



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:44 PM UTC

PDB ID : 6YE3 / pdb_00006ye3
Title : IL-2 in complex with a Fab fragment from UFKA-20
Authors : Karakus, U.; Mittl, P.; Boyman, O.
Deposited on : 2020-03-23
Resolution : 2.89 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

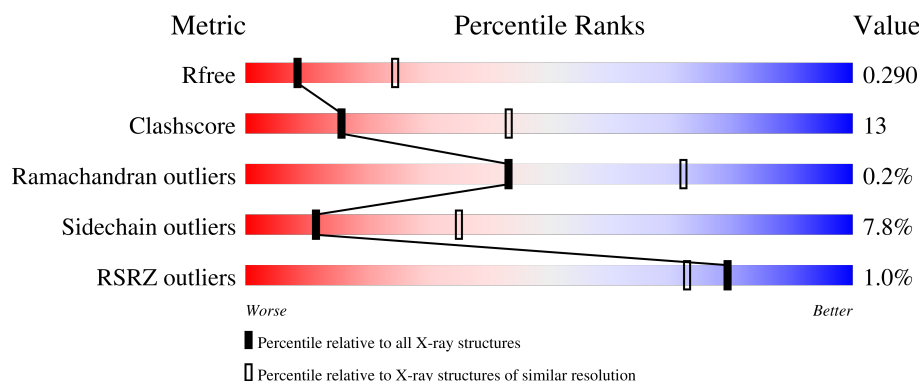
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	447	35% 13% • 50%
1	D	447	33% 15% • 50%
1	G	447	34% 15% • 50%
2	B	219	68% 29% •
2	E	219	% 71% 28% •

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Mol	Chain	Length	Quality of chain
2	H	219	% 66%33%
3	C	134	71%26%
3	F	134	% 60%34%
3	I	134	4% 56%39%
4	J	2	50%50%
4	K	2	50%50%
4	L	2	100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13559 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 Chains: A,D,G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1692	1074	281	327	10			
1	D	225	Total	C	N	O	S	0	0	0
			1702	1079	283	329	11			
1	G	225	Total	C	N	O	S	0	0	0
			1702	1079	283	329	11			

- Molecule 2 is a protein called Chains: B,E,H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	0	0	0
			1697	1061	284	345	7			
2	E	219	Total	C	N	O	S	0	0	0
			1697	1061	284	345	7			
2	H	219	Total	C	N	O	S	0	0	0
			1697	1061	284	345	7			

- Molecule 3 is a protein called Interleukin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	131	Total	C	N	O	S	0	0	0
			1068	685	176	200	7			
3	F	130	Total	C	N	O	S	0	0	0
			1061	681	175	198	7			
3	I	131	Total	C	N	O	S	0	0	0
			1068	686	176	199	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	MET	-	initiating methionine	UNP P60568
F	-5	MET	-	initiating methionine	UNP P60568

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-5	MET	-	initiating methionine	UNP P60568

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

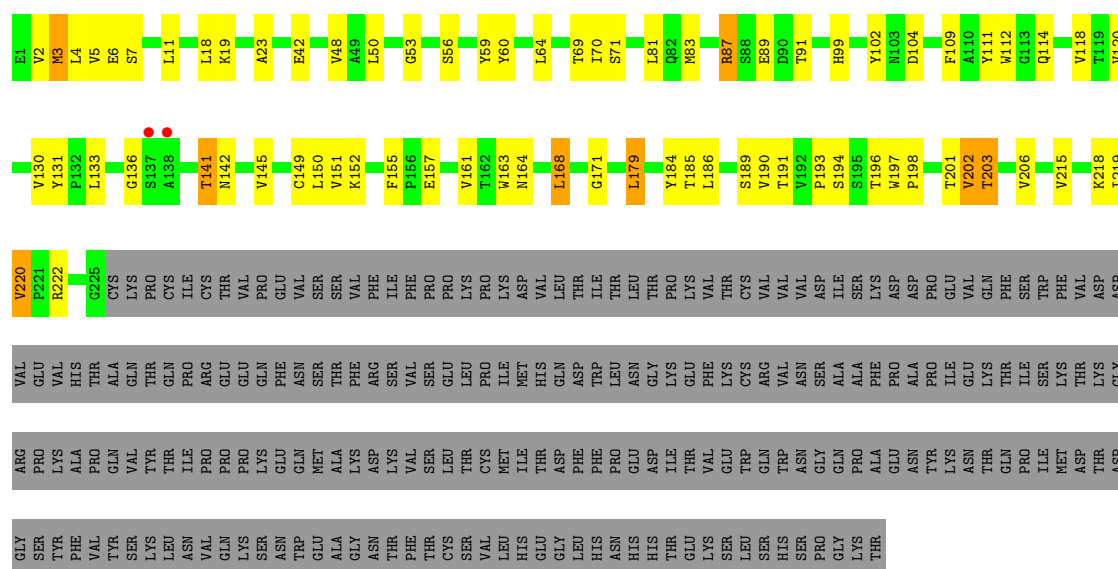
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	18	Total	O	0	0
			18	18		
5	C	6	Total	O	0	0
			6	6		
5	D	9	Total	O	0	0
			9	9		
5	E	6	Total	O	0	0
			6	6		
5	F	7	Total	O	0	0
			7	7		
5	G	14	Total	O	0	0
			14	14		
5	H	17	Total	O	0	0
			17	17		
5	I	3	Total	O	0	0
			3	3		

GLY	ASP
ARG	GLY
PRO	SER
LYS	PHE
TYR	VAL
ALA	THR
PRO	GLN
GLN	VAL
VAL	SER
TYR	LYS
THR	LEU
ILE	ASN
PRO	VAL
PRO	GLN
PRO	LYS
LYS	SER
GLU	ASN
GLN	TRP
MET	GLU
ALA	ALA
LYS	LYS
ASP	ASN
VAL	THR
VAL	PHE
SER	THR
LEU	CYS
THR	LEU
CYS	THR
THR	CYS
THR	LEU
ILE	MET
THR	GLU
THR	GLY
ASP	PHE
PHE	PHE
GLU	ASN
PRO	ASN
ASP	HIS
ILE	HIS
THR	THR
THR	THR
VAL	GLY
THR	LYS
VAL	SER
GLU	LEU
TRP	TRP
GLN	SER
TRP	GLN
ASN	TRP
GLY	SER
GLN	GLY
PRO	GLY
PRO	LYS
ALA	LYS
ALA	THR
ASN	THR
TYR	THR
LYS	LYS
LYS	THR
THR	THR
ILE	THR
PRO	THR
MET	THR
ASP	THR
THR	THR

