



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:37 AM UTC

PDB ID : 1HZH / pdb_00001hzh
Title : CRYSTAL STRUCTURE OF THE INTACT HUMAN IGG B12 WITH BROAD AND POTENT ACTIVITY AGAINST PRIMARY HIV-1 ISOLATES: A TEMPLATE FOR HIV VACCINE DESIGN
Authors : Sapphire, E.O.; Burton, D.R.; Wilson, I.A.
Deposited on : 2001-01-24
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

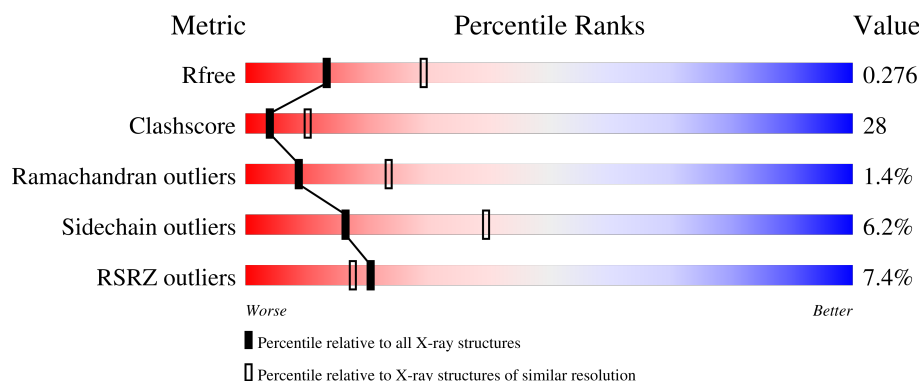
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	H	457	12% 48% 45% 6%
1	K	457	5% 60% 33%
2	L	215	3% 57% 40%
2	M	215	6% 47% 47% 6%
3	A	9	33% 33% 33%

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Mol	Chain	Length	Quality of chain
4	B	9	44% 33% 22%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10647 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 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	457	Total	C	N	O	S	0	0	0
			3553	2252	600	685	16			
1	K	444	Total	C	N	O	S	0	0	0
			3466	2202	583	665	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	225	ALA	VAL	conflict	UNP P0DOX5
K	225	ALA	VAL	conflict	UNP P0DOX5

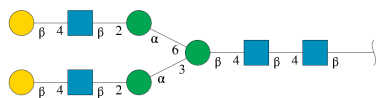
- Molecule 2 is a protein called IMMUNOGLOBULIN LIGHT CHAIN, Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	215	Total	C	N	O	S	0	0	0
			1668	1036	297	330	5			
2	M	215	Total	C	N	O	S	0	0	0
			1668	1036	297	330	5			

There are 2 discrepancies between the modelled and reference sequences:

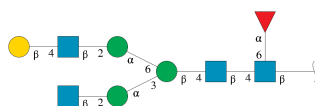
Chain	Residue	Modelled	Actual	Comment	Reference
L	202	ARG	SER	conflict	UNP Q8TCD0
M	202	ARG	SER	conflict	UNP Q8TCD0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	9	Total	C	N	O	0	0	0
			111	62	4	45			

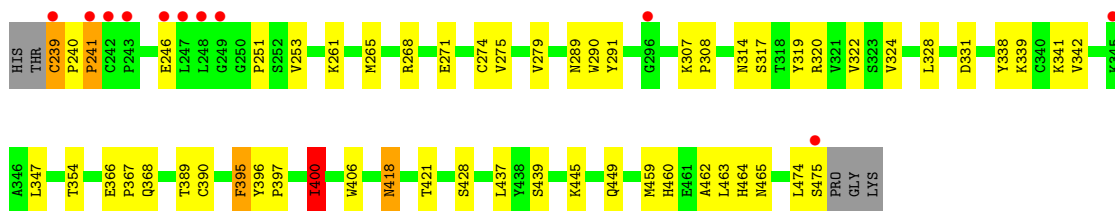
- Molecule 4 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose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



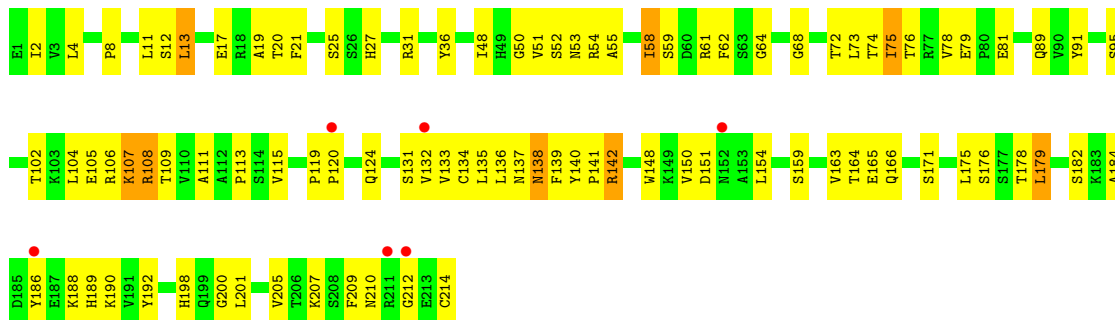
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	9	Total	C	N	O	0	0	0
			110	62	4	44			

- Molecule 5 is water.

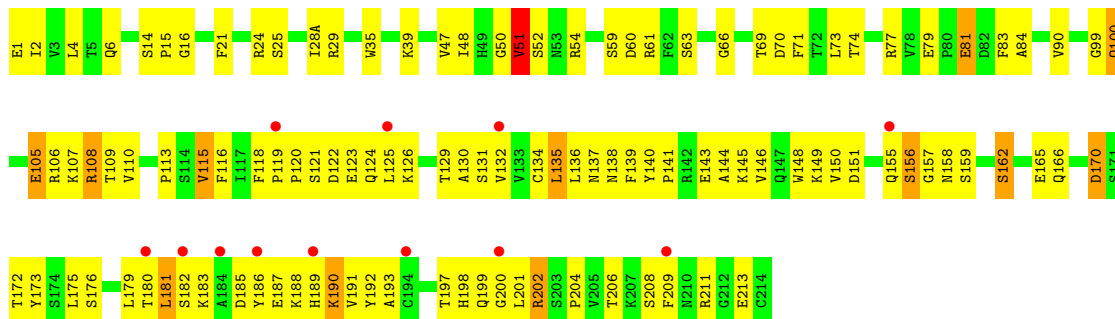
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	15	Total	O	0	0
			15	15		
5	K	38	Total	O	0	0
			38	38		
5	L	6	Total	O	0	0
			6	6		
5	M	12	Total	O	0	0
			12	12		



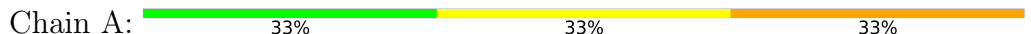
• Molecule 2: IMMUNOGLOBULIN LIGHT CHAIN, Uncharacterized protein



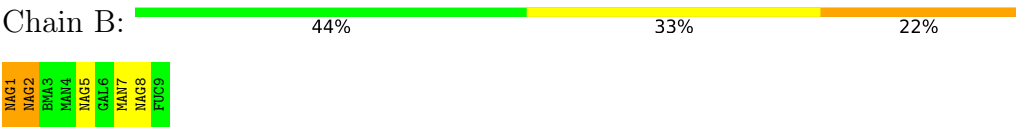
• Molecule 2: IMMUNOGLOBULIN LIGHT CHAIN, Uncharacterized protein



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



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	271.32Å 271.32Å 175.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.65 – 2.70 29.65 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.7 (29.65-2.70) 91.6 (29.65-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.61Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.229 , 0.273 0.233 , 0.276	Depositor DCC
R_{free} test set	6926 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 67.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for $-1/3^*h+1/3^*k+4/3^*l,-k,2/3^*h+1/3^*k+1/3^*l$ 0.012 for $-2/3^*h-1/3^*k-4/3^*l,-1/3^*h-2/3^*k+4/3^*l,-1/3^*h+1/3^*k+1/3^*l$ 0.006 for $-h,1/3^*h-1/3^*k-4/3^*l,-1/3^*h-2/3^*k+1/3^*l$	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10647	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: GAL, MAN, BMA, FUC, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	H	0.45	0/3654	1.00	16/4983 (0.3%)
1	K	0.50	2/3563 (0.1%)	0.93	10/4859 (0.2%)
2	L	0.41	0/1704	0.87	3/2306 (0.1%)
2	M	0.46	0/1704	0.93	6/2306 (0.3%)
All	All	0.46	2/10625 (0.0%)	0.95	35/14454 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	100(J)	MET	SD-CE	-5.87	1.64	1.79
1	K	400	ILE	CA-CB	5.73	1.59	1.55

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	239	CYS	CA-C-N	17.74	132.61	119.66
1	H	239	CYS	C-N-CA	17.74	132.61	119.66
1	H	240	PRO	N-CA-C	10.76	120.80	110.47
1	K	418	ASN	N-CA-C	7.51	121.33	109.39
1	H	244	ALA	CA-C-N	7.36	127.28	120.21
1	H	244	ALA	C-N-CA	7.36	127.28	120.21
1	H	240	PRO	CA-C-N	7.05	126.98	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	240	PRO	C-N-CA	7.05	126.98	120.21
2	M	190	LYS	N-CA-C	6.51	118.26	111.03
1	K	240	PRO	N-CA-C	6.34	118.43	110.70
2	L	138	ASN	N-CA-C	6.25	119.98	111.17
1	H	146	ASP	N-CA-C	5.95	117.86	110.91
1	K	66	ARG	N-CA-C	5.92	119.82	112.59
1	K	317	SER	N-CA-C	5.89	119.67	111.90
2	M	138	ASN	N-CA-C	5.89	119.47	111.17
1	H	29	PHE	N-CA-C	5.88	118.17	111.11
1	K	428	SER	N-CA-C	5.87	119.27	111.75
2	M	115	VAL	N-CA-C	5.77	116.45	108.84
2	L	137	ASN	N-CA-C	5.76	119.02	109.46
2	M	99	GLY	N-CA-C	-5.45	104.08	112.85
1	H	418	ASN	N-CA-C	5.45	122.40	110.80
1	K	395	PHE	N-CA-C	5.42	118.82	110.42
1	H	124	LEU	N-CA-C	-5.33	102.19	109.71
1	K	366	GLU	CA-C-N	5.28	125.18	119.85
1	K	366	GLU	C-N-CA	5.28	125.18	119.85
1	K	389	THR	N-CA-C	5.24	117.95	109.40
1	K	7	SER	N-CA-C	5.23	117.43	110.53
1	H	363	GLN	CA-C-N	5.22	125.14	119.76
1	H	363	GLN	C-N-CA	5.22	125.14	119.76
2	L	142	ARG	N-CA-C	5.21	116.64	111.07
2	M	137	ASN	N-CA-C	5.21	117.97	109.59
1	H	269	THR	CA-C-N	5.15	125.06	119.76
1	H	269	THR	C-N-CA	5.15	125.06	119.76
1	H	104	GLY	N-CA-C	-5.06	103.66	112.06
2	M	156	SER	N-CA-C	5.05	115.82	108.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	136	GLY	Mainchain

