	N-CA-C	6.29	119.20	109.07
2	D	19	ALA	C-N-CD	5.85	133.46	120.60
1	A	137	TRP	CA-C-N	5.79	132.12	121.70
1	A	137	TRP	C-N-CA	5.79	132.12	121.70
3	E	101	THR	CB-CA-C	5.70	118.80	109.90
2	D	145	GLY	N-CA-C	5.66	117.99	111.36
3	G	48	ASP	CA-C-N	5.66	128.14	120.38
3	G	48	ASP	C-N-CA	5.66	128.14	120.38
4	J	108	TYR	O-C-N	-5.66	115.11	122.97
4	F	118	GLN	N-CA-C	5.64	117.12	110.97
2	B	18	ASP	N-CA-C	5.60	118.01	109.62
2	B	20	PRO	CA-N-CD	-5.54	103.75	111.50
1	A	140	LEU	N-CA-C	-5.49	105.38	111.36
2	B	74	VAL	N-CA-CB	5.45	116.47	110.53
5	I	61	ALA	N-CA-C	-5.45	101.79	109.96
1	C	11	TRP	N-CA-C	5.39	117.58	111.11
1	C	105	LEU	CA-C-N	5.34	127.44	120.28
1	C	105	LEU	C-N-CA	5.34	127.44	120.28
3	E	119	THR	CB-CA-C	5.32	118.97	109.65
3	G	51	ASP	CA-CB-CG	5.31	117.91	112.60
2	D	37	THR	CB-CA-C	5.22	119.35	109.37
1	A	49	VAL	CA-C-N	-5.16	115.03	120.66
1	A	49	VAL	C-N-CA	-5.16	115.03	120.66
2	B	281	ASN	CA-CB-CG	5.16	117.76	112.60
2	B	230	VAL	N-CA-C	5.13	116.75	108.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	76	GLU	N-CA-C	-5.13	106.86	113.01
1	C	68	GLN	N-CA-C	5.12	116.86	111.28
2	B	299	GLU	N-CA-C	-5.10	103.80	110.53
2	D	301	ALA	N-CA-C	-5.08	100.96	109.24
1	A	29	HIS	CB-CA-C	5.07	116.24	109.65
4	J	30	ASP	CA-CB-CG	5.07	117.67	112.60
3	E	28	THR	CB-CA-C	5.04	118.45	109.38
4	J	43	LYS	CA-C-N	5.03	129.36	120.87
4	J	43	LYS	C-N-CA	5.03	129.36	120.87
3	G	97	THR	CB-CA-C	5.02	118.06	109.72
3	G	25	SER	CA-C-N	5.02	130.73	121.70
3	G	25	SER	C-N-CA	5.02	130.73	121.70
3	E	52	ASP	CA-C-N	5.01	127.50	120.28
3	E	52	ASP	C-N-CA	5.01	127.50	120.28

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	ALA	Peptide
1	A	30	PRO	Peptide
1	A	47	ASN	Peptide
2	B	143	PRO	Peptide
4	F	112	GLU	Peptide
4	F	113	TYR	Peptide
5	H	65	LYS	Peptide
5	H	66	ASP	Peptide
5	I	17	SER	Peptide
4	J	108	TYR	Mainchain
4	J	115	TYR	Peptide
4	J	116	TRP	Peptide
4	J	117	GLY	Peptide
4	J	23	ALA	Peptide
4	J	24	ALA	Peptide
4	J	25	SER	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	1010	0	1006	31	0
1	C	1002	0	1001	5	0
2	B	2331	0	2244	33	0
2	D	2319	0	2215	37	0
3	E	938	0	890	8	0
3	G	937	0	887	9	0
4	F	954	0	888	32	0
4	J	932	0	869	25	0
5	H	938	0	893	11	0
5	I	938	0	893	18	0
6	K	61	0	52	3	0
6	L	61	0	52	7	0
7	A	24	0	0	0	0
7	B	143	0	0	1	0
7	C	48	0	0	1	0
7	D	187	0	0	2	0
7	E	67	0	0	0	0
7	F	38	0	0	0	0
7	G	57	0	0	0	0
7	H	50	0	0	0	0
7	I	73	0	0	1	0
7	J	23	0	0	0	0
All	All	13131	0	11890	194	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 8.

