Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 06:53 PM EDT

PDB ID	:	4JTV
Title	:	Crystal structure of 2009 pandemic influenza virus hemagglutinin complexed with human receptor analogue LSTc
Authors	:	Zhang, W.; Shi, Y.; Qi, J.; Gao, F.; Li, Q.; Fan, Z.; Yan, J.; Gao, G.F.
Deposited on	:	2013-03-24
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

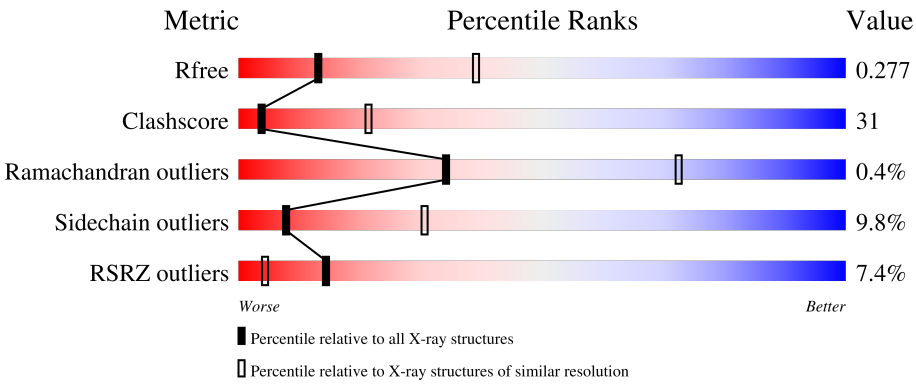
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	321	3% 48% 45% 7%
1	C	321	6% 52% 40% 7% •
1	E	321	2% 56% 38% 5% •
1	G	321	5% 60% 36% • •
1	I	321	3% 52% 40% 7% •

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Mol	Chain	Length	Quality of chain
1	K	321	6% 55% 40%
2	B	162	9% 59% 36% 6%
2	D	162	9% 60% 34% 6%
2	F	162	17% 66% 28% 5%
2	H	162	10% 61% 35%
2	J	162	2% 62% 35%
2	L	162	35% 51% 43% 6%
3	M	3	67% 33%
3	Q	3	67% 33%
3	R	3	67% 33%
4	N	4	75% 25%
4	P	4	75% 25%
5	O	2	100%

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
6	NAG	G	601	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 23528 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.

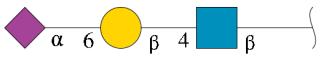
- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	321	2505	1584	433	477	11	0	0	0
1	C	321	2509	1586	433	479	11	0	0	0
1	E	321	2509	1586	433	479	11	0	0	0
1	G	321	2505	1584	433	477	11	0	0	0
1	I	321	2510	1587	433	479	11	0	0	0
1	K	321	2509	1586	433	479	11	0	0	0

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	162	1305	822	220	257	6	0	0	0
2	D	162	1300	818	219	257	6	0	0	0
2	F	161	1302	821	219	256	6	0	0	0
2	H	162	1305	822	220	257	6	0	0	0
2	J	162	1300	818	219	257	6	0	0	0
2	L	161	1302	821	219	256	6	0	0	0

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto pyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	M	3	45	25	2	18	0	0	0
3	Q	3	45	25	2	18	0	0	0
3	R	3	45	25	2	18	0	0	0

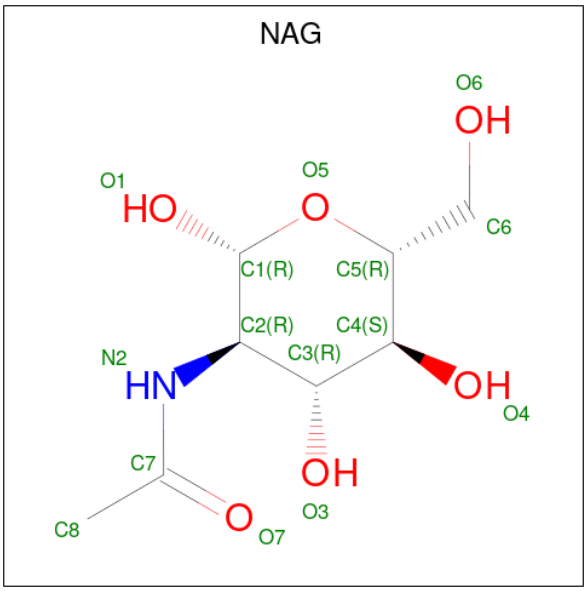
- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto pyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	N	4	56	31	2	23	0	0	0
4	P	4	56	31	2	23	0	0	0

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

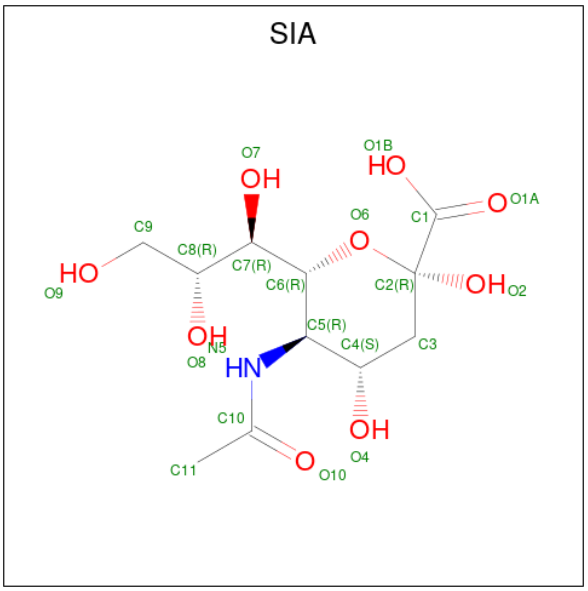
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	O	2	28	16	2	10	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	G	1	20	11	1	8	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	40	40	40	0	0
			Total	O		
8	B	13	13	13	0	0
			Total	O		
8	C	29	29	29	0	0
			Total	O		
8	D	13	13	13	0	0
			Total	O		
8	E	31	31	31	0	0
			Total	O		
8	F	7	7	7	0	0
			Total	O		
8	G	19	19	19	0	0
			Total	O		
8	H	13	13	13	0	0
			Total	O		
8	I	35	35	35	0	0
			Total	O		
8	J	18	18	18	0	0
			Total	O		
8	K	25	25	25	0	0

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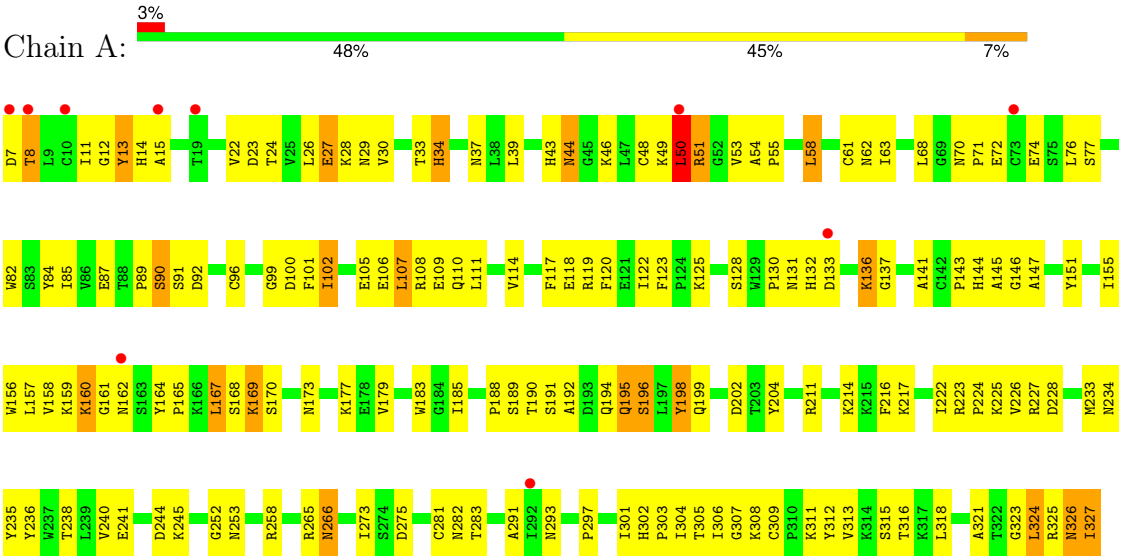
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	L	31	31	31	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

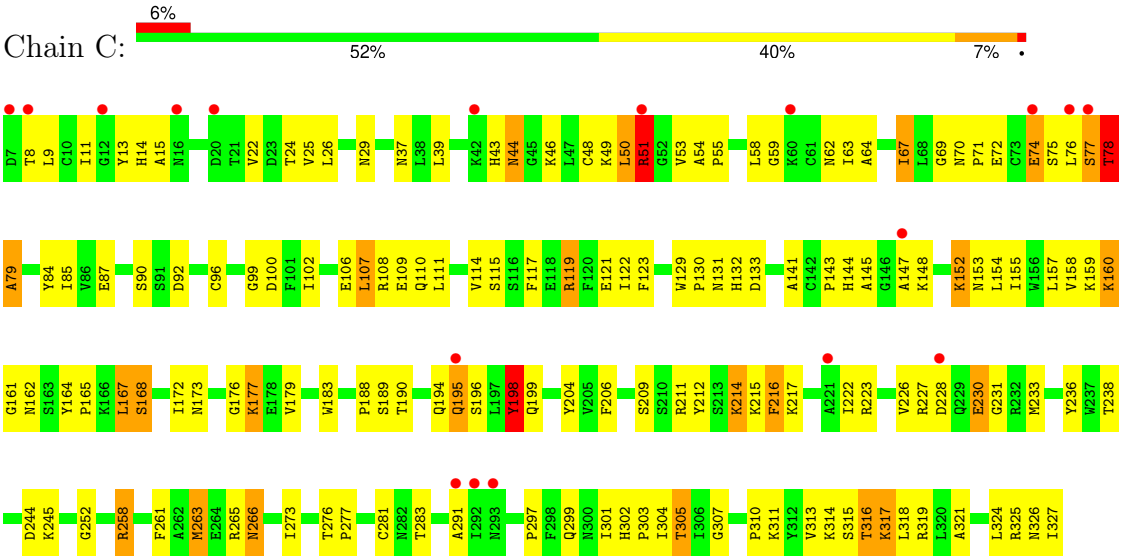
• Molecule 1: Hemagglutinin

Chain A:



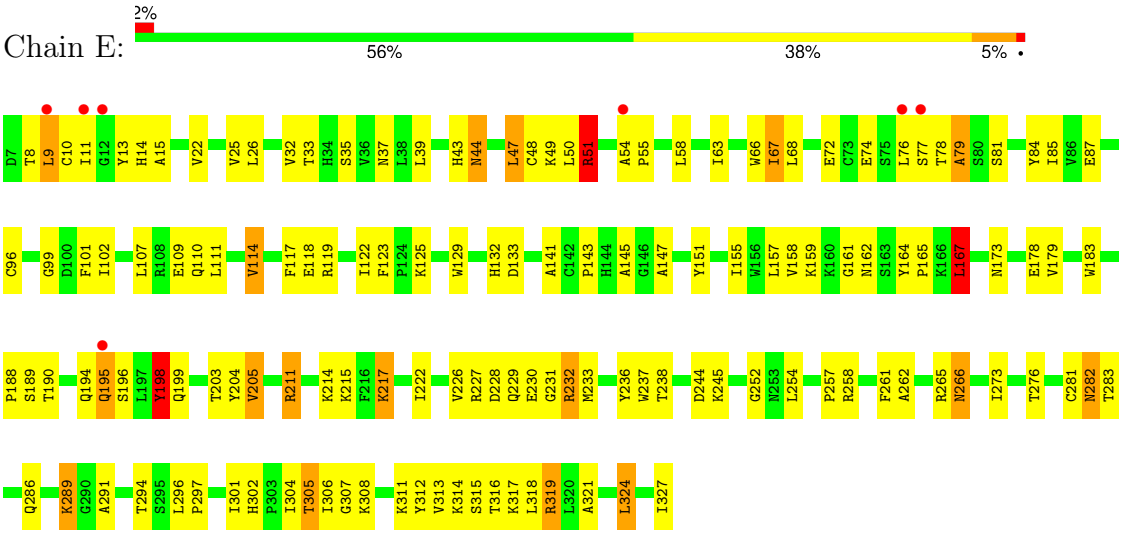
• Molecule 1: Hemagglutinin

Chain C:



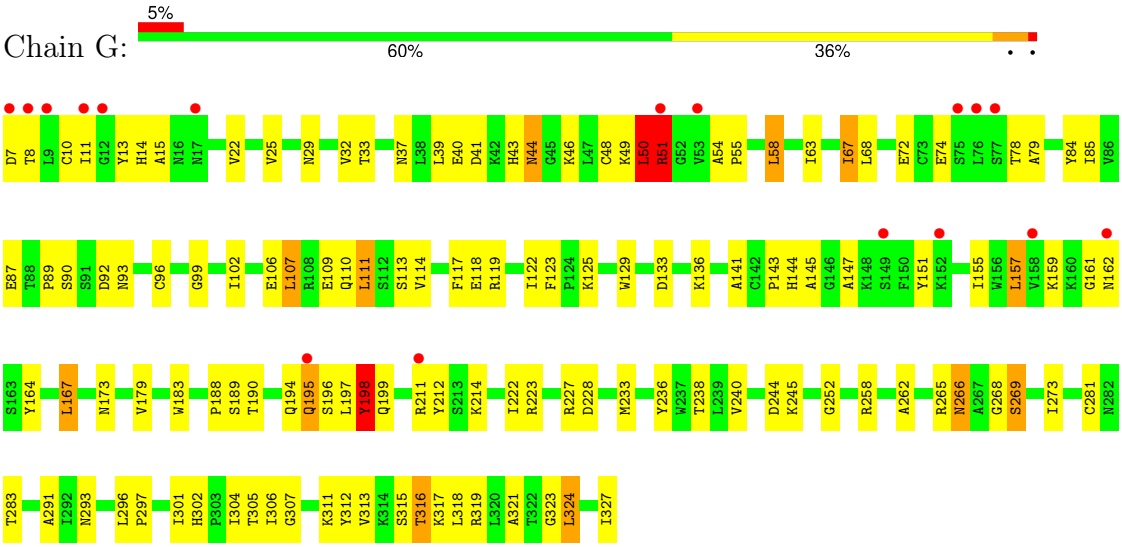
• Molecule 1: Hemagglutinin

Chain E:



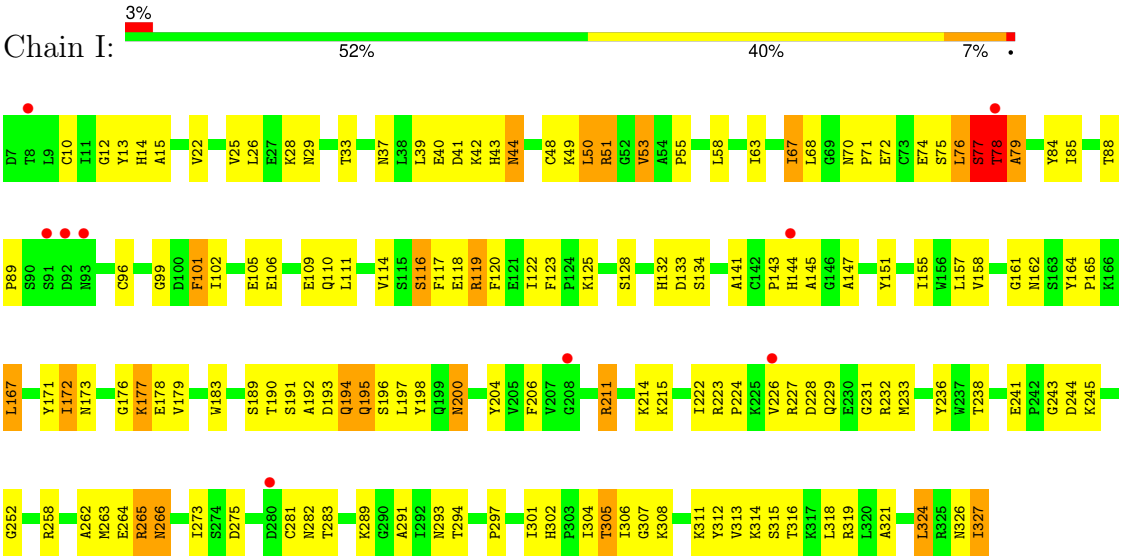
- Molecule 1: Hemagglutinin

Chain G:



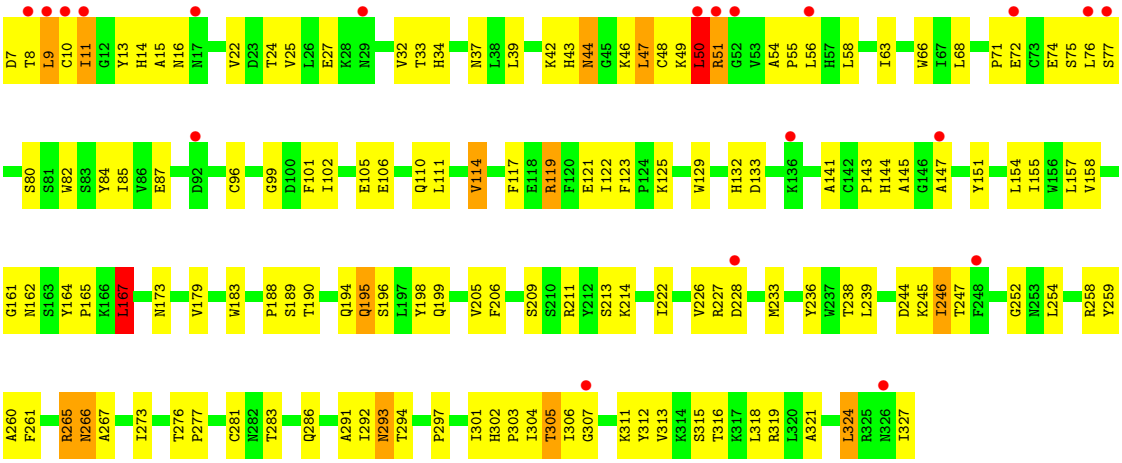
- Molecule 1: Hemagglutinin

Chain I:



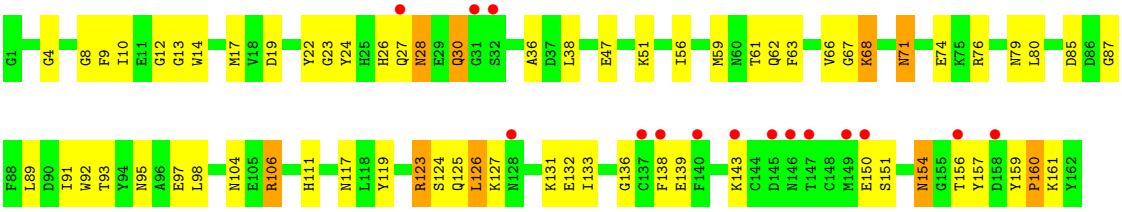
- Molecule 1: Hemagglutinin

Chain K:



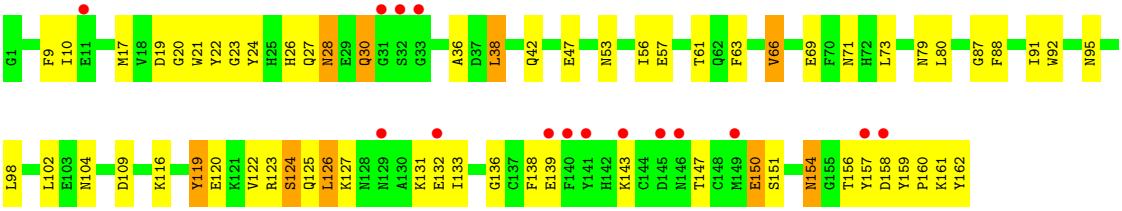
- Molecule 2: Hemagglutinin

Chain B:



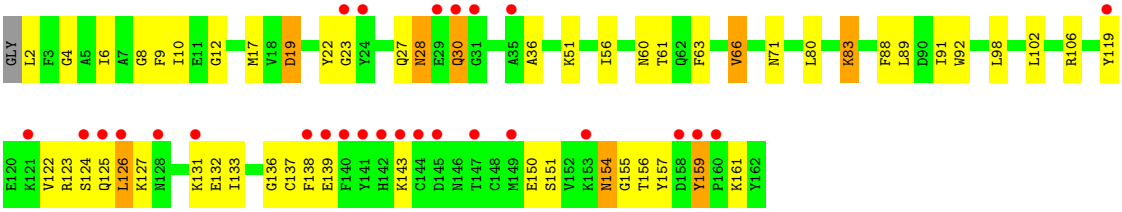
- Molecule 2: Hemagglutinin

Chain D:



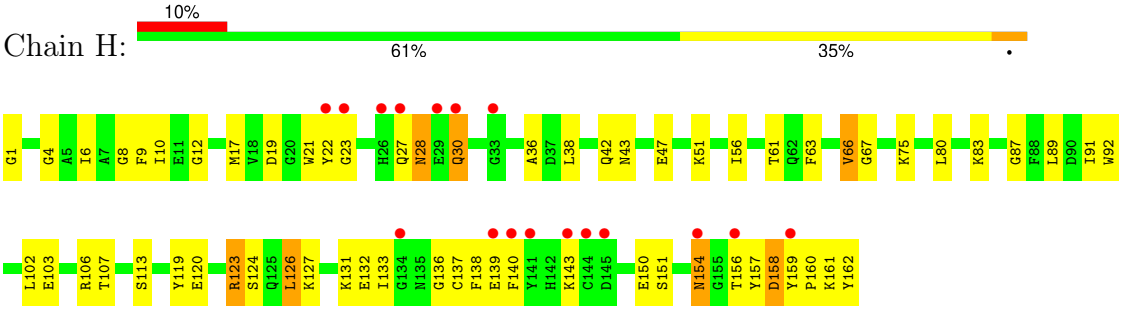
- Molecule 2: Hemagglutinin

Chain F:



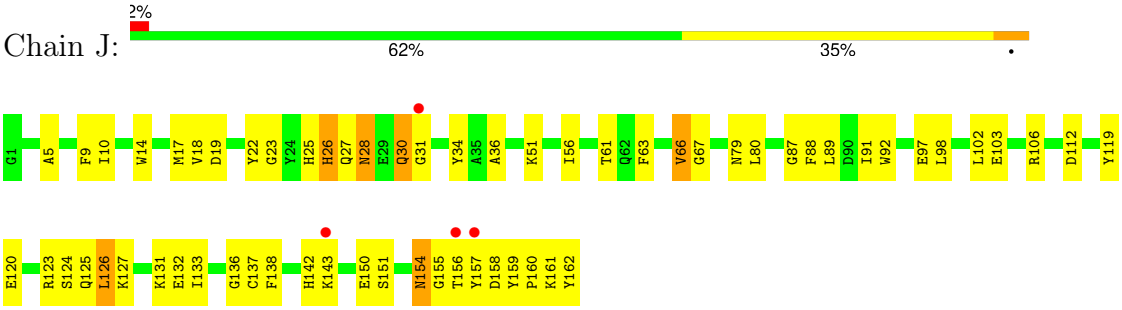
• Molecule 2: Hemagglutinin

Chain H:



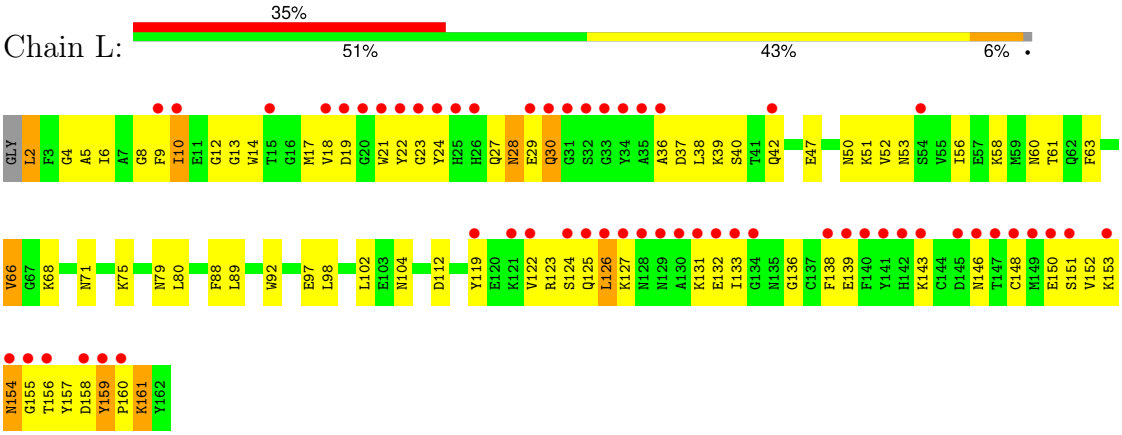
• Molecule 2: Hemagglutinin

Chain J:



• Molecule 2: Hemagglutinin

Chain L:

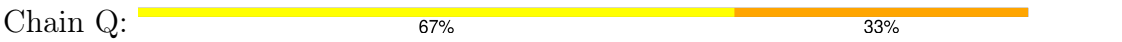


• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

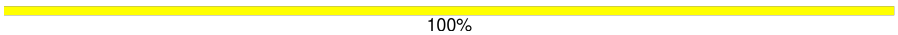
• Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain N:

• Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain P:

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

Chain O: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.72Å 117.32Å 117.39Å 61.78° 81.82° 77.42°	Depositor
Resolution (Å)	38.39 – 3.00 49.68 – 3.00	Depositor EDS
% Data completeness (in resolution range)	81.5 (38.39-3.00) 87.5 (49.68-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.224 , 0.275 0.229 , 0.277	Depositor DCC
R_{free} test set	2711 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	55.4	Xtriage
Anisotropy	0.701	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 58.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	23528	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SIA, NAG, GAL

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	0.57	0/2568	0.75	5/3488 (0.1%)
1	C	0.55	0/2572	0.69	8/3493 (0.2%)
1	E	0.39	0/2572	0.58	4/3493 (0.1%)
1	G	0.33	0/2568	0.77	9/3488 (0.3%)
1	I	0.47	0/2573	0.63	3/3495 (0.1%)
1	K	0.33	0/2572	0.63	5/3493 (0.1%)
2	B	0.48	0/1333	0.54	1/1797 (0.1%)
2	D	0.38	0/1328	0.45	0/1791
2	F	0.26	0/1330	0.46	0/1794
2	H	0.26	0/1333	0.49	1/1797 (0.1%)
2	J	0.43	0/1328	0.48	0/1791
2	L	0.26	0/1330	0.53	1/1794 (0.1%)
All	All	0.42	0/23407	0.62	37/31714 (0.1%)

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

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

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	119	ARG	NE-CZ-NH1	-16.56	112.02	120.30
1	A	119	ARG	NE-CZ-NH2	16.50	128.55	120.30
1	A	119	ARG	NE-CZ-NH1	-16.32	112.14	120.30
1	G	119	ARG	NE-CZ-NH2	15.97	128.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	212	TYR	N-CA-CB	11.91	132.04	110.60
1	G	211	ARG	CB-CA-C	-11.01	88.39	110.40
1	I	78	THR	N-CA-CB	-10.87	89.66	110.30
2	L	10	ILE	CB-CA-C	10.73	133.07	111.60
1	C	74	GLU	CB-CA-C	-10.72	88.96	110.40
1	C	78	THR	N-CA-CB	-9.71	91.85	110.30
1	G	50	LEU	CB-CA-C	-8.91	93.28	110.20
1	A	50	LEU	CB-CA-C	-8.80	93.47	110.20
1	C	50	LEU	CB-CA-C	-8.59	93.88	110.20
1	C	75	SER	N-CA-C	-8.45	88.19	111.00
1	I	119	ARG	NE-CZ-NH2	-8.39	116.10	120.30
1	K	119	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	A	119	ARG	CD-NE-CZ	8.15	135.01	123.60
1	G	119	ARG	CD-NE-CZ	8.06	134.89	123.60
1	K	119	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	I	119	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	C	198	TYR	N-CA-C	-7.07	91.92	111.00
1	E	51	ARG	N-CA-C	-7.04	91.98	111.00
1	C	51	ARG	N-CA-C	-6.90	92.38	111.00
1	C	212	TYR	CB-CA-C	-6.32	97.76	110.40
1	A	51	ARG	N-CA-C	-6.16	94.36	111.00
1	K	167	LEU	CA-CB-CG	5.94	128.97	115.30
1	E	167	LEU	CA-CB-CG	5.83	128.70	115.30
1	G	212	TYR	N-CA-C	-5.81	95.31	111.00
1	G	51	ARG	N-CA-C	-5.80	95.33	111.00
2	B	66	VAL	CB-CA-C	-5.77	100.43	111.40
1	G	198	TYR	N-CA-C	-5.77	95.42	111.00
2	H	66	VAL	CB-CA-C	-5.69	100.59	111.40
1	E	167	LEU	CB-CG-CD2	5.34	120.07	111.00
1	C	50	LEU	N-CA-C	5.18	125.00	111.00
1	K	167	LEU	CB-CG-CD2	5.10	119.67	111.00
1	E	198	TYR	N-CA-C	-5.04	97.38	111.00
1	K	50	LEU	CB-CA-C	-5.00	100.70	110.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	77	SER	Peptide

5.2 Too-close contacts (i)

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	2505	0	2444	227	0
1	C	2509	0	2451	186	0
1	E	2509	0	2451	159	4
1	G	2505	0	2445	137	0
1	I	2510	0	2456	183	0
1	K	2509	0	2452	188	0
2	B	1305	0	1228	97	0
2	D	1300	0	1216	81	0
2	F	1302	0	1226	65	0
2	H	1305	0	1228	73	0
2	J	1300	0	1216	89	0
2	L	1302	0	1226	126	4
3	M	45	0	38	4	0
3	Q	45	0	38	3	0
3	R	45	0	38	0	0
4	N	56	0	47	1	0
4	P	56	0	47	2	0
5	O	28	0	25	3	0
6	A	56	0	52	6	0
6	C	14	0	13	2	0
6	G	28	0	26	5	0
7	G	20	0	17	1	0
8	A	40	0	0	59	0
8	B	13	0	0	11	0
8	C	29	0	0	34	0
8	D	13	0	0	6	0
8	E	31	0	0	27	0
8	F	7	0	0	6	0
8	G	19	0	0	22	0
8	H	13	0	0	22	0
8	I	35	0	0	32	0
8	J	18	0	0	22	0
8	K	25	0	0	47	0
8	L	31	0	0	48	0
All	All	23528	0	22380	1414	4

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 31.