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	H	3553	0	3460	240	1
1	K	3466	0	3373	161	0
2	L	1668	0	1621	71	0
2	M	1668	0	1621	117	0
3	A	111	0	94	11	0
4	B	110	0	94	7	0
5	H	15	0	0	2	0
5	K	38	0	0	0	0
5	L	6	0	0	0	0
5	M	12	0	0	1	0
All	All	10647	0	10263	583	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (583) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:400:ILE:HD11	1:H:458:VAL:HG13	1.38	1.05
1:K:221:LYS:HE3	1:K:221:LYS:HA	1.39	1.04
2:M:1:GLU:HG3	2:M:2:ILE:H	1.18	1.03
2:M:100:GLN:H	2:M:100:GLN:NE2	1.56	1.03
1:H:277:VAL:HG11	3:A:2:NAG:O7	1.59	1.02
1:H:145:LYS:HE3	1:H:179:GLN:HE22	1.23	1.00
1:K:314:ASN:HD21	4:B:1:NAG:C1	1.75	0.98
1:H:27:TYR:HB2	1:H:28:ARG:HH21	1.30	0.95
1:K:28:ARG:H	1:K:28:ARG:HE	1.11	0.95
2:M:149:LYS:HB2	2:M:193:ALA:HB3	1.44	0.95
1:H:124:LEU:HD11	1:H:143:LEU:HB2	1.47	0.94
2:M:100:GLN:H	2:M:100:GLN:HE21	0.95	0.94
1:H:367:PRO:HB3	1:H:395:PHE:HB3	1.49	0.94
1:H:150:GLU:HB2	1:H:151:PRO:HA	1.50	0.94
2:L:11:LEU:HG	2:L:13:LEU:HD11	1.48	0.94
1:H:347:LEU:HD23	1:H:348:PRO:HD2	1.49	0.93
2:M:100:GLN:HE21	2:M:100:GLN:N	1.69	0.91
2:M:190:LYS:O	2:M:211:ARG:HB3	1.73	0.89
1:H:28:ARG:H	1:H:28:ARG:HE	0.89	0.88
1:H:28:ARG:H	1:H:28:ARG:NE	1.71	0.88
1:K:28:ARG:H	1:K:28:ARG:NE	1.72	0.88
1:H:121:VAL:HG21	1:H:219:VAL:HG11	1.52	0.88
2:M:16:GLY:HA2	2:M:77:ARG:HG3	1.57	0.87
1:K:212:HIS:HD2	1:K:214:PRO:HD2	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:261:LYS:HE2	1:K:265:MET:CE	2.05	0.85
2:M:39:LYS:HD3	2:M:84:ALA:HB2	1.56	0.85
1:H:28:ARG:HE	1:H:28:ARG:N	1.73	0.85
1:H:35:HIS:HD2	1:H:47:TRP:HE1	1.22	0.84
1:H:187:LEU:HD13	1:H:188:SER:N	1.93	0.84
2:M:188:LYS:N	2:M:211:ARG:HH12	1.74	0.84
1:H:339:LYS:HG2	1:H:354:THR:HG22	1.58	0.84
1:K:3:GLN:HB2	1:K:25:SER:HB2	1.58	0.83
1:K:100(I):TYR:C	1:K:100(J):MET:HE3	2.04	0.82
2:L:55:ALA:O	2:L:58:ILE:HD13	1.80	0.81
1:H:314:ASN:HD21	3:A:1:NAG:C1	1.94	0.81
1:K:314:ASN:ND2	4:B:1:NAG:C1	2.45	0.79
1:K:275:VAL:HG22	1:K:322:VAL:HG22	1.64	0.79
1:K:54:ASN:ND2	1:K:56:ASN:H	1.80	0.78
1:K:94:ARG:HD3	1:K:95:VAL:O	1.83	0.78
1:H:460:HIS:CD2	1:H:462:ALA:H	2.00	0.78
1:H:66:ARG:HH21	1:H:82:LEU:HD11	1.49	0.77
1:K:63:PHE:HB3	1:K:67:VAL:HG21	1.64	0.77
3:A:5:NAG:H61	3:A:6:GAL:C1	2.15	0.77
1:H:400:ILE:HD13	1:H:401:ALA:N	1.98	0.77
2:M:1:GLU:HG3	2:M:2:ILE:N	1.98	0.77
1:K:126:PRO:HG3	1:K:140:LEU:HB3	1.67	0.77
2:M:105:GLU:HG3	2:M:173:TYR:OH	1.85	0.76
1:H:163:SER:H	1:H:209:ASN:HD21	1.30	0.76
1:H:212:HIS:HD2	1:H:214:PRO:HD2	1.50	0.75
1:H:51:ILE:HD13	1:H:52:ASN:N	2.02	0.75
1:K:320:ARG:NE	4:B:2:NAG:H81	2.02	0.75
2:L:19:ALA:HB3	2:L:75:ILE:HG12	1.69	0.75
1:K:400:ILE:HD12	1:K:460:HIS:HB2	1.68	0.74
1:H:256:PHE:CE2	3:A:8:NAG:H5	2.22	0.73
1:K:228:LYS:HE2	2:M:213:GLU:OE2	1.88	0.73
2:L:108:ARG:HD3	2:L:109:THR:O	1.89	0.73
1:K:261:LYS:HG2	1:K:265:MET:HE2	1.71	0.73
1:K:289:ASN:HB2	1:K:341:LYS:HB3	1.70	0.73
1:K:87:THR:HG23	1:K:110:ILE:HA	1.71	0.72
2:L:17:GLU:O	2:L:78:VAL:HG23	1.89	0.72
2:M:151:ASP:HB2	2:M:189:HIS:HB3	1.70	0.72
1:K:145:LYS:HG2	1:K:146:ASP:OD1	1.90	0.71
1:H:30:SER:HA	1:H:52(A):PRO:HB2	1.70	0.71
2:M:202:ARG:O	2:M:202:ARG:HD3	1.91	0.71
1:H:35:HIS:CD2	1:H:47:TRP:HE1	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:145:LYS:HE3	1:H:179:GLN:NE2	2.01	0.71
1:H:256:PHE:CD2	3:A:8:NAG:H5	2.26	0.70
1:H:38:ARG:HD2	1:H:46:GLU:OE1	1.92	0.70
1:K:63:PHE:HB3	1:K:67:VAL:CG2	2.22	0.70
1:H:117:LYS:HG2	1:H:118:GLY:H	1.56	0.70
2:M:143:GLU:H	2:M:143:GLU:CD	2.00	0.70
2:L:175:LEU:HD23	2:L:176:SER:N	2.07	0.69
1:K:100(J):MET:HE3	1:K:100(J):MET:N	2.07	0.69
2:M:181:LEU:HD12	2:M:185:ASP:HB2	1.74	0.69
1:H:193:VAL:HG22	1:H:194:PRO:HD2	1.74	0.69
1:H:162:ASN:ND2	1:H:207:ILE:H	1.91	0.69
2:M:6:GLN:H	2:M:100:GLN:HE22	1.40	0.69
2:M:187:GLU:HA	2:M:211:ARG:CZ	2.22	0.69
1:H:330:GLN:CD	1:H:330:GLN:H	2.01	0.69
2:L:186:TYR:HA	2:L:192:TYR:OH	1.92	0.69
2:L:124:GLN:HE22	2:L:131:SER:HB2	1.58	0.69
1:K:261:LYS:HE2	1:K:265:MET:HE2	1.73	0.69
1:K:193:VAL:HG13	1:K:194:PRO:HD2	1.75	0.68
1:K:265:MET:HE3	1:K:268:ARG:HG3	1.76	0.68
1:H:33:VAL:HB	1:H:95:VAL:HG21	1.75	0.68
1:H:6:GLN:HE21	1:H:107:THR:HG23	1.57	0.68
1:K:261:LYS:HE2	1:K:265:MET:HE1	1.74	0.68
1:K:63:PHE:O	1:K:67:VAL:HG23	1.93	0.67
1:K:139:ALA:HB2	1:K:192:THR:HG22	1.74	0.67
1:K:367:PRO:HB3	1:K:395:PHE:HB3	1.75	0.67
1:H:82:LEU:HD13	1:H:82(A):ARG:N	2.10	0.67
1:H:119:PRO:HD3	1:H:212:HIS:ND1	2.10	0.67
1:H:193:VAL:CG2	1:H:194:PRO:HD2	2.24	0.67
2:L:12:SER:HB3	2:L:105:GLU:CG	2.24	0.67
1:H:23:GLN:HG2	1:H:77:THR:OG1	1.95	0.66
1:H:63:PHE:HB3	1:H:67:VAL:CG2	2.25	0.66
1:H:163:SER:N	1:H:209:ASN:HD21	1.93	0.66
1:H:212:HIS:CD2	1:H:214:PRO:HD2	2.30	0.66
2:M:28(A):ILE:HD13	2:M:71:PHE:HE2	1.60	0.66
1:H:33:VAL:HB	1:H:95:VAL:CG2	2.25	0.66
1:H:66:ARG:HA	1:H:82(A):ARG:NH1	2.11	0.66
1:H:117:LYS:HG2	1:H:118:GLY:N	2.11	0.66
2:M:135:LEU:HD12	2:M:136:LEU:N	2.11	0.66
1:H:63:PHE:HB3	1:H:67:VAL:HG23	1.78	0.65
1:H:54:ASN:CG	1:H:56:ASN:HD22	2.05	0.65
1:H:95:VAL:HG12	1:H:96:GLY:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:189:HIS:O	2:M:211:ARG:HD3	1.96	0.65
1:H:122:PHE:CD1	2:L:124:GLN:HB2	2.32	0.65
1:K:35:HIS:ND1	1:K:100(J):MET:HE2	2.11	0.65
1:H:100(B):ASP:HB2	1:H:100(F):ASP:HB2	1.79	0.64
1:K:117:LYS:HE3	1:K:146:ASP:O	1.97	0.64
1:H:2:VAL:HG12	1:H:27:TYR:HB3	1.78	0.64
2:M:125:LEU:O	2:M:183:LYS:HD2	1.98	0.64
1:K:261:LYS:HD3	1:K:268:ARG:NH2	2.12	0.64
2:L:132:VAL:HB	2:L:179:LEU:HB3	1.80	0.64
2:M:188:LYS:H	2:M:211:ARG:HH12	1.43	0.64
1:K:35:HIS:HD2	1:K:47:TRP:HE1	1.43	0.64
1:K:54:ASN:HD21	1:K:56:ASN:HB2	1.63	0.64
2:L:55:ALA:C	2:L:58:ILE:HD13	2.23	0.64
1:K:52:ASN:C	1:K:52:ASN:HD22	2.04	0.64
1:K:178:LEU:HD13	1:K:185:TYR:CE2	2.33	0.64
2:M:155:GLN:NE2	2:M:158:ASN:HD21	1.96	0.64
1:K:137:THR:HG23	1:K:193:VAL:O	1.98	0.63
1:H:309:ARG:HG2	1:H:321:VAL:HG22	1.80	0.63
1:H:110:ILE:HD12	1:H:110:ILE:H	1.64	0.63
1:K:119:PRO:HD2	1:K:217:THR:HG21	1.79	0.63
2:M:200:GLY:O	2:M:201:LEU:HD12	1.98	0.63
1:H:145:LYS:CE	1:H:179:GLN:HE22	2.06	0.63
2:M:175:LEU:HD23	2:M:176:SER:N	2.14	0.63
1:K:212:HIS:CD2	1:K:214:PRO:HD2	2.31	0.62
2:M:113:PRO:HB3	2:M:139:PHE:HB3	1.81	0.62
1:K:162:ASN:HB2	1:K:165:ALA:HB3	1.81	0.62
1:H:6:GLN:NE2	1:H:107:THR:HG23	2.14	0.62
2:M:108:ARG:HD3	2:M:109:THR:O	1.99	0.62
2:M:151:ASP:CB	2:M:189:HIS:HB3	2.29	0.62
1:H:255:LEU:HD12	1:H:273:THR:O	2.00	0.61
1:H:278:ASP:OD1	3:A:1:NAG:H3	2.00	0.61
1:H:87:THR:HG23	1:H:110:ILE:HA	1.82	0.61
1:K:6:GLN:HE21	1:K:104:GLY:HA3	1.65	0.61
1:K:328:LEU:HD12	1:K:331:ASP:OD2	2.01	0.61
1:K:274:CYS:HB2	1:K:290:TRP:CH2	2.36	0.61
2:L:4:LEU:HD23	2:L:25:SER:HB3	1.83	0.61
1:H:258:PRO:HD3	1:H:272:VAL:HG22	1.83	0.61
1:H:390:CYS:HB2	1:H:406:TRP:CZ2	2.35	0.61
2:M:202:ARG:HD3	2:M:202:ARG:C	2.26	0.61
1:H:256:PHE:HE1	1:H:275:VAL:HG12	1.65	0.61
2:M:155:GLN:CD	2:M:179:LEU:HD11	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:5:NAG:C6	3:A:6:GAL:C1	2.78	0.61
1:H:328:LEU:HB2	1:H:331:ASP:OD2	2.01	0.61
1:H:314:ASN:ND2	3:A:1:NAG:C1	2.64	0.60
1:H:279:VAL:HB	1:H:319:TYR:HB2	1.83	0.60
2:L:12:SER:HB3	2:L:105:GLU:HG2	1.83	0.60
2:L:36:TYR:CE1	2:L:89:GLN:HG2	2.36	0.60
1:H:238:THR:O	1:H:239:CYS:HB2	2.00	0.60
1:H:82:LEU:HD12	1:H:82(C):LEU:HD23	1.82	0.60
2:L:201:LEU:HD13	2:L:205:VAL:HG23	1.82	0.60
1:K:54:ASN:C	1:K:54:ASN:HD22	2.08	0.60
1:K:122:PHE:HB3	2:M:121:SER:OG	2.02	0.60
1:K:460:HIS:CD2	1:K:462:ALA:H	2.19	0.60
1:K:47:TRP:CZ2	1:K:49:GLY:HA2	2.36	0.60
1:K:100(D):PRO:O	1:K:100(E):GLN:HB2	2.01	0.60
1:H:40:ALA:HA	1:H:88:ALA:HB2	1.84	0.60
1:K:339:LYS:HB2	1:K:354:THR:HG22	1.84	0.59
1:K:83:ARG:O	1:K:111:VAL:HG11	2.03	0.59
1:H:360:LYS:HE2	1:H:360:LYS:HA	1.84	0.59
2:M:124:GLN:HE22	2:M:131:SER:N	2.01	0.59
2:M:175:LEU:HD23	2:M:175:LEU:C	2.27	0.59
1:H:100:TRP:CD1	1:H:100:TRP:H	2.18	0.59
1:K:175:PRO:HG2	2:M:162:SER:OG	2.03	0.59
2:M:150:VAL:HG23	2:M:155:GLN:HB2	1.83	0.59
2:M:48:ILE:HD13	2:M:54:ARG:HA	1.83	0.59
2:M:105:GLU:HG2	2:M:106:ARG:N	2.17	0.59
1:K:1:GLN:O	1:K:1:GLN:HG3	2.02	0.59
2:M:145:LYS:HB2	2:M:197:THR:HB	1.85	0.58
1:H:126:PRO:HD3	1:H:140:LEU:HB3	1.84	0.58
1:H:437:LEU:C	1:H:437:LEU:HD12	2.29	0.58
2:L:59:SER:C	2:L:61:ARG:H	2.11	0.58
1:H:187:LEU:HD13	1:H:188:SER:H	1.65	0.58
2:M:24:ARG:HD2	2:M:70:ASP:OD1	2.02	0.58
1:H:331:ASP:O	1:H:336:LYS:HB2	2.04	0.58
1:H:207:ILE:O	1:H:207:ILE:HG13	2.02	0.58
2:M:113:PRO:HD3	2:M:198:HIS:CD2	2.39	0.58
1:H:153:THR:OG1	1:H:211:ASN:HB3	2.04	0.57
2:M:16:GLY:HA2	2:M:77:ARG:CG	2.33	0.57
1:H:144:VAL:HB	1:H:187:LEU:HB3	1.84	0.57
1:H:207:ILE:HG22	1:H:222:LYS:HA	1.86	0.57
1:H:400:ILE:HD11	1:H:458:VAL:CG1	2.25	0.57
1:H:59:PHE:CD2	1:H:64:GLN:HA	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:72:THR:HG22	2:L:73:LEU:N	2.19	0.57