All (194) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:200:ASN:HD21	6:L:1:NAG:C1	1.31	1.44
2:B:200:ASN:HD21	6:K:1:NAG:C1	1.36	1.30
4:J:22:CYS:SG	4:J:96:CYS:SG	1.30	1.29
1:A:137:TRP:HB3	1:A:138:GLN:HB3	1.18	1.18
1:A:137:TRP:HB3	1:A:138:GLN:CB	1.79	1.11
2:D:19:ALA:HB1	2:D:20:PRO:CA	1.82	1.10
2:B:19:ALA:HB1	2:B:20:PRO:HA	1.30	1.05
1:A:135:GLN:HE21	1:A:135:GLN:HA	1.14	1.05
2:D:19:ALA:CB	2:D:20:PRO:HA	1.78	1.04
5:H:104:THR:HG21	5:H:109:HIS:HD2	1.23	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:104:THR:HG21	5:H:109:HIS:CD2	1.98	0.99
5:I:104:THR:HG21	5:I:109:HIS:HD2	1.28	0.98
5:I:104:THR:HG21	5:I:109:HIS:CD2	2.01	0.96
4:F:104:ARG:NH1	4:F:113:TYR:CB	2.31	0.93
4:J:73:ASP:HB2	4:J:80:TYR:HE2	1.34	0.93
1:A:137:TRP:CB	1:A:138:GLN:HB3	1.99	0.92
2:D:19:ALA:HB1	2:D:20:PRO:HA	0.93	0.92
1:A:137:TRP:HB3	1:A:138:GLN:CA	2.01	0.90
1:A:135:GLN:HA	1:A:135:GLN:NE2	1.87	0.88
1:A:136:PRO:O	1:A:137:TRP:HB2	1.75	0.87
2:B:19:ALA:CB	2:B:20:PRO:HA	2.07	0.83
5:H:104:THR:CG2	5:H:109:HIS:HD2	1.91	0.83
4:F:67:ARG:NH2	4:F:90:ASP:OD2	2.14	0.81
5:I:104:THR:CG2	5:I:109:HIS:HD2	1.92	0.81
4:F:109:TYR:CZ	4:F:111:GLY:HA2	2.16	0.80
2:B:200:ASN:HD22	6:K:1:NAG:C1	1.93	0.79
4:J:115:TYR:HB3	4:J:116:TRP:O	1.82	0.78
4:F:104:ARG:HH12	4:F:113:TYR:CB	1.96	0.77
4:J:63:SER:O	4:J:67:ARG:NH1	2.18	0.77
4:F:103:TYR:O	4:F:108:TYR:O	2.04	0.75
2:B:253:VAL:HB	2:B:267:VAL:HG13	1.68	0.74
3:G:79:MET:HE1	3:G:117:VAL:HG21	1.68	0.74
2:D:16:TYR:HB2	2:D:17:PRO:CD	2.18	0.73
1:A:47:ASN:OD1	2:D:277:ILE:HD11	1.89	0.73
4:J:73:ASP:HB2	4:J:80:TYR:CE2	2.22	0.72
4:F:109:TYR:CE1	4:F:111:GLY:HA2	2.26	0.70
1:C:54:CYS:HG	2:D:177:CYS:HG	1.38	0.70
4:F:112:GLU:OE2	4:F:112:GLU:HA	1.91	0.69
4:J:22:CYS:CB	4:J:96:CYS:SG	2.78	0.69
2:D:219:LEU:HD11	2:D:301:ALA:HB1	1.74	0.69
4:J:4:LEU:HA	4:J:23:ALA:O	1.93	0.69
4:F:104:ARG:HD3	4:F:110:ASN:HB2	1.73	0.69
5:H:40:ALA:HB3	5:H:43:LYS:HG3	1.76	0.68
4:F:109:TYR:CZ	4:F:111:GLY:CA	2.77	0.68
2:B:280:LYS:O	2:B:281:ASN:HB2	1.95	0.67
2:B:144:GLN:NE2	2:B:144:GLN:HA	2.11	0.65
2:B:145:GLY:O	2:B:174:ASP:N	2.27	0.65
5:I:27:ARG:NH1	5:I:77:ASN:OD1	2.31	0.64
2:D:16:TYR:HB2	2:D:17:PRO:HD2	1.78	0.64
2:D:221:LEU:HB2	2:D:230:VAL:HG11	1.79	0.63
4:F:29:LEU:HD23	4:F:32:LEU:HD12	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:PRO:HD3	1:A:80:PHE:CD2	2.34	0.62
2:B:13:LEU:CD1	2:B:15:TRP:HB2	2.30	0.62
1:A:137:TRP:CB	1:A:138:GLN:CB	2.66	0.62
2:B:215:PRO:HG3	2:B:299:GLU:HG2	1.82	0.62
1:A:136:PRO:HG2	1:A:137:TRP:CD1	2.34	0.62
1:A:135:GLN:HE21	1:A:135:GLN:CA	2.03	0.61
4:J:67:ARG:NH2	4:J:90:ASP:OD2	2.34	0.61
3:G:8:GLY:O	3:G:18:LEU:HD21	2.00	0.60
1:A:137:TRP:HB3	1:A:138:GLN:C	2.27	0.60
2:B:138:ARG:O	2:B:143:PRO:HB2	2.02	0.59
4:J:5:VAL:N	4:J:23:ALA:O	2.32	0.59
2:B:19:ALA:HB1	2:B:20:PRO:CA	2.19	0.58
2:D:19:ALA:CB	2:D:20:PRO:CA	2.57	0.58
2:B:278:CYS:SG	2:B:284:ILE:HD11	2.44	0.58
4:F:109:TYR:CE1	4:F:111:GLY:CA	2.86	0.58
2:D:172:GLN:HE22	3:E:103:TRP:HH2	1.52	0.58
5:H:64:VAL:HG11	5:H:68:PHE:CD2	2.39	0.57
1:A:47:ASN:N	1:A:48:ASP:HB2	2.19	0.57
2:B:13:LEU:HD13	2:B:15:TRP:HB2	1.85	0.57
1:A:48:ASP:HB2	2:D:277:ILE:HD13	1.85	0.56
2:D:37:THR:HG22	2:D:69:HIS:HB2	1.87	0.56
4:F:104:ARG:CD	4:F:110:ASN:HB2	2.34	0.56
4:F:115:TYR:CD1	4:F:116:TRP:N	2.73	0.56
2:D:278:CYS:SG	2:D:284:ILE:HD11	2.46	0.56
4:J:50:CYS:HB2	4:J:105:VAL:HG21	1.88	0.55
4:F:103:TYR:C	4:F:108:TYR:O	2.48	0.55
5:I:43:LYS:HD3	5:I:44:GLU:H	1.71	0.55
4:J:3:GLN:HB3	4:J:25:SER:O	2.06	0.55
1:A:94:PRO:CG	1:A:140:LEU:HD21	2.37	0.55
2:B:187:GLU:HB2	2:B:189:MET:HE2	1.89	0.55
1:A:136:PRO:O	1:A:137:TRP:CB	2.50	0.54
1:A:8:SER:N	1:A:9:PRO:HD3	2.22	0.54
1:A:94:PRO:HG2	1:A:140:LEU:HD21	1.89	0.54
4:J:51:VAL:HG13	4:J:70:ILE:HG23	1.87	0.54
2:B:19:ALA:CB	2:B:20:PRO:CA	2.83	0.54
2:B:108:ARG:HD2	2:B:121:TRP:CZ2	2.41	0.54
1:C:64:ARG:HG3	3:E:31:ASP:OD2	2.08	0.54
5:I:1:GLU:HA	7:I:247:HOH:O	2.07	0.54
1:A:137:TRP:CG	1:A:138:GLN:HB3	2.42	0.54
2:B:224:LEU:HD12	2:B:229:GLN:HG2	1.90	0.54
3:G:13:GLN:NE2	3:G:13:GLN:H	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:93:ALA:HB3	3:G:108:MET:HE2	1.91	0.52
2:B:143:PRO:O	2:B:145:GLY:N	2.42	0.52
1:C:12:THR:HG22	7:C:225:HOH:O	2.10	0.52
4:J:26:GLY:N	4:J:27:PHE:CD1	2.78	0.52
7:D:572:HOH:O	5:I:109:HIS:HE1	1.92	0.52
4:J:3:GLN:HA	4:J:3:GLN:OE1	2.10	0.52
4:F:51:VAL:HG13	4:F:70:ILE:HG23	1.91	0.52
1:C:30:PRO:O	1:C:31:LEU:HB2	2.10	0.52
4:J:25:SER:OG	4:J:26:GLY:HA2	2.09	0.51
2:D:115:SER:HB2	3:E:103:TRP:CE2	2.45	0.51
1:A:47:ASN:N	1:A:48:ASP:CB	2.74	0.51