All (1414) 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:C:11:ILE:HD13	2:D:24:TYR:CD2	1.53	1.42
1:I:190:THR:HG21	1:I:193:ASP:OD1	1.24	1.35
1:K:106:GLU:HB3	8:K:915:HOH:O	1.20	1.34
2:L:19:ASP:HA	8:L:228:HOH:O	1.33	1.28
1:A:8:THR:HG22	2:B:138:PHE:O	1.18	1.27
1:A:8:THR:CG2	2:B:138:PHE:O	1.86	1.24
1:E:281:CYS:SG	8:E:709:HOH:O	1.92	1.23
2:L:56:ILE:HB	8:L:214:HOH:O	1.32	1.23
1:G:7:ASP:N	2:H:140:PHE:H	1.36	1.22
1:A:7:ASP:O	2:B:27:GLN:O	1.58	1.22
2:B:97:GLU:CB	8:B:213:HOH:O	1.88	1.22
1:K:122:ILE:HG22	8:K:914:HOH:O	1.40	1.20
1:C:258:ARG:HB3	8:C:717:HOH:O	1.34	1.20
1:I:145:ALA:HB3	8:I:903:HOH:O	1.44	1.17
1:I:190:THR:CG2	1:I:193:ASP:OD1	1.92	1.17
1:A:326:ASN:O	1:A:327:ILE:HG12	1.43	1.17
1:C:11:ILE:CD1	2:D:24:TYR:CD2	2.28	1.16
1:A:305:THR:CG2	1:A:309:CYS:SG	2.33	1.16
1:I:190:THR:HG23	1:I:193:ASP:N	1.60	1.16
1:E:178:GLU:OE1	1:E:265:ARG:NH1	1.77	1.16
1:A:108:ARG:HB2	8:A:734:HOH:O	0.98	1.15
1:C:11:ILE:CD1	2:D:24:TYR:CE2	2.27	1.15
1:K:14:HIS:CG	1:K:15:ALA:H	1.65	1.15
1:A:326:ASN:C	1:A:327:ILE:HG12	1.59	1.14
1:E:203:THR:O	1:E:217:LYS:HE2	1.46	1.13
2:L:38:LEU:C	8:L:207:HOH:O	1.86	1.12
1:E:66:TRP:HE1	1:E:77:SER:HB2	1.02	1.12
2:H:67:GLY:N	8:H:205:HOH:O	1.82	1.12
2:B:97:GLU:HB2	8:B:213:HOH:O	1.46	1.11
1:I:88:THR:HB	8:I:908:HOH:O	1.49	1.11
1:I:190:THR:CG2	1:I:193:ASP:H	1.62	1.11
1:K:14:HIS:CE1	1:K:15:ALA:O	2.04	1.11
1:K:162:ASN:OD1	1:K:199:GLN:NE2	1.81	1.10
2:L:39:LYS:N	8:L:207:HOH:O	1.82	1.09
2:L:4:GLY:C	8:L:216:HOH:O	1.91	1.08
1:A:8:THR:CG2	2:B:139:GLU:HA	1.82	1.08
1:K:56:LEU:CA	8:K:913:HOH:O	2.02	1.07
2:B:98:LEU:N	8:B:213:HOH:O	1.83	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:19:ASP:CA	8:L:228:HOH:O	1.89	1.07
1:A:305:THR:HG21	1:A:309:CYS:SG	1.93	1.07
2:J:124:SER:HB3	8:J:213:HOH:O	1.54	1.07
1:C:76:LEU:O	1:C:77:SER:HB2	1.54	1.06
1:C:121:GLU:OE2	1:C:258:ARG:NH1	1.88	1.06
2:H:66:VAL:HA	8:H:205:HOH:O	1.55	1.06
2:H:66:VAL:CA	8:H:205:HOH:O	2.04	1.05
1:K:34:HIS:CE1	8:K:908:HOH:O	2.09	1.05
1:K:213:SER:O	8:K:910:HOH:O	1.73	1.05
1:C:258:ARG:N	8:C:717:HOH:O	1.88	1.05
1:C:327:ILE:O	1:C:327:ILE:HG22	1.55	1.05
1:K:14:HIS:NE2	1:K:15:ALA:O	1.90	1.05
1:G:324:LEU:N	8:G:717:HOH:O	1.86	1.05
1:I:211:ARG:NH2	8:I:923:HOH:O	1.90	1.04
1:K:56:LEU:N	8:K:913:HOH:O	1.91	1.04
1:A:234:ASN:N	8:A:733:HOH:O	1.89	1.03
1:A:167:LEU:HD12	1:A:167:LEU:C	1.77	1.03
1:I:327:ILE:HG22	1:I:327:ILE:O	1.55	1.03
2:L:4:GLY:HA2	8:L:216:HOH:O	1.58	1.02
2:L:4:GLY:CA	8:L:216:HOH:O	2.08	1.02
1:K:154:LEU:HA	8:K:902:HOH:O	1.57	1.02
2:B:71:ASN:H	2:B:71:ASN:ND2	1.55	1.02
2:B:71:ASN:ND2	2:B:74:GLU:OE1	1.93	1.01
1:A:233:MET:CA	8:A:733:HOH:O	2.07	1.01
2:J:142:HIS:CE1	2:J:161:LYS:HD3	1.95	1.01
1:K:292:ILE:O	1:K:292:ILE:HG22	1.56	1.01
1:C:51:ARG:N	8:C:715:HOH:O	1.69	1.01
1:G:90:SER:CA	8:G:719:HOH:O	2.06	1.01
2:H:75:LYS:HD2	8:H:204:HOH:O	1.60	1.01
1:K:14:HIS:CD2	1:K:15:ALA:H	1.79	1.01
1:A:8:THR:HG23	2:B:139:GLU:HA	1.44	1.00
1:A:30:VAL:N	8:A:719:HOH:O	1.93	1.00
1:E:119:ARG:O	1:E:119:ARG:HG2	1.60	0.99
1:G:324:LEU:CA	8:G:717:HOH:O	2.06	0.99
1:K:33:THR:HB	8:K:908:HOH:O	1.60	0.99
1:I:190:THR:HG23	1:I:190:THR:O	1.59	0.98
1:K:14:HIS:CD2	1:K:15:ALA:N	2.30	0.98
1:A:118:GLU:OE2	8:A:720:HOH:O	1.81	0.98
1:K:13:TYR:N	8:K:925:HOH:O	1.89	0.97
1:C:245:LYS:NZ	1:I:264:GLU:OE2	1.97	0.97
1:G:324:LEU:C	8:G:717:HOH:O	2.02	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:74:GLU:O	8:K:905:HOH:O	1.81	0.97
2:B:71:ASN:HD22	2:B:71:ASN:N	1.59	0.97
1:A:91:SER:OG	8:A:732:HOH:O	1.83	0.97
1:G:317:LYS:O	8:G:710:HOH:O	1.82	0.97
1:I:190:THR:HG22	1:I:193:ASP:HB2	1.43	0.96
1:E:51:ARG:CD	8:E:718:HOH:O	2.11	0.96
1:E:294:THR:O	8:E:725:HOH:O	1.83	0.95
1:A:133:ASP:OD2	1:A:136:LYS:HD3	1.64	0.95
2:B:97:GLU:C	8:B:213:HOH:O	1.97	0.95
1:C:258:ARG:CB	8:C:717:HOH:O	1.99	0.95
1:A:102:ILE:HD12	1:A:102:ILE:N	1.79	0.95
1:C:159:LYS:HZ2	1:C:199:GLN:HE21	1.12	0.95
2:L:52:VAL:O	8:L:214:HOH:O	1.83	0.95
1:I:305:THR:H	2:J:66:VAL:HG13	1.30	0.94
1:A:12:GLY:N	2:B:14:TRP:CH2	2.36	0.94
1:A:185:ILE:O	8:A:733:HOH:O	1.84	0.94
2:J:106:ARG:HD3	8:J:214:HOH:O	1.65	0.94
2:H:103:GLU:O	8:H:211:HOH:O	1.86	0.94
1:A:91:SER:CB	8:A:717:HOH:O	2.15	0.94
1:E:66:TRP:HE1	1:E:77:SER:CB	1.80	0.93
1:K:8:THR:OG1	2:L:27:GLN:HB3	1.69	0.93
1:A:89:PRO:O	8:A:711:HOH:O	1.84	0.93
2:H:154:ASN:OD1	8:H:203:HOH:O	1.85	0.93
1:I:44:ASN:HD22	1:I:44:ASN:H	1.17	0.93
1:E:51:ARG:HG2	8:E:718:HOH:O	1.69	0.92
1:I:190:THR:HG23	1:I:193:ASP:H	0.76	0.92
1:E:66:TRP:NE1	1:E:77:SER:HB2	1.82	0.92
2:J:162:TYR:CD2	8:J:216:HOH:O	2.22	0.92
1:C:153:ASN:O	8:C:717:HOH:O	1.86	0.92
1:G:7:ASP:N	2:H:140:PHE:N	2.17	0.92
1:C:74:GLU:O	1:C:74:GLU:HG2	1.69	0.92
1:K:14:HIS:CG	1:K:15:ALA:N	2.29	0.92
2:J:106:ARG:HB2	8:J:206:HOH:O	1.67	0.91
1:A:105:GLU:O	8:A:734:HOH:O	1.88	0.91
2:J:26:HIS:HD2	2:J:26:HIS:O	1.52	0.91
1:A:29:ASN:N	8:A:719:HOH:O	2.03	0.91
1:A:133:ASP:OD2	1:A:136:LYS:CE	2.19	0.91
1:G:90:SER:N	8:G:719:HOH:O	2.04	0.90
2:L:138:PHE:O	8:L:231:HOH:O	1.89	0.90
1:E:305:THR:CB	8:E:719:HOH:O	2.20	0.90
2:J:142:HIS:CE1	2:J:161:LYS:HE2	2.07	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ASN:ND2	6:A:602:NAG:O7	2.04	0.90
1:E:282:ASN:HD22	1:E:283:THR:N	1.69	0.90
1:I:120:PHE:HB3	8:I:924:HOH:O	1.71	0.90
2:L:19:ASP:O	8:L:228:HOH:O	1.89	0.90
2:L:30:GLN:NE2	8:L:212:HOH:O	2.05	0.90
2:J:103:GLU:OE1	8:J:214:HOH:O	1.89	0.90
1:K:15:ALA:HB1	8:K:904:HOH:O	1.71	0.90
1:A:102:ILE:N	1:A:102:ILE:CD1	2.30	0.90
2:D:161:LYS:O	8:D:204:HOH:O	1.90	0.89
1:K:266:ASN:H	1:K:266:ASN:ND2	1.68	0.89
1:I:190:THR:CG2	1:I:193:ASP:HB2	2.01	0.89
1:K:106:GLU:OE1	8:K:915:HOH:O	1.89	0.89
1:A:293:ASN:ND2	8:A:708:HOH:O	1.82	0.89
1:E:51:ARG:NE	8:E:718:HOH:O	2.05	0.89
1:A:102:ILE:CD1	1:A:102:ILE:H	1.85	0.89
1:A:233:MET:HA	8:A:733:HOH:O	1.66	0.89
1:I:190:THR:CG2	1:I:193:ASP:CB	2.50	0.88
1:A:133:ASP:OD2	1:A:136:LYS:CD	2.21	0.88
1:A:233:MET:C	8:A:733:HOH:O	2.07	0.88
1:C:71:PRO:HA	1:C:152:LYS:NZ	1.86	0.88
1:G:307:GLY:O	8:G:703:HOH:O	1.92	0.88
1:G:324:LEU:O	8:G:717:HOH:O	1.92	0.88
1:A:28:LYS:C	8:A:719:HOH:O	2.12	0.88
1:G:96:CYS:O	1:G:227:ARG:HD2	1.74	0.87
1:G:133:ASP:OD2	1:G:136:LYS:HG3	1.75	0.87
2:B:91:ILE:O	2:B:95:ASN:OD1	1.92	0.87
2:L:37:ASP:C	8:L:207:HOH:O	2.13	0.87
2:D:150:GLU:O	2:D:154:ASN:HB2	1.74	0.87
2:L:8:GLY:HA3	8:L:216:HOH:O	1.74	0.87
1:A:143:PRO:HD2	6:A:603:NAG:H62	1.56	0.87
1:A:308:LYS:NZ	8:A:723:HOH:O	2.06	0.87
1:C:11:ILE:CD1	2:D:24:TYR:HE2	1.82	0.87
1:C:62:ASN:OD1	8:C:729:HOH:O	1.92	0.86
1:K:66:TRP:HE1	1:K:77:SER:HB2	1.39	0.86
1:A:241:GLU:HG2	8:A:715:HOH:O	1.75	0.86
1:A:167:LEU:HD12	1:A:167:LEU:O	1.75	0.86
1:E:305:THR:OG1	8:E:719:HOH:O	1.94	0.85
1:A:185:ILE:N	8:A:721:HOH:O	2.08	0.85
1:C:204:TYR:HD2	8:C:711:HOH:O	1.59	0.85
2:L:4:GLY:O	8:L:216:HOH:O	1.90	0.85
1:I:44:ASN:HD21	1:I:291:ALA:HB3	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:265:ARG:O	8:K:909:HOH:O	1.94	0.85
1:G:114:VAL:HG11	1:G:117:PHE:HB2	1.57	0.84
1:A:114:VAL:HG11	1:A:117:PHE:HB2	1.59	0.84
1:A:133:ASP:OD2	1:A:136:LYS:HE2	1.77	0.84
1:C:114:VAL:HG11	1:C:117:PHE:HB2	1.58	0.84
1:G:293:ASN:ND2	8:G:706:HOH:O	2.09	0.84
1:I:172:ILE:O	1:I:172:ILE:HG23	1.78	0.84
1:C:327:ILE:N	1:C:327:ILE:HD12	1.92	0.84
1:K:260:ALA:N	8:K:914:HOH:O	2.10	0.84
1:G:315:SER:HA	8:H:207:HOH:O	1.78	0.84
1:I:114:VAL:HG11	1:I:117:PHE:HB2	1.57	0.84
1:I:145:ALA:O	8:I:903:HOH:O	1.96	0.84
1:I:194:GLN:OE1	1:I:200:ASN:O	1.96	0.84
2:L:150:GLU:O	2:L:154:ASN:HB2	1.78	0.84
1:I:114:VAL:CG1	1:I:116:SER:O	2.27	0.83
1:I:118:GLU:OE1	8:I:913:HOH:O	1.95	0.83
2:H:127:LYS:H	2:H:127:LYS:HD2	1.43	0.83
2:L:53:ASN:HA	8:L:214:HOH:O	1.77	0.83
1:A:159:LYS:NZ	1:A:195:GLN:O	2.11	0.83
1:C:11:ILE:HD12	2:D:24:TYR:CE2	2.12	0.83
2:F:136:GLY:N	8:F:201:HOH:O	2.11	0.83
2:H:150:GLU:O	2:H:154:ASN:HB2	1.79	0.83
2:H:1:GLY:HA2	8:H:209:HOH:O	1.77	0.83
1:I:144:HIS:O	8:I:903:HOH:O	1.96	0.83
2:J:132:GLU:OE1	8:J:212:HOH:O	1.95	0.83
8:H:213:HOH:O	2:J:66:VAL:HG23	1.78	0.82
1:C:59:GLY:N	8:C:712:HOH:O	2.11	0.82
2:F:127:LYS:H	2:F:127:LYS:HD2	1.44	0.82
2:J:150:GLU:O	2:J:154:ASN:HB2	1.79	0.82
1:I:76:LEU:O	1:I:77:SER:HB2	1.79	0.82
2:J:127:LYS:H	2:J:127:LYS:HD2	1.42	0.82
2:F:150:GLU:O	2:F:154:ASN:HB2	1.79	0.82
1:I:74:GLU:OE1	8:I:914:HOH:O	1.97	0.82
1:K:74:GLU:C	8:K:905:HOH:O	2.13	0.82
2:J:123:ARG:NH1	8:J:213:HOH:O	2.11	0.82
1:A:326:ASN:C	1:A:327:ILE:CG1	2.46	0.82
2:B:127:LYS:H	2:B:127:LYS:HD2	1.42	0.82
1:K:266:ASN:H	1:K:266:ASN:HD22	1.24	0.82
2:B:150:GLU:O	2:B:154:ASN:HB2	1.79	0.81
2:L:19:ASP:N	8:L:226:HOH:O	2.10	0.81
1:C:305:THR:H	2:D:66:VAL:HG13	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:GLY:O	1:E:232:ARG:HD3	1.80	0.81
2:J:26:HIS:C	2:J:26:HIS:CD2	2.54	0.81
1:E:13:TYR:CE2	2:F:6:ILE:HA	2.16	0.81
1:K:259:TYR:CZ	8:K:906:HOH:O	2.33	0.81
1:K:114:VAL:HG21	1:K:117:PHE:HB2	1.63	0.80
2:H:120:GLU:OE1	2:H:123:ARG:CZ	2.30	0.80
1:C:62:ASN:CG	8:C:729:HOH:O	2.20	0.80
2:D:127:LYS:H	2:D:127:LYS:HD2	1.43	0.80
1:K:11:ILE:HG22	1:K:11:ILE:O	1.81	0.80
1:C:69:GLY:O	1:C:152:LYS:HG2	1.82	0.80
1:K:258:ARG:N	8:K:902:HOH:O	2.12	0.80
1:C:195:GLN:HA	1:C:198:TYR:O	1.82	0.80
2:H:106:ARG:HB2	8:H:211:HOH:O	1.80	0.80
1:A:132:HIS:HD2	8:A:729:HOH:O	1.64	0.80
2:D:124:SER:O	2:D:127:LYS:HE3	1.81	0.80
1:I:190:THR:HG21	1:I:193:ASP:CG	2.02	0.80
1:K:51:ARG:HB3	1:K:51:ARG:NH1	1.96	0.80
1:G:41:ASP:O	8:G:708:HOH:O	1.98	0.80
1:I:190:THR:CG2	1:I:190:THR:O	2.30	0.80
1:E:114:VAL:HG21	1:E:117:PHE:HB2	1.63	0.80
1:I:172:ILE:O	1:I:172:ILE:CG2	2.30	0.80
1:K:7:ASP:O	8:K:911:HOH:O	2.00	0.79
1:C:172:ILE:O	8:C:722:HOH:O	2.00	0.79
1:E:244:ASP:OD1	8:E:728:HOH:O	1.99	0.79
2:L:148:CYS:O	8:L:223:HOH:O	1.99	0.79
1:A:195:GLN:HG2	8:A:704:HOH:O	1.82	0.79
1:C:326:ASN:C	1:C:327:ILE:HD12	2.03	0.79
1:E:319:ARG:HH11	1:E:319:ARG:CG	1.94	0.79
1:A:167:LEU:C	1:A:167:LEU:CD1	2.50	0.79
1:C:159:LYS:NZ	1:C:199:GLN:HE21	1.79	0.79
1:E:11:ILE:HD12	2:F:119:TYR:HA	1.62	0.79
2:F:123:ARG:NH2	8:F:204:HOH:O	1.96	0.79
1:C:100:ASP:OD1	8:C:720:HOH:O	2.00	0.79
1:E:72:GLU:HG2	5:O:1:NAG:H82	1.62	0.79
1:E:110:GLN:OE1	8:E:731:HOH:O	2.01	0.79
8:A:706:HOH:O	3:M:1:NAG:O7	2.01	0.78
1:C:50:LEU:CA	8:C:715:HOH:O	2.32	0.78
1:G:7:ASP:N	1:G:8:THR:HA	1.98	0.78
2:B:14:TRP:HE3	2:B:17:MET:HE2	1.48	0.78
1:K:266:ASN:ND2	1:K:266:ASN:N	2.30	0.78
1:A:185:ILE:HG12	8:A:721:HOH:O	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:190:THR:CG2	1:I:193:ASP:CG	2.51	0.78
1:A:61:CYS:O	8:A:717:HOH:O	2.00	0.78
1:G:143:PRO:HD2	6:G:602:NAG:H62	1.66	0.78
1:E:203:THR:O	1:E:217:LYS:CE	2.31	0.78
1:K:13:TYR:O	8:K:925:HOH:O	2.01	0.77
2:J:142:HIS:CE1	2:J:161:LYS:CD	2.67	0.77
2:L:127:LYS:H	2:L:127:LYS:HD2	1.47	0.77
1:C:76:LEU:O	1:C:77:SER:CB	2.29	0.77
1:I:244:ASP:OD1	8:I:925:HOH:O	2.01	0.77
1:E:11:ILE:CD1	2:F:119:TYR:HA	2.15	0.77
1:E:282:ASN:OD1	8:E:710:HOH:O	2.03	0.77
1:A:185:ILE:CB	8:A:721:HOH:O	2.33	0.77
2:D:109:ASP:OD2	8:F:205:HOH:O	2.02	0.77
2:J:18:VAL:HB	8:J:211:HOH:O	1.85	0.77
1:C:59:GLY:O	8:C:712:HOH:O	2.01	0.77
2:D:150:GLU:OE2	2:D:150:GLU:CA	2.30	0.77
1:K:11:ILE:O	1:K:11:ILE:CG2	2.33	0.77
1:E:47:LEU:HD12	1:E:286:GLN:NE2	2.00	0.77
2:J:18:VAL:O	8:J:211:HOH:O	2.02	0.77
2:J:26:HIS:O	2:J:26:HIS:CD2	2.36	0.76
1:I:114:VAL:HG13	1:I:116:SER:O	1.86	0.76
1:K:294:THR:N	8:K:916:HOH:O	1.82	0.76
1:A:107:LEU:C	1:A:107:LEU:CD2	2.53	0.76
1:E:319:ARG:HH11	1:E:319:ARG:HG2	1.49	0.76
2:H:6:ILE:O	8:H:209:HOH:O	2.01	0.76
1:I:89:PRO:HD2	8:I:908:HOH:O	1.85	0.76
1:A:192:ALA:O	1:A:196:SER:OG	2.03	0.76
1:E:51:ARG:CG	8:E:718:HOH:O	2.23	0.76
1:K:27:GLU:OE2	8:K:921:HOH:O	2.04	0.76
1:K:56:LEU:HB2	8:K:913:HOH:O	1.85	0.76
1:C:64:ALA:N	8:C:729:HOH:O	2.12	0.75
1:I:105:GLU:O	8:I:906:HOH:O	2.02	0.75
1:K:246:ILE:HG13	1:K:247:THR:N	2.00	0.75
1:I:190:THR:HG22	1:I:193:ASP:CB	2.13	0.75
1:A:130:PRO:HD2	8:A:729:HOH:O	1.87	0.75
1:A:159:LYS:NZ	1:A:199:GLN:NE2	2.33	0.75
1:K:7:ASP:HA	2:L:27:GLN:O	1.86	0.75
1:K:305:THR:H	2:L:66:VAL:HG13	1.50	0.75
1:I:120:PHE:CA	8:I:924:HOH:O	2.33	0.75
1:I:241:GLU:HG2	8:I:925:HOH:O	1.87	0.75
1:K:24:THR:HG22	2:L:104:ASN:HB3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:ILE:HD13	2:D:24:TYR:HD2	1.00	0.74
2:H:107:THR:N	8:H:211:HOH:O	2.20	0.74
2:J:106:ARG:CB	8:J:206:HOH:O	2.29	0.74
1:A:8:THR:HG21	2:B:138:PHE:O	1.87	0.74
1:C:222:ILE:HG23	1:C:230:GLU:HG2	1.69	0.74
1:I:119:ARG:NH1	8:I:919:HOH:O	2.21	0.74
1:A:76:LEU:O	8:A:739:HOH:O	2.05	0.74
1:I:282:ASN:ND2	8:I:902:HOH:O	2.18	0.74
1:A:7:ASP:C	2:B:27:GLN:O	2.26	0.73
1:A:102:ILE:H	1:A:102:ILE:HD13	1.51	0.73
1:G:315:SER:CA	8:H:207:HOH:O	2.34	0.73
2:H:162:TYR:OH	8:H:206:HOH:O	2.05	0.73
1:A:82:TRP:O	8:A:740:HOH:O	2.05	0.73
1:C:71:PRO:HA	1:C:152:LYS:HZ2	1.53	0.73
1:G:90:SER:HA	8:G:719:HOH:O	1.76	0.73
1:E:8:THR:OG1	8:E:712:HOH:O	2.06	0.73
1:I:327:ILE:O	1:I:327:ILE:CG2	2.30	0.73
1:C:119:ARG:HB2	1:C:261:PHE:CD2	2.24	0.72
2:B:4:GLY:CA	8:B:212:HOH:O	2.37	0.72
2:H:83:LYS:NZ	8:H:213:HOH:O	1.91	0.72
2:J:142:HIS:CE1	2:J:161:LYS:CE	2.72	0.72
1:I:189:SER:HB2	1:I:222:ILE:HD13	1.71	0.72
2:F:106:ARG:NH2	8:F:205:HOH:O	1.86	0.72
1:K:294:THR:O	8:K:916:HOH:O	2.08	0.72
1:A:305:THR:HG21	1:A:309:CYS:CB	2.19	0.72
2:B:123:ARG:HD2	2:B:132:GLU:OE1	1.89	0.72
1:A:24:THR:HG22	2:B:104:ASN:HB3	1.72	0.72
1:G:323:GLY:C	8:G:717:HOH:O	2.24	0.72
2:J:103:GLU:HA	8:J:206:HOH:O	1.90	0.72
1:K:55:PRO:C	8:K:913:HOH:O	2.19	0.72
1:C:46:LYS:NZ	8:C:719:HOH:O	2.23	0.72
1:I:275:ASP:OD2	8:I:908:HOH:O	2.07	0.72
1:C:71:PRO:HA	1:C:152:LYS:HZ1	1.54	0.71
2:D:150:GLU:OE2	2:D:150:GLU:HA	1.90	0.71
1:I:118:GLU:CD	8:I:913:HOH:O	2.29	0.71
1:E:10:CYS:HA	2:F:137:CYS:HA	1.72	0.71
1:I:120:PHE:CB	8:I:924:HOH:O	2.32	0.71
2:D:132:GLU:HG2	2:D:138:PHE:HE2	1.55	0.71
1:C:130:PRO:O	1:C:160:LYS:NZ	2.23	0.71
2:B:14:TRP:HE3	2:B:17:MET:CE	2.04	0.71
2:L:132:GLU:HG2	2:L:138:PHE:HE2	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:GLY:O	8:B:202:HOH:O	2.07	0.71
2:J:103:GLU:O	8:J:206:HOH:O	2.08	0.71
2:J:142:HIS:HE1	2:J:161:LYS:HE2	1.54	0.71
2:B:22:TYR:OH	2:B:111:HIS:ND1	2.20	0.70
2:B:132:GLU:HG2	2:B:138:PHE:HE2	1.56	0.70
1:A:11:ILE:C	2:B:14:TRP:CH2	2.64	0.70
2:F:132:GLU:HG2	2:F:138:PHE:HE2	1.55	0.70
2:J:132:GLU:HG2	2:J:138:PHE:HE2	1.55	0.70
1:K:10:CYS:O	2:L:24:TYR:HA	1.91	0.70
2:D:71:ASN:C	2:D:71:ASN:OD1	2.29	0.70
2:L:157:TYR:CD1	8:L:223:HOH:O	2.44	0.70
2:H:132:GLU:HG2	2:H:138:PHE:HE2	1.56	0.70
1:A:196:SER:HB2	3:M:1:NAG:H82	1.73	0.70
2:B:71:ASN:H	2:B:71:ASN:HD22	0.79	0.70
1:A:145:ALA:C	1:A:147:ALA:H	1.95	0.70
1:G:11:ILE:HD12	2:H:119:TYR:HA	1.73	0.70
1:K:292:ILE:HD11	1:K:301:ILE:HD12	1.73	0.70
1:K:51:ARG:HB3	1:K:51:ARG:HH11	1.57	0.70
1:E:282:ASN:HD22	1:E:283:THR:H	1.40	0.70
1:A:191:SER:O	8:A:704:HOH:O	2.09	0.69
1:A:313:VAL:HG12	1:A:315:SER:H	1.57	0.69
2:J:18:VAL:CA	8:J:211:HOH:O	2.40	0.69
1:A:27:GLU:OE1	1:A:325:ARG:NH2	2.25	0.69
1:A:30:VAL:HG23	8:A:719:HOH:O	1.92	0.69
1:C:327:ILE:O	1:C:327:ILE:CG2	2.30	0.69
1:A:236:TYR:OH	8:A:726:HOH:O	2.08	0.69
1:G:7:ASP:N	2:H:140:PHE:HB2	2.07	0.69
1:A:202:ASP:OD1	1:A:202:ASP:C	2.30	0.69
1:G:89:PRO:C	8:G:719:HOH:O	2.29	0.69
1:G:313:VAL:HG12	1:G:315:SER:H	1.58	0.69
1:I:101:PHE:O	8:I:920:HOH:O	2.11	0.69
1:A:204:TYR:CD1	1:A:204:TYR:C	2.65	0.69
1:E:282:ASN:ND2	1:E:283:THR:N	2.40	0.69
2:L:139:GLU:HB3	8:L:225:HOH:O	1.91	0.69
1:A:74:GLU:HA	8:A:737:HOH:O	1.92	0.69
1:A:233:MET:CG	8:A:733:HOH:O	2.41	0.68
1:K:313:VAL:HG12	1:K:315:SER:H	1.58	0.68
1:C:102:ILE:HG13	1:C:236:TYR:CE2	2.28	0.68
1:E:313:VAL:HG12	1:E:315:SER:H	1.59	0.68
1:G:102:ILE:HG13	1:G:236:TYR:CE2	2.29	0.68
1:C:50:LEU:CB	8:C:715:HOH:O	2.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:ARG:O	1:E:119:ARG:CG	2.32	0.68
1:K:259:TYR:OH	8:K:906:HOH:O	2.09	0.68
2:L:97:GLU:OE2	8:L:220:HOH:O	2.12	0.68
1:K:102:ILE:HG13	1:K:236:TYR:CE2	2.29	0.68
1:I:15:ALA:O	8:I:909:HOH:O	2.11	0.68
1:A:49:LYS:O	1:A:283:THR:HG22	1.94	0.68
1:I:313:VAL:HG12	1:I:315:SER:H	1.58	0.68
1:A:120:PHE:HB3	8:A:720:HOH:O	1.93	0.68
1:E:245:LYS:NZ	8:E:721:HOH:O	2.22	0.67
1:C:11:ILE:CD1	2:D:24:TYR:HD2	1.83	0.67
8:E:712:HOH:O	2:F:27:GLN:HB3	1.95	0.67
1:I:190:THR:HG22	1:I:193:ASP:OD1	1.93	0.67
2:H:42:GLN:OE1	8:H:201:HOH:O	2.12	0.67
1:K:324:LEU:HD21	2:L:21:TRP:CD1	2.30	0.67
1:A:185:ILE:HB	8:A:721:HOH:O	1.92	0.67
1:A:305:THR:HG23	1:A:309:CYS:SG	2.31	0.67
1:A:132:HIS:CD2	8:A:729:HOH:O	2.43	0.67
1:E:119:ARG:HB2	1:E:261:PHE:CD2	2.30	0.67
1:I:172:ILE:HD12	1:I:245:LYS:HB3	1.76	0.67
2:L:38:LEU:N	8:L:207:HOH:O	2.25	0.67
1:C:313:VAL:HG12	1:C:315:SER:H	1.59	0.67
1:E:102:ILE:HG13	1:E:236:TYR:CE2	2.28	0.67
1:G:13:TYR:CE2	2:H:6:ILE:HA	2.28	0.67
1:A:128:SER:O	1:A:130:PRO:HD3	1.94	0.67
1:G:268:GLY:HA2	8:G:709:HOH:O	1.95	0.67
1:C:223:ARG:O	1:C:230:GLU:HG3	1.95	0.66
1:A:107:LEU:C	1:A:107:LEU:HD22	2.15	0.66
1:A:217:LYS:O	8:A:735:HOH:O	2.13	0.66
2:H:51:LYS:NZ	8:H:211:HOH:O	2.26	0.66
1:A:105:GLU:HA	1:A:108:ARG:HD3	1.78	0.66
1:C:49:LYS:O	1:C:283:THR:HG22	1.96	0.66
2:F:83:LYS:O	8:F:207:HOH:O	2.13	0.66
1:E:178:GLU:CD	1:E:265:ARG:NH1	2.48	0.66
1:I:194:GLN:HG3	1:I:195:GLN:N	2.10	0.66
1:I:311:LYS:HG3	2:J:92:TRP:CE2	2.31	0.66
2:L:37:ASP:O	8:L:207:HOH:O	2.11	0.66
1:A:102:ILE:HD13	1:A:235:TYR:O	1.96	0.66
2:B:71:ASN:HD21	2:B:74:GLU:CD	1.99	0.66
1:K:49:LYS:O	1:K:283:THR:HG22	1.95	0.66
1:A:76:LEU:N	8:A:738:HOH:O	1.80	0.66
1:A:33:THR:HG23	1:A:324:LEU:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ASN:OD1	8:A:724:HOH:O	2.13	0.65
1:I:102:ILE:HG13	1:I:236:TYR:CE2	2.30	0.65
1:G:109:GLU:OE2	2:L:79:ASN:ND2	2.29	0.65
1:I:44:ASN:HD22	1:I:44:ASN:N	1.89	0.65
1:I:307:GLY:HA2	2:J:63:PHE:CE1	2.31	0.65
1:C:24:THR:HG22	2:D:104:ASN:HB3	1.78	0.65
1:I:190:THR:CG2	1:I:193:ASP:N	2.38	0.65
1:I:265:ARG:NE	8:I:910:HOH:O	2.28	0.65
2:J:162:TYR:CE2	8:J:216:HOH:O	2.43	0.65
1:I:25:VAL:HG12	2:L:51:LYS:HA	1.77	0.65
1:I:297:PRO:HG3	2:J:56:ILE:HA	1.78	0.65
1:I:49:LYS:O	1:I:283:THR:HG22	1.96	0.65
2:B:51:LYS:HG3	1:E:25:VAL:HG12	1.78	0.65
2:J:103:GLU:C	8:J:206:HOH:O	2.35	0.65
1:C:25:VAL:CG2	2:D:102:LEU:HD12	2.26	0.65
1:C:50:LEU:N	8:C:715:HOH:O	2.30	0.65
1:E:178:GLU:CD	1:E:265:ARG:HH12	1.98	0.65
1:I:145:ALA:CB	8:I:903:HOH:O	2.16	0.65
1:I:44:ASN:HD21	1:I:291:ALA:CB	2.09	0.65
1:K:43:HIS:HB3	1:K:301:ILE:HD13	1.79	0.65
1:A:307:GLY:HA2	2:B:63:PHE:CE1	2.32	0.65
1:E:119:ARG:HB2	1:E:261:PHE:CE2	2.32	0.65
1:A:13:TYR:HD1	8:A:730:HOH:O	1.80	0.64
1:C:155:ILE:HD11	1:C:258:ARG:HD3	1.80	0.64
1:G:11:ILE:CD1	2:H:119:TYR:HA	2.27	0.64
1:G:49:LYS:O	1:G:283:THR:HG22	1.98	0.64
2:L:139:GLU:N	8:L:225:HOH:O	2.21	0.64
1:C:74:GLU:O	1:C:74:GLU:CG	2.28	0.64
1:C:231:GLY:HA3	8:C:701:HOH:O	1.96	0.64
1:E:294:THR:O	8:E:704:HOH:O	2.15	0.64
1:K:16:ASN:ND2	8:K:908:HOH:O	2.05	0.64
1:K:293:ASN:O	1:K:293:ASN:ND2	2.30	0.64
1:A:107:LEU:CD2	1:A:107:LEU:O	2.46	0.64
1:E:319:ARG:CG	1:E:319:ARG:NH1	2.55	0.64
2:J:159:TYR:N	2:J:160:PRO:CD	2.61	0.64
2:L:157:TYR:CE1	8:L:223:HOH:O	2.50	0.64
1:C:131:ASN:HD21	1:I:243:GLY:HA3	1.62	0.64
2:F:19:ASP:N	2:F:19:ASP:OD1	2.30	0.64
1:E:50:LEU:HD21	1:E:306:ILE:HG22	1.80	0.64
1:K:82:TRP:HB3	8:K:913:HOH:O	1.97	0.64
1:I:25:VAL:CG1	2:L:51:LYS:HG3	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:PRO:HB3	8:E:726:HOH:O	1.98	0.64
2:L:131:LYS:O	8:L:225:HOH:O	2.16	0.64
1:C:204:TYR:CD2	8:C:711:HOH:O	2.41	0.63
1:A:108:ARG:NH1	8:A:709:HOH:O	2.10	0.63
1:I:14:HIS:HE1	2:J:18:VAL:HA	1.64	0.63
1:C:119:ARG:HB2	1:C:261:PHE:CE2	2.33	0.63
1:K:66:TRP:NE1	1:K:77:SER:HB2	2.12	0.63
2:L:123:ARG:C	8:L:205:HOH:O	2.36	0.63
1:C:59:GLY:CA	8:C:712:HOH:O	2.45	0.63
2:J:18:VAL:CB	8:J:211:HOH:O	2.45	0.63
1:C:133:ASP:O	8:C:728:HOH:O	2.15	0.63
1:K:66:TRP:HE1	1:K:77:SER:CB	2.09	0.63
2:B:14:TRP:CE3	2:B:17:MET:CE	2.82	0.63
1:C:327:ILE:N	1:C:327:ILE:CD1	2.60	0.63
1:E:43:HIS:HB3	1:E:301:ILE:HD13	1.80	0.62
1:C:194:GLN:O	1:C:198:TYR:O	2.17	0.62
1:A:43:HIS:HB3	1:A:301:ILE:HD13	1.81	0.62
1:A:224:PRO:HG2	1:C:209:SER:HA	1.79	0.62
1:C:64:ALA:HB3	8:C:729:HOH:O	1.98	0.62
1:I:43:HIS:HB3	1:I:301:ILE:HD13	1.80	0.62
1:K:106:GLU:O	1:K:110:GLN:HG2	2.00	0.62
1:A:159:LYS:HZ2	1:A:199:GLN:NE2	1.95	0.62
1:I:231:GLY:O	1:I:232:ARG:NH1	2.32	0.62
2:L:131:LYS:HG3	8:L:225:HOH:O	2.00	0.62
1:A:131:ASN:O	1:A:132:HIS:CG	2.53	0.62
1:A:145:ALA:O	1:A:147:ALA:N	2.32	0.62
1:A:305:THR:HG22	1:A:309:CYS:SG	2.37	0.62
1:E:13:TYR:CD2	2:F:6:ILE:HG12	2.35	0.62
1:E:229:GLN:NE2	4:P:4:SIA:O1A	2.30	0.62