1:K:54:ASN:HD22	1:K:56:ASN:H	1.52	0.57
2:M:192:TYR:HB2	2:M:209:PHE:CE1	2.40	0.57
1:H:162:ASN:HD21	1:H:206:TYR:HA	1.68	0.57
2:M:155:GLN:OE1	2:M:179:LEU:HD11	2.04	0.57
1:H:400:ILE:HD13	1:H:401:ALA:C	2.30	0.56
1:K:28:ARG:HG2	1:K:31:ASN:HB2	1.88	0.56
1:H:4:LEU:HD23	1:H:92:CYS:O	2.06	0.56
1:K:119:PRO:HB2	1:K:144:VAL:HG13	1.88	0.56
1:H:347:LEU:HD22	1:H:349:ALA:O	2.05	0.56
2:M:100:GLN:NE2	2:M:100:GLN:N	2.38	0.56
2:M:189:HIS:O	2:M:211:ARG:NH1	2.39	0.56
1:K:28:ARG:HE	1:K:28:ARG:N	1.92	0.56
1:K:166:LEU:HD21	1:K:191:VAL:HG21	1.88	0.56
1:H:162:ASN:HD21	1:H:207:ILE:H	1.52	0.56
1:H:270:PRO:HD3	1:H:329:HIS:CE1	2.41	0.56
1:H:329:HIS:HB2	1:H:330:GLN:OE1	2.05	0.56
1:H:339:LYS:HE2	1:H:354:THR:HG21	1.88	0.56
1:H:32:PHE:CG	1:H:94:ARG:HD2	2.41	0.55
1:H:121:VAL:CG2	1:H:219:VAL:HG11	2.31	0.55
1:H:400:ILE:HD13	1:H:401:ALA:H	1.71	0.55
1:H:347:LEU:HD23	1:H:348:PRO:CD	2.31	0.55
1:K:207:ILE:HG12	1:K:222:LYS:HA	1.88	0.55
2:M:115:VAL:O	2:M:116:PHE:HD2	1.89	0.55
1:H:235:LYS:O	1:H:236:THR:C	2.50	0.55
1:K:6:GLN:HB2	1:K:107:THR:CG2	2.37	0.55
2:M:124:GLN:NE2	2:M:131:SER:N	2.55	0.55
2:M:155:GLN:HG2	2:M:156:SER:N	2.22	0.55
1:K:27:TYR:CB	1:K:28:ARG:HH21	2.19	0.55
1:K:140:LEU:HD21	1:K:206:TYR:HD1	1.72	0.55
1:K:221:LYS:HA	1:K:221:LYS:CE	2.24	0.54
2:M:131:SER:HA	2:M:179:LEU:O	2.07	0.54
1:H:82:LEU:HD12	1:H:82(C):LEU:CD2	2.36	0.54
1:H:178:LEU:HD13	1:H:185:TYR:CE1	2.43	0.54
1:H:266:ILE:C	1:H:266:ILE:HD13	2.32	0.54
1:K:239:CYS:O	1:K:239:CYS:SG	2.65	0.54
1:H:177:VAL:HG12	1:H:177:VAL:O	2.08	0.54
1:K:163:SER:HA	1:K:209:ASN:OD1	2.08	0.54
1:K:187:LEU:HD12	1:K:188:SER:N	2.22	0.54
1:K:141:GLY:HA2	1:K:157:TRP:CH2	2.42	0.54
2:L:4:LEU:CD2	2:L:25:SER:HB3	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:52:SER:HB3	2:L:64:GLY:O	2.06	0.54
2:L:108:ARG:NH1	2:L:111:ALA:HB2	2.22	0.54
1:H:95:VAL:HG13	1:H:100(G):ASN:O	2.07	0.54
1:K:52:ASN:ND2	1:K:53:TYR:H	2.06	0.54
1:H:110:ILE:HD12	1:H:110:ILE:N	2.23	0.54
1:H:19:LYS:HE2	1:H:79:TYR:CD2	2.43	0.54
1:H:251:PRO:HG2	1:H:347:LEU:HD12	1.90	0.54
2:L:19:ALA:O	2:L:74:THR:HA	2.08	0.54
2:M:165:GLU:O	2:M:166:GLN:C	2.49	0.53
1:H:140:LEU:HD21	1:H:206:TYR:CD2	2.44	0.53
1:K:27:TYR:HB2	1:K:28:ARG:HH21	1.73	0.53
1:K:193:VAL:CG1	1:K:194:PRO:HD2	2.38	0.53
1:K:208:CYS:C	1:K:209:ASN:HD22	2.16	0.53
2:L:135:LEU:C	2:L:136:LEU:HD12	2.33	0.53
1:K:190:VAL:HG21	2:M:135:LEU:HD22	1.90	0.53
2:M:130:ALA:HB3	2:M:181:LEU:O	2.09	0.53
1:H:12:LYS:HB3	1:H:16:ALA:HB3	1.89	0.53
1:H:314:ASN:HD21	3:A:1:NAG:C2	2.22	0.53
1:H:4:LEU:HD12	1:H:24:ALA:HB2	1.91	0.53
1:H:37:VAL:HG13	1:H:46:GLU:O	2.09	0.53
1:K:56:ASN:C	1:K:57:LYS:HG3	2.34	0.53
1:H:7:SER:OG	1:H:20:VAL:HG13	2.09	0.53
1:K:52:ASN:HB3	1:K:54:ASN:HD21	1.73	0.53
1:H:35:HIS:HD2	1:H:47:TRP:NE1	1.99	0.52
1:H:38:ARG:HG3	1:H:46:GLU:HB2	1.90	0.52
1:H:99:SER:HB2	1:H:100(B):ASP:OD2	2.08	0.52
1:K:110:ILE:HD12	1:K:110:ILE:N	2.24	0.52
1:H:67:VAL:HG12	1:H:68:THR:N	2.24	0.52
1:H:255:LEU:HD23	1:H:355:ILE:HB	1.90	0.52
1:H:280:SER:HB2	1:H:282:GLU:OE1	2.08	0.52
2:M:141:PRO:HB2	2:M:143:GLU:OE2	2.08	0.52
2:L:31:ARG:NH2	2:L:51:VAL:HG11	2.24	0.52
2:M:6:GLN:H	2:M:100:GLN:NE2	2.06	0.52
2:M:123:GLU:HA	2:M:126:LYS:HE2	1.92	0.52
2:M:191:VAL:HG12	2:M:192:TYR:N	2.25	0.52
2:M:202:ARG:O	2:M:204:PRO:HD3	2.09	0.52
1:K:10:GLU:HG3	1:K:18:VAL:CG2	2.40	0.52
2:L:62:PHE:CE2	2:L:75:ILE:HD12	2.44	0.52
2:L:140:TYR:CE1	2:L:141:PRO:HG3	2.45	0.52
1:H:66:ARG:HA	1:H:82(A):ARG:HH12	1.74	0.52
1:H:174:PHE:O	1:H:187:LEU:HD22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:248:LEU:C	1:H:250:GLY:H	2.18	0.52
1:H:27:TYR:CB	1:H:28:ARG:HH21	2.12	0.52
1:H:95:VAL:CG1	1:H:96:GLY:N	2.73	0.52
1:H:226:GLU:HG3	1:H:227:PRO:HD2	1.91	0.52
2:L:79:GLU:HB3	2:L:81:GLU:OE1	2.10	0.52
2:M:188:LYS:H	2:M:211:ARG:NH1	2.06	0.51
1:K:400:ILE:CD1	1:K:460:HIS:HB2	2.38	0.51
2:L:201:LEU:HD13	2:L:205:VAL:CG2	2.40	0.51
3:A:5:NAG:H5	3:A:6:GAL:O2	2.10	0.51
2:L:184:ALA:O	2:L:188:LYS:HG3	2.09	0.51
1:H:100:TRP:CZ3	1:H:100(A):ASP:HB3	2.45	0.51
1:K:279:VAL:HB	1:K:319:TYR:HB2	1.93	0.51
1:H:141:GLY:HA2	1:H:157:TRP:CH2	2.46	0.51
1:H:13:LYS:HB3	1:H:14:PRO:HD2	1.92	0.51
1:H:35:HIS:CD2	1:H:50:TRP:HB3	2.46	0.51
1:H:339:LYS:CG	1:H:354:THR:HG22	2.34	0.51
1:H:330:GLN:OE1	1:H:330:GLN:N	2.40	0.51
2:L:107:LYS:HD3	2:L:140:TYR:OH	2.11	0.51
1:K:24:ALA:HB1	1:K:27:TYR:CE1	2.46	0.51
1:K:68:THR:HB	1:K:81:GLU:HB3	1.92	0.51
1:K:140:LEU:HD21	1:K:206:TYR:CD1	2.46	0.51
1:K:191:VAL:O	1:K:191:VAL:HG13	2.11	0.51
1:K:154:VAL:HG12	1:K:210:VAL:HG22	1.92	0.51
2:L:190:LYS:O	2:L:210:ASN:HA	2.11	0.51
1:H:11:VAL:HG22	1:H:110:ILE:HD13	1.92	0.50
2:L:165:GLU:O	2:L:166:GLN:C	2.55	0.50
1:H:140:LEU:HD12	1:H:140:LEU:C	2.36	0.50
1:H:475:SER:O	1:H:476:PRO:C	2.53	0.50
1:K:100(E):GLN:HG2	1:K:100(H):TYR:CD2	2.47	0.50
2:L:115:VAL:O	2:L:207:LYS:HE3	2.10	0.50
2:L:159:SER:HA	2:L:178:THR:O	2.11	0.50
2:M:28(A):ILE:HD13	2:M:71:PHE:CE2	2.43	0.50
2:M:144:ALA:C	2:M:145:LYS:HG3	2.35	0.50
2:L:59:SER:C	2:L:61:ARG:N	2.69	0.50
1:H:266:ILE:HD13	1:H:266:ILE:O	2.12	0.50
1:H:314:ASN:OD1	3:A:1:NAG:C1	2.59	0.50
1:H:100(J):MET:SD	1:H:100(J):MET:N	2.83	0.50
1:H:27:TYR:HB2	1:H:28:ARG:NH2	2.13	0.50
1:H:258:PRO:HD2	1:H:332:TRP:CH2	2.47	0.50
1:H:464:HIS:O	1:H:465:ASN:HB2	2.11	0.50
1:K:14:PRO:HD3	1:K:112:SER:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:40:ALA:HA	1:K:88:ALA:HB2	1.92	0.50
2:M:28(A):ILE:HD12	2:M:28(A):ILE:N	2.26	0.50
2:M:134:CYS:HB2	2:M:148:TRP:CH2	2.47	0.50
2:M:188:LYS:N	2:M:211:ARG:NH1	2.51	0.50
1:K:120:SER:HB3	1:K:122:PHE:CZ	2.47	0.50
1:K:72:ASP:HB3	1:K:75:ALA:HB3	1.94	0.49
1:H:211:ASN:ND2	1:H:218:LYS:HE2	2.26	0.49
2:M:59:SER:OG	2:M:61:ARG:HG3	2.11	0.49
1:H:163:SER:HA	1:H:209:ASN:ND2	2.28	0.49
1:K:193:VAL:HG11	1:K:206:TYR:OH	2.12	0.49
2:L:2:ILE:HD12	2:L:2:ILE:N	2.27	0.49
2:M:198:HIS:CD2	2:M:200:GLY:H	2.30	0.49
1:H:344:ASN:HD22	1:H:345:LYS:H	1.60	0.49
1:K:339:LYS:CB	1:K:354:THR:HG22	2.42	0.49
2:L:19:ALA:HB3	2:L:75:ILE:CG1	2.39	0.49
2:M:125:LEU:C	2:M:183:LYS:HD2	2.37	0.49
1:H:35:HIS:CD2	1:H:47:TRP:NE1	2.77	0.49
1:H:51:ILE:HD13	1:H:52:ASN:C	2.37	0.49
1:H:54:ASN:OD1	1:H:56:ASN:ND2	2.43	0.49
2:L:13:LEU:C	2:L:107:LYS:HB2	2.37	0.49
1:H:19:LYS:HE2	1:H:79:TYR:HD2	1.78	0.49
1:H:40:ALA:HA	1:H:88:ALA:CB	2.43	0.49
1:H:157:TRP:CZ3	1:H:208:CYS:HB3	2.48	0.49
1:K:437:LEU:HD12	1:K:437:LEU:C	2.37	0.49
1:H:193:VAL:HG22	1:H:194:PRO:CD	2.41	0.49
2:L:89:GLN:NE2	2:L:91:TYR:HB3	2.27	0.49
1:H:4:LEU:CD1	1:H:24:ALA:HB2	2.43	0.49
2:M:47:VAL:HG12	2:M:48:ILE:HG12	1.94	0.49
1:K:52:ASN:HB3	1:K:54:ASN:ND2	2.28	0.48
2:L:13:LEU:HD12	2:L:13:LEU:N	2.28	0.48
1:H:150:GLU:HB2	1:H:151:PRO:CA	2.33	0.48
1:H:391:LEU:HD12	1:H:392:VAL:N	2.28	0.48
2:L:198:HIS:CD2	2:L:200:GLY:H	2.31	0.48
1:H:10:GLU:HB3	1:H:12:LYS:NZ	2.29	0.48
2:M:25:SER:OG	2:M:28(A):ILE:HD11	2.13	0.48
1:H:324:VAL:HG23	1:H:324:VAL:O	2.12	0.48
1:K:52:ASN:ND2	1:K:53:TYR:HB3	2.28	0.48
2:M:83:PHE:CE2	2:M:106:ARG:HA	2.49	0.48
2:M:150:VAL:HG13	2:M:192:TYR:HE1	1.79	0.48
1:K:122:PHE:O	1:K:143:LEU:HB3	2.14	0.48
1:K:209:ASN:N	1:K:209:ASN:ND2	2.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:221:LYS:HE3	1:K:221:LYS:CA	2.26	0.48
2:L:120:PRO:HD2	2:L:186:TYR:OH	2.14	0.48
1:H:401:ALA:HB3	1:H:459:MET:HB2	1.95	0.48
1:K:141:GLY:HA2	1:K:157:TRP:HH2	1.78	0.48
2:M:50:GLY:C	2:M:51:VAL:HG13	2.39	0.48
1:H:440:LYS:HE2	5:H:491:HOH:O	2.12	0.48
2:M:183:LYS:HA	2:M:186:TYR:HB3	1.96	0.48
1:K:140:LEU:HD12	1:K:140:LEU:O	2.14	0.48
2:L:150:VAL:O	2:L:151:ASP:HB2	2.14	0.48
1:H:9:ALA:C	1:H:10:GLU:HG3	2.39	0.48
1:H:87:THR:O	1:H:88:ALA:HB2	2.14	0.48
1:K:28:ARG:CG	1:K:31:ASN:HB2	2.44	0.48
1:K:40:ALA:HB3	1:K:43:GLN:HG3	1.94	0.48
1:H:59:PHE:HD2	1:H:64:GLN:HA	1.77	0.47
1:H:275:VAL:HG23	1:H:322:VAL:HG22	1.95	0.47
1:K:123:PRO:HD3	1:K:221:LYS:HG2	1.95	0.47
1:H:339:LYS:HG2	1:H:354:THR:CG2	2.38	0.47
1:K:140:LEU:HD11	1:K:206:TYR:CD1	2.49	0.47
1:K:209:ASN:HD22	1:K:209:ASN:N	2.11	0.47
2:L:119:PRO:HB3	2:L:209:PHE:CE2	2.49	0.47
1:H:314:ASN:O	1:H:317:SER:HB3	2.15	0.47
2:L:21:PHE:O	2:L:72:THR:HG23	2.14	0.47
2:M:115:VAL:C	2:M:116:PHE:HD2	2.23	0.47
1:H:51:ILE:HD13	1:H:51:ILE:C	2.40	0.47
1:K:251:PRO:HD2	1:K:347:LEU:CD2	2.44	0.47
2:L:163:VAL:CG1	2:L:164:THR:N	2.78	0.47
2:M:150:VAL:HG13	2:M:192:TYR:CE1	2.50	0.47
1:H:147:TYR:CE2	1:H:152:VAL:HG13	2.49	0.47
1:K:14:PRO:HD3	1:K:112:SER:C	2.39	0.47
1:K:314:ASN:CG	4:B:1:NAG:C1	2.88	0.47
2:L:36:TYR:HE1	2:L:89:GLN:HG2	1.79	0.47
2:L:72:THR:HG22	2:L:73:LEU:H	1.79	0.47
2:L:4:LEU:HD23	2:L:25:SER:CB	2.45	0.47
2:L:113:PRO:HB3	2:L:139:PHE:HB3	1.97	0.47