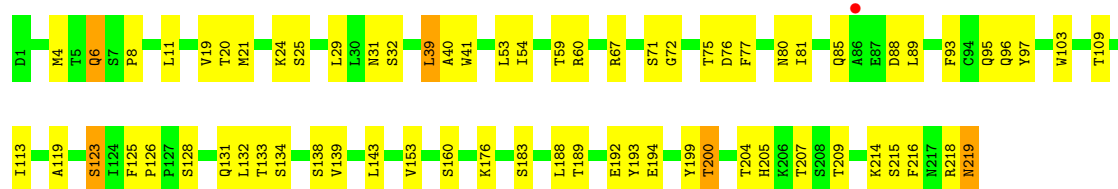
• Molecule 1: Chains: A,D,G

Chain G:  34% 15% 50%



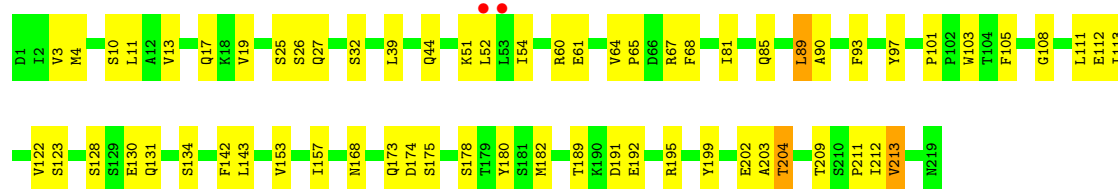
• Molecule 2: Chains: B,E,H

Chain B:  68% 29%



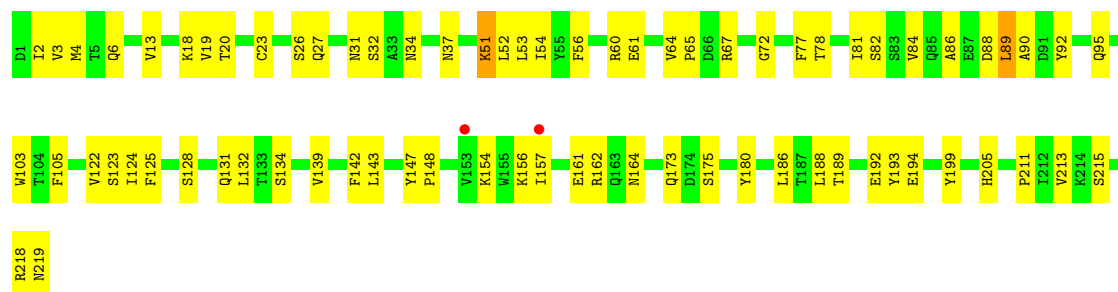
• Molecule 2: Chains: B,E,H

Chain E:  71% 28%



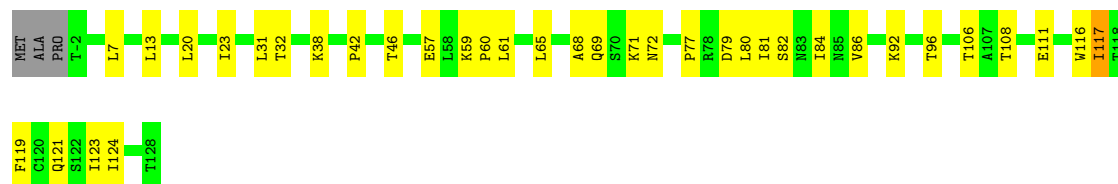
• Molecule 2: Chains: B,E,H

Chain H:  66% 33%



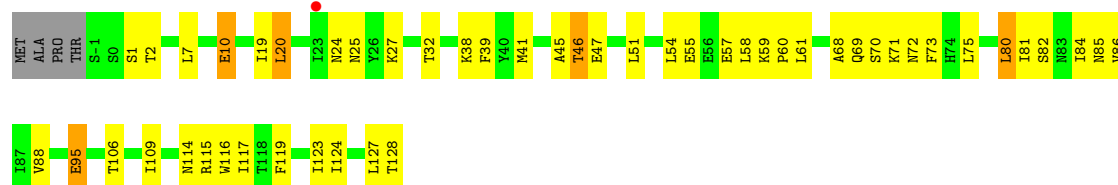
- Molecule 3: Interleukin-2

Chain C: 71% 26% ..



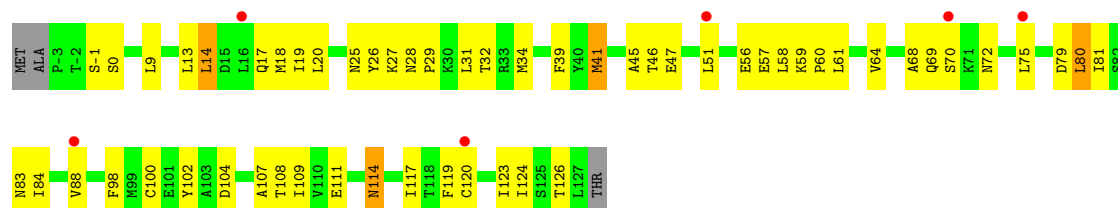
- Molecule 3: Interleukin-2

Chain F: 60% 34% ..



- Molecule 3: Interleukin-2

Chain I: 56% 39% ..



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

Chain J: 50% 50%

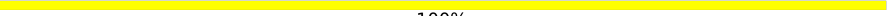


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%

MAG1
MAG2

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

Chain L:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	238.38Å 92.55Å 121.89Å 90.00° 100.11° 90.00°	Depositor
Resolution (Å)	49.40 – 2.89 49.40 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.40-2.89) 99.8 (49.40-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.91Å)	Xtriage
Refinement program	BUSTER, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.215 , 0.283 0.226 , 0.290	Depositor DCC
R_{free} test set	2933 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	99.5	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 93.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13559	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/1739	0.82	2/2374 (0.1%)
1	D	0.43	0/1749	0.76	0/2387
1	G	0.42	0/1749	0.77	0/2387
2	B	0.47	0/1736	0.79	0/2357
2	E	0.39	0/1736	0.69	0/2357
2	H	0.43	0/1736	0.71	0/2357
3	C	0.42	0/1085	0.73	0/1465
3	F	0.41	0/1078	0.75	0/1455
3	I	0.41	0/1086	0.73	0/1466
All	All	0.43	0/13694	0.75	2/18605 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	42	GLU	CA-C-N	-5.34	111.62	122.31
1	A	42	GLU	C-N-CA	-5.34	111.62	122.31

There are no chirality outliers.

There are no planarity outliers.

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	1692	0	1646	46	0
1	D	1702	0	1654	55	0
1	G	1702	0	1654	47	0
2	B	1697	0	1629	46	0
2	E	1697	0	1629	45	0
2	H	1697	0	1629	54	0
3	C	1068	0	1106	25	0
3	F	1061	0	1099	28	0
3	I	1068	0	1106	34	0
4	J	28	0	25	3	0
4	K	28	0	25	0	0
4	L	28	0	25	0	0
5	A	11	0	0	0	0
5	B	18	0	0	1	0
5	C	6	0	0	0	0
5	D	9	0	0	0	0
5	E	6	0	0	0	0
5	F	7	0	0	0	0
5	G	14	0	0	0	0
5	H	17	0	0	1	0
5	I	3	0	0	1	0
All	All	13559	0	13227	354	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 13.

