



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:17 PM UTC

PDB ID : 1QFU / pdb_00001qfu
Title : INFLUENZA VIRUS HEMAGGLUTININ COMPLEXED WITH A NEUTRALIZING ANTIBODY
Authors : Fleury, D.; Gigant, B.; Bizebard, T.; Daniels, R.S.; Skehel, J.J.; Knossow, M.
Deposited on : 1999-04-14
Resolution : 2.80 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

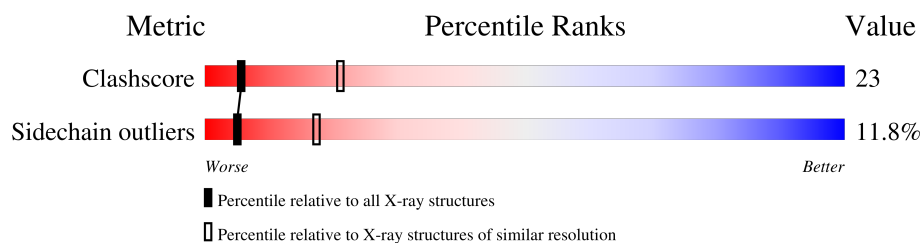
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	328	55% 37% 5% .
2	B	175	61% 34% . ..
3	L	217	43% 43% 12% .
4	H	223	48% 40% 12%
5	C	2	100%
6	D	3	100%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7439 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 PROTEIN (HEMAGGLUTININ (HA1 CHAIN)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	1
			2447	1532	430	472	13			

- Molecule 2 is a protein called PROTEIN (HEMAGGLUTININ (HA2 CHAIN)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	174	Total	C	N	O	S	0	0	1
			1408	874	248	280	6			

- Molecule 3 is a protein called PROTEIN (IMMUNOGLOBULIN IGG1-KAPPA ANTIBODY (LIGHT CHAIN)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	217	Total	C	N	O	S	0	0	0
			1687	1056	289	336	6			

- Molecule 4 is a protein called PROTEIN (IMMUNOGLOBULIN IGG1-KAPPA ANTIBODY (HEAVY CHAIN)).

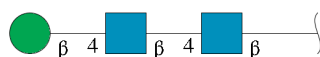
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	223	Total	C	N	O	S	0	0	0
			1718	1089	281	340	8			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



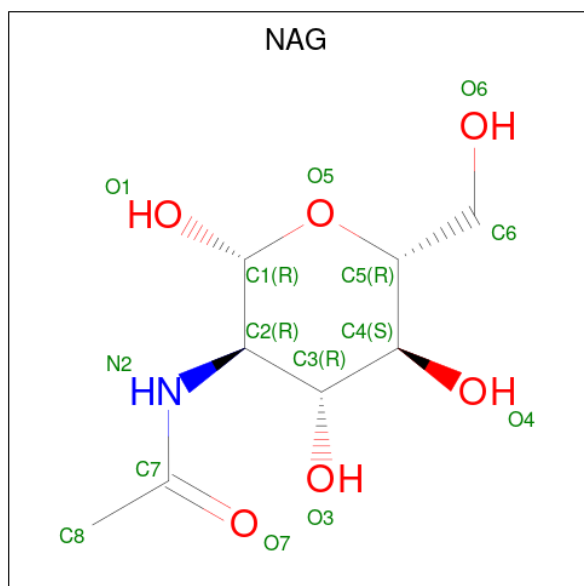
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called 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	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is water.

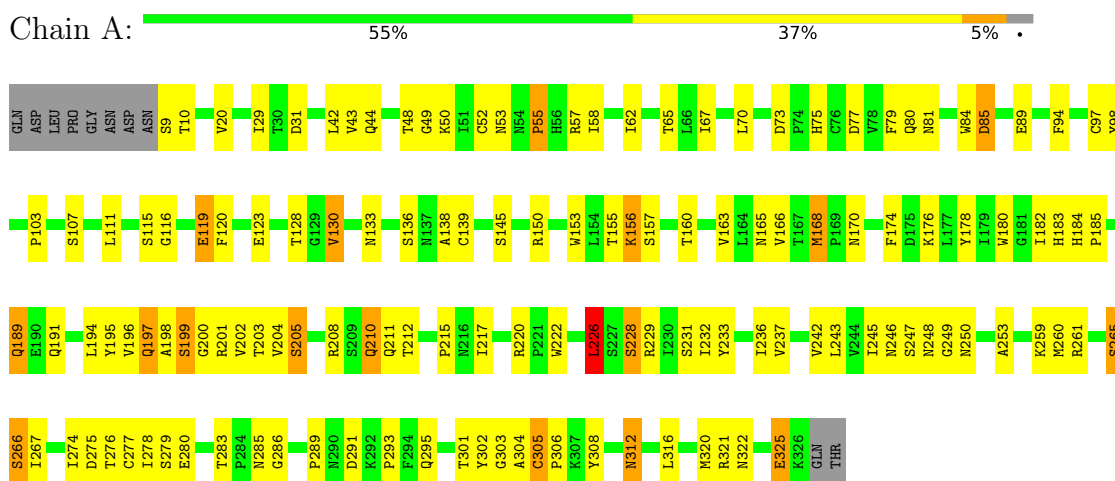
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	28	Total 28	O 28	0	0
8	B	30	Total 30	O 30	0	0
8	L	3	Total 3	O 3	0	0
8	H	9	Total 9	O 9	0	0

3 Residue-property plots

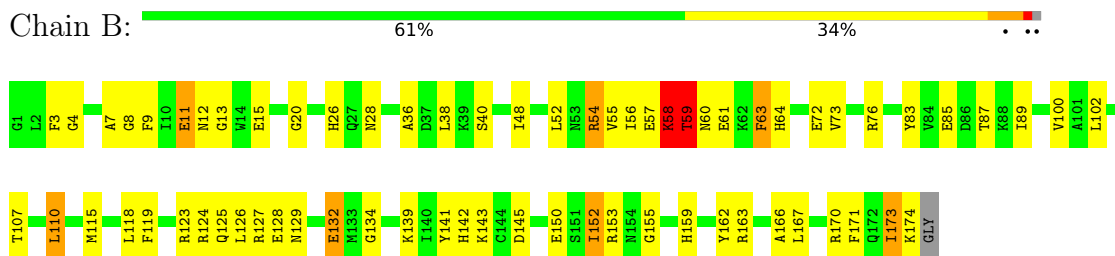
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

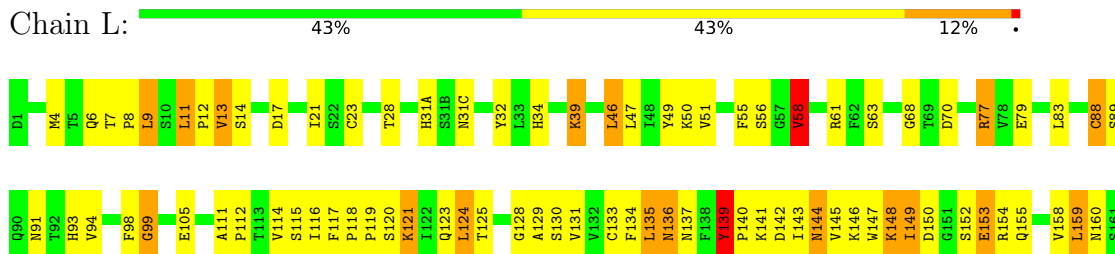
• Molecule 1: PROTEIN (HEMAGGLUTININ (HA1 CHAIN))