2:L:175:LEU:HD23	2:L:175:LEU:C	2.39	0.47
1:K:70:THR:OG1	1:K:79:TYR:HB2	2.15	0.47
1:K:213:LYS:HB2	1:K:214:PRO:HD3	1.96	0.47
1:K:367:PRO:HG2	1:K:463:LEU:HD21	1.97	0.47
2:L:2:ILE:HD12	2:L:2:ILE:H	1.80	0.47
1:H:54:ASN:OD1	1:H:56:ASN:HB2	2.14	0.46
1:H:312:GLN:NE2	1:H:320:ARG:HB2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:241:PRO:O	1:H:242:CYS:SG	2.71	0.46
1:H:339:LYS:HE2	1:H:354:THR:CG2	2.45	0.46
1:K:291:TYR:CD1	1:K:339:LYS:HD2	2.50	0.46
1:K:314:ASN:OD1	4:B:1:NAG:C1	2.63	0.46
1:H:230:CYS:O	2:L:214:CYS:SG	2.73	0.46
1:K:35:HIS:CE1	1:K:100(J):MET:HE2	2.50	0.46
1:K:52:ASN:C	1:K:52:ASN:ND2	2.72	0.46
1:H:10:GLU:HB3	1:H:12:LYS:HZ2	1.80	0.46
1:H:100(B):ASP:HB2	1:H:100(F):ASP:CB	2.45	0.46
1:K:261:LYS:HE3	1:K:459:MET:HE1	1.96	0.46
1:K:265:MET:HE3	1:K:268:ARG:CG	2.43	0.46
1:H:124:LEU:N	1:H:124:LEU:HD12	2.30	0.46
1:K:10:GLU:HG3	1:K:18:VAL:HG23	1.96	0.46
1:K:474:LEU:HG	1:K:475:SER:N	2.30	0.46
1:H:336:LYS:HB3	1:H:338:TYR:CE1	2.51	0.46
2:L:58:ILE:N	2:L:58:ILE:HD12	2.31	0.46
1:H:216:ASN:HD22	1:H:216:ASN:HA	1.53	0.46
2:M:146:VAL:O	2:M:146:VAL:HG13	2.16	0.46
1:H:82:LEU:HD13	1:H:82(A):ARG:H	1.80	0.45
1:K:52:ASN:HD22	1:K:53:TYR:H	1.64	0.45
1:H:338:TYR:O	1:H:354:THR:HA	2.16	0.45
1:K:32:PHE:O	1:K:34:ILE:HD12	2.16	0.45
2:M:120:PRO:HD3	2:M:132:VAL:HG22	1.99	0.45
1:K:230:CYS:O	1:K:232:ASP:HB2	2.16	0.45
2:L:106:ARG:HG2	2:L:171:SER:OG	2.15	0.45
1:H:50:TRP:O	1:H:57:LYS:HA	2.16	0.45
1:K:261:LYS:CG	1:K:265:MET:HE2	2.44	0.45
2:M:14:SER:O	2:M:15:PRO:C	2.60	0.45
1:K:51:ILE:HG13	1:K:57:LYS:HG2	1.99	0.45
2:M:21:PHE:HB3	5:M:218:HOH:O	2.15	0.45
2:M:124:GLN:NE2	2:M:131:SER:H	2.14	0.45
1:K:251:PRO:HD2	1:K:347:LEU:HD21	1.98	0.45
1:K:307:LYS:HE3	1:K:324:VAL:CG2	2.47	0.45
2:L:48:ILE:HG23	2:L:53:ASN:H	1.81	0.45
2:M:155:GLN:NE2	2:M:179:LEU:HD11	2.31	0.45
2:L:163:VAL:HG12	2:L:164:THR:N	2.31	0.45
1:H:150:GLU:HG2	1:H:185:TYR:CE2	2.52	0.45
1:H:367:PRO:HG2	1:H:463:LEU:HD21	1.98	0.45
1:K:146:ASP:HB3	1:K:184:LEU:HD13	1.99	0.45
1:K:390:CYS:HB2	1:K:406:TRP:CZ2	2.52	0.45
2:L:48:ILE:HD13	2:L:54:ARG:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:115:VAL:C	2:M:116:PHE:CD2	2.95	0.45
1:H:240:PRO:HA	1:H:241:PRO:HD3	1.69	0.45
1:K:126:PRO:HD2	1:K:227:PRO:HA	1.99	0.45
2:L:8:PRO:O	2:L:102:THR:HG23	2.16	0.45
1:H:197:SER:HA	1:H:200:THR:OG1	2.17	0.44
1:H:256:PHE:HE1	1:H:275:VAL:CG1	2.30	0.44
1:H:302:HIS:C	1:H:304:ALA:H	2.26	0.44
2:M:4:LEU:HD11	2:M:90:VAL:HG23	1.98	0.44
2:M:129:THR:HA	2:M:182:SER:HA	1.99	0.44
1:H:100:TRP:CE3	1:H:100(A):ASP:HB3	2.52	0.44
1:H:163:SER:CA	1:H:209:ASN:HD21	2.30	0.44
1:H:184:LEU:N	1:H:184:LEU:HD22	2.33	0.44
2:M:50:GLY:O	2:M:51:VAL:HG13	2.18	0.44
2:M:66:GLY:HA3	2:M:71:PHE:HA	1.98	0.44
1:H:154:VAL:HG11	1:H:189:SER:CB	2.48	0.44
1:H:449:GLN:HA	1:H:474:LEU:HD22	1.99	0.44
1:K:193:VAL:HG11	1:K:206:TYR:CE1	2.53	0.44
1:H:133:THR:O	1:H:135:GLY:N	2.51	0.44
1:K:52:ASN:HD21	1:K:53:TYR:HB3	1.82	0.44
1:K:67:VAL:HA	1:K:81:GLU:O	2.18	0.44
1:K:124:LEU:HB3	2:M:118:PHE:CD1	2.52	0.44
2:L:150:VAL:HG12	2:L:189:HIS:CD2	2.53	0.44
2:M:187:GLU:HA	2:M:211:ARG:NH2	2.33	0.44
1:H:248:LEU:C	1:H:250:GLY:N	2.76	0.44
1:K:54:ASN:HD22	1:K:55:GLY:N	2.16	0.44
2:L:135:LEU:HD12	2:L:136:LEU:H	1.83	0.44
2:M:159:SER:HB3	2:M:179:LEU:CD1	2.48	0.44
2:M:198:HIS:CG	2:M:199:GLN:H	2.35	0.44
1:H:163:SER:HA	1:H:209:ASN:HD21	1.83	0.44
1:H:261:LYS:HE2	5:H:496:HOH:O	2.16	0.44
1:K:139:ALA:HB3	2:M:116:PHE:CD1	2.53	0.44
1:K:320:ARG:HE	4:B:2:NAG:H81	1.81	0.44
1:K:396:TYR:HA	1:K:397:PRO:C	2.43	0.44
2:M:107:LYS:HA	2:M:140:TYR:OH	2.17	0.44
2:M:135:LEU:HD12	2:M:135:LEU:C	2.43	0.44
1:H:37:VAL:HG13	1:H:46:GLU:C	2.43	0.43
1:H:63:PHE:HB3	1:H:67:VAL:HG21	1.99	0.43
1:H:437:LEU:C	1:H:437:LEU:CD1	2.91	0.43
1:K:54:ASN:ND2	1:K:54:ASN:C	2.73	0.43
2:M:1:GLU:CG	2:M:2:ILE:H	2.04	0.43
1:K:307:LYS:HE3	1:K:324:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:273:THR:HG23	1:H:322:VAL:CG1	2.48	0.43
1:K:62:LYS:HB2	1:K:63:PHE:CD1	2.54	0.43
1:K:156:SER:HB2	1:K:209:ASN:HB2	2.00	0.43
1:K:307:LYS:HB3	1:K:308:PRO:HD2	1.99	0.43
2:L:120:PRO:HD2	2:L:186:TYR:CZ	2.53	0.43
1:H:54:ASN:CG	1:H:56:ASN:ND2	2.76	0.43
1:K:100(C):SER:O	1:K:100(D):PRO:C	2.61	0.43
1:K:177:VAL:HG22	1:K:186:SER:O	2.18	0.43
1:K:445:LYS:O	1:K:449:GLN:HG2	2.18	0.43
2:M:159:SER:HB3	2:M:179:LEU:HD12	2.00	0.43
1:H:312:GLN:HB2	1:H:318:THR:OG1	2.19	0.43
1:K:75:ALA:CB	1:K:77:THR:HG22	2.49	0.43
1:K:474:LEU:O	1:K:475:SER:HB3	2.18	0.43
2:M:170:ASP:OD2	2:M:172:THR:OG1	2.36	0.43
2:M:198:HIS:CG	2:M:199:GLN:N	2.85	0.43
1:K:397:PRO:O	1:K:460:HIS:HE1	2.02	0.43
2:L:50:GLY:O	2:L:51:VAL:HB	2.18	0.43
1:H:30:SER:OG	1:H:53:TYR:HA	2.19	0.43
1:H:343:SER:OG	1:H:350:PRO:HB3	2.19	0.43
1:K:39:GLN:O	1:K:88:ALA:HB1	2.18	0.43
2:M:155:GLN:CG	2:M:158:ASN:HD21	2.32	0.43
1:H:66:ARG:NH2	1:H:82:LEU:HD11	2.26	0.43
1:H:121:VAL:HG23	1:H:121:VAL:O	2.19	0.43
1:H:325:LEU:O	1:H:327:VAL:HG13	2.18	0.43
1:H:445:LYS:O	1:H:449:GLN:HG3	2.19	0.43
1:K:207:ILE:HG12	1:K:222:LYS:HG2	1.99	0.43
1:H:33:VAL:HB	1:H:95:VAL:HG23	1.99	0.43
1:H:95:VAL:HG13	1:H:100(H):TYR:HA	2.00	0.43
1:H:100(D):PRO:O	1:H:100(E):GLN:HB2	2.18	0.43
1:H:117:LYS:CG	1:H:118:GLY:N	2.81	0.43
1:H:120:SER:O	1:H:144:VAL:HA	2.19	0.43
1:H:239:CYS:HA	1:H:240:PRO:HD2	1.71	0.43
1:H:348:PRO:HB3	2:M:202:ARG:HB3	2.00	0.43
1:K:207:ILE:CG1	1:K:222:LYS:HG2	2.48	0.43
1:K:464:HIS:O	1:K:465:ASN:HB2	2.19	0.43
2:M:187:GLU:HA	2:M:211:ARG:NH1	2.33	0.43
1:H:33:VAL:HG13	1:H:51:ILE:O	2.19	0.43
1:H:172:HIS:HE1	2:L:138:ASN:OD1	2.02	0.43
2:L:140:TYR:CD1	2:L:140:TYR:C	2.96	0.43
2:M:35:TRP:CD2	2:M:73:LEU:HB2	2.54	0.42
2:M:180:THR:O	2:M:181:LEU:HD22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:364:PRO:HA	1:H:396:TYR:O	2.19	0.42
2:L:31:ARG:O	2:L:51:VAL:HG23	2.18	0.42
1:H:476:PRO:O	1:H:477:GLY:C	2.62	0.42
2:L:148:TRP:CG	2:L:179:LEU:HD23	2.55	0.42
2:M:179:LEU:HD12	2:M:179:LEU:HA	1.88	0.42
1:H:236:THR:O	1:H:237:HIS:C	2.62	0.42
1:H:284:PRO:HB3	1:H:319:TYR:CE2	2.55	0.42
2:M:118:PHE:HA	2:M:119:PRO:HD3	1.77	0.42
1:H:211:ASN:HD21	1:H:218:LYS:HE2	1.83	0.42
2:M:81:GLU:CD	2:M:81:GLU:H	2.26	0.42
2:M:155:GLN:HE21	2:M:158:ASN:HD21	1.64	0.42
2:M:29:ARG:HA	2:M:29:ARG:HD3	1.85	0.42
1:H:344:ASN:HD22	1:H:345:LYS:N	2.18	0.42
2:L:182:SER:C	2:L:184:ALA:N	2.78	0.42
1:H:121:VAL:HG11	1:H:219:VAL:CG1	2.50	0.42
2:M:151:ASP:CG	2:M:189:HIS:HB3	2.45	0.42
1:H:148:PHE:CE2	1:H:149:PRO:HB3	2.55	0.42
2:M:155:GLN:CD	2:M:158:ASN:HD21	2.27	0.42
1:K:125:ALA:HA	1:K:126:PRO:HD3	1.89	0.41
1:H:9:ALA:O	1:H:10:GLU:HG3	2.20	0.41
1:H:38:ARG:HB3	1:H:90:TYR:CD2	2.55	0.41
1:H:269:THR:HA	1:H:270:PRO:HD3	1.83	0.41
1:H:388:LEU:HD13	1:H:472:LEU:HD23	2.01	0.41
2:M:109:THR:O	2:M:110:VAL:C	2.62	0.41
2:M:155:GLN:CG	2:M:156:SER:N	2.83	0.41
2:M:208:SER:OG	2:M:209:PHE:N	2.53	0.41
1:H:179:GLN:C	1:H:182:SER:N	2.76	0.41
1:H:474:LEU:O	1:H:475:SER:C	2.63	0.41
2:L:20:THR:HG22	2:L:74:THR:HG22	2.03	0.41
2:M:50:GLY:C	2:M:51:VAL:CG1	2.93	0.41
1:H:32:PHE:O	1:H:52(A):PRO:HD2	2.21	0.41
1:H:36:TRP:CE3	1:H:80:MET:HB2	2.56	0.41
1:K:291:TYR:HB2	1:K:339:LYS:HB3	2.03	0.41
1:H:119:PRO:HA	1:H:147:TYR:HB3	2.01	0.41
1:H:274:CYS:HB2	1:H:290:TRP:CH2	2.56	0.41
1:K:421:THR:HA	1:K:439:SER:HA	2.02	0.41
2:L:133:VAL:HG12	2:L:134:CYS:N	2.34	0.41
1:H:57:LYS:HG2	1:H:59:PHE:HE1	1.86	0.41
1:H:331:ASP:HB3	1:H:338:TYR:OH	2.21	0.41
1:K:119:PRO:HD2	1:K:217:THR:CG2	2.48	0.41
2:M:199:GLN:C	2:M:201:LEU:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2:VAL:HG23	1:H:2:VAL:O	2.21	0.41
1:H:67:VAL:CG1	1:H:68:THR:N	2.84	0.41
1:H:174:PHE:HA	1:H:175:PRO:HD3	1.90	0.41
1:H:253:VAL:HB	1:H:351:ILE:HG21	2.02	0.41
2:M:124:GLN:HE21	2:M:130:ALA:HA	1.86	0.41
1:H:4:LEU:HG	1:H:22:CYS:SG	2.60	0.41
1:H:123:PRO:HG3	1:H:221:LYS:HD3	2.03	0.41
1:H:369:VAL:HG21	1:H:468:THR:CG2	2.51	0.41
2:M:61:ARG:CZ	2:M:79:GLU:HG2	2.51	0.41
1:K:54:ASN:ND2	1:K:56:ASN:HB2	2.33	0.40
2:L:25:SER:OG	2:L:27:HIS:O	2.32	0.40
1:H:363:GLN:O	1:H:396:TYR:HD2	2.04	0.40
1:H:18:VAL:HG23	1:H:82(C):LEU:CD1	2.52	0.40
1:H:242:CYS:SG	1:H:242:CYS:O	2.79	0.40
1:K:338:TYR:O	1:K:354:THR:HA	2.21	0.40
4:B:8:NAG:HO3	4:B:8:NAG:C7	2.33	0.40
1:H:27:TYR:CE2	1:H:94:ARG:HD3	2.56	0.40
1:H:94:ARG:O	1:H:101:ASP:HB3	2.22	0.40
1:H:121:VAL:HG21	1:H:219:VAL:CG1	2.38	0.40
1:K:40:ALA:HA	1:K:88:ALA:CB	2.51	0.40
1:K:253:VAL:HG22	1:K:342:VAL:HG21	2.03	0.40
2:M:50:GLY:O	2:M:52:SER:N	2.50	0.40
1:H:266:ILE:O	1:H:268:ARG:N	2.55	0.40
1:K:10:GLU:OE1	1:K:12:LYS:NZ	2.55	0.40
1:K:148:PHE:CE2	1:K:149:PRO:HB3	2.56	0.40
1:K:239:CYS:O	1:K:241:PRO:HD3	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:136:GLY:CA	1:H:136:GLY:CA[4_557]	1.86	0.34