1:G:43:HIS:HB3	1:G:301:ILE:HD13	1.82	0.62
1:I:106:GLU:O	1:I:110:GLN:HG2	1.99	0.62
2:L:158:ASP:O	2:L:160:PRO:HD3	2.00	0.62
1:G:32:VAL:HB	8:G:717:HOH:O	2.00	0.62
1:G:106:GLU:O	1:G:110:GLN:HG2	2.00	0.62
1:K:25:VAL:CG2	2:L:102:LEU:HD12	2.29	0.62
1:C:43:HIS:HB3	1:C:301:ILE:HD13	1.80	0.61
2:B:85:ASP:OD1	2:F:83:LYS:NZ	2.33	0.61
1:G:10:CYS:HA	2:H:137:CYS:HA	1.82	0.61
1:E:49:LYS:O	1:E:283:THR:HG22	2.01	0.61
1:G:297:PRO:HG3	2:H:56:ILE:HA	1.81	0.61
1:K:8:THR:HG1	2:L:27:GLN:HB3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:THR:CG2	2:B:139:GLU:CA	2.72	0.61
1:I:141:ALA:O	1:I:143:PRO:HD3	2.00	0.61
1:K:239:LEU:CD1	1:K:265:ARG:NH1	2.63	0.61
1:K:105:GLU:OE2	2:L:71:ASN:HB3	1.99	0.61
2:L:139:GLU:CB	8:L:225:HOH:O	2.47	0.61
1:C:11:ILE:HD11	2:D:24:TYR:CE2	2.31	0.61
1:G:195:GLN:HA	1:G:198:TYR:O	2.00	0.61
2:B:62:GLN:OE1	1:E:314:LYS:NZ	2.20	0.61
2:B:79:ASN:ND2	1:C:109:GLU:OE2	2.34	0.61
2:D:159:TYR:N	2:D:160:PRO:CD	2.64	0.61
1:G:133:ASP:OD2	1:G:136:LYS:CG	2.48	0.61
6:A:602:NAG:O7	6:A:602:NAG:C1	2.49	0.60
1:I:50:LEU:HD11	1:I:306:ILE:HG22	1.83	0.60
1:A:77:SER:N	8:A:738:HOH:O	2.30	0.60
1:E:161:GLY:O	1:E:162:ASN:HB2	2.00	0.60
1:G:161:GLY:O	1:G:162:ASN:HB2	2.01	0.60
1:I:145:ALA:C	8:I:903:HOH:O	2.36	0.60
1:K:9:LEU:HD21	2:L:153:LYS:HE2	1.83	0.60
2:D:19:ASP:HB2	2:D:36:ALA:HB3	1.84	0.60
1:G:90:SER:HB2	8:G:719:HOH:O	2.01	0.60
2:L:152:VAL:O	8:L:227:HOH:O	2.17	0.60
2:B:95:ASN:HD21	2:D:95:ASN:HD22	1.49	0.60
2:D:162:TYR:CZ	8:D:205:HOH:O	2.51	0.60
1:A:326:ASN:O	1:A:327:ILE:CG1	2.35	0.60
2:D:71:ASN:ND2	8:D:207:HOH:O	2.33	0.60
1:E:25:VAL:CG2	2:F:102:LEU:HD12	2.31	0.60
1:G:141:ALA:O	1:G:143:PRO:HD3	2.01	0.60
2:L:124:SER:HA	8:L:205:HOH:O	2.01	0.60
1:E:141:ALA:O	1:E:143:PRO:HD3	2.02	0.60
1:K:76:LEU:N	8:K:905:HOH:O	2.22	0.60
1:E:211:ARG:HD2	8:E:728:HOH:O	2.00	0.59
1:G:8:THR:HG22	2:H:139:GLU:HA	1.84	0.59
1:I:14:HIS:CE1	2:J:18:VAL:HA	2.37	0.59
2:J:161:LYS:O	8:J:207:HOH:O	2.16	0.59
1:K:141:ALA:O	1:K:143:PRO:HD3	2.02	0.59
1:C:299:GLN:HG2	1:C:310:PRO:HB2	1.83	0.59
2:H:43:ASN:O	2:H:47:GLU:HG3	2.02	0.59
1:K:312:TYR:CD2	2:L:89:LEU:HD13	2.36	0.59
1:C:141:ALA:O	1:C:143:PRO:HD3	2.02	0.59
2:D:150:GLU:OE2	2:D:150:GLU:N	2.35	0.59
1:I:44:ASN:ND2	1:I:291:ALA:HB3	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:19:ASP:HB2	2:J:36:ALA:HB3	1.85	0.59
1:K:56:LEU:CB	8:K:913:HOH:O	2.32	0.59
1:C:168:SER:HB3	1:I:176:GLY:HA2	1.85	0.59
2:L:23:GLY:HA3	2:L:36:ALA:HA	1.84	0.59
1:C:25:VAL:HG22	2:D:102:LEU:HD12	1.84	0.59
1:E:58:LEU:HD11	1:E:63:ILE:HD13	1.84	0.59
1:A:214:LYS:HG2	1:A:216:PHE:CZ	2.36	0.59
1:E:265:ARG:HG3	8:E:720:HOH:O	2.02	0.59
1:A:131:ASN:C	1:A:132:HIS:CD2	2.77	0.59
1:E:8:THR:O	8:E:712:HOH:O	2.17	0.59
1:I:25:VAL:HG12	2:L:51:LYS:HG3	1.85	0.59
2:B:19:ASP:HB2	2:B:36:ALA:HB3	1.84	0.59
2:B:67:GLY:C	2:B:68:LYS:HG2	2.23	0.59
1:C:107:LEU:HD12	1:C:107:LEU:O	2.03	0.59
2:H:19:ASP:HB2	2:H:36:ALA:HB3	1.84	0.59
1:A:26:LEU:HB3	2:D:47:GLU:HB3	1.85	0.58
2:B:159:TYR:N	2:B:160:PRO:HD3	2.18	0.58
1:C:231:GLY:CA	8:C:701:HOH:O	2.51	0.58
1:I:312:TYR:CD2	2:J:89:LEU:HD13	2.38	0.58
1:E:281:CYS:N	8:E:709:HOH:O	2.35	0.58
1:G:315:SER:CB	8:H:207:HOH:O	2.51	0.58
1:K:13:TYR:OH	2:L:12:GLY:N	2.32	0.58
1:I:58:LEU:HD11	1:I:63:ILE:HD13	1.85	0.58
2:L:2:LEU:N	8:L:222:HOH:O	2.36	0.58
2:L:19:ASP:HB2	2:L:36:ALA:HB3	1.85	0.58
5:O:1:NAG:H61	5:O:2:NAG:C7	2.33	0.58
2:L:132:GLU:HG2	2:L:138:PHE:CE2	2.38	0.58
1:E:8:THR:HG22	2:F:139:GLU:HA	1.84	0.58
1:G:92:ASP:HB2	6:G:602:NAG:H81	1.86	0.58
2:L:123:ARG:HD2	2:L:132:GLU:OE1	2.04	0.58
1:C:25:VAL:HG12	2:F:51:LYS:HG3	1.85	0.58
1:C:162:ASN:HD22	1:C:199:GLN:NE2	2.02	0.58
1:I:161:GLY:O	1:I:162:ASN:HB2	2.02	0.58
4:N:4:SIA:O1A	4:N:4:SIA:H6	2.03	0.58
1:E:44:ASN:HD21	1:E:291:ALA:H	1.51	0.58
1:A:50:LEU:HD11	1:A:306:ILE:HG22	1.86	0.58
2:D:123:ARG:HD2	2:D:132:GLU:OE1	2.03	0.58
1:I:40:GLU:OE1	1:I:294:THR:OG1	2.19	0.58
1:C:158:VAL:HG22	8:C:728:HOH:O	2.03	0.58
1:G:44:ASN:HD21	1:G:291:ALA:H	1.52	0.58
1:G:50:LEU:HD11	1:G:306:ILE:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:58:LEU:HD11	1:K:63:ILE:HD13	1.85	0.58
1:A:29:ASN:C	8:A:719:HOH:O	2.34	0.57
1:A:185:ILE:CG1	8:A:721:HOH:O	2.42	0.57
1:C:11:ILE:HD12	2:D:24:TYR:HE2	1.54	0.57
1:I:44:ASN:H	1:I:44:ASN:ND2	1.96	0.57
1:K:245:LYS:HG3	1:K:246:ILE:N	2.18	0.57
1:A:15:ALA:HB2	8:A:712:HOH:O	2.04	0.57
1:A:107:LEU:C	1:A:107:LEU:HD23	2.24	0.57
2:B:51:LYS:HG3	1:E:25:VAL:CG1	2.34	0.57
2:B:123:ARG:O	2:B:123:ARG:HG2	2.00	0.57
1:K:312:TYR:HD2	2:L:89:LEU:HD13	1.70	0.57
1:A:107:LEU:O	1:A:107:LEU:HD23	2.05	0.57
1:A:161:GLY:O	1:A:162:ASN:HB2	2.03	0.57
1:C:107:LEU:HD12	1:C:107:LEU:C	2.24	0.57
1:I:293:ASN:ND2	8:I:905:HOH:O	2.36	0.57
1:K:302:HIS:CE1	1:K:304:ILE:HB	2.40	0.57
1:A:225:LYS:NZ	3:M:2:GAL:O3	2.37	0.57
1:C:106:GLU:O	1:C:110:GLN:HG2	2.05	0.57
1:C:153:ASN:C	8:C:717:HOH:O	2.36	0.57
1:C:172:ILE:CG2	8:C:722:HOH:O	2.52	0.57
2:J:159:TYR:N	2:J:160:PRO:HD2	2.20	0.57
1:K:75:SER:CA	8:K:905:HOH:O	2.52	0.57
2:L:18:VAL:CA	8:L:226:HOH:O	2.52	0.57
1:C:14:HIS:N	2:D:21:TRP:O	2.37	0.57
2:L:123:ARG:HD2	8:L:217:HOH:O	2.05	0.57
1:A:145:ALA:C	1:A:147:ALA:N	2.58	0.57
1:K:13:TYR:CE1	2:L:12:GLY:O	2.58	0.57
1:A:28:LYS:NZ	6:A:602:NAG:O6	2.32	0.57
1:A:44:ASN:HD21	1:A:291:ALA:H	1.52	0.57
1:A:91:SER:HB3	8:A:717:HOH:O	1.94	0.57
1:A:313:VAL:CG1	1:A:315:SER:H	2.18	0.57
2:B:26:HIS:HD2	2:B:26:HIS:O	1.88	0.57
2:B:26:HIS:O	2:B:26:HIS:CD2	2.58	0.57
2:D:23:GLY:HA3	2:D:36:ALA:HA	1.86	0.57
2:D:69:GLU:N	8:D:208:HOH:O	1.86	0.57
1:I:25:VAL:O	2:L:51:LYS:HA	2.05	0.57
1:I:327:ILE:N	1:I:327:ILE:CD1	2.67	0.57
2:J:23:GLY:HA3	2:J:36:ALA:HA	1.87	0.57
1:K:44:ASN:HD21	1:K:291:ALA:H	1.51	0.57
1:A:188:PRO:HG2	1:A:194:GLN:NE2	2.20	0.56
1:C:58:LEU:HD11	1:C:63:ILE:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:CYS:HB3	1:E:281:CYS:O	2.04	0.56
1:I:173:ASN:ND2	1:I:179:VAL:HG23	2.19	0.56
2:L:124:SER:CA	8:L:205:HOH:O	2.53	0.56
2:H:23:GLY:HA3	2:H:36:ALA:HA	1.87	0.56
1:C:297:PRO:HG3	2:D:56:ILE:HA	1.87	0.56
2:D:160:PRO:O	2:D:161:LYS:HG2	2.05	0.56
1:E:305:THR:H	2:F:66:VAL:HG13	1.70	0.56
1:K:10:CYS:O	2:L:24:TYR:CA	2.53	0.56
1:K:13:TYR:CE1	2:L:12:GLY:C	2.78	0.56
2:L:19:ASP:C	8:L:228:HOH:O	2.11	0.56
1:C:155:ILE:HG22	1:C:157:LEU:CD1	2.36	0.56
1:E:11:ILE:O	2:F:10:ILE:HD13	2.05	0.56
2:F:123:ARG:HD2	2:F:132:GLU:OE1	2.05	0.56
1:K:259:TYR:HA	8:K:914:HOH:O	2.05	0.56
2:B:4:GLY:N	8:B:212:HOH:O	2.37	0.56
1:K:155:ILE:HD11	1:K:258:ARG:HD2	1.87	0.56
1:K:13:TYR:O	2:L:13:GLY:HA2	2.05	0.56
1:K:259:TYR:CA	8:K:914:HOH:O	2.54	0.56
1:C:29:ASN:ND2	8:C:706:HOH:O	2.09	0.56
1:E:188:PRO:HG2	1:E:194:GLN:NE2	2.21	0.56
1:E:305:THR:HB	8:E:719:HOH:O	1.98	0.56
1:G:188:PRO:HG2	1:G:194:GLN:NE2	2.21	0.56
1:I:133:ASP:HB3	1:I:158:VAL:HG23	1.88	0.56
1:I:224:PRO:HG2	1:K:209:SER:HA	1.88	0.56
1:K:44:ASN:ND2	1:K:291:ALA:H	2.04	0.56
1:A:23:ASP:O	2:B:104:ASN:ND2	2.22	0.56
1:A:106:GLU:O	1:A:110:GLN:HG2	2.06	0.56
1:A:302:HIS:CE1	1:A:304:ILE:HB	2.41	0.56
1:I:302:HIS:CE1	1:I:304:ILE:HB	2.41	0.56
1:I:307:GLY:HA2	2:J:63:PHE:CD1	2.41	0.56
1:C:131:ASN:ND2	1:I:243:GLY:HA3	2.21	0.56
3:Q:1:NAG:H83	3:Q:3:SIA:H112	1.88	0.56
1:A:29:ASN:OD1	6:A:602:NAG:O5	2.19	0.55
1:A:92:ASP:HB2	6:A:603:NAG:H82	1.88	0.55
1:A:266:ASN:H	1:A:266:ASN:ND2	2.05	0.55
1:C:48:CYS:HB3	1:C:281:CYS:O	2.06	0.55
1:K:133:ASP:HB3	1:K:158:VAL:HG23	1.88	0.55
2:B:119:TYR:CE1	2:B:136:GLY:HA2	2.42	0.55
1:G:302:HIS:CE1	1:G:304:ILE:HB	2.42	0.55
2:J:132:GLU:HG2	2:J:138:PHE:CE2	2.40	0.55
1:K:244:ASP:OD2	1:K:245:LYS:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ILE:N	8:A:712:HOH:O	2.40	0.55
2:F:23:GLY:HA3	2:F:36:ALA:HA	1.87	0.55
1:G:7:ASP:N	1:G:8:THR:CA	2.65	0.55
1:G:143:PRO:HD2	6:G:602:NAG:C6	2.36	0.55
1:I:48:CYS:HB3	1:I:281:CYS:O	2.06	0.55
2:B:117:ASN:ND2	8:B:209:HOH:O	2.02	0.55
1:E:313:VAL:CG1	1:E:315:SER:H	2.20	0.55
1:A:44:ASN:ND2	1:A:291:ALA:H	2.04	0.55
1:A:107:LEU:HD22	1:A:107:LEU:O	2.07	0.55
1:C:9:LEU:HD12	2:D:26:HIS:HA	1.88	0.55
1:C:133:ASP:HB3	1:C:158:VAL:HG23	1.88	0.55
1:C:159:LYS:NZ	1:C:199:GLN:NE2	2.53	0.55
1:G:7:ASP:N	2:H:140:PHE:CB	2.69	0.55
1:G:141:ALA:C	1:G:143:PRO:HD3	2.27	0.55
1:I:313:VAL:CG1	1:I:315:SER:H	2.20	0.55
2:D:159:TYR:H	2:D:160:PRO:CD	2.19	0.55
2:L:40:SER:N	8:L:207:HOH:O	2.39	0.55
1:A:11:ILE:CA	2:B:14:TRP:HH2	2.20	0.55
1:A:155:ILE:HD11	1:A:258:ARG:HD2	1.89	0.55
1:C:46:LYS:CD	8:C:719:HOH:O	2.55	0.55
1:G:311:LYS:HG3	2:H:92:TRP:CE2	2.42	0.55
1:C:119:ARG:O	1:C:119:ARG:HG2	2.04	0.55
1:G:44:ASN:ND2	1:G:291:ALA:H	2.05	0.55
2:H:132:GLU:HG2	2:H:138:PHE:CE2	2.40	0.55
1:K:56:LEU:HA	8:K:913:HOH:O	1.86	0.55
2:L:131:LYS:CG	8:L:225:HOH:O	2.55	0.55
1:A:297:PRO:HG3	2:B:56:ILE:HA	1.88	0.55
1:C:188:PRO:HG2	1:C:194:GLN:NE2	2.22	0.55
1:E:114:VAL:CG2	1:E:117:PHE:HB2	2.35	0.55
1:E:302:HIS:CE1	1:E:304:ILE:HB	2.41	0.55
2:J:79:ASN:HB3	2:L:68:LYS:HE3	1.89	0.55
1:A:133:ASP:HB3	1:A:158:VAL:HG23	1.89	0.55
1:C:44:ASN:HD21	1:C:291:ALA:H	1.53	0.55
1:E:51:ARG:NH2	8:E:703:HOH:O	2.39	0.55
1:E:266:ASN:HB2	8:E:714:HOH:O	2.06	0.55
1:G:90:SER:CB	8:G:719:HOH:O	2.43	0.55
1:K:239:LEU:HD13	1:K:265:ARG:NH1	2.22	0.55
2:D:132:GLU:HG2	2:D:138:PHE:CE2	2.39	0.54
1:E:155:ILE:HD11	1:E:258:ARG:HD2	1.89	0.54
1:G:7:ASP:CB	2:H:140:PHE:HB2	2.38	0.54
1:K:48:CYS:HB3	1:K:281:CYS:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLY:HA3	1:A:233:MET:O	2.08	0.54
1:C:8:THR:OG1	2:D:27:GLN:HB3	2.07	0.54
1:C:14:HIS:HB2	2:D:20:GLY:O	2.07	0.54
1:I:99:GLY:HA3	1:I:233:MET:O	2.08	0.54
1:I:266:ASN:H	1:I:266:ASN:ND2	2.05	0.54
1:K:63:ILE:HD11	1:K:85:ILE:HG21	1.90	0.54
1:A:324:LEU:N	1:A:324:LEU:HD23	2.21	0.54
1:E:44:ASN:ND2	1:E:291:ALA:H	2.04	0.54
1:E:99:GLY:HA3	1:E:233:MET:O	2.07	0.54
1:I:155:ILE:HD11	1:I:258:ARG:HD2	1.89	0.54
1:K:114:VAL:CG2	1:K:117:PHE:HB2	2.36	0.54
2:L:119:TYR:CE1	2:L:136:GLY:HA2	2.42	0.54
2:L:155:GLY:N	8:L:227:HOH:O	2.34	0.54
2:B:47:GLU:HB3	1:E:26:LEU:HB3	1.90	0.54
1:C:59:GLY:C	8:C:712:HOH:O	2.43	0.54
1:K:188:PRO:HG2	1:K:194:GLN:NE2	2.22	0.54
1:A:189:SER:HB2	1:A:222:ILE:HD13	1.90	0.54
1:A:311:LYS:HE2	2:B:61:THR:HG22	1.87	0.54
1:C:313:VAL:CG1	1:C:315:SER:H	2.20	0.54
1:G:313:VAL:CG1	1:G:315:SER:H	2.19	0.54
1:G:189:SER:HB2	1:G:222:ILE:HD13	1.90	0.54
1:I:141:ALA:C	1:I:143:PRO:HD3	2.27	0.54
2:J:119:TYR:CE1	2:J:136:GLY:HA2	2.43	0.54
1:K:189:SER:HB2	1:K:222:ILE:HD13	1.90	0.54
1:K:313:VAL:CG1	1:K:315:SER:H	2.20	0.54
2:L:155:GLY:CA	8:L:227:HOH:O	2.55	0.54
1:A:62:ASN:HA	1:A:87:GLU:OE1	2.07	0.54
1:A:183:TRP:HZ3	1:A:238:THR:HG22	1.73	0.54
2:B:95:ASN:HD21	2:D:95:ASN:ND2	2.05	0.54
1:C:72:GLU:HG2	6:C:601:NAG:H82	1.89	0.54
1:K:121:GLU:CD	8:K:906:HOH:O	2.45	0.54
1:K:141:ALA:C	1:K:143:PRO:HD3	2.28	0.54
1:E:39:LEU:HB2	1:E:318:LEU:HB2	1.90	0.54
1:G:327:ILE:HD12	2:H:12:GLY:HA2	1.89	0.54
1:I:29:ASN:ND2	8:I:901:HOH:O	2.22	0.54
1:I:96:CYS:O	1:I:227:ARG:HD3	2.08	0.54
1:I:116:SER:OG	1:I:264:GLU:CB	2.56	0.54
1:A:90:SER:HA	8:A:711:HOH:O	2.06	0.54
2:B:132:GLU:HG2	2:B:138:PHE:CE2	2.40	0.54
1:C:141:ALA:C	1:C:143:PRO:HD3	2.28	0.54
1:C:222:ILE:HG23	1:C:230:GLU:CG	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:SER:OG	1:E:319:ARG:NH1	2.41	0.54
1:E:133:ASP:HB3	1:E:158:VAL:HG23	1.89	0.54
1:G:48:CYS:HB3	1:G:281:CYS:O	2.08	0.54
2:H:119:TYR:CE1	2:H:136:GLY:HA2	2.43	0.54
1:K:25:VAL:HG22	2:L:102:LEU:HD12	1.89	0.54
1:K:122:ILE:CB	8:K:914:HOH:O	2.52	0.54
1:K:324:LEU:HD23	1:K:324:LEU:N	2.23	0.54
1:C:316:THR:HG23	1:C:317:LYS:N	2.22	0.54
1:G:13:TYR:CD2	2:H:6:ILE:HG12	2.43	0.54
1:G:312:TYR:HD2	2:H:89:LEU:HD13	1.73	0.54
1:A:48:CYS:HB3	1:A:281:CYS:O	2.08	0.53
1:C:63:ILE:HD11	1:C:85:ILE:HG21	1.90	0.53
1:C:172:ILE:HG22	8:C:722:HOH:O	2.06	0.53
1:G:183:TRP:HZ3	1:G:238:THR:HG22	1.73	0.53
2:H:66:VAL:C	8:H:205:HOH:O	2.11	0.53
1:I:44:ASN:HD21	1:I:291:ALA:H	1.56	0.53
1:K:14:HIS:NE2	1:K:15:ALA:C	2.61	0.53
1:C:314:LYS:NZ	2:F:60:ASN:O	2.42	0.53
1:G:155:ILE:HD11	1:G:258:ARG:HD2	1.91	0.53
1:G:266:ASN:H	1:G:266:ASN:ND2	2.05	0.53
1:C:44:ASN:ND2	1:C:291:ALA:H	2.06	0.53
1:E:96:CYS:O	1:E:227:ARG:HD3	2.08	0.53
1:E:141:ALA:C	1:E:143:PRO:HD3	2.28	0.53
1:E:324:LEU:N	1:E:324:LEU:HD23	2.23	0.53
2:B:127:LYS:H	2:B:127:LYS:CD	2.19	0.53
1:C:64:ALA:CB	8:C:729:HOH:O	2.54	0.53
1:C:99:GLY:HA3	1:C:233:MET:O	2.09	0.53
1:C:183:TRP:HZ3	1:C:238:THR:HG22	1.73	0.53
1:I:190:THR:O	1:I:193:ASP:N	2.42	0.53
1:K:99:GLY:HA3	1:K:233:MET:O	2.08	0.53
1:A:141:ALA:C	1:A:143:PRO:HD3	2.29	0.53
1:A:312:TYR:CD2	2:B:89:LEU:HD13	2.43	0.53
1:E:297:PRO:HG3	2:F:56:ILE:HA	1.90	0.53
1:K:292:ILE:CD1	1:K:301:ILE:HD12	2.39	0.53
1:E:266:ASN:C	8:E:714:HOH:O	2.46	0.53
1:I:44:ASN:ND2	1:I:291:ALA:H	2.07	0.53
1:A:133:ASP:CG	1:A:136:LYS:HD3	2.28	0.53
1:A:214:LYS:HG2	1:A:216:PHE:CE2	2.43	0.53
2:F:119:TYR:CE1	2:F:136:GLY:HA2	2.42	0.53
1:I:63:ILE:HD11	1:I:85:ILE:HG21	1.90	0.53
2:J:79:ASN:CB	2:L:68:LYS:HE3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ASN:CA	1:A:87:GLU:OE1	2.57	0.53
1:G:63:ILE:HD11	1:G:85:ILE:HG21	1.90	0.53
1:G:99:GLY:HA3	1:G:233:MET:O	2.09	0.53
1:G:107:LEU:HD22	1:G:111:LEU:HD22	1.91	0.53
1:I:183:TRP:HZ3	1:I:238:THR:HG22	1.74	0.53
1:K:75:SER:N	8:K:905:HOH:O	2.36	0.53
1:K:96:CYS:O	1:K:227:ARG:HD3	2.09	0.53
1:A:96:CYS:O	1:A:227:ARG:HD3	2.09	0.53
2:D:9:PHE:CD1	2:D:10:ILE:HG13	2.44	0.53
1:I:33:THR:HG22	1:I:326:ASN:OD1	2.09	0.53
2:B:76:ARG:NH1	2:D:69:GLU:O	2.40	0.52
2:F:159:TYR:CD1	2:F:161:LYS:HE3	2.43	0.52
1:K:14:HIS:O	1:K:15:ALA:HB2	2.09	0.52
1:E:63:ILE:HD11	1:E:85:ILE:HG21	1.91	0.52
1:I:305:THR:H	2:J:66:VAL:CG1	2.12	0.52
1:K:259:TYR:C	8:K:914:HOH:O	2.44	0.52
1:C:96:CYS:O	1:C:227:ARG:HD3	2.09	0.52
1:C:154:LEU:HA	8:C:717:HOH:O	2.08	0.52
1:C:302:HIS:CE1	1:C:304:ILE:HB	2.43	0.52
2:F:9:PHE:CD1	2:F:10:ILE:HG13	2.44	0.52
1:I:324:LEU:HD23	1:I:324:LEU:N	2.24	0.52
1:K:183:TRP:HZ3	1:K:238:THR:HG22	1.74	0.52
1:E:189:SER:HB2	1:E:222:ILE:HD13	1.91	0.52
2:F:132:GLU:HG2	2:F:138:PHE:CE2	2.39	0.52
1:G:324:LEU:N	1:G:324:LEU:HD23	2.24	0.52
1:I:312:TYR:HD2	2:J:89:LEU:HD13	1.75	0.52
1:C:266:ASN:ND2	1:C:266:ASN:H	2.06	0.52
1:E:72:GLU:CG	5:O:1:NAG:H82	2.34	0.52
1:E:281:CYS:CB	8:E:709:HOH:O	2.41	0.52
1:G:113:SER:HB2	1:G:269:SER:HB2	1.92	0.52
1:G:315:SER:HB3	8:H:207:HOH:O	2.08	0.52
1:C:311:LYS:HG3	2:D:92:TRP:CE2	2.45	0.52
1:E:312:TYR:HD2	2:F:89:LEU:HD13	1.74	0.52
1:I:50:LEU:HD13	2:J:63:PHE:CZ	2.45	0.52
1:A:62:ASN:HB2	8:A:709:HOH:O	2.09	0.52
1:A:159:LYS:HZ1	1:A:199:GLN:NE2	2.08	0.52
2:B:13:GLY:HA2	8:B:202:HOH:O	2.09	0.52
1:C:177:LYS:HB3	1:C:177:LYS:HZ2	1.75	0.52
1:E:317:LYS:O	1:E:318:LEU:HD23	2.10	0.52
1:I:327:ILE:N	1:I:327:ILE:HD13	2.25	0.52
1:C:189:SER:HB2	1:C:222:ILE:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:40:GLU:OE1	1:I:294:THR:CB	2.58	0.52
1:K:305:THR:HG22	2:L:66:VAL:HG12	1.91	0.52
1:A:62:ASN:OD1	1:A:62:ASN:N	2.30	0.51
1:G:7:ASP:N	2:H:140:PHE:HD1	2.08	0.51
1:G:312:TYR:CD2	2:H:89:LEU:HD13	2.45	0.51
2:J:106:ARG:HG3	8:J:206:HOH:O	2.10	0.51
1:A:63:ILE:HD11	1:A:85:ILE:HG21	1.91	0.51
1:C:77:SER:O	1:C:79:ALA:N	2.44	0.51
2:L:18:VAL:N	8:L:226:HOH:O	2.42	0.51
1:A:102:ILE:HG12	1:A:236:TYR:CE2	2.45	0.51
1:C:307:GLY:HA2	2:D:63:PHE:CE1	2.45	0.51
1:G:25:VAL:HG12	2:J:51:LYS:HG3	1.92	0.51
1:G:162:ASN:HD22	1:G:199:GLN:HE21	1.57	0.51
2:J:120:GLU:OE1	2:J:123:ARG:NH1	2.44	0.51
1:K:50:LEU:HD21	1:K:306:ILE:HG22	1.92	0.51
1:C:155:ILE:HG22	1:C:157:LEU:HD13	1.93	0.51
1:G:55:PRO:HB3	1:G:84:TYR:CE2	2.46	0.51
2:H:143:LYS:HA	2:H:143:LYS:HE2	1.93	0.51
1:K:82:TRP:CB	8:K:913:HOH:O	2.55	0.51
1:E:195:GLN:HA	1:E:198:TYR:O	2.11	0.51
8:H:213:HOH:O	2:J:67:GLY:N	2.04	0.51
1:I:120:PHE:HA	8:I:924:HOH:O	2.06	0.51
1:C:159:LYS:CD	1:C:199:GLN:HG2	2.40	0.51
1:E:183:TRP:HZ3	1:E:238:THR:HG22	1.74	0.51
2:H:113:SER:CB	2:L:2:LEU:HD22	2.40	0.51
1:A:223:ARG:HG3	1:C:206:PHE:HZ	1.76	0.51
1:C:44:ASN:C	1:C:44:ASN:HD22	2.13	0.51
1:E:63:ILE:HG12	1:E:87:GLU:OE1	2.11	0.51
2:L:9:PHE:CD1	2:L:10:ILE:HG13	2.46	0.51
1:A:55:PRO:HB3	1:A:84:TYR:CE2	2.46	0.51
1:E:312:TYR:CD2	2:F:89:LEU:HD13	2.46	0.51
2:H:9:PHE:CD1	2:H:10:ILE:HG13	2.46	0.51
1:I:224:PRO:O	1:I:232:ARG:NH2	2.43	0.51
1:E:13:TYR:CZ	2:F:6:ILE:HG23	2.46	0.50
1:E:55:PRO:HB3	1:E:84:TYR:CE2	2.46	0.50
1:G:307:GLY:HA2	2:H:63:PHE:CE1	2.46	0.50
1:I:231:GLY:C	1:I:232:ARG:HG2	2.32	0.50
2:J:25:HIS:HB2	2:J:34:TYR:CD2	2.46	0.50
2:L:29:GLU:HB2	8:L:212:HOH:O	2.10	0.50
1:E:33:THR:HG23	1:E:324:LEU:O	2.11	0.50
1:K:162:ASN:HA	1:K:199:GLN:HE21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ASN:C	1:A:132:HIS:CG	2.84	0.50
2:B:28:ASN:HD22	2:B:28:ASN:H	1.60	0.50
2:D:139:GLU:CG	8:D:212:HOH:O	2.59	0.50
1:C:63:ILE:HG12	1:C:87:GLU:OE1	2.12	0.50
2:L:139:GLU:OE2	8:L:211:HOH:O	2.20	0.50
1:A:58:LEU:HD21	1:A:63:ILE:HD13	1.94	0.50
1:A:159:LYS:HD3	1:A:199:GLN:H	1.77	0.50
1:G:93:ASN:ND2	6:G:602:NAG:O7	2.44	0.50
1:I:223:ARG:HG3	1:K:206:PHE:HZ	1.77	0.50
1:K:27:GLU:HB2	8:K:921:HOH:O	2.10	0.50
2:B:9:PHE:CD1	2:B:10:ILE:HG13	2.46	0.50
1:C:167:LEU:C	1:C:167:LEU:HD12	2.32	0.50
2:D:122:VAL:O	2:D:125:GLN:HB2	2.11	0.50
1:G:7:ASP:N	2:H:140:PHE:CD1	2.80	0.50
1:K:25:VAL:HG21	2:L:102:LEU:HD12	1.93	0.50
2:B:87:GLY:HA3	2:D:88:PHE:CZ	2.47	0.50
1:G:122:ILE:HG23	1:G:123:PHE:N	2.27	0.50
1:I:55:PRO:HB3	1:I:84:TYR:CE2	2.47	0.50
1:I:311:LYS:HE2	2:J:61:THR:HG22	1.94	0.50
1:K:239:LEU:CD1	1:K:265:ARG:HH11	2.24	0.50
2:B:14:TRP:CE3	2:B:17:MET:HE2	2.36	0.50
2:J:151:SER:HB2	2:J:156:THR:O	2.12	0.50
2:L:143:LYS:HE2	2:L:143:LYS:HA	1.94	0.50
1:A:33:THR:OG1	1:A:34:HIS:ND1	2.30	0.49
1:A:159:LYS:HZ2	1:A:199:GLN:HE21	1.57	0.49
1:C:74:GLU:OE1	1:C:144:HIS:CE1	2.64	0.49
1:E:311:LYS:HG3	2:F:92:TRP:CE2	2.47	0.49
1:C:206:PHE:HD2	1:C:215:LYS:HB2	1.77	0.49
2:F:143:LYS:HA	2:F:143:LYS:HE2	1.93	0.49
1:G:167:LEU:C	1:G:167:LEU:HD12	2.33	0.49
1:I:40:GLU:OE1	1:I:294:THR:HB	2.12	0.49
1:I:190:THR:C	1:I:192:ALA:N	2.66	0.49
1:K:15:ALA:HB1	1:K:327:ILE:O	2.12	0.49
1:A:33:THR:HB	1:A:34:HIS:CE1	2.47	0.49
2:J:9:PHE:CD1	2:J:10:ILE:HG13	2.47	0.49
2:J:28:ASN:H	2:J:28:ASN:HD22	1.60	0.49
2:B:143:LYS:HE2	2:B:143:LYS:HA	1.93	0.49
2:D:143:LYS:HE2	2:D:143:LYS:HA	1.93	0.49
1:E:162:ASN:HD22	1:E:199:GLN:HE21	1.59	0.49
1:E:266:ASN:ND2	1:E:266:ASN:H	2.09	0.49
1:E:282:ASN:ND2	1:E:282:ASN:C	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:40:GLU:OE1	8:G:718:HOH:O	2.20	0.49
1:G:63:ILE:HG12	1:G:87:GLU:OE1	2.13	0.49
1:K:44:ASN:C	1:K:44:ASN:HD22	2.15	0.49
3:Q:3:SIA:H6	3:Q:3:SIA:O1A	2.11	0.49
2:L:28:ASN:H	2:L:28:ASN:HD22	1.60	0.49
2:L:151:SER:HB2	2:L:156:THR:O	2.13	0.49
2:B:27:GLN:O	2:B:27:GLN:HG3	2.13	0.49
1:I:116:SER:OG	1:I:264:GLU:HB2	2.13	0.49
1:A:305:THR:HG22	1:A:306:ILE:N	2.27	0.49
2:D:38:LEU:O	2:D:42:GLN:HB2	2.12	0.49
1:K:55:PRO:HB3	1:K:84:TYR:CE2	2.47	0.49
1:A:12:GLY:HA3	2:B:14:TRP:CZ2	2.47	0.49
1:C:25:VAL:HG21	2:D:102:LEU:HD12	1.94	0.49
2:D:9:PHE:CE1	2:D:10:ILE:HG13	2.48	0.49
2:H:126:LEU:HB3	2:H:157:TYR:CE2	2.48	0.49
2:H:151:SER:HB2	2:H:156:THR:O	2.12	0.49
2:L:27:GLN:O	2:L:27:GLN:HG3	2.12	0.49
1:A:122:ILE:HG23	1:A:123:PHE:N	2.28	0.49
1:A:305:THR:CG2	1:A:306:ILE:N	2.76	0.49
1:C:55:PRO:HB3	1:C:84:TYR:CE2	2.47	0.49
1:G:155:ILE:HG13	1:G:258:ARG:HB2	1.94	0.49
1:I:116:SER:OG	1:I:264:GLU:HB3	2.13	0.49
2:J:126:LEU:HB3	2:J:157:TYR:CE2	2.47	0.49
4:P:4:SIA:O1A	4:P:4:SIA:H6	2.13	0.49
1:A:155:ILE:HG13	1:A:258:ARG:HB2	1.95	0.48
1:E:155:ILE:HG13	1:E:258:ARG:HB2	1.95	0.48
2:F:151:SER:HB2	2:F:156:THR:O	2.13	0.48
1:G:33:THR:HG23	1:G:324:LEU:O	2.13	0.48
1:K:122:ILE:CG2	8:K:914:HOH:O	2.18	0.48
1:A:44:ASN:C	1:A:44:ASN:HD22	2.16	0.48
1:C:92:ASP:HB2	6:C:601:NAG:O6	2.12	0.48
1:E:122:ILE:HG23	1:E:123:PHE:N	2.28	0.48
1:G:44:ASN:C	1:G:44:ASN:HD22	2.15	0.48
2:H:28:ASN:H	2:H:28:ASN:HD22	1.61	0.48
1:I:14:HIS:NE2	8:I:909:HOH:O	2.34	0.48
1:I:167:LEU:HD12	1:I:167:LEU:C	2.33	0.48
2:J:132:GLU:CD	8:J:212:HOH:O	2.45	0.48
1:K:305:THR:HG22	2:L:66:VAL:CG1	2.43	0.48
1:A:62:ASN:CB	1:A:87:GLU:OE1	2.61	0.48
2:B:123:ARG:O	2:B:123:ARG:CG	2.62	0.48
2:B:151:SER:HB2	2:B:156:THR:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:ASN:O	1:C:46:LYS:HG3	2.13	0.48
1:I:308:LYS:HE2	2:J:61:THR:O	2.12	0.48
1:K:63:ILE:HG12	1:K:87:GLU:OE1	2.12	0.48
2:L:126:LEU:HB3	2:L:157:TYR:CE2	2.47	0.48
1:A:55:PRO:HB3	1:A:84:TYR:CZ	2.49	0.48
2:H:158:ASP:C	2:H:160:PRO:HD3	2.34	0.48
1:K:47:LEU:HD22	1:K:276:THR:O	2.14	0.48