4:J:26:GLY:N	4:J:27:PHE:HD1	2.08	0.51
5:H:12:VAL:HG11	5:H:18:LEU:HD23	1.93	0.50
3:E:97:ALA:HB3	3:E:112:MET:HE2	1.92	0.50
1:A:75:HIS:CE1	1:A:117:GLN:HB2	2.47	0.50
2:D:19:ALA:HB3	7:D:521:HOH:O	2.11	0.50
1:A:47:ASN:HB2	2:D:277:ILE:CD1	2.42	0.50
4:F:67:ARG:HH22	4:F:90:ASP:CG	2.20	0.49
2:D:86:GLU:OE1	5:I:52:ARG:NH2	2.46	0.49
2:D:117:ARG:HB2	2:D:172:GLN:NE2	2.28	0.49
3:G:87:THR:HG23	3:G:118:THR:HA	1.93	0.49
3:E:12:VAL:HG11	3:E:86:LEU:HD23	1.96	0.48
2:D:200:ASN:HD22	6:L:1:NAG:C1	2.09	0.48
4:F:110:ASN:C	4:F:112:GLU:H	2.20	0.48
2:B:217:LYS:NZ	3:G:54:ALA:O	2.46	0.48
2:D:101:PRO:HG2	2:D:105:THR:HG21	1.95	0.48
2:D:113:ASN:HD22	2:D:115:SER:H	1.61	0.47
4:F:110:ASN:C	4:F:112:GLU:N	2.69	0.47
5:I:18:LEU:CD1	5:I:83:MET:HE3	2.44	0.47
4:F:111:GLY:C	4:F:113:TYR:H	2.22	0.47
5:H:64:VAL:HG11	5:H:68:PHE:CE2	2.49	0.47
1:A:94:PRO:HB3	4:J:108:TYR:CZ	2.49	0.47
2:B:100:GLU:HA	2:B:101:PRO:C	2.40	0.47
5:H:64:VAL:CG1	5:H:68:PHE:CD2	2.98	0.47
5:H:95:LEU:HD12	5:H:116:GLY:CA	2.45	0.47
2:D:200:ASN:ND2	6:L:1:NAG:H82	2.30	0.47
5:I:104:THR:CG2	5:I:109:HIS:CD2	2.78	0.47
2:B:16:TYR:CD1	4:F:41:PRO:HB2	2.51	0.46
2:D:68:CYS:HB2	2:D:76:SER:O	2.15	0.46
1:C:30:PRO:HD2	4:F:100:PRO:HG3	1.96	0.46
2:B:266:ARG:NH2	4:J:25:SER:OG	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:27:PHE:CD1	4:J:27:PHE:N	2.84	0.46
2:B:237:PRO:HG2	2:B:240:TRP:HB2	1.96	0.46
2:D:68:CYS:HB3	2:D:75:LEU:HB2	1.97	0.46
2:D:117:ARG:HB2	2:D:172:GLN:HE21	1.81	0.46
4:F:111:GLY:C	4:F:113:TYR:N	2.73	0.45
1:A:137:TRP:CB	1:A:138:GLN:CA	2.84	0.45
4:F:22:CYS:HB2	4:F:36:TRP:CZ2	2.52	0.45
5:I:28:THR:HG22	5:I:98:GLU:OE1	2.16	0.45
3:G:14:PRO:HG2	3:G:121:SER:HA	1.99	0.45
2:D:18:ASP:O	2:D:19:ALA:HB3	2.17	0.45
4:F:32:LEU:O	4:F:72:ARG:NH1	2.46	0.45
5:H:34:VAL:HB	5:H:79:VAL:HG21	1.99	0.45
5:I:88:PRO:HA	5:I:121:VAL:HB	1.99	0.45
5:I:95:LEU:HD12	5:I:116:GLY:CA	2.47	0.45
6:L:3:BMA:H61	6:L:5:MAN:H2	1.60	0.45
5:I:27:ARG:HD2	5:I:53:TRP:CD1	2.52	0.44
1:A:49:VAL:HG23	1:A:51:HIS:CE1	2.52	0.44
2:D:279:ARG:HB2	2:D:282:ALA:HB2	1.99	0.44
4:F:91:THR:HG23	4:F:123:THR:HA	1.99	0.44
5:I:67:ARG:C	5:I:68:PHE:HD1	2.25	0.44
4:J:25:SER:CB	4:J:26:GLY:HA2	2.47	0.44
2:D:237:PRO:HG2	2:D:240:TRP:HB2	2.00	0.44
2:B:30:THR:HG21	2:B:75:LEU:HD13	1.99	0.43
2:D:2:TRP:CH2	6:L:1:NAG:H2	2.52	0.43
2:D:30:THR:HG21	2:D:75:LEU:HD13	2.01	0.43
2:D:126:ILE:HG21	2:D:194:HIS:CD2	2.54	0.43
2:D:200:ASN:HD21	6:L:1:NAG:H82	1.84	0.43
2:D:108:ARG:HD3	2:D:121:TRP:CZ2	2.53	0.43
3:E:19:ARG:HG3	3:E:82:GLN:NE2	2.34	0.42
5:I:68:PHE:N	5:I:68:PHE:CD1	2.86	0.42
1:A:47:ASN:HB2	2:D:277:ILE:HD12	2.00	0.42
4:J:64:VAL:HA	4:J:67:ARG:NH1	2.34	0.42
2:B:64:GLY:HA2	2:B:196:LEU:HD21	2.01	0.42
4:J:4:LEU:CA	4:J:23:ALA:O	2.66	0.42
4:F:116:TRP:HA	4:F:116:TRP:CE3	2.55	0.42
1:A:82:GLU:OE2	1:A:106:HIS:HE1	2.03	0.41
4:F:83:MET:HE1	4:F:122:VAL:HG21	2.02	0.41
5:I:34:VAL:HB	5:I:79:VAL:HG21	2.01	0.41
6:L:1:NAG:H83	6:L:1:NAG:H3	2.02	0.41
2:D:221:LEU:HD23	2:D:221:LEU:H	1.84	0.41
5:I:83:MET:HE1	5:I:119:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:PRO:HG3	4:J:32:LEU:HD21	2.03	0.41
4:F:115:TYR:HD1	4:F:116:TRP:H	1.67	0.41
4:F:93:VAL:HG22	4:F:121:GLN:HG2	2.03	0.41
4:F:110:ASN:ND2	4:F:112:GLU:HB2	2.36	0.41
2:B:36:ILE:HA	2:B:69:HIS:O	2.20	0.41
1:A:143:ARG:NH1	4:J:103:TYR:OH	2.51	0.40
2:B:88:GLY:HA3	4:F:121:GLN:CD	2.47	0.40
7:B:627:HOH:O	6:K:1:NAG:H82	2.21	0.40
3:G:13:GLN:H	3:G:13:GLN:HE21	1.69	0.40
5:H:91:THR:HG23	5:H:120:THR:HA	2.03	0.40
2:B:16:TYR:CE1	4:F:41:PRO:HB2	2.56	0.40
2:B:133:SER:HB3	2:B:191:ASP:HB2	2.03	0.40
2:B:215:PRO:CG	2:B:299:GLU:HG2	2.51	0.40
2:B:266:ARG:HD3	2:B:268:PHE:CE2	2.56	0.40
3:E:108:PRO:HG2	3:E:110:TYR:CZ	2.56	0.40
1:A:167:THR:OG1	1:A:168:LEU:HD12	2.22	0.40
2:B:13:LEU:HD11	2:B:15:TRP:HB2	2.04	0.40
3:E:68:PHE:HA	3:E:82:GLN:O	2.21	0.40
3:G:95:VAL:HG22	3:G:108:MET:HE1	2.02	0.40
4:J:26:GLY:H	4:J:27:PHE:HD1	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	124/189 (66%)	118 (95%)	2 (2%)	4 (3%)	3	2
1	C	123/189 (65%)	120 (98%)	3 (2%)	0	100	100
2	B	285/328 (87%)	269 (94%)	14 (5%)	2 (1%)	18	25
2	D	284/328 (87%)	268 (94%)	13 (5%)	3 (1%)	11	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	123/125 (98%)	123 (100%)	0	0	100	100
3	G	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
4	F	123/126 (98%)	118 (96%)	5 (4%)	0	100	100
4	J	118/126 (94%)	109 (92%)	7 (6%)	2 (2%)	7	8
5	H	121/123 (98%)	118 (98%)	2 (2%)	1 (1%)	16	22
5	I	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
All	All	1545/1782 (87%)	1485 (96%)	48 (3%)	12 (1%)	16	22