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	H	455/457 (100%)	400 (88%)	48 (10%)	7 (2%)	8	22
1	K	438/457 (96%)	402 (92%)	30 (7%)	6 (1%)	9	23
2	L	213/215 (99%)	193 (91%)	17 (8%)	3 (1%)	9	23
2	M	213/215 (99%)	195 (92%)	15 (7%)	3 (1%)	9	23
All	All	1319/1344 (98%)	1190 (90%)	110 (8%)	19 (1%)	9	23

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	99	SER
1	H	239	CYS
1	H	476	PRO
1	H	477	GLY
1	K	16	ALA
1	K	146	ASP
1	K	191	VAL
2	L	154	LEU
2	M	51	VAL
2	M	157	GLY
1	H	267	SER
1	K	29	PHE
1	K	232	ASP
1	K	241	PRO
1	H	134	SER
2	L	212	GLY
2	M	162	SER
1	H	14	PRO
2	L	68	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	405/405 (100%)	374 (92%)	31 (8%)	12	30
1	K	395/405 (98%)	378 (96%)	17 (4%)	26	54
2	L	187/187 (100%)	177 (95%)	10 (5%)	20	46
2	M	187/187 (100%)	172 (92%)	15 (8%)	11	28
All	All	1174/1184 (99%)	1101 (94%)	73 (6%)	16	39

