



Full wwPDB X-ray Structure Validation Report

Mar 9, 2026 – 04:58 PM UTC

PDB ID : 6EA5 / pdb_00006ea5
Title : Structure of BDBV GPcl in complex with the pan-ebolavirus mAb ADI-15878
Authors : King, L.B.; West, B.R.; Moyer, C.L.; Fusco, M.L.; Milligan, J.C.; Hui, S.;
Saphire, E.O.
Deposited on : 2018-08-02
Resolution : 4.75 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

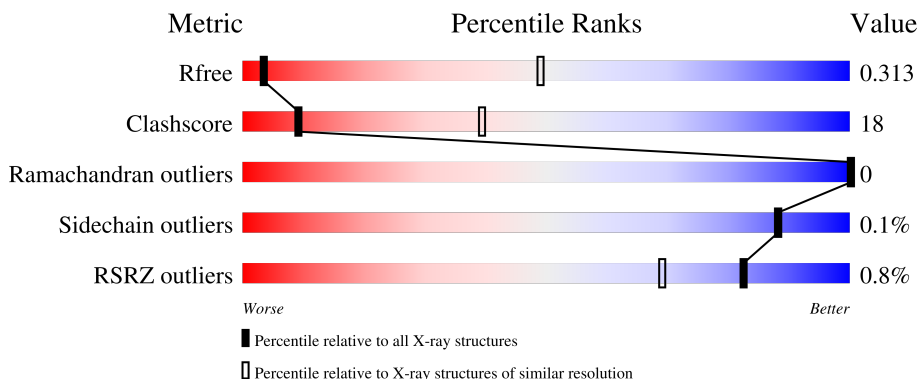
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.75 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	1016 (5.58-3.94)
Clashscore	190562	1039 (5.56-3.96)
Ramachandran outliers	187476	1100 (5.58-3.90)
Sidechain outliers	187428	1081 (5.58-3.90)
RSRZ outliers	180081	1011 (5.58-3.94)

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	162	 67% 32% .
1	C	162	 56% 40% ..
1	E	162	 58% 38% .
2	B	111	 44% 48% . 6%
2	D	111	 57% 35% . 6%

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Mol	Chain	Length	Quality of chain
2	F	111	
3	H	233	
3	M	233	
3	Q	233	
4	L	213	
4	N	213	
4	R	213	
5	G	6	
6	I	5	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	G	1	-	-	X	-
6	BMA	I	3	-	-	X	-
7	NAG	A	201	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15944 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 Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	162	1251	798	213	235	5	0	0	0
1	C	158	1208	767	207	229	5	0	0	0
1	E	155	1187	755	204	223	5	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	ALA	LYS	conflict	UNP B8XCN0
C	64	ALA	LYS	conflict	UNP B8XCN0
E	64	ALA	LYS	conflict	UNP B8XCN0

- Molecule 2 is a protein called Glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	104	813	518	142	147	6	0	0	0
2	D	104	813	518	142	147	6	0	0	0
2	F	103	808	515	141	146	6	0	0	0

- Molecule 3 is a protein called ADI-15878 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	213	1598	1016	269	307	6	0	0	0
3	M	217	1625	1031	274	314	6	0	0	0

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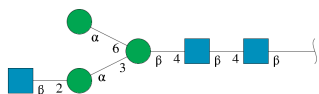
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	Q	222	Total 1655	C 1047	N 280	O 322	S 6	0	0	0

- Molecule 4 is a protein called ADI-15878 Fab Light Chain.

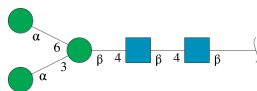
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	L	210	Total 1597	C 999	N 261	O 333	S 4	0	0	0
4	N	212	Total 1617	C 1011	N 267	O 335	S 4	0	0	0
4	R	211	Total 1608	C 1006	N 266	O 332	S 4	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	G	6	Total 75	C 42	N 3	O 30	0	0	0

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



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

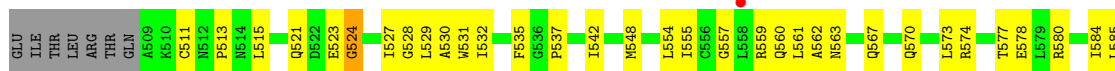
- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



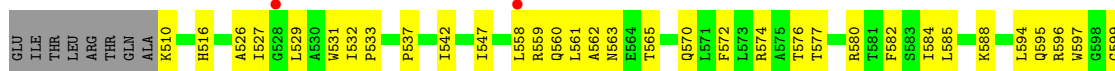
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		



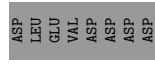
• Molecule 2: Glycoprotein



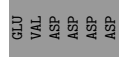
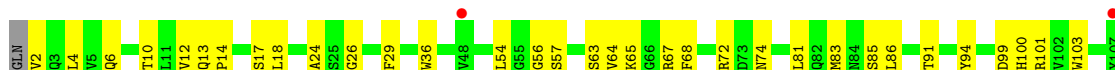
• Molecule 2: Glycoprotein



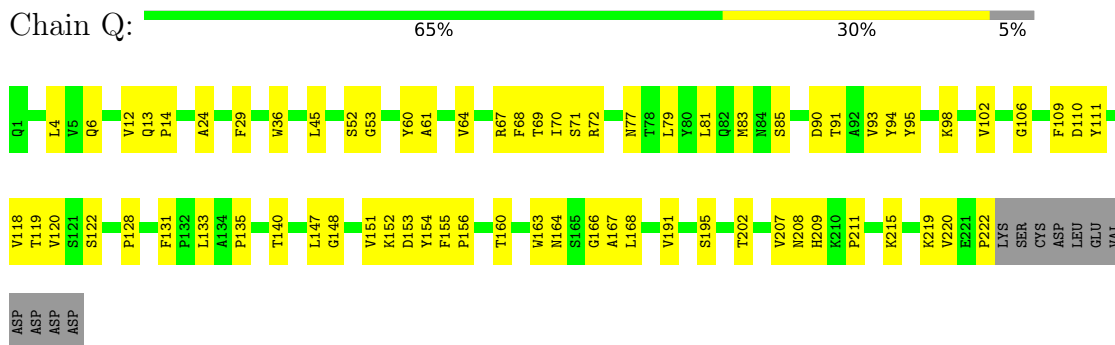
• Molecule 3: ADI-15878 Fab Heavy Chain



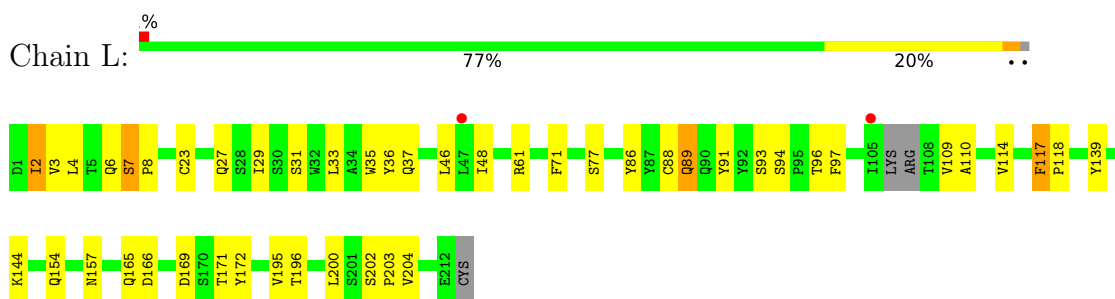
• Molecule 3: ADI-15878 Fab Heavy Chain



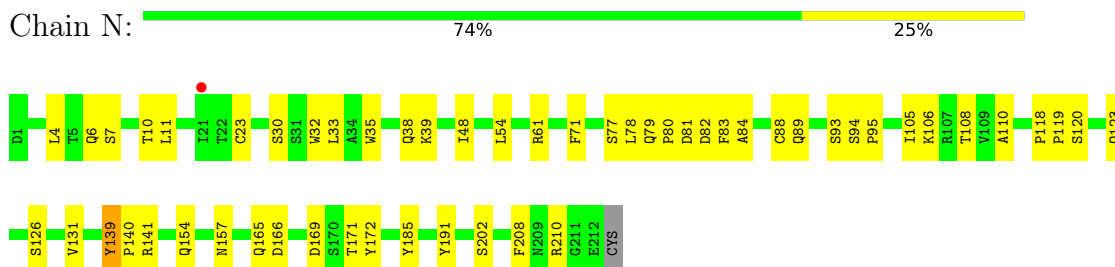
- Molecule 3: ADI-15878 Fab Heavy Chain



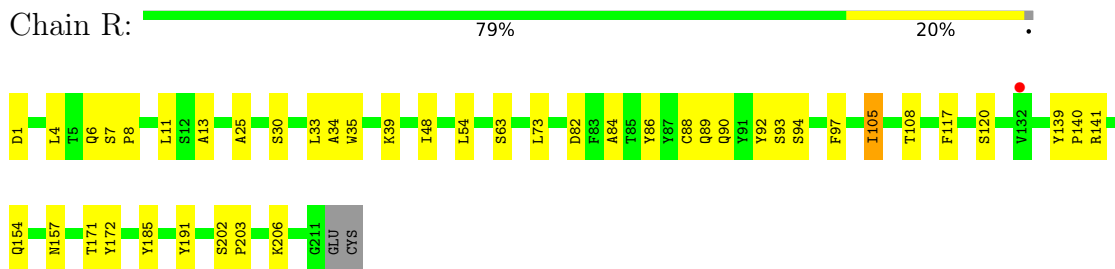
- Molecule 4: ADI-15878 Fab Light Chain



- Molecule 4: ADI-15878 Fab Light Chain



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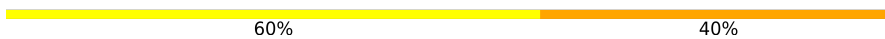
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





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

Chain I:



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.62Å 151.62Å 247.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.26 – 4.75 41.26 – 4.75	Depositor EDS
% Data completeness (in resolution range)	99.4 (41.26-4.75) 99.2 (41.26-4.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 4.85Å)	Xtrriage
Refinement program	PHENIX DEV_1539	Depositor
R, R_{free}	0.295 , 0.305 0.309 , 0.313	Depositor DCC
R_{free} test set	850 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	259.4	Xtrriage
Anisotropy	0.392	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 366.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.075 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15944	wwPDB-VP
Average B, all atoms (Å ²)	203.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, 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	0.53	0/1282	1.06	6/1741 (0.3%)
1	C	0.53	0/1237	1.17	7/1683 (0.4%)
1	E	0.50	0/1216	0.95	2/1654 (0.1%)
2	B	0.47	0/833	0.98	2/1134 (0.2%)
2	D	0.47	0/833	1.01	3/1134 (0.3%)
2	F	0.51	0/828	0.98	1/1127 (0.1%)
3	H	0.39	0/1639	0.87	4/2236 (0.2%)
3	M	0.44	0/1666	0.88	2/2271 (0.1%)
3	Q	0.39	0/1697	0.88	3/2314 (0.1%)
4	L	0.42	0/1631	0.88	6/2218 (0.3%)
4	N	0.41	0/1652	0.87	4/2246 (0.2%)
4	R	0.38	0/1643	0.90	5/2234 (0.2%)
All	All	0.45	0/16157	0.94	45/21992 (0.2%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	ILE	N-CA-C	8.21	118.30	110.42
4	L	89	GLN	N-CA-C	7.43	121.02	108.90
3	M	134	ALA	CA-C-N	7.14	127.06	119.85
3	M	134	ALA	C-N-CA	7.14	127.06	119.85
2	B	558	LEU	N-CA-C	6.98	118.68	111.14
1	A	33	ILE	CA-C-N	6.90	126.87	119.76
1	A	33	ILE	C-N-CA	6.90	126.87	119.76
3	Q	13	GLN	CA-C-N	-6.90	112.66	119.90
3	Q	13	GLN	C-N-CA	-6.90	112.66	119.90
2	D	523	GLU	N-CA-C	-6.84	104.14	113.30
3	H	127	GLY	CA-C-N	6.75	126.51	119.76
3	H	127	GLY	C-N-CA	6.75	126.51	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	92	TYR	N-CA-C	6.72	118.60	111.28
1	C	48	ILE	N-CA-C	6.71	117.47	110.62
1	E	181	VAL	N-CA-C	6.51	117.85	108.48
3	H	13	GLN	CA-C-N	-6.51	113.07	119.90
3	H	13	GLN	C-N-CA	-6.51	113.07	119.90
4	R	117	PHE	CA-C-N	6.45	127.02	120.38
4	R	117	PHE	C-N-CA	6.45	127.02	120.38
1	C	41	ASN	N-CA-C	6.42	120.41	112.58
4	R	105	ILE	N-CA-C	6.34	115.85	106.85
1	E	66	VAL	N-CA-C	6.34	117.00	107.75
2	F	585	LEU	N-CA-C	-6.29	104.51	111.36
2	D	597	TRP	N-CA-C	6.25	119.07	111.82
1	C	66	VAL	N-CA-C	6.17	116.76	107.75
2	D	524	GLY	N-CA-C	-6.11	105.41	112.50
4	L	117	PHE	CA-C-N	6.02	126.58	120.38
4	L	117	PHE	C-N-CA	6.02	126.58	120.38
1	C	79	VAL	CB-CA-C	-5.94	108.06	113.70
2	B	527	ILE	N-CA-C	5.88	118.44	111.09
4	L	7	SER	CA-C-N	-5.85	112.52	119.84
4	L	7	SER	C-N-CA	-5.85	112.52	119.84
1	A	111	LEU	N-CA-C	5.84	117.94	108.41
4	L	2	ILE	N-CA-C	5.64	116.07	108.17
1	C	142	SER	N-CA-C	5.59	117.80	108.02
4	N	7	SER	CA-C-N	-5.50	112.97	119.84
4	N	7	SER	C-N-CA	-5.50	112.97	119.84
4	N	30	SER	CB-CA-C	-5.47	110.29	116.63
4	N	139	TYR	CB-CA-C	5.21	116.95	108.87
3	Q	52	SER	N-CA-C	5.17	117.36	110.53
1	C	149	GLU	N-CA-C	5.13	116.78	109.14
1	C	147	CYS	N-CA-C	-5.11	102.14	109.24
4	R	30	SER	CB-CA-C	-5.06	110.76	116.63
1	A	79	VAL	CB-CA-C	-5.05	107.38	114.00
1	A	155	LYS	N-CA-C	5.01	116.55	111.14

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	1251	0	1223	58	0
1	C	1208	0	1180	72	0
1	E	1187	0	1163	70	0
2	B	813	0	790	77	0
2	D	813	0	790	64	1
2	F	808	0	785	58	0
3	H	1598	0	1560	49	0
3	M	1625	0	1588	63	0
3	Q	1655	0	1618	55	0
4	L	1597	0	1537	36	0
4	N	1617	0	1564	57	0
4	R	1608	0	1558	32	1
5	G	75	0	64	11	0
6	I	61	0	52	11	0
7	A	14	0	13	7	0
7	B	14	0	13	4	0
All	All	15944	0	15498	571	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 18.