2:L:124:SER:N	8:L:205:HOH:O	2.45	0.48
2:B:126:LEU:HB3	2:B:157:TYR:CE2	2.49	0.48
1:C:176:GLY:C	1:C:177:LYS:CG	2.82	0.48
2:H:159:TYR:N	2:H:160:PRO:HD3	2.28	0.48
1:I:76:LEU:O	1:I:77:SER:CB	2.52	0.48
1:A:159:LYS:NZ	1:A:199:GLN:HE21	2.12	0.48
2:B:125:GLN:NE2	2:B:157:TYR:HB3	2.28	0.48
2:F:9:PHE:CE1	2:F:10:ILE:HG13	2.49	0.48
2:F:28:ASN:HD22	2:F:28:ASN:H	1.60	0.48
2:F:126:LEU:HB3	2:F:157:TYR:CE2	2.48	0.48
1:G:113:SER:HB2	1:G:269:SER:CB	2.43	0.48
1:I:55:PRO:HB3	1:I:84:TYR:CZ	2.49	0.48
2:J:159:TYR:H	2:J:160:PRO:CD	2.25	0.48
2:J:162:TYR:O	8:J:216:HOH:O	2.20	0.48
2:B:93:THR:O	2:B:97:GLU:HG2	2.14	0.48
2:B:124:SER:O	2:B:127:LYS:HE3	2.13	0.48
1:G:25:VAL:HG21	2:H:102:LEU:HD22	1.95	0.48
1:G:58:LEU:HD21	1:G:63:ILE:HD13	1.95	0.48
1:I:33:THR:HG23	1:I:324:LEU:O	2.14	0.48
2:D:28:ASN:HD22	2:D:28:ASN:H	1.61	0.48
2:J:97:GLU:HB3	2:L:58:LYS:HD2	1.95	0.48
2:J:143:LYS:HE2	2:J:143:LYS:HA	1.94	0.48
1:K:121:GLU:OE2	8:K:906:HOH:O	2.20	0.48
2:L:124:SER:O	2:L:127:LYS:HE3	2.13	0.48
1:A:74:GLU:CA	8:A:737:HOH:O	2.58	0.48
1:A:137:GLY:HA3	1:A:156:TRP:HB3	1.95	0.48
1:A:188:PRO:HG2	1:A:194:GLN:HE21	1.78	0.48
1:C:55:PRO:HB3	1:C:84:TYR:CZ	2.49	0.48
2:D:151:SER:HB2	2:D:156:THR:O	2.13	0.48
1:E:55:PRO:HB3	1:E:84:TYR:CZ	2.49	0.48
1:I:128:SER:N	8:I:911:HOH:O	2.47	0.48
1:A:33:THR:OG1	1:A:323:GLY:HA3	2.14	0.47
1:A:109:GLU:N	8:A:734:HOH:O	2.45	0.47
1:A:188:PRO:HD3	1:A:253:ASN:ND2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:126:LEU:HB3	2:D:157:TYR:CE2	2.49	0.47
1:E:11:ILE:HD13	2:F:119:TYR:HA	1.95	0.47
2:J:142:HIS:NE2	2:J:161:LYS:HD3	2.24	0.47
1:A:312:TYR:HD2	2:B:89:LEU:HD13	1.78	0.47
1:C:122:ILE:HG23	1:C:123:PHE:N	2.28	0.47
1:C:216:PHE:CD1	1:C:216:PHE:N	2.82	0.47
1:E:25:VAL:HG21	2:F:102:LEU:HD12	1.94	0.47
1:I:155:ILE:HG13	1:I:258:ARG:HB2	1.96	0.47
1:K:122:ILE:HG23	1:K:123:PHE:N	2.29	0.47
2:L:17:MET:HG2	8:L:226:HOH:O	2.13	0.47
1:C:167:LEU:HD12	1:C:167:LEU:O	2.14	0.47
1:E:9:LEU:N	2:F:138:PHE:O	2.42	0.47
2:F:124:SER:O	2:F:127:LYS:HE3	2.13	0.47
1:G:55:PRO:HB3	1:G:84:TYR:CZ	2.49	0.47
2:H:27:GLN:O	2:H:27:GLN:HG3	2.15	0.47
2:H:87:GLY:HA3	2:J:88:PHE:CZ	2.49	0.47
2:H:124:SER:O	2:H:127:LYS:HE3	2.14	0.47
1:I:167:LEU:HD12	1:I:167:LEU:O	2.14	0.47
1:A:34:HIS:ND1	1:A:34:HIS:N	2.61	0.47
1:A:313:VAL:HG12	1:A:315:SER:N	2.28	0.47
1:C:223:ARG:O	1:C:230:GLU:CG	2.62	0.47
2:J:124:SER:O	2:J:127:LYS:HE3	2.15	0.47
1:C:129:TRP:CG	1:C:157:LEU:HD21	2.49	0.47
1:E:44:ASN:C	1:E:44:ASN:HD22	2.16	0.47
1:I:122:ILE:HG23	1:I:123:PHE:N	2.29	0.47
1:C:217:LYS:N	8:C:727:HOH:O	2.06	0.47
1:K:13:TYR:O	2:L:14:TRP:N	2.44	0.47
1:K:155:ILE:HG13	1:K:258:ARG:HB2	1.97	0.47
1:A:12:GLY:N	2:B:14:TRP:CZ3	2.82	0.47
1:A:33:THR:HG1	1:A:34:HIS:CE1	2.28	0.47
1:A:141:ALA:O	1:A:227:ARG:NH1	2.42	0.47
2:B:9:PHE:CE1	2:B:10:ILE:HG13	2.50	0.47
1:C:117:PHE:CD2	1:C:263:MET:HG3	2.49	0.47
2:D:161:LYS:O	2:D:162:TYR:HB2	2.15	0.47
1:E:14:HIS:CD2	1:E:15:ALA:N	2.82	0.47
2:L:17:MET:SD	2:L:23:GLY:HA3	2.55	0.47
1:A:195:GLN:HG3	1:A:196:SER:N	2.30	0.47
1:K:44:ASN:O	1:K:46:LYS:HG3	2.15	0.47
1:K:55:PRO:HB3	1:K:84:TYR:CZ	2.50	0.47
8:K:925:HOH:O	2:L:13:GLY:HA2	2.15	0.47
2:L:9:PHE:CE1	2:L:10:ILE:HG13	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LEU:HD23	1:A:107:LEU:HA	1.69	0.47
1:A:131:ASN:O	1:A:132:HIS:CD2	2.68	0.47
1:A:173:ASN:ND2	1:A:179:VAL:HG23	2.30	0.47
1:C:226:VAL:HG12	1:C:227:ARG:HG3	1.97	0.47
1:G:44:ASN:O	1:G:46:LYS:HG3	2.15	0.47
1:A:12:GLY:CA	2:B:14:TRP:CH2	2.98	0.47
1:A:195:GLN:CG	8:A:704:HOH:O	2.54	0.47
1:C:14:HIS:CD2	1:C:15:ALA:N	2.83	0.47
1:C:311:LYS:HE2	2:D:61:THR:HG22	1.96	0.47
2:D:159:TYR:O	2:D:161:LYS:N	2.48	0.47
2:F:27:GLN:O	2:F:27:GLN:HG3	2.15	0.47
1:I:44:ASN:HD21	1:I:291:ALA:N	2.12	0.47
1:I:226:VAL:HG12	1:I:227:ARG:HG3	1.97	0.47
1:K:13:TYR:O	2:L:13:GLY:CA	2.62	0.47
1:A:132:HIS:HE1	1:A:165:PRO:O	1.98	0.46
1:K:14:HIS:CD2	1:K:15:ALA:O	2.65	0.46
1:K:188:PRO:HG2	1:K:194:GLN:HE21	1.80	0.46
1:E:125:LYS:HB2	1:E:258:ARG:NH1	2.30	0.46
1:E:132:HIS:HE1	1:E:165:PRO:O	1.98	0.46
1:G:14:HIS:CD2	1:G:15:ALA:N	2.83	0.46
1:G:188:PRO:HG2	1:G:194:GLN:HE21	1.80	0.46
1:G:316:THR:N	8:H:207:HOH:O	2.46	0.46
1:K:39:LEU:HB2	1:K:318:LEU:HB2	1.96	0.46
1:K:132:HIS:HE1	1:K:165:PRO:O	1.98	0.46
1:A:311:LYS:HG3	2:B:92:TRP:CE2	2.50	0.46
1:C:141:ALA:O	1:C:227:ARG:NH1	2.41	0.46
2:D:87:GLY:HA3	2:F:88:PHE:CZ	2.50	0.46
1:C:177:LYS:HZ3	1:C:177:LYS:HG2	1.43	0.46
1:G:125:LYS:HB2	1:G:258:ARG:NH1	2.29	0.46
2:J:27:GLN:HG3	2:J:27:GLN:O	2.15	0.46
1:K:162:ASN:OD1	1:K:199:GLN:CD	2.51	0.46
2:B:28:ASN:H	2:B:28:ASN:ND2	2.14	0.46
1:G:268:GLY:N	8:G:709:HOH:O	2.48	0.46
2:H:9:PHE:CE1	2:H:10:ILE:HG13	2.50	0.46
1:K:213:SER:N	8:K:910:HOH:O	2.38	0.46
1:A:11:ILE:C	2:B:14:TRP:HH2	2.18	0.46
1:A:198:TYR:O	1:A:199:GLN:C	2.54	0.46
2:D:27:GLN:O	2:D:27:GLN:HG3	2.14	0.46
1:A:44:ASN:O	1:A:46:LYS:HG3	2.16	0.46
1:E:25:VAL:HG22	2:F:102:LEU:HD12	1.98	0.46
1:G:197:LEU:HD11	7:G:603:SIA:H91	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:132:HIS:HE1	1:I:165:PRO:O	1.99	0.46
1:A:164:TYR:CZ	1:A:252:GLY:HA2	2.51	0.46
2:D:71:ASN:OD1	2:D:73:LEU:N	2.39	0.46
1:I:171:TYR:CE2	1:I:173:ASN:HA	2.51	0.46
1:C:51:ARG:NH1	1:C:51:ARG:HB3	2.30	0.46
1:C:74:GLU:OE1	1:C:144:HIS:HE1	1.99	0.46
1:I:26:LEU:HD23	2:L:47:GLU:OE1	2.16	0.46
1:I:125:LYS:HB2	1:I:258:ARG:NH1	2.31	0.46
1:K:33:THR:HG23	1:K:324:LEU:O	2.14	0.46
1:E:159:LYS:HD2	1:E:199:GLN:HG2	1.98	0.45
1:A:22:VAL:HG21	1:A:321:ALA:HB2	1.98	0.45
1:E:244:ASP:OD2	1:E:245:LYS:N	2.48	0.45
1:K:14:HIS:CD2	1:K:15:ALA:CA	2.98	0.45
2:B:91:ILE:HD13	2:D:91:ILE:HG21	1.98	0.45
1:E:8:THR:HG22	2:F:139:GLU:CA	2.46	0.45
1:E:188:PRO:HG2	1:E:194:GLN:HE21	1.79	0.45
1:E:289:LYS:HB3	1:E:289:LYS:HE3	1.40	0.45
1:G:7:ASP:HB2	2:H:140:PHE:HB2	1.97	0.45
1:G:167:LEU:HD12	1:G:167:LEU:O	2.15	0.45
2:J:9:PHE:CE1	2:J:10:ILE:HG13	2.51	0.45
1:K:226:VAL:HG12	1:K:227:ARG:HG3	1.98	0.45
2:L:28:ASN:H	2:L:28:ASN:ND2	2.14	0.45
1:C:132:HIS:HE1	1:C:165:PRO:O	2.00	0.45
1:E:226:VAL:HG12	1:E:227:ARG:HG3	1.97	0.45
2:H:91:ILE:HD13	2:J:91:ILE:HG21	1.97	0.45
2:H:120:GLU:OE1	2:H:123:ARG:NH1	2.49	0.45
1:K:10:CYS:O	2:L:24:TYR:HB3	2.17	0.45
1:C:316:THR:HG23	1:C:317:LYS:HG2	1.97	0.45
1:G:106:GLU:OE1	2:L:75:LYS:N	2.50	0.45
1:G:122:ILE:HG23	1:G:123:PHE:H	1.81	0.45
1:I:44:ASN:HD21	1:I:291:ALA:CA	2.29	0.45
1:K:311:LYS:HE2	2:L:61:THR:HG22	1.98	0.45
1:A:39:LEU:HB2	1:A:318:LEU:HB2	1.99	0.45
2:D:28:ASN:H	2:D:28:ASN:ND2	2.15	0.45
1:E:266:ASN:ND2	1:E:266:ASN:N	2.64	0.45
1:I:10:CYS:HA	2:J:137:CYS:HA	1.99	0.45
2:J:17:MET:SD	2:J:23:GLY:HA3	2.56	0.45
1:K:129:TRP:CD2	1:K:157:LEU:HD11	2.52	0.45
1:K:254:LEU:N	8:K:917:HOH:O	2.48	0.45
1:A:74:GLU:N	8:A:737:HOH:O	2.49	0.45
1:A:266:ASN:ND2	1:A:266:ASN:N	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:266:ASN:HD22	1:K:266:ASN:N	1.94	0.45
1:C:39:LEU:HB2	1:C:318:LEU:HB2	1.98	0.45
1:C:159:LYS:HZ2	1:C:199:GLN:NE2	1.96	0.45
2:D:53:ASN:O	2:D:57:GLU:HB2	2.17	0.45
2:F:28:ASN:H	2:F:28:ASN:ND2	2.15	0.45
1:G:164:TYR:CZ	1:G:252:GLY:HA2	2.52	0.45
1:I:145:ALA:CA	8:I:903:HOH:O	2.54	0.45
1:I:164:TYR:CZ	1:I:252:GLY:HA2	2.52	0.45
1:K:7:ASP:HA	2:L:28:ASN:HA	1.97	0.45
1:K:195:GLN:HG3	1:K:196:SER:N	2.31	0.45
2:B:51:LYS:HA	1:E:25:VAL:O	2.16	0.45
1:C:214:LYS:HZ2	1:C:214:LYS:HG2	1.67	0.45
2:D:87:GLY:HA3	2:F:88:PHE:CE1	2.52	0.45
1:E:164:TYR:CZ	1:E:252:GLY:HA2	2.52	0.45
1:E:327:ILE:HD12	2:F:12:GLY:HA2	1.98	0.45
2:H:28:ASN:H	2:H:28:ASN:ND2	2.15	0.45
1:I:28:LYS:HG3	2:L:50:ASN:OD1	2.16	0.45
1:K:106:GLU:CB	8:K:915:HOH:O	2.04	0.45
2:H:17:MET:SD	2:H:23:GLY:HA3	2.57	0.45
2:J:18:VAL:C	8:J:211:HOH:O	2.43	0.45
1:K:22:VAL:HG21	1:K:321:ALA:HB2	1.98	0.45
1:K:141:ALA:O	1:K:227:ARG:NH1	2.41	0.45
2:D:147:THR:HA	2:D:150:GLU:HB2	1.99	0.44
1:G:39:LEU:HB2	1:G:318:LEU:HB2	1.98	0.44
1:G:266:ASN:ND2	1:G:266:ASN:N	2.65	0.44
2:J:28:ASN:H	2:J:28:ASN:ND2	2.15	0.44
1:K:22:VAL:HG12	1:K:319:ARG:HG2	1.98	0.44
1:C:22:VAL:HG21	1:C:321:ALA:HB2	1.99	0.44
2:F:17:MET:SD	2:F:23:GLY:HA3	2.57	0.44
2:F:28:ASN:HD22	2:F:28:ASN:N	2.16	0.44
1:G:29:ASN:OD1	6:G:601:NAG:N2	2.50	0.44
1:G:78:THR:O	1:G:79:ALA:C	2.55	0.44
1:K:13:TYR:CE2	2:L:10:ILE:HG22	2.52	0.44
1:K:324:LEU:CD2	2:L:21:TRP:CD1	2.98	0.44
1:A:14:HIS:CD2	1:A:15:ALA:N	2.85	0.44
1:E:54:ALA:HB1	1:E:55:PRO:HD2	1.98	0.44
1:G:114:VAL:CG1	1:G:117:PHE:HB2	2.40	0.44
1:K:164:TYR:CZ	1:K:252:GLY:HA2	2.52	0.44
1:A:33:THR:CB	1:A:34:HIS:ND1	2.79	0.44
1:A:76:LEU:CA	8:A:738:HOH:O	2.48	0.44
2:B:23:GLY:HA3	2:B:36:ALA:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:159:LYS:HD2	1:G:199:GLN:HG2	1.98	0.44
1:I:51:ARG:HB2	1:I:53:VAL:CG1	2.48	0.44
1:I:195:GLN:HG3	1:I:196:SER:N	2.31	0.44
1:K:54:ALA:HB1	1:K:55:PRO:HD2	2.00	0.44
1:A:226:VAL:HG12	1:A:227:ARG:HG3	1.99	0.44
2:B:87:GLY:HA3	2:D:88:PHE:CE1	2.53	0.44
1:C:231:GLY:N	8:C:701:HOH:O	2.50	0.44
1:E:22:VAL:HG21	1:E:321:ALA:HB2	2.00	0.44
1:K:47:LEU:HD12	1:K:286:GLN:NE2	2.32	0.44
1:K:266:ASN:O	1:K:267:ALA:C	2.55	0.44
1:A:7:ASP:HA	1:A:8:THR:HA	1.79	0.44
1:A:72:GLU:C	1:A:74:GLU:H	2.21	0.44
1:A:108:ARG:CB	8:A:734:HOH:O	1.88	0.44
1:C:164:TYR:CZ	1:C:252:GLY:HA2	2.52	0.44
2:H:160:PRO:HD2	2:H:161:LYS:HG3	2.00	0.44
1:K:125:LYS:HB2	1:K:258:ARG:NH1	2.33	0.44
1:C:14:HIS:HB2	2:D:21:TRP:HA	2.00	0.44
1:C:305:THR:HG22	2:D:66:VAL:HG12	1.99	0.44
1:E:129:TRP:CD2	1:E:157:LEU:HD11	2.53	0.44
1:G:22:VAL:HG21	1:G:321:ALA:HB2	1.99	0.44
1:I:53:VAL:O	1:I:53:VAL:HG22	2.18	0.44
1:K:51:ARG:HB3	1:K:51:ARG:CZ	2.48	0.44
1:K:105:GLU:OE2	8:K:920:HOH:O	2.21	0.44
1:C:188:PRO:HG2	1:C:194:GLN:HE21	1.81	0.44
1:E:307:GLY:HA2	2:F:63:PHE:CE1	2.52	0.44
2:J:125:GLN:HE22	2:J:155:GLY:C	2.21	0.44
1:K:311:LYS:HG3	2:L:92:TRP:CE2	2.52	0.44
2:B:14:TRP:CE3	2:B:17:MET:HE1	2.53	0.43
1:E:205:VAL:HG21	1:E:254:LEU:HD13	2.00	0.43
2:H:30:GLN:H	2:H:30:GLN:HE21	1.66	0.43
2:J:28:ASN:HD22	2:J:28:ASN:N	2.16	0.43
2:J:123:ARG:HB2	2:J:138:PHE:HZ	1.83	0.43
2:L:131:LYS:HE3	2:L:133:ILE:HD13	2.00	0.43
1:A:122:ILE:HG23	1:A:123:PHE:H	1.83	0.43
1:A:204:TYR:CD1	1:A:204:TYR:O	2.71	0.43
1:A:233:MET:HB2	1:A:233:MET:HE3	1.91	0.43
2:B:160:PRO:HD2	2:B:161:LYS:HG3	2.00	0.43
1:C:76:LEU:HB3	1:C:77:SER:H	1.47	0.43
1:G:145:ALA:C	1:G:147:ALA:H	2.22	0.43
1:I:265:ARG:NH2	8:I:910:HOH:O	2.50	0.43
1:K:122:ILE:HG23	1:K:123:PHE:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:3:SIA:O1A	3:M:3:SIA:H6	2.17	0.43
1:C:22:VAL:HG12	1:C:319:ARG:HG2	1.99	0.43
1:E:313:VAL:HG12	1:E:315:SER:N	2.30	0.43
1:G:72:GLU:C	1:G:74:GLU:H	2.21	0.43
1:I:72:GLU:C	1:I:74:GLU:H	2.22	0.43
2:L:159:TYR:CD1	2:L:161:LYS:HD2	2.53	0.43
1:A:302:HIS:HA	1:A:303:PRO:HD3	1.84	0.43
1:I:41:ASP:C	1:I:41:ASP:OD1	2.56	0.43
1:I:314:LYS:NZ	2:L:60:ASN:O	2.46	0.43
1:K:13:TYR:CZ	2:L:12:GLY:O	2.71	0.43
2:B:30:GLN:H	2:B:30:GLN:HE21	1.66	0.43
2:B:71:ASN:ND2	2:B:71:ASN:N	2.30	0.43
2:D:28:ASN:HD22	2:D:28:ASN:N	2.16	0.43
2:F:125:GLN:HE22	2:F:155:GLY:C	2.21	0.43
1:I:313:VAL:HG12	1:I:315:SER:N	2.30	0.43
1:A:159:LYS:HZ1	1:A:199:GLN:HE22	1.67	0.43
1:A:214:LYS:HE3	1:A:216:PHE:CE2	2.53	0.43
1:C:107:LEU:O	1:C:108:ARG:C	2.55	0.43
1:C:173:ASN:ND2	1:C:179:VAL:HG23	2.33	0.43
1:C:195:GLN:HG3	1:C:196:SER:N	2.31	0.43
2:D:120:GLU:O	2:D:124:SER:OG	2.37	0.43
1:E:122:ILE:HG23	1:E:123:PHE:H	1.83	0.43
1:E:195:GLN:HG3	1:E:196:SER:N	2.31	0.43
1:G:54:ALA:HB1	1:G:55:PRO:HD2	2.00	0.43
1:I:12:GLY:N	2:J:14:TRP:CH2	2.87	0.43
1:I:42:LYS:HE3	1:I:42:LYS:HB2	1.87	0.43
1:K:14:HIS:O	2:L:13:GLY:HA3	2.18	0.43
1:K:16:ASN:N	8:K:904:HOH:O	2.30	0.43
1:C:117:PHE:HD2	1:C:263:MET:HG3	1.82	0.43
1:E:47:LEU:HD22	1:E:276:THR:O	2.19	0.43
1:E:296:LEU:HA	1:E:296:LEU:HD23	1.70	0.43
1:E:319:ARG:NH1	1:E:319:ARG:HG3	2.30	0.43
2:J:159:TYR:O	2:J:161:LYS:N	2.52	0.43
2:L:30:GLN:H	2:L:30:GLN:HE21	1.67	0.43
1:C:122:ILE:HG23	1:C:123:PHE:H	1.83	0.43
1:E:173:ASN:ND2	1:E:179:VAL:HG23	2.34	0.43
2:F:30:GLN:HE21	2:F:30:GLN:H	1.67	0.43
1:G:311:LYS:HE2	2:H:61:THR:HG22	2.00	0.43
1:I:39:LEU:HB2	1:I:318:LEU:HB2	2.01	0.43
1:K:276:THR:HA	1:K:277:PRO:HD3	1.87	0.43
2:D:79:ASN:ND2	1:E:109:GLU:OE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:195:GLN:HG3	1:G:196:SER:N	2.32	0.43
1:G:313:VAL:HG12	1:G:315:SER:N	2.30	0.43
1:I:76:LEU:N	1:I:76:LEU:HD23	2.34	0.43
1:I:78:THR:O	1:I:79:ALA:C	2.57	0.43
2:J:26:HIS:NE2	2:J:31:GLY:O	2.52	0.43
2:B:26:HIS:CD2	2:B:26:HIS:C	2.91	0.43
1:I:197:LEU:HD11	3:Q:3:SIA:H91	2.01	0.43
2:J:30:GLN:H	2:J:30:GLN:HE21	1.67	0.43
1:K:307:GLY:HA2	2:L:63:PHE:CE1	2.54	0.43
2:L:152:VAL:HG23	8:L:223:HOH:O	2.18	0.43
1:A:33:THR:C	1:A:34:HIS:ND1	2.73	0.42
1:C:72:GLU:C	1:C:74:GLU:H	2.21	0.42
2:D:30:GLN:H	2:D:30:GLN:HE21	1.67	0.42
1:K:173:ASN:ND2	1:K:179:VAL:HG23	2.33	0.42
2:B:17:MET:HE2	2:B:17:MET:HB2	1.76	0.42
1:C:273:ILE:N	1:C:273:ILE:HD12	2.33	0.42
2:F:71:ASN:O	8:F:203:HOH:O	2.21	0.42
1:G:11:ILE:O	2:H:10:ILE:HD13	2.19	0.42
1:G:223:ARG:HG3	1:I:206:PHE:HZ	1.84	0.42
1:I:51:ARG:HB3	1:I:51:ARG:NH1	2.34	0.42
1:K:114:VAL:CA	1:K:266:ASN:HD21	2.32	0.42
1:C:78:THR:O	1:C:79:ALA:C	2.58	0.42
1:C:159:LYS:HD2	1:C:199:GLN:HG2	2.01	0.42
1:C:266:ASN:ND2	1:C:266:ASN:N	2.65	0.42
1:G:268:GLY:CA	8:G:709:HOH:O	2.59	0.42
1:I:22:VAL:HG21	1:I:321:ALA:HB2	2.00	0.42
1:A:169:LYS:HG3	1:A:170:SER:H	1.84	0.42
1:C:11:ILE:HD11	2:D:24:TYR:HE2	1.73	0.42
1:E:318:LEU:HD23	1:E:318:LEU:HA	1.75	0.42
1:I:145:ALA:C	1:I:147:ALA:H	2.22	0.42
1:K:72:GLU:C	1:K:74:GLU:H	2.22	0.42
1:K:167:LEU:C	1:K:167:LEU:HD23	2.40	0.42
2:L:5:ALA:HB3	2:L:112:ASP:OD2	2.20	0.42
1:A:54:ALA:HB1	1:A:55:PRO:HD2	2.01	0.42
1:A:167:LEU:HD12	1:A:168:SER:N	2.32	0.42
1:A:266:ASN:N	1:A:266:ASN:HD22	2.18	0.42
1:A:273:ILE:HD12	1:A:273:ILE:N	2.35	0.42
1:A:62:ASN:HB2	1:A:87:GLU:OE1	2.19	0.42
1:A:324:LEU:HD23	1:A:324:LEU:H	1.84	0.42
1:C:145:ALA:C	1:C:147:ALA:H	2.23	0.42
1:E:8:THR:HA	2:F:138:PHE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:LEU:O	1:E:76:LEU:HD11	2.19	0.42
2:F:4:GLY:O	2:F:8:GLY:HA3	2.20	0.42
1:I:176:GLY:C	1:I:177:LYS:HG2	2.39	0.42
1:K:13:TYR:CE2	2:L:6:ILE:HA	2.53	0.42
1:K:145:ALA:C	1:K:147:ALA:H	2.23	0.42
2:D:116:LYS:O	2:D:119:TYR:HB3	2.20	0.42
1:E:8:THR:CA	2:F:138:PHE:O	2.68	0.42
1:E:68:LEU:O	1:E:151:TYR:HB3	2.19	0.42
1:E:305:THR:HG21	8:E:719:HOH:O	2.18	0.42
2:H:75:LYS:HG3	1:I:109:GLU:HG2	2.01	0.42
2:H:131:LYS:HE3	2:H:133:ILE:HD13	2.02	0.42
1:E:72:GLU:C	1:E:74:GLU:H	2.22	0.42
1:E:273:ILE:N	1:E:273:ILE:HD12	2.34	0.42
1:I:125:LYS:CB	1:I:258:ARG:NH1	2.83	0.42
1:I:229:GLN:HB3	8:I:922:HOH:O	2.19	0.42
1:K:68:LEU:O	1:K:151:TYR:HB3	2.19	0.42
1:A:91:SER:OG	8:A:717:HOH:O	2.21	0.42
1:C:313:VAL:HG12	1:C:315:SER:N	2.30	0.42
1:E:8:THR:HA	2:F:139:GLU:HA	2.02	0.42
1:G:68:LEU:O	1:G:151:TYR:HB3	2.20	0.42
1:I:244:ASP:OD2	1:I:245:LYS:N	2.53	0.42
2:J:102:LEU:O	2:J:106:ARG:HG3	2.20	0.42
2:L:125:GLN:HE22	2:L:155:GLY:C	2.23	0.42
2:F:127:LYS:H	2:F:127:LYS:CD	2.21	0.42
1:A:125:LYS:HB2	1:A:258:ARG:NH1	2.35	0.41
1:A:236:TYR:HE1	8:A:721:HOH:O	2.03	0.41
2:B:106:ARG:HH21	2:F:106:ARG:NH1	2.17	0.41
1:C:69:GLY:O	1:C:152:LYS:CG	2.62	0.41
1:C:77:SER:O	1:C:78:THR:C	2.59	0.41
1:E:145:ALA:C	1:E:147:ALA:H	2.23	0.41
1:E:233:MET:HB2	1:E:233:MET:HE3	1.91	0.41
2:F:127:LYS:HD2	2:F:127:LYS:N	2.24	0.41
1:G:125:LYS:CB	1:G:258:ARG:NH1	2.83	0.41
1:I:50:LEU:HD13	2:J:63:PHE:HZ	1.83	0.41
1:K:239:LEU:HD13	1:K:265:ARG:HH11	1.84	0.41
2:L:18:VAL:C	8:L:226:HOH:O	2.49	0.41
1:A:141:ALA:O	1:A:143:PRO:HD3	2.20	0.41
1:A:327:ILE:CB	8:A:712:HOH:O	2.68	0.41
2:B:59:MET:O	2:B:59:MET:HG3	2.19	0.41
2:D:131:LYS:HE3	2:D:133:ILE:HD13	2.01	0.41
1:G:173:ASN:ND2	1:G:179:VAL:HG23	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:231:GLY:O	1:I:232:ARG:HG2	2.20	0.41
2:J:5:ALA:HB3	2:J:112:ASP:OD2	2.20	0.41
1:K:313:VAL:HG12	1:K:315:SER:N	2.30	0.41
1:A:100:ASP:O	1:A:102:ILE:CD1	2.68	0.41
2:B:4:GLY:O	2:B:8:GLY:HA3	2.19	0.41
2:B:123:ARG:HB2	2:B:138:PHE:HZ	1.84	0.41
1:C:70:ASN:HA	1:C:71:PRO:HD3	1.96	0.41
2:F:131:LYS:HE3	2:F:133:ILE:HD13	2.02	0.41
1:G:144:HIS:HE1	8:G:716:HOH:O	2.03	0.41
1:I:122:ILE:HG23	1:I:123:PHE:H	1.84	0.41
1:I:190:THR:CG2	1:I:193:ASP:CA	2.98	0.41
1:A:244:ASP:OD2	1:A:245:LYS:N	2.54	0.41
2:B:91:ILE:HG21	2:F:91:ILE:HD13	2.01	0.41
1:C:51:ARG:HB3	1:C:51:ARG:HH11	1.86	0.41
1:C:244:ASP:OD2	1:C:245:LYS:N	2.54	0.41
1:E:13:TYR:HE2	2:F:6:ILE:HA	1.78	0.41
1:G:269:SER:N	8:G:702:HOH:O	1.85	0.41
1:G:273:ILE:HD12	1:G:273:ILE:N	2.36	0.41
1:I:125:LYS:HB2	1:I:258:ARG:HH11	1.85	0.41
2:B:131:LYS:HE3	2:B:133:ILE:HD13	2.02	0.41
1:C:222:ILE:CG2	1:C:230:GLU:HG2	2.46	0.41
1:E:167:LEU:C	1:E:167:LEU:HD23	2.41	0.41
1:G:51:ARG:NH1	1:G:51:ARG:HB3	2.35	0.41
1:I:13:TYR:HB2	1:I:324:LEU:HD11	2.03	0.41
1:K:144:HIS:O	1:K:145:ALA:HB3	2.21	0.41
1:K:161:GLY:O	1:K:162:ASN:HB3	2.20	0.41
1:C:258:ARG:HH11	1:C:258:ARG:HD2	1.72	0.41
1:E:51:ARG:NH1	1:E:51:ARG:HB3	2.35	0.41
1:G:25:VAL:CG1	2:J:51:LYS:HG3	2.51	0.41
1:I:70:ASN:HA	1:I:71:PRO:HD3	1.93	0.41
1:I:200:ASN:OD1	1:I:200:ASN:N	2.54	0.41
1:K:266:ASN:O	1:K:267:ALA:O	2.38	0.41
1:K:302:HIS:HA	1:K:303:PRO:HD3	1.85	0.41
1:A:8:THR:CG2	2:B:138:PHE:C	2.80	0.41
1:A:160:LYS:O	1:A:161:GLY:C	2.59	0.41
1:E:118:GLU:CG	1:E:262:ALA:HB3	2.51	0.41
1:E:311:LYS:HE2	2:F:61:THR:HG22	2.02	0.41
1:G:118:GLU:CG	1:G:262:ALA:HB3	2.50	0.41
1:G:125:LYS:HB2	1:G:258:ARG:HH11	1.84	0.41
1:I:141:ALA:O	1:I:227:ARG:NH1	2.42	0.41
1:A:114:VAL:O	8:A:740:HOH:O	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:HIS:O	1:A:145:ALA:HB3	2.21	0.41
1:C:13:TYR:HA	2:D:21:TRP:O	2.20	0.41
2:D:159:TYR:N	2:D:160:PRO:HD2	2.36	0.41
2:H:28:ASN:HD22	2:H:28:ASN:N	2.16	0.41
1:I:25:VAL:HG11	2:L:51:LYS:HG3	1.98	0.41
2:J:87:GLY:HA3	2:L:88:PHE:CZ	2.56	0.41
1:K:297:PRO:HG3	2:L:56:ILE:HA	2.03	0.41
1:A:70:ASN:HA	1:A:71:PRO:HD3	1.95	0.41
1:A:327:ILE:CA	8:A:712:HOH:O	2.69	0.41
1:C:77:SER:C	1:C:79:ALA:N	2.74	0.41
1:E:125:LYS:CB	1:E:258:ARG:NH1	2.83	0.41
1:E:141:ALA:O	1:E:227:ARG:NH1	2.41	0.41
1:E:294:THR:HG22	8:E:704:HOH:O	2.20	0.41
1:G:162:ASN:HD22	1:G:162:ASN:HA	1.74	0.41
1:G:296:LEU:HA	1:G:297:PRO:HD3	1.87	0.41
2:H:4:GLY:O	2:H:8:GLY:HA3	2.21	0.41
1:I:26:LEU:HG	2:L:47:GLU:HB3	2.03	0.41
1:I:41:ASP:OD1	1:I:41:ASP:N	2.49	0.41
2:J:131:LYS:HE3	2:J:133:ILE:HD13	2.03	0.41
1:K:292:ILE:CG2	1:K:294:THR:HG22	2.51	0.41
2:B:4:GLY:HA2	8:B:212:HOH:O	2.12	0.41
2:H:127:LYS:HD2	2:H:127:LYS:N	2.23	0.41
1:C:276:THR:HA	1:C:277:PRO:HD3	1.87	0.40
1:C:302:HIS:HA	1:C:303:PRO:HD3	1.85	0.40
2:D:139:GLU:HG3	8:D:212:HOH:O	2.18	0.40
1:E:63:ILE:O	1:E:67:ILE:HG12	2.21	0.40
1:E:107:LEU:HB2	1:E:237:TRP:CE2	2.57	0.40
1:G:14:HIS:N	2:H:21:TRP:O	2.54	0.40
2:H:51:LYS:HG3	1:K:25:VAL:HG12	2.02	0.40
1:I:68:LEU:O	1:I:151:TYR:HB3	2.20	0.40
1:A:51:ARG:HH21	1:A:53:VAL:HG21	1.86	0.40
1:A:68:LEU:O	1:A:151:TYR:HB3	2.21	0.40
1:C:157:LEU:HA	1:C:157:LEU:HD12	1.81	0.40
1:G:13:TYR:CZ	2:H:6:ILE:HG23	2.56	0.40
1:G:118:GLU:HG3	1:G:262:ALA:HB3	2.03	0.40
1:G:155:ILE:HG22	1:G:157:LEU:HD13	2.03	0.40
1:I:63:ILE:O	1:I:67:ILE:HG12	2.22	0.40
1:I:118:GLU:CG	1:I:262:ALA:HB3	2.51	0.40
1:K:71:PRO:O	1:K:74:GLU:HB2	2.21	0.40
1:K:125:LYS:HB2	1:K:258:ARG:HH11	1.87	0.40
1:C:54:ALA:HB1	1:C:55:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:308:LYS:HE3	1:E:308:LYS:HB2	1.93	0.40
1:G:244:ASP:OD2	1:G:245:LYS:N	2.55	0.40
1:I:173:ASN:HD21	1:I:179:VAL:HG23	1.87	0.40
1:I:273:ILE:N	1:I:273:ILE:HD12	2.36	0.40
1:K:42:LYS:HB2	1:K:42:LYS:HE3	1.88	0.40
1:K:119:ARG:HB2	1:K:261:PHE:CD2	2.56	0.40
2:L:4:GLY:O	2:L:8:GLY:HA3	2.21	0.40
2:B:97:GLU:CA	8:B:213:HOH:O	2.24	0.40
1:C:63:ILE:O	1:C:67:ILE:HG12	2.21	0.40
2:D:161:LYS:O	2:D:162:TYR:CB	2.70	0.40
1:E:78:THR:O	1:E:79:ALA:C	2.59	0.40
1:G:129:TRP:CG	1:G:157:LEU:HD21	2.57	0.40
1:I:204:TYR:CD1	1:I:215:LYS:HE3	2.57	0.40
2:J:87:GLY:HA3	2:L:88:PHE:CE1	2.57	0.40
1:K:24:THR:HG22	2:L:104:ASN:CB	2.47	0.40
1:K:273:ILE:HD12	1:K:273:ILE:N	2.36	0.40
2:L:157:TYR:HD1	8:L:223:HOH:O	1.89	0.40
2:D:119:TYR:CE1	2:D:136:GLY:HA2	2.56	0.40
1:E:204:TYR:CD1	1:E:215:LYS:HE3	2.56	0.40
1:E:266:ASN:N	1:E:266:ASN:HD22	2.18	0.40
1:G:63:ILE:O	1:G:67:ILE:HG12	2.21	0.40
1:I:120:PHE:N	8:I:924:HOH:O	2.50	0.40
2:J:136:GLY:HA3	8:J:208:HOH:O	2.20	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:ARG:NH2	2:L:38:LEU:CD2[1_565]	1.96	0.24
1:E:79:ALA:N	2:L:150:GLU:OE2[1_565]	2.01	0.19
1:E:258:ARG:NH2	2:L:42:GLN:OE1[1_565]	2.04	0.16
1:E:81:SER:OG	2:L:146:ASN:OD1[1_565]	2.12	0.08