• Molecule 2: PROTEIN (HEMAGGLUTININ (HA2 CHAIN))

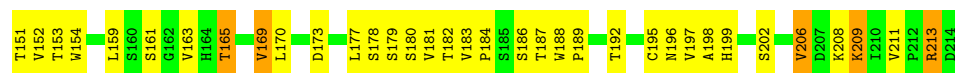
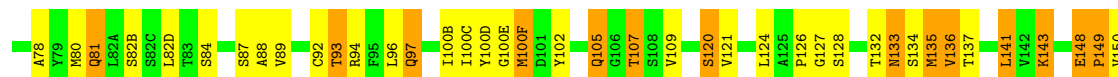
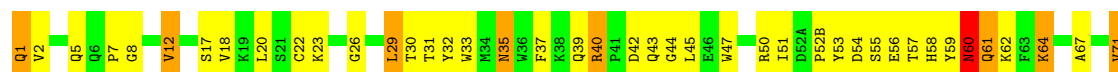


• Molecule 3: PROTEIN (IMMUNOGLOBULIN IGG1-KAPPA ANTIBODY (LIGHT CHAIN))





• Molecule 4: PROTEIN (IMMUNOGLOBULIN IGG1-KAPPA ANTIBODY (HEAVY CHAIN))



• Molecule 5: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 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

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.00Å 138.00Å 135.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 2.80	Depositor
% Data completeness (in resolution range)	98.0 (7.00-2.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.84	Depositor
R, R_{free}	0.198 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7439	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NDG, BMA, 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	0.67	1/2503 (0.0%)	1.16	18/3412 (0.5%)
2	B	0.83	2/1432 (0.1%)	1.18	10/1925 (0.5%)
3	L	0.58	0/1726	1.18	20/2342 (0.9%)
4	H	0.63	1/1764 (0.1%)	1.10	13/2413 (0.5%)
All	All	0.68	4/7425 (0.1%)	1.15	61/10092 (0.6%)

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
3	L	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	100(F)	MET	SD-CE	-5.96	1.64	1.79
1	A	325	GLU	C-N	-5.55	1.25	1.33
2	B	63	PHE	CA-C	5.42	1.55	1.52
2	B	173	ILE	C-N	-5.25	1.26	1.33

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	58	LYS	N-CA-C	10.92	126.00	108.41
1	A	197	GLN	N-CA-C	10.78	126.22	113.18
4	H	213	ARG	N-CA-C	-10.54	98.72	111.69
1	A	85	ASP	N-CA-C	-10.18	99.39	112.93
4	H	60	ASN	N-CA-C	-7.75	98.33	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	GLN	N-CA-C	-7.36	102.95	110.97
3	L	137	ASN	N-CA-C	7.34	121.57	112.47
1	A	199	SER	N-CA-C	-7.22	98.87	109.63
3	L	152	SER	N-CA-C	7.10	125.93	110.80
1	A	286	GLY	N-CA-C	-6.98	103.61	111.63
3	L	148	LYS	N-CA-C	6.89	122.10	112.93
1	A	128	THR	N-CA-C	6.78	118.92	109.15
2	B	3	PHE	N-CA-C	6.72	121.80	112.45
1	A	133	ASN	N-CA-C	6.64	120.58	111.54
4	H	161	SER	N-CA-C	6.58	124.83	110.80
1	A	305	CYS	N-CA-C	6.58	120.30	109.58
3	L	189	ASN	N-CA-C	-6.48	97.50	108.26
1	A	168	MET	CA-C-N	6.44	127.41	120.13
1	A	168	MET	C-N-CA	6.44	127.41	120.13
4	H	5	GLN	N-CA-C	6.42	119.07	109.25
3	L	58	VAL	CA-C-N	6.29	126.20	119.85
3	L	58	VAL	C-N-CA	6.29	126.20	119.85
1	A	138	ALA	N-CA-C	-6.28	103.72	112.45
2	B	163	ARG	N-CA-C	6.10	118.46	111.02
2	B	55	VAL	N-CA-C	6.04	116.15	110.30
3	L	139	TYR	CA-C-N	-5.98	112.36	119.84
3	L	139	TYR	C-N-CA	-5.98	112.36	119.84
4	H	7	PRO	N-CA-C	5.97	124.76	112.47
2	B	76	ARG	N-CA-C	5.82	123.19	110.80
1	A	247	SER	N-CA-C	5.81	117.62	108.96
2	B	118	LEU	N-CA-C	-5.79	104.97	111.28
3	L	9	LEU	N-CA-C	-5.79	106.25	113.55
4	H	165	THR	N-CA-C	-5.75	99.92	109.46
2	B	171	PHE	N-CA-C	5.71	118.50	108.56
3	L	153	GLU	N-CA-C	5.70	117.77	108.76
4	H	143	LYS	N-CA-C	5.66	118.63	109.40
4	H	121	VAL	N-CA-C	5.64	115.45	106.88
3	L	39	LYS	N-CA-C	-5.61	102.97	109.93
4	H	148	GLU	N-CA-C	-5.60	101.89	110.01
4	H	206	VAL	N-CA-C	5.58	116.63	108.53
3	L	121	LYS	N-CA-C	-5.49	105.30	111.28
2	B	152	ILE	N-CA-C	-5.46	105.39	110.53
3	L	88	CYS	N-CA-C	-5.43	100.17	109.24
3	L	193	CYS	N-CA-C	-5.42	98.94	108.20
2	B	7	ALA	N-CA-C	-5.39	104.79	111.90
1	A	205	SER	N-CA-C	5.38	116.45	108.60
1	A	226	LEU	N-CA-C	5.38	122.25	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	SER	N-CA-C	-5.36	102.26	110.14
3	L	58	VAL	N-CA-C	5.36	114.80	108.96
1	A	253	ALA	CA-C-N	5.31	126.66	120.98
1	A	253	ALA	C-N-CA	5.31	126.66	120.98
3	L	125	THR	N-CA-C	-5.30	105.58	111.36
3	L	51	VAL	N-CA-C	5.26	120.29	109.34
3	L	99	GLY	N-CA-C	-5.26	104.58	112.89
2	B	59	THR	N-CA-C	5.22	121.91	110.80
1	A	65	THR	N-CA-C	-5.21	103.16	110.35
4	H	100(E)	GLY	N-CA-C	-5.14	103.25	110.75
3	L	144	ASN	N-CA-C	5.12	116.99	108.02
4	H	120	SER	N-CA-C	-5.08	100.23	108.52
4	H	92	CYS	N-CA-C	-5.02	101.69	109.72
3	L	136	ASN	N-CA-C	5.00	117.72	110.17

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	139	TYR	Sidechain
3	L	191	TYR	Sidechain

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	2447	0	2393	100	0
2	B	1408	0	1329	52	0
3	L	1687	0	1640	117	0
4	H	1718	0	1680	105	0
5	C	28	0	24	0	0
6	D	39	0	34	0	0
7	A	28	0	26	0	0
7	B	14	0	13	1	0
8	A	28	0	0	1	0
8	B	30	0	0	3	0
8	H	9	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L	3	0	0	0	0
All	All	7439	0	7139	338	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 23.