All (571) 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:A:41:ASN:HB2	7:A:201:NAG:C8	1.57	1.32
1:E:57:LEU:HD12	1:E:62:GLN:NE2	1.50	1.26
2:F:563:ASN:HD21	5:G:1:NAG:C1	1.50	1.23
1:A:41:ASN:HB2	7:A:201:NAG:H81	1.23	1.11
3:M:12:VAL:HG12	3:M:13:GLN:H	1.16	1.09
3:H:12:VAL:HG12	3:H:13:GLN:H	1.21	1.04
3:M:12:VAL:CG1	3:M:13:GLN:H	1.70	1.04
1:A:41:ASN:HB2	7:A:201:NAG:H82	1.37	1.02
3:M:12:VAL:HG12	3:M:13:GLN:N	1.69	1.00
2:F:563:ASN:OD1	5:G:1:NAG:C7	2.11	0.99
3:H:12:VAL:HG12	3:H:13:GLN:N	1.76	0.95
1:E:124:GLU:HG3	1:E:172:ARG:NH1	1.81	0.94
1:E:57:LEU:HD12	1:E:62:GLN:HE21	1.05	0.94
3:H:12:VAL:CG1	3:H:13:GLN:H	1.81	0.92
1:C:77:THR:HB	1:C:107:ASN:HD22	1.32	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:563:ASN:ND2	5:G:1:NAG:C1	2.33	0.91
1:A:41:ASN:CB	7:A:201:NAG:H81	1.99	0.91
1:C:164:ARG:HB2	2:F:577:THR:HG21	1.52	0.90
2:F:563:ASN:OD1	5:G:1:NAG:H82	1.73	0.89
4:R:7:SER:OG	4:R:8:PRO:HD3	1.74	0.88
2:F:527:ILE:HG13	4:L:94:SER:H	1.39	0.87
2:D:531:TRP:CZ3	2:D:532:ILE:HG22	2.10	0.87
1:E:124:GLU:HG3	1:E:172:ARG:HH12	1.36	0.87
1:E:57:LEU:CD1	1:E:62:GLN:HE21	1.86	0.86
1:E:72:GLY:HA3	2:F:559:ARG:NH2	1.91	0.85
1:E:124:GLU:CG	1:E:172:ARG:HH12	1.88	0.85
1:C:94:PRO:HB3	1:C:169:ILE:HD12	1.59	0.85
2:F:563:ASN:OD1	5:G:1:NAG:C8	2.26	0.84
4:N:39:LYS:HE2	4:N:81:ASP:OD1	1.79	0.83
1:E:57:LEU:HA	1:E:62:GLN:HE22	1.43	0.82
2:B:592:PHE:CZ	2:B:596:ARG:NH1	2.49	0.81
3:Q:120:VAL:HG12	3:Q:120:VAL:O	1.79	0.81
1:E:47:ASP:HB3	1:E:50:LYS:HG2	1.63	0.80
3:H:128:PRO:HB3	3:H:154:TYR:HB3	1.62	0.80
2:B:551:GLN:HG2	2:B:554:LEU:HD12	1.64	0.80
1:C:72:GLY:HA3	2:D:559:ARG:NH2	1.97	0.80
1:A:34:PRO:HD2	2:B:565:THR:HG23	1.65	0.79
2:B:599:GLY:HA3	1:E:56:LYS:NZ	1.97	0.79
1:C:184:LEU:HD11	2:D:561:LEU:HD23	1.65	0.79
1:A:88:PHE:HB3	1:A:149:GLU:HB2	1.62	0.78
4:N:39:LYS:CE	4:N:81:ASP:OD1	2.31	0.78
1:E:94:PRO:HB3	1:E:169:ILE:HD12	1.65	0.78
1:E:184:LEU:HD11	2:F:558:LEU:HD13	1.63	0.78
1:E:50:LYS:O	2:F:595:GLN:NE2	2.16	0.78
1:E:72:GLY:HA3	2:F:559:ARG:HH22	1.44	0.78
4:N:33:LEU:HD22	4:N:71:PHE:CD2	2.16	0.78
2:D:531:TRP:HZ3	1:E:157:GLY:HA3	1.49	0.78
2:D:560:GLN:O	2:D:563:ASN:HB3	1.83	0.78
4:R:6:GLN:NE2	4:R:88:CYS:SG	2.57	0.78
2:B:557:GLY:O	2:B:560:GLN:HB2	1.83	0.77
1:E:124:GLU:CG	1:E:172:ARG:NH1	2.49	0.76
4:N:33:LEU:CD2	4:N:71:PHE:CG	2.69	0.75
1:A:41:ASN:CB	7:A:201:NAG:C8	2.52	0.75
1:C:43:LEU:O	1:C:43:LEU:HD12	1.85	0.75
3:H:10:THR:HB	3:H:18:LEU:HD21	1.66	0.75
3:Q:128:PRO:HB3	3:Q:154:TYR:HB3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:532:ILE:HD11	2:D:535:PHE:HB2	1.69	0.75
1:C:164:ARG:HB2	2:F:577:THR:CG2	2.17	0.75
1:C:99:TYR:OH	1:C:162:TYR:O	2.04	0.74
1:E:113:ILE:HG23	1:E:121:CYS:HB2	1.69	0.74
4:N:154:GLN:HB3	4:N:157:ASN:HD21	1.52	0.74
4:N:108:THR:HB	4:N:139:TYR:CE2	2.22	0.74
1:A:42:THR:HG22	1:A:44:GLN:NE2	2.03	0.73
3:Q:53:GLY:O	3:Q:72:ARG:NH2	2.21	0.73
2:F:563:ASN:O	5:G:1:NAG:H82	1.89	0.73
4:L:110:ALA:H	4:L:139:TYR:HB2	1.54	0.72
1:A:51:LEU:HD21	2:B:596:ARG:HG2	1.71	0.72
3:H:61:ALA:HB3	3:H:64:VAL:HG22	1.70	0.72
2:B:592:PHE:CE1	2:B:596:ARG:NH1	2.58	0.71
1:C:58:SER:OG	1:C:62:GLN:NE2	2.23	0.71
3:Q:67:ARG:NH2	3:Q:90:ASP:OD2	2.23	0.71
1:C:88:PHE:HB3	1:C:149:GLU:HB2	1.72	0.71
3:H:12:VAL:HG12	3:H:13:GLN:O	1.91	0.70
2:D:521:GLN:NE2	2:D:524:GLY:HA3	2.06	0.70
1:C:77:THR:CB	1:C:107:ASN:HD22	2.04	0.70
4:L:4:LEU:HD12	4:L:4:LEU:C	2.16	0.70
4:N:33:LEU:HD23	4:N:71:PHE:CD1	2.26	0.70
1:A:184:LEU:HD21	2:B:558:LEU:HD13	1.74	0.70
1:A:39:HIS:HB3	1:A:42:THR:HB	1.72	0.70
2:F:527:ILE:HG13	4:L:94:SER:N	2.05	0.70
4:R:35:TRP:HB2	4:R:48:ILE:HG22	1.73	0.70
3:H:2:VAL:N	3:H:27:PHE:HB2	2.07	0.70
2:D:531:TRP:CH2	2:D:532:ILE:HG22	2.27	0.69
2:F:563:ASN:OD1	5:G:1:NAG:N2	2.25	0.69
4:L:89:GLN:OE1	4:L:97:PHE:CE1	2.46	0.69
4:L:144:LYS:HB3	4:L:196:THR:HB	1.73	0.69
2:D:554:LEU:C	2:D:554:LEU:HD23	2.17	0.68
3:M:101:ARG:NH1	6:I:3:BMA:C6	2.57	0.68
4:N:105:ILE:HG13	4:N:165:GLN:OE1	1.94	0.68
1:E:99:TYR:OH	1:E:162:TYR:O	2.12	0.68
2:F:529:LEU:HD22	4:L:91:TYR:CE1	2.29	0.68
3:Q:163:TRP:O	3:Q:166:GLY:N	2.26	0.67
1:E:122:LEU:HB2	1:E:172:ARG:HG3	1.76	0.67
2:F:563:ASN:CG	5:G:1:NAG:C7	2.66	0.67
3:M:12:VAL:HG11	3:M:86:LEU:HD12	1.77	0.66
4:L:35:TRP:HB2	4:L:48:ILE:HG22	1.77	0.66
1:A:40:ASN:O	7:A:201:NAG:H82	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:72:ARG:NH1	3:M:74:ASN:OD1	2.29	0.66
2:F:529:LEU:HD11	3:H:106:GLY:HA2	1.78	0.65
3:H:102:VAL:HG11	3:H:106:GLY:HA3	1.77	0.65
1:C:51:LEU:HD22	2:D:595:GLN:HG3	1.78	0.65
3:Q:90:ASP:O	3:Q:94:TYR:OH	2.14	0.65
2:D:532:ILE:CD1	2:D:535:PHE:HB2	2.27	0.65
2:D:531:TRP:CZ3	1:E:157:GLY:HA3	2.31	0.64
4:N:106:LYS:HB2	4:N:139:TYR:HB2	1.78	0.64
2:D:593:LEU:HD21	2:F:594:LEU:HD23	1.79	0.64
2:B:599:GLY:HA3	1:E:56:LYS:HZ3	1.62	0.64
4:N:119:PRO:HD3	4:N:131:VAL:HG22	1.79	0.64
1:C:69:ASN:ND2	1:C:105:ALA:HB2	2.13	0.64
1:C:152:ALA:O	1:C:169:ILE:HA	1.97	0.64
1:E:147:CYS:N	1:E:148:PRO:HD3	2.12	0.64
2:B:533:PRO:HB2	1:C:153:PHE:CD2	2.33	0.63
3:M:135:PRO:HG3	3:M:147:LEU:HB3	1.80	0.63
1:C:43:LEU:HD21	2:D:557:GLY:HA3	1.80	0.63
1:E:52:VAL:O	2:F:596:ARG:NH2	2.30	0.63
4:R:108:THR:H	4:R:139:TYR:HE2	1.45	0.63
1:E:111:LEU:HD12	1:E:170:ILE:HG21	1.81	0.63
1:C:45:VAL:HG21	3:M:54:LEU:HG	1.80	0.63
1:C:71:GLU:OE2	1:C:107:ASN:N	2.21	0.63
3:M:36:TRP:CE2	3:M:81:LEU:HB2	2.34	0.63
3:H:10:THR:CB	3:H:18:LEU:HD21	2.29	0.62
3:H:83:MET:HB3	3:H:86:LEU:HD21	1.81	0.62
1:A:66:VAL:HG22	1:A:101:ALA:HB3	1.81	0.62
4:N:33:LEU:HD22	4:N:71:PHE:CG	2.32	0.62
1:E:104:TRP:CD1	2:F:516:HIS:HD1	2.18	0.62
1:A:45:VAL:HG21	3:H:56:GLY:CA	2.29	0.62
2:B:576:THR:HG21	2:B:581:THR:HG21	1.79	0.62
7:B:701:NAG:H83	2:F:531:TRP:HH2	1.62	0.62
3:Q:140:THR:HG23	3:Q:140:THR:O	1.99	0.62
2:D:537:PRO:HG2	2:D:542:ILE:HG22	1.82	0.61
1:A:99:TYR:OH	1:A:162:TYR:O	2.12	0.61
1:A:99:TYR:CZ	1:A:161:LEU:HD22	2.37	0.60
3:M:144:THR:N	3:M:195:SER:HG	1.99	0.60
2:B:536:GLY:O	1:C:89:ARG:NH2	2.31	0.60
1:A:40:ASN:O	1:A:40:ASN:OD1	2.20	0.60
3:H:147:LEU:HB2	3:H:220:VAL:HG11	1.84	0.60
1:A:182:ALA:HB2	2:B:562:ALA:HB2	1.83	0.60
4:L:4:LEU:HD12	4:L:4:LEU:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:105:ILE:HG13	4:N:105:ILE:O	2.01	0.60
2:F:558:LEU:HD12	2:F:558:LEU:O	2.01	0.60
3:M:101:ARG:HH12	6:I:3:BMA:H62	1.68	0.59
1:E:55:ASP:OD1	2:F:596:ARG:NH2	2.35	0.59
4:R:4:LEU:HA	4:R:25:ALA:HA	1.85	0.59
1:A:103:GLU:HA	2:B:517:TYR:HA	1.84	0.59
2:B:563:ASN:HD21	7:B:701:NAG:C1	2.14	0.59
4:R:108:THR:HG1	4:R:139:TYR:HH	1.43	0.59
3:Q:120:VAL:O	3:Q:120:VAL:CG1	2.50	0.59
2:B:599:GLY:HA3	1:E:56:LYS:HZ2	1.68	0.59
2:D:532:ILE:HD12	2:D:535:PHE:HD2	1.67	0.58
2:D:561:LEU:HD13	3:M:54:LEU:HD23	1.85	0.58
4:L:169:ASP:OD2	4:L:171:THR:OG1	2.21	0.58
1:C:97:VAL:HG23	2:D:584:ILE:HD12	1.84	0.58
2:B:599:GLY:O	2:B:600:THR:C	2.46	0.58
3:M:125:THR:HG22	3:M:156:PRO:HD3	1.86	0.58
3:M:101:ARG:NH1	6:I:3:BMA:H62	2.19	0.58
4:N:35:TRP:HB2	4:N:48:ILE:HG22	1.85	0.57
3:M:103:TRP:HB3	6:I:1:NAG:H62	1.86	0.57
1:A:107:ASN:OD1	1:A:139:HIS:NE2	2.36	0.57
4:N:106:LYS:HD2	4:N:141:ARG:H	1.68	0.57
1:C:69:ASN:HD22	1:C:105:ALA:HB2	1.69	0.57
2:F:576:THR:HG23	2:F:576:THR:O	2.05	0.57
1:A:130:ARG:NH2	2:D:577:THR:OG1	2.38	0.57
1:E:57:LEU:HD12	1:E:62:GLN:HE22	1.61	0.57
1:E:89:ARG:HB3	1:E:153:PHE:CD1	2.39	0.57
3:H:102:VAL:HB	3:H:106:GLY:H	1.70	0.57
2:B:551:GLN:HG2	2:B:554:LEU:CD1	2.34	0.56
2:F:516:HIS:HA	2:F:547:ILE:HG22	1.87	0.56
3:M:135:PRO:HD2	3:M:222:PRO:HB3	1.87	0.56
2:B:528:GLY:O	2:B:531:TRP:NE1	2.38	0.56
2:B:539:ALA:HB2	1:C:93:PRO:HD3	1.87	0.56
2:B:548:MET:HG3	2:B:555:ILE:HD11	1.88	0.56
2:D:521:GLN:NE2	2:D:524:GLY:C	2.64	0.56
4:R:1:ASP:HB2	4:R:94:SER:CB	2.35	0.56
1:C:154:HIS:CD2	1:C:156:GLU:HB2	2.41	0.56
1:C:51:LEU:HD11	2:D:596:ARG:CZ	2.35	0.56
2:D:532:ILE:HG13	2:D:532:ILE:O	2.06	0.56
1:E:88:PHE:HB3	1:E:149:GLU:HB2	1.88	0.56
1:E:96:VAL:HB	2:F:580:ARG:HG2	1.87	0.56
4:N:105:ILE:CG1	4:N:165:GLN:OE1	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ALA:O	1:A:169:ILE:HA	2.06	0.56
3:Q:168:LEU:HD21	3:Q:191:VAL:HG21	1.88	0.56
1:C:115:LYS:HD3	1:C:147:CYS:H	1.70	0.55
2:B:582:PHE:CE2	2:D:578:GLU:HG2	2.40	0.55
1:E:57:LEU:HA	1:E:62:GLN:NE2	2.17	0.55
4:R:1:ASP:HB2	4:R:94:SER:HB2	1.89	0.55
1:C:162:TYR:HB2	1:C:165:LEU:O	2.05	0.55
4:L:29:ILE:HD11	4:L:33:LEU:HD12	1.88	0.55
3:Q:147:LEU:HB2	3:Q:220:VAL:HG11	1.89	0.55
3:Q:164:ASN:CB	3:Q:167:ALA:HB3	2.36	0.55