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	A	136	PRO
2	B	19	ALA
2	D	19	ALA
4	J	116	TRP
1	A	137	TRP
2	D	280	LYS
5	H	66	ASP
2	B	101	PRO
2	D	195	LYS
1	A	92	GLY
4	J	88	PRO

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	109/159 (69%)	99 (91%)	10 (9%)	8	10
1	C	108/159 (68%)	101 (94%)	7 (6%)	15	22
2	B	263/297 (89%)	232 (88%)	31 (12%)	5	5
2	D	262/297 (88%)	231 (88%)	31 (12%)	5	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	96/97 (99%)	83 (86%)	13 (14%)	4	3
3	G	95/97 (98%)	84 (88%)	11 (12%)	5	6
4	F	100/103 (97%)	87 (87%)	13 (13%)	4	4
4	J	97/103 (94%)	73 (75%)	24 (25%)	1	0
5	H	98/99 (99%)	78 (80%)	20 (20%)	1	1
5	I	98/99 (99%)	82 (84%)	16 (16%)	2	2
All	All	1326/1510 (88%)	1150 (87%)	176 (13%)	4	4

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	17	LEU
1	A	29	HIS
1	A	73	ARG
1	A	82	GLU
1	A	88	ASP
1	A	110	LEU
1	A	135	GLN
1	A	141	LEU
1	A	142	LEU
2	B	6	LYS
2	B	13	LEU
2	B	20	PRO
2	B	23	MET
2	B	47	LEU
2	B	52	THR
2	B	59	GLU
2	B	100	GLU
2	B	102	LYS
2	B	104	LYS
2	B	108	ARG
2	B	112	LYS
2	B	123	LEU
2	B	130	LEU
2	B	135	LYS
2	B	158	VAL
2	B	163	LYS
2	B	164	GLU
2	B	172	GLN

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Mol	Chain	Res	Type
2	B	187	GLU
2	B	202	THR
2	B	204	SER
2	B	227	SER
2	B	231	GLU
2	B	256	GLN
2	B	267	VAL
2	B	275	THR
2	B	278	CYS
2	B	279	ARG
2	B	299	GLU
2	B	303	VAL
1	C	31	LEU
1	C	48	ASP
1	C	54	CYS
1	C	64	ARG
1	C	82	GLU
1	C	135	GLN
1	C	148	ARG
2	D	6	LYS
2	D	20	PRO
2	D	33	GLU
2	D	37	THR
2	D	42	GLN
2	D	47	LEU
2	D	59	GLU
2	D	68	CYS
2	D	73	GLU
2	D	85	LYS
2	D	99	LYS
2	D	103	ASN
2	D	113	ASN
2	D	130	LEU
2	D	141	SER
2	D	156	GLU
2	D	157	ARG
2	D	172	GLN
2	D	177	CYS
2	D	196	LEU
2	D	204	SER
2	D	220	GLN
2	D	221	LEU