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

Mol	Chain	Res	Type
1	H	28	ARG
1	H	38	ARG
1	H	51	ILE
1	H	80	MET
1	H	82	LEU
1	H	82(A)	ARG
1	H	82(B)	SER
1	H	82(C)	LEU
1	H	108	THR
1	H	110	ILE
1	H	144	VAL
1	H	153	THR
1	H	166	LEU
1	H	177	VAL
1	H	187	LEU
1	H	216	ASN
1	H	237	HIS
1	H	238	THR
1	H	239	CYS
1	H	266	ILE
1	H	269	THR
1	H	311	GLU
1	H	313	TYR
1	H	330	GLN
1	H	347	LEU
1	H	400	ILE
1	H	418	ASN
1	H	420	LYS
1	H	440	LYS
1	H	457	SER
1	H	476	PRO
1	K	4	LEU
1	K	28	ARG

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Mol	Chain	Res	Type
1	K	31	ASN
1	K	38	ARG
1	K	54	ASN
1	K	67	VAL
1	K	94	ARG
1	K	107	THR
1	K	187	LEU
1	K	209	ASN
1	K	221	LYS
1	K	239	CYS
1	K	246	GLU
1	K	271	GLU
1	K	368	GLN
1	K	400	ILE
1	K	418	ASN
2	L	13	LEU
2	L	58	ILE
2	L	75	ILE
2	L	76	THR
2	L	95	SER
2	L	104	LEU
2	L	107	LYS
2	L	108	ARG
2	L	142	ARG
2	L	179	LEU
2	M	51	VAL
2	M	60	ASP
2	M	63	SER
2	M	69	THR
2	M	74	THR
2	M	81	GLU
2	M	100	GLN
2	M	105	GLU
2	M	108	ARG
2	M	122	ASP
2	M	135	LEU
2	M	170	ASP
2	M	181	LEU
2	M	202	ARG
2	M	206	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	3	GLN
1	H	31	ASN
1	H	35	HIS
1	H	56	ASN
1	H	76	ASN
1	H	162	ASN
1	H	172	HIS
1	H	179	GLN
1	H	209	ASN
1	H	216	ASN
1	H	289	ASN
1	H	312	GLN
1	H	344	ASN
1	H	384	ASN
1	H	414	GLN
1	H	418	ASN
1	H	452	ASN
1	H	460	HIS
1	K	31	ASN
1	K	35	HIS
1	K	52	ASN
1	K	54	ASN
1	K	172	HIS
1	K	179	GLN
1	K	289	ASN
1	K	314	ASN
1	K	344	ASN
1	K	368	GLN
1	K	418	ASN
1	K	450	GLN
1	K	452	ASN
1	K	460	HIS
1	K	465	ASN
2	L	37	GLN
2	L	42	GLN
2	L	49	HIS
2	L	89	GLN
2	L	137	ASN
2	L	147	GLN
2	L	198	HIS
2	M	37	GLN
2	M	100	GLN
2	M	124	GLN

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Mol	Chain	Res	Type
2	M	137	ASN
2	M	158	ASN
2	M	198	HIS
2	M	199	GLN
2	M	210	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