1:A:42:THR:CG2	1:A:44:GLN:NE2	2.70	0.55
4:N:106:LYS:HA	4:N:139:TYR:CD2	2.42	0.55
1:E:159:PHE:CZ	2:F:570:GLN:NE2	2.75	0.54
3:M:91:THR:HG23	3:M:119:THR:HA	1.90	0.54
2:D:521:GLN:NE2	2:D:524:GLY:CA	2.69	0.54
2:D:531:TRP:CH2	2:D:532:ILE:CG2	2.90	0.54
1:A:70:LEU:HD21	1:A:75:VAL:HG11	1.88	0.54
2:F:560:GLN:O	2:F:563:ASN:HB3	2.08	0.54
3:M:110:ASP:OD1	3:M:111:TYR:N	2.40	0.54
1:E:36:GLY:HA3	2:F:561:LEU:HD21	1.89	0.54
4:R:33:LEU:HD22	4:R:89:GLN:O	2.08	0.54
3:M:36:TRP:CZ2	3:M:81:LEU:HB2	2.43	0.54
1:A:111:LEU:HD12	1:A:170:ILE:HG21	1.90	0.54
1:C:183:PHE:C	1:C:184:LEU:HD12	2.33	0.54
2:D:521:GLN:HB3	2:D:524:GLY:HA3	1.90	0.53
3:H:110:ASP:OD1	3:H:111:TYR:N	2.40	0.53
3:M:2:VAL:O	3:M:2:VAL:HG13	2.08	0.53
3:Q:94:TYR:HE2	3:Q:118:VAL:HB	1.73	0.53
3:M:6:GLN:HB3	3:M:116:ALA:HB2	1.89	0.53
3:M:198:LEU:HD21	3:M:222:PRO:HG3	1.90	0.53
4:R:154:GLN:HB3	4:R:157:ASN:HD21	1.74	0.53
1:A:45:VAL:HG21	3:H:56:GLY:HA3	1.90	0.53
4:L:2:ILE:CG2	4:L:27:GLN:CD	2.82	0.53
4:N:202:SER:HB3	4:R:11:LEU:HD13	1.91	0.53
2:B:531:TRP:CD1	2:D:567:GLN:HG3	2.44	0.53
3:M:4:LEU:CD2	3:M:24:ALA:HA	2.39	0.53
1:E:112:ASP:O	1:E:142:SER:HA	2.08	0.53
4:N:48:ILE:HG13	4:N:54:LEU:HD23	1.91	0.53
1:A:94:PRO:HB3	1:A:169:ILE:HD13	1.90	0.52
1:A:130:ARG:HH11	1:C:93:PRO:CB	2.21	0.52
1:A:95:LYS:NZ	2:B:574:ARG:HA	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:30:SER:HB3	3:H:74:ASN:HB3	1.90	0.52
3:M:10:THR:OG1	3:M:117:LEU:O	2.27	0.52
1:C:96:VAL:HB	2:D:580:ARG:HA	1.91	0.52
3:Q:6:GLN:OE1	3:Q:6:GLN:HA	2.08	0.52
1:A:159:PHE:CE2	2:B:566:THR:HG23	2.43	0.52
2:B:531:TRP:HE3	2:D:570:GLN:HG3	1.74	0.52
4:R:108:THR:OG1	4:R:139:TYR:OH	2.21	0.52
2:D:597:TRP:CE2	2:F:597:TRP:HB3	2.44	0.52
1:C:77:THR:CB	1:C:107:ASN:ND2	2.73	0.52
3:H:95:TYR:HB3	3:H:112:TRP:HE3	1.74	0.52
4:L:36:TYR:CZ	4:L:46:LEU:HD23	2.45	0.52
3:M:202:THR:HB	3:M:219:LYS:HE3	1.90	0.52
1:E:151:TYR:CG	1:E:169:ILE:HD13	2.45	0.52
4:R:1:ASP:HB2	4:R:94:SER:OG	2.09	0.52
3:H:160:THR:OG1	3:H:208:ASN:HB3	2.10	0.52
2:D:531:TRP:CH2	1:E:156:GLU:O	2.63	0.51
4:N:185:TYR:HA	4:N:191:TYR:OH	2.10	0.51
4:R:185:TYR:HA	4:R:191:TYR:OH	2.10	0.51
3:Q:93:VAL:HG11	3:Q:95:TYR:OH	2.09	0.51
3:Q:164:ASN:HB2	3:Q:167:ALA:HB3	1.92	0.51
1:A:72:GLY:O	2:B:512:ASN:HB2	2.10	0.51
3:H:12:VAL:CG1	3:H:16:GLY:HA3	2.39	0.51
3:H:35:SER:HB3	3:H:109:PHE:CZ	2.46	0.51
3:Q:12:VAL:HG23	3:Q:120:VAL:HA	1.92	0.51
2:B:563:ASN:ND2	7:B:701:NAG:C1	2.73	0.51
1:E:113:ILE:HG12	1:E:121:CYS:SG	2.50	0.51
4:N:108:THR:HB	4:N:139:TYR:CZ	2.45	0.51
1:A:78:ASP:OD1	1:A:78:ASP:N	2.43	0.51
1:A:104:TRP:N	2:B:516:HIS:O	2.37	0.51
3:M:64:VAL:HB	3:M:68:PHE:CD2	2.46	0.51
4:N:165:GLN:HB2	4:N:172:TYR:CZ	2.46	0.51
2:F:510:LYS:HE3	5:G:2:NAG:H82	1.92	0.51
4:N:39:LYS:HE3	4:N:81:ASP:OD1	2.08	0.51
4:R:82:ASP:O	4:R:86:TYR:OH	2.24	0.51
1:C:95:LYS:NZ	2:D:574:ARG:HA	2.26	0.51
3:M:14:PRO:HD3	3:M:122:SER:HB2	1.93	0.51
1:E:33:ILE:HB	2:F:588:LYS:CE	2.41	0.51
4:N:11:LEU:HD13	4:R:202:SER:HB3	1.93	0.50
2:B:528:GLY:C	2:B:531:TRP:HE1	2.19	0.50
2:D:515:LEU:CB	2:D:555:ILE:HD12	2.42	0.50
3:Q:110:ASP:OD1	3:Q:111:TYR:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:93:VAL:CG1	3:Q:95:TYR:CZ	2.94	0.50
1:A:39:HIS:HB2	1:A:44:GLN:OE1	2.12	0.50
4:N:6:GLN:NE2	4:N:88:CYS:SG	2.85	0.50
4:L:6:GLN:NE2	4:L:88:CYS:SG	2.84	0.50
4:L:31:SER:HA	4:L:71:PHE:HZ	1.76	0.50
3:M:94:TYR:HE2	3:M:118:VAL:HB	1.76	0.50
2:B:544:THR:HG22	2:B:545:GLU:N	2.26	0.50
1:C:77:THR:HB	1:C:107:ASN:ND2	2.14	0.50
3:M:99:ASP:HA	3:M:108:HIS:O	2.12	0.50
1:C:34:PRO:HG3	3:M:57:SER:OG	2.12	0.50
1:E:182:ALA:HB2	2:F:562:ALA:HB2	1.93	0.50
3:Q:202:THR:HB	3:Q:219:LYS:HE3	1.94	0.50
1:C:182:ALA:HB2	2:D:562:ALA:HA	1.94	0.49
3:M:12:VAL:CG1	3:M:13:GLN:N	2.34	0.49
2:B:603:ILE:HG12	2:B:610:ILE:HG21	1.94	0.49
2:D:528:GLY:O	2:D:529:LEU:HB3	2.12	0.49
2:B:594:LEU:HD22	1:E:57:LEU:HB3	1.93	0.49
4:L:3:VAL:HG23	4:L:96:THR:HG21	1.93	0.49
1:A:45:VAL:CG2	3:H:56:GLY:CA	2.90	0.49
4:N:38:GLN:O	4:N:84:ALA:HB1	2.12	0.49
2:B:593:LEU:HD21	2:D:594:LEU:HD23	1.94	0.49
1:C:97:VAL:HG13	1:C:166:ALA:HB3	1.95	0.49
3:M:12:VAL:HG13	3:M:13:GLN:H	1.71	0.49
2:B:513:PRO:O	2:B:555:ILE:HG21	2.13	0.49
3:Q:93:VAL:HG12	3:Q:95:TYR:CZ	2.47	0.49
4:N:139:TYR:HA	4:N:140:PRO:C	2.38	0.49
3:Q:207:VAL:O	3:Q:215:LYS:HA	2.13	0.49
3:H:10:THR:HB	3:H:18:LEU:CD2	2.39	0.49
4:L:109:VAL:HA	4:L:139:TYR:HB2	1.95	0.49
3:Q:12:VAL:CG2	3:Q:120:VAL:HG22	2.42	0.49
4:R:1:ASP:CB	4:R:94:SER:OG	2.61	0.49
2:B:527:ILE:HG12	4:N:94:SER:N	2.28	0.48
1:C:38:VAL:O	1:C:187:PRO:HG3	2.13	0.48
1:E:160:PHE:CE2	1:E:170:ILE:HG12	2.48	0.48
4:N:139:TYR:CE1	4:N:171:THR:HG22	2.48	0.48
1:A:184:LEU:HD21	2:B:558:LEU:CD1	2.42	0.48
2:B:529:LEU:HD21	4:N:32:TRP:CG	2.47	0.48
3:M:100:HIS:HB3	3:M:108:HIS:HB3	1.95	0.48
3:Q:156:PRO:HD2	3:Q:211:PRO:HG2	1.94	0.48
2:D:531:TRP:CZ3	2:D:532:ILE:CG2	2.91	0.48
4:L:165:GLN:HG2	4:L:172:TYR:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:TYR:HB2	1:A:165:LEU:O	2.14	0.48
1:C:33:ILE:HB	2:D:588:LYS:CE	2.43	0.48
3:M:67:ARG:HB2	3:M:85:SER:HB2	1.94	0.48
1:E:99:TYR:CZ	1:E:161:LEU:HD22	2.49	0.48
3:M:83:MET:HB3	3:M:86:LEU:HD21	1.94	0.48
3:Q:91:THR:HG23	3:Q:119:THR:HA	1.94	0.48
3:H:64:VAL:HB	3:H:68:PHE:CD2	2.48	0.48
2:B:527:ILE:HG12	4:N:94:SER:HA	1.96	0.48
2:F:572:PHE:CE2	2:F:584:ILE:HG12	2.48	0.48
4:N:108:THR:O	4:N:139:TYR:CD2	2.66	0.48
3:Q:14:PRO:HD3	3:Q:122:SER:HB2	1.96	0.48
4:R:90:GLN:NE2	4:R:94:SER:O	2.47	0.48
4:N:10:THR:O	4:R:203:PRO:HD2	2.14	0.48
1:C:33:ILE:HB	2:D:588:LYS:HE3	1.95	0.48
3:Q:147:LEU:HD13	3:Q:220:VAL:HG21	1.94	0.48
4:N:4:LEU:HD12	4:N:4:LEU:C	2.39	0.47
6:I:3:BMA:H62	6:I:5:MAN:H2	1.49	0.47
1:C:99:TYR:HD2	1:C:101:ALA:O	1.97	0.47
3:Q:4:LEU:HD23	3:Q:24:ALA:HA	1.95	0.47
1:A:165:LEU:HG	2:D:577:THR:HG21	1.97	0.47
2:B:560:GLN:HG2	3:H:103:TRP:CZ2	2.49	0.47
2:B:563:ASN:ND2	3:H:103:TRP:CZ3	2.82	0.47
2:B:567:GLN:HA	2:F:531:TRP:CD2	2.49	0.47
2:B:571:LEU:CD1	2:F:526:ALA:HB2	2.44	0.47
1:A:130:ARG:HD3	1:A:163:ASP:OD2	2.14	0.47
3:Q:135:PRO:HG2	3:Q:222:PRO:HB3	1.95	0.47
3:Q:163:TRP:O	3:Q:164:ASN:C	2.55	0.47
2:B:551:GLN:HG2	2:B:554:LEU:CG	2.45	0.47
2:D:511:CYS:O	2:D:513:PRO:HD3	2.15	0.47
1:E:98:ASN:HB3	2:F:582:PHE:CE2	2.50	0.47
3:H:4:LEU:HA	3:H:23:ALA:O	2.15	0.47
3:H:40:ALA:HB3	3:H:43:LYS:HB2	1.96	0.47
2:D:531:TRP:CZ3	1:E:156:GLU:O	2.67	0.47
5:G:3:BMA:H62	5:G:6:MAN:H2	1.49	0.47
3:H:61:ALA:HB3	3:H:64:VAL:CG2	2.44	0.47
4:N:106:LYS:HD2	4:N:140:PRO:HA	1.97	0.47
3:Q:60:TYR:CZ	3:Q:70:ILE:HG22	2.49	0.47
1:E:89:ARG:HA	1:E:149:GLU:HG3	1.97	0.47
3:M:63:SER:O	3:M:67:ARG:NH1	2.47	0.47
2:D:554:LEU:C	2:D:554:LEU:CD2	2.85	0.46
4:L:200:LEU:HD13	4:L:204:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:131:PHE:HB3	4:N:120:SER:OG	2.15	0.46
4:N:78:LEU:HD12	4:N:82:ASP:OD2	2.15	0.46
4:N:118:PRO:HB3	4:N:208:PHE:CE2	2.51	0.46
1:C:51:LEU:HD21	2:D:596:ARG:HG2	1.98	0.46
3:H:202:THR:HB	3:H:219:LYS:HE3	1.96	0.46
3:M:101:ARG:CZ	6:I:3:BMA:H61	2.46	0.46
1:A:69:ASN:ND2	1:A:105:ALA:HB2	2.30	0.46
2:B:570:GLN:HB2	2:F:531:TRP:HB2	1.97	0.46
1:C:65:SER:HB3	2:D:585:LEU:HD21	1.96	0.46
2:D:554:LEU:HD23	2:D:554:LEU:O	2.16	0.46
1:E:57:LEU:CD1	1:E:62:GLN:NE2	2.45	0.46
3:M:101:ARG:NH1	6:I:3:BMA:C5	2.78	0.46
4:N:110:ALA:N	4:N:139:TYR:O	2.43	0.46
1:C:111:LEU:HD12	1:C:170:ILE:HG21	1.97	0.46
1:E:35:LEU:HD21	1:E:185:ILE:HD11	1.97	0.46
3:H:51:ILE:HD13	3:H:72:ARG:HG2	1.97	0.46
3:M:14:PRO:HD3	3:M:122:SER:CB	2.46	0.46
3:Q:29:PHE:CD2	3:Q:77:ASN:HA	2.51	0.46
4:R:48:ILE:HG13	4:R:54:LEU:HD23	1.96	0.46
4:N:33:LEU:CD2	4:N:71:PHE:CD1	2.93	0.46
2:B:572:PHE:O	2:B:576:THR:HG22	2.16	0.46
4:R:141:ARG:HB2	4:R:172:TYR:CE1	2.50	0.46
2:B:570:GLN:HG3	2:F:531:TRP:HE3	1.80	0.46
2:F:588:LYS:HA	2:F:588:LYS:HD3	1.74	0.46
3:H:128:PRO:HB2	3:H:151:VAL:HG13	1.98	0.46
1:E:162:TYR:HB2	1:E:165:LEU:O	2.15	0.46
3:H:91:THR:HG23	3:H:119:THR:HA	1.97	0.46
3:Q:67:ARG:HD2	3:Q:85:SER:HB2	1.97	0.46
1:A:70:LEU:N	1:A:178:GLU:O	2.44	0.46
4:L:109:VAL:HA	4:L:139:TYR:CB	2.46	0.46
1:E:113:ILE:CG2	1:E:121:CYS:HB2	2.44	0.45
1:C:182:ALA:HB2	2:D:562:ALA:CA	2.46	0.45
3:Q:14:PRO:HD3	3:Q:122:SER:CB	2.45	0.45
2:B:531:TRP:HB2	2:D:570:GLN:HB2	1.97	0.45
2:B:564:GLU:OE1	3:H:52:SER:HB2	2.17	0.45
2:F:537:PRO:HG2	2:F:542:ILE:HG22	1.97	0.45
3:Q:128:PRO:HB2	3:Q:151:VAL:HG13	1.99	0.45
3:Q:154:TYR:HB2	3:Q:209:HIS:CD2	2.52	0.45
1:E:34:PRO:HD2	2:F:565:THR:HG23	1.98	0.45