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Mol	Chain	Res	Type
2	D	229	GLN
2	D	230	VAL
2	D	231	GLU
2	D	275	THR
2	D	277	ILE
2	D	278	CYS
2	D	283	SER
2	D	303	VAL
3	E	3	GLN
3	E	18	LEU
3	E	28	THR
3	E	38	ARG
3	E	44	GLU
3	E	45	ARG
3	E	78	THR
3	E	86	LEU
3	E	87	ARG
3	E	98	ARG
3	E	101	THR
3	E	105	LEU
3	E	125	SER
4	F	2	VAL
4	F	12	VAL
4	F	18	LEU
4	F	28	THR
4	F	38	ARG
4	F	44	GLU
4	F	51	VAL
4	F	65	LYS
4	F	77	SER
4	F	87	LYS
4	F	108	TYR
4	F	112	GLU
4	F	118	GLN
3	G	11	LEU
3	G	12	VAL
3	G	13	GLN
3	G	34	ARG
3	G	41	ARG
3	G	49	SER
3	G	73	ASN
3	G	74	THR

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Mol	Chain	Res	Type
3	G	77	LEU
3	G	101	LEU
3	G	118	THR
5	H	3	GLN
5	H	11	LEU
5	H	12	VAL
5	H	13	GLN
5	H	27	ARG
5	H	28	THR
5	H	38	ARG
5	H	39	GLN
5	H	43	LYS
5	H	63	SER
5	H	64	VAL
5	H	65	LYS
5	H	67	ARG
5	H	95	LEU
5	H	98	GLU
5	H	104	THR
5	H	115	GLN
5	H	120	THR
5	H	121	VAL
5	H	122	SER
5	I	3	GLN
5	I	4	LEU
5	I	11	LEU
5	I	12	VAL
5	I	17	SER
5	I	18	LEU
5	I	19	ARG
5	I	27	ARG
5	I	28	THR
5	I	43	LYS
5	I	45	ARG
5	I	52	ARG
5	I	69	THR
5	I	95	LEU
5	I	104	THR
5	I	123	SER
4	J	3	GLN
4	J	4	LEU
4	J	7	SER

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Mol	Chain	Res	Type
4	J	11	LEU
4	J	12	VAL
4	J	17	SER
4	J	18	LEU
4	J	22	CYS
4	J	25	SER
4	J	28	THR
4	J	31	TYR
4	J	38	ARG
4	J	39	GLN
4	J	44	GLU
4	J	45	ARG
4	J	51	VAL
4	J	56	GLN
4	J	65	LYS
4	J	67	ARG
4	J	69	THR
4	J	74	ASN
4	J	76	GLU
4	J	89	GLU
4	J	118	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	75	HIS
1	A	76	GLN
1	A	104	GLN
1	A	106	HIS
1	A	135	GLN
2	B	77	HIS
2	B	200	ASN
2	B	229	GLN
2	B	256	GLN
1	C	19	GLN
1	C	72	GLN
1	C	104	GLN
1	C	138	GLN
2	D	65	GLN
2	D	98	GLN
2	D	113	ASN

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Mol	Chain	Res	Type
2	D	172	GLN
2	D	200	ASN
2	D	220	GLN
2	D	256	GLN
3	E	77	ASN
3	E	82	GLN
4	F	3	GLN
4	F	82	GLN
4	F	110	ASN
4	F	118	GLN
3	G	13	GLN
3	G	70	ASN
3	G	73	ASN
3	G	78	GLN
3	G	80	ASN
5	H	3	GLN
5	H	39	GLN
5	H	77	ASN
5	H	109	HIS
5	I	82	GLN
5	I	109	HIS
4	J	82	GLN
4	J	121	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 ⓘ

10 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	$\# Z > 2$
6	NAG	K	1	6,2	14,14,15	0.38	0	17,19,21	2.50	5 (29%)
6	NAG	K	2	6	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
6	BMA	K	3	6	11,11,12	0.46	0	15,15,17	1.17	1 (6%)
6	MAN	K	4	6	11,11,12	0.51	0	15,15,17	1.18	1 (6%)
6	MAN	K	5	6	11,11,12	0.49	0	15,15,17	1.17	1 (6%)
6	NAG	L	1	6,2	14,14,15	0.38	0	17,19,21	2.52	4 (23%)
6	NAG	L	2	6	14,14,15	0.46	0	17,19,21	1.07	2 (11%)
6	BMA	L	3	6	11,11,12	0.41	0	15,15,17	1.24	2 (13%)
6	MAN	L	4	6	11,11,12	0.47	0	15,15,17	1.13	2 (13%)
6	MAN	L	5	6	11,11,12	0.42	0	15,15,17	1.38	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	K	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
6	BMA	K	3	6	-	2/2/19/22	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	0/1/1/1
6	NAG	L	1	6,2	-	6/6/23/26	0/1/1/1
6	NAG	L	2	6	-	2/6/23/26	0/1/1/1
6	BMA	L	3	6	-	2/2/19/22	0/1/1/1
6	MAN	L	4	6	-	0/2/19/22	0/1/1/1
6	MAN	L	5	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1	NAG	C2-N2-C7	6.94	132.19	122.90
6	K	1	NAG	C1-C2-N2	-6.40	100.35	110.43
6	L	1	NAG	C4-C3-C2	-5.90	102.38	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	1	NAG	O5-C1-C2	4.86	118.82	111.29
6	L	5	MAN	C1-O5-C5	4.62	118.38	112.19
6	K	1	NAG	C1-O5-C5	4.23	117.86	112.19
6	K	3	BMA	C1-O5-C5	3.83	117.33	112.19
6	K	5	MAN	C1-O5-C5	3.67	117.11	112.19
6	L	3	BMA	O5-C5-C6	2.97	113.45	107.66
6	L	1	NAG	C1-O5-C5	2.88	116.04	112.19
6	K	2	NAG	C1-C2-N2	-2.87	105.91	110.43
6	L	1	NAG	O5-C1-C2	2.58	115.28	111.29
6	K	1	NAG	C4-C3-C2	-2.55	107.28	111.02
6	L	2	NAG	O7-C7-C8	-2.46	117.68	122.05
6	K	4	MAN	C3-C4-C5	2.40	114.58	110.23
6	L	4	MAN	C3-C4-C5	2.39	114.56	110.23
6	K	1	NAG	C2-N2-C7	2.32	126.01	122.90
6	L	2	NAG	C1-C2-N2	-2.27	106.85	110.43
6	L	3	BMA	C3-C4-C5	2.20	114.23	110.23
6	L	4	MAN	C1-O5-C5	2.19	115.11	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