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	319/321 (99%)	295 (92%)	23 (7%)	1 (0%)	41	76
1	C	319/321 (99%)	296 (93%)	19 (6%)	4 (1%)	12	45
1	E	319/321 (99%)	295 (92%)	23 (7%)	1 (0%)	41	76
1	G	319/321 (99%)	292 (92%)	27 (8%)	0	100	100
1	I	319/321 (99%)	291 (91%)	26 (8%)	2 (1%)	25	64
1	K	319/321 (99%)	290 (91%)	29 (9%)	0	100	100
2	B	160/162 (99%)	146 (91%)	13 (8%)	1 (1%)	25	64
2	D	160/162 (99%)	143 (89%)	16 (10%)	1 (1%)	25	64
2	F	159/162 (98%)	145 (91%)	14 (9%)	0	100	100
2	H	160/162 (99%)	146 (91%)	14 (9%)	0	100	100
2	J	160/162 (99%)	144 (90%)	16 (10%)	0	100	100
2	L	159/162 (98%)	145 (91%)	13 (8%)	1 (1%)	25	64
All	All	2872/2898 (99%)	2628 (92%)	233 (8%)	11 (0%)	34	72

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	160	PRO
1	A	146	GLY
1	C	77	SER
1	C	78	THR
1	C	161	GLY
1	I	78	THR
1	C	79	ALA
2	L	161	LYS
2	D	119	TYR
1	E	79	ALA
1	I	79	ALA