All (354) 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:H:194:GLU:HA	2:H:218:ARG:HH12	1.34	0.91
2:H:53:LEU:HB3	2:H:54:ILE:HD12	1.50	0.91
1:D:40:THR:HG21	1:D:44:ARG:HH21	1.34	0.91
2:E:89:LEU:HD21	2:E:175:SER:HA	1.54	0.89
1:G:91:THR:HG22	1:G:120:VAL:H	1.40	0.87
2:B:80:ASN:HD21	4:J:1:NAG:H4	1.46	0.81
1:A:91:THR:HG22	1:A:120:VAL:H	1.48	0.79
1:D:223:ASP:N	1:D:223:ASP:OD1	2.18	0.77
1:G:163:TRP:HZ3	1:G:219:ILE:HD11	1.50	0.76
2:B:67:ARG:NH1	2:B:88:ASP:OD2	2.18	0.76
1:D:172:VAL:HG12	1:D:190:VAL:HG12	1.68	0.75
1:A:67:ARG:HD3	1:A:85:SER:HB2	1.68	0.74
1:A:157:GLU:HG2	1:A:184:TYR:CZ	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:GLN:HG2	1:D:142:ASN:HB2	1.71	0.72
1:G:130:VAL:HG21	1:G:206:VAL:HG21	1.71	0.72
1:G:136:GLY:HA2	1:G:222:ARG:HD2	1.71	0.72
2:E:13:VAL:HG11	2:E:19:VAL:HG12	1.72	0.72
2:B:131:GLN:O	2:B:134:SER:OG	2.10	0.69
1:A:12:VAL:HG12	1:A:120:VAL:HG22	1.74	0.69
1:G:179:LEU:HB2	1:G:184:TYR:CE1	2.28	0.69
1:G:164:ASN:HB2	1:G:168:LEU:HG	1.76	0.67
2:B:67:ARG:HH12	2:B:88:ASP:CG	2.02	0.67
1:D:59:TYR:OH	3:F:59:LYS:HE2	1.95	0.66
2:E:204:THR:HG22	2:E:211:PRO:HB3	1.77	0.66
3:I:13:LEU:O	3:I:17:GLN:HG2	1.95	0.66
2:H:162:ARG:HH12	2:H:188:LEU:HD13	1.61	0.66
2:B:123:SER:HB2	2:B:125:PHE:HE1	1.61	0.65
1:G:202:VAL:HB	1:G:219:ILE:HD13	1.79	0.65
1:G:152:LYS:HA	1:G:185:THR:HG23	1.78	0.64
1:G:5:VAL:HG13	1:G:23:ALA:HB3	1.80	0.64
1:G:130:VAL:HG22	1:G:151:VAL:HG12	1.79	0.64
1:A:36:TRP:NE1	1:A:81:LEU:HB2	2.13	0.64
1:A:36:TRP:CG	1:A:81:LEU:HD22	2.32	0.63
1:A:91:THR:CG2	1:A:120:VAL:H	2.10	0.63
2:H:52:LEU:HD23	2:H:61:GLU:HB2	1.81	0.63
3:I:25:ASN:O	3:I:27:LYS:N	2.32	0.63
3:C:92:LYS:HZ2	3:C:96:THR:HG21	1.65	0.62
3:C:92:LYS:NZ	3:C:96:THR:HG21	2.15	0.61
3:I:25:ASN:C	3:I:27:LYS:H	2.07	0.61
2:B:72:GLY:HA3	2:B:77:PHE:HA	1.81	0.61
2:B:123:SER:HB2	2:B:125:PHE:CE1	2.36	0.61
1:D:91:THR:HG23	1:D:119:THR:HA	1.82	0.61
1:G:163:TRP:CZ3	1:G:219:ILE:HD11	2.33	0.61
1:G:163:TRP:HZ3	1:G:219:ILE:CD1	2.13	0.61
1:D:136:GLY:HA2	1:D:222:ARG:HD2	1.83	0.61
1:D:179:LEU:HB2	1:D:184:TYR:CE1	2.36	0.61
2:E:202:GLU:HG3	2:E:213:VAL:HG13	1.83	0.61
1:D:151:VAL:HG11	1:D:206:VAL:HG11	1.83	0.60
1:G:164:ASN:HA	1:G:203:THR:HG23	1.84	0.60
2:H:31:ASN:OD1	3:I:79:ASP:HB3	2.01	0.60
1:A:68:PHE:HA	1:A:82:GLN:O	2.01	0.60
3:F:61:LEU:HD23	3:F:81:ILE:HD12	1.83	0.59
3:I:29:PRO:HG2	3:I:69:GLN:HE22	1.66	0.59
1:D:142:ASN:O	1:D:194:SER:OG	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:60:ARG:HB3	2:E:64:VAL:CG2	2.33	0.59
1:D:189:SER:HB2	2:E:142:PHE:CE2	2.38	0.59
2:E:101:PRO:HG3	2:E:103:TRP:CZ2	2.38	0.58
2:H:60:ARG:HB3	2:H:64:VAL:CG2	2.33	0.58
1:G:133:LEU:HD21	1:G:150:LEU:HB2	1.86	0.58
1:D:157:GLU:HG2	1:D:184:TYR:CZ	2.39	0.58
2:H:51:LYS:HD3	2:H:52:LEU:H	1.69	0.58
1:D:2:VAL:CG2	1:D:27:PHE:HD1	2.17	0.57
2:E:61:GLU:O	2:E:64:VAL:HG22	2.04	0.57
2:E:65:PRO:HD2	2:E:68:PHE:CE2	2.39	0.57
1:D:151:VAL:HG23	1:D:186:LEU:HB3	1.86	0.57
3:I:58:LEU:HD22	3:I:81:ILE:HG23	1.86	0.57
2:H:13:VAL:HG11	2:H:19:VAL:HG12	1.88	0.56
2:H:173:GLN:HB2	2:H:180:TYR:CZ	2.39	0.56
2:H:194:GLU:HA	2:H:218:ARG:NH1	2.13	0.56
2:B:19:VAL:HG22	2:B:81:ILE:HB	1.88	0.56
1:A:36:TRP:CD1	1:A:81:LEU:HB2	2.41	0.56
1:D:11:LEU:HD12	1:D:12:VAL:H	1.71	0.55
2:H:189:THR:HG22	2:H:192:GLU:OE1	2.06	0.55
3:I:14:LEU:HD23	3:I:18:MET:HE3	1.89	0.55
3:C:65:LEU:HD12	3:C:81:ILE:HD11	1.89	0.55
2:H:157:ILE:HG22	2:H:199:TYR:HE1	1.70	0.55
1:A:6:GLU:N	1:A:6:GLU:OE1	2.40	0.54
2:E:157:ILE:O	2:E:157:ILE:HG13	2.06	0.54
2:B:80:ASN:HD21	4:J:1:NAG:C4	2.19	0.54
3:C:77:PRO:HA	3:C:80:LEU:HD12	1.88	0.54
3:C:121:GLN:O	3:C:124:ILE:HG13	2.07	0.54
2:B:119:ALA:HA	2:B:207:THR:HG21	1.90	0.54
2:E:19:VAL:HG22	2:E:81:ILE:HB	1.90	0.54
1:A:201:THR:HG21	2:H:211:PRO:O	2.08	0.54
2:E:25:SER:OG	2:E:27:GLN:O	2.20	0.54
1:G:60:TYR:CE1	1:G:70:ILE:HG22	2.42	0.54
2:H:89:LEU:HD21	2:H:175:SER:HA	1.89	0.53
3:C:108:THR:HG23	3:C:111:GLU:H	1.73	0.53
1:D:67:ARG:HD3	1:D:85:SER:HB2	1.89	0.53
1:G:202:VAL:O	1:G:219:ILE:HD12	2.09	0.53
2:H:131:GLN:O	2:H:134:SER:OG	2.26	0.53
2:B:95:GLN:HG2	2:B:96:GLN:N	2.23	0.53
3:C:80:LEU:O	3:C:84:ILE:HG13	2.09	0.53
2:H:34:ASN:HB3	3:I:83:ASN:OD1	2.09	0.53
1:A:161:VAL:HB	1:A:206:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:157:ILE:HG22	2:H:199:TYR:CE1	2.43	0.53
1:G:59:TYR:OH	3:I:59:LYS:HE2	2.08	0.53
3:C:77:PRO:O	3:C:81:ILE:HG12	2.08	0.53
3:I:29:PRO:HG2	3:I:69:GLN:NE2	2.24	0.53
3:I:-1:SER:OG	3:I:0:SER:N	2.43	0.52
1:G:91:THR:CG2	1:G:120:VAL:H	2.18	0.52
3:C:61:LEU:HD23	3:C:81:ILE:HD12	1.91	0.52
1:D:2:VAL:HG21	1:D:27:PHE:HD1	1.74	0.52
2:H:156:LYS:HA	2:H:161:GLU:HA	1.92	0.51
3:I:56:GLU:OE1	3:I:102:TYR:OH	2.21	0.51
3:I:57:GLU:C	3:I:60:PRO:HD2	2.36	0.51
1:A:12:VAL:CG1	1:A:120:VAL:HG22	2.39	0.51
1:A:60:TYR:CE1	1:A:70:ILE:HG22	2.46	0.51
1:D:42:GLU:H	1:D:42:GLU:CD	2.19	0.51
3:F:2:THR:HG22	3:F:127:LEU:HD12	1.91	0.51
3:F:57:GLU:C	3:F:60:PRO:HD2	2.36	0.51
1:G:151:VAL:CG2	1:G:186:LEU:HB3	2.40	0.51
1:D:128:PRO:HB3	1:D:154:TYR:HB3	1.92	0.51
3:F:25:ASN:ND2	3:F:27:LYS:HB2	2.26	0.51
1:G:201:THR:HG22	1:G:218:LYS:HE2	1.91	0.51
3:I:80:LEU:O	3:I:84:ILE:HG13	2.10	0.51
1:G:189:SER:HB2	2:H:142:PHE:CE2	2.46	0.51
1:A:12:VAL:HG11	1:A:86:LEU:HD13	1.91	0.51
3:C:108:THR:CG2	3:C:111:GLU:H	2.23	0.51
3:F:68:ALA:HB1	3:F:72:ASN:HD21	1.76	0.51
2:H:142:PHE:C	2:H:143:LEU:HD12	2.36	0.51
2:B:131:GLN:CD	2:B:138:SER:H	2.18	0.50
2:B:189:THR:HG23	2:B:192:GLU:H	1.77	0.50
1:D:83:MET:HE1	1:D:118:VAL:HG21	1.92	0.50
2:E:189:THR:HG23	2:E:192:GLU:H	1.76	0.50