18 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	1	3	14,14,15	0.45	0	17,19,21	0.87	0
3	NAG	A	2	3	14,14,15	0.37	0	17,19,21	0.89	1 (5%)
3	BMA	A	3	3	11,11,12	0.49	0	15,15,17	0.79	1 (6%)
3	MAN	A	4	3	11,11,12	0.57	0	15,15,17	0.69	0
3	NAG	A	5	3	14,14,15	0.64	0	17,19,21	0.86	1 (5%)
3	GAL	A	6	3	11,11,12	0.46	0	15,15,17	0.37	0
3	MAN	A	7	3	11,11,12	0.70	0	15,15,17	0.57	0
3	NAG	A	8	3	14,14,15	0.65	0	17,19,21	1.02	1 (5%)
3	GAL	A	9	3	11,11,12	0.56	0	15,15,17	0.29	0
4	NAG	B	1	4	14,14,15	0.43	0	17,19,21	1.02	1 (5%)
4	NAG	B	2	4	14,14,15	0.49	0	17,19,21	0.88	1 (5%)
4	BMA	B	3	4	11,11,12	0.67	0	15,15,17	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	B	4	4	11,11,12	0.79	0	15,15,17	0.57	0
4	NAG	B	5	4	14,14,15	0.53	0	17,19,21	1.04	1 (5%)
4	GAL	B	6	4	11,11,12	0.55	0	15,15,17	0.33	0
4	MAN	B	7	4	11,11,12	0.57	0	15,15,17	1.10	1 (6%)
4	NAG	B	8	4	14,14,15	0.59	0	17,19,21	0.67	0
4	FUC	B	9	4	10,10,11	0.58	0	14,14,16	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1	3	-	0/6/23/26	0/1/1/1
3	NAG	A	2	3	-	2/6/23/26	0/1/1/1
3	BMA	A	3	3	-	0/2/19/22	0/1/1/1
3	MAN	A	4	3	-	0/2/19/22	0/1/1/1
3	NAG	A	5	3	-	0/6/23/26	0/1/1/1
3	GAL	A	6	3	-	2/2/19/22	0/1/1/1
3	MAN	A	7	3	-	2/2/19/22	0/1/1/1
3	NAG	A	8	3	-	2/6/23/26	0/1/1/1
3	GAL	A	9	3	-	2/2/19/22	0/1/1/1
4	NAG	B	1	4	-	4/6/23/26	0/1/1/1
4	NAG	B	2	4	-	1/6/23/26	0/1/1/1
4	BMA	B	3	4	-	0/2/19/22	0/1/1/1
4	MAN	B	4	4	-	0/2/19/22	0/1/1/1
4	NAG	B	5	4	-	2/6/23/26	0/1/1/1
4	GAL	B	6	4	-	0/2/19/22	0/1/1/1
4	MAN	B	7	4	-	2/2/19/22	0/1/1/1
4	NAG	B	8	4	-	3/6/23/26	0/1/1/1
4	FUC	B	9	4	-	-	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	8	NAG	C2-N2-C7	-3.04	118.82	122.90
4	B	5	NAG	C2-N2-C7	-2.91	119.00	122.90
4	B	1	NAG	C2-N2-C7	-2.89	119.03	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2	NAG	C2-N2-C7	-2.69	119.30	122.90
3	A	2	NAG	C2-N2-C7	-2.64	119.36	122.90
4	B	7	MAN	C1-O5-C5	2.51	115.56	112.19
3	A	5	NAG	C2-N2-C7	-2.28	119.84	122.90
3	A	3	BMA	O3-C3-C2	-2.06	105.86	110.05

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	8	NAG	C3-C2-N2-C7
4	B	8	NAG	C8-C7-N2-C2
4	B	8	NAG	O7-C7-N2-C2
4	B	7	MAN	O5-C5-C6-O6
3	A	6	GAL	C4-C5-C6-O6
3	A	9	GAL	O5-C5-C6-O6
4	B	7	MAN	C4-C5-C6-O6
3	A	6	GAL	O5-C5-C6-O6
4	B	5	NAG	C8-C7-N2-C2
3	A	9	GAL	C4-C5-C6-O6
3	A	2	NAG	C8-C7-N2-C2
4	B	1	NAG	C8-C7-N2-C2
4	B	5	NAG	O7-C7-N2-C2
3	A	7	MAN	C4-C5-C6-O6
3	A	7	MAN	O5-C5-C6-O6
3	A	2	NAG	O7-C7-N2-C2
4	B	1	NAG	O7-C7-N2-C2
4	B	2	NAG	O5-C5-C6-O6
3	A	8	NAG	C8-C7-N2-C2
4	B	1	NAG	C4-C5-C6-O6
3	A	8	NAG	O7-C7-N2-C2
4	B	1	NAG	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 18 short contacts:

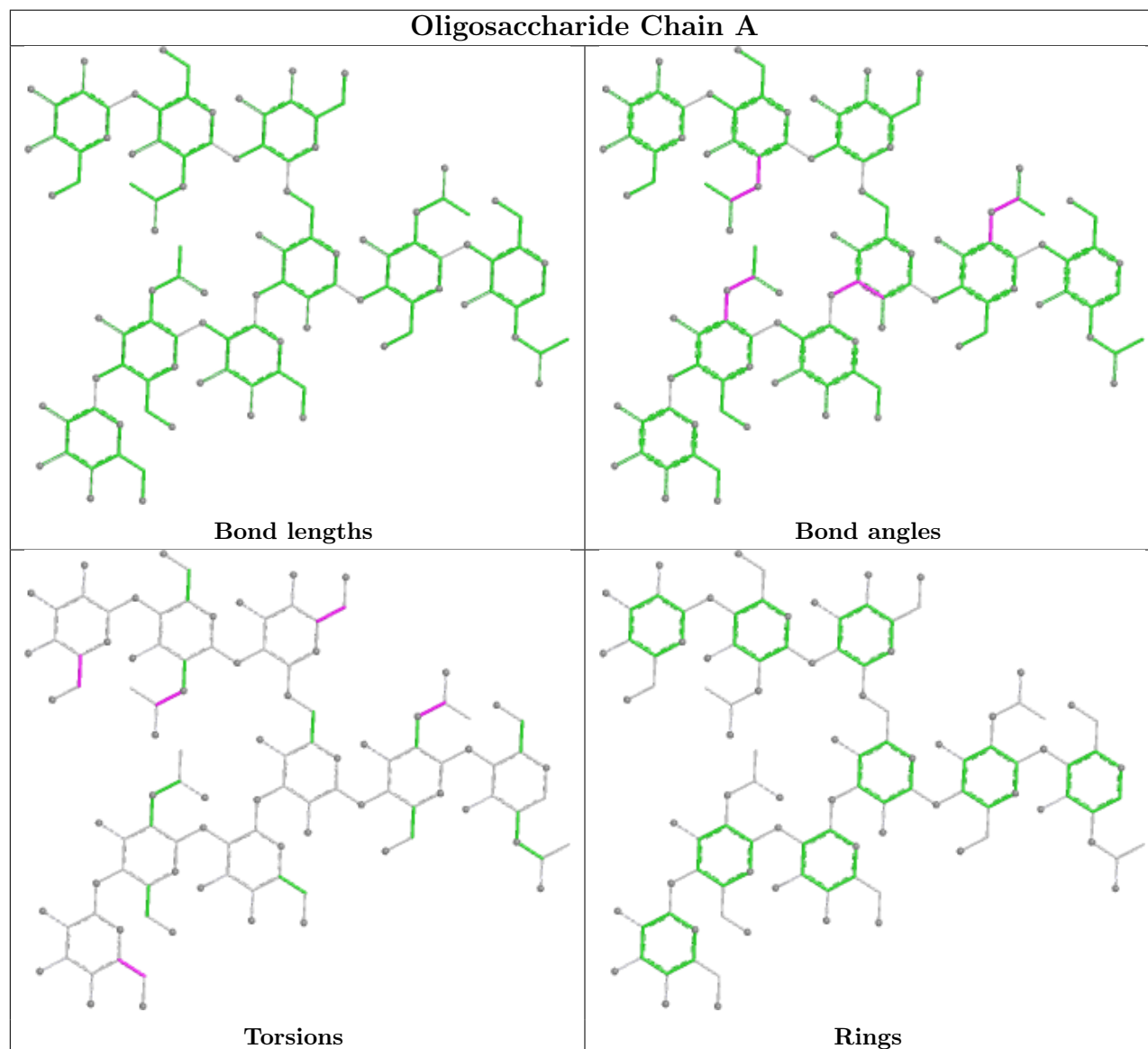
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2	NAG	2	0
3	A	2	NAG	1	0
4	B	1	NAG	4	0
3	A	5	NAG	3	0

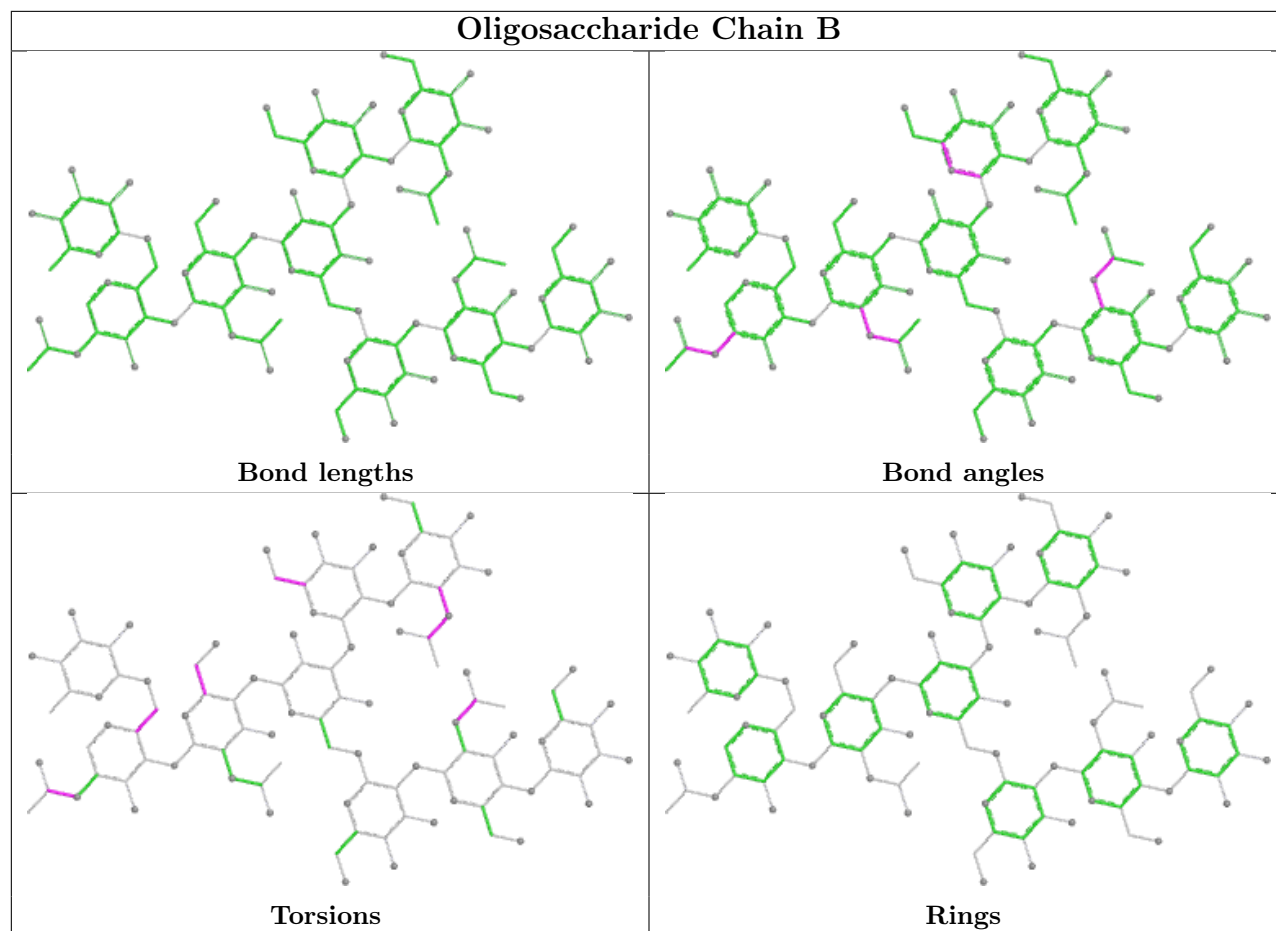
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	8	NAG	1	0
3	A	1	NAG	5	0
3	A	8	NAG	2	0
3	A	6	GAL	3	0