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	281/282 (100%)	248 (88%)	33 (12%)	5 22
1	C	282/282 (100%)	248 (88%)	34 (12%)	5 21
1	E	282/282 (100%)	254 (90%)	28 (10%)	8 30
1	G	281/282 (100%)	258 (92%)	23 (8%)	11 39
1	I	282/282 (100%)	247 (88%)	35 (12%)	4 20
1	K	282/282 (100%)	255 (90%)	27 (10%)	8 32
2	B	139/139 (100%)	128 (92%)	11 (8%)	12 41
2	D	138/139 (99%)	125 (91%)	13 (9%)	8 32
2	F	139/139 (100%)	126 (91%)	13 (9%)	8 32
2	H	139/139 (100%)	130 (94%)	9 (6%)	17 50
2	J	138/139 (99%)	128 (93%)	10 (7%)	14 45
2	L	139/139 (100%)	128 (92%)	11 (8%)	12 41
All	All	2522/2526 (100%)	2275 (90%)	247 (10%)	8 30

All (247) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	13	TYR
1	A	27	GLU
1	A	34	HIS
1	A	37	ASN
1	A	44	ASN
1	A	50	LEU
1	A	58	LEU
1	A	90	SER
1	A	101	PHE
1	A	102	ILE
1	A	107	LEU
1	A	111	LEU
1	A	136	LYS
1	A	157	LEU
1	A	160	LYS
1	A	167	LEU
1	A	169	LYS
1	A	177	LYS
1	A	190	THR

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Mol	Chain	Res	Type
1	A	195	GLN
1	A	196	SER
1	A	198	TYR
1	A	211	ARG
1	A	228	ASP
1	A	240	VAL
1	A	265	ARG
1	A	266	ASN
1	A	275	ASP
1	A	316	THR
1	A	324	LEU
1	A	326	ASN
1	A	327	ILE
2	B	24	TYR
2	B	28	ASN
2	B	30	GLN
2	B	38	LEU
2	B	68	LYS
2	B	71	ASN
2	B	80	LEU
2	B	106	ARG
2	B	123	ARG
2	B	126	LEU
2	B	154	ASN
1	C	26	LEU
1	C	37	ASN
1	C	44	ASN
1	C	51	ARG
1	C	53	VAL
1	C	67	ILE
1	C	90	SER
1	C	107	LEU
1	C	111	LEU
1	C	115	SER
1	C	119	ARG
1	C	148	LYS
1	C	152	LYS
1	C	160	LYS
1	C	167	LEU
1	C	168	SER
1	C	177	LYS
1	C	190	THR

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Mol	Chain	Res	Type
1	C	195	GLN
1	C	198	TYR
1	C	211	ARG
1	C	214	LYS
1	C	216	PHE
1	C	228	ASP
1	C	230	GLU
1	C	258	ARG
1	C	263	MET
1	C	265	ARG
1	C	266	ASN
1	C	305	THR
1	C	316	THR
1	C	317	LYS
1	C	324	LEU
1	C	325	ARG
2	D	17	MET
2	D	22	TYR
2	D	28	ASN
2	D	30	GLN
2	D	38	LEU
2	D	66	VAL
2	D	80	LEU
2	D	98	LEU
2	D	124	SER
2	D	126	LEU
2	D	150	GLU
2	D	154	ASN
2	D	158	ASP
1	E	9	LEU
1	E	32	VAL
1	E	37	ASN
1	E	44	ASN
1	E	47	LEU
1	E	51	ARG
1	E	67	ILE
1	E	101	PHE
1	E	111	LEU
1	E	114	VAL
1	E	167	LEU
1	E	190	THR
1	E	195	GLN

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Mol	Chain	Res	Type
1	E	198	TYR
1	E	205	VAL
1	E	211	ARG
1	E	214	LYS
1	E	217	LYS
1	E	228	ASP
1	E	230	GLU
1	E	232	ARG
1	E	266	ASN
1	E	282	ASN
1	E	289	LYS
1	E	305	THR
1	E	316	THR
1	E	319	ARG
1	E	324	LEU
2	F	2	LEU
2	F	19	ASP
2	F	22	TYR
2	F	28	ASN
2	F	30	GLN
2	F	66	VAL
2	F	80	LEU
2	F	83	LYS
2	F	98	LEU
2	F	122	VAL
2	F	126	LEU
2	F	154	ASN
2	F	159	TYR
1	G	37	ASN
1	G	44	ASN
1	G	50	LEU
1	G	51	ARG
1	G	58	LEU
1	G	67	ILE
1	G	107	LEU
1	G	111	LEU
1	G	157	LEU
1	G	167	LEU
1	G	190	THR
1	G	195	GLN
1	G	198	TYR
1	G	214	LYS

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Mol	Chain	Res	Type
1	G	228	ASP
1	G	240	VAL
1	G	265	ARG
1	G	266	ASN
1	G	269	SER
1	G	305	THR
1	G	316	THR
1	G	319	ARG
1	G	324	LEU
2	H	22	TYR
2	H	28	ASN
2	H	30	GLN
2	H	38	LEU
2	H	80	LEU
2	H	123	ARG
2	H	126	LEU
2	H	154	ASN
2	H	158	ASP
1	I	37	ASN
1	I	44	ASN
1	I	50	LEU
1	I	51	ARG
1	I	53	VAL
1	I	67	ILE
1	I	75	SER
1	I	76	LEU
1	I	77	SER
1	I	101	PHE
1	I	111	LEU
1	I	116	SER
1	I	134	SER
1	I	157	LEU
1	I	167	LEU
1	I	172	ILE
1	I	177	LYS
1	I	178	GLU
1	I	191	SER
1	I	194	GLN
1	I	195	GLN
1	I	198	TYR
1	I	200	ASN
1	I	211	ARG

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Mol	Chain	Res	Type
1	I	214	LYS
1	I	228	ASP
1	I	263	MET
1	I	265	ARG
1	I	266	ASN
1	I	289	LYS
1	I	305	THR
1	I	316	THR
1	I	319	ARG
1	I	324	LEU
1	I	327	ILE
2	J	22	TYR
2	J	26	HIS
2	J	28	ASN
2	J	30	GLN
2	J	66	VAL
2	J	80	LEU
2	J	98	LEU
2	J	126	LEU
2	J	154	ASN
2	J	158	ASP
1	K	9	LEU
1	K	11	ILE
1	K	32	VAL
1	K	37	ASN
1	K	44	ASN
1	K	47	LEU
1	K	50	LEU
1	K	51	ARG
1	K	80	SER
1	K	101	PHE
1	K	111	LEU
1	K	114	VAL
1	K	167	LEU
1	K	190	THR
1	K	195	GLN
1	K	198	TYR
1	K	205	VAL
1	K	211	ARG
1	K	214	LYS
1	K	228	ASP
1	K	246	ILE

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Mol	Chain	Res	Type
1	K	265	ARG
1	K	266	ASN
1	K	293	ASN
1	K	305	THR
1	K	316	THR
1	K	324	LEU
2	L	2	LEU
2	L	22	TYR
2	L	28	ASN
2	L	30	GLN
2	L	66	VAL
2	L	80	LEU
2	L	98	LEU
2	L	122	VAL
2	L	126	LEU
2	L	154	ASN
2	L	159	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	44	ASN
1	A	132	HIS
1	A	162	ASN
1	A	194	GLN
1	A	195	GLN
1	A	199	GLN
1	A	266	ASN
2	B	26	HIS
2	B	27	GLN
2	B	28	ASN
2	B	71	ASN
2	B	125	GLN
2	B	129	ASN
2	B	146	ASN
1	C	14	HIS
1	C	37	ASN
1	C	44	ASN
1	C	131	ASN
1	C	132	HIS
1	C	144	HIS

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Mol	Chain	Res	Type
1	C	162	ASN
1	C	194	GLN
1	C	199	GLN
1	C	253	ASN
1	C	266	ASN
2	D	27	GLN
2	D	28	ASN
2	D	95	ASN
2	D	129	ASN
2	D	142	HIS
2	D	146	ASN
1	E	14	HIS
1	E	37	ASN
1	E	44	ASN
1	E	132	HIS
1	E	162	ASN
1	E	194	GLN
1	E	199	GLN
1	E	253	ASN
1	E	266	ASN
1	E	282	ASN
2	F	27	GLN
2	F	28	ASN
2	F	125	GLN
2	F	129	ASN
2	F	146	ASN
1	G	14	HIS
1	G	37	ASN
1	G	44	ASN
1	G	162	ASN
1	G	194	GLN
1	G	199	GLN
1	G	253	ASN
1	G	266	ASN
2	H	27	GLN
2	H	28	ASN
2	H	95	ASN
2	H	129	ASN
2	H	146	ASN
1	I	37	ASN
1	I	44	ASN
1	I	93	ASN

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Mol	Chain	Res	Type
1	I	132	HIS
1	I	162	ASN
1	I	194	GLN
1	I	199	GLN
1	I	253	ASN
1	I	266	ASN
2	J	26	HIS
2	J	27	GLN
2	J	28	ASN
2	J	125	GLN
2	J	129	ASN
2	J	142	HIS
2	J	146	ASN
1	K	37	ASN
1	K	44	ASN
1	K	93	ASN
1	K	132	HIS
1	K	194	GLN
1	K	199	GLN
1	K	253	ASN
1	K	266	ASN
1	K	293	ASN
2	L	27	GLN
2	L	28	ASN
2	L	125	GLN
2	L	128	ASN
2	L	129	ASN
2	L	146	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

19 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	M	1	3	14,14,15	0.60	0	17,19,21	0.96	0
3	GAL	M	2	3	11,11,12	0.62	0	15,15,17	0.78	0
3	SIA	M	3	3	20,20,21	0.73	0	21,28,31	3.60	2 (9%)
4	GAL	N	1	4	11,11,12	0.70	0	15,15,17	0.91	1 (6%)
4	NAG	N	2	4	14,14,15	0.58	0	17,19,21	1.27	2 (11%)
4	GAL	N	3	4	11,11,12	0.57	0	15,15,17	0.93	1 (6%)
4	SIA	N	4	4	20,20,21	0.66	0	21,28,31	3.85	2 (9%)
5	NAG	O	1	5,1	14,14,15	0.57	0	17,19,21	0.75	0
5	NAG	O	2	5	14,14,15	0.45	0	17,19,21	0.78	0
4	GAL	P	1	4	11,11,12	0.63	0	15,15,17	0.54	0
4	NAG	P	2	4	14,14,15	0.61	0	17,19,21	0.76	0
4	GAL	P	3	4	11,11,12	0.68	0	15,15,17	0.75	0
4	SIA	P	4	4	20,20,21	0.74	0	21,28,31	3.33	2 (9%)
3	NAG	Q	1	3	14,14,15	0.49	0	17,19,21	0.69	0
3	GAL	Q	2	3	11,11,12	0.71	0	15,15,17	1.11	2 (13%)
3	SIA	Q	3	3	20,20,21	0.63	0	21,28,31	3.53	3 (14%)
3	NAG	R	1	3	14,14,15	0.51	0	17,19,21	0.67	0
3	GAL	R	2	3	11,11,12	0.60	0	15,15,17	0.78	0
3	SIA	R	3	3	20,20,21	0.62	0	21,28,31	3.57	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	1	3	-	0/6/23/26	0/1/1/1
3	GAL	M	2	3	-	0/2/19/22	0/1/1/1
3	SIA	M	3	3	-	3/18/34/38	0/1/1/1
4	GAL	N	1	4	-	1/2/19/22	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
4	GAL	N	3	4	-	0/2/19/22	0/1/1/1
4	SIA	N	4	4	-	3/18/34/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	O	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
4	GAL	P	1	4	-	0/2/19/22	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
4	GAL	P	3	4	-	0/2/19/22	0/1/1/1
4	SIA	P	4	4	-	3/18/34/38	0/1/1/1
3	NAG	Q	1	3	-	0/6/23/26	0/1/1/1
3	GAL	Q	2	3	-	0/2/19/22	0/1/1/1
3	SIA	Q	3	3	-	2/18/34/38	0/1/1/1
3	NAG	R	1	3	-	0/6/23/26	0/1/1/1
3	GAL	R	2	3	-	2/2/19/22	0/1/1/1
3	SIA	R	3	3	-	4/18/34/38	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	N	4	SIA	O6-C2-C3	-15.23	90.09	110.56
3	M	3	SIA	O6-C2-C3	-13.85	91.93	110.56
3	R	3	SIA	O6-C2-C3	-13.53	92.37	110.56
3	Q	3	SIA	O6-C2-C3	-13.51	92.39	110.56
4	P	4	SIA	O6-C2-C3	-12.98	93.11	110.56
3	R	3	SIA	O6-C2-C1	8.52	123.80	107.72
3	M	3	SIA	O6-C2-C1	8.34	123.47	107.72
4	N	4	SIA	O6-C2-C1	8.27	123.34	107.72
3	Q	3	SIA	O6-C2-C1	8.11	123.03	107.72
4	P	4	SIA	O6-C2-C1	7.54	121.95	107.72
4	N	2	NAG	C1-O5-C5	3.09	116.33	112.19
4	N	2	NAG	C4-C3-C2	2.54	114.74	111.02
4	N	3	GAL	O5-C5-C6	2.43	112.40	107.66
3	Q	2	GAL	C1-C2-C3	2.41	113.15	109.64
4	N	1	GAL	C3-C4-C5	2.28	114.37	110.23
3	Q	3	SIA	O1B-C1-C2	2.11	118.19	112.71
3	R	3	SIA	C8-C7-C6	-2.09	109.13	113.05
3	Q	2	GAL	C1-O5-C5	-2.03	109.46	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	R	2	GAL	C4-C5-C6-O6
3	R	2	GAL	O5-C5-C6-O6
3	M	3	SIA	C11-C10-N5-C5
3	M	3	SIA	O10-C10-N5-C5
3	Q	3	SIA	C11-C10-N5-C5
3	Q	3	SIA	O10-C10-N5-C5
3	R	3	SIA	C11-C10-N5-C5
3	R	3	SIA	O10-C10-N5-C5
4	N	4	SIA	C11-C10-N5-C5
4	N	4	SIA	O10-C10-N5-C5
4	P	4	SIA	C11-C10-N5-C5
4	P	4	SIA	O10-C10-N5-C5
3	R	3	SIA	O8-C8-C9-O9
3	R	3	SIA	C7-C8-C9-O9
3	M	3	SIA	O1A-C1-C2-O6
4	N	4	SIA	O1A-C1-C2-O6
4	P	4	SIA	O1A-C1-C2-O6
4	N	1	GAL	O5-C5-C6-O6

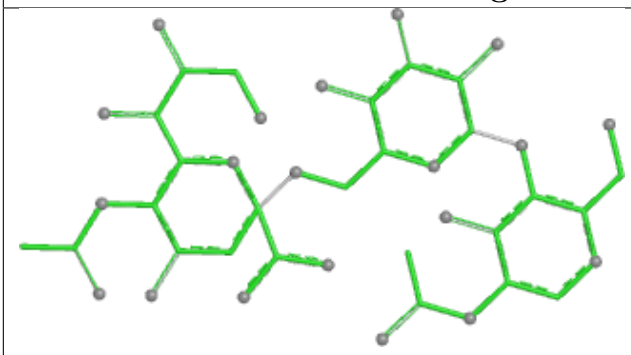
There are no ring outliers.