All (338) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:194:GLU:HG3	3:L:205:VAL:HG22	1.34	1.08
3:L:189:ASN:HD21	3:L:209:ASN:HA	1.21	1.04
1:A:53:ASN:OD1	1:A:276:THR:HA	1.72	0.87
3:L:8:PRO:HG3	3:L:11:LEU:HD23	1.56	0.87
3:L:189:ASN:ND2	3:L:209:ASN:HA	1.93	0.84
3:L:131:VAL:HB	3:L:178:LEU:HB3	1.60	0.84
2:B:123:ARG:NH1	2:B:124:ARG:HG3	1.95	0.82
3:L:195:ALA:HB3	3:L:204:ILE:HG23	1.63	0.81
2:B:132:GLU:HG3	2:B:134:GLY:H	1.45	0.80
3:L:77:ARG:NH1	3:L:79:GLU:HG2	1.98	0.79
4:H:17:SER:HB3	4:H:82(B):SER:HA	1.65	0.79
3:L:188:HIS:O	3:L:210:ARG:HG3	1.82	0.78
1:A:304:ALA:HB1	2:B:59:THR:HG21	1.66	0.77
3:L:143:ILE:HG13	3:L:197:HIS:HB2	1.66	0.77
4:H:37:PHE:CE2	4:H:100(F):MET:HE2	2.21	0.75
3:L:118:PRO:HG2	4:H:213:ARG:HH22	1.51	0.75
4:H:188:TRP:HB3	4:H:189:PRO:HD3	1.68	0.74
3:L:146:LYS:HG3	3:L:194:GLU:HB3	1.68	0.74
4:H:135:MET:HE2	4:H:184:PRO:HA	1.70	0.73
1:A:312:ASN:H	1:A:312:ASN:HD22	1.34	0.73
2:B:83:TYR:O	2:B:87:THR:HG23	1.89	0.73
1:A:156:LYS:HG3	1:A:196:VAL:HG23	1.71	0.72
4:H:33:TRP:CE3	4:H:50:ARG:HD2	2.25	0.71
3:L:134:PHE:CE2	4:H:180:SER:HB3	2.24	0.71
4:H:96:LEU:O	4:H:100(D):TYR:HA	1.91	0.71
4:H:32:TYR:HA	4:H:97:GLN:HE22	1.56	0.71
4:H:126:PRO:HD2	4:H:188:TRP:CH2	2.26	0.70
2:B:123:ARG:HH12	2:B:124:ARG:HG3	1.56	0.70
3:L:149:ILE:HA	3:L:190:SER:O	1.91	0.70
1:A:205:SER:HB3	1:A:210:GLN:HA	1.73	0.69
3:L:31(A):HIS:HB3	3:L:31(C):ASN:OD1	1.91	0.69
2:B:58:LYS:HD3	2:B:59:THR:N	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:148:GLU:OE1	4:H:149:PRO:HA	1.92	0.69
3:L:194:GLU:HG3	3:L:205:VAL:CG2	2.19	0.68
1:A:312:ASN:HD22	1:A:312:ASN:N	1.91	0.67
1:A:191:GLN:HG3	1:A:198:ALA:HA	1.77	0.67
3:L:146:LYS:CG	3:L:194:GLU:HB3	2.24	0.67
4:H:50:ARG:HG2	4:H:51:ILE:N	2.09	0.66
1:A:226:LEU:HD23	1:A:226:LEU:N	2.09	0.66
3:L:114:VAL:HG13	3:L:133:CYS:SG	2.37	0.65
4:H:133:ASN:HD22	4:H:133:ASN:H	1.43	0.65
3:L:134:PHE:CD1	3:L:175:SER:HB2	2.32	0.65
3:L:34:HIS:HD2	3:L:49:TYR:HA	1.62	0.65
1:A:20:VAL:HG22	1:A:322:ASN:OD1	1.97	0.65
2:B:4:GLY:O	2:B:8:GLY:HA3	1.97	0.65
2:B:20:GLY:HA3	2:B:36:ALA:HB1	1.77	0.65
4:H:32:TYR:HA	4:H:97:GLN:NE2	2.12	0.65
4:H:87:SER:HA	4:H:109:VAL:O	1.97	0.64
1:A:220:ARG:HB3	1:A:229:ARG:NH2	2.12	0.64
1:A:308:TYR:CE1	2:B:89:ILE:HD13	2.33	0.63
4:H:60:ASN:HD22	4:H:62:LYS:H	1.46	0.63
3:L:117:PHE:HZ	4:H:137:THR:HG22	1.61	0.63
3:L:116:ILE:HG22	3:L:133:CYS:SG	2.39	0.63
3:L:135:LEU:HD22	3:L:145:VAL:HG22	1.82	0.62
4:H:12:VAL:HG21	4:H:82(D):LEU:HD13	1.81	0.62
1:A:89:GLU:HG3	1:A:267:ILE:HD11	1.81	0.62
1:A:312:ASN:H	1:A:312:ASN:ND2	1.96	0.62
1:A:52:CYS:HB3	1:A:277:CYS:O	2.00	0.62
4:H:37:PHE:HE2	4:H:100(F):MET:HE2	1.64	0.62
3:L:123:GLN:HG2	3:L:128:GLY:O	2.00	0.61
3:L:192:THR:HG23	3:L:207:SER:OG	1.99	0.61
1:A:276:THR:HG23	1:A:276:THR:O	2.01	0.61
4:H:20:LEU:HD12	4:H:80:MET:HE2	1.82	0.61
3:L:11:LEU:CD1	3:L:13:VAL:HG13	2.31	0.60
4:H:2:VAL:HA	4:H:26:GLY:HA3	1.84	0.60
1:A:283:THR:HG22	1:A:301:THR:HG22	1.83	0.60
3:L:121:LYS:HA	3:L:124:LEU:HD11	1.84	0.60
4:H:153:THR:HG23	4:H:196:ASN:HB2	1.82	0.59
3:L:169:ASP:HB3	3:L:171:THR:OG1	2.02	0.59
2:B:58:LYS:HD3	2:B:59:THR:H	1.68	0.59
3:L:4:MET:HE3	3:L:23:CYS:SG	2.42	0.59
3:L:46:LEU:HD13	3:L:55:PHE:CD1	2.38	0.59
2:B:115:MET:HE3	2:B:115:MET:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:131:VAL:HG12	3:L:147:TRP:CZ3	2.37	0.58
1:A:182:ILE:HD11	1:A:215:PRO:HD3	1.84	0.58
2:B:124:ARG:HD2	8:B:426:HOH:O	2.02	0.58
4:H:37:PHE:CZ	4:H:100(F):MET:HE2	2.38	0.58
3:L:167:SER:C	3:L:168:LYS:HG3	2.29	0.58
4:H:64:LYS:HB2	4:H:64:LYS:NZ	2.19	0.57
1:A:29:ILE:HD11	2:B:102:LEU:HD23	1.86	0.57
1:A:97:CYS:HA	1:A:139:CYS:HA	1.86	0.57
4:H:159:LEU:HD21	4:H:181:VAL:HG21	1.87	0.57
1:A:94:PHE:CE1	4:H:1:GLN:HB2	2.39	0.57
2:B:153:ARG:HD3	8:B:434:HOH:O	2.03	0.57
4:H:50:ARG:HG2	4:H:51:ILE:H	1.69	0.57
3:L:119:PRO:HG2	3:L:129:ALA:HB1	1.87	0.57
3:L:28:THR:O	3:L:93:HIS:HE1	1.87	0.56
1:A:200:GLY:HA2	1:A:248:ASN:OD1	2.05	0.56
1:A:44:GLN:NE2	1:A:289:PRO:HG2	2.20	0.56
3:L:189:ASN:HD22	3:L:190:SER:N	2.03	0.56
2:B:110:LEU:HD23	2:B:110:LEU:C	2.30	0.56
1:A:97:CYS:SG	1:A:98:TYR:N	2.73	0.55
3:L:34:HIS:CD2	3:L:50:LYS:H	2.24	0.55
4:H:93:THR:HG22	4:H:102:TYR:O	2.07	0.55
1:A:73:ASP:OD1	1:A:75:HIS:HD2	1.89	0.55
3:L:94:VAL:HG11	4:H:58:HIS:NE2	2.21	0.55
3:L:198:LYS:CD	3:L:198:LYS:H	2.20	0.54
1:A:182:ILE:HG22	1:A:231:SER:HB2	1.88	0.54
4:H:188:TRP:CB	4:H:189:PRO:HD3	2.36	0.54
4:H:64:LYS:HB2	4:H:64:LYS:HZ2	1.72	0.54
2:B:125:GLN:NE2	2:B:155:GLY:HA2	2.22	0.54
3:L:160:ASN:ND2	3:L:174:MET:HE2	2.23	0.54
4:H:127:GLY:HA3	4:H:213:ARG:NH2	2.23	0.54
2:B:141:TYR:CD2	2:B:170:ARG:HG2	2.43	0.54
4:H:61:GLN:HA	4:H:64:LYS:NZ	2.23	0.54
3:L:159:LEU:HD13	4:H:169:VAL:HG13	1.89	0.53
1:A:231:SER:HB3	1:A:233:TYR:CE1	2.42	0.53
3:L:135:LEU:HD12	3:L:135:LEU:H	1.72	0.53
4:H:67:ALA:HA	4:H:81:GLN:O	2.08	0.53
4:H:209:LYS:HE3	4:H:211:VAL:CG1	2.39	0.53
3:L:174:MET:HG2	3:L:175:SER:N	2.24	0.53
4:H:150:VAL:HA	4:H:198:ALA:O	2.09	0.53
2:B:56:ILE:HG13	2:B:56:ILE:O	2.08	0.52