4:L:117:PHE:HA	4:L:118:PRO:HD3	1.72	0.45
4:N:4:LEU:HD13	4:N:23:CYS:SG	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:164:ASN:HB3	3:Q:167:ALA:HB3	1.99	0.45
2:D:596:ARG:HD3	2:D:609:CYS:SG	2.57	0.45
3:H:164:ASN:HB3	3:H:167:ALA:HB3	1.98	0.45
3:M:10:THR:HB	3:M:18:LEU:HD21	1.99	0.45
4:N:33:LEU:HD12	4:N:89:GLN:O	2.17	0.45
4:N:106:LYS:O	4:N:106:LYS:HG3	2.17	0.45
3:Q:69:THR:O	3:Q:81:LEU:HD12	2.17	0.45
1:C:86:TRP:CD1	1:C:154:HIS:ND1	2.85	0.45
1:A:34:PRO:HB2	2:B:561:LEU:HD11	1.99	0.45
2:B:551:GLN:HG2	2:B:554:LEU:HB2	1.97	0.45
2:B:587:ARG:HG3	1:E:60:THR:HG21	1.99	0.45
1:C:49:ASP:OD1	1:C:50:LYS:N	2.50	0.45
3:H:94:TYR:HE1	3:H:118:VAL:HB	1.81	0.45
3:M:67:ARG:HD2	3:M:85:SER:O	2.17	0.45
1:C:70:LEU:HD12	1:C:178:GLU:OE1	2.17	0.45
4:L:4:LEU:C	4:L:4:LEU:CD1	2.85	0.45
3:M:128:PRO:HB2	3:M:151:VAL:HG13	1.98	0.45
3:M:178:VAL:HG22	3:M:186:SER:O	2.16	0.45
1:C:132:PHE:HB3	1:C:135:CYS:SG	2.57	0.45
2:D:531:TRP:CE2	2:D:532:ILE:HG23	2.51	0.45
1:A:41:ASN:CG	7:A:201:NAG:H81	2.41	0.44
1:A:133:PRO:HB3	2:B:543:TYR:CE2	2.52	0.44
3:M:2:VAL:N	3:M:26:GLY:HA3	2.32	0.44
4:R:13:ALA:O	4:R:105:ILE:HA	2.17	0.44
1:C:37:VAL:HG22	1:C:44:GLN:O	2.17	0.44
4:R:33:LEU:HD13	4:R:34:ALA:N	2.33	0.44
3:M:6:GLN:HE22	3:M:36:TRP:HZ3	1.66	0.44
4:N:166:ASP:HB2	4:N:169:ASP:OD1	2.16	0.44
3:M:160:THR:OG1	3:M:208:ASN:HB3	2.17	0.44
3:Q:155:PHE:HA	3:Q:156:PRO:HA	1.76	0.44
4:R:63:SER:O	4:R:73:LEU:HD12	2.18	0.44
1:A:54:ARG:O	1:A:55:ASP:C	2.60	0.44
2:B:578:GLU:HG3	2:F:582:PHE:CE1	2.52	0.44
2:D:515:LEU:HB2	2:D:555:ILE:HD12	1.98	0.44
1:E:130:ARG:HH21	1:E:164:ARG:HH11	1.65	0.44
4:N:33:LEU:HD23	4:N:71:PHE:CG	2.46	0.44
2:D:521:GLN:HE21	2:D:524:GLY:C	2.25	0.44
3:M:13:GLN:HB3	3:M:14:PRO:HD2	1.99	0.44
4:R:39:LYS:HG2	4:R:84:ALA:HB2	1.99	0.44
1:C:35:LEU:HD21	1:C:185:ILE:HD11	2.00	0.44
1:C:45:VAL:CG2	3:M:54:LEU:HG	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:123:GLN:O	4:N:126:SER:OG	2.27	0.44
1:A:191:LYS:HE2	3:M:65:LYS:NZ	2.32	0.44
2:B:539:ALA:O	2:B:542:ILE:HG12	2.17	0.44
2:B:567:GLN:HG3	2:F:531:TRP:CD1	2.53	0.44
3:Q:152:LYS:HG2	3:Q:153:ASP:OD1	2.17	0.44
7:B:701:NAG:C8	2:F:531:TRP:HH2	2.30	0.44
1:C:94:PRO:CB	1:C:169:ILE:HD12	2.39	0.44
4:L:166:ASP:HB2	4:L:169:ASP:OD1	2.17	0.44
3:Q:133:LEU:HD12	3:Q:148:GLY:HA3	2.00	0.44
2:B:527:ILE:HG12	4:N:93:SER:C	2.42	0.43
1:E:86:TRP:CD1	1:E:154:HIS:HD1	2.36	0.43
3:Q:160:THR:HG23	3:Q:208:ASN:HB3	2.00	0.43
2:D:548:MET:HE3	2:D:548:MET:HB3	1.92	0.43
3:Q:131:PHE:HB3	4:R:120:SER:OG	2.17	0.43
4:R:206:LYS:HA	4:R:206:LYS:HD3	1.83	0.43
3:Q:98:LYS:O	3:Q:109:PHE:HA	2.19	0.43
2:B:528:GLY:C	2:B:531:TRP:NE1	2.76	0.43
1:C:99:TYR:CZ	1:C:161:LEU:HD22	2.53	0.43
4:N:80:PRO:HA	4:N:83:PHE:CE2	2.52	0.43
2:B:523:GLU:OE1	2:B:526:ALA:HB2	2.17	0.43
2:D:563:ASN:HD21	6:I:1:NAG:C1	2.32	0.43
4:L:61:ARG:HD2	4:L:77:SER:O	2.19	0.43
3:M:17:SER:HA	3:M:83:MET:O	2.19	0.43
2:B:527:ILE:HG13	4:N:95:PRO:HD3	2.00	0.43
2:B:558:LEU:C	2:B:560:GLN:N	2.75	0.43
1:C:77:THR:OG1	1:C:107:ASN:ND2	2.52	0.43
1:E:78:ASP:OD1	1:E:78:ASP:N	2.51	0.43
4:N:154:GLN:HB3	4:N:157:ASN:ND2	2.27	0.43
2:B:531:TRP:CD2	2:D:567:GLN:HA	2.54	0.43
3:H:155:PHE:HA	3:H:156:PRO:HA	1.72	0.43
3:Q:12:VAL:HG21	3:Q:120:VAL:HG22	2.00	0.43
2:F:527:ILE:HG13	4:L:93:SER:HA	2.01	0.43
1:A:68:LEU:HD11	2:B:558:LEU:HG	2.01	0.43
4:R:202:SER:HA	4:R:203:PRO:HD2	1.89	0.43
1:E:69:ASN:ND2	1:E:105:ALA:HB2	2.34	0.43
1:A:74:GLY:HA3	2:B:510:LYS:HB2	2.00	0.42
1:C:156:GLU:HG2	6:I:2:NAG:H61	2.01	0.42
2:D:521:GLN:HE21	2:D:524:GLY:HA3	1.82	0.42
1:E:33:ILE:HD11	2:F:572:PHE:CG	2.52	0.42
4:L:7:SER:OG	4:L:8:PRO:HD3	2.18	0.42
3:Q:68:PHE:CE1	3:Q:83:MET:HB3	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:517:TYR:CZ	2:B:546:GLY:HA3	2.54	0.42
2:B:592:PHE:CE2	2:B:596:ARG:NH1	2.79	0.42
1:C:88:PHE:CB	1:C:149:GLU:HB2	2.47	0.42
1:C:108:CYS:HB3	1:C:175:THR:CG2	2.50	0.42
1:A:51:LEU:HD13	2:B:595:GLN:CD	2.43	0.42
2:B:577:THR:HG21	1:E:164:ARG:O	2.19	0.42
4:L:2:ILE:HG21	4:L:27:GLN:CD	2.44	0.42
1:E:49:ASP:OD1	1:E:50:LYS:N	2.52	0.42
3:H:36:TRP:CZ2	3:H:79:LEU:HG	2.55	0.42
3:Q:36:TRP:CE2	3:Q:81:LEU:HB2	2.54	0.42
1:A:39:HIS:CB	1:A:44:GLN:HE22	2.32	0.42
4:N:61:ARG:HD2	4:N:77:SER:O	2.20	0.42
2:F:532:ILE:HA	2:F:533:PRO:HD3	1.86	0.42
3:H:157:GLU:HB3	3:H:158:PRO:HA	2.01	0.42
3:Q:61:ALA:HB3	3:Q:64:VAL:HG22	2.01	0.42
3:Q:91:THR:HG23	3:Q:118:VAL:O	2.20	0.42
2:F:531:TRP:CD1	2:F:531:TRP:H	2.37	0.42
3:M:12:VAL:CG2	3:M:18:LEU:HD22	2.50	0.42
3:Q:60:TYR:OH	3:Q:70:ILE:HG22	2.20	0.42
3:Q:140:THR:HB	3:Q:195:SER:CB	2.50	0.42
1:A:33:ILE:HA	1:A:34:PRO:HD3	1.75	0.42
1:A:39:HIS:HB2	1:A:44:GLN:HE22	1.85	0.42
1:E:132:PHE:HA	1:E:133:PRO:HD3	1.91	0.42
3:H:147:LEU:HD13	3:H:220:VAL:HG21	2.01	0.42
3:M:29:PHE:HE1	3:M:72:ARG:NH1	2.18	0.42
1:A:89:ARG:HB3	1:A:153:PHE:CD1	2.55	0.42
1:C:90:ALA:N	1:C:149:GLU:HG2	2.35	0.42
1:C:114:LYS:HE3	1:C:120:GLU:OE2	2.20	0.42
1:A:45:VAL:CG2	3:H:56:GLY:HA3	2.50	0.42
1:E:147:CYS:N	1:E:148:PRO:CD	2.82	0.42
1:E:151:TYR:CB	1:E:169:ILE:HD13	2.50	0.42
4:N:106:LYS:NZ	4:N:140:PRO:HB3	2.35	0.42
4:R:139:TYR:CE1	4:R:171:THR:HG22	2.55	0.42
1:A:51:LEU:HD11	2:B:596:ARG:CG	2.50	0.41
1:C:69:ASN:N	1:C:69:ASN:OD1	2.53	0.41
1:C:165:LEU:HD21	2:F:577:THR:OG1	2.20	0.41
2:D:561:LEU:HD13	3:M:54:LEU:CD2	2.50	0.41
4:L:4:LEU:HD21	4:L:88:CYS:O	2.19	0.41
4:L:139:TYR:CZ	4:L:171:THR:HG22	2.55	0.41
2:B:525:ALA:HB1	2:B:527:ILE:HD13	2.02	0.41
1:C:156:GLU:OE2	6:I:1:NAG:O3	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:530:ALA:HB1	2:D:537:PRO:HD3	2.02	0.41
3:H:161:VAL:HG11	3:H:189:SER:CB	2.51	0.41
4:N:78:LEU:HD11	4:N:82:ASP:HB2	2.02	0.41
1:C:45:VAL:HG11	3:M:56:GLY:CA	2.51	0.41
3:M:2:VAL:O	3:M:2:VAL:HG22	2.19	0.41
1:C:33:ILE:HA	1:C:34:PRO:HD3	1.87	0.41
1:C:45:VAL:HG11	3:M:56:GLY:HA3	2.02	0.41
1:E:182:ALA:HB2	2:F:562:ALA:CB	2.50	0.41
3:H:30:SER:HA	3:H:72:ARG:NH2	2.36	0.41
5:G:5:NAG:O7	5:G:5:NAG:H3	2.20	0.41
2:B:531:TRP:HB2	2:D:570:GLN:CB	2.49	0.41
2:B:551:GLN:CG	2:B:554:LEU:HB2	2.50	0.41
1:E:151:TYR:HB3	1:E:169:ILE:HD13	2.02	0.41
3:H:86:LEU:CB	3:H:120:VAL:HG11	2.51	0.41
4:N:61:ARG:CZ	4:N:79:GLN:HG3	2.51	0.41
1:A:147:CYS:N	1:A:148:PRO:CD	2.84	0.41
1:E:89:ARG:NE	1:E:90:ALA:O	2.53	0.41
3:H:14:PRO:HD3	3:H:122:SER:HB2	2.03	0.41
3:M:134:ALA:HA	3:M:135:PRO:HD3	1.75	0.41
4:R:139:TYR:HA	4:R:140:PRO:C	2.45	0.41
1:A:96:VAL:HB	2:B:580:ARG:HG2	2.02	0.41
2:D:532:ILE:HD12	2:D:535:PHE:CD2	2.52	0.41
2:F:527:ILE:CG1	4:L:93:SER:HA	2.51	0.41
3:H:208:ASN:OD1	3:H:215:LYS:HG2	2.21	0.41
1:E:33:ILE:HB	2:F:588:LYS:HE3	2.01	0.41
1:E:95:LYS:NZ	2:F:574:ARG:HA	2.36	0.41
1:E:125:ALA:HA	1:E:126:PRO:HD3	1.84	0.41
4:L:33:LEU:HD21	4:L:88:CYS:HB2	2.02	0.41
4:L:114:VAL:HG22	4:L:195:VAL:HG21	2.03	0.41
3:M:12:VAL:HG23	3:M:18:LEU:HD22	2.02	0.41
4:N:78:LEU:CD1	4:N:82:ASP:HB2	2.50	0.41
3:Q:45:LEU:HB2	4:R:97:PHE:CG	2.56	0.41
4:R:82:ASP:N	4:R:82:ASP:OD1	2.53	0.41
1:C:57:LEU:HD12	1:C:62:GLN:OE1	2.21	0.41
4:L:4:LEU:HD22	4:L:23:CYS:SG	2.61	0.41
4:L:37:GLN:HB2	4:L:86:TYR:HE1	1.86	0.41
3:M:12:VAL:HG12	3:M:13:GLN:O	2.21	0.41
3:Q:64:VAL:HB	3:Q:68:PHE:CD2	2.56	0.41
3:Q:102:VAL:HG21	3:Q:106:GLY:CA	2.51	0.41
2:B:527:ILE:HG12	4:N:94:SER:CA	2.51	0.40
1:C:72:GLY:HA3	2:D:559:ARG:HH22	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:PRO:O	1:C:95:LYS:HD3	2.21	0.40
4:L:202:SER:HA	4:L:203:PRO:HD2	1.89	0.40
4:N:39:LYS:HG2	4:N:84:ALA:HB2	2.03	0.40
2:B:512:ASN:HA	2:B:513:PRO:HD3	1.87	0.40
1:C:56:LYS:HG2	2:F:599:GLY:HA2	2.03	0.40
1:C:148:PRO:HB2	1:C:149:GLU:OE1	2.20	0.40
1:C:161:LEU:HD23	1:C:161:LEU:HA	1.92	0.40
2:F:529:LEU:HD21	3:H:106:GLY:HA2	2.04	0.40
3:M:29:PHE:CE1	3:M:72:ARG:HD2	2.56	0.40
1:C:95:LYS:HB3	2:D:573:LEU:HB3	2.04	0.40
3:M:101:ARG:CZ	6:I:3:BMA:C6	2.99	0.40
3:Q:36:TRP:CZ2	3:Q:79:LEU:HG	2.56	0.40
1:A:194:PHE:CE1	2:B:519:THR:HG21	2.57	0.40
2:D:537:PRO:HD2	2:F:574:ARG:NH2	2.37	0.40
1:E:52:VAL:HB	1:E:55:ASP:OD2	2.21	0.40
3:H:6:GLN:HE22	3:H:95:TYR:HA	1.87	0.40
4:L:154:GLN:HB3	4:L:157:ASN:HD21	1.86	0.40
3:Q:71:SER:O	3:Q:79:LEU:HD12	2.22	0.40
2:B:531:TRP:CE3	2:D:570:GLN:HG3	2.56	0.40
1:C:183:PHE:O	1:C:184:LEU:HD12	2.21	0.40
1:E:149:GLU:HA	1:E:149:GLU:OE1	2.22	0.40
3:M:128:PRO:HB3	3:M:154:TYR:HB3	2.03	0.40
4:N:185:TYR:CZ	4:N:210:ARG:HG3	2.57	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)
2:D:527:ILE:CB	4:R:93:SER:O[2_565]	1.99	0.21