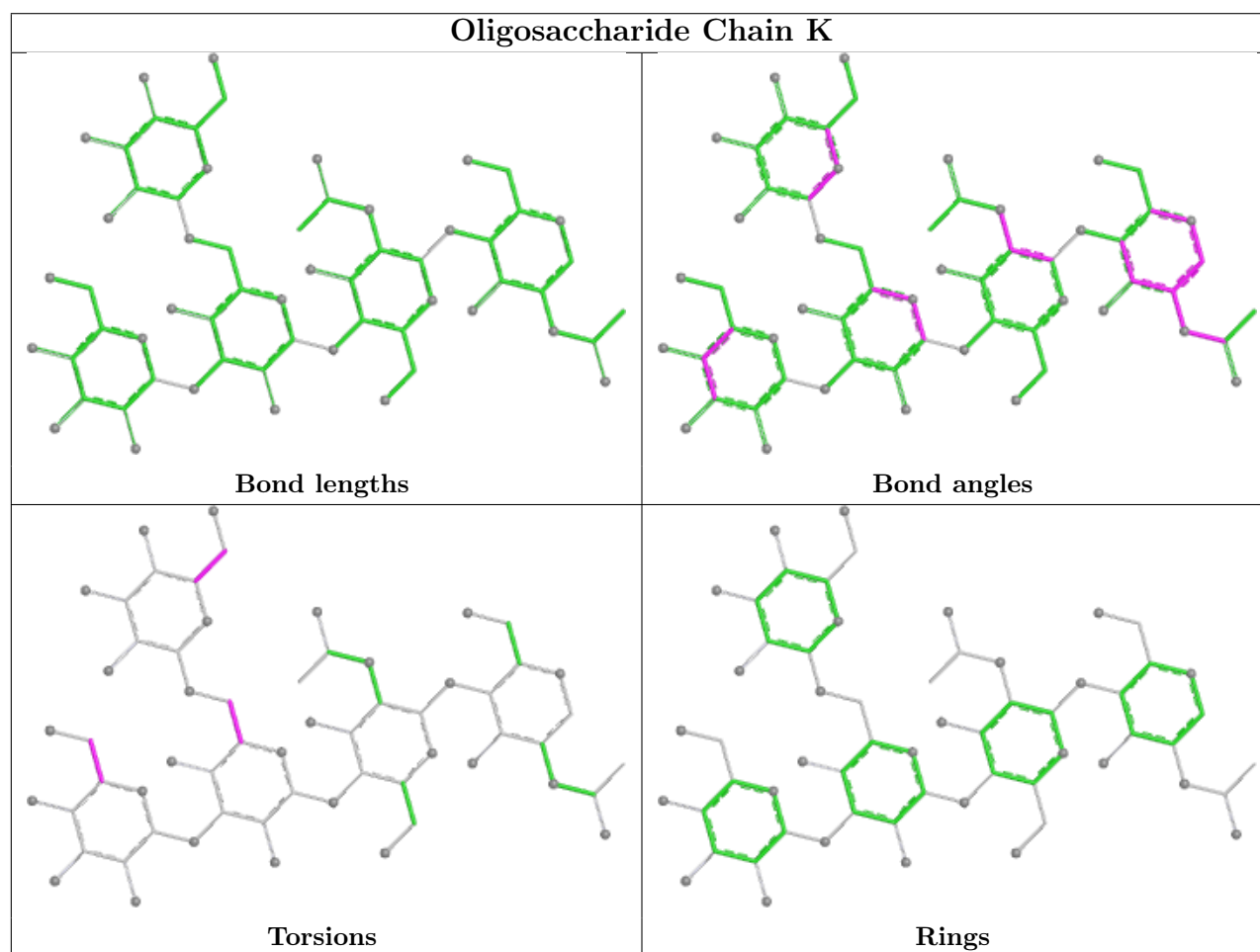
Mol	Chain	Res	Type	Atoms
6	K	5	MAN	C4-C5-C6-O6
6	L	3	BMA	O5-C5-C6-O6
6	K	5	MAN	O5-C5-C6-O6
6	K	3	BMA	O5-C5-C6-O6
6	L	3	BMA	C4-C5-C6-O6
6	K	4	MAN	O5-C5-C6-O6
6	K	3	BMA	C4-C5-C6-O6
6	K	4	MAN	C4-C5-C6-O6
6	L	1	NAG	C8-C7-N2-C2
6	L	1	NAG	O7-C7-N2-C2
6	L	2	NAG	C4-C5-C6-O6
6	L	2	NAG	O5-C5-C6-O6
6	L	1	NAG	C4-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6
6	L	1	NAG	C1-C2-N2-C7
6	L	1	NAG	C3-C2-N2-C7