1:A:197:GLN:C	1:A:199:SER:H	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:184:GLU:OE1	3:L:188:HIS:HE1	1.93	0.52
2:B:11:GLU:HG2	2:B:12:ASN:OD1	2.08	0.52
3:L:186:GLU:HA	3:L:210:ARG:NE	2.25	0.52
4:H:61:GLN:HA	4:H:64:LYS:HZ3	1.75	0.52
3:L:134:PHE:CE1	3:L:175:SER:HB2	2.45	0.52
3:L:11:LEU:HD11	3:L:13:VAL:HG13	1.92	0.51
1:A:84:TRP:CE2	1:A:116:GLY:HA2	2.45	0.51
1:A:208:ARG:NH1	1:A:208:ARG:HB2	2.26	0.51
3:L:119:PRO:HG3	3:L:130:SER:N	2.26	0.51
4:H:133:ASN:CG	4:H:134:SER:H	2.19	0.51
4:H:141:LEU:HD13	4:H:143:LYS:HB2	1.92	0.51
1:A:120:PHE:CD2	1:A:150:ARG:HD2	2.46	0.50
1:A:77:ASP:O	1:A:80:GLN:HG3	2.11	0.50
2:B:142:HIS:CE1	2:B:162:TYR:CD2	3.00	0.50
2:B:129:ASN:HA	2:B:166:ALA:HB1	1.94	0.50
2:B:141:TYR:O	2:B:166:ALA:HA	2.11	0.50
4:H:165:THR:HA	4:H:179:SER:HA	1.94	0.50
3:L:98:PHE:HE1	4:H:37:PHE:CE1	2.30	0.50
1:A:295:GLN:CG	1:A:306:PRO:HB2	2.42	0.50
4:H:12:VAL:HG21	4:H:82(D):LEU:CD1	2.41	0.49
1:A:184:HIS:O	1:A:228:SER:HB2	2.11	0.49
3:L:120:SER:O	3:L:124:LEU:HG	2.11	0.49
1:A:156:LYS:HG3	1:A:196:VAL:CG2	2.41	0.49
3:L:134:PHE:CD2	4:H:180:SER:HB3	2.48	0.49
3:L:146:LYS:HG2	3:L:194:GLU:O	2.12	0.49
3:L:187:ARG:HG3	3:L:187:ARG:HH11	1.78	0.49
2:B:125:GLN:HE22	2:B:155:GLY:HA2	1.77	0.49
1:A:200:GLY:O	1:A:215:PRO:HD2	2.13	0.49
3:L:198:LYS:H	3:L:198:LYS:HD3	1.78	0.49
1:A:123:GLU:HB3	1:A:168:MET:HE3	1.95	0.49
3:L:61:ARG:HD2	3:L:77:ARG:HD2	1.95	0.49
4:H:42:ASP:O	4:H:43:GLN:HB2	2.12	0.49
3:L:32:TYR:CE1	4:H:100(D):TYR:HD2	2.30	0.48
3:L:189:ASN:O	3:L:190:SER:CB	2.61	0.48
1:A:94:PHE:CD1	4:H:1:GLN:HB2	2.48	0.48
1:A:312:ASN:N	1:A:312:ASN:ND2	2.58	0.48
4:H:126:PRO:HD2	4:H:188:TRP:CZ3	2.47	0.48
4:H:136:VAL:HG23	4:H:183:VAL:O	2.14	0.48
1:A:49:GLY:HA2	1:A:285:ASN:O	2.13	0.48
3:L:32:TYR:HB3	3:L:91:ASN:HB2	1.94	0.48
4:H:159:LEU:HG	4:H:159:LEU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLN:O	1:A:81:ASN:HB2	2.11	0.48
2:B:119:PHE:HZ	2:B:132:GLU:CD	2.22	0.48
1:A:153:TRP:CZ2	1:A:183:HIS:CD2	3.01	0.48
3:L:146:LYS:HD2	3:L:194:GLU:OE2	2.13	0.48
3:L:159:LEU:HB2	3:L:177:THR:HB	1.96	0.48
1:A:62:ILE:HA	4:H:32:TYR:OH	2.13	0.48
1:A:191:GLN:HE22	1:A:195:TYR:HB2	1.78	0.48
4:H:100(F):MET:SD	4:H:100(F):MET:N	2.87	0.48
4:H:35:ASN:ND2	4:H:47:TRP:HE1	2.11	0.48
1:A:202:VAL:O	1:A:212:THR:HA	2.13	0.47
3:L:123:GLN:OE1	3:L:130:SER:HB3	2.14	0.47
4:H:40:ARG:HD2	4:H:44:GLY:O	2.13	0.47
3:L:134:PHE:HD1	3:L:175:SER:HB2	1.78	0.47
4:H:89:VAL:HA	4:H:107:THR:O	2.14	0.47
4:H:94:ARG:O	4:H:100(F):MET:HA	2.15	0.47
4:H:153:THR:CG2	4:H:196:ASN:HB2	2.44	0.47
4:H:78:ALA:HB1	8:H:218:HOH:O	2.13	0.47
1:A:119:GLU:OE2	1:A:259:LYS:HD3	2.15	0.47
1:A:304:ALA:CB	2:B:59:THR:HG21	2.41	0.47
3:L:135:LEU:HD22	3:L:145:VAL:CG2	2.44	0.47
3:L:115:SER:O	3:L:133:CYS:HA	2.15	0.47
3:L:118:PRO:HD2	4:H:213:ARG:NH2	2.29	0.47
1:A:203:THR:HA	1:A:211:GLN:O	2.15	0.47
1:A:170:ASN:HB2	1:A:237:VAL:HG12	1.95	0.47
1:A:280:GLU:HB3	8:A:466:HOH:O	2.15	0.47
3:L:183:ASP:CG	3:L:187:ARG:HH22	2.23	0.46
1:A:165:ASN:OD1	1:A:246:ASN:ND2	2.48	0.46
1:A:111:LEU:HD13	1:A:260:MET:HE1	1.97	0.46
1:A:320:MET:HG3	1:A:321:ARG:O	2.15	0.46
3:L:112:PRO:HG3	3:L:143:ILE:HD11	1.98	0.46
4:H:8:GLY:HA2	4:H:105:GLN:HE22	1.81	0.46
1:A:185:PRO:O	1:A:217:ILE:HA	2.16	0.46
2:B:150:GLU:HG3	7:B:410:NAG:O5	2.16	0.46
3:L:119:PRO:CG	3:L:129:ALA:HB1	2.46	0.46
4:H:188:TRP:CD1	4:H:188:TRP:C	2.94	0.46
2:B:26:HIS:C	2:B:26:HIS:CD2	2.94	0.45
3:L:192:THR:HA	3:L:206:LYS:O	2.16	0.45
1:A:295:GLN:NE2	1:A:308:TYR:HB2	2.31	0.45
4:H:133:ASN:HD22	4:H:133:ASN:N	2.13	0.45
1:A:115:SER:HA	1:A:261:ARG:O	2.16	0.45
4:H:51:ILE:HD13	4:H:71:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:42:ASP:O	4:H:43:GLN:CB	2.64	0.45
1:A:85:ASP:O	1:A:265:SER:HA	2.17	0.45
3:L:192:THR:HG22	3:L:205:VAL:CG1	2.47	0.45
3:L:189:ASN:ND2	3:L:210:ARG:H	2.14	0.45
4:H:184:PRO:O	4:H:186:SER:N	2.49	0.45
2:B:40:SER:HB2	8:B:411:HOH:O	2.15	0.45
4:H:18:VAL:HG22	4:H:82(D):LEU:HD11	1.98	0.45
1:A:10:THR:HG21	2:B:139:LYS:HE2	1.99	0.45
1:A:176:LYS:O	1:A:236:ILE:HA	2.17	0.45
3:L:191:TYR:C	3:L:192:THR:HG1	2.25	0.45
4:H:100(B):ILE:HG13	4:H:100(C):ILE:HG13	1.97	0.45
4:H:136:VAL:O	4:H:182:THR:HA	2.17	0.45
3:L:141:LYS:HB2	3:L:172:TYR:CE2	2.52	0.45
3:L:165:GLN:HE21	3:L:170:SER:HB3	1.82	0.44
3:L:61:ARG:CZ	3:L:79:GLU:HG3	2.47	0.44
3:L:150:ASP:OD2	3:L:188:HIS:HD2	2.01	0.44
1:A:304:ALA:HB1	2:B:59:THR:CG2	2.42	0.44
4:H:127:GLY:O	4:H:128:SER:C	2.61	0.44
1:A:103:PRO:HD2	1:A:232:ILE:O	2.17	0.44
1:A:119:GLU:OE1	1:A:261:ARG:NH2	2.50	0.44
3:L:198:LYS:H	3:L:198:LYS:HE3	1.82	0.44
1:A:183:HIS:ND1	1:A:184:HIS:N	2.65	0.44
2:B:127:ARG:HG3	2:B:159:HIS:CE1	2.52	0.44
2:B:173:ILE:HG22	2:B:174:LYS:N	2.33	0.44
4:H:137:THR:OG1	4:H:182:THR:HG22	2.18	0.44
1:A:50:LYS:HG2	1:A:275:ASP:HB2	1.99	0.44
1:A:308:TYR:HE1	2:B:89:ILE:HD13	1.81	0.44
1:A:231:SER:HB3	1:A:233:TYR:HE1	1.83	0.44
3:L:159:LEU:HD13	4:H:169:VAL:CG1	2.48	0.44
4:H:54:ASP:O	4:H:55:SER:HB2	2.17	0.44
1:A:166:VAL:CG2	1:A:245:ILE:HB	2.48	0.44
3:L:47:LEU:HA	3:L:58:VAL:HG11	2.00	0.44
4:H:153:THR:HG22	4:H:196:ASN:O	2.17	0.44
1:A:55:PRO:HD2	1:A:279:SER:O	2.18	0.43