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	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
1	C	156/162 (96%)	152 (97%)	4 (3%)	0	100	100
1	E	153/162 (94%)	147 (96%)	6 (4%)	0	100	100
2	B	102/111 (92%)	96 (94%)	6 (6%)	0	100	100
2	D	102/111 (92%)	98 (96%)	4 (4%)	0	100	100
2	F	101/111 (91%)	97 (96%)	4 (4%)	0	100	100
3	H	209/233 (90%)	204 (98%)	5 (2%)	0	100	100
3	M	213/233 (91%)	206 (97%)	7 (3%)	0	100	100
3	Q	220/233 (94%)	214 (97%)	6 (3%)	0	100	100
4	L	206/213 (97%)	198 (96%)	8 (4%)	0	100	100
4	N	210/213 (99%)	201 (96%)	9 (4%)	0	100	100
4	R	209/213 (98%)	205 (98%)	4 (2%)	0	100	100
All	All	2041/2157 (95%)	1974 (97%)	67 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	135/135 (100%)	135 (100%)	0	100	100
1	C	130/135 (96%)	130 (100%)	0	100	100
1	E	128/135 (95%)	128 (100%)	0	100	100
2	B	84/91 (92%)	84 (100%)	0	100	100
2	D	84/91 (92%)	83 (99%)	1 (1%)	63	73
2	F	84/91 (92%)	84 (100%)	0	100	100
3	H	176/194 (91%)	176 (100%)	0	100	100
3	M	180/194 (93%)	180 (100%)	0	100	100
3	Q	183/194 (94%)	183 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L	184/187 (98%)	184 (100%)	0	100	100
4	N	186/187 (100%)	186 (100%)	0	100	100
4	R	185/187 (99%)	185 (100%)	0	100	100
All	All	1739/1821 (96%)	1738 (100%)	1 (0%)	88	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	601	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	HIS
2	B	521	GLN
2	B	563	ASN
2	B	567	GLN
1	C	62	GLN
1	C	107	ASN
2	D	521	GLN
1	E	39	HIS
1	E	62	GLN
3	H	6	GLN
4	L	37	GLN
3	M	100	HIS
3	M	180	GLN
4	N	159	GLN
3	Q	13	GLN
3	Q	108	HIS