1:D:107:ALA:HB3	2:E:97:TYR:HB2	1.92	0.50
1:A:91:THR:HG22	1:A:120:VAL:N	2.22	0.50
2:B:199:TYR:HB2	2:B:216:PHE:CE1	2.46	0.50
3:C:68:ALA:HB1	3:C:72:ASN:HB2	1.93	0.50
3:I:25:ASN:C	3:I:27:LYS:N	2.69	0.50
3:I:123:ILE:HA	3:I:126:THR:HG22	1.93	0.50
1:D:157:GLU:HG2	1:D:184:TYR:CE2	2.47	0.50
3:F:19:ILE:HD11	3:F:80:LEU:HD22	1.93	0.50
1:G:142:ASN:O	1:G:194:SER:OG	2.29	0.50
2:H:90:ALA:HB3	2:H:92:TYR:CE1	2.46	0.50
1:A:156:PRO:C	1:A:158:PRO:HD2	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:ILE:HD13	2:B:60:ARG:HA	1.94	0.49
3:F:119:PHE:O	3:F:123:ILE:HG12	2.11	0.49
2:E:3:VAL:HB	2:E:26:SER:HB3	1.94	0.49
1:A:59:TYR:OH	3:C:59:LYS:HE2	2.12	0.49
1:G:5:VAL:HA	1:G:114:GLN:OE1	2.12	0.49
1:G:111:TYR:HA	2:H:51:LYS:HZ3	1.77	0.49
2:B:39:LEU:HG	2:B:40:ALA:N	2.26	0.49
2:E:203:ALA:HB3	2:E:212:ILE:HG23	1.95	0.49
2:H:61:GLU:O	2:H:64:VAL:HG22	2.12	0.49
2:H:139:VAL:HG13	2:H:186:LEU:HB3	1.93	0.49
2:E:51:LYS:HD3	2:E:52:LEU:N	2.28	0.49
3:F:38:LYS:HB3	3:F:106:THR:HB	1.94	0.49
3:I:61:LEU:HD23	3:I:81:ILE:HD12	1.94	0.49
3:F:55:GLU:HA	3:F:58:LEU:HG	1.94	0.49
1:G:109:PHE:O	1:G:112:TRP:NE1	2.42	0.49
1:G:218:LYS:HD3	1:G:220:VAL:HG13	1.94	0.49
1:A:157:GLU:HG2	1:A:184:TYR:CE2	2.48	0.48
1:G:104:ASP:HB2	2:H:103:TRP:CH2	2.48	0.48
2:H:147:TYR:CD1	2:H:148:PRO:HA	2.49	0.48
1:A:131:TYR:HD2	1:A:150:LEU:HD12	1.77	0.48
2:B:31:ASN:OD1	3:C:79:ASP:HB3	2.13	0.48
1:G:193:PRO:O	1:G:196:THR:HG22	2.14	0.48
2:E:157:ILE:HG22	2:E:199:TYR:CE1	2.49	0.48
2:E:4:MET:HE1	2:E:39:LEU:HD12	1.96	0.48
1:G:145:VAL:O	1:G:191:THR:HA	2.13	0.48
1:D:6:GLU:N	1:D:6:GLU:OE1	2.47	0.48
1:D:201:THR:OG1	1:D:218:LYS:HE2	2.14	0.48
2:H:86:ALA:HB3	5:H:405:HOH:O	2.14	0.48
3:C:82:SER:O	3:C:86:VAL:HG23	2.13	0.48
1:D:2:VAL:HG21	1:D:27:PHE:CD1	2.49	0.48
1:D:218:LYS:HD3	1:D:220:VAL:HG13	1.95	0.48
3:F:71:LYS:O	3:F:71:LYS:HD3	2.14	0.48
3:C:69:GLN:C	3:C:71:LYS:H	2.22	0.48
3:F:45:ALA:HB1	3:F:119:PHE:CD1	2.49	0.48
3:I:9:LEU:HD21	3:I:123:ILE:HB	1.96	0.48
1:D:48:VAL:HG13	1:D:64:LEU:HD21	1.95	0.47
2:H:18:LYS:HD3	2:H:82:SER:HA	1.96	0.47
1:A:43:ARG:HA	1:A:43:ARG:HD2	1.76	0.47
1:A:106:LEU:HB3	1:A:108:TRP:CZ3	2.49	0.47
1:D:131:TYR:HB3	2:E:128:SER:OG	2.15	0.47
3:I:19:ILE:HG13	3:I:80:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:ASN:OD1	2:B:219:ASN:N	2.46	0.47
3:I:47:GLU:HB3	5:I:201:HOH:O	2.13	0.47
2:H:19:VAL:HG13	2:H:84:VAL:HG21	1.95	0.47
2:B:131:GLN:OE1	2:B:138:SER:N	2.48	0.47
1:G:164:ASN:ND2	1:G:168:LEU:HD21	2.30	0.47
2:H:147:TYR:O	2:H:205:HIS:HE1	1.98	0.47
1:A:42:GLU:CD	1:A:42:GLU:H	2.23	0.47
2:B:21:MET:HG2	2:B:109:THR:HG21	1.97	0.47
2:B:24:LYS:HA	2:B:75:THR:O	2.15	0.47
2:E:11:LEU:HD22	2:E:111:LEU:CD1	2.45	0.47
1:A:133:LEU:HB2	1:A:148:GLY:CA	2.45	0.47
2:E:112:GLU:HG3	2:E:180:TYR:OH	2.15	0.47
1:A:145:VAL:O	1:A:191:THR:HA	2.15	0.46
1:G:50:LEU:HD12	1:G:99:HIS:NE2	2.30	0.46
2:H:19:VAL:HG22	2:H:81:ILE:HB	1.96	0.46
1:D:68:PHE:HB3	1:D:81:LEU:HD11	1.98	0.46
3:F:69:GLN:O	3:F:71:LYS:N	2.49	0.46
3:F:82:SER:O	3:F:86:VAL:HG23	2.16	0.46
1:A:179:LEU:HB2	1:A:184:TYR:CE1	2.51	0.46
1:D:133:LEU:HB2	1:D:148:GLY:CA	2.45	0.46
2:B:200:THR:HB	2:B:215:SER:HB3	1.97	0.46
2:H:132:LEU:HD23	2:H:132:LEU:HA	1.82	0.46
1:D:104:ASP:HB2	2:E:103:TRP:CH2	2.50	0.46
1:A:126:THR:OG1	1:A:183:LEU:HD11	2.16	0.45
3:C:38:LYS:HB3	3:C:106:THR:OG1	2.16	0.45
2:E:143:LEU:HD11	2:E:153:VAL:HG22	1.99	0.45
1:A:20:LEU:HD13	1:A:83:MET:HE3	1.99	0.45
2:B:193:TYR:CE1	2:B:199:TYR:CE2	3.05	0.45
3:C:119:PHE:O	3:C:123:ILE:HG12	2.17	0.45
1:D:27:PHE:CE2	1:D:98:ARG:HD2	2.52	0.45
1:G:83:MET:HE1	1:G:118:VAL:HG21	1.99	0.45
2:H:88:ASP:O	2:H:92:TYR:OH	2.23	0.45
2:B:132:LEU:HA	2:B:132:LEU:HD23	1.68	0.45
1:D:189:SER:HB2	2:E:142:PHE:CD2	2.52	0.45
2:B:194:GLU:C	2:B:218:ARG:HH12	2.22	0.45
1:D:50:LEU:HD13	2:E:103:TRP:CH2	2.52	0.45
2:H:188:LEU:HD12	2:H:188:LEU:HA	1.89	0.45
1:A:36:TRP:CE2	1:A:81:LEU:HB2	2.52	0.45
1:D:20:LEU:HG	1:D:83:MET:HE2	1.99	0.45
1:D:130:VAL:HA	1:D:150:LEU:O	2.16	0.45
1:A:40:THR:HB	1:A:41:PRO:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:89:LEU:CD2	2:H:175:SER:HA	2.47	0.44
1:A:83:MET:HB2	1:A:86:LEU:HD11	1.99	0.44
2:B:25:SER:O	2:B:75:THR:HB	2.17	0.44
2:B:41:TRP:O	2:B:53:LEU:HB2	2.17	0.44
2:H:60:ARG:HD2	2:H:64:VAL:HG23	1.99	0.44
1:A:183:LEU:HD12	1:A:183:LEU:HA	1.84	0.44
1:D:68:PHE:HA	1:D:82:GLN:O	2.17	0.44
2:E:122:VAL:HG22	2:E:143:LEU:HD22	2.00	0.44
2:H:122:VAL:HA	2:H:142:PHE:O	2.17	0.44
1:A:152:LYS:HB2	1:A:185:THR:HG23	1.99	0.44
1:A:175:PHE:CD1	1:A:175:PHE:N	2.85	0.44
2:E:65:PRO:HD2	2:E:68:PHE:HE2	1.80	0.44
2:H:162:ARG:NH1	2:H:188:LEU:HD13	2.30	0.44
1:A:36:TRP:O	1:A:48:VAL:HG22	2.18	0.44
1:D:57:TYR:OH	1:D:103:ASN:HB3	2.17	0.44
2:E:4:MET:HB2	2:E:105:PHE:O	2.18	0.44
2:E:52:LEU:HD23	2:E:61:GLU:OE1	2.18	0.44
1:A:108:TRP:HE3	2:B:97:TYR:CE2	2.35	0.44
2:B:80:ASN:ND2	4:J:1:NAG:H4	2.20	0.44
2:B:126:PRO:HB3	2:B:216:PHE:CE2	2.52	0.44
2:E:54:ILE:CD1	2:E:60:ARG:HG2	2.48	0.44
1:G:42:GLU:CD	1:G:42:GLU:H	2.24	0.44
1:G:53:GLY:HA3	1:G:102:TYR:CD1	2.53	0.44
3:I:39:PHE:CE1	3:I:109:ILE:HB	2.53	0.44
2:B:24:LYS:HE3	2:B:76:ASP:OD1	2.18	0.44
2:B:53:LEU:HD23	2:B:53:LEU:HA	1.80	0.44
2:B:125:PHE:O	2:B:139:VAL:HG23	2.18	0.44
3:F:54:LEU:HD13	3:F:116:TRP:CD1	2.53	0.44
3:I:28:ASN:ND2	3:I:31:LEU:HB2	2.33	0.44
3:I:98:PHE:HE1	3:I:100:CYS:HA	1.83	0.44
1:D:130:VAL:HG22	1:D:217:LYS:HE3	1.99	0.43
2:H:2:ILE:HG12	2:H:27:GLN:HB2	1.99	0.43
1:D:105:TYR:HD2	3:F:85:ASN:ND2	2.17	0.43
1:A:67:ARG:HB3	1:A:84:SER:O	2.18	0.43
2:H:72:GLY:HA3	2:H:77:PHE:HA	2.00	0.43