3:L:114:VAL:CG1	3:L:133:CYS:SG	3.05	0.43
3:L:197:HIS:CD2	3:L:199:THR:HG21	2.52	0.43
1:A:325:GLU:HG2	2:B:13:GLY:O	2.17	0.43
3:L:34:HIS:CD2	3:L:49:TYR:HA	2.47	0.43
3:L:140:PRO:C	3:L:142:ASP:N	2.74	0.43
1:A:302:TYR:CE1	2:B:63:PHE:HD1	2.36	0.43
2:B:9:PHE:CD1	2:B:9:PHE:C	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:150:ASP:N	3:L:190:SER:OG	2.48	0.43
4:H:183:VAL:HB	4:H:187:THR:OG1	2.18	0.43
1:A:191:GLN:CG	1:A:198:ALA:HA	2.46	0.43
1:A:308:TYR:CD1	2:B:89:ILE:HD13	2.53	0.43
1:A:156:LYS:HB3	1:A:194:LEU:O	2.19	0.43
1:A:293:PRO:HD3	2:B:56:ILE:HG22	2.00	0.43
4:H:39:GLN:HA	4:H:44:GLY:O	2.19	0.43
1:A:178:TYR:CD2	1:A:243:LEU:HD22	2.54	0.43
1:A:295:GLN:HG2	1:A:306:PRO:HB2	2.01	0.43
4:H:170:LEU:HD21	4:H:173:ASP:HA	2.01	0.43
1:A:163:VAL:HG22	1:A:248:ASN:HB3	2.01	0.43
1:A:303:GLY:O	2:B:61:GLU:HA	2.18	0.43
3:L:197:HIS:O	3:L:199:THR:HG22	2.19	0.43
1:A:79:PHE:CE1	4:H:100(B):ILE:HD13	2.54	0.42
3:L:158:VAL:HA	3:L:177:THR:O	2.19	0.42
4:H:154:TRP:CZ3	4:H:195:CYS:HB3	2.53	0.42
1:A:9:SER:N	2:B:143:LYS:HG2	2.34	0.42
3:L:149:ILE:HG23	3:L:191:TYR:CE1	2.55	0.42
4:H:39:GLN:O	4:H:88:ALA:HB1	2.19	0.42
4:H:184:PRO:HG2	4:H:187:THR:CG2	2.49	0.42
1:A:57:ARG:O	1:A:85:ASP:HB2	2.19	0.42
1:A:180:TRP:CE2	1:A:204:VAL:HG21	2.53	0.42
2:B:85:GLU:O	2:B:89:ILE:HG13	2.20	0.42
3:L:49:TYR:HD1	3:L:50:LYS:HG3	1.84	0.42
3:L:121:LYS:HA	3:L:124:LEU:CD1	2.49	0.42
1:A:266:SER:OG	2:B:64:HIS:HA	2.20	0.42
3:L:12:PRO:HA	3:L:105:GLU:O	2.18	0.42
3:L:61:ARG:NH1	3:L:61:ARG:HG3	2.34	0.42
4:H:17:SER:CB	4:H:82(B):SER:HA	2.43	0.42
4:H:40:ARG:HD2	4:H:40:ARG:H	1.85	0.42
1:A:50:LYS:HE3	4:H:53:TYR:CD2	2.55	0.42
3:L:112:PRO:HA	3:L:136:ASN:O	2.20	0.42
4:H:137:THR:HA	4:H:182:THR:HG22	2.01	0.42
2:B:126:LEU:HD21	2:B:152:ILE:HD13	2.01	0.42
3:L:88:CYS:O	3:L:99:GLY:N	2.52	0.42
4:H:40:ARG:HD3	4:H:42:ASP:OD1	2.20	0.42
1:A:210:GLN:HE21	1:A:210:GLN:HB3	1.65	0.42
1:A:275:ASP:OD1	1:A:276:THR:N	2.53	0.42
3:L:139:TYR:HB3	3:L:140:PRO:HD3	2.02	0.42
4:H:29:LEU:HD22	4:H:52(B):PRO:HG2	2.01	0.42
4:H:61:GLN:HG3	4:H:64:LYS:HZ1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:188:TRP:HB3	4:H:189:PRO:CD	2.45	0.42
3:L:135:LEU:HD21	3:L:145:VAL:CG1	2.50	0.42
3:L:184:GLU:HA	3:L:187:ARG:NH2	2.34	0.42
3:L:14:SER:O	3:L:17:ASP:HB2	2.20	0.41
3:L:136:ASN:HB2	3:L:173:SER:CB	2.50	0.41
3:L:46:LEU:HD13	3:L:55:PHE:CG	2.55	0.41
3:L:55:PHE:CG	3:L:56:SER:N	2.88	0.41
3:L:89:SER:HB3	3:L:98:PHE:CD2	2.55	0.41
1:A:136:SER:C	1:A:145:SER:HB2	2.45	0.41
3:L:144:ASN:HB3	3:L:196:THR:HB	2.01	0.41
1:A:174:PHE:CD1	1:A:174:PHE:C	2.98	0.41
1:A:205:SER:CB	1:A:210:GLN:HA	2.47	0.41
1:A:249:GLY:O	1:A:250:ASN:HB2	2.20	0.41
1:A:304:ALA:HA	2:B:61:GLU:HA	2.01	0.41
3:L:50:LYS:NZ	4:H:100(B):ILE:O	2.50	0.41
4:H:55:SER:O	4:H:57:THR:HG23	2.21	0.41
4:H:196:ASN:HA	4:H:206:VAL:O	2.20	0.41
4:H:33:TRP:CD2	4:H:50:ARG:HD2	2.55	0.41
3:L:28:THR:HA	3:L:68:GLY:O	2.21	0.41
3:L:116:ILE:CD1	3:L:208:PHE:HD1	2.33	0.41
3:L:118:PRO:CG	4:H:213:ARG:HH22	2.25	0.41
4:H:127:GLY:N	4:H:213:ARG:HH21	2.18	0.41
4:H:152:VAL:HG11	4:H:179:SER:CB	2.51	0.41
3:L:189:ASN:CG	3:L:210:ARG:H	2.28	0.41
4:H:208:LYS:HD2	4:H:208:LYS:HA	1.79	0.41
1:A:52:CYS:HB3	1:A:277:CYS:C	2.45	0.41
1:A:67:ILE:O	1:A:70:LEU:HB3	2.20	0.41
1:A:130:VAL:HA	1:A:157:SER:HB2	2.02	0.41
2:B:48:ILE:HD11	2:B:107:THR:HG23	2.02	0.41
2:B:54:ARG:O	2:B:57:GLU:HB2	2.21	0.41
3:L:111:ALA:HA	3:L:197:HIS:HD2	1.85	0.41
3:L:139:TYR:O	3:L:141:LYS:N	2.54	0.41
3:L:160:ASN:HB3	3:L:162:TRP:CH2	2.56	0.41
4:H:60:ASN:ND2	4:H:62:LYS:H	2.16	0.41
4:H:134:SER:O	4:H:135:MET:HE3	2.21	0.41
4:H:159:LEU:CD2	4:H:181:VAL:HG21	2.50	0.41
4:H:199:HIS:ND1	4:H:202:SER:OG	2.47	0.41
1:A:58:ILE:HG21	1:A:274:ILE:HD13	2.03	0.41
1:A:301:THR:HB	1:A:305:CYS:SG	2.61	0.41
1:A:316:LEU:HD23	2:B:52:LEU:CD1	2.51	0.41
3:L:98:PHE:CE1	4:H:37:PHE:CE1	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:LEU:HD23	2:B:167:LEU:HA	1.89	0.40
3:L:140:PRO:O	3:L:141:LYS:C	2.64	0.40
4:H:35:ASN:HD22	4:H:35:ASN:HA	1.71	0.40
1:A:42:LEU:HD12	2:B:100:VAL:CG2	2.51	0.40
1:A:43:VAL:O	1:A:43:VAL:HG12	2.20	0.40
2:B:28:ASN:ND2	2:B:145:ASP:C	2.79	0.40
3:L:6:GLN:HE21	3:L:21:ILE:HG21	1.86	0.40
4:H:59:TYR:CD1	4:H:59:TYR:N	2.89	0.40
3:L:34:HIS:HD2	3:L:49:TYR:CA	2.31	0.40
4:H:22:CYS:O	4:H:22:CYS:SG	2.79	0.40
1:A:170:ASN:HB2	1:A:237:VAL:CG1	2.52	0.40
1:A:201:ARG:HG2	1:A:201:ARG:HH11	1.86	0.40
2:B:52:LEU:HA	2:B:52:LEU:HD12	1.75	0.40
2:B:127:ARG:HB3	2:B:128:GLU:H	1.66	0.40
3:L:55:PHE:HE1	4:H:100(C):ILE:HD13	1.85	0.40
3:L:117:PHE:HA	3:L:118:PRO:HD3	1.76	0.40
3:L:135:LEU:HD21	3:L:145:VAL:HG13	2.04	0.40
3:L:147:TRP:O	3:L:153:GLU:O	2.39	0.40
3:L:182:LYS:O	3:L:186:GLU:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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	279/289 (96%)	260 (93%)	19 (7%)	14	42
2	B	148/149 (99%)	137 (93%)	11 (7%)	13	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	195/195 (100%)	164 (84%)	31 (16%)	2	9
4	H	197/197 (100%)	161 (82%)	36 (18%)	2	6
All	All	819/830 (99%)	722 (88%)	97 (12%)	5	17