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 i

11 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	G	1	5	14,14,15	0.36	0	17,19,21	0.47	0
5	NAG	G	2	5	14,14,15	0.33	0	17,19,21	0.52	0
5	BMA	G	3	5	11,11,12	0.62	0	15,15,17	0.91	1 (6%)
5	MAN	G	4	5	11,11,12	0.74	0	15,15,17	1.18	2 (13%)
5	NAG	G	5	5	14,14,15	0.32	0	17,19,21	1.07	1 (5%)
5	MAN	G	6	5	11,11,12	0.93	1 (9%)	15,15,17	1.06	2 (13%)
6	NAG	I	1	6	14,14,15	0.37	0	17,19,21	0.46	0
6	NAG	I	2	6	14,14,15	0.34	0	17,19,21	0.53	0
6	BMA	I	3	6	11,11,12	0.62	0	15,15,17	0.90	1 (6%)
6	MAN	I	4	6	11,11,12	0.73	0	15,15,17	1.18	2 (13%)
6	MAN	I	5	6	11,11,12	0.92	1 (9%)	15,15,17	1.07	2 (13%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	6	MAN	C1-C2	2.62	1.58	1.52
6	I	5	MAN	C1-C2	2.58	1.58	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	5	NAG	C2-N2-C7	3.65	127.79	122.90
5	G	4	MAN	C1-O5-C5	3.27	116.57	112.19
6	I	4	MAN	C1-O5-C5	3.26	116.56	112.19
5	G	3	BMA	C1-O5-C5	2.55	115.60	112.19
6	I	3	BMA	C1-O5-C5	2.52	115.56	112.19
5	G	4	MAN	O2-C2-C3	-2.42	105.14	110.15
6	I	4	MAN	O2-C2-C3	-2.41	105.16	110.15
5	G	6	MAN	C1-O5-C5	2.30	115.26	112.19
6	I	5	MAN	C1-O5-C5	2.29	115.26	112.19
6	I	5	MAN	O2-C2-C3	-2.26	105.47	110.15
5	G	6	MAN	O2-C2-C3	-2.25	105.50	110.15

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	5	NAG	C3-C2-N2-C7
5	G	3	BMA	C4-C5-C6-O6
6	I	3	BMA	C4-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
6	I	3	BMA	O5-C5-C6-O6
5	G	5	NAG	O5-C5-C6-O6
5	G	4	MAN	O5-C5-C6-O6
6	I	4	MAN	O5-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
5	G	5	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 22 short contacts:

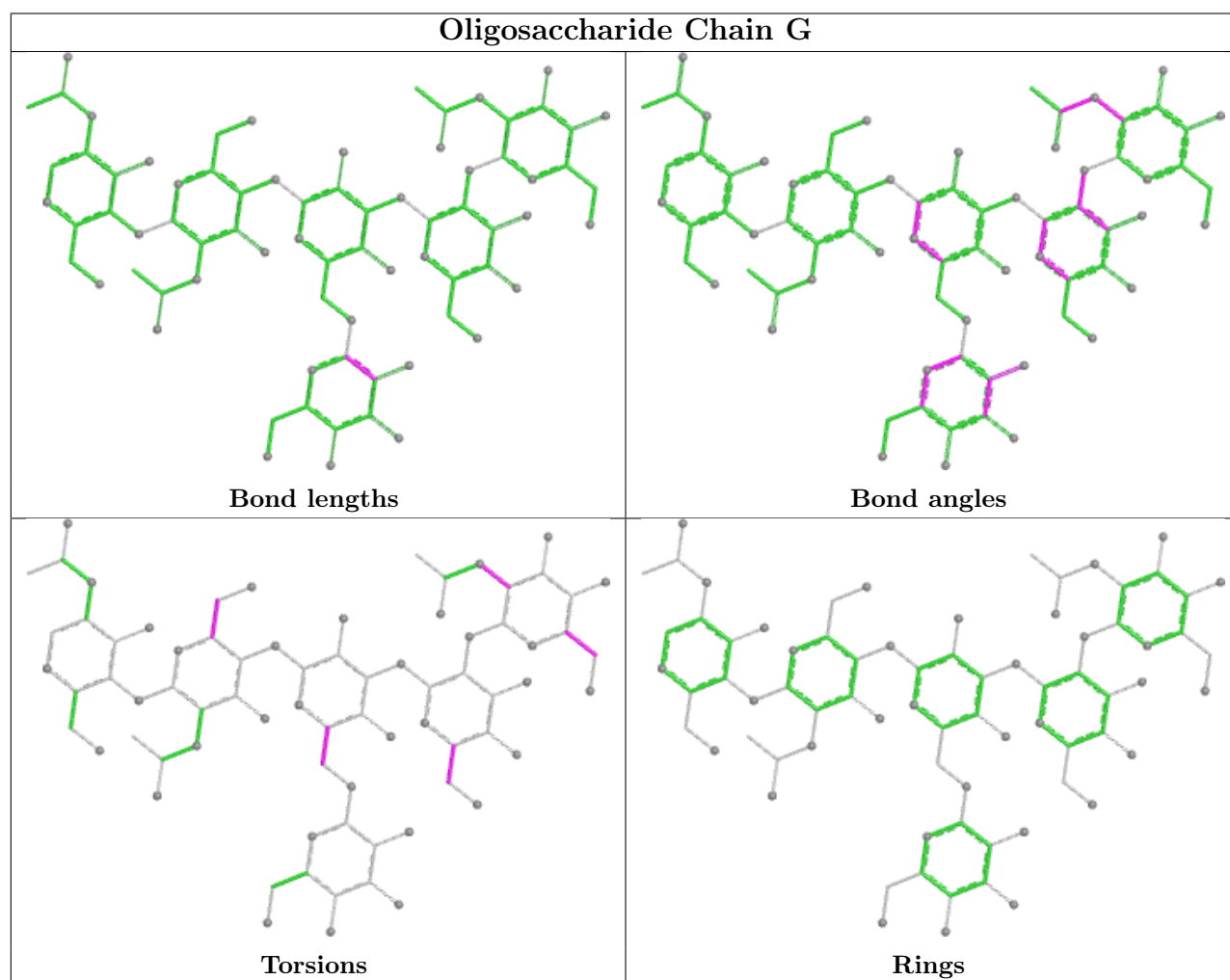
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	1	NAG	8	0
6	I	5	MAN	1	0