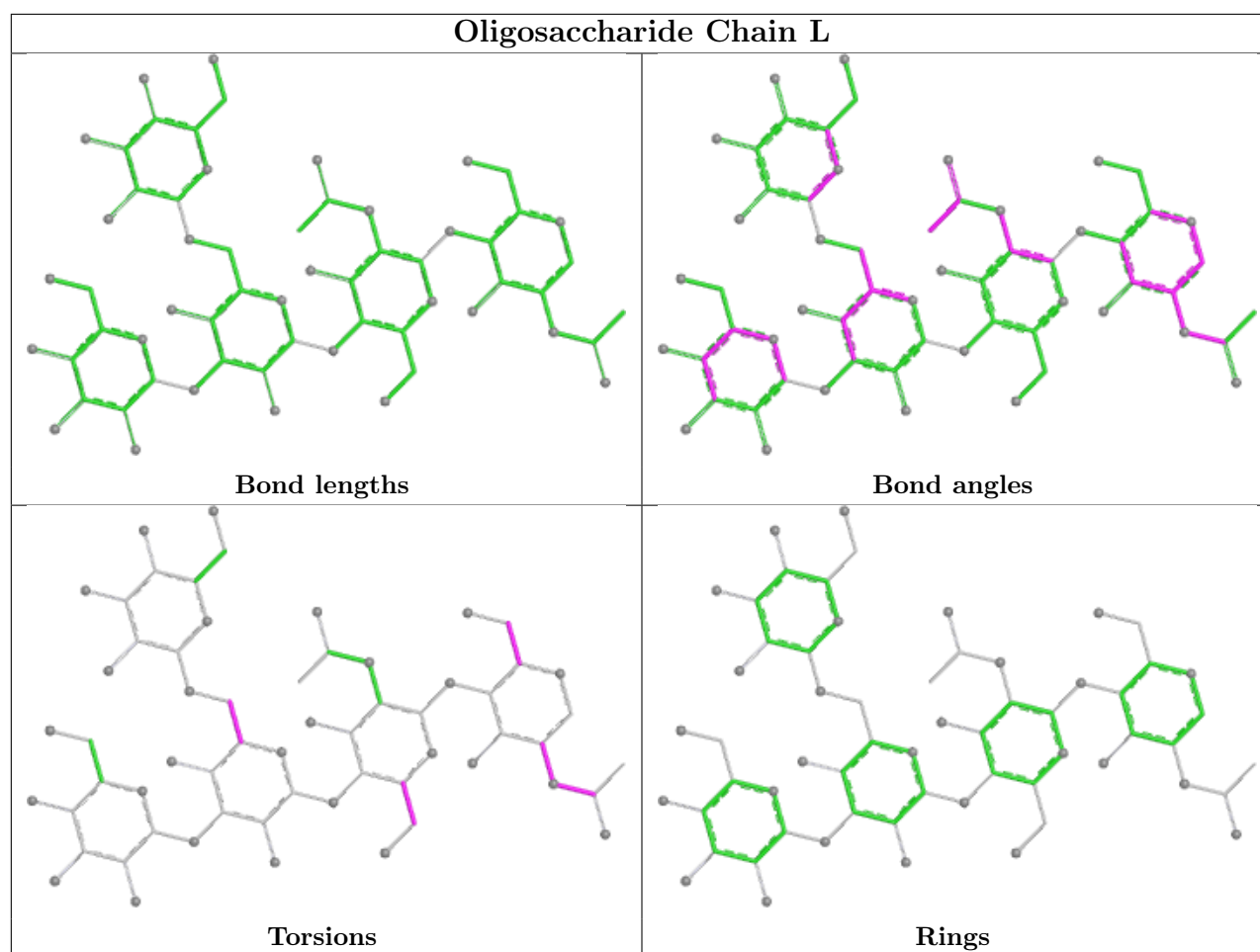
There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	3	BMA	1	0
6	L	5	MAN	1	0
6	K	1	NAG	3	0
6	L	1	NAG	6	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	130/189 (68%)	0.42	9 (6%) 23 22	33, 54, 87, 109	0
1	C	129/189 (68%)	0.04	4 (3%) 51 52	29, 42, 68, 102	0
2	B	293/328 (89%)	0.06	11 (3%) 44 45	28, 45, 83, 126	0
2	D	292/328 (89%)	-0.06	9 (3%) 51 52	24, 40, 84, 130	0
3	E	125/125 (100%)	-0.46	0 100 100	26, 37, 55, 94	0
3	G	125/125 (100%)	-0.04	1 (0%) 82 84	33, 44, 63, 109	0
4	F	125/126 (99%)	0.30	9 (7%) 21 20	28, 51, 85, 113	0
4	J	122/126 (96%)	1.12	19 (15%) 5 4	40, 73, 102, 118	0
5	H	123/123 (100%)	0.12	1 (0%) 82 84	28, 48, 78, 100	0
5	I	123/123 (100%)	-0.07	1 (0%) 82 84	25, 41, 68, 104	0
All	All	1587/1782 (89%)	0.11	64 (4%) 42 43	24, 45, 86, 130	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	121	SER	5.2
4	J	114	ASP	5.1
2	B	159	ARG	4.6
2	B	162	ASN	4.2
4	J	126	SER	3.9
1	A	47	ASN	3.8
2	B	163	LYS	3.7
2	D	257	GLY	3.7
4	J	23	ALA	3.6
4	J	111	GLY	3.6
1	A	137	TRP	3.5
1	A	31	LEU	3.4
2	B	143	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
4	F	43	LYS	3.3
4	F	116	TRP	3.2
4	J	75	ALA	3.2
4	J	31	TYR	3.2
4	F	115	TYR	3.2
4	F	113	TYR	3.1
4	J	41	PRO	3.1
4	F	114	ASP	3.1
1	A	8	SER	3.0
4	J	22	CYS	3.0
5	I	123	SER	3.0
1	C	31	LEU	2.9
4	J	43	LYS	2.9
4	J	117	GLY	2.8
1	A	168	LEU	2.8
1	C	170	PRO	2.8
2	D	17	PRO	2.7
1	A	136	PRO	2.7
4	J	29	LEU	2.7
4	F	110	ASN	2.7
2	D	158	VAL	2.7
2	D	100	GLU	2.6
4	J	116	TRP	2.6
2	B	257	GLY	2.6
1	C	117	GLN	2.6
4	J	67	ARG	2.5
2	D	162	ASN	2.5
1	A	54	CYS	2.5
2	B	144	GLN	2.5
2	B	305	CYS	2.4
2	B	139	GLY	2.3
2	D	159	ARG	2.3
4	J	28	THR	2.3
2	D	101	PRO	2.3
4	F	126	SER	2.2
1	A	48	ASP	2.2
2	B	228	ARG	2.2
4	J	27	PHE	2.2
4	J	40	ALA	2.2
1	A	138	GLN	2.2
4	J	115	TYR	2.2
2	B	278	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	120	CYS	2.2
2	D	19	ALA	2.1
4	J	42	GLY	2.1
1	C	49	VAL	2.1
4	F	2	VAL	2.1
5	H	123	SER	2.1
4	J	109(A)	TYR	2.0
2	B	23	MET	2.0
4	F	125	SER	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](#)