9 monomers are involved in 13 short contacts:

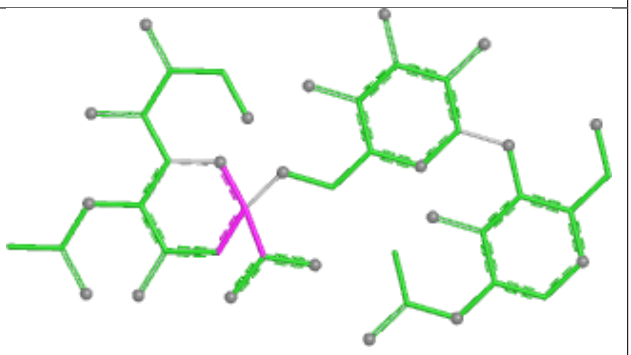
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	2	GAL	1	0
3	Q	1	NAG	1	0
4	P	4	SIA	2	0
5	O	1	NAG	3	0
3	M	1	NAG	2	0
4	N	4	SIA	1	0
3	M	3	SIA	1	0
3	Q	3	SIA	3	0
5	O	2	NAG	1	0

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

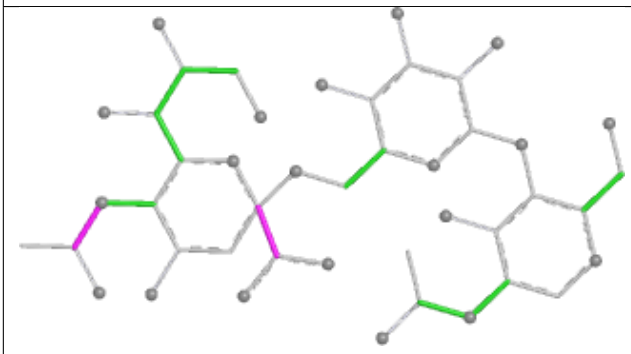
Oligosaccharide Chain M



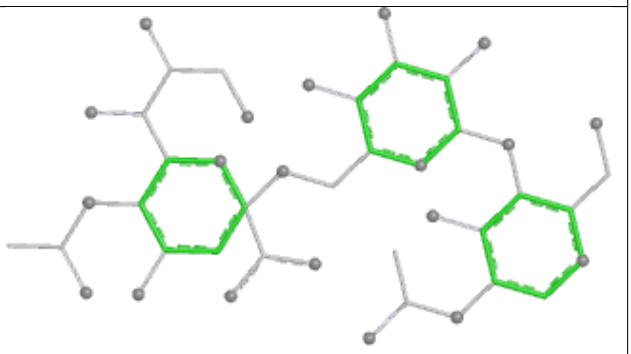
Bond lengths



Bond angles

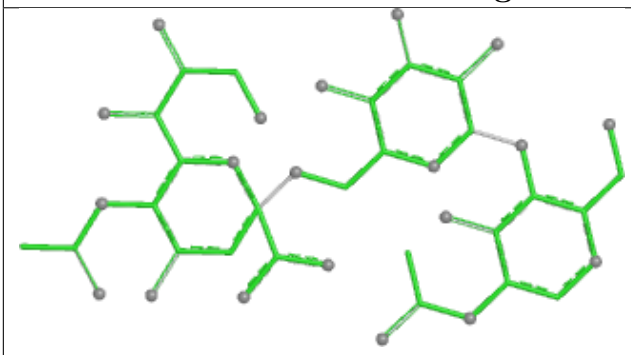


Torsions

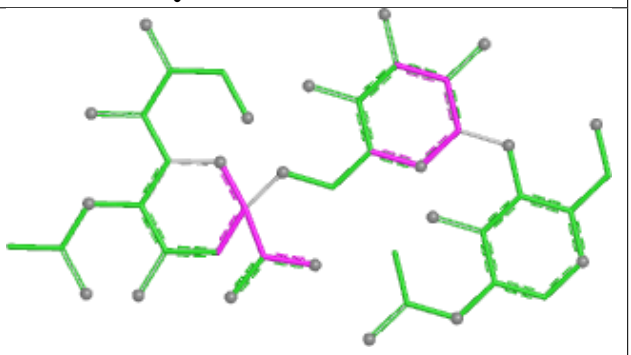


Rings

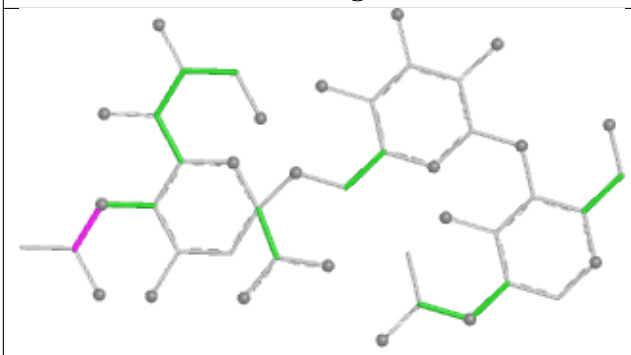
Oligosaccharide Chain Q



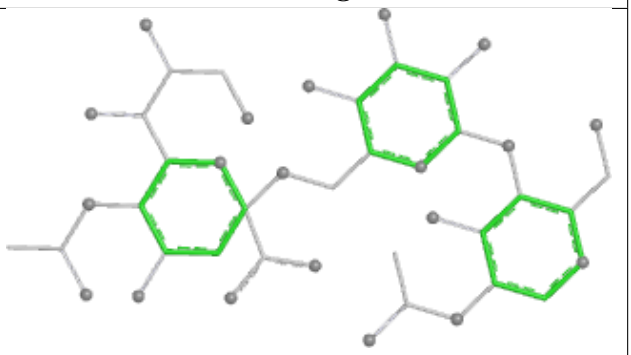
Bond lengths



Bond angles

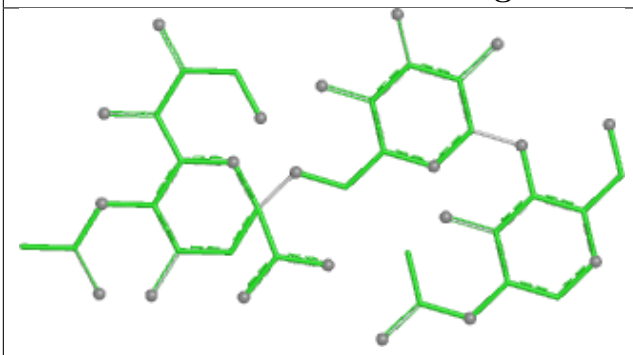


Torsions

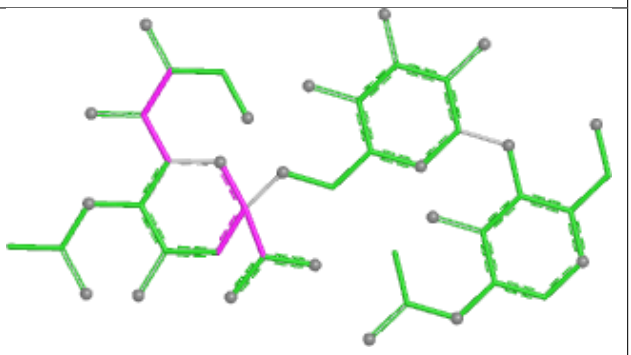


Rings

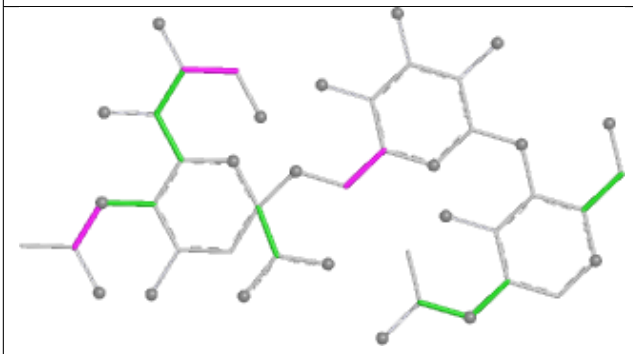
Oligosaccharide Chain R



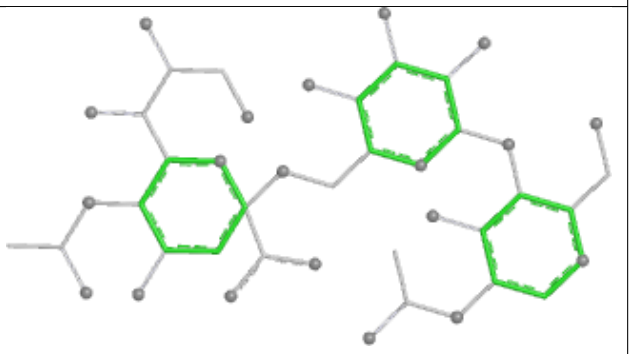
Bond lengths



Bond angles

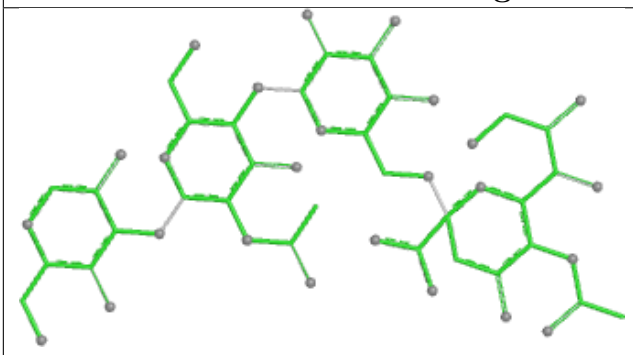


Torsions

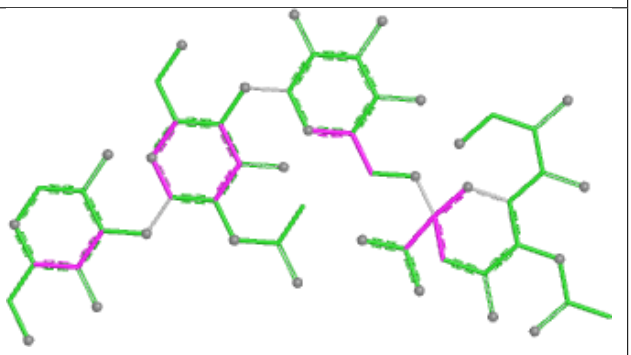


Rings

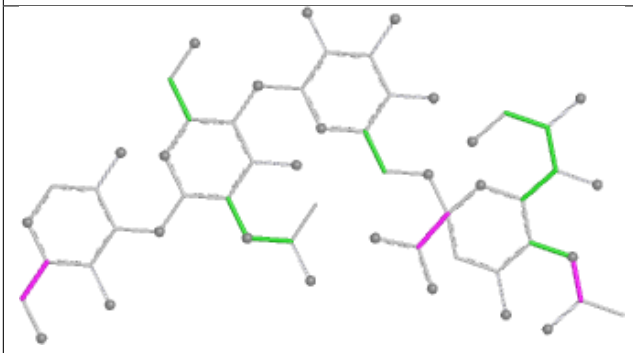
Oligosaccharide Chain N



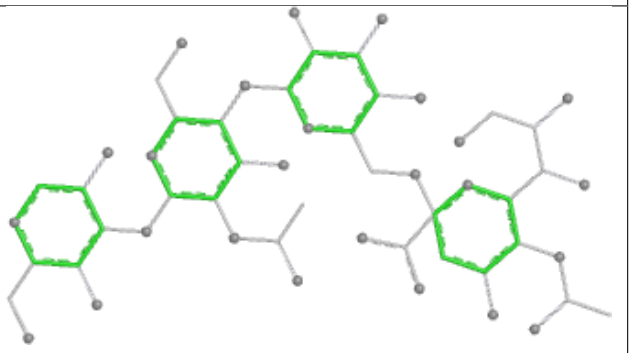
Bond lengths



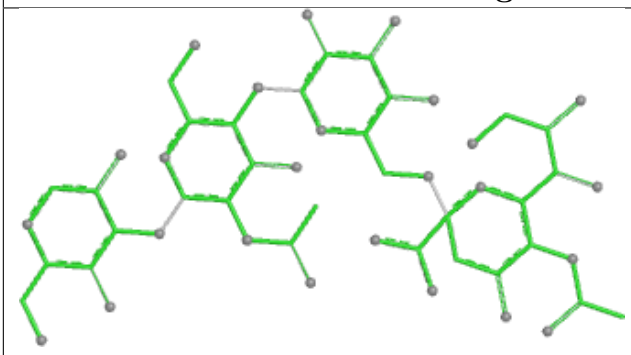
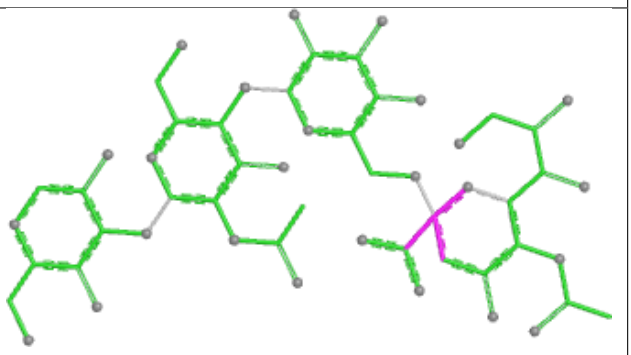
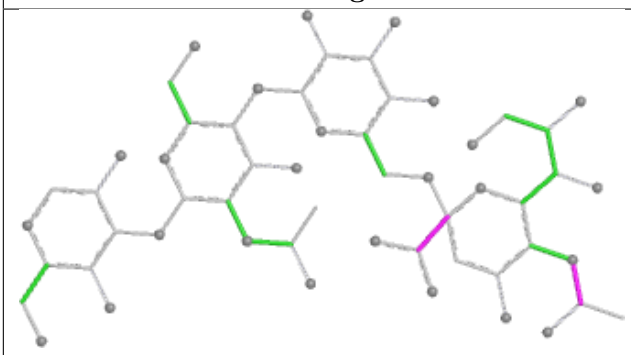
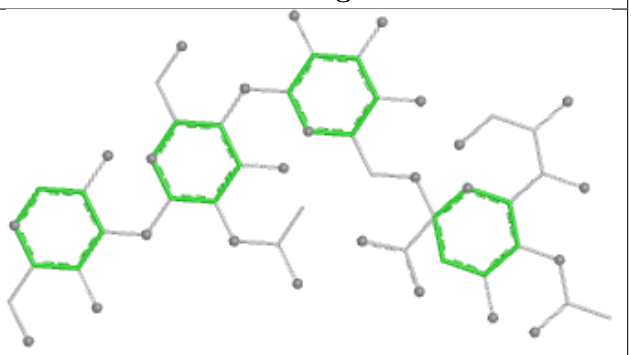
Bond angles



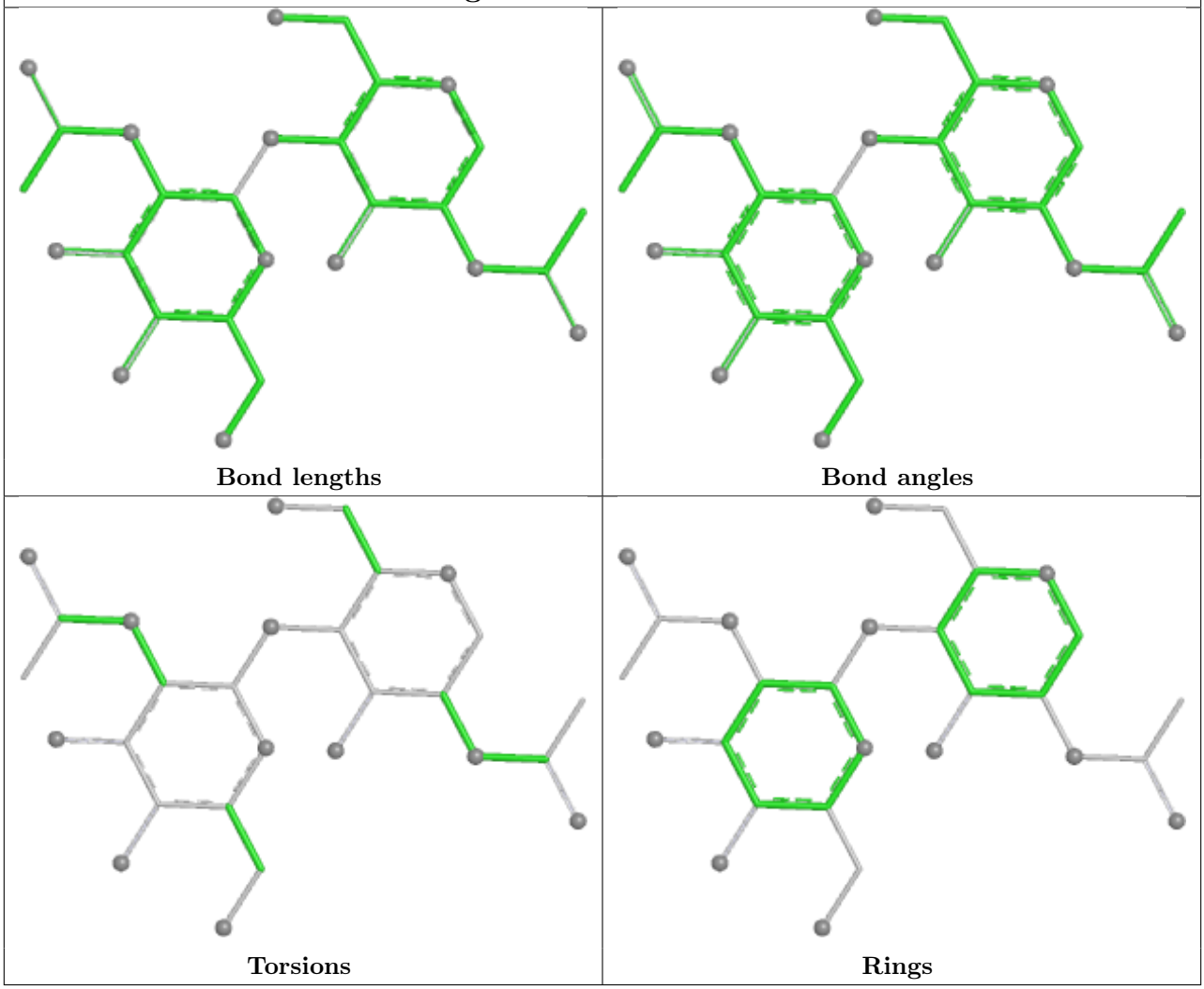
Torsions



Rings

Oligosaccharide Chain P	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain O



5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
6	NAG	A	603	1	14,14,15	0.53	0	17,19,21	0.56	0
6	NAG	G	602	1	14,14,15	0.77	0	17,19,21	1.72	3 (17%)
6	NAG	A	604	1	14,14,15	0.56	0	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	A	602	1	14,14,15	0.55	0	17,19,21	0.61	0
6	NAG	G	601	1	14,14,15	0.29	0	17,19,21	0.56	0
6	NAG	C	601	1	14,14,15	0.46	0	17,19,21	1.04	1 (5%)
7	SIA	G	603	-	20,20,21	0.65	0	21,28,31	1.21	3 (14%)
6	NAG	A	601	1	14,14,15	0.52	0	17,19,21	0.81	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
6	NAG	A	603	1	-	0/6/23/26	0/1/1/1
6	NAG	G	602	1	-	1/6/23/26	0/1/1/1
6	NAG	A	604	1	-	2/6/23/26	0/1/1/1
6	NAG	A	602	1	-	1/6/23/26	0/1/1/1
6	NAG	G	601	1	-	2/6/23/26	0/1/1/1
6	NAG	C	601	1	-	2/6/23/26	0/1/1/1
7	SIA	G	603	-	-	3/18/34/38	0/1/1/1
6	NAG	A	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	602	NAG	C2-N2-C7	4.30	128.67	122.90
7	G	603	SIA	O6-C2-C3	4.03	115.98	110.56
6	C	601	NAG	C1-O5-C5	3.21	116.49	112.19
6	G	602	NAG	C1-C2-N2	2.66	114.62	110.43
6	G	602	NAG	C4-C3-C2	2.19	114.22	111.02
7	G	603	SIA	O1B-C1-C2	2.11	118.20	112.71
7	G	603	SIA	O1A-C1-C2	-2.04	118.45	122.85

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	602	NAG	C1-C2-N2-C7
6	G	602	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
6	C	601	NAG	O5-C5-C6-O6
6	A	601	NAG	O5-C5-C6-O6
6	A	601	NAG	C4-C5-C6-O6
6	A	604	NAG	O5-C5-C6-O6
6	C	601	NAG	C4-C5-C6-O6
6	G	601	NAG	O5-C5-C6-O6
6	G	601	NAG	C4-C5-C6-O6
6	A	604	NAG	C4-C5-C6-O6
7	G	603	SIA	C11-C10-N5-C5
7	G	603	SIA	O10-C10-N5-C5
7	G	603	SIA	O8-C8-C9-O9

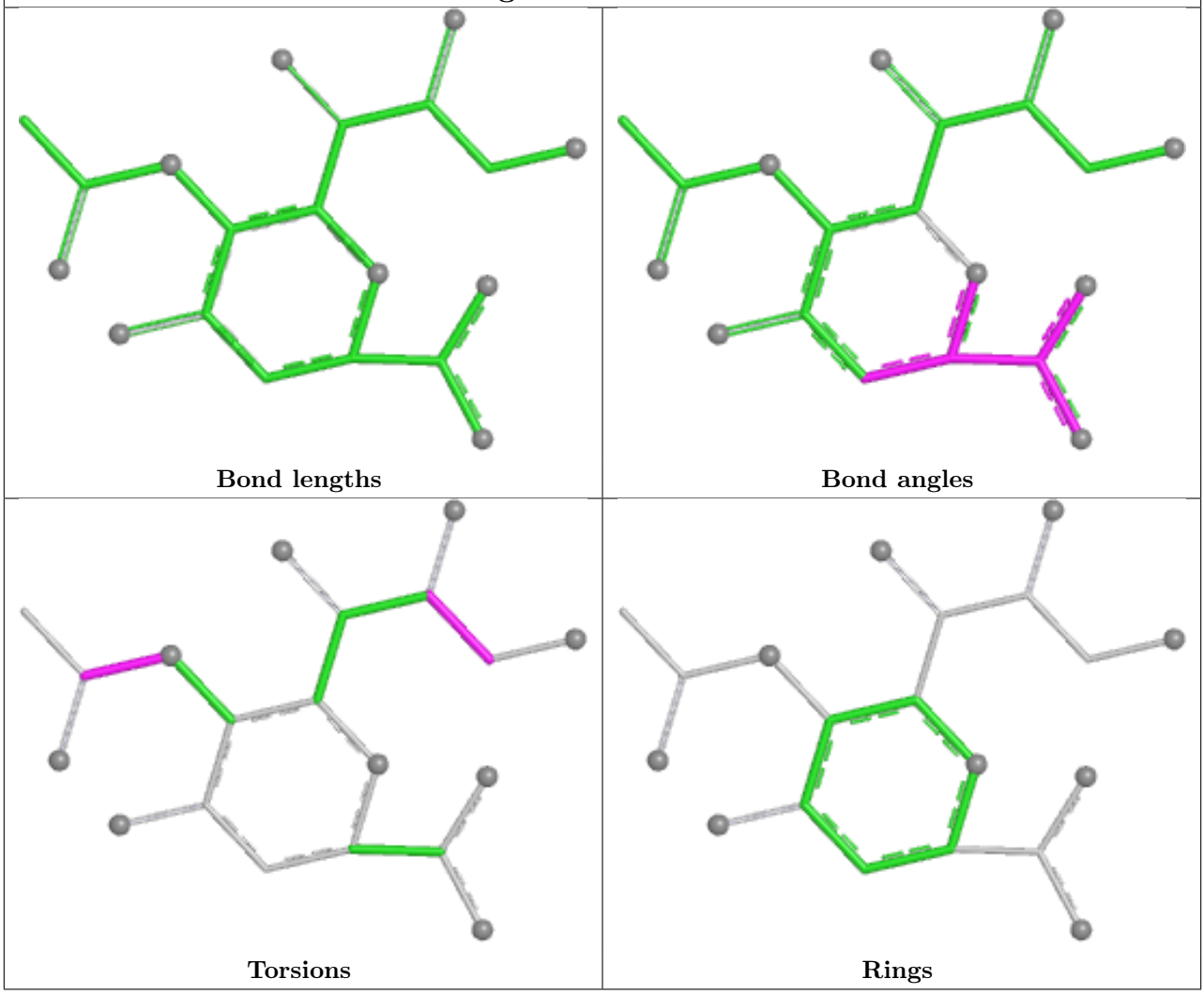
There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	603	NAG	2	0
6	G	602	NAG	4	0
6	A	602	NAG	4	0
6	G	601	NAG	1	0
6	C	601	NAG	2	0
7	G	603	SIA	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SIA G 603