3:I:114:ASN:O	3:I:117:ILE:HG13	2.18	0.43
1:A:57:TYR:OH	1:A:103:ASN:HB3	2.18	0.43
2:B:143:LEU:HD12	2:B:143:LEU:N	2.33	0.43
1:D:11:LEU:HD12	1:D:12:VAL:N	2.34	0.43
1:D:153:GLY:HA2	1:D:183:LEU:HG	2.00	0.43
2:E:65:PRO:HB2	2:E:67:ARG:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:39:PHE:CE1	3:F:109:ILE:HB	2.53	0.43
2:H:147:TYR:O	2:H:205:HIS:CE1	2.72	0.43
2:B:205:HIS:HB3	2:B:207:THR:HG22	2.00	0.43
2:E:10:SER:OG	2:E:11:LEU:N	2.52	0.43
3:F:84:ILE:O	3:F:88:VAL:HG23	2.19	0.43
2:H:65:PRO:HB2	2:H:67:ARG:HG2	2.00	0.43
2:B:4:MET:HE1	2:B:29:LEU:HD11	2.01	0.43
2:B:194:GLU:O	2:B:218:ARG:NH1	2.28	0.43
1:A:105:TYR:OH	3:C:59:LYS:HD2	2.19	0.43
1:D:147:LEU:HD11	1:D:197:TRP:CG	2.53	0.43
3:F:20:LEU:O	3:F:24:ASN:HB2	2.19	0.43
3:F:51:LEU:HB3	3:F:88:VAL:HG13	2.01	0.43
3:C:13:LEU:CD1	3:C:117:ILE:HG23	2.49	0.43
1:G:131:TYR:HB3	2:H:128:SER:OG	2.19	0.43
2:B:218:ARG:H	2:B:218:ARG:HG2	1.60	0.42
1:D:53:GLY:O	1:D:72:ARG:NH2	2.52	0.42
2:E:191:ASP:O	2:E:195:ARG:HG3	2.19	0.42
1:G:151:VAL:HG22	1:G:186:LEU:HB3	2.01	0.42
3:I:28:ASN:HD21	3:I:31:LEU:HB2	1.84	0.42
2:E:44:GLN:O	2:E:90:ALA:HB1	2.19	0.42
3:F:45:ALA:HB3	3:F:115:ARG:HH12	1.84	0.42
2:H:147:TYR:CG	2:H:148:PRO:HA	2.54	0.42
2:B:176:LYS:NZ	5:B:401:HOH:O	2.51	0.42
2:E:173:GLN:HG2	2:E:178:SER:HA	2.02	0.42
1:A:131:TYR:HB3	2:B:128:SER:OG	2.20	0.42
1:A:108:TRP:CE3	2:B:97:TYR:CE2	3.08	0.42
2:B:8:PRO:HG2	2:B:11:LEU:HD12	2.02	0.42
3:I:120:CYS:O	3:I:124:ILE:HG23	2.19	0.42
1:D:2:VAL:HG23	1:D:26:GLY:C	2.44	0.42
2:H:3:VAL:HB	2:H:26:SER:HB3	2.02	0.42
1:D:152:LYS:HA	1:D:185:THR:HG23	2.01	0.42
1:D:215:VAL:HG21	1:D:217:LYS:HE2	2.00	0.42
2:E:93:PHE:CD1	2:E:108:GLY:HA3	2.53	0.42
3:F:114:ASN:O	3:F:117:ILE:HG13	2.19	0.42
3:I:34:MET:HE1	3:I:68:ALA:HB2	2.02	0.42
1:A:36:TRP:CB	1:A:81:LEU:HD22	2.50	0.42
3:F:75:LEU:HD23	3:F:80:LEU:HD12	2.00	0.42
1:A:35:SER:HA	1:A:49:ALA:O	2.19	0.42
1:D:130:VAL:HB	1:D:151:VAL:HG12	2.01	0.42
1:D:207:ALA:HB2	1:D:214:LYS:HD3	2.02	0.41
1:G:141:THR:HG22	1:G:142:ASN:H	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:200:THR:CB	2:B:215:SER:HB3	2.49	0.41
1:D:142:ASN:OD1	1:D:143:SER:N	2.53	0.41
1:G:171:GLY:O	1:G:190:VAL:HA	2.20	0.41
3:I:60:PRO:O	3:I:64:VAL:HG23	2.19	0.41
3:C:61:LEU:O	3:C:65:LEU:HG	2.20	0.41
1:G:5:VAL:CG1	1:G:23:ALA:HB3	2.48	0.41
2:H:6:GLN:NE2	2:H:92:TYR:O	2.51	0.41
2:H:157:ILE:HG13	2:H:157:ILE:O	2.19	0.41
3:I:84:ILE:O	3:I:88:VAL:HG23	2.21	0.41
1:D:105:TYR:HD2	3:F:85:ASN:HD22	1.68	0.41
3:I:108:THR:HG23	3:I:111:GLU:H	1.84	0.41
3:C:23:ILE:O	3:C:31:LEU:HD13	2.21	0.41
1:D:106:LEU:HD21	3:F:86:VAL:HG22	2.02	0.41
1:G:3:MET:O	1:G:4:LEU:HD23	2.20	0.41
1:G:81:LEU:HD12	1:G:81:LEU:HA	1.61	0.41
2:E:128:SER:HB2	2:E:130:GLU:OE1	2.21	0.41
1:G:11:LEU:HD22	1:G:155:PHE:CE1	2.56	0.41
1:A:149:CYS:HB2	1:A:163:TRP:CZ2	2.55	0.41
2:E:67:ARG:HH11	2:E:67:ARG:HD2	1.71	0.41
2:E:174:ASP:O	2:E:178:SER:HA	2.20	0.41
3:I:51:LEU:HB3	3:I:88:VAL:HG13	2.01	0.41
3:C:42:PRO:HG3	3:C:116:TRP:CH2	2.56	0.41
3:C:57:GLU:C	3:C:60:PRO:HD2	2.46	0.41
3:C:71:LYS:O	3:C:71:LYS:HD3	2.20	0.41
1:D:12:VAL:CG2	1:D:18:LEU:HD22	2.51	0.41
2:E:168:ASN:HB3	2:E:182:MET:HE3	2.01	0.41
1:G:18:LEU:HD12	1:G:19:LYS:H	1.86	0.41
1:G:136:GLY:HA2	1:G:222:ARG:CD	2.47	0.41
2:H:4:MET:HE3	2:H:23:CYS:SG	2.60	0.41
2:H:193:TYR:O	2:H:218:ARG:NH1	2.53	0.41
1:A:104:ASP:HB2	2:B:103:TRP:CH2	2.56	0.41
1:D:131:TYR:CE2	2:E:131:GLN:HG3	2.56	0.41
3:F:95:GLU:H	3:F:95:GLU:CD	2.28	0.41
2:H:125:PHE:O	2:H:139:VAL:HG23	2.21	0.41
2:H:199:TYR:C	2:H:215:SER:HG	2.26	0.41
1:G:197:TRP:HB3	1:G:198:PRO:HD3	2.03	0.40
3:I:41:MET:SD	3:I:107:ALA:HB3	2.60	0.40
3:I:68:ALA:HB1	3:I:72:ASN:HD21	1.86	0.40
3:F:46:THR:OG1	3:F:47:GLU:HG3	2.21	0.40
1:A:11:LEU:HB2	1:A:156:PRO:HG3	2.04	0.40
3:C:38:LYS:HD2	3:C:106:THR:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:93:PHE:CE1	2:E:108:GLY:HA3	2.56	0.40
2:E:142:PHE:C	2:E:143:LEU:HD23	2.46	0.40
1:G:87:ARG:HD2	1:G:89:GLU:OE2	2.20	0.40
3:I:45:ALA:HB1	3:I:119:PHE:CD1	2.57	0.40
1:G:6:GLU:OE1	1:G:6:GLU:N	2.55	0.40
2:H:162:ARG:CZ	2:H:164:ASN:HB2	2.51	0.40
2:B:6:GLN:OE1	2:B:93:PHE:HA	2.22	0.40
2:B:54:ILE:HG23	2:B:59:THR:O	2.22	0.40
1:D:68:PHE:CD1	1:D:68:PHE:N	2.89	0.40
2:E:112:GLU:HG2	2:E:113:ILE:N	2.36	0.40
3:F:7:LEU:HA	3:F:10:GLU:HB2	2.04	0.40
2:H:37:ASN:O	2:H:56:PHE:HA	2.22	0.40
2:H:95:GLN:HB2	2:H:105:PHE:CD2	2.56	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	221/447 (49%)	212 (96%)	8 (4%)	1 (0%)	24	54
1	D	223/447 (50%)	213 (96%)	10 (4%)	0	100	100
1	G	223/447 (50%)	210 (94%)	13 (6%)	0	100	100
2	B	217/219 (99%)	211 (97%)	6 (3%)	0	100	100
2	E	217/219 (99%)	210 (97%)	7 (3%)	0	100	100
2	H	217/219 (99%)	210 (97%)	7 (3%)	0	100	100
3	C	129/134 (96%)	127 (98%)	2 (2%)	0	100	100
3	F	128/134 (96%)	123 (96%)	4 (3%)	1 (1%)	16	44
3	I	129/134 (96%)	123 (95%)	5 (4%)	1 (1%)	16	44
All	All	1704/2400 (71%)	1639 (96%)	62 (4%)	3 (0%)	43	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	26	TYR
3	F	70	SER
1	A	136	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	188/396 (48%)	170 (90%)	18 (10%)	8	26
1	D	189/396 (48%)	172 (91%)	17 (9%)	9	28
1	G	189/396 (48%)	170 (90%)	19 (10%)	7	24
2	B	194/194 (100%)	175 (90%)	19 (10%)	7	25
2	E	194/194 (100%)	185 (95%)	9 (5%)	24	57
2	H	194/194 (100%)	184 (95%)	10 (5%)	21	52
3	C	125/127 (98%)	120 (96%)	5 (4%)	28	62
3	F	124/127 (98%)	113 (91%)	11 (9%)	9	28
3	I	125/127 (98%)	115 (92%)	10 (8%)	11	34
All	All	1522/2151 (71%)	1404 (92%)	118 (8%)	11	35