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASP
1	A	48	THR
1	A	55	PRO
1	A	107	SER
1	A	119	GLU
1	A	130	VAL
1	A	155	THR
1	A	156	LYS
1	A	160	THR
1	A	189	GLN
1	A	210	GLN
1	A	222	TRP
1	A	226	LEU
1	A	242	VAL
1	A	265	SER
1	A	266	SER
1	A	278	ILE
1	A	291	ASP
1	A	312	ASN
2	B	11	GLU
2	B	15	GLU
2	B	38	LEU
2	B	54	ARG
2	B	58	LYS
2	B	59	THR
2	B	60	ASN
2	B	72	GLU
2	B	73	VAL
2	B	110	LEU
2	B	132	GLU
3	L	7	THR
3	L	9	LEU
3	L	11	LEU
3	L	13	VAL

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Mol	Chain	Res	Type
3	L	39	LYS
3	L	46	LEU
3	L	58	VAL
3	L	63	SER
3	L	70	ASP
3	L	77	ARG
3	L	83	LEU
3	L	124	LEU
3	L	135	LEU
3	L	148	LYS
3	L	149	ILE
3	L	154	ARG
3	L	155	GLN
3	L	159	LEU
3	L	167	SER
3	L	171	THR
3	L	175	SER
3	L	180	LEU
3	L	181	THR
3	L	183	ASP
3	L	187	ARG
3	L	189	ASN
3	L	192	THR
3	L	198	LYS
3	L	199	THR
3	L	203	PRO
3	L	211	ASN
4	H	1	GLN
4	H	12	VAL
4	H	23	LYS
4	H	29	LEU
4	H	30	THR
4	H	31	THR
4	H	35	ASN
4	H	40	ARG
4	H	45	LEU
4	H	56	GLU
4	H	60	ASN
4	H	61	GLN
4	H	64	LYS
4	H	71	VAL
4	H	81	GLN