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	321/321 (100%)	0.14	10 (3%) 49 21	35, 69, 111, 154	0
1	C	321/321 (100%)	0.22	18 (5%) 24 8	36, 68, 118, 223	0
1	E	321/321 (100%)	0.15	7 (2%) 62 33	41, 71, 121, 203	0
1	G	321/321 (100%)	0.29	17 (5%) 26 10	39, 76, 124, 154	0
1	I	321/321 (100%)	0.25	9 (2%) 53 25	39, 75, 117, 169	0
1	K	321/321 (100%)	0.48	20 (6%) 20 7	52, 91, 136, 187	0
2	B	162/162 (100%)	0.41	15 (9%) 8 3	35, 84, 142, 180	0
2	D	162/162 (100%)	0.51	15 (9%) 8 3	39, 86, 163, 220	0
2	F	161/162 (99%)	0.72	27 (16%) 1 0	43, 86, 160, 246	0
2	H	162/162 (100%)	0.46	17 (10%) 6 2	40, 85, 149, 181	0
2	J	162/162 (100%)	0.26	4 (2%) 57 29	47, 80, 129, 156	0
2	L	161/162 (99%)	1.82	56 (34%) 0 0	43, 101, 223, 362	0
All	All	2896/2898 (99%)	0.40	215 (7%) 14 4	35, 78, 142, 362	0

All (215) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	129	ASN	11.9
2	L	146	ASN	10.3
2	L	130	ALA	9.2
2	L	147	THR	9.0
2	L	149	MET	8.5
1	G	9	LEU	8.1
2	L	154	ASN	8.1
2	L	159	TYR	7.2
1	K	77	SER	7.2
2	L	23	GLY	7.0
2	L	138	PHE	6.8

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Mol	Chain	Res	Type	RSRZ
2	L	158	ASP	6.7
2	L	160	PRO	6.3
1	G	75	SER	6.0
2	D	31	GLY	5.9
2	F	139	GLU	5.9
2	L	153	LYS	5.7
2	F	159	TYR	5.6
2	L	24	TYR	5.6
1	K	9	LEU	5.6
2	D	129	ASN	5.6
2	L	133	ILE	5.5
1	E	11	ILE	5.5
1	G	76	LEU	5.5
2	L	156	THR	5.4
2	L	31	GLY	5.3
2	L	32	SER	5.3
2	L	143	LYS	5.2
2	H	33	GLY	5.1
1	C	74	GLU	5.0
2	L	141	TYR	5.0
2	L	150	GLU	4.9
2	L	122	VAL	4.9
1	K	147	ALA	4.9
2	L	124	SER	4.9
2	L	35	ALA	4.8
2	F	23	GLY	4.8
2	L	121	LYS	4.8
2	L	126	LEU	4.7
2	F	29	GLU	4.7
1	K	10	CYS	4.7
1	C	7	ASP	4.7
2	F	144	CYS	4.6
2	L	140	PHE	4.6
2	F	158	ASP	4.6
2	D	143	LYS	4.5
2	D	158	ASP	4.5
2	D	139	GLU	4.3
2	L	29	GLU	4.2
2	F	35	ALA	4.2
2	L	125	GLN	4.1
1	E	12	GLY	4.1
1	G	211	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
2	L	145	ASP	4.0
1	I	78	THR	3.9
2	F	128	ASN	3.9
2	F	143	LYS	3.8
2	L	127	LYS	3.7
2	H	141	TYR	3.7
1	C	12	GLY	3.7
2	L	20	GLY	3.7
2	H	27	GLN	3.7
1	K	11	ILE	3.7
2	F	30	GLN	3.6
2	L	139	GLU	3.6
2	H	134	GLY	3.6
1	G	162	ASN	3.6
1	I	91	SER	3.6
2	F	138	PHE	3.6
1	K	50	LEU	3.6
1	K	76	LEU	3.6
2	D	141	TYR	3.5
2	L	131	LYS	3.5
1	A	50	LEU	3.5
2	B	140	PHE	3.5
2	B	156	THR	3.4
1	K	8	THR	3.4
1	G	12	GLY	3.4
2	L	42	GLN	3.4
2	F	141	TYR	3.4
2	F	142	HIS	3.3
2	L	155	GLY	3.3
1	G	77	SER	3.3
2	B	31	GLY	3.3
2	H	156	THR	3.3
2	L	36	ALA	3.3
1	A	19	THR	3.3
2	L	132	GLU	3.2
1	C	8	THR	3.2
2	B	138	PHE	3.2
2	L	134	GLY	3.2
2	L	142	HIS	3.2
1	G	11	ILE	3.1
2	D	146	ASN	3.1
1	E	76	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	H	23	GLY	3.1
1	A	15	ALA	3.1
2	F	121	LYS	3.1
1	I	93	ASN	3.1
2	J	157	TYR	3.1
2	H	144	CYS	3.1
1	K	326	ASN	3.0
2	L	25	HIS	3.0
2	L	34	TYR	3.0
1	C	16	ASN	3.0
1	E	9	LEU	3.0
1	C	293	ASN	2.9
2	B	32	SER	2.9
2	L	15	THR	2.9
2	L	151	SER	2.9
2	B	143	LYS	2.8
2	L	128	ASN	2.8
2	D	132	GLU	2.8
2	L	19	ASP	2.8
1	C	77	SER	2.8
2	L	26	HIS	2.8
2	F	31	GLY	2.8
2	H	145	ASP	2.8
2	L	148	CYS	2.8
1	A	8	THR	2.7
2	L	119	TYR	2.7
2	L	21	TRP	2.7
1	C	195	GLN	2.7
2	J	31	GLY	2.7
2	H	139	GLU	2.7
1	I	8	THR	2.7
1	K	56	LEU	2.7
2	F	149	MET	2.6
2	F	24	TYR	2.6
2	L	10	ILE	2.6
2	B	147	THR	2.6
2	D	33	GLY	2.6
2	H	30	GLN	2.6
1	G	8	THR	2.6
2	F	145	ASP	2.6
2	L	18	VAL	2.6
2	H	26	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	92	ASP	2.6
1	A	162	ASN	2.6
1	I	226	VAL	2.6
2	L	22	TYR	2.6
2	H	154	ASN	2.6
2	B	145	ASP	2.5
2	B	158	ASP	2.5
1	G	17	ASN	2.5
2	H	29	GLU	2.5
2	D	157	TYR	2.5
1	K	248	PHE	2.5
2	F	140	PHE	2.5
2	F	131	LYS	2.5
2	J	156	THR	2.5
1	C	291	ALA	2.4
2	B	128	ASN	2.4
2	F	153	LYS	2.4
2	J	143	LYS	2.4
1	E	77	SER	2.4
2	B	146	ASN	2.4
2	L	30	GLN	2.4
1	C	51	ARG	2.4
2	B	27	GLN	2.4
2	B	137	CYS	2.4
1	C	42	LYS	2.4
2	L	9	PHE	2.3
1	K	307	GLY	2.3
2	L	33	GLY	2.3
1	G	158	VAL	2.3
2	H	22	TYR	2.3
2	B	150	GLU	2.3
1	C	76	LEU	2.3
1	K	52	GLY	2.3
2	D	140	PHE	2.3
2	F	160	PRO	2.3
1	C	60	LYS	2.3
1	A	133	ASP	2.3
2	D	32	SER	2.3
1	G	195	GLN	2.3
2	H	159	TYR	2.2
2	F	147	THR	2.2
1	C	228	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	228	ASP	2.2
2	L	54	SER	2.2
1	A	73	CYS	2.2
2	F	124	SER	2.2
1	C	147	ALA	2.2
1	A	10	CYS	2.2
1	A	7	ASP	2.2
1	G	152	LYS	2.2
1	E	54	ALA	2.1
2	D	11	GLU	2.1
1	C	292	ILE	2.1
1	E	195	GLN	2.1
1	G	53	VAL	2.1
1	I	144	HIS	2.1
1	K	72	GLU	2.1
1	C	221	ALA	2.1
2	D	149	MET	2.1
2	H	140	PHE	2.1
2	D	145	ASP	2.1
1	G	51	ARG	2.1
2	B	149	MET	2.1
1	I	280	ASP	2.1
2	F	119	TYR	2.1
1	K	29	ASN	2.1
1	A	292	ILE	2.0
1	C	20	ASP	2.0
1	K	51	ARG	2.0
1	I	208	GLY	2.0
1	K	17	ASN	2.0
2	F	125	GLN	2.0
1	K	92	ASP	2.0
1	K	136	LYS	2.0
2	F	126	LEU	2.0
1	G	7	ASP	2.0
1	G	149	SER	2.0
2	H	143	LYS	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)

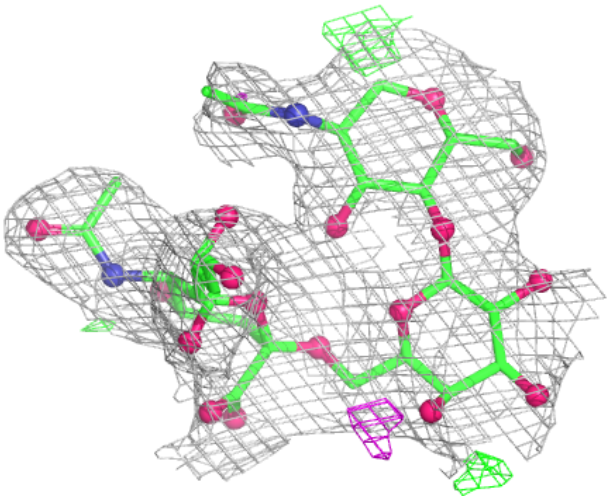
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

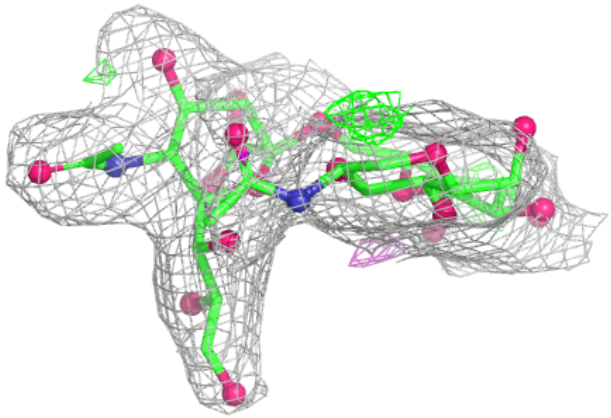
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GAL	N	1	11/12	0.64	0.26	104,129,151,153	0
4	GAL	P	1	11/12	0.75	0.26	110,139,162,174	0
5	NAG	O	2	14/15	0.79	0.34	88,113,132,144	0
3	GAL	R	2	11/12	0.80	0.23	96,131,149,169	0
3	NAG	R	1	14/15	0.83	0.23	110,146,159,172	0
4	NAG	N	2	14/15	0.83	0.25	75,106,127,128	0
3	NAG	M	1	14/15	0.85	0.23	65,80,89,96	0
4	NAG	P	2	14/15	0.86	0.32	120,126,146,147	0
3	NAG	Q	1	14/15	0.86	0.27	111,129,140,142	0
3	GAL	Q	2	11/12	0.87	0.23	61,95,108,114	0
5	NAG	O	1	14/15	0.92	0.16	74,82,98,102	0
4	SIA	P	4	20/21	0.92	0.22	42,65,87,99	0
4	GAL	P	3	11/12	0.93	0.15	78,95,110,122	0
4	SIA	N	4	20/21	0.93	0.20	48,71,90,97	0
3	GAL	M	2	11/12	0.93	0.12	53,93,104,109	0
3	SIA	Q	3	20/21	0.93	0.18	61,77,95,96	0
3	SIA	R	3	20/21	0.94	0.21	64,83,91,91	0
4	GAL	N	3	11/12	0.94	0.17	56,84,92,100	0
3	SIA	M	3	20/21	0.94	0.17	37,53,76,80	0

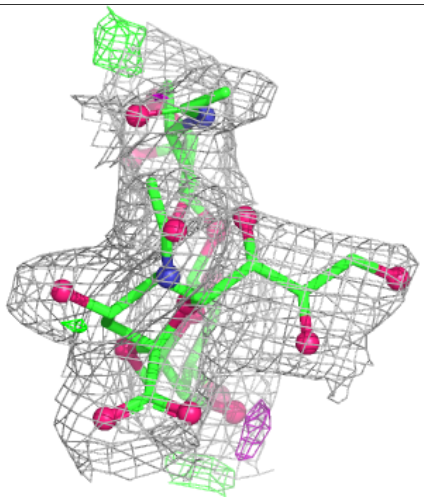
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain M:

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

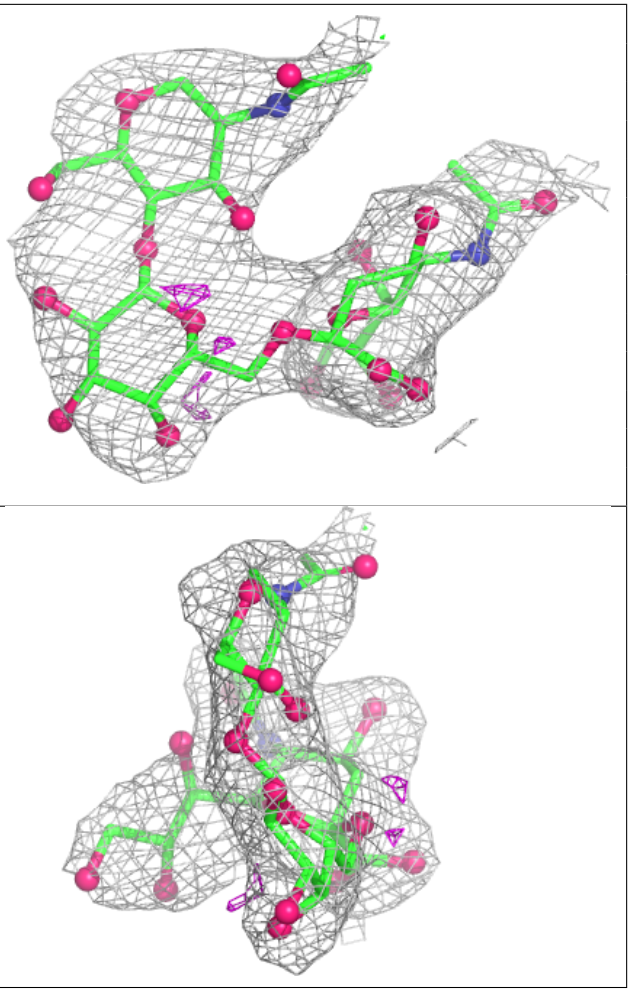






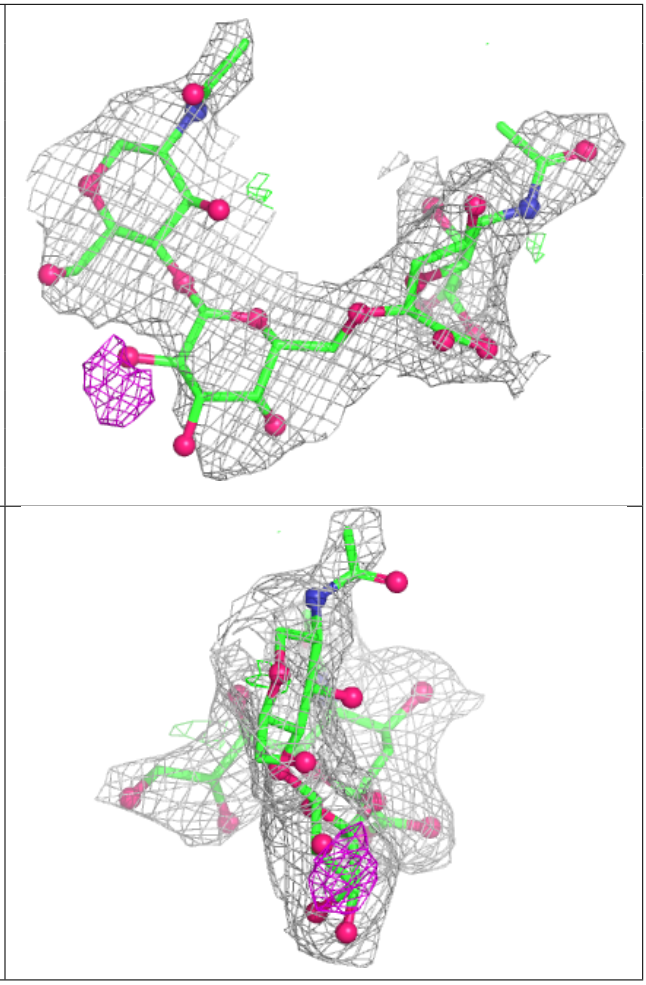
Electron density around Chain Q:

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



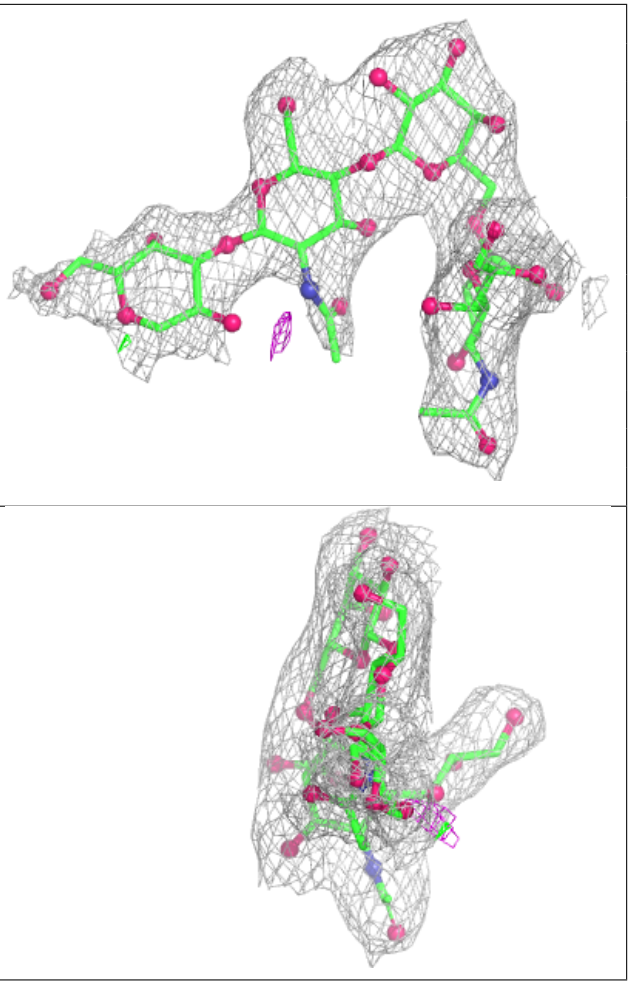
Electron density around Chain R:

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



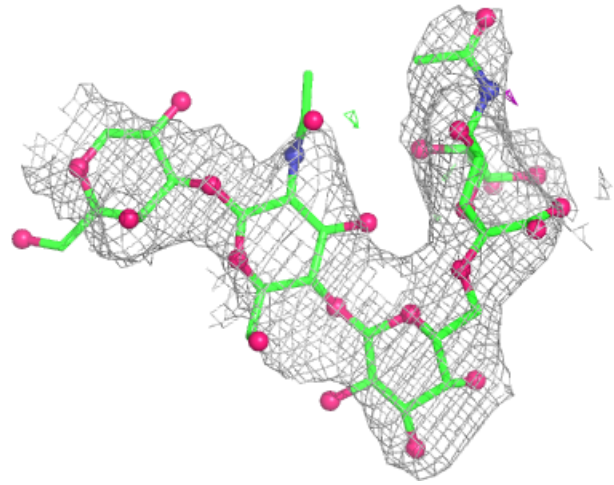
Electron density around Chain N:

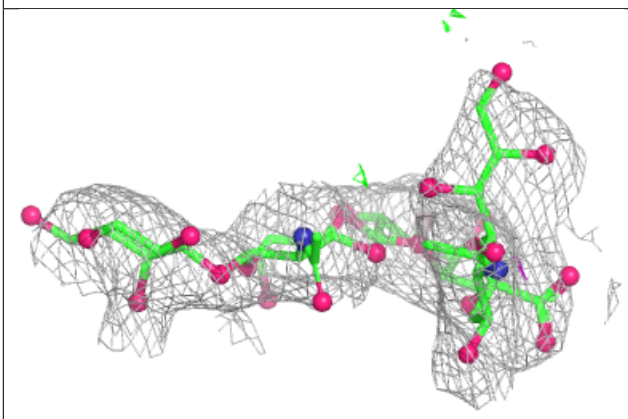
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

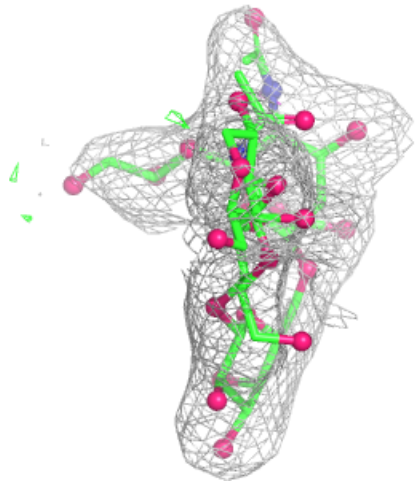


Electron density around Chain P:

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

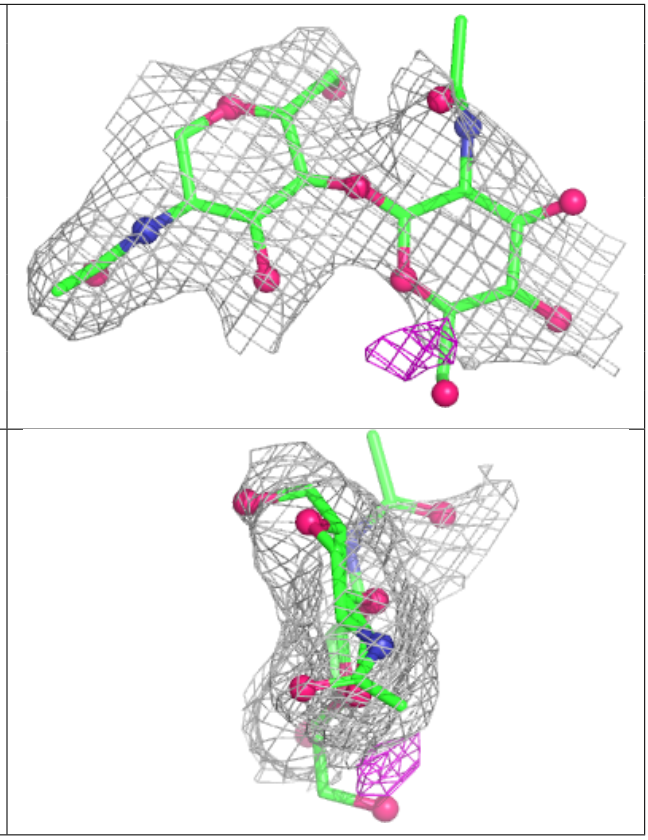






Electron density around Chain O:

$2mF_o$-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)

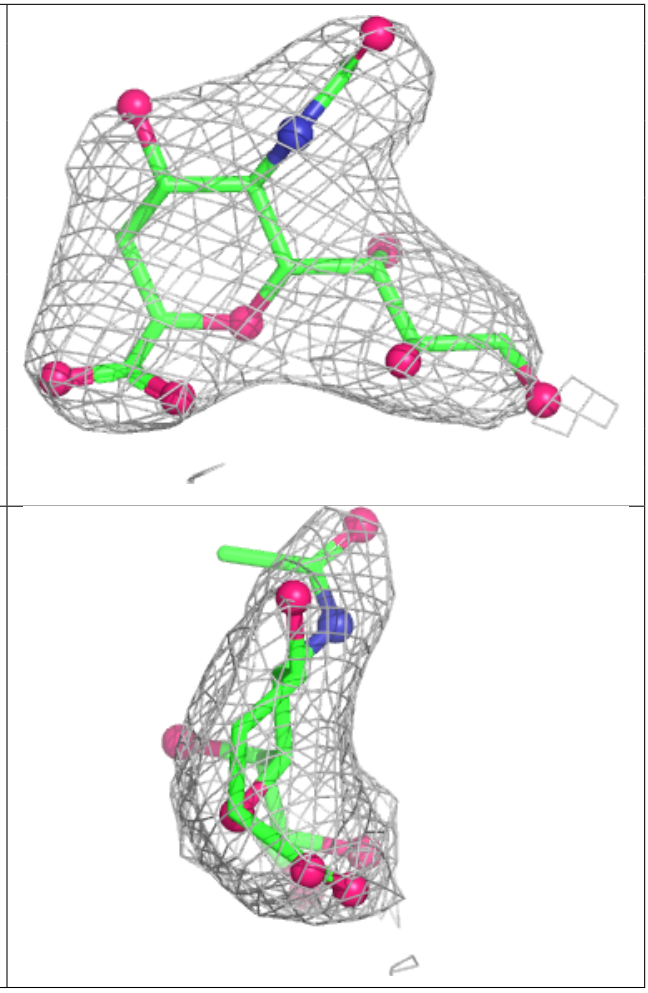
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	G	601	14/15	0.52	0.48	119,147,162,173	0
6	NAG	A	601	14/15	0.67	0.35	142,168,177,178	0
6	NAG	A	602	14/15	0.69	0.30	146,167,182,187	0
6	NAG	A	604	14/15	0.72	0.26	99,145,158,161	0
6	NAG	C	601	14/15	0.81	0.23	70,86,97,103	0
6	NAG	G	602	14/15	0.82	0.28	100,121,147,149	0
6	NAG	A	603	14/15	0.89	0.27	70,102,144,146	0
7	SIA	G	603	20/21	0.89	0.28	65,86,119,122	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SIA G 603:

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



6.5 Other polymers (i)

There are no such residues in this entry.