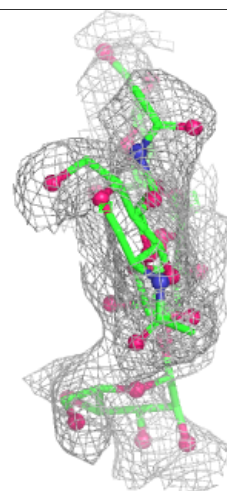
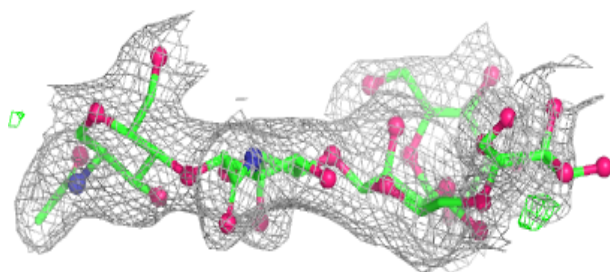
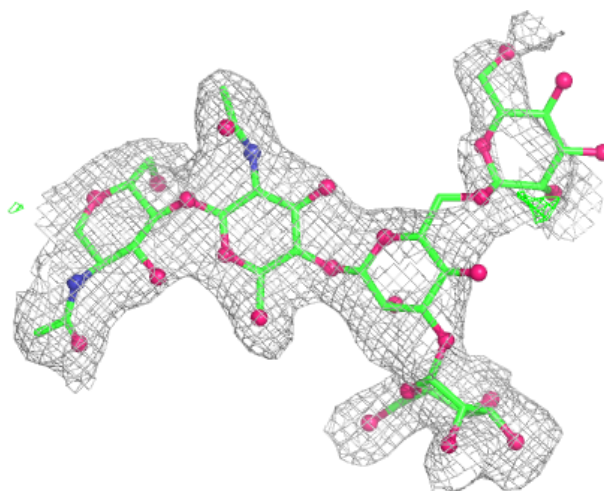
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

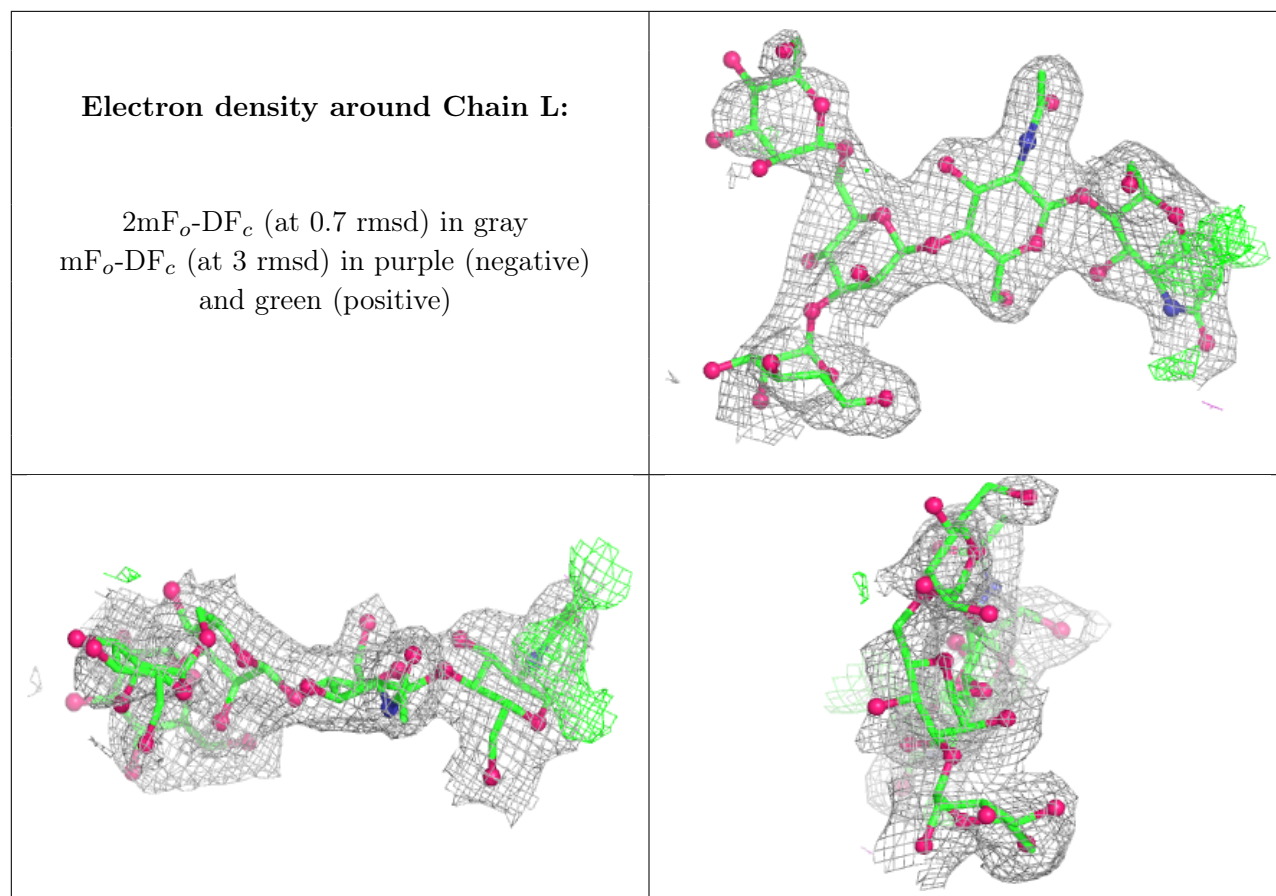
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MAN	K	5	11/12	0.43	0.14	84,130,146,150	0
6	MAN	L	5	11/12	0.56	0.15	81,105,128,138	0
6	BMA	K	3	11/12	0.76	0.12	51,106,130,136	0
6	MAN	K	4	11/12	0.78	0.11	62,92,147,148	0
6	MAN	L	4	11/12	0.80	0.12	43,98,120,127	0
6	BMA	L	3	11/12	0.85	0.10	54,95,123,128	0
6	NAG	L	1	14/15	0.91	0.12	16,40,89,96	0
6	NAG	K	1	14/15	0.95	0.07	20,44,57,82	0
6	NAG	K	2	14/15	0.95	0.08	24,39,72,93	0
6	NAG	L	2	14/15	0.95	0.07	25,41,58,76	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 K:

$2mF_o-DF_c$ (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.