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	3	MET
1	A	7	SER
1	A	48	VAL
1	A	56	SER
1	A	64	LEU
1	A	69	THR
1	A	114	GLN
1	A	117	LEU
1	A	119	THR

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Mol	Chain	Res	Type
1	A	150	LEU
1	A	152	LYS
1	A	157	GLU
1	A	161	VAL
1	A	189	SER
1	A	202	VAL
1	A	215	VAL
1	A	222	ARG
2	B	6	GLN
2	B	20	THR
2	B	32	SER
2	B	39	LEU
2	B	71	SER
2	B	85	GLN
2	B	89	LEU
2	B	113	ILE
2	B	123	SER
2	B	133	THR
2	B	153	VAL
2	B	160	SER
2	B	183	SER
2	B	188	LEU
2	B	200	THR
2	B	204	THR
2	B	209	THR
2	B	214	LYS
2	B	219	ASN
3	C	7	LEU
3	C	20	LEU
3	C	32	THR
3	C	46	THR
3	C	117	ILE
1	D	7	SER
1	D	56	SER
1	D	64	LEU
1	D	119	THR
1	D	124	LYS
1	D	130	VAL
1	D	145	VAL
1	D	151	VAL
1	D	157	GLU
1	D	160	THR

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Mol	Chain	Res	Type
1	D	179	LEU
1	D	187	SER
1	D	201	THR
1	D	203	THR
1	D	215	VAL
1	D	222	ARG
1	D	223	ASP
2	E	17	GLN
2	E	32	SER
2	E	85	GLN
2	E	89	LEU
2	E	123	SER
2	E	134	SER
2	E	204	THR
2	E	209	THR
2	E	213	VAL
3	F	1	SER
3	F	10	GLU
3	F	20	LEU
3	F	32	THR
3	F	41	MET
3	F	46	THR
3	F	73	PHE
3	F	80	LEU
3	F	95	GLU
3	F	124	ILE
3	F	128	THR
1	G	2	VAL
1	G	3	MET
1	G	7	SER
1	G	48	VAL
1	G	56	SER
1	G	64	LEU
1	G	69	THR
1	G	71	SER
1	G	87	ARG
1	G	141	THR
1	G	149	CYS
1	G	157	GLU
1	G	161	VAL
1	G	168	LEU
1	G	179	LEU

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Mol	Chain	Res	Type
1	G	202	VAL
1	G	203	THR
1	G	215	VAL
1	G	220	VAL
2	H	20	THR
2	H	32	SER
2	H	51	LYS
2	H	78	THR
2	H	89	LEU
2	H	123	SER
2	H	124	ILE
2	H	154	LYS
2	H	213	VAL
2	H	219	ASN
3	I	14	LEU
3	I	20	LEU
3	I	32	THR
3	I	41	MET
3	I	46	THR
3	I	70	SER
3	I	75	LEU
3	I	80	LEU
3	I	104	ASP
3	I	114	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
2	B	85	GLN
2	B	217	ASN
2	E	197	ASN
2	E	217	ASN
3	F	25	ASN
3	F	66	ASN
3	F	114	ASN
2	H	37	ASN
2	H	85	GLN
3	I	21	ASN
3	I	69	GLN
3	I	72	ASN
3	I	114	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 ⓘ

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NAG	J	1	4,2	14,14,15	0.94	1 (7%)	17,19,21	1.03	1 (5%)
4	NAG	J	2	4	14,14,15	0.66	1 (7%)	17,19,21	0.66	0
4	NAG	K	1	4,2	14,14,15	1.04	1 (7%)	17,19,21	0.75	0
4	NAG	K	2	4	14,14,15	0.57	0	17,19,21	0.43	0
4	NAG	L	1	4,2	14,14,15	0.84	2 (14%)	17,19,21	1.12	1 (5%)
4	NAG	L	2	4	14,14,15	2.51	2 (14%)	17,19,21	1.69	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	J	1	4,2	-	1/6/23/26	0/1/1/1
4	NAG	J	2	4	-	3/6/23/26	0/1/1/1
4	NAG	K	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	NAG	L	1	4,2	-	1/6/23/26	0/1/1/1
4	NAG	L	2	4	-	4/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	2	NAG	O5-C1	7.84	1.56	1.43
4	L	2	NAG	C1-C2	5.01	1.59	1.52
4	K	1	NAG	C1-C2	3.56	1.57	1.52
4	J	1	NAG	O5-C1	2.63	1.48	1.43
4	J	2	NAG	C1-C2	2.33	1.55	1.52
4	L	1	NAG	O5-C1	2.15	1.47	1.43
4	L	1	NAG	C1-C2	2.03	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	2	NAG	C1-O5-C5	6.23	120.53	112.19
4	L	1	NAG	C1-O5-C5	3.77	117.23	112.19
4	J	1	NAG	C1-O5-C5	3.15	116.40	112.19
4	L	2	NAG	C3-C4-C5	-2.24	106.17	110.23

There are no chirality outliers.

All (11) torsion outliers are listed below:

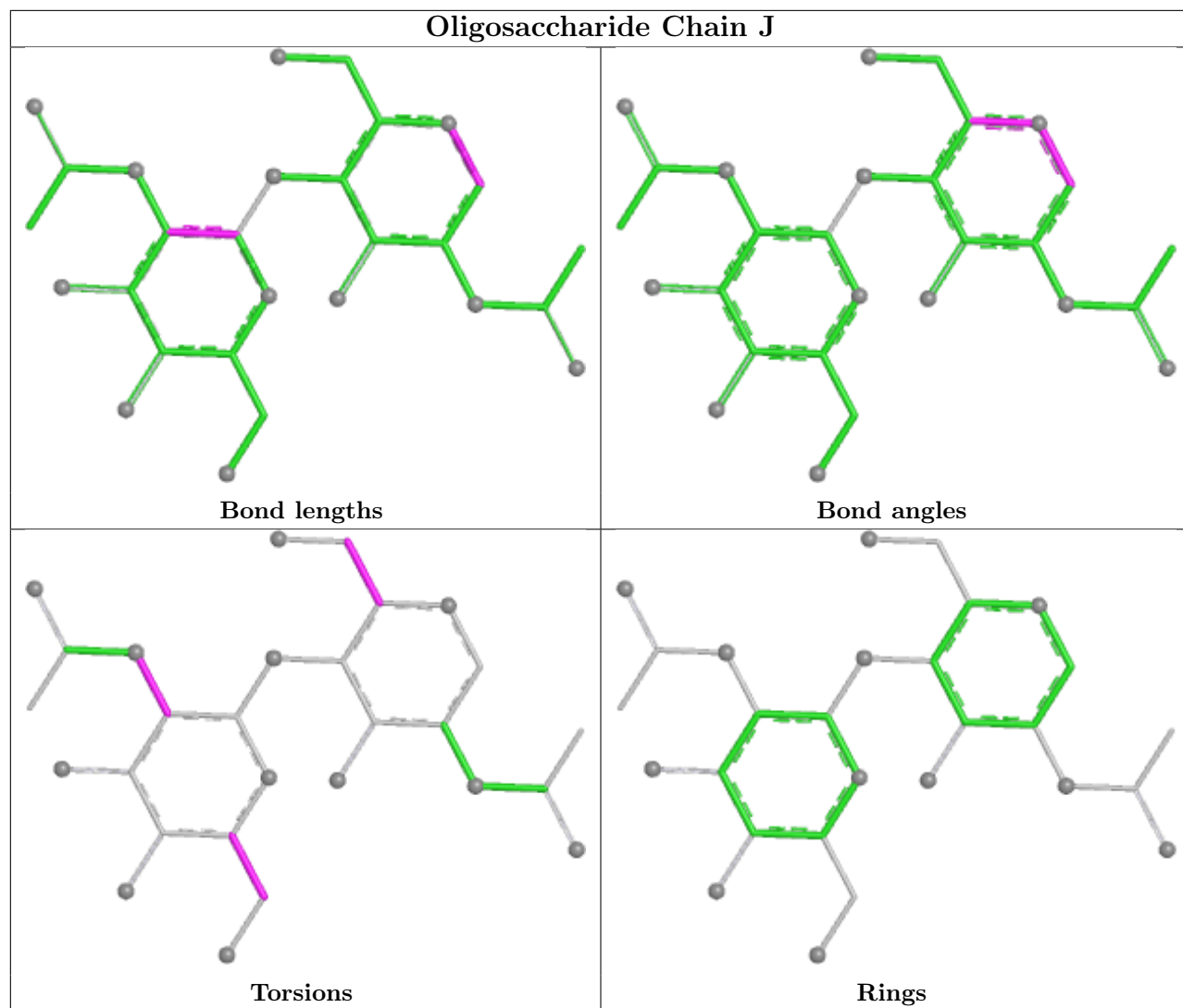
Mol	Chain	Res	Type	Atoms
4	L	2	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	L	2	NAG	C1-C2-N2-C7
4	K	1	NAG	O5-C5-C6-O6
4	J	2	NAG	C3-C2-N2-C7
4	L	2	NAG	C3-C2-N2-C7
4	L	1	NAG	C4-C5-C6-O6

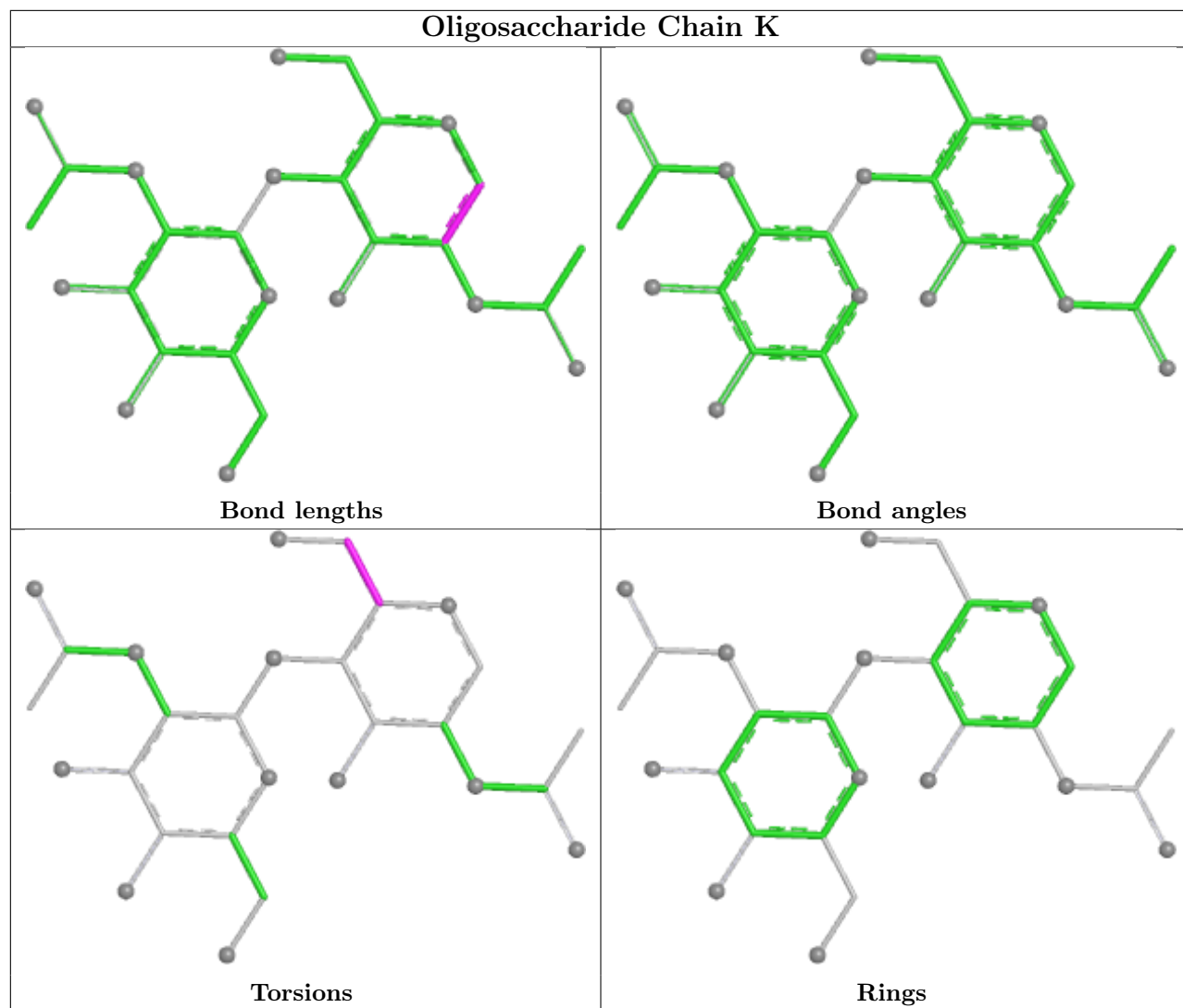
There are no ring outliers.

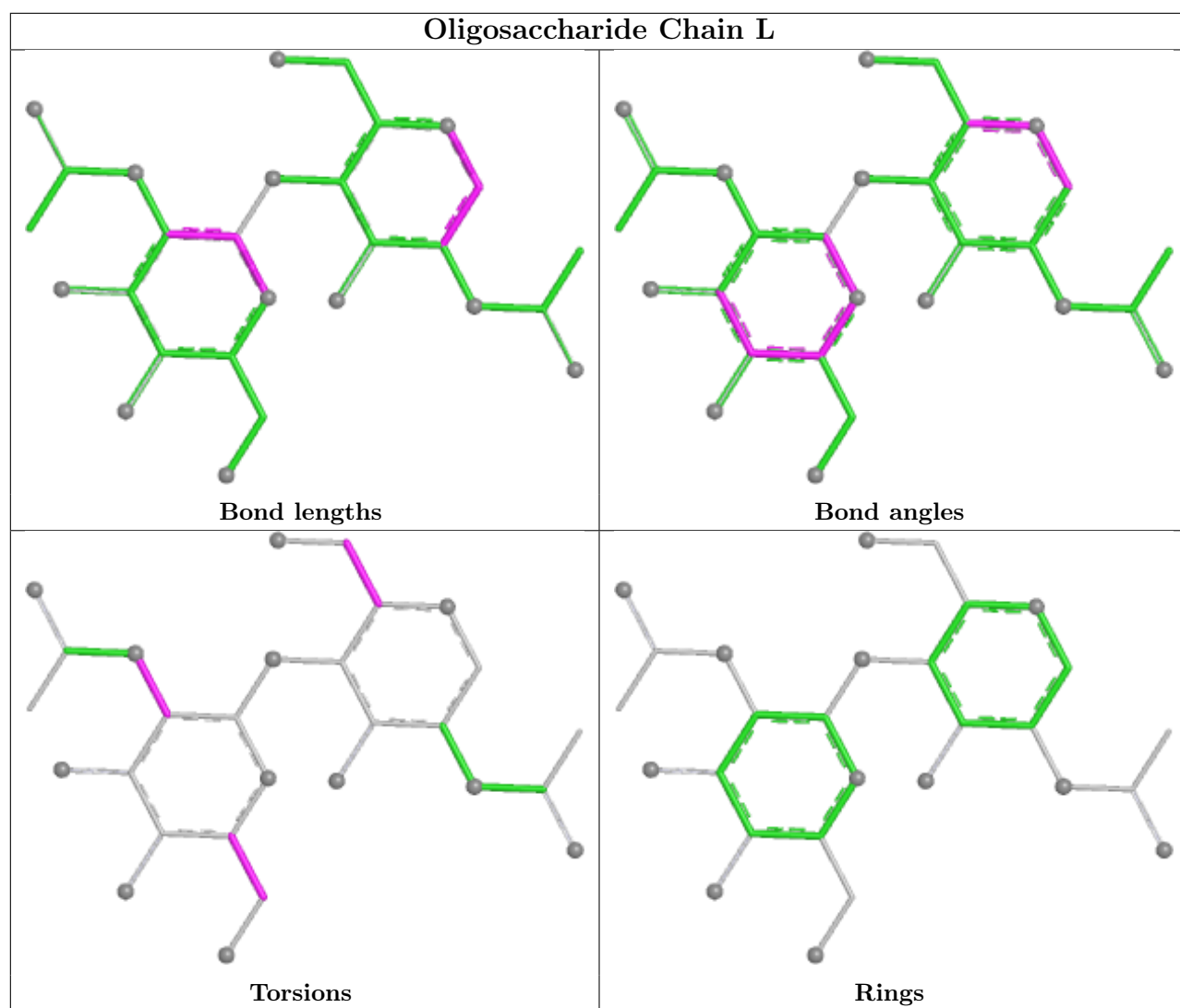
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	1	NAG	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	A	223/447 (49%)	-0.03	2 (0%) 81 75	65, 104, 168, 232	0
1	D	225/447 (50%)	0.00	2 (0%) 81 75	70, 116, 163, 188	0
1	G	225/447 (50%)	-0.06	2 (0%) 81 75	61, 102, 194, 240	0
2	B	219/219 (100%)	-0.22	1 (0%) 87 83	70, 99, 133, 173	0
2	E	219/219 (100%)	-0.10	2 (0%) 81 75	81, 116, 162, 187	0
2	H	219/219 (100%)	-0.01	2 (0%) 81 75	66, 112, 176, 199	0
3	C	131/134 (97%)	0.02	0 100 100	77, 114, 180, 201	0
3	F	130/134 (97%)	0.02	1 (0%) 82 77	71, 114, 192, 230	0
3	I	131/134 (97%)	0.24	6 (4%) 37 29	86, 141, 194, 236	0
All	All	1722/2400 (71%)	-0.03	18 (1%) 79 73	61, 112, 176, 240	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	120	CYS	3.7
2	H	153	VAL	2.5
1	A	131	TYR	2.4
1	A	56	SER	2.4
3	I	88	VAL	2.4
1	D	48	VAL	2.3
2	E	53	LEU	2.2
1	G	137	SER	2.2
3	I	75	LEU	2.2
3	I	16	LEU	2.2
1	D	221	PRO	2.1
3	I	51	LEU	2.1
2	E	52	LEU	2.1
3	F	23	ILE	2.1
2	B	86	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	I	70	SER	2.0
2	H	157	ILE	2.0
1	G	138	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

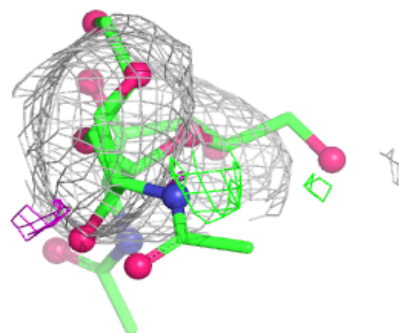
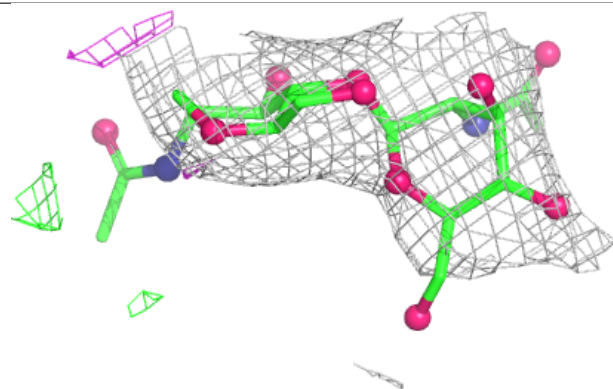
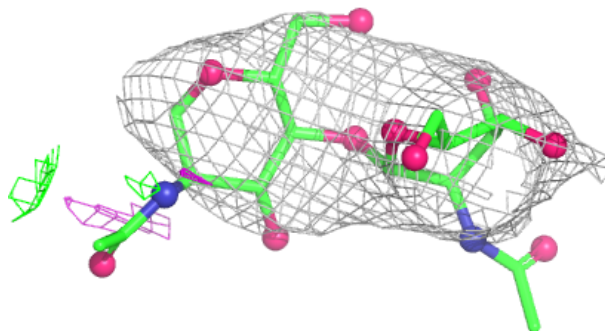
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	K	2	14/15	0.26	0.11	222,229,234,234	0
4	NAG	L	1	14/15	0.54	0.17	176,192,202,216	0
4	NAG	J	2	14/15	0.58	0.11	178,188,203,206	0
4	NAG	K	1	14/15	0.63	0.11	149,179,195,210	0
4	NAG	L	2	14/15	0.66	0.10	205,222,225,227	0
4	NAG	J	1	14/15	0.68	0.16	139,157,170,170	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.

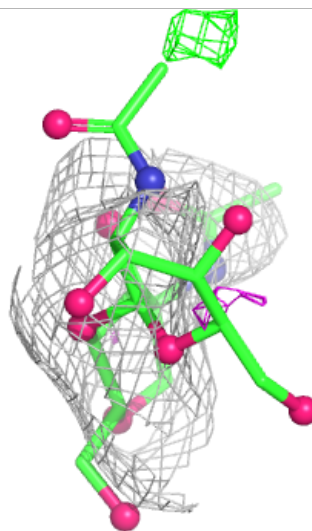
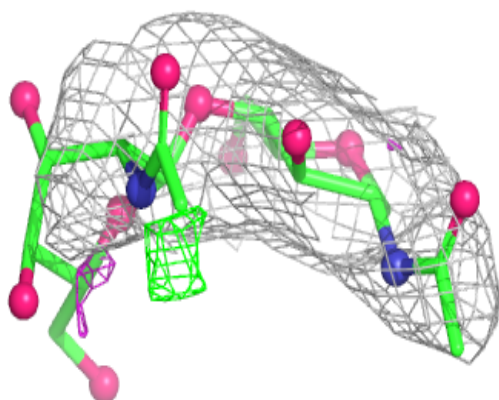
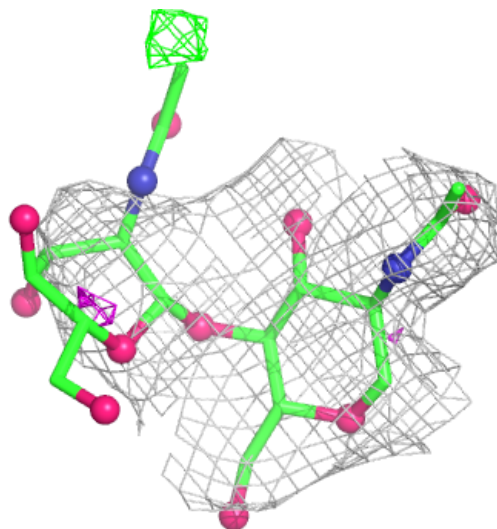
Electron density around Chain J:

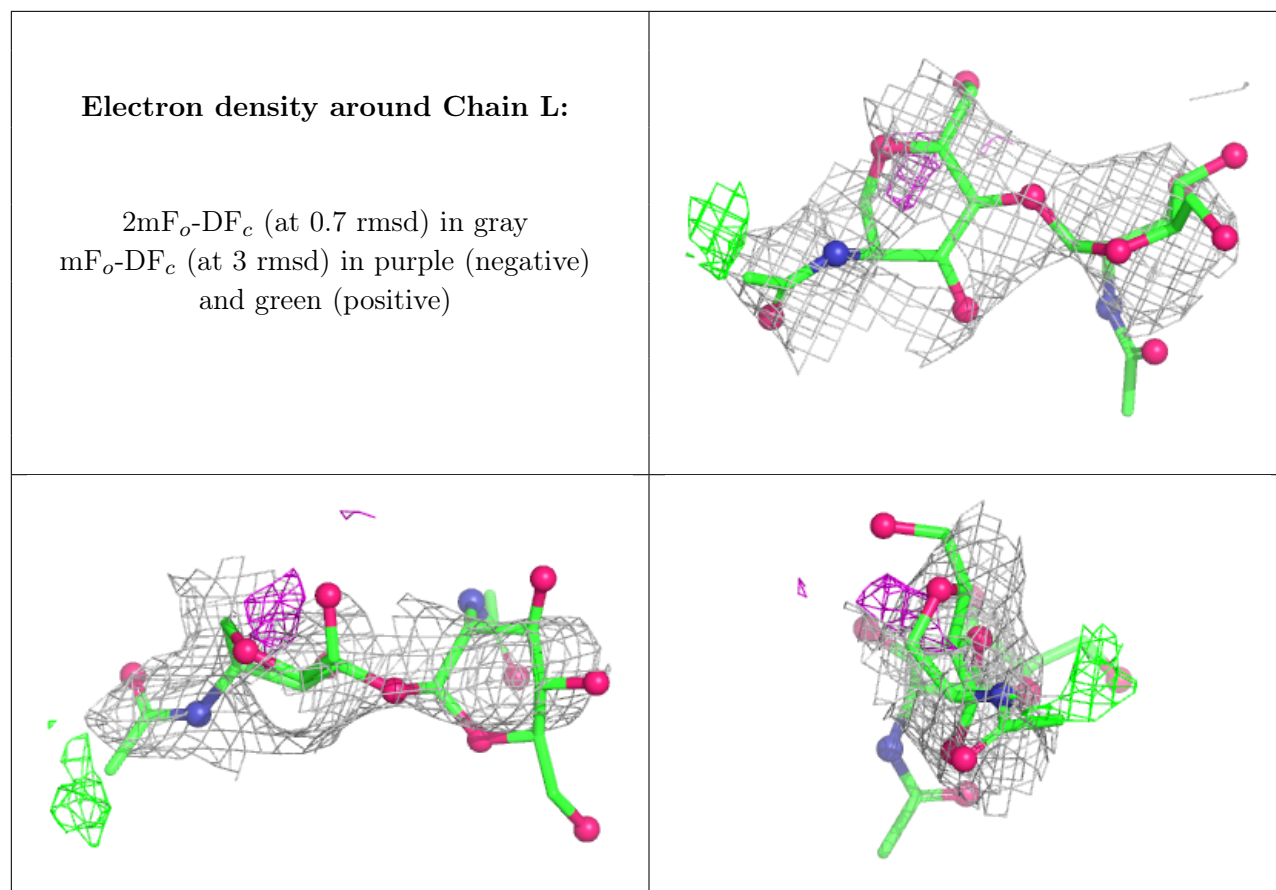
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.