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Mol	Chain	Res	Type
4	H	84	SER
4	H	93	THR
4	H	97	GLN
4	H	105	GLN
4	H	107	THR
4	H	120	SER
4	H	124	LEU
4	H	132	THR
4	H	133	ASN
4	H	135	MET
4	H	136	VAL
4	H	141	LEU
4	H	149	PRO
4	H	151	THR
4	H	163	VAL
4	H	169	VAL
4	H	177	LEU
4	H	178	SER
4	H	192	THR
4	H	197	VAL
4	H	209	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	75	HIS
1	A	171	ASN
1	A	210	GLN
1	A	211	GLN
1	A	312	ASN
2	B	26	HIS
2	B	53	ASN
2	B	60	ASN
2	B	125	GLN
2	B	168	ASN
3	L	18	GLN
3	L	27	GLN
3	L	34	HIS
3	L	93	HIS
3	L	160	ASN
3	L	165	GLN

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Mol	Chain	Res	Type
3	L	188	HIS
3	L	189	ASN
3	L	209	ASN
4	H	43	GLN
4	H	60	ASN
4	H	81	GLN
4	H	105	GLN
4	H	133	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 ⓘ

5 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	$\# Z > 2$
5	NAG	C	1	1,5	14,14,15	1.06	2 (14%)	17,19,21	2.36	4 (23%)
5	NDG	C	2	5	14,14,15	2.72	3 (21%)	17,19,21	3.05	5 (29%)
6	NAG	D	1	1,6	14,14,15	1.02	1 (7%)	17,19,21	1.72	5 (29%)
6	NAG	D	2	6	14,14,15	0.80	1 (7%)	17,19,21	1.02	1 (5%)
6	BMA	D	3	6	11,11,12	1.25	1 (9%)	15,15,17	1.38	3 (20%)

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
5	NAG	C	1	1,5	-	2/6/23/26	0/1/1/1
5	NDG	C	2	5	-	2/6/23/26	0/1/1/1
6	NAG	D	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	2	6	-	0/6/23/26	0/1/1/1
6	BMA	D	3	6	-	0/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2	NDG	C1-C2	8.45	1.63	1.52
5	C	2	NDG	O5-C1	3.49	1.49	1.43
6	D	3	BMA	C4-C5	2.52	1.58	1.53
6	D	1	NAG	C1-C2	2.51	1.55	1.52
5	C	2	NDG	C4-C5	2.48	1.58	1.53
6	D	2	NAG	C4-C5	-2.46	1.47	1.53
5	C	1	NAG	C6-C5	2.16	1.59	1.51
5	C	1	NAG	O5-C1	-2.02	1.40	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2	NDG	C1-O5-C5	9.29	124.64	112.19
5	C	1	NAG	C1-O5-C5	7.43	122.15	112.19
5	C	2	NDG	C6-C5-C4	5.11	125.57	113.02
5	C	2	NDG	C1-C2-N2	4.41	117.38	110.43
5	C	1	NAG	C6-C5-C4	3.76	122.25	113.02
6	D	1	NAG	C6-C5-C4	3.37	121.29	113.02
6	D	1	NAG	C1-C2-N2	3.05	115.24	110.43
5	C	1	NAG	O4-C4-C3	-3.03	103.23	110.38
6	D	1	NAG	O5-C1-C2	-2.85	106.88	111.29
6	D	3	BMA	C3-C4-C5	2.80	115.30	110.23
6	D	3	BMA	O4-C4-C3	-2.60	104.25	110.38
6	D	3	BMA	C6-C5-C4	2.43	118.99	113.02
6	D	1	NAG	C1-O5-C5	2.33	115.31	112.19
6	D	2	NAG	C2-N2-C7	2.32	126.02	122.90
5	C	2	NDG	O7-C7-C8	-2.14	118.25	122.05
6	D	1	NAG	O4-C4-C3	-2.12	105.37	110.38
5	C	2	NDG	O4-C4-C3	-2.11	105.39	110.38
5	C	1	NAG	O6-C6-C5	2.08	118.42	111.33

There are no chirality outliers.

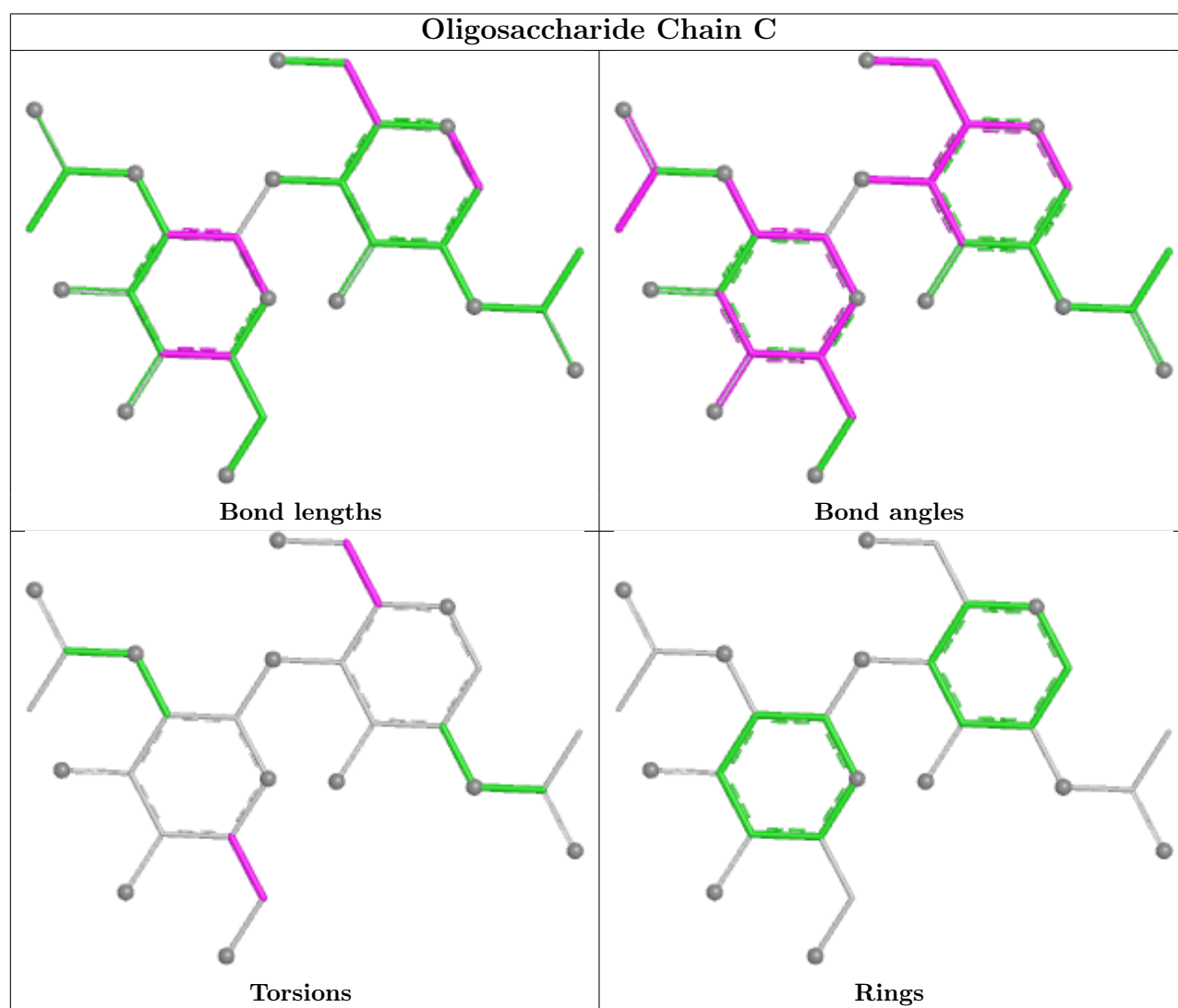
All (4) torsion outliers are listed below:

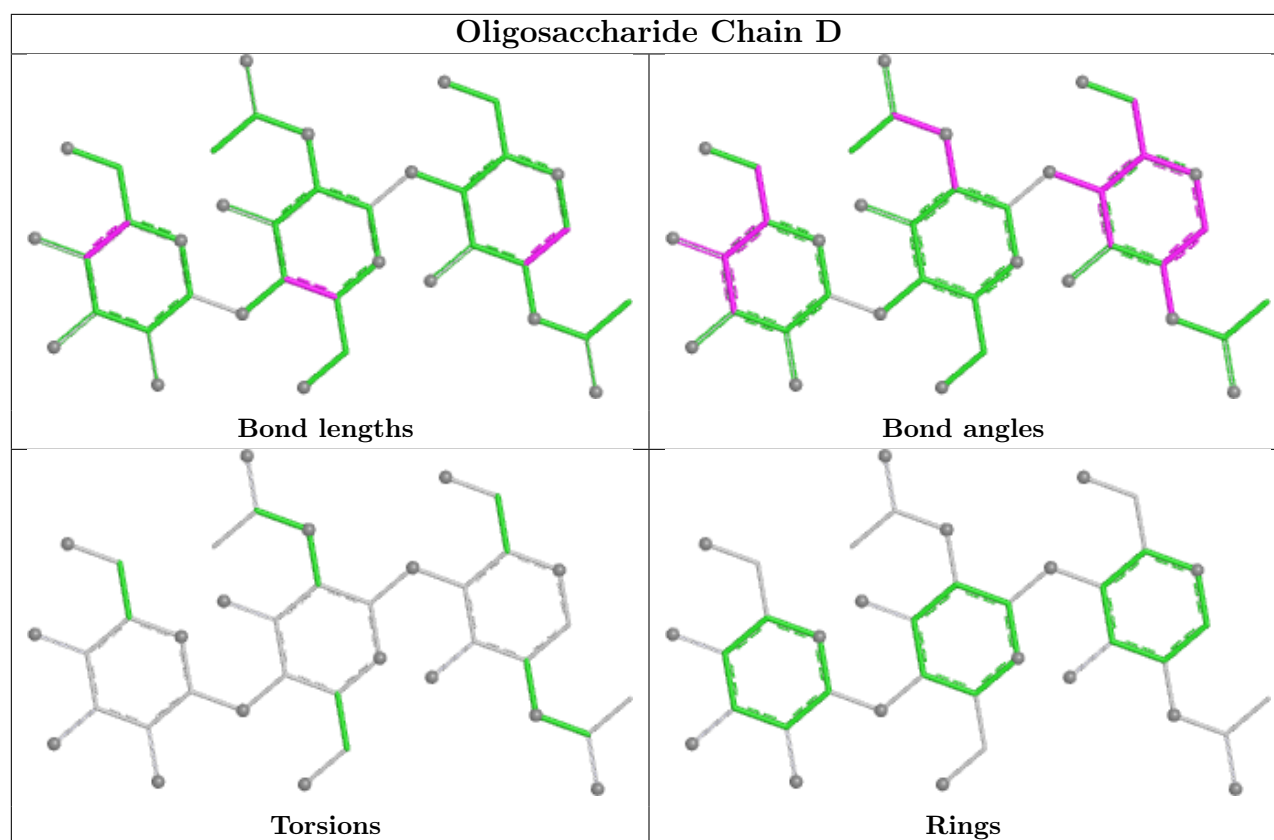
Mol	Chain	Res	Type	Atoms
5	C	2	NDG	O5-C5-C6-O6
5	C	1	NAG	C4-C5-C6-O6
5	C	1	NAG	O5-C5-C6-O6
5	C	2	NDG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	B	410	2	14,14,15	1.55	2 (14%)	17,19,21	2.05	3 (17%)
7	NAG	A	430	1	14,14,15	1.79	4 (28%)	17,19,21	1.46	4 (23%)
7	NAG	A	460	1	14,14,15	1.82	4 (28%)	17,19,21	2.67	7 (41%)

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
7	NAG	B	410	2	-	0/6/23/26	0/1/1/1
7	NAG	A	430	1	-	0/6/23/26	0/1/1/1
7	NAG	A	460	1	-	2/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	430	NAG	C1-C2	-4.39	1.46	1.52
7	B	410	NAG	C1-C2	3.94	1.57	1.52
7	A	460	NAG	C1-C2	3.90	1.57	1.52
7	A	460	NAG	O5-C1	-3.22	1.38	1.43
7	A	430	NAG	O5-C1	-3.09	1.38	1.43
7	B	410	NAG	C4-C5	3.05	1.59	1.53
7	A	460	NAG	C4-C5	2.55	1.58	1.53
7	A	430	NAG	C4-C3	2.44	1.58	1.52
7	A	460	NAG	C4-C3	2.39	1.58	1.52
7	A	430	NAG	C8-C7	2.02	1.54	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	460	NAG	C1-O5-C5	7.26	121.92	112.19
7	B	410	NAG	C1-O5-C5	6.30	120.63	112.19
7	A	460	NAG	O5-C5-C6	-4.47	98.97	107.66
7	A	430	NAG	C3-C4-C5	3.46	116.50	110.23
7	A	460	NAG	O7-C7-C8	-3.43	115.95	122.05
7	A	460	NAG	C8-C7-N2	3.19	121.40	116.12
7	B	410	NAG	C1-C2-N2	3.18	115.44	110.43
7	A	460	NAG	C2-N2-C7	-3.17	118.65	122.90
7	A	430	NAG	C1-C2-N2	-2.85	105.94	110.43
7	A	430	NAG	C2-N2-C7	-2.33	119.77	122.90
7	A	430	NAG	O4-C4-C5	-2.29	103.67	109.32
7	A	460	NAG	C4-C3-C2	-2.18	107.82	111.02
7	A	460	NAG	O5-C1-C2	2.17	114.64	111.29
7	B	410	NAG	O6-C6-C5	2.02	118.20	111.33

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	460	NAG	O5-C5-C6-O6
7	A	460	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	410	NAG	1	0

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.