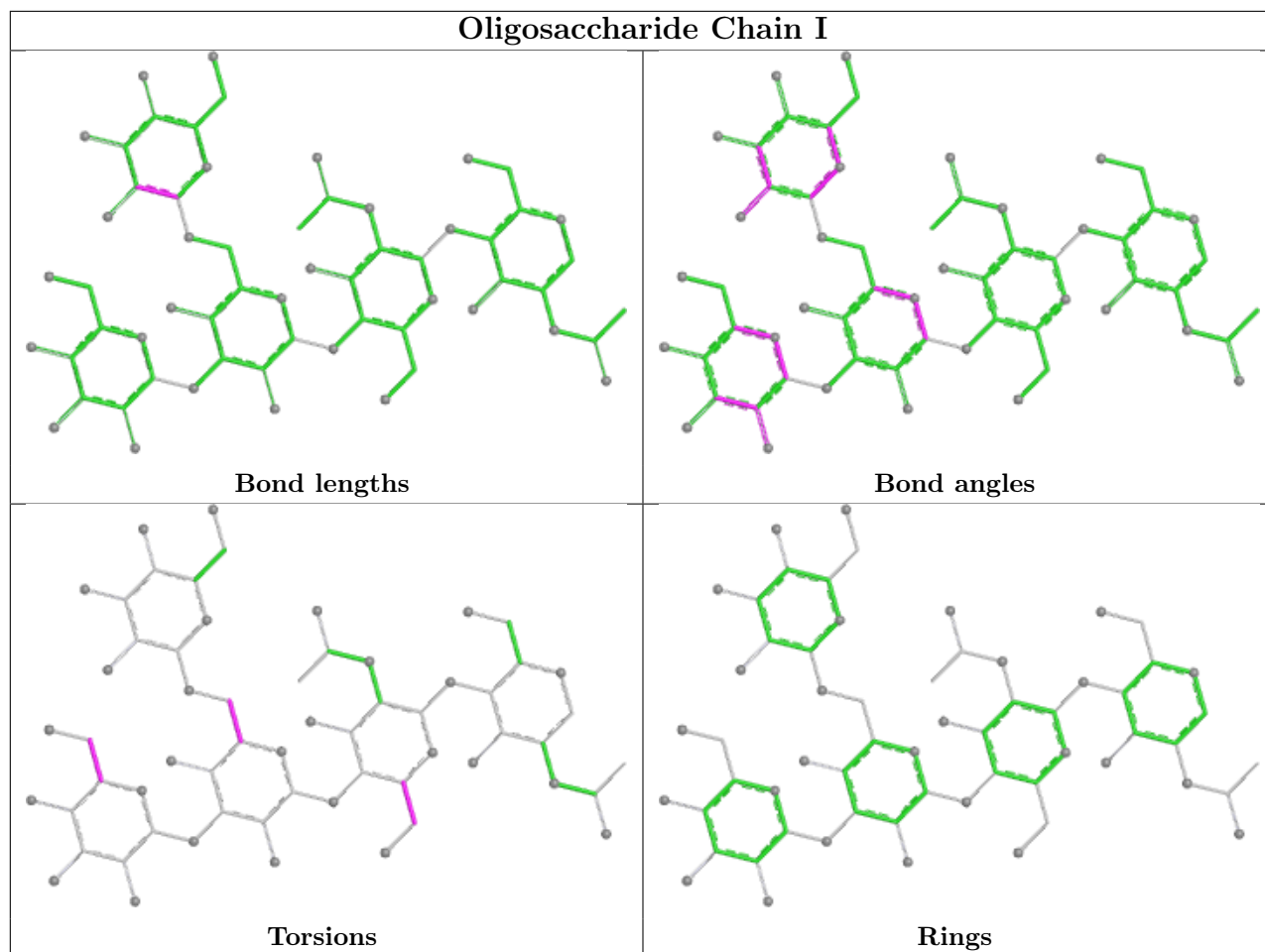
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	1	NAG	3	0
5	G	5	NAG	1	0
5	G	3	BMA	1	0
6	I	3	BMA	7	0
6	I	2	NAG	1	0
5	G	2	NAG	1	0
5	G	6	MAN	1	0

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





5.6 Ligand geometry [i](#)

2 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	701	-	14,14,15	0.39	0	17,19,21	0.49	0
7	NAG	A	201	1	14,14,15	0.38	0	17,19,21	0.47	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
7	NAG	B	701	-	-	2/6/23/26	0/1/1/1
7	NAG	A	201	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	701	NAG	O5-C5-C6-O6
7	B	701	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	701	NAG	4	0
7	A	201	NAG	7	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

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	162/162 (100%)	-0.42	1 (0%) 85 73	98, 203, 245, 274	0
1	C	158/162 (97%)	-0.51	1 (0%) 85 73	30, 196, 237, 291	0
1	E	155/162 (95%)	-0.42	3 (1%) 66 53	95, 221, 252, 315	0
2	B	104/111 (93%)	-0.54	1 (0%) 79 64	129, 206, 258, 272	0
2	D	104/111 (93%)	-0.29	1 (0%) 79 64	105, 194, 260, 298	0
2	F	103/111 (92%)	-0.35	2 (1%) 66 53	130, 214, 267, 293	0
3	H	213/233 (91%)	-0.54	2 (0%) 81 67	160, 219, 253, 265	0
3	M	217/233 (93%)	-0.53	2 (0%) 81 67	157, 187, 223, 253	0
3	Q	222/233 (95%)	-0.57	0 100 100	157, 195, 227, 256	0
4	L	210/213 (98%)	-0.49	2 (0%) 79 64	197, 236, 260, 267	0
4	N	212/213 (99%)	-0.47	1 (0%) 87 75	30, 187, 215, 232	0
4	R	211/213 (99%)	-0.44	1 (0%) 87 75	156, 190, 220, 243	0
All	All	2071/2157 (96%)	-0.48	17 (0%) 82 69	30, 203, 251, 315	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	558	LEU	5.6
3	M	48	VAL	5.2
4	L	47	LEU	5.0
3	M	107	TYR	4.4
4	R	132	VAL	4.4
2	F	558	LEU	4.3
1	A	68	LEU	3.6
1	C	68	LEU	3.3
3	H	149	CYS	3.2
1	E	66	VAL	3.0
3	H	189	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	528	GLY	2.6
2	B	558	LEU	2.5
1	E	181	VAL	2.3
4	L	105	ILE	2.1
4	N	21	ILE	2.1
1	E	42	THR	2.0

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

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

6.3 Carbohydrates [i](#)

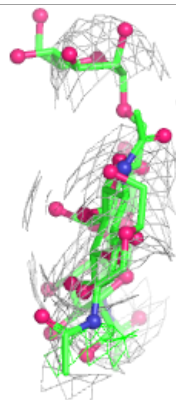
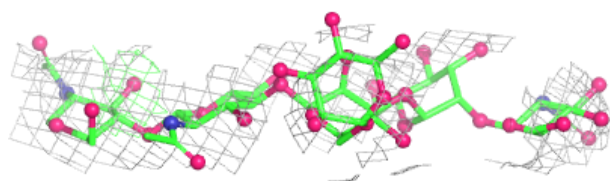
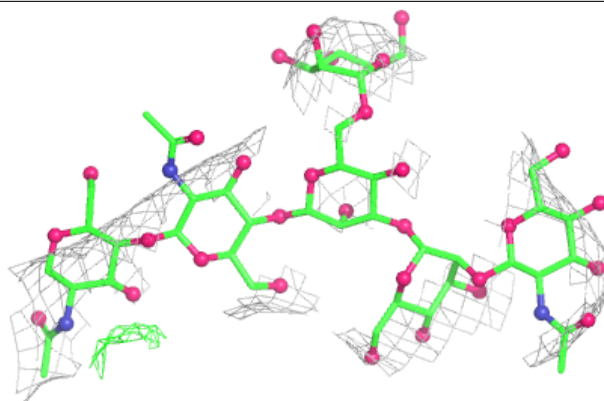
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	G	1	14/15	-	-	152,172,182,183	0
5	NAG	G	2	14/15	-	-	194,201,218,220	0
5	BMA	G	3	11/12	-	-	194,203,224,231	0
5	MAN	G	4	11/12	-	-	178,189,203,209	0
5	NAG	G	5	14/15	-	-	163,213,218,220	0
5	MAN	G	6	11/12	-	-	158,242,249,266	0
6	NAG	I	1	14/15	-	-	152,172,182,183	0
6	NAG	I	2	14/15	-	-	194,201,218,220	0
6	BMA	I	3	11/12	-	-	194,203,224,231	0
6	MAN	I	4	11/12	-	-	178,189,203,209	0
6	MAN	I	5	11/12	-	-	158,242,249,266	0

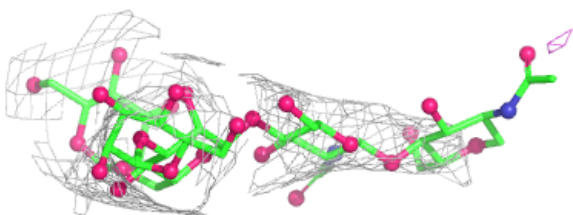
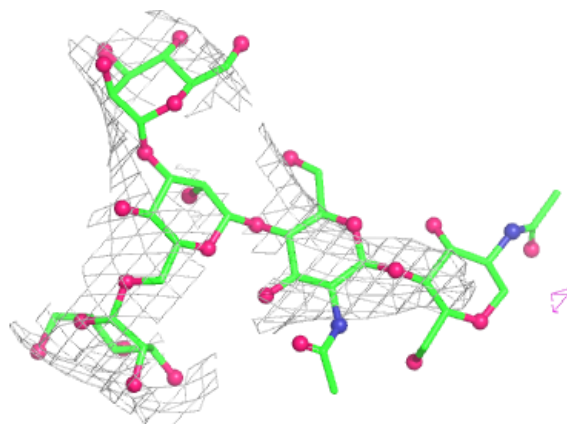
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

**Electron density around Chain I:**

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



6.4 Ligands [i](#)

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
7	NAG	A	201	14/15	0.34	0.08	152,172,182,183	0
7	NAG	B	701	14/15	0.68	0.15	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.