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	H	457/457 (100%)	0.76	56 (12%) 8 7	29, 97, 181, 199	0
1	K	444/457 (97%)	0.22	25 (5%) 30 26	28, 67, 159, 197	0
2	L	215/215 (100%)	0.48	6 (2%) 55 51	43, 89, 146, 164	0
2	M	215/215 (100%)	0.43	12 (5%) 30 26	36, 77, 167, 193	0
All	All	1331/1344 (99%)	0.48	99 (7%) 20 18	28, 83, 167, 199	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	134	SER	7.0
1	H	288	PHE	4.6
1	H	265	MET	4.4
1	H	267	SER	4.3
1	K	219	VAL	4.2
1	K	248	LEU	4.1
1	K	475	SER	4.1
1	K	225	ALA	4.0
1	H	326	THR	3.8
1	K	235	LYS	3.7
1	H	264	LEU	3.7
2	M	186	TYR	3.7
1	H	241	PRO	3.6
1	H	30	SER	3.5
1	K	198	LEU	3.5
1	H	121	VAL	3.5
1	K	122	PHE	3.5
1	H	133	THR	3.4
1	K	232	ASP	3.4
2	M	119	PRO	3.4
1	H	266	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	K	242	CYS	3.2
1	H	236	THR	3.2
2	L	186	TYR	3.2
1	K	239	CYS	3.2
1	H	478	LYS	3.1
1	K	125	ALA	3.1
1	H	271	GLU	3.1
1	H	67	VAL	3.1
1	H	272	VAL	3.1
2	M	155	GLN	3.0
2	M	125	LEU	3.0
1	H	122	PHE	2.9
2	M	182	SER	2.9
2	M	194	CYS	2.9
1	K	246	GLU	2.9
1	K	247	LEU	2.9
1	H	24	ALA	2.8
1	H	247	LEU	2.8
1	H	349	ALA	2.8
1	K	186	SER	2.8
1	H	269	THR	2.7
1	K	92	CYS	2.7
2	L	132	VAL	2.6
1	H	291	TYR	2.6
1	H	324	VAL	2.6
1	H	92	CYS	2.5
2	M	132	VAL	2.5
2	L	152	ASN	2.5
1	H	4	LEU	2.5
1	K	140	LEU	2.5
1	H	100(A)	ASP	2.5
1	K	296	GLY	2.5
2	M	209	PHE	2.5
1	H	313	TYR	2.4
1	H	79	TYR	2.4
1	H	110	ILE	2.4
1	H	277	VAL	2.4
1	H	317	SER	2.4
1	H	342	VAL	2.4
1	H	100(B)	ASP	2.3
1	H	214	PRO	2.3
2	M	200	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	286	VAL	2.3
2	L	120	PRO	2.3
2	L	211	ARG	2.3
1	H	477	GLY	2.3
1	K	123	PRO	2.2
1	K	30	SER	2.2
2	L	212	GLY	2.2
1	H	321	VAL	2.2
2	M	180	THR	2.2
1	K	345	LYS	2.2
1	H	114	ALA	2.2
1	H	346	ALA	2.2
1	H	245	PRO	2.2
1	H	259	LYS	2.2
1	H	296	GLY	2.2
1	H	33	VAL	2.2
1	H	32	PHE	2.2
1	H	78	ALA	2.2
1	H	31	ASN	2.2
1	H	243	PRO	2.2
1	K	110	ILE	2.2
1	H	125	ALA	2.1
1	K	241	PRO	2.1
1	H	325	LEU	2.1
1	K	249	GLY	2.1
1	H	123	PRO	2.1
2	M	189	HIS	2.1
1	H	253	VAL	2.1
1	K	243	PRO	2.1
1	H	52(A)	PRO	2.0
1	H	126	PRO	2.0
1	H	240	PRO	2.0
1	K	142	CYS	2.0
2	M	184	ALA	2.0
1	H	149	PRO	2.0
1	H	143	LEU	2.0

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

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

6.3 Carbohydrates

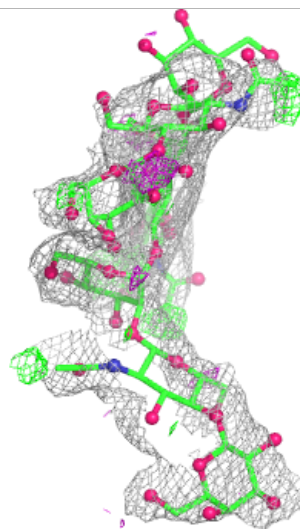
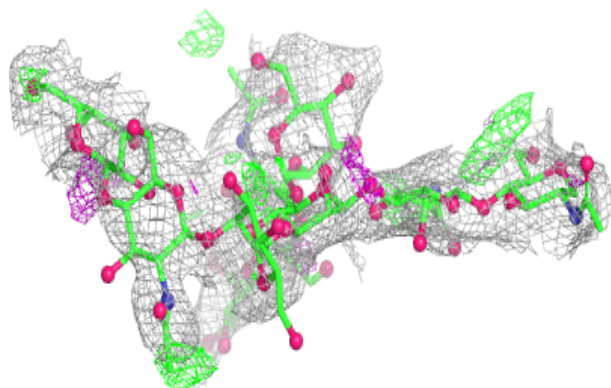
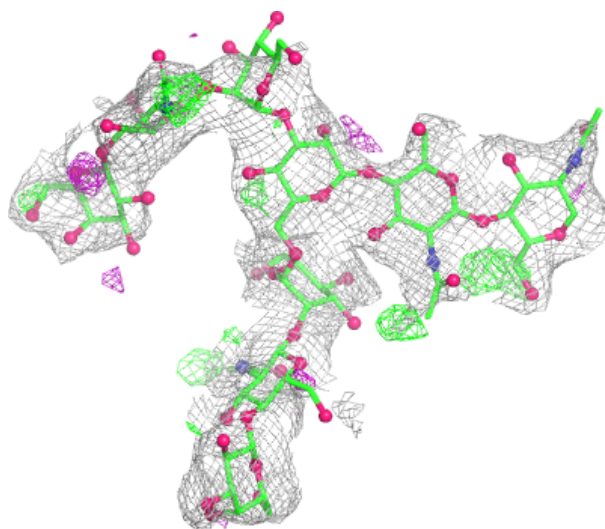
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

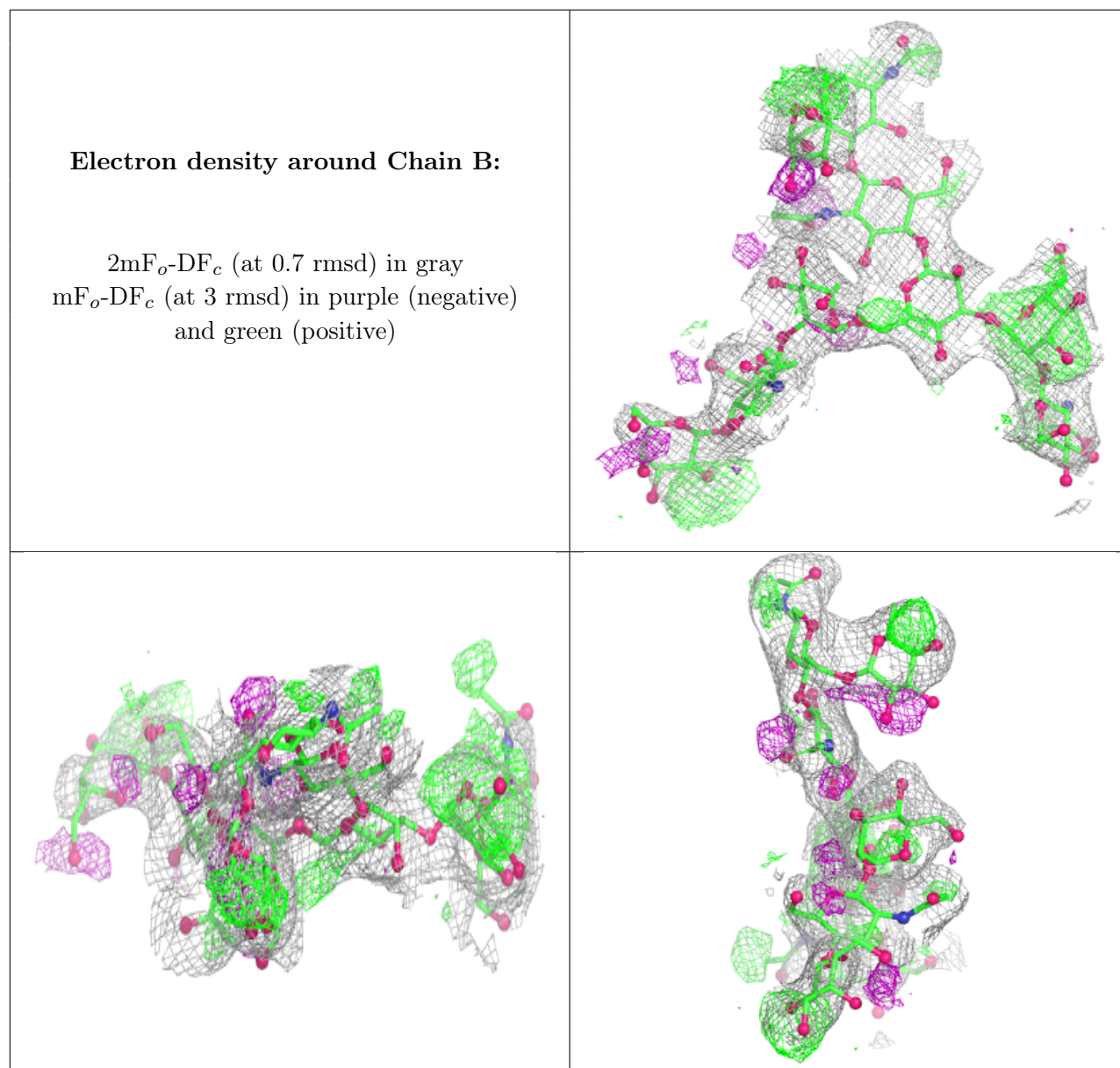
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	1	14/15	-	-	90,146,146,146	0
3	NAG	A	2	14/15	-	-	168,168,168,168	0
3	BMA	A	3	11/12	-	-	130,130,130,130	0
3	MAN	A	4	11/12	-	-	191,191,191,191	0
3	NAG	A	5	14/15	-	-	172,172,172,172	0
3	GAL	A	6	11/12	-	-	198,198,198,198	0
3	MAN	A	7	11/12	-	-	164,164,164,164	0
3	NAG	A	8	14/15	-	-	136,136,136,136	0
3	GAL	A	9	11/12	-	-	151,151,151,151	0
4	NAG	B	1	14/15	-	-	95,95,95,95	0
4	NAG	B	2	14/15	-	-	84,84,84,84	0
4	BMA	B	3	11/12	-	-	77,77,77,77	0
4	MAN	B	4	11/12	-	-	97,97,97,97	0
4	NAG	B	5	14/15	-	-	110,110,110,110	0
4	GAL	B	6	11/12	-	-	168,168,168,168	0
4	MAN	B	7	11/12	-	-	154,154,154,154	0
4	NAG	B	8	14/15	-	-	157,157,157,157	0
4	FUC	B	9	10/11	-	-	133,133,133,133	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 A:

$2mF_o-DF_c